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Research Article

Phonon–nuclear Coupling for Anomalies in Condensed Matter Nuclear Science

Peter L. Hagelstein *

Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA

Irfan U. Chaudhary

Department of Computer Science and Engineering, University of Engineering and Technology. Lahore, Pakistan

Abstract

Excess heat in the Fleischmann–Pons experiment is thought to have a nuclear origin, yet there are no energetic particles observed in amounts commensurate with the energy produced. This in our view is the most fundamental issue in connection with theory. In earlier work we developed a mathematical model (the lossy spin–boson model) which shows coherent energy exchange between two-level systems and an oscillator under conditions of fractionation. Recently, we have found an interesting physical model that is closely connected, and which is capable of coherent energy exchange with fractionation; this model is based on a relativistic description of composite nuclei in a lattice. In this work we present a much stronger development of the model directly from field theory than given previously. In the lossy spin–boson model, the ability of the model to fractionate a large quantum depends on the presence of suitable loss mechanisms; the same is true in the case of the new physical model. The new model predicts anomalies such as excess heat without energetic nuclear radiation, ^{4}He production, low-level gamma emission, and collimated X-ray emission in the Karabut experiment; however, as yet we have not demonstrated agreement between theory and experiment. Last summer we concluded (erroneously) that coupling with strong static transitions might impact the fractionation power of the model on dynamic transitions, and the resulting model appeared to be in agreement with our interpretation of the experiment. Here we review this kind of model more carefully, and find that no such enhancement is present. Our conclusion in the end is that the theory, model, and interpretation are "close" to the experimental results in the case of the Karabut experiment, but some problem remains.

Keywords: Phonon theory, fractionation, Fleischmann-Pons experiment, Karabut experiment, fundamental Hamiltonian

1. Introduction

Excess heat in the Fleischmann–Pons experiment [1,2] is an effect that should probably not occur, at least according to how nuclear physics and condensed matter physics are currently understood in text books and in the literature.

*E-mail: plh@mit.edu

Nevertheless, there are a sufficient number of experiments showing positive results [3,4] that we consider the effect to be very real, and very much worth understanding theoretically. How many positive confirmation experiments will be required in order to convince the scientific community generally to take an interest is one of the imponderable questions in the field. The situation at this time is almost beyond comprehension, as experiments in the case of the Piantelli group and the Swartz effort have reached the point where the possible commercialization of the associated technology could be contemplated [and other groups (Rossi, and Defkalion) are currently claiming to have already made substantial progress toward the commercialization of relevant technology].

The amount of excess energy produced in the Fleischmann–Pons experiment is prodigious, yet there is no commensurate level of chemical products observed. This observation led Fleischmann to conjecture that the origin of the energy might be nuclear. In the case of PdD experiments, ^{4}He has been observed in amount commensurate with the energy produced, and correlated with energy production (the effect was first studied by Bush, Miles, and coworkers [5–8]). Unfortunately, no similar results are available for the NiH experiments (where ^{3}He measurements are badly needed). Measurements of the amount of ^{4}He produced to energy generated are consistent with the 24 MeV mass difference between two deuterium atoms and ^{4}He [3], but further measurements are needed to be sure.

In normal nuclear reactions, the energy produced is expressed through energetic nuclear particles. If this were the case in the Fleischmann–Pons experiment, we would be able to study the reaction mechanism using conventional nuclear techniques. For example, fusion between two deuterons leads to p+t and n+^{3}He as energetic products in roughly equal amounts; but as is well known neither channel occurs in amounts commensurate with the energy produced in Fleischmann–Pons experiment. Since ^{4}He is considered to be a product in the case of PdD experiments, we might expect it to carry away some fraction of the reaction energy in a Rutherford scenario. If we consider the PdD itself to constitute a nuclear detector, then from a theoretical calibration we conclude that it is an exquisitely sensitive detector of fast alphas [9,10]. From data reported for simultaneous neutron and excess power production, we conclude that the alphas are born confidently with an energy less than 20 keV [10,11], under conditions where the reaction energy is thought to be 24 MeV. This is inconsistent with any sensible Rutherford picture reaction mechanism.

Huizenga considered the absence of 24 MeV gammas in connection with ^{4}He as a product to be one of his three “miracles” [12]. From our perspective Huizenga did not come close to capturing what is really significant in connection with this “hidden product miracle;” instead of focusing on the absence of gamma emission, the real headache in these experiments is the complete absence of any energetic nuclear emission at a level commensurate with the energy produced. For example, if energetic electrons or gammas were present at the watt level, then it would be obvious (as a health hazard if for no other reason); and if energetic neutrons, protons, alphas, or other low-mass nuclei were present there would be a corresponding large penetrating neutron signal (which is not seen). We note that there have been a very large number of theoretical mechanisms put forth over the years to account for excess energy in the Fleischmann–Pons experiment. Since the vast majority of these are based ultimately on Rutherford picture reaction mechanisms (that is, that the reaction energy comes out as energetic nuclear radiation in amounts commensurate with the energy produced), we can conclude that nearly all of these theoretical proposals can be discounted as being inconsistent with experiment (because nuclear radiation at levels commensurate with the energy produced is not seen in the PdD experiments). This point has generally not been appreciated within the condensed matter nuclear science community, as new proposals and models continue to be put forth which would ultimately lead to orders of magnitude more nuclear radiation than is observed in experiment.

If the energy produced does not go into the generation of energetic nuclear radiation, then we might reasonably ask: where does it go? For example, one can see in Schwinger’s ICCF4 paper his focus on this problem, which he recognized as perhaps the most significant theoretical issue [13]. Preparata was of the opinion that the nuclear energy coupled to plasmons [14] or various low energy channels [15]. The focus of our efforts for a great many years now has centered on the possibility that the nuclear energy is coupled into vibrations.

Although this has clearly been the key theoretical issue in our view since the beginning, there is very little in the way of experimental measurements that shed light on how it works. The singular exception is in the case of the Letts two-laser experiment [16,17]. In this experiment, excess heat is triggered when two weak laser beams at different wavelengths overlap in p-polarization on the surface of a Fleischmann–Pons cathode held just below threshold for excess heat production. The excess power produced is seen to be largest at three resonances; the lower two of which correspond to the Γ-point and L-point of the optical phonon mode dispersion relation (which are points where the group velocity for the compressional optical phonon modes go to zero). By itself, this implicates the participation of these optical phonon modes in excess heat production. In single-laser experiments [18–23] excess heat is also triggered by a weak laser beam; however, in this case it goes away when the laser is turned off. In the two-laser experiment, the excess heat is observed to persists after the lasers are switched off. It has been argued [17] that this provides indirect evidence that the nuclear energy is going into these vibrational modes to sustain them (an argument that has not been universally accepted). In a more recent report [24], the excess heat in at least one case was seen to die off slowly after the lasers are switched off.

Of course, once one goes down this particular road, the immediate issue that arises has to do with how a very large MeV quantum gets split up into the large number of low-energy quanta associated with a condensed matter degree of freedom. Up-conversion from the optical regime to the X-ray regime is known in high-harmonic generation [25], where several thousand low-energy quanta are combined to make a more energetic X-ray quantum. However, for the Fleischmann–Pons experiment, the conversion of a 24 MeV quantum into optical phonons near 8 THz would require a fractionation of the large nuclear quantum into roughly 7×10^8 phonons. No mechanism is recognized in physics that is capable of this level of fractionation. It was this problem that we expect motivated Schwinger's early exploratory phonon models; and the somewhat smaller number of plasmons (in the vicinity of a few million) for Preparata's model for multi-photon exchange [14].

In the first several years of our efforts in the field we pursued all manner of schemes, in an effort on the one hand seeking an understanding of the lay of the theoretical landscape, and on the other hand looking for a mechanism that could fractionate a large quantum. After a very large number of failures (most not published), we decided to focus on the fractionation mechanism as a mathematical problem divorced from any physical scheme. To be honest, things were sufficiently discouraging at this point in the research effort that the problem had boiled down to determining whether fractionation was possible with any kind of model, with the expectation that it could be shown to be impossible. In this kind of analysis, the nuclei were reduced to equivalent two-level systems, and the modes of the condensed matter system were turned into linear and nonlinear oscillators. The models at the outset showed some weak ability to fractionate a large quantum, but resisted efforts generally to try to make the effect stronger. Ultimately, the question came down to what prevented the models from fractionating more effectively (since at the nuts and bolts level it seemed that it should have been possible to do better).

We found that the issue was destructive interference. This could be seen most readily in perturbation theory, where the problem of coherent energy exchange under conditions of fractionation was found to be equivalent to that of indirect coupling between distant states that were degenerate. In general there are a large number of paths connecting the two states, and to within near precision the contributions from all the different paths cancelled out. Hence, the only way to increase the fractionation power of the models was to find a mechanism that distinguished broadly between the paths that contributed with a positive sign from those that contributed with a negative sign. In the end, it became clear that loss mechanisms were the most likely candidate. Sure enough, when models were constructed which were augmented with loss (which was discussed at ICCF9 in 2002 [26]), the resulting rate of coherent energy exchange under conditions of fractionation showed orders of magnitude increase. These results were discussed in conference proceedings; however it took many years before a systematic exposition of the new model was published [27–33]. Although the mathematical models focused on coherent energy exchange between sets of two-level systems and an oscillator, the basic mechanism is sufficiently general that it would also apply in the case of two-level systems (or more level systems) coupling to an oscillator, or to other two-level systems (or more level systems).

However, being able to demonstrate coherent energy exchange under conditions of fractionation in a mathematical model is not the same as having a physical model. For example, it is a straightforward calculation to determine the parameters in the mathematical model that would allow fractionation, but it is another thing altogether to specify a physical system in which those parameters can be obtained. We know this well, since over the course of a decade we made several major attempts to identify the physical system in terms of energy levels and coupling mechanism. In all cases, we met with nothing but failure when we carried out calculations with the candidate physical systems. Ultimately we put together a computer code to carry out a systematic evaluation of the important parameters relevant to the system including several hundred candidate transitions, pretty much including all which might conceivably be relevant; and in less than a second the program reported back that none of them calculated out to be suitable candidates. In essence, we could eliminate every atomic, molecular and nuclear transition that we tried as being a suitable receiver transition the donor–receiver model of Ref. [32].

The basic problem in all cases was that the coupling was too weak to do the job. For the requirements of the donor–receiver model to be satisfied, the strength of the coupling for a particular transition to a vibrational mode of the lattice had to be very strong. Meanwhile, all the different coupling mechanisms that we identified, and developed estimates for the coupling strength, resulted in coupling orders of magnitude too weak give sufficient fractionation power. This was very discouraging.

Keep in mind that just because we were not able to make a connection with the existing experimental results with these models, they described effects qualitatively very similar to experiment. For example, we could model excess heat production from deuterons reacting to make ^{4}He, with the energy going into optical phonon modes; however, the conditions required within the model to make it work involved orders of magnitude more deuterons, and orders of magnitude more phonon excitation, than could possible be present in the experiments. In a sense, the models worked and predicted anomalies similar to what was seen in experiment, except that the numbers were all wrong.

We decided to calculate out a model for excitation transfer between vibrations and the lowest energy nuclear transition from the ground state of a stable nucleus (1565 eV transition in ^{201}Hg). The idea here was that according to the models this should be one of the easiest anomalies to implement experimentally. For example, we could design an experiment to demonstrate coherent energy exchange of this kind based on couplings that are understood; the presumption is that if some additional coupling existed that we didn't understand, it should only make the experiment work better. At the end of this exercise, the design required very strong optical phonon excitation over square meters of surface area, but suggested that we should be able to excite the ^{201}Hg nuclei. Ultimately we understood that if it worked we would expect collimated X-ray emission normal from the surface if optical phonon excitation at the Γ-point were used.

At this point we recognized that the effect under consideration would be consistent with collimated emission near 1.5 keV in Karabut's high-current density glow discharge experiment [34–39] . We could use our model to analyze Karabut's data, and we should be able to extract information about the coupling strength directly from the experiment. When we did so, the coupling strength that resulted was enormous. And it was immediately clear that only direct phonon-nuclear coupling could produce such a large coupling strength.

Note that we had considered direct phonon-nuclear coupling over the years (it seems like a dozen times), and each time we concluded that such an effect was impossible. The basic issue is that there is a clean separation of the center of mass motion of a composite (which would be involved in the vibrations), and the internal relative degrees of freedom of a composite (which would be involved in the internal nuclear transition) in nonrelativistic mechanics. The relativistic problem is more complicated, but our understanding was that the separation was equally clean in the relativistic problem (otherwise there should be sections in the text books explaining the consequences of such a coupling).

A lot of thought went into this problem (over a decade altogether, since this problem had been on the radar screen for years prior to the connection with the Karabut experiment). There is a very strong coupling initially in the relativistic model between the center of mass motion and internal transitions. This coupling disappears when we take the nonrelativistic limit, but we know that it was there initially in the relativistic version of the problem. For an isolated composite, we know that a generalized Foldy–Wouthuysen transformation eliminates this strong first-order coupling, which then allows us to take the nonrelativistic limit. Our interpretation of the Karabut experiment then directly points to issues involved with the generalized Foldy–Wouthuysen transformation.

It seems useful here to summarize the resulting situation. We have mathematical models that describe coherent energy exchange under conditions of fractionation, and these models point to the Karabut collimated X-ray experiment as perhaps the most fundamental experiment in the field. From a comparison of the model and experiment, we are forced to conclude that transitions are mediated by very strong direct phonon-nuclear coupling. Coupling that is of sufficient strength is present initially in the relativistic version of the problem. But we know that a generalized Foldy–Wouthuysen transformation eliminates this coupling (and hence the game is over). But collimated X-rays are seen in Karabut's experiment! You might predict the outcome if you suggest to your colleagues that the generalized Foldy–Wouthuysen transformation breaks (this is not a good way to impress one's physics colleagues!).

After some reflection, we realized that we have encountered a very similar situation previously. If we go back to our mathematical model for two-level systems coupled to an oscillator, we find an analogy. In the lossless version of the spin–boson model, we can apply a generalized Foldy–Wouthuysen transformation, which eliminates the first-order coupling. A weak higher-order coupling remains in the rotated version of the problem, and we found that matrix elements of this residual coupling describes coherent energy exchange in the multi-phonon version of the problem accurately [40]. However, when the model is augmented with loss the resulting behavior of the model changes qualitatively; the rate for coherent energy exchange is increased by many orders of magnitude. In this case the strong first-order coupling which is normally rotated out by the Foldy–Wouthuysen transformation seems to stick around to mediate coherent energy exchange under conditions of fractionation. Conclusions in this case that we might make based on the Foldy–Wouthuysen rotated version of the lossless version of the problem just do not match with the results of direct calculations in the presence of loss. It is as if the Foldy–Wouthuysen transformation "breaks." Note that it is impossible for a unitary transformation to "break" in that it is just a change of basis. However, it is very much possible for a change of basis to be unhelpful in the analysis of a problem. And this seems to be the situation here.

In what follows, we consider a fundamental relativistic model for condensed matter nuclear science (see [41] for our earlier effort), and examine the model under conditions where the generalized Foldy–Wouthuysen transformation is unhelpful. Not long ago we were convinced that the resulting model could account for the anomalies, and that we finally had a model relevant to experiment. For example, last year we discussed results from a version of this model, where we found that the model seemed to be consistent quantitatively with the experimental parameters in the Karabut experiment [42,43]. We also found a degree of consistency with gamma emission, and with rates for energy generation and ^{4}He production in the Letts experiment.

Unfortunately, while documenting the model of last summer, we found an error (which we explain and correct in this work). At issue was the question of whether the presence of a large number of very strong static transitions impacts the dynamics on a weak low-energy transition which undergoes coherent dynamics. In the model of last summer, we concluded that there was a very strong impact. With the error corrected, the conclusion now is that there is essentially no impact. This is important, since it means that when we analyze coherent dynamics on a single transition, we know that all of the other transitions act as if the generalized Foldy–Wouthuysen transformation had been successful (in essence, they are decoupled). Rather than having to re-analyze the entire system with all possible transitions each time, we can focus only on those transitions likely to exhibit coherent dynamics.

2. Dirac Model for Interacting Protons

The issues that we must deal with in the development of our model are subtle, so it makes sense to begin with an introductory example that focuses on a particularly simple version of the problem. As it turns out, our intuition about the nonrelativistic limit of a relativistic problem depends critically on the Foldy–Wouthuysen transformation [44] in the case of Dirac particles. Even though the Foldy–Wouthuysen transformation is usually thought of as providing for the nonrelativistic limit of the Dirac model, what it actually does is to rotate out the strong first-order coupling with the proton momentum. This produces a transformed model in which this first-order interaction has been removed, which then allows an easy development of the nonrelativistic approximation subsequently.

Since this example is so simple, we are able to construct the rotation explicitly; we can see clearly how things work in every step of the computation; and we see that this coupled lattice and Dirac proton model has a mathematical structure very closely related to the spin–boson model. Unfortunately, the analogy in this case is not quite as close as we might like, as the negative energy states are mathematical states and not physical states in this example; however, in the more general case to be considered later on, coupling to physical states does occur. By laying out the development explicitly for this simple version of the model, we can see how things work, and we can understand how fundamental the Foldy–Wouthuysen transformation is in this development.

2.1. Idealized model for a lattice made of Dirac protons

We begin with an idealized lattice model with relativistic protons described using a Dirac Hamiltonian

$$\hat{H} = \sum_j \left(\boldsymbol{\alpha}_j \cdot c\hat{\mathbf{P}}_j + \beta_j Mc^2 \right) + \sum_{j<k} V(|\mathbf{R}_j - \mathbf{R}_k|), \tag{1}$$

where a Born–Oppenheimer approximation has been adopted for the electrons resulting in an effective proton-proton potential. Such a model can of course be criticized since at low pressure hydrogen crystallizes into an HCP lattice of H_2 molecules, and at high pressure it is expected to form more complicated lattice structures [45]; which would require a more complicated effective proton–proton potential than are included here. We are interested here in an idealized model in which the Dirac protons make up a simple crystal lattice, rather than a molecular solid. Nevertheless, although its applicability to a physical system is limited, this simple model is useful to us since we can use it to study the reduction of the relativistic model to a nonrelativistic one.

It will be convenient to rewrite the Hamiltonian in the form

$$\hat{H} = \sum_j \left\{ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j Mc^2 + \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_j (\boldsymbol{\sigma} \cdot c\hat{\mathbf{P}})_j \right\} + \sum_{j<k} V(|\mathbf{R}_j - \mathbf{R}_k|). \tag{2}$$

Doing so brings out the coupling between the large and small components, and provides us with a notation that we can take advantage of in connection with the unitary operator for the transformation which follows.

2.2. Foldy–Wouthuysen rotation and nonrelativistic limit

As discussed above, the Foldy–Wouthuysen transformation was introduced to address the reduction of the relativistic Dirac electron problem to obtain the nonrelativistic limit; however, from our perspective the critical issue is that it removes a strong first-order coupling term. We make use of the Foldy–Wouthuysen transform to write

$$\hat{H}' = \hat{\mathcal{U}}^\dagger \hat{H} \hat{\mathcal{U}} = \sum_j \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j \sqrt{(Mc^2)^2 + c^2|\hat{\mathbf{P}}_j|^2} + \sum_{j<k} V(|\hat{\mathbf{R}}'_j - \hat{\mathbf{R}}'_k|), \tag{3}$$

where the unitary transformation is given explicitly by

$$\hat{\mathcal{U}} \ = \ \exp \frac{i}{2} \left\{ \sum_j \text{Arctan} \left(\frac{(\boldsymbol{\sigma} \cdot c\hat{\mathbf{P}})_j}{Mc^2} \right) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_j \right\}. \tag{4}$$

The rotated position operator is

$$\hat{\mathbf{R}}'_j \ = \ \hat{\mathcal{U}}^\dagger \hat{\mathbf{R}}_j \hat{\mathcal{U}} \ = \ \mathbf{R}_j + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_j \frac{(Mc^2)^2}{(Mc^2)^2 + c^2 |\hat{\mathbf{P}}_j|^2} \frac{\hat{\mathbf{s}}_j}{Mc}. \tag{5}$$

In the rotated version of the problem the strong first-order $\boldsymbol{\alpha} \cdot c\mathbf{P}$ interaction has been eliminated.

2.3. Nonrelativistic limit and discussion

It is possible to recover the nonrelativistic limit by retaining lowest order terms in the momentum, while at the same time eliminating the negative energy sector; this leads to

$$\hat{H}' \ \to \ \sum_j \left(Mc^2 + \frac{|\hat{\mathbf{P}}_j|^2}{2M} \right) + \sum_{j<k} V(|\mathbf{R}_j - \mathbf{R}_k|). \tag{6}$$

This simple example is important because it makes explicit the arguments and steps that take us from an idealized relativistic model to a rotated version of the model, and then to the nonrelativistic limit. It makes clear just how central the Foldy–Wouthuysen transformation itself is in connection with the discussion. In this idealized model there is a strong relativistic coupling between the proton momentum and internal degrees of freedom (in this case, a positive to negative energy state transition); which is eliminated by the rotation. We see that the Foldy–Wouthuysen transformation (and later on its generalization) provides the foundation generally upon which our intuition of how the world works rests.

3. Lattice Model with Dirac Protons

The next step in this introductory discussion is to revisit the Foldy–Wouthuysen rotation under conditions where the protons interact harmonically, so that the associated position and momentum variables become operators of the lattice problem. We encounter this situation in the more general version of the problem to follow, so it is worth studying here in the context of the simpler idealized proton model where we can construct the rotation explicitly.

3.1. Harmonic lattice with Dirac protons

For a displacement around the equilibrium position of a proton $\mathbf{R}_j^{(0)}$ we write

$$\mathbf{R}_j \ = \ \mathbf{R}_j^{(0)} + \mathbf{r}_j. \tag{7}$$

With this notation the potential can be expanded in the vicinity of equilibrium

$$V_{jk} \ = \ V_{jk}^{(0)} + (\mathbf{r}_j - \mathbf{r}_k) \cdot \mathbf{K}_{jk} \cdot (\mathbf{r}_j - \mathbf{r}_k) + \cdots \tag{8}$$

where $\mathbf{K}_{jk}$ is the associated force constant matrix. Keeping only the second order terms, we may write

$$\hat{H} = \sum_j \left(\boldsymbol{\alpha}_j \cdot c\hat{\mathbf{P}}_j + \beta_j Mc^2 \right) + V_0 + \sum_{j<k} (\mathbf{r}_j - \mathbf{r}_k) \cdot \mathbf{K}_{jk} \cdot (\mathbf{r}_j - \mathbf{r}_k). \tag{9}$$

We would expect that this model would behave very nearly like a conventional harmonic lattice model since we recognize that the protons should act nonrelativistically in a lattice setting. However, instead of carrying out a Foldy–Wouthuysen transformation here, we would like instead to first develop a description of the problem in terms of phonon modes prior to the rotation.

3.2. Hamiltonian written in terms of phonon modes

To carry out the approach mentioned above, we make use of a mathematical device that allows us to develop a harmonic lattice while keeping the Dirac proton description intact; we add and subtract nonrelativistic kinetic energy terms to obtain

$$\begin{aligned} \hat{H} = &\sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M} + V_0 + \sum_{j<k} (\mathbf{r}_j - \mathbf{r}_k) \cdot \mathbf{K}_{jk} \cdot (\mathbf{r}_j - \mathbf{r}_k) \\ &+ \sum_j \left(\boldsymbol{\alpha}_j \cdot c\hat{\mathbf{P}}_j + \beta_j Mc^2 \right) - \sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M}. \end{aligned} \tag{10}$$

Written in this form, we see a harmonic lattice model, and the relativistic part of the Hamiltonian appears separately, augmented with a counter term. We recast the harmonic lattice part of the problem into phonon mode operators

$$\sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M} + \sum_{j<k} (\mathbf{r}_j - \mathbf{r}_k) \cdot \mathbf{K}_{jk} \cdot (\mathbf{r}_j - \mathbf{r}_k) = \sum_i \hbar\omega_i \left(\hat{a}_i^\dagger \hat{a}_i + \frac{1}{2} \right). \tag{11}$$

In what follows we will need to make use of proton position and momentum operators written in terms of phonon mode creation and annihilation operators; the relations will be written as

$$\hat{\mathbf{R}}_j = \mathbf{R}_j^{(0)} + \sum_\mu \frac{\mathrm{d}\mathbf{R}_j}{\mathrm{d}a_\mu} (\hat{a}_\mu + \hat{a}_\mu^\dagger), \tag{12}$$

$$\hat{\mathbf{P}}_j = \sum_\mu \frac{\mathrm{d}\mathbf{P}_j}{\mathrm{d}a_\mu} \left(\frac{\hat{a}_\mu - \hat{a}_\mu^\dagger}{i} \right), \tag{13}$$

where the derivatives $\mathrm{d}\mathbf{R}_j/\mathrm{d}a_\mu$ and $\mathrm{d}\mathbf{P}_j/\mathrm{d}a_\mu$ here are intended as a kind of shorthand to keep track of different terms which make up the mode operators. With these relations we can write the model as

$$\hat{H} = \sum_{\mu} \hbar\omega_{\mu} \left(\hat{a}_{\mu}^{\dagger}\hat{a}_{\mu} + \frac{1}{2}\right) + Mc^2 \sum_{j} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j + V_0$$
$$+ \sum_{j} \sum_{\mu} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_j \boldsymbol{\sigma}_j \cdot c \frac{\mathrm{d}\,\hat{\mathbf{P}}_j}{\mathrm{d}a_{\mu}} \left(\frac{\hat{a}_{\mu} - \hat{a}_{\mu}^{\dagger}}{i}\right) - \sum_{j} \frac{|\hat{\mathbf{P}}_j|^2}{2M}. \tag{14}$$

We have succeeded in implementing a harmonic lattice model for the interacting protons, while retaining the strong first-order relativistic coupling between the proton momentum (now written in terms of phonon operators) and internal transitions between the large and small Dirac components. As a result of the mathematical device mentioned above, we retain a counter term for the Dirac mass and kinetic energy terms. The problem is now set up so that we can examine cleanly the implementation of a Foldy–Wouthuysen transformation.

3.3. Foldy–Wouthuysen rotation for the spin–boson problem

It probably comes as no surprise that we are able to carry out a Foldy–Wouthuysen transformation in this case as well, since this new model can be thought of as a special case of the more general version of the model discussed above. In fact, the unitary transformation that eliminates the linear coupling term is formally the same is in the case above, although we write it now in terms of the phonon mode operators

$$\hat{\mathcal{U}} = \exp\left\{\frac{i}{2}\sum_{j} \mathrm{Arctan}\left(\sum_{i} \frac{1}{Mc}\boldsymbol{\sigma}_j \cdot \frac{\mathrm{d}\mathbf{P}_j}{\mathrm{d}a_i}(\hat{a}_i + \hat{a}_i^{\dagger})\right) \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_j \right\}. \tag{15}$$

The rotated Hamiltonian can be written as

$$\hat{H}' = \hat{\mathcal{U}}^{\dagger}\hat{H}\hat{\mathcal{U}}$$
$$= \sum_{j} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j \sqrt{(Mc^2)^2 + c^2|\hat{\mathbf{P}}_j|^2} - \sum_{j} \frac{|\hat{\mathbf{P}}_j|^2}{2M} + \sum_{\mu} \hbar\omega_{\mu}\left(\hat{a}_{\mu}^{\dagger}\hat{a}_{\mu} + \frac{1}{2}\right)$$
$$+ V_0 + \sum_{j<k} (\hat{\mathbf{r}}'_j - \hat{\mathbf{r}}'_k) \cdot \mathbf{K}_{jk} \cdot (\hat{\mathbf{r}}'_j - \hat{\mathbf{r}}'_k) - \sum_{j<k} (\mathbf{r}_j - \mathbf{r}_k) \cdot \mathbf{K}_{jk} \cdot (\mathbf{r}_j - \mathbf{r}_k), \tag{16}$$

where the transformed position operators are

$$\hat{\mathbf{r}}'_j = \hat{\mathcal{U}}^{\dagger}\hat{\mathbf{r}}_j\hat{\mathcal{U}}$$
$$= \mathbf{r}_j + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_j \frac{(Mc^2)^2}{(Mc^2)^2 + c^2 \left|\sum_{\mu} \frac{\mathrm{d}\mathbf{P}_j}{\mathrm{d}a_{\mu}}\left(\frac{\hat{a}_{\mu} - \hat{a}_{\mu}}{i}\right)\right|^2} \frac{\hat{\mathbf{s}}_j}{Mc}. \tag{17}$$

Similar to the case considered earlier, the Foldy–Wouthuysen transformation in this case has eliminated the first-order coupling between the phonon and internal Dirac degrees of freedom. We see that the Foldy–Wouthuysen transformation that we have used in the two different examples is essentially the same; working in the context of a lattice with phonon modes has not impeded our ability to implement the rotation.

3.4. Nonrelativistic limit

Taking the nonrelativistic limit now becomes straightforward; we may write

$$\hat{H}' \rightarrow \sum_j \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j (Mc^2)^2 + \sum_\mu \hbar\omega_\mu \left(\hat{a}_\mu^\dagger \hat{a}_\mu + \frac{1}{2}\right) + V_0$$

$$+ \sum_{j<k} (\hat{\mathbf{r}}'_j - \hat{\mathbf{r}}'_k) \cdot \mathbf{K}_{jk} \cdot (\hat{\mathbf{r}}'_j - \hat{\mathbf{r}}'_k) - \sum_{j<k} (\mathbf{r}_j - \mathbf{r}_k) \cdot \mathbf{K}_{jk} \cdot (\mathbf{r}_j - \mathbf{r}_k), \tag{18}$$

where we recognize the residual nuclear spin interactions denoted by the second line of the rotated Hamiltonian to be small. The kinetic energy counter term in this case has eliminated the second-order kinetic energy contribution from the expansion of the relativistic energy; and we have dropped higher-order terms.

3.5. Discussion

There are a variety of issues to consider in this discussion, and we have made some progress in providing some illumination with these idealized example models. We have seen that in both cases that there appears a first-order coupling between proton momentum and internal Dirac degrees of freedom; and we recognize that the problems would be much more difficult to solve and understand if we had to work with this first-order coupling in place. From these examples, we view the Foldy–Wouthuysen transformation as most importantly removing this first-order coupling; the problem that we end up with in both cases has a nearly clean separation between proton momentum and internal Dirac degrees of freedom. We see additionally that the Foldy–Wouthuysen transformation is effective in both examples on equal footing; when the momentum to be made up of phonon mode operators there is no fundamental difference in the associated unitary operator, or in the rotated version of the problem.

When the interacting protons in this model are worked into a harmonic lattice description, the resulting problem is closely related mathematically (but not so closely related physically) to the spin–boson model. As mentioned above, we are able to make use of the Foldy–Wouthuysen transformation in the spin–boson model in the same way as done here, which allows us to eliminate the first-order coupling (and the residual high-order coupling gives rise to known results for coherent energy exchange when many quanta are exchanged) [40]. Also as discussed above, the spin–boson model behaves very differently in regard to coherent energy exchange when substantial loss is present (since loss removes the destructive interference that inhibits energy exchange) [27–31].

This motivates us to consider what the idealized Dirac proton lattice model might look like if augmented with loss. Note that protons cannot have real occupation of the negative energy state, so there are some differences with the lossy spin-boson problem. The idea here is to examine briefly here the situation that would result in this idealized problem if the Foldy-Wouthusyen transformation were to become unhelpful due to the inclusion of a strong loss model.

The Hamiltonian for the lossy spin–boson model can be written as

$$\hat{H} = \hbar\omega_0 \hat{a}^\dagger \hat{a} + \frac{\Delta E}{2} \sum_j \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_j + V \sum_j \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_j (\hat{a} + \hat{a}^\dagger) - i\frac{\hbar\hat{\Gamma}(E)}{2}. \tag{19}$$

There is no problem in using a Foldy–Wouthuysen type of transformation as a mathematical operation for such a model; and by doing so one eliminates the first-order coupling between the oscillator and two-level system, similar to the situation above. However, the loss operator in this case is transformed as well, and the rotated version of the loss operator is nearly impossible to work with. We have found that for this kind of problem we are much better off simply working with the unrotated version of the model.

As commented upon previously, the lossy spin–boson model is closely related to the lattice and Dirac proton model discussed above, and we expect an analogous situation if the model is similarly augmented with loss. In this case we might write

$$\hat{H} \rightarrow \sum_{\mu} \hbar\omega_{\mu}\left(\hat{a}_{\mu}^{\dagger}\hat{a}_{\mu}+\frac{1}{2}\right)+Mc^2\sum_j \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}_j + V_0 + \sum_j\sum_{\mu}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}_j \boldsymbol{\sigma}_j\cdot c\frac{\mathrm{d}\hat{\mathbf{P}}_j}{\mathrm{d}a_{\mu}}\left(\frac{\hat{a}_{\mu}-\hat{a}_{\mu}^{\dagger}}{i}\right)-\sum_j\frac{|\hat{\mathbf{P}}_j|^2}{2M}-i\frac{\hbar\hat{\Gamma}(E)}{2}, \tag{20}$$

then we would encounter the same difficulty. In this case, under the Foldy–Wouthuysen transformation we would be able to write down a nonrelativistic limit for the basic model

$$\hat{H}' \rightarrow \sum_{\mu} \hbar\omega_{\mu}\left(\hat{a}_{\mu}^{\dagger}\hat{a}_{\mu}+\frac{1}{2}\right)+V_0+\sum_j \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}_j (Mc^2)^2 + \sum_{j<k}(\hat{\mathbf{r}}_j'-\hat{\mathbf{r}}_k')\cdot\mathbf{K}_{jk}\cdot(\hat{\mathbf{r}}_j'-\hat{\mathbf{r}}_k')-\sum_{j<k}(\mathbf{r}_j-\mathbf{r}_k)\cdot\mathbf{K}_{jk}\cdot(\mathbf{r}_j-\mathbf{r}_k)-i\frac{\hbar\hat{\Gamma}'(E)}{2}, \tag{21}$$

However, the loss is also transformed under the Foldy–Wouthuysen transformation

$$\hat{\Gamma}'(E)=\hat{\mathcal{U}}^{\dagger}\hat{\Gamma}(E)\hat{\mathcal{U}}. \tag{22}$$

Under conditions where the loss is extremely fast in accessible regimes, then the rotated version of the loss operator becomes extremely difficult to work with; in such cases we are much better off analyzing the problem in the original frame. Strong loss in accessible regimes can produce a modification of the phonon distribution which ruins the entanglement between the phonon and nuclear degrees of freedom that the Foldy–Wouthuysen rotation seeks to simplify.

4. Coupling between Momentum and Internal Nuclear Degrees of Freedom

By now we have made several attempts at specifying a fundamental Hamiltonian that we might be able to use as a starting point for modeling the new effects [46,41,42], and in each case the resulting Hamiltonian could be criticized for one reason or another. In [46] we worked with nonrelativistic models (where the first-order coupling under discussion is eliminated); in [41] we proposed using a many-particle Dirac Hamiltonian for nucleons, which is not covariant; and in [42] we discussed a Dirac Hamiltonian for quarks, where such a model does not provide even a useful starting place for nucleons, much less nuclei made up of several nucleons. This motivates us to return once again to this problem, and to try to develop an improved foundation for the model.

4.1. The problem of the basic description

We might consider adopting as a starting point QED to describe electrons and the electromagnetic field, and QCD to describe quarks and gluons; in this case our fundamental Hamiltonian takes the form

$$\hat{H} = \hat{H}_{\rm QED} + \hat{H}_{\rm QCD}. \tag{23}$$

Surely such a starting place must be free of all such criticisms. Such a model would be appropriately relativistically covariant; we would now have a useful starting point capable at least in principle of describing nucleons appropriately and leading ultimately to compound nuclei.

Even so, we still recognize deficiencies. We need to make sure that our QCD Hamiltonian has photon exchange so that interactions between nuclei and other nuclei or electrons is included. Eventually we will want to describe weak interactions, so perhaps only a standard model Hamiltonian will do the job. On the practical side, now that we have decided on a sufficiently general Hamiltonian, we have little hope of carrying out specific calculations, in part because we have now enlarged our model to include pretty much everything. We inherit the headache that bound state QCD has not yet reached the stage that it can be used routinely for nuclei with many nucleons.

In light of this, it may be time to adopt a different strategy altogether for the problem. Since the effects that we are interested in depend only on the changes in the relativistic nuclear wavefunction when it moves (slowly), it might be better to start over and to focus on the modification of the internal nuclear that occurs in connection with motion, and recast the problem in terms of the associated coupling matrix elements. In this way we might better focus attention on the part of the problem most relevant to the model, and by doing so cast the relevant coupling matrix elements into a form that might allow for suitable approximations later on. In what follows this is the approach that we will take.

4.2. Rest frame basis states

We begin then by presuming the existence of a complete set of rest frame basis states for a compound nucleus that are eigenfunctions of a relevant relativistic Hamiltonian

$$M_j c^2 \Phi_j = \hat{H}_{\rm QCD} \Phi_j. \tag{24}$$

Sadly, we already run into a technical issue in such a proposition. These eigenfunctions include those we need that correspond to physical states, along with a great many solutions that involve particles in negative energy states. At this stage, formally we are going to need all of them as mathematical solutions; later we are going to have to be careful to make sure that we end up with solutions that we can identify as being in the positive energy sector, which will correspond to physical states.

4.3. Boosted wavefunctions in terms of a rest frame basis

Next, we consider boosted versions of the state constructed according to

$$\Phi'_j(\mathbf{P}) = \exp\left\{ i\frac{\mathbf{P}}{\hbar} \cdot \mathbf{R} \right\} \hat{\mathcal{U}}(\mathbf{P}) \Phi_j(0). \tag{25}$$

The idea here is that the dependence on the center of mass coordinate $\mathbf{R}$ here is a pure plane wave $\exp\{i\mathbf{P}\cdot\mathbf{R}/\hbar\}$, which constitutes the only $\mathbf{R}$-dependence in the problem. The internal nuclear wavefunction undergoes a rearrangement relative to the rest frame in order to be consistent with relativity. Note that we are interested in stationary states in this discussion, and in what follows; hence the $\exp(-iEt/\hbar)$ terms that might appear in a space-time description is not present.

Since QCD is Lorentz invariant, we the energy of the boosted basis state satisfies

$$\sqrt{(M_j c^2)^2 + c^2|\mathbf{P}|^2}\ \Phi'_j(\mathbf{P}) = \hat{H}_{\mathrm{QCD}}\Phi'_j(\mathbf{P}). \tag{26}$$

Since we are working with a complete set of (mathematical) states, we can expand the boosted state in terms of the rest frame basis

$$\Phi'_j(\mathbf{P}) = \exp\left\{i\frac{\mathbf{P}}{\hbar}\cdot\mathbf{R}\right\}\sum_k \langle\Phi_k(0)|\Phi'_j(\mathbf{P})\rangle\Phi_k(0). \tag{27}$$

Since there is no center of mass dependence outside of the explicit plane wave dependence, it is possible to expand the rearranged internal nuclear wavefunction in terms of rest frame basis states.

4.4. Linearization around the rest frame

For nuclei in the lattice, the coherent energy transfer effects of interest to us will occur under conditions where the nuclei individually are moving slowly. Consequently, we would like to develop an approximate relativistic model that will be useful in the vicinity of the rest frame. To proceed, we probably need to extract the rest frame part of $\hat{H}_{\mathrm{QCD}}$. To do so, we can make use (at least formally) of the rest frame basis states in order to construct a rest frame version of the Hamiltonian

$$\hat{H}_0 = \sum_j |\Phi_j(0)\rangle M_j c^2\langle\Phi_j(0)|. \tag{28}$$

Next, we assume that we can obtain a reasonable boosted wavefunction keeping terms only up to first order in the rotation

$$\Phi'_j(\mathbf{P}) = \exp\left\{i\frac{\mathbf{P}}{\hbar}\cdot\mathbf{R}\right\}\left[\Phi_j(0) + \left(\nabla_{\mathbf{P}}\hat{\mathcal{U}}\right)_{\mathbf{P}=0}\cdot\mathbf{P}\Phi_j(0) + \cdots\right]. \tag{29}$$

We would expect this approximate boost to produce an approximate solution to the Schrödinger equation (26); this we might expand as

$$\begin{aligned}\left[M_j c^2 + \frac{|\mathbf{P}|^2}{2M_j} + \cdots\right]\exp\left\{i\frac{\mathbf{P}}{\hbar}\cdot\mathbf{R}\right\}\left[\Phi_j(0) + \left(\nabla_{\mathbf{P}}\hat{\mathcal{U}}\right)_{\mathbf{P}=0}\cdot\mathbf{P}\Phi_j(0) + \cdots\right]\\ = \left[\hat{H}_0 + \left(\nabla_{\mathbf{P}}\hat{H}_{\mathrm{QCD}}\right)_{\mathbf{P}=0}\cdot\hat{\mathbf{P}} + \cdots\right]\exp\left\{i\frac{\mathbf{P}}{\hbar}\cdot\mathbf{R}\right\}\left[\Phi_j(0) + (\nabla_{\mathbf{P}}\hat{\mathcal{U}})_{\mathbf{P}=0}\cdot\mathbf{P}\Phi_j(0) + \cdots\right].\end{aligned} \tag{30}$$

There are some subtleties associated with such an equation. Since we needed to make use of the rest frame basis functions to construct the rest frame Hamiltonian, probably we need to do something similar in order to construct the gradient of the Hamiltonian. If we begin with $\nabla_{\mathbf{P}}\hat{H}_{\mathrm{QCD}}$, then it would follow that we can develop a rest frame version of it also by taking advantage of the rest frame basis

$$\left(\nabla_{\mathbf{P}}\hat{H}_{\mathrm{QCD}}\right)_{\mathbf{P}=0} = \sum_j\sum_k |\langle\Phi_j(0)\rangle\langle\Phi_j(0)|\nabla_{\mathbf{P}}\hat{H}_{\mathrm{QCD}}|\Phi_k(0)\rangle\langle\Phi_k(0)|. \tag{31}$$

We can isolate the rest frame part of the boost operator similarly. In the end, we match terms linear in **P** to obtain a relation between the gradient of the unitary operator and the gradient of the Hamiltonian

$$\left(\nabla_{\mathbf{P}}\hat{\mathcal{U}}\right)_{\mathbf{P}=0} = \left(M_j c^2 - \hat{H}_0\right)^{-1} \left(\nabla_{\mathbf{P}}\hat{H}_{\text{QCD}}\right)_{\mathbf{P}=0}. \tag{32}$$

Note that this discussion has been focused on what happens to a single basis state, so that in this equation the operator on the LHS is specific to Φ_j. We could obtain a more general version of the operator by replacing the rest frame mass M_j with the rest frame mass matrix.

4.5. Reduction to matrix form

Our discussion so far has been pretty general, but now we need to attend to the problem of developing a model that we can use in the context of a lattice Hamiltonian. In essence, the point of the development above was to achieve a separation between the center of mass dynamics and the internal dynamics in a way that will be useful in what follows. The linearized Hamiltonian is now expressed completely in terms of rest frame basis states and the center of mass momentum operator. It will be convenient to write this as

$$\begin{aligned} &\hat{H}_0 + \left(\nabla_{\mathbf{P}}\hat{H}_{\text{QCD}}\right)_{\mathbf{P}=0} \cdot \hat{\mathbf{P}} + \cdots \\ &\quad = \sum_j |\Phi_j(0)\rangle M_j c^2 \langle\Phi_j(0)| + \sum_{j,k} |\Phi_j(0)\rangle\langle\Phi_j(0)|\nabla_{\mathbf{P}}\hat{H}_{\text{QCD}} \cdot \hat{\mathbf{P}}|\Phi_k(0)\rangle\langle\Phi_k(0)| + \cdots \end{aligned} \tag{33}$$

It will be convenient to define the vector $\mathbf{a}_{jk}$ according to

$$\mathbf{a}_{jk} = \frac{1}{c}\langle\Phi_j(0)|\nabla_{\mathbf{P}}\hat{H}_{\text{QCD}}|\Phi_k(0)\rangle. \tag{34}$$

This allows us to recast the Hamiltonian as

$$\hat{H}_0 + \left(\nabla_{\mathbf{P}}\hat{H}_{\text{QCD}}\right)_{\mathbf{P}=0} \cdot \hat{\mathbf{P}} + \cdots = \sum_j |\Phi_j(0)\rangle M_j c^2 \langle\Phi_j(0)| + \sum_{j,k} |\Phi_j(0)\rangle \mathbf{a}_{jk} \cdot c\hat{\mathbf{P}}\langle\Phi_k(0)| + \cdots \tag{35}$$

Since we have made use of the rest frame basis in the construction of the rest frame Hamiltonian, as well as for isolating the linear part, we can make use of a basis expansion in terms of rest frame states to construct a solution

$$\Psi = \exp\left\{i\frac{\mathbf{P}}{\hbar}\cdot\mathbf{R}\right\}\sum_j c_j \Phi_j(0). \tag{36}$$

The expansion coefficients satisfy a matrix version of the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\mathbf{c}(t) = \mathbf{H}\cdot\mathbf{c}(t) \tag{37}$$

with

$$\mathbf{H} = \mathbf{M}c^2 + \mathbf{a} \cdot c\hat{\mathbf{P}} + \cdots \tag{38}$$

Note that there are an infinite number of rest frame basis states, so these matrices are correspondingly infinitely large. It may be that a reasonable approximation can be developed in principle with a finite number of basis states; adopting a matrix form is convenient for such a finite basis approximation.

4.6. Quadratic relation

We can square the matrix version of the Hamiltonian operator to write

$$\hat{\mathbf{H}}^2 = (\mathbf{M}c^2)^2 + (\mathbf{M}c^2)(\mathbf{a} \cdot c\hat{\mathbf{P}}) + (\mathbf{a} \cdot c\hat{\mathbf{P}})(\mathbf{M}c^2) + (\mathbf{a} \cdot c\hat{\mathbf{P}})^2 + \cdots \tag{39}$$

Since the square of the total energy has no linear dependence on momentum, it follows that

$$(\mathbf{M}c^2)(\mathbf{a} \cdot c\hat{\mathbf{P}}) + (\mathbf{a} \cdot c\hat{\mathbf{P}})(\mathbf{M}c^2) = 0. \tag{40}$$

Since the square of the energy depends on the square of the momentum with no higher order terms appearing, if follows that

$$\hat{\mathbf{H}} = \mathbf{M}c^2 + \mathbf{a} \cdot c\hat{\mathbf{P}} \tag{41}$$

with no higher-order terms (the $\cdots$ above must be zero). In addition, the **a**-matrix must satisfy

$$(\mathbf{a} \cdot c\hat{\mathbf{P}})^2 = c^2|\hat{\mathbf{P}}|^2. \tag{42}$$

4.7. Dirac-like formalism for composite nuclei

In essence, the argument here is that if we work with the rest frame basis states, the the form of the associated matrix Hamiltonian must be analogous to the free-space Dirac Hamiltonian

$$\mathbf{M}c^2 + \mathbf{a} \cdot (c\hat{\mathbf{P}}) \;\leftrightarrow\; \beta M c^2 + \boldsymbol{\alpha} \cdot (c\hat{\mathbf{P}}). \tag{43}$$

The Dirac matrices are very simple, and the mass matrix for the composite nucleus using the rest frame basis is diagonal. The **a**-matrix for the composite nucleus will be enormously complicated; fortunately we will need only a small number of matrix elements in working with the model that results.

4.8. Discussion

When we began these studies our focus was on many-nucleon Dirac models primarily because such models were the simplest one that were likely to contain the effects we sought [and these models resulted in a free composite Hamiltonian of the form $\mathbf{M}c^2 + \mathbf{a} \cdot (c\hat{\mathbf{P}})$]. Now that we have some experience working with these earlier models, the path forward to generalize the approach to more sophisticated models seems clearer.

In all cases the basic issue is that a rest frame state is modified according to relativity when boosted, although how this works is different in a Dirac model versus a Lorentz covariant model such as QCD. Now we have a better formulation that can be used systematically for either approach, and we are able to have a consistent formulation that can be used with a covariant field theory.

There remain issues that are worth some additional thought. In view of the discussion of the previous section, we understand that the complete set of basis states includes positive energy states, as well as states in other sectors where some components involve negative energy states. This is a necessary feature of the formulation (as it was in the previous section) since in general the construction of a positive energy boosted wavefunction will require pieces that are from sectors with negative energy components in the rest frame.

5. Lattice Model with Internal Nuclear Degrees of Freedom

We now have a starting place for a general description of nuclei embedded in a lattice that takes into account changes in the internal nuclear wavefunction due to relativity when it moves. In the event that we make use of a Born–Oppenheimer approximation, we end up with a model that describes the interaction between interacting nuclei, including the coupling between the nuclear momentum and internal degrees of freedom. The resulting problem constitutes the generalization of the Dirac proton lattice model of Section 3, and the issues that arise are analogous. In this section we consider the model itself, the use of a generalized Foldy–Wouthuysen transformation for the elimination of the first-order coupling, the nonrelativistic limit of the model, and the possibility that regimes exist where the Foldy–Wouthuysen transformation is not useful.

5.1. A model for nuclei in the lattice

We make use of the matrix Hamiltonian of the previous section to construct a many-nucleon Hamiltonian that interact through effective potentials that arise from a Born–Oppenheimer treatment of the electrons

$$\hat{H} = \sum_j \left(\mathbf{M}c^2 + \mathbf{a} \cdot c\hat{\mathbf{P}} \right)_j + \sum_{j<k} V(|\mathbf{R}_j - \mathbf{R}_k|). \quad (44)$$

This model constitutes a direct generalization of the idealized model of Section 2. Once again we have adopted a simple effective potential for interactions between nuclei which is easily generalized to more complicated models which better describe physical systems.

Although this model is of the same form as earlier coupled lattice and nuclear models that we have put forth previously [41,42], this one is different. The basis states that provide the foundation for the construction of the matrices are now eigenstates of the rest frame QCD problem. We recognize now that the dominant coupling of the $\mathbf{a} \cdot c\mathbf{P}$ interaction is with states that have explicit negative energy components, generalizing the situation encounter with the Dirac phenomenology of Section 2. Although our discussion of the previous section focused on a QCD description for the nuclei, we might have used any other covariant model with similar results.

5.2. Generalized Foldy–Wouthuysen transformation

As was the case with the Dirac proton model, we see in this model a first-order coupling between the center of mass momentum of the nuclei and their internal degrees of freedom. And as before we are able to carry out a rotation that eliminates this first-order coupling which leads to

$$\hat{H}' = \hat{\mathcal{U}}^\dagger \hat{H} \hat{\mathcal{U}} = \sum_j \left(\mathbf{M}c^2 \sqrt{1 + \frac{c^2|\hat{\mathbf{P}}|^2}{(\mathbf{M}c^2)^2}} \right)_j + \sum_{j<k} \hat{V}'_{jk}, \quad (45)$$

where

$$\hat{V}'_{jk} = \hat{\mathcal{U}}^{\dagger} V(|\mathbf{R}_j - \mathbf{R}_k|)\hat{\mathcal{U}}. \tag{46}$$

We recognize the rotation that accomplished this as a generalized Foldy–Wouthuysen transformation; one which diagonalizes in this case very large matrices, rather than simple two by two matrices of Section 2. The specific unitary operator $\hat{\mathcal{U}}$ that does this is very complicated, and can be obtained formally from rest frame matrix elements of the boost operator of the previous section. We note that generalizations of the Foldy–Wouthuysen rotation beyond the single Dirac particle have been discussed in the literature (e.g., see [47], [48,49]).

5.3. Discussion and nonrelativistic limit

In the original Hamiltonian of equation (44) we see a strong first-order $\mathbf{a} \cdot c\mathbf{P}$ coupling between the two degrees of freedom that produces mixing between the different degrees of freedom. Note that the generalized Foldy–Wouthuysen transformation has removed the first-order coupling between the momentum and internal nuclear transitions in the rotated version of the problem. In the transformed Hamiltonian, the two degrees of freedom are very nearly independent. We might think of the original Hamiltonian as describing the "physical" system, and the rotated Hamiltonian as describing a "dressed" version of the system. The "dressed" system is free of the strong coupling between the composite motion and internal degrees of freedom; it is this situation upon which our intuition about how the world works in solid state physics (that the nuclei effective don't notice lattice vibrations).

From this perspective, the situation that occurs when the generalized Foldy–Wouthuysen transform becomes inappropriate perhaps makes more sense. In both regimes there occurs strong mixing between the nuclear and vibrational system; we have grown so used to the conventional regime where the generalized Foldy–Wouthuysen transform works that the "dressed" version of the system looks like reality to us; consequently we are amazed when we see a regime where the generalized Foldy–Wouthuysen transform doesn't work and the mixing between the two degrees of freedom lead to anomalies.

As was the case previously, when the generalized Foldy–Wouthuysen transformation can be used we are able to develop the nonrelativistic approximation

$$\hat{H}' \;\rightarrow\; \sum_j \left(\mathbf{M}c^2 + \frac{|\hat{\mathbf{P}}|^2}{2\mathbf{M}}\right)_j + \sum_{j<k} \hat{V}'_{jk}. \tag{47}$$

6. Composite Nuclei in a Harmonic Lattice

At this point we have assembled a foundation sufficient to allow us to take the next step, which is to consider composite nuclei interacting in a harmonic lattice. This problem is closely related to the idealized model for Dirac protons in a harmonic lattice considered above; hence, from the discussion above we anticipate that a generalized Foldy–Wouthuysen transformation will be able to eliminate the first-order coupling between the composite center of mass momentum and internal degrees of freedom. On the other hand, we also know that the problem is also closely related to the lossy spin–boson model mentioned above and described in earlier works; consequently, we expect that under some conditions a Foldy–Wouthuysen transformation will be unhelpful.

6.1. Composite nuclei in a harmonic lattice

Composite nuclei in a harmonic lattice (again within a Born–Oppenheimer approximation) are described then by a Hamiltonian of the form

$$\hat{H} = \sum_j \left(\mathbf{M}c^2 + \mathbf{a} \cdot c\hat{\mathbf{P}} \right)_j + V_0 + \sum_{j<k} (\mathbf{r}_j - \mathbf{r}_k) \cdot \mathbf{K}_{jk} \cdot (\mathbf{r}_j - \mathbf{r}_k). \tag{48}$$

We would like to work with lattice position and momentum operators as for the Dirac proton version of the problem. For this, we make use of the same mathematical device of adding and subtracting nonrelativistic kinetic energy terms to obtain

$$\begin{aligned}\hat{H} =& \sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M_j} + V_0 + \sum_{j<k} (\mathbf{r}_j - \mathbf{r}_k) \cdot \mathbf{K}_{jk} \cdot (\mathbf{r}_j - \mathbf{r}_k) \\ &+ \sum_j \left(\mathbf{M}c^2 + \mathbf{a} \cdot c\hat{\mathbf{P}} \right)_j - \sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M_j},\end{aligned} \tag{49}$$

where we adopt ground state nuclear masses for the nonrelativistic kinetic energy terms. As before, the associated harmonic lattice problem is recast in terms of phonon mode operators

$$\sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M_j} + \sum_{j<k} (\mathbf{r}_j - \mathbf{r}_k) \cdot \mathbf{K}_{jk} \cdot (\mathbf{r}_j - \mathbf{r}_k) \ \rightarrow \ \sum_\mu \hbar\omega_\mu \left(\hat{a}_\mu^\dagger \hat{a}_\mu + \frac{1}{2} \right). \tag{50}$$

We may write for the coupled harmonic lattice and nuclei problem the Hamiltonian

$$\hat{H} = \sum_\mu \hbar\omega_\mu \left(\hat{a}_\mu^\dagger \hat{a}_\mu + \frac{1}{2} \right) + V_0 + \sum_j \left(\mathbf{M}c^2 + \mathbf{a} \cdot c\hat{\mathbf{P}} \right)_j - \sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M_j}. \tag{51}$$

6.2. Generalized Foldy–Wouthuysen transformation

In a conventional regime (where strong loss terms are absent) we can carry out a generalized Foldy–Wouthuysen transformation for this Hamiltonian leading to

$$\hat{H}' = \sum_\mu \hbar\omega_\mu \left(\hat{a}_\mu^\dagger \hat{a}_\mu + \frac{1}{2} \right) + V_0 + \sum_j \left(\mathbf{M}c^2 \sqrt{1 + \frac{c^2 |\hat{\mathbf{P}}|^2}{(\mathbf{M}c^2)^2}} \right)_j - \sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M_j} + \sum_{j<k} \Delta \hat{V}'_{jk}, \tag{52}$$

where

$$\Delta \hat{V}'_{jk} = \left[(\mathbf{r}'_j - \mathbf{r}'_k) \cdot \mathbf{K}_{jk} \cdot (\mathbf{r}'_j - \mathbf{r}'_k) \right] - \left[(\mathbf{r}_j - \mathbf{r}_k) \cdot \mathbf{K}_{jk} \cdot (\mathbf{r}_j - \mathbf{r}_k) \right]. \tag{53}$$

In this case we worked with quantized vibrations and an appropriate relativistic nuclear model, and once again we have removed the strong first-order coupling between the vibrational and internal nuclear degrees of freedom. We recognize that we must add to this the constraint that we want to take the positive energy sector states to correspond to physical nuclei; and we would like further to match the nuclear state mass to the mass used in the kinetic energy terms used for the construction of the phonon mode. In the resulting "dressed" version of the problem, we recognize that the system is very nearly decoupled, and we would not expect to see anomalies.

We are able to develop a nonrelativistic model from this rotated Hamiltonian; we may write

$$\hat{H}' \rightarrow \sum_j M_j c^2 + \sum_\mu \hbar\omega_\mu \left(\hat{a}^\dagger_\mu \hat{a}_\mu + \frac{1}{2}\right) + V_0, \tag{54}$$

where we have eliminated higher-order terms, and further assumed (positive energy) ground state occupation of the dressed composite nuclear states.

6.3. Loss mechanisms

As discussed above, we know that in the presence of strong loss the lossy spin–boson model predicts efficient coherent energy exchange under conditions of fractionation, which is qualitatively different from what we see in the normal spin–boson model. Because of the close connection between the lossy spin–boson model, and the models under discussion here, we anticipate a similar difference for composite nuclei in a harmonic lattice when loss is present.

The issue relevant here then is what loss mechanisms should be considered in this context. Usually when loss is considered in the context of a simple harmonic oscillator, the discussion is focused on dissipation effects that provide "friction;" which is the most important loss in many applications. Here, the issue is more subtle. For example, such friction losses are hardly going to impact the utility of a generalized Foldy–Wouthuysen transformation. What would make a real difference is a massive loss of state occupation for states critical to the separation of degrees of freedom accomplished by the Foldy–Wouthuysen transformation.

In general we would not expect a significant impact on this state occupation for a thermal lattice, or even for localized excitations. The situation is different in the event that a single mode is very highly excited. For the spin–boson case the Hamiltonian provides coupling which results in massive coupling between the different unrotated states. All of this coupling is of course sorted out under the Foldy–Wouthuysen transformation. However, if fast loss channels are present then the situation changes drastically. Many of the states coupled to in the unrotated spin–boson model are basis states driven very far off of resonance, which have much less energy than the system has (as measured by the eigenvalue of the overall state under consideration). Such states might be considered to have an energy surplus, and the decay rate can become greatly enhanced on account of this energy surplus. Basis states at higher energy suffer an energy deficit, so the associated decay rate is reduced. This describes the mechanism responsible for removing destructive interference in the lossy spin–boson model, which leads to a large increase in coherent energy exchange under conditions of fractionation.

In a metal, phonon loss to electron promotion would be expected to be the dominant energy loss mechanism for the coupled phonon–nuclear system. A highly-excited vibrational mode will similarly lose energy rapidly if a strong vibrational nonlinearity is present. These are the most important loss mechanisms under consideration in this discussion.

6.4. Lossy coupled lattice–nuclear model

In light of this discussion, we might augment the model with these loss channels and write

$$\hat{H} = \sum_\mu \hbar\omega_\mu \left(\hat{a}^\dagger_\mu \hat{a}_\mu + \frac{1}{2}\right) + V_0 + \sum_j \left(\mathbf{M}c^2 + \mathbf{a}\cdot c\hat{\mathbf{P}}\right)_j - \sum_j \frac{|\hat{\mathbf{P}}|^2}{2M} - i\frac{\hbar\hat{\Gamma}(E)}{2}. \tag{55}$$

We have used such a notation in previous work to denote the augmentation of similar models with loss. We recognized the operator $\hat{\Gamma}(E)$ as a loss operator in an infinite-order Brillouin–Wigner formalism [27,50]. In such a formalism one works with a Hermitian model, and then divides the state space into sectors. If we focus on a single sector, then interactions which couple from one sector to another appear not to be Hermitian with respect to that sector. If the associated loss produces an exponential decay of the sector probability, then such a description is very useful since one can carry out an approximate evaluation of the decay rate within the formalism to obtain the Golden Rule estimate. Consequently, we recognize this Hamiltonian as describing a relevant sector of interest, with the loss operator keeping track of the associated decay mechanisms (such as those described above).

Note that it is straightforward to write down relevant Hermitian models. For example, in the case of anharmonic coupling and atomic ejection, we could add atomic continuum states explicitly and describe the associated nonlinear coupling. Some nuclear excitation (and disintegration) in principle is already described since we have the $\mathbf{a} \cdot c\mathbf{P}$ coupling present. Coupling to electrons could be modeled using an appropriate electron Hamiltonian and adding electron-phonon interaction terms.

6.5. Discussion

As discussed above, when accessible fast loss channels are available that are sufficiently strong to impact the state occupation, then the generalized Foldy–Wouthuysen transformation becomes inappropriate. We are still able to carry out the rotation mathematically, but the implementation of the loss operator becomes problematic, and the resulting picture is not useful. In this case we need to work with unrotated problem with its strong first-order coupling and strong loss directly. In this regime the strong first-order coupling between vibrational and internal nuclear degrees of freedom (which is normally hidden from us because we are used to the rotated frame where it is eliminated) has the potential to produce anomalies observed in experiments.

Previously we would have considered the model of Eq. (55) to constitute the basic model that describes anomalies in condensed matter nuclear science. By now we know that this model is at the same time successful and unsuccessful. The model is known to be successful in that it describes new effects such as collimated X-rays in the Karabut experiment; excess heat generation and nonenergetic ^{4}He production in the Fleischmann–Pons experiment; it resolves Huizenga's three miracles; it sheds light on the origin of low-level gamma emission in the Gozzi experiment [51] and in Piantelli's experiment [52]; and it provides a basis to understand some transmutation effects. Sadly, the model is unsuccessful in that the conditions where these effects are predicted in the analysis done so far do not match with those of the experiments.

In a sense, we are close. But something is still missing from the model (and our effort to remedy this will be dealt with in following publications).

7. Lattice-induced Nuclear Excitation

As we have seen from many years of developing and analyzing models, models for excess heat production within the approach we have pursued are complicated (in that there are donor transitions and receiver transitions); there are uncertainties (we do not know from experiment in general which transitions operate as receiver transitions in the model); and in the end it is hard to be certain that the model is correct (due to the absence of relevant observables in the experiments). Much better would be a simpler effect with only one set of transitions, and even better if there was a clean diagnostic to tell from experiment what is going on in more detail.

In light of these difficulties, in recent years our focus has shifted to Karabut's collimated X-rays. These we have interpreted as due to direct excitation of the 1565 eV transition in a small number of ^{201}Hg impurities on the cathode surface. If this interpretation is correct, then the situation is very different. Instead of two transitions (donor and receiver), only one would be involved here (very much reducing the model). For completeness, we note that there is also the possibility of a donor and receiver scheme leading to excitation of the ^{201}Hg, a possibility that will be considered in a subsequent paper. Although the identity of the transition has not been confirmed experimentally, it seems likely since it is the only nuclear transition from the ground state of a stable nucleus anywhere close to the energy observed in experiment. And finally if the 1565 eV ^{201}Hg transition is excited, we would expect electron emission, X-ray emission, and most importantly collimated X-ray emission if phase coherence is established.

7.1. Previous work

The problem of coherent energy exchange between a highly-excited oscillator and two-level systems in the lossy spin–boson model was considered as a mathematical problem in [27,29–31]. As a result, we might consider this to be a known problem that has been analyzed and solved within the framework of the lossy spin–boson model. However, as mentioned above there is a difference between the (toy) mathematical model (of the lossy spin–boson model), and a physical model (such as that of composite nuclei in a harmonic lattice as discussed above). While the mathematical model clarifies how the physical mechanism works, we expect a physical model to predict the physical conditions under which the effect should be observed.

The situation at present is then that we have relevant mathematical models based on the lossy spin–boson model that we can solve, and which give results which seem to be connected to experiment. By now we also have experience with a number of physical models, all of which we can analyze with sufficient accuracy to ascertain whether they agree with experiment or not. For models based on electron–nuclear coupling as a basis for phonon–nuclear interaction, there are orders of magnitude between the predictions and experiment. In the case of a donor and receiver model based on electron–electron coupling for fractionation, there are again orders of magnitude difference (but fewer) between the model and experiment.

Now that we have a much improved model for phonon–nuclear coupling as described by Eq. (55), which is based on a much stronger coupling between vibrations and the internal nuclear degrees of freedom, of interest is whether this model agrees with experiment. Sadly, our initial efforts at predicting the Karabut experiment with this model showed some deficiency remained, either in the fundamental theory, or else in the particular model examined for the Karabut experiment. Although collimated X-ray emission is predicted, the fractionation power in this model seems to be short of what the experiment seems to be doing by at least two orders of magnitude. While far superior to earlier models (in that the numbers are now very much closer), some problem remains.

During the summer of last year, we had a brainstorm as to how this problem might be resolved. The idea was that perhaps the transitions that are coupled to most strongly would produce additional phonon fluctuations which might make up the difference. Under the gun before the ICCF17 we analyzed a model of this kind, and found (errantly) that these additional fluctuations could provide an enhancement to the fractionation power, resulting in general agreement between our proposed model for the Karabut experiment and our interpretation of the experimental conditions. For a while things were very exciting, since we were able for the first time to work with a physical model that seemed to give good results for the Karabut experiment [42], and at the same time could make sense of excess heat experiments, and also gamma emission [43]. After the conference while writing up the model, we found the error. We now know that this approach that we had tried doesn't work.

In what follows in this section, we consider the basic arguments of last summer's model more carefully. At issue here is the question of what happens in the case of a relatively weak low-energy transitions when a great many much stronger (and lossy) high-energy transitions are present. The issue is relevant generally if we are to make use of this kind of model, and since the models are new we have little intuition *a priori*. The result of the analysis is that we would expect essentially no contribution from all of these much stronger lossy transitions. This resolves the issues raised last summer; sadly, this also takes away the good agreement between the new theory and Karabut model, and experiment, that had for a few months been elating. Even so, there is good news in the result, and that is that even when we can't use Foldy–Woutuysen transformation, the result that we obtain for all transitions not involved in the coherent dynamics is the same as if we had been able to use the transformation. This means that we are free to focus on those transitions involved in phonon-nuclear coherent dynamics, which simplifies what we need to do when analyzing the model considerably.

However, in spite of all that is good about it, the new theory and our particular Karabut model is still not in agreement with our interpretation of the experiment. This will motivate us to re-examine the theory, the model, and the interpretation of the experiment, in following works.

7.2. The model

We are interested then in a model for lattice-induced nuclear excitation relevant to collimated X-ray emission in the Karabut experiment. Our starting place for this analysis will be the fundamental phonon–nuclear Hamiltonian developed in the last section

$$\hat{H} = \sum_{\mu} \hbar\omega_{\mu} \left(\hat{a}^{\dagger}_{\mu}\hat{a}_{\mu} + \frac{1}{2} \right) + V_0 + \sum_j \left(\mathbf{M}c^2 + \mathbf{a} \cdot c\hat{\mathbf{P}} \right)_j - \sum_j \frac{|\hat{\mathbf{P}}|^2}{2M} - i\frac{\hbar\hat{\Gamma}(E)}{2}.$$

Here, all the phonon modes and all transitions in all nuclei are accounted for. Our job in what follows will be to bring out the dynamics associated with the highly excited phonon mode and preferred nuclear transition.

7.3. The coupled lattice-nuclear problem

We assume that the sufficiently fast decay channels restrict us from using a generalized Foldy–Wouthuysen transformation, in which case we need to pursue solutions for the coupled lattice and nuclear problem. The strongest coupling occurs with basis states that have negative energy components, and also with internal nucleon degrees of freedom (isobars). Consequently, we would like to deal with the coupling with these degrees of freedom first.

In previous work we proposed to make up separate $\mathbf{M}c^2$ and $\mathbf{a} \cdot c\mathbf{P}$ terms for the preferred transitions, and for all other transitions. Such an approach has the advantage that it is conceptually easy to explain and to work with; but it has the disadvantage that it doesn't provide such a good match to the physical system. Here we will use a different approach where we work with the Hamiltonian as given rather than splitting it up. Instead here we split up the transition matrix into separate parts

$$\left(\mathbf{a} \cdot c\hat{\mathbf{P}} \right)_j = \left(\overline{\mathbf{a}} \cdot c\hat{\mathbf{P}} \right)_j + \left(\mathbf{a}_{\text{preferred}} \cdot c\hat{\mathbf{P}} \right)_j, \tag{56}$$

where the preferred transition is separated from all others. The idea is that we are interested in describing coherent dynamics on the preferred transition, while conditions on the other transitions are more nearly static. If we wish to be precise, we should also extract the contribution of this transition from the counter term, and write

$$\sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M_j} = \overline{\sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M_j}} + \left(\sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M_j} \right)_{\text{preferred}}. \tag{57}$$

In practice the contribution of the preferred transition to the counter term is trivially small (e.g., in the case of nonlinear Rabi oscillations), so that we might reasonably make use of the full kinetic energy counter term for the rest of the problem. Also, from previous work we know that the counter term plays very little role under conditions where coherent dynamics occurs, so that it could be neglected away from threshold.

In light of these comments we seek eigenfunctions and eigenvalues of the coupled lattice and nuclear problem (in the absence of the preferred transition) given by

$$E\Upsilon = \left\{ \sum_{\mu} \hbar\omega_{\mu} \left(\hat{a}_{\mu}^{\dagger}\hat{a}_{\mu} + \frac{1}{2} \right) + V_0 + \sum_{j} \left(\mathbf{M}c^2 + \overline{\mathbf{a}} \cdot c\hat{\mathbf{P}} \right)_j - \sum_{j} \frac{|\hat{\mathbf{P}}|^2}{2M} - i\frac{\hbar\hat{\Gamma}(E)}{2} \right\} \Upsilon. \tag{58}$$

The eigenfunctions that result from this calculation are very close to the states of the transformed system (but expressed in the unrotated frame) were we able to make use of the Foldy–Wouthuysen transformation. If there were no preferred transition and we used the full transition matrix **a** (instead of the reduced $\overline{\mathbf{a}}$), and if loss could be neglected, then the eigenfunctions are the same (to within a unitary transformation) as the states of the separated problem following the Foldy–Wouthuysen transformation. In the unconventional regime where the Foldy–Wouthuysen transformation is not helpful, this calculation takes its place in the description of most of the coupled system.

We have recently studied a similar model in which a highly excited mode is coupled to N-level transitions initially in the ground state, with highly unstable excited states [50]. Our present model is different in that there are many states at lower energy that involve negative energy components. However, since these cannot have real occupation, the extension of the model to such states involves no modifications that will end up producing a different answer in interactions with the highly excited mode. We found that approximate product solutions gave results very similar to exact numerical solutions for a highly excited oscillator as long as the coupling is strong.

Interactions with unexcited modes or thermal modes produces mixing which matches the contribution to the counter term to second order exactly on a mode by mode basis. The detailed analysis of this problem would require a minor modification of the approach used in [50] to adapt it to low n, but essentially the same product state approximation would be effective.

7.4. Finite basis expansion for the low-energy dynamic transition

Next we focus on the coupling between the preferred low-energy nuclear transition and the highly excited mode. In previous work we found that we could develop good estimates for the rate of coherent energy exchange by working with a finite basis expansion for product states of the oscillator number states and two-level system Dicke states. Unfortunately in this problem the oscillator is now strongly-coupled to the internal nuclear transitions, and this needs to be taken into account in our analysis.

In view of these comments, we adopt a global solution of the form

$$\Psi = \sum_j c_j \Upsilon_j, \tag{59}$$

where the coupled nuclear and lattice states Υ_j includes excitations of the lattice, the preferred transition, as well as all other states. In general these states are too complicated to work with, so we need to simplify things to proceed. Since our focus is on the dynamics of the the preferred transition, and on energy exchange with the highly excited phonon mode, it seems sensible to bring out the associated indices of these systems and suppress those not immediately involved. To accomplish this we adopt the notation

$$\Upsilon_j \;\rightarrow\; \Upsilon_{m,n}, \tag{60}$$

where n is essentially the number of oscillator quanta in the highly excited mode, and where m is a Dicke index associated with the Dicke states $|S, m\rangle$ of the two-level system. It may not be obvious that such a notation is appropriate, given that we are dealing with a system that involves substantial coupling between the vibrational and nuclear degrees of freedom. These states are complicated, so we might expect that more is needed to describe them.

However, we recall that the coupled vibrational and nuclear system we are dealing with would be described by

$$E\Upsilon' = \left\{ \sum_\mu \hbar\omega_\mu \left(\hat{a}^\dagger_\mu \hat{a}_\mu + \frac{1}{2} \right) + V_0 + \sum_j \left(\mathbf{M}c^2 \sqrt{1 + \frac{c^2 |\hat{\mathbf{P}}|^2}{(\mathbf{M}c^2)^2}} \right)_j - \sum_j \frac{|\hat{\mathbf{P}}_j|^2}{2M_j} + \sum_{j<k} \Delta \hat{V}'_{jk} \right\} \Upsilon' \tag{61}$$

if we could make use of the Foldy–Wouthuysen transformation. In the unconventional regime we cannot make use of the transformation, but nonetheless the coupled lattice and nuclear states are, for the most part, not very different from what we would compute in the conventional regime. Since there is no difficulty with the assignment of n or m for the conventional regime, it should probably not be surprised that the same indices are appropriate in the unconventional regime.

It will be useful to take another step along these lines. In the conventional regime we would have no difficulty in using a product wavefunction for the highly excited mode and Dicke system

$$\Upsilon_{m,n} \ \rightarrow \ \overline{\Upsilon}|n\rangle|S, m\rangle. \tag{62}$$

For the unconventional regime we can reasonably separate out the Dicke system, but for now we will keep the background coupled vibrational and nuclear states together keeping in mind the mixing; in this case we write

$$\Upsilon_{m,n} \ \rightarrow \ \overline{\Upsilon}_n |S, m\rangle \qquad \text{(conventional)}. \tag{63}$$

In the end our finite basis expansion is of the form

$$\Psi = \sum_m \sum_n c_{m,n} \overline{\Upsilon}_n |S, m\rangle. \tag{64}$$

7.5. Resonant versus off-resonant states

Before continuing there remains on last issue to address; this involves whether the basis states are resonant (real) or off-resonant (virtual) states. It is this issue which led to problems in our earlier analysis of lattice-induced nuclear excitation in Refs. [42,43], so we are motivated to focus some attention on the issue here.

The case of real states probably corresponds best to our intuition, so this would be the place to start. The issue here is that the energy we would use to evaluate the loss operator would be the same as the energy eigenvalue; we might denote this situation as

$$E_{m,n}\Upsilon_{m,n} = \left\{ \sum_{\mu} \hbar\omega_\mu \left(\hat{a}_\mu^\dagger \hat{a}_\mu + \frac{1}{2} \right) + V_0 + \sum_j \left(\mathbf{M}c^2 + \overline{\mathbf{a}} \cdot c\hat{\mathbf{P}} \right)_j - \sum_j \frac{|\hat{\mathbf{P}}|^2}{2M} - i\frac{\hbar\hat{\Gamma}(E_{m,n})}{2} \right\} \Upsilon_{m,n} \qquad \text{(real)}. \tag{65}$$

Alternatively, we might be interested in the computation of the coupled lattice and nuclear states in the off-resonant case. For example, in a finite basis calculation we might have basis states of the coupled lattice and nuclear problem for which the part of the system energy available is very different than the basis state energy. In this case, we might indicate this as

$$E_{m,n}\Upsilon_{m,n} = \left\{ \sum_{\mu} \hbar\omega_\mu \left(\hat{a}_\mu^\dagger \hat{a}_\mu + \frac{1}{2} \right) + V_0 + \sum_j \left(\mathbf{M}c^2 + \overline{\mathbf{a}} \cdot c\hat{\mathbf{P}} \right)_j - \sum_j \frac{|\hat{\mathbf{P}}|^2}{2M} - i\frac{\hbar\hat{\Gamma}(E)}{2} \right\} \Upsilon_{m,n} \qquad \text{(virtual)}. \tag{66}$$

These two problems are very different, especially since the unconventional regime is one where the loss is presumed to be extremely fast for some of the accessible states. As we are using state exclusion as a way to take into account the very fast loss, a different set of states would be excluded in the two calculations. We need to make sure that the correct ones are used in for the computations that follow.

7.6. Eigenvalue equation for the expansion coefficients

We can take our finite basis expansion and insert into the model to obtain an eigenvalue equation for the expansion coefficients; this produces

$$\begin{aligned} Ec_{m,n} =& E_{m,n}c_{m,n} \\ & - i\left(\mathbf{a}_0 \cdot c\frac{\mathrm{d}\hat{\mathbf{P}}}{\mathrm{d}a}\right)\sqrt{(S-m)(S+m+1)}\sum_{\Delta n_1}\langle\overline{\Upsilon}_{m,n}|\hat{a}|\overline{\Upsilon}_{m+1,n+\Delta n_1}\rangle c_{m+1,n+\Delta n_1} \\ & + i\left(\mathbf{a}_0 \cdot c\frac{\mathrm{d}\hat{\mathbf{P}}}{\mathrm{d}a}\right)\sqrt{(S-m)(S+m+1)}\sum_{\Delta n_1}\langle\overline{\Upsilon}_{m,n}|\hat{a}^\dagger|\overline{\Upsilon}_{m+1,n+\Delta n_1}\rangle c_{m+1,n+\Delta n_1} \\ & - i\left(\mathbf{a}_0 \cdot c\frac{\mathrm{d}\hat{\mathbf{P}}}{\mathrm{d}a}\right)\sqrt{(S+m)(S-m+1)}\sum_{\Delta n_1}\langle\overline{\Upsilon}_{m,n}|\hat{a}|\overline{\Upsilon}_{m-1,n+\Delta n_1}\rangle c_{m-1,n+\Delta n_1} \\ & + i\left(\mathbf{a}_0 \cdot c\frac{\mathrm{d}\hat{\mathbf{P}}}{\mathrm{d}a}\right)\sqrt{(S+m)(S-m+1)}\sum_{\Delta n_1}\langle\overline{\Upsilon}_{m,n}|\hat{a}^\dagger|\overline{\Upsilon}_{m-1,n+\Delta n_1}\rangle c_{m-1,n+\Delta n_1}. \end{aligned} \tag{67}$$

As in our previous work, we implement loss through the removal of highly unstable states. The idea is that when the associated decay rate of a state is fast in a sector Hamiltonian, faster than can be replenished by transitions to that state, then the occupation of the state is reduced. We have found in previous work that only minor differences in the coherent energy exchange rate occur between models with accurate loss models and those where the unstable states are removed.

7.7. Approximate eigenvalue equation

It will be convenient to take the limit where S is large, but where $|m|$ is not close to S; in this case we approximate

$$\sqrt{(S-m)(S+m+1)} \ \rightarrow\ \sqrt{S^2-m^2},$$
$$\sqrt{(S+m)(S-m+1)} \ \rightarrow\ \sqrt{S^2-m^2}. \tag{68}$$

Under conventional conditions where the Foldy–Wouthuysen transformation can be used, we can write for the phonon exchange matrix elements

$$\langle \overline{\Upsilon}_{m,n}|\hat{a}|\overline{\Upsilon}_{m\pm 1,n+\Delta n_1}\rangle \ \rightarrow\ \sqrt{n_0}\,\delta_{\Delta n_1,1} \qquad \text{(conventional)},$$
$$\langle \overline{\Upsilon}_{m,n}|\hat{a}^\dagger|\overline{\Upsilon}_{m\pm 1,n+\Delta n_1}\rangle \ \rightarrow\ \sqrt{n_0}\,\delta_{\Delta n_1,-1} \qquad \text{(conventional)}, \tag{69}$$

where we have assumed that the oscillator is highly excited, so that n_0 is very large, and n is near n_0. In the unconventional regime this remains the case for the majority of the n states; because of this, it is convenient to write the eigenvalue equation as

$$\begin{aligned} Ec_{m,n} =& E_{m,n}c_{m,n} - i\left(\mathbf{a}_0\cdot c\frac{\mathrm{d}\hat{\mathbf{P}}}{\mathrm{d}a}\right)\sqrt{n_0}\sqrt{S^2-m^2} \\ &\times\left\{\sum_{\Delta n_1}\frac{\langle \overline{\Upsilon}_{m,n}|\hat{a}-\hat{a}^\dagger|\overline{\Upsilon}_{m+1,n+\Delta n_1}\rangle}{\sqrt{n_0}}\,c_{m+1,n+\Delta n_1}\right. \\ &\left.+\sum_{\Delta n_1}\frac{\langle \overline{\Upsilon}_{m,n}|\hat{a}-\hat{a}^\dagger|\overline{\Upsilon}_{m-1,n+\Delta n_1}\rangle}{\sqrt{n_0}}\,c_{m-1,n+\Delta n_1}\right\}. \end{aligned} \tag{70}$$

We now have an eigenvalue equation that is similar to eigenvalue equations that we have encountered previously, and which we can analyze using the same methods as before. What is different here is that the energies of the basis states are not equi-spaced in n, and the coupling between the different states is now more complicated.

7.8. Periodic approximation

We found in previous work that we could reduce the two-dimensional problem down to a one-dimensional problem by taking advantage of the fact that when the resonance condition is satisfied

$$\Delta E = \Delta n\hbar\omega_0, \tag{71}$$

the system is nearly periodic for large S away from the boundaries (where $|m|$ is close to S). In this case

$$\left(\mathbf{a}_0 \cdot c\frac{\mathrm{d}\hat{\mathbf{P}}}{\mathrm{d}a}\right)\sqrt{n_0}\sqrt{S^2-m^2} \ \rightarrow \ g_v\hbar\omega_0 = \text{constant}. \tag{72}$$

We can construct approximate eigenfunctions of the locally periodic model using

$$c_{m,n} = \mathrm{e}^{im\phi}v_{n-m\Delta n}(\phi). \tag{73}$$

The v expansion coefficients then satisfy

$$E(\phi)v_n \ = \ E_n v_n - i\hbar\omega_0 g_v \left\{ \mathrm{e}^{i\phi}\sum_{\Delta n_1} \frac{\langle \overline{\Upsilon}_{m,n}|\hat{a}-\hat{a}^\dagger|\overline{\Upsilon}_{m+1,n+\Delta n_1}\rangle}{\sqrt{n_0}}\ v_{n+\Delta n_1-\Delta n} \right.$$
$$\left. -i\mathrm{e}^{-i\phi}\sum_{\Delta n_1} \frac{\langle \overline{\Upsilon}_{m,n}|\hat{a}-\hat{a}^\dagger|\overline{\Upsilon}_{m-1,n+\Delta n_1}\rangle}{\sqrt{n_0}}\ v_{n+\Delta n_1+\Delta n} \right\}, \tag{74}$$

where we implement loss through the elimination of states for negative n

$$v_n = 0 \quad \text{for } n < 0. \tag{75}$$

The index n is incremental in this case. The matrix elements for the $\overline{\Upsilon}$ states of the underlying coupled lattice nuclear problem is analyzed as in Ref. [50], and we take g_u for the associated dimensionless coupling constant.

From previous work we know that for large Δn we can estimate the indirect coupling matrix element from the difference between the energy eigenvalue for two phases

$$V_{\text{eff}} \ \rightarrow \ \frac{E(0)-E(\pi)}{4}. \tag{76}$$

7.9. Results

We have obtained numerical solutions for this model for representative cases, with the result that the model is only weakly dependent on the coupling strength associated with the mixed lattice and nuclear system. Results from a calculation with $\Delta n = 41$ are shown in Fig. 1. In essence the indirect matrix element depends only on g_v unless g_u gets to be sufficiently large that the underlying coupled lattice and nuclear system has the strength to fractionate the quantum by itself. This behavior is consistent between many computations we have done with various different values of Δn.

This means that it is a reasonable approximation to replace the complicated eigenvalue equation for the locally periodic approximation with a much simpler model

$$\frac{E(\phi)}{\hbar\omega_0}v_n = nv_n - ig_v\left\{\mathrm{e}^{i\phi}\left[v_{n+\Delta n-1} - v_{n+\Delta n+1}\right] + \mathrm{e}^{-i\phi}\left[v_{n-\Delta n-1} - v_{n-\Delta n+1}\right]\right\}. \tag{77}$$

The indirect coupling matrix element that results is

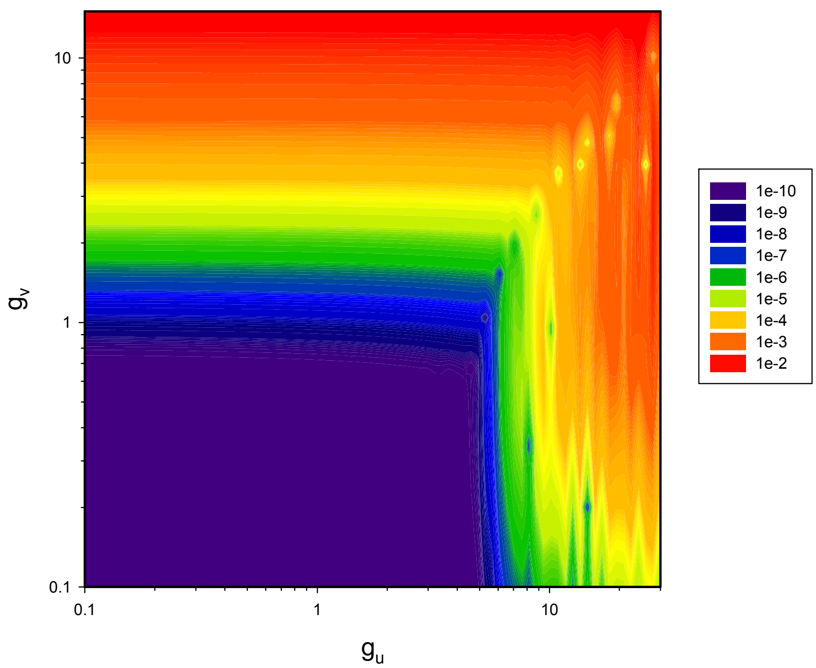

Figure 1. Indirect coupling strength $V_{\text{eff}}/\Delta E$ as a function of the two dimensionless coupling strengths g_u and g_v, for $\Delta n = 41$.

$$\frac{V_{\text{eff}}}{\Delta E} = 4 g_v \Phi(g_v), \tag{78}$$

where $\Phi(g)$ has been calculated, discussed, and fitted in Ref. [31].

7.10. Discussion

There are a number of conclusions that we can draw from this result. Perhaps the most important is that we seem to be getting pretty much the same result for the indirect coupling matrix element as we would have if the lattice and nuclear problem for all the other transitions were rotated using a Foldy–Wouthuysen transformation. This is important since it provides a major simplification for the analysis of indirect coupling matrix elements and the associated dynamics within the theory.

Another result from this is that our earlier analysis of this problem [42,43] which gave an enhancement in the indirect coupling matrix element is in error. In the earlier analysis we made use of intermediate states calculated as real states, instead of calculating them as virtual states. When done correctly (as in this section) the problems noted in the earlier calculation are resolved.

8. Summary and Conclusions

Accounting for excess heat in the Fleischmann–Pons experiment has proven to be a tough theoretical problem over the years. By now a very large number of theoretical proposals have been put forward, but even more than 24 years after the effect was first announced there is no consensus within the community as to how it might work.

From our perspective the biggest theoretical issue has to do with where the energy goes, since energetic nuclear particles are not present in amounts commensurate with the energy produced. For example, if coherent energy exchange could proceed efficiently under conditions where the large (MeV) nuclear quantum is fractionated into small (eV) quanta of the condensed matter system, then there would be no difficulty in accounting for the anomalies. In earlier work we showed that the lossy spin–boson model as a toy mathematical model describes exactly such an effect. The difficulty has been in the identification of a relevant physical model which makes use of this mechanism.

From a comparison of different models with experiment in the case of Karabut's collimated X-ray emission, we have evolved to focus now on a model for phonon–nuclear coupling mediated by relativistic coupling (under conditions where the Foldy–Wouthuysen transformation is unhelpful). From the discussion of Sections 2–4 in this work, we have argued that the new model is on a solid theoretical foundation. We know that it implements coherent energy exchange under conditions of fractionation based on the same mechanism demonstrated previously in the lossy spin–boson model; and in addition it has the strongest phonon–nuclear coupling possible (stronger by orders of magnitude than indirect coupling mechanisms).

The new model is in addition elegant, in that it describes a straightforward relativistic generalization of the condensed matter system to include coupling with internal nuclear degrees of freedom in a very fundamental and obvious formulation. In a Born–Oppenheimer picture, we can describe physical systems now using a Hamiltonian of the form

$$\hat{H} = \sum_j \left(\mathbf{M}c^2 + \mathbf{a}\cdot c\hat{\mathbf{P}}\right)_j + \sum_{j<k} V(|\mathbf{R}_j - \mathbf{R}_k|) - i\frac{\hbar}{2}\hat{\Gamma}(E). \tag{79}$$

There is no difficulty in working with a more fundamental version of the problem where the electrons are included explicitly, as in

$$\begin{aligned}\hat{H} = &\sum_j \left(\mathbf{M}c^2 + \mathbf{a}\cdot c\hat{\mathbf{P}}\right)_j + \sum_k \frac{|\hat{\mathbf{p}}_k|^2}{2m} + \sum_{j<j'} \frac{Z_j Z_{j'} e^2}{4\pi\epsilon_0|\mathbf{R}_{j'} - \mathbf{R}_j|} \\ &+ \sum_{k<k'} \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_{k'} - \mathbf{r}_k|} - \sum j,k \frac{Z_j e^2}{4\pi\epsilon_0|\mathbf{r}_k - \mathbf{R}_j|}.\end{aligned} \tag{80}$$

In this case, electron loss would emerge in a systematic treatment, so that we no longer would have to include a loss Hamiltonian explicitly. In the case of a highly excited phonon mode, we would expect this model to describe coherent energy exchange under conditions of fractionation.

This is interesting for many reasons. These new models under discussion constitute a clear improvement over text book models, since they greatly extend the realm of physics under discussion, while retaining (including) a basic description of known results in both condensed matter physics and in nuclear physics. In addition we are able to work with the new models, and carry out calculations without undo heroics. These models describe coupling of vibrational energy to the nuclear system, qualitatively consistent with collimated X-ray emission in the Karabut experiment; excess heat in PdD with ^{4}He production; and low-level gamma emission effects. In all cases the effects predicted are qualitatively very much like experiment.

Unfortunately, in our use of the models we have as yet not obtained quantitative agreement between theory and experiment. For example, if we make use of a result from the lossy spin–boson model [31], we obtain an approximate constraint for coherent energy exchange which should give us a threshold for nuclear excitation in the Karabut experiment; this constraint can be written as

$$\frac{g}{\Delta n^2} \rightarrow \frac{1}{\Delta n^2}\left(\frac{acP\sqrt{S^2-m^2}}{\Delta E}\right) > 5\times 10^{-4}, \tag{81}$$

where g is the dimensionless coupling constant, Δn is the number of phonons exchanged, a is the coupling matrix element for the $\Delta E = 1565$ eV transition, P is the Hg atom momentum matrix element, and where $\sqrt{S^2-m^2}$ is the Dicke number. We have so far been unable to find model parameters for the Karabut experiment consistent with our interpretation of the experiment which allow this constraint to be satisfied.

Our conclusion then is that we are in a sense "close," in that we have new models which have a good physical basis, which describe the phenomena observed in experiment, and which can fractionate a large quantum. But because we do not obtain consistency so far with the experimental parameters of our interpretation of the Karabut experiment, we know that something important is missing. There is a problem either in the theory, in the particular model, or in the interpretation.

We have understood within the past year that in metals that electron-phonon coupling can lead to phonon fluctuations, and that these phonon fluctuations have the potential for increasing the fractionation power in the phonon–nuclear problem. This effect would be included in the model of Eq. (80) ([ut not in models of the form of Eq. (79)). Our efforts over the past several months have been focused on the analysis of this problem; we will describe our efforts in a forthcoming paper.

Appendix A.

A thoughtful reviewer has taken the time to read some of our papers, and offer a criticism which in our view gets at some key issues that are important. This is the case in our model, and also in other models that seek to account for excess heat in the Fleischmann–Pons experiment based on deuteron-deuteron fusion reactions. Because of this, we felt that it would be of interest to others to include some of the reviewer's comments in this Appendix, and to provide a response in what follows.

Appendix A.1. Reviewer's argument

The main assumption of this and other papers in this rather extensive line of research by the authors is that there is direct coupling at the Hamiltonion level between the nuclear states and various oscillatory modes (phonons, plasmons, etc.) of a condensed matter system. Let us refer to these oscillatory modes as simply phonons. This assumption then allows the authors to examine different forms of coupling and loss mechanisms, and to seek ways to explain "fractionation" of a nuclear reaction like a fusion event's Q energy into a large number ($\sim 7\times 10^8$) of small quanta of these phonons. They are also interested in explaining X-ray production in the Karabut experiment. The key assumption is that a Hamiltonian of this form, which directly couples phonons to the nuclear states, is a valid theory. There are two ways to look at this. First, the authors have in mind that the standard model of particle physics lies at the basis of the nuclear structure and reactions, and that their Hamiltonian is an effective Hamiltonian which will ultimately be found to be compatible with the standard model, and hopefully can be derived from it. The second possibility is that the authors may wish to imply that the standard model is simply wrong, and does not apply to the nuclear structure or reactions that have been observed in LENR expriments.

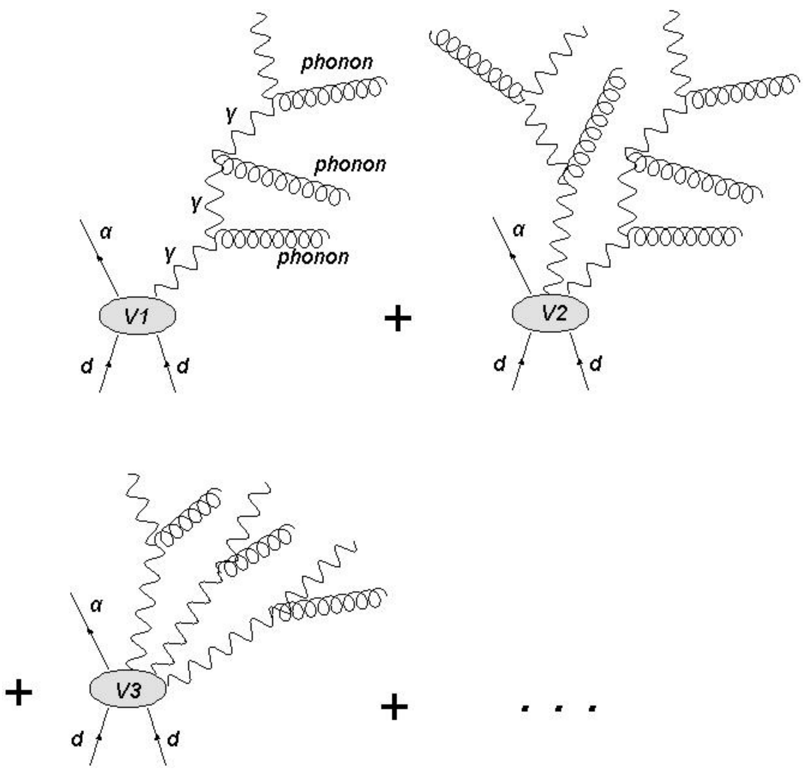

Figure 2. Feynman diagrams for phonon excitation in a standard model description of d + d + phonons + photons. The phonons are produced when the photon lines interact with charged particles (not shown) in the lattice.

If the authors wish to present a theory which does not contradict the standard model of particle physics, then I believe the basic assumption that a Hamiltonian which directly couples phonons to nuclear states is not plausible, at least for deuterium cold fusion. The reason is that the standard model requires that a nuclear fusion event that couples fusion with the lattice when ^{4}He is being produced should be mediated by the electromagnetic force, ie. by photons. The principle coupling in the standard model (or in just plain QED for that matter) between a fusion reaction and phonons in a solid is via photon exchange. The photons are exchanged between the fusion event and various charged particles in the solid. The following Feynman diagrams illustrate this situation for the production of ^{4}He.

Each photon emitted from the vertex brings a factor of the fine structure constant to the probability of the diagrams in Figure 1. So, the probability of emitting a large number of photons is vanishingly small, unless the vertex functions Vn were to have anomalous behavior for large number of photons n, which has not been observed in other fusion experiments. We must therefore limit the number of photons being emitted. So each photon emitted would be expected to be a gamma ray, and the largest contribution should come from single photon emission. But then we know from many experiments how a gamma ray will react with a solid. Yes, they will produce some phonons, but they will also have a range of motion, and many should be observed in the LENR experiments that have been performed. So these

Feynman diagrams would seem to rule out the possibility that a direct Hamiltonian coupling between the nuclear state and phonons is a good approximation to the standard model in the case of deuterium fusion. You need to have photons to transfer energy from the nuclear event to the lattice, and this system does not seem to be well approximated by any direct phonon to nuclear state coupling.

The time reverse situation is also in effect. In order for a phonon to excite a nucleus, it must do so by causing a virtual photon be be created in the lattice which can then be absorbed by the nucleus. There is expected to be a factor of α (fine structure constant) for each such photon. Although this situation might be better approximated by a direct nuclear–phonon interaction in the standard model or in QED, it's not clear from the current paper how to justify this or to justify the magnitude of the coupling constant needed for appreciable fractionation.

The standard model also predicts the reactions

$$\mathrm{d} + \mathrm{d} \quad\rightarrow\quad \mathrm{t} + \mathrm{p}$$

and

$$\mathrm{d} + \mathrm{d} \quad\rightarrow\quad \mathrm{n} + {}^{3}\mathrm{He}.$$

Although the energetic charged particles produced could produce some phonons, it is very hard to see how these channels might be suppressed to the rates observed in LENR experiments which would be required in order for a direct phonon-nucleus interaction to be a good approximation.

So, if we then assume that the standard model is inconsistent with direct phonon coupling, and we still insist that we will consider a direct coupling of phonons to nuclear states, then that begs the question how exactly does the energy from the nuclear event get communicated to the charged particles of the lattice which is the only mechanism to excite a phonon. There needs to be some local but long range field that mediates this force. The only fundamental long range forces in nature are electromagnetism and gravitation. It we eliminate gravity due to its extremely weak coupling, then electromagnetism is the only known way for a force to be communicated from the nuclear event to the charge particles of the solid (including electrons). But we must avoid photons in order to avoid gamma rays (in some reactions at least). One possibility that might be considered is action at a distance theory, like that of Fokker–Tetrode–Wheeler–Feynman for the electromagnetic force [53]. But these theories can violate causality and are a "hard sell" to most physicists. Moreover, they are difficult to solve as the Cauchy problem is non trivial for them. Still, it might be the only way for a direct nuclear-phonon interaction Hamiltonian to fit into "conventional" theoretical physics.

Appendix A.2. Response

We are generally of the opinion that if a model (for excess heat in the Fleischmann–Pons experiment, or for other anomalies) is inconsistent with the standard model in the area that the standard model applies, then it will likely have issues being consistent with the large body of conventional experimental results. Having the standard model in this sense is a good thing, since it gives a starting place that we and others can have some confidence in. We are of the opinion that our model lies within the standard model generally.

From the reviewer's comments it might seem that if we would like ^{4}He as a reaction product from a deuteron-deuteron fusion reaction (which is the subject of other papers, but not so much this one), then we are stuck with an electromagnetic interaction, and will have to face the consequences of producing an energetic gamma. According to the reviewer, "*The reason is that the standard model requires that a nuclear fusion event that couples fusion with the lattice when* ^{4}*He is being produced should be mediated by the electromagnetic force, ie. by photons.*" Seemingly it could not be any simpler; if a model is to be consistent with the standard model, then it must be an electromagnetic interaction that mediates the deuteron-deuteron to ^{4}He reaction. If the interaction is not mediated by electromagnetic interaction, then it lies outside of the standard model (by this criterion). What follows from this argument is a highly unlikely picture in which phonon emission comes about from subsequent interactions involving the gamma; a picture that we are in complete agreement with the reviewer has sufficient associated headaches that there is little chance things actually could work this way.

On the other hand, a deuteron–deuteron reaction leading to ^{4}He mediated by phonon exchange as we have proposed is not something that you see every day in nuclear physics texts. If we make use of the requirement put forth by the reviewer, that the reaction must be mediated by photon exchange in order to be consistent with the standard model, then it is hard to see how a phonon-mediated version of the reaction could be consistent. This then is what we need to think about, and to address here, in response to the reviewer's comments.

In a sense, the resolution is pretty simple; in our view it has to do with the difference between the viewpoint taken in particle physics or nuclear physics, and the viewpoint taken in condensed matter physics. For example, suppose we think about a QHD type of model (plausibly derivable from the standard model) in which nucleons interact with each other through pion exchange and photon exchange; then we envision a Hamiltonian of the general form

$$\hat{H} = \hat{H}_{\text{nucleon}} + \hat{H}_{\pi} + \hat{H}_{\text{EM}} + \hat{V}_{\pi-\text{n}} + \hat{V}_{\text{phot-n}} \tag{A.1}$$

except that a particle physicist would work with a Lagrangian instead of a Hamiltonian. In such a model we have Dirac nucleons, Hamiltonians for pions and photons, with single pion exchange and single photon exchange terms. If we start with two deuterons in free space, and hope to end up with a ^{4}He in free space, then the lowest-order interaction that is going to make it work is single photon exchange. If there happen to be other atoms around, then they are far away, and we expect little impact from them. Any residual interactions in such a view can be dealt with through perturbation theory.

Next, a particle physicist would begin writing out Feynman diagrams, since the mathematical machinery for computations with this kind of model have all been automated. However, here we will adopt a much more pedestrian approach and focus on how photon exchange comes into the problem in the case of a single nucleon that we focus on; the relevant Hamiltonian for this part of the problem might be written as

$$\hat{H} = \boldsymbol{\alpha} \cdot c[\hat{\mathbf{p}} - q\hat{\mathbf{A}}(\mathbf{r})] + \beta Mc^2 + \sum_j \hat{V}_{\pi}(\mathbf{r} - \mathbf{r}_j) + \sum_j \frac{qq_j}{4\pi\epsilon_0|\mathbf{r} - \mathbf{r}_j|}. \tag{A.2}$$

Pion exchange here is accounted for through an equivalent nuclear potential as was done in years past (since our focus is on the electromagnetic interaction and not on pion exchange). In this kind of model, the only relevant propagating degree of freedom capable of dealing with the relevant large energy quantum is electromagnetic. We can expand out the vector potential operator

$$\hat{A}(\mathbf{r}) = \sum_{\mathbf{k},\sigma} \hat{\mathbf{i}}_{\sigma} \sqrt{\frac{\hbar}{2\omega_{\mathbf{k}}\epsilon_0 L^3}} \left[\frac{\hat{a}_{\mathbf{k},\sigma} \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}} - \hat{a}^{\dagger}_{\mathbf{k},\sigma} \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}}{i} \right] \tag{A.3}$$

and see creation and annihilation operators for the photons appearing explicitly. The construction of the theory itself helps us keep track of photon creation as an independent quantum degree of freedom.

Phonon exchange was not important in nuclear reactions generally historically, so we have no phonon modes in this kind of formulation. Since phonons in a metal come about due in part to Coulomb interactions between the nucleons, and in part due to the electronic degrees of freedom, one knows that they are described within a sufficiently general Hamiltonian (the standard model includes electrons and photon exchange, so phonons are consistent with the standard model). Phonon exchange comes into this kind of picture after the fact; either as a result of interactions with the gamma as proposed by the reviewer, or perhaps as a consequence of soft photon exchange with the lattice as an external system, in which case one could argue that in this picture the associated perturbation is small.

Now let us consider the problem from a condensed matter viewpoint. In this case, the deuterons are presumed to be inside the solid, and the lattice vibrations which we are interested in (for thinking about phonon exchange) include the deuterons of the initial state, and the ^{4}He of the final state. As such, the center of mass position and momentum of the nuclei are now lattice operators. In general the lattice is disordered, so that the vibrational modes are a mess; we might write in this case

$$\hat{\mathbf{R}}_j = \mathbf{R}_j^{(0)} + \sum_\mu \frac{d\mathbf{R}_j}{da_\mu}\left[\hat{a}_j + \hat{a}_j^\dagger\right], \tag{A.4}$$

$$\frac{\hat{\mathbf{P}}_j}{m_j} = \sum_\mu \frac{d\mathbf{P}_j}{da_\mu}\left[\frac{\hat{a}_j - \hat{a}_j^\dagger}{i}\right], \tag{A.5}$$

where the capital position and momentum operators refer to the nuclear center of mass degrees of freedom. In place of the QHD-type of Hamiltonian, we will have a new one which looks like

$$\hat{H} = \hat{H}_{\text{vib}} + \hat{H}'_{\text{nucleon}} + \hat{H}_\pi + \hat{H}_{\text{EM}} + \hat{V}_{\pi-\text{n}} + \hat{V}_{\text{phot-n}}, \tag{A.6}$$

where we now have a vibrational Hamiltonian to keep track of the relevant lattice degrees of freedom. Since the nuclear center of mass coordinates are now part of the vibrational Hamiltonian, we have to remove them from the nucleon Hamiltonian, which is indicated by $\hat{H}_{\text{nucleon}} \to \hat{H}'_{\text{nucleon}}$. On the face of it, there seems to be little change in the nucleon interactions, since we have not added any distinct phonon interaction terms. However, there are now all kinds of places where phonon exchange comes in, primarily since the nucleon positions and momenta have acquired phonon operator components. To see this, we revisit the simple one-nucleon Hamiltonian

$$\hat{H} = \boldsymbol{\alpha}\cdot c[\hat{\mathbf{p}} - q\hat{\mathbf{A}}(\hat{\mathbf{r}})] + \beta M c^2 + \sum_j \hat{V}_\pi(\hat{\mathbf{r}} - \hat{\mathbf{r}}_j) + \sum_j \frac{q q_j}{4\pi\epsilon_0|\hat{\mathbf{r}} - \hat{\mathbf{r}}_j|} \tag{A.7}$$

and view it with new eyes. Since the nucleon position operators now include phonon operators, we find that phonon exchange can occur in connection with Coulomb interactions, transverse photon exchange, and with the strong-force interaction (however, phonon exchange in the latter case requires the nucleons to be associated with different nuclei, so we can get phonon exchange when one nucleus tunnels close to another).

Having spent time analyzing phonon exchange in all of these cases, we can conclude that phonon exchange generally is a very small effect for these terms, which can be treated as minor perturbations consistent with the view described above. However, there remains the $\boldsymbol{\alpha}\cdot c\hat{\mathbf{p}}$ term which is now in part a phonon operator, and which can mediate phonon exchange now. Normally this operator is rotated out in a Foldy–Wouthuysen transformation, where it loses whatever teeth it had. However, under conditions where a Foldy–Wouthuysen transformation is unhelpful, then the associated interaction strength is quite large. In this simple example, we can think of transverse photon exchange for a single nucleon as mediated by the interaction

$$\hat{h}_{\text{int}}^{(\text{photon})} = -\boldsymbol{\alpha}\cdot cq\hat{\mathbf{A}}(\hat{\mathbf{r}}), \tag{A.8}$$

We can relate the nucleon momentum operator to the center of mass operator according to

$$\hat{\mathbf{p}} = \frac{\hat{\mathbf{P}}}{N} + \hat{\boldsymbol{\pi}}, \tag{A.9}$$

where N is the number of nucleons in the nucleus, and where $\hat{\boldsymbol{\pi}}$ is relative momentum operator. Because of this, the $\boldsymbol{\alpha} \cdot \hat{\mathbf{p}}$ operator contains a part that is a roughly equivalent phonon operator

$$\hat{h}_{\text{int}}^{(\text{phonon})} = \boldsymbol{\alpha} \cdot c\frac{\hat{\mathbf{P}}}{N}. \tag{A.10}$$

Perhaps in this context it is useful to examine phonon exchange and photon exchange in the context of the idealized relativistic composite model discussed in the text. In this case we may write

$$\hat{H} = \sum_j \left(\mathbf{M}c^2 + \mathbf{a}_M \cdot c\hat{\mathbf{P}} - q\mathbf{a}_q \cdot c\hat{\mathbf{A}}\right)_j + \sum_{j<k} V(\mathbf{R}_j - \mathbf{R}_k). \tag{A.11}$$

This corrects an error in [54] where we followed the suggestion of a reviewer that we make use of the formulation to add the coupling to the electromagnetic field by analogy with the electron case (we note in addition that the model in [54] suffers additionally from the problem that nucleons are not Dirac particles, and that the matrix element is too low by more than an order of magnitude as a direct result of this approximation). However, in general the mass weighted **a**-matrix ($\mathbf{a}_M$) is different than the charge weighted **a**-matrix ($\mathbf{a}_q$); so in writing this we have distinguished between the two. So, if we wished to describe deuteron–deuteron fusion mediate by photon exchange within this formalism, the interaction would be

$$\hat{h}_{\text{int}}^{(\text{photon})} = -q\mathbf{a}_q \cdot c\hat{\mathbf{A}}, \tag{A.12}$$

which is similar in form to the equivalent phonon interaction

$$\hat{h}_{\text{int}}^{(\text{phonon})} = \mathbf{a}_M \cdot c\hat{\mathbf{P}}. \tag{A.13}$$

Some modification of the photon exchange interaction in this form would be required for interactions beyond the dipole interaction, since the relativistic composite operators deal with transitions appropriate for long wavelength radiation; new operators will be needed to deal with higher multipoles where the wavelength is on the order of the nuclear size.

Consistent with the discussion here, there is no reason to exclude phonon exchange from interactions within the standard model; for interactions between nuclei embedded in a lattice, working with position and momentum operators that are phonon operators is the more natural and more useful description. Unfortunately, in general the problem becomes more complicated when this is done, so one gives up some of the advantage that the simpler free-space formalism provides for computations.

The assertion of the reviewer that phonon exchange cannot mediate an electromagnetic transition and remain within the standard model is simply incorrect (although a very understandable misconception). It is true that one cannot satisfy energy and momentum conservation for the deuteron–deuteron to ^{4}He transition, since there is no way a single phonon can take away 24 MeV. This is why we have explored alternative schemes in which the 24 MeV excitation is transferred elsewhere to a different system capable of fractionating the large quantum. In this kind of scheme, we require a single phonon exchange interaction to mediate the $D_2/^4$He virtual transition, and then deal with the fractionation as a separate part of the problem.

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