COHERENT AND SEMICOHERENT NEUTRON TRANSFER REACTIONS III: PHONON FREQUENCY SHIFTS

COLD FUSION

TECHNICAL NOTE

KEYWORDS: *cold fusion theory, neutron transfer reactions, solid-state nuclear physics*

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Received August 11, 1992
Accepted for Publication October 14, 1992

A new model describing the transfer of neutrons to and from nuclei embedded in a lattice was recently proposed. The coupling between the nuclei and lattice phonons is now explored, focusing on the question of whether it is possible under any conditions for anomalously large energy transfer to or from the lattice to occur during a neutron transfer reaction.

By studying the gamma line shape, no anomalies are expected for a ground-state lattice or for a thermal lattice. Under certain conditions, the frequency of a phonon mode can be shifted significantly in a neutron transfer reaction; phonons initially present in that mode are shifted in frequency during the reaction. This effect produces an anomalous energy shift in the event that the mode is initially strongly excited.

I. INTRODUCTION

In two previous papers,[1,2] we formulated a theory that describes neutron capture and neutron ionization from nuclei embedded in a lattice. The seminal treatments of this basic problem are due to Lamb,[3,4] and much use has been made of the model following the discovery of the Mossbauer effect.[5] Much more use of Lamb's theory has been made for resonant transitions than for gamma emission due to neutron capture; as presented, Lamb's theory is actually deficient for describing neutron capture in that effects associated with the recoil of the neutron during the capture process are not included. Although the literature is replete with theory papers containing formulations, calculations, discussions, and reviews of resonant processes that are really quite sophisticated, little effort appears to have been devoted to the capture problem.

The model we developed has improved on Lamb's work by including, at least formally, all recoil effects associated with the neutron and with the lattice. In the process, we developed phonon operators that describe two primary effects beyond the primary $\exp(i\boldsymbol{k}\cdot\boldsymbol{R})$ neutron recoil term: (a) a large effect that accounts for the change in the lattice mode definitions in the before and after lattice states (we term this effect a Duschinsky effect following nomenclature from an analogous effect that occurs in electronic transitions in polyatomic molecules) and (b) a rather weak effect due ultimately to a microscopic difference between the initial and final nuclei center-of-mass positions.

In this technical note, we focus on the primary Duschinsky term to gain an understanding of phonon generation in the presence of "mismatched" initial- and final-state lattices. The higher order non-Duschinsky effects are neglected in this technical note. It can be arranged for the recoil due to the neutron and gamma ray to cancel through a suitable choice of experimental setup, specifically one that collects measurements only for collinear neutron and gamma momenta of equal magnitude; this would have the effect of isolating Duschinsky effects from other recoil effects. In our earlier works, we considered this sort of experimental arrangement to discuss the possible observation of Duschinsky and non-Duschinsky effects for the model problem of neutron capture on H_2.

A primary motivation for the research described in this and in previous works has been to explore possible theoretical explanations for some of the anomalous effects that have been observed in deuterated metals. In this work, we begin to address what is probably the key issue facing any model that seeks to address the reported anomalies, specifically the possibility of the transfer of significant energy between the lattice on the macroscopic scale and nuclear constituents on the microscopic scale.

The energy spacing between the nuclear energy levels that would be involved in neutron ionization is multiple mega-electron-volts, assuming that the nucleus is initially in the ground state. The lattice phonon modes are of low energy, typically on the order of tens of milli-electron-volts. Coupling of energy between the nucleus and the lattice then requires a mechanism capable of transferring an astonishingly large amount of energy between nucleons and the lattice.

Large numbers of phonons can of course be transferred to a lattice; a lattice that is struck with a hammer can absorb a large number of phonons, but this involves a transfer of energy that starts and finishes in small sub-electron-volt-sized quanta. A fast mega-electron-volt particle that slows down in a lattice transfers a large amount of energy, but once again, the actual transfer is done essentially through a sequence of interactions, each of which results in the generation of a small number of phonons. Transferring energy a few phonons at a time to ionize a neutron does not work since there are not enough intermediate nuclear states; the theory for such processes gives transition probabilities on the order of $(H_{if}/\Delta E)^{2n}$, which is vanishingly small unless the coupling matrix element H_{if} is on the order of ΔE. The coupling of a nucleus and the surrounding lattice is very weak, and the transition probability for processes involving the sequential generation of small numbers of phonons can simply be taken to be zero.

Nevertheless, the lattice does possess states that can be resonant with the nuclear states, and all that is lacking is a matrix element with which to couple them nonperturbatively. Currently, no mechanisms are known that can do the job, and no new mechanisms have been anticipated that would ever do it under any circumstances.

We have found an interesting new mechanism that appears to be capable of anomalously large energy transfer during a neutron transfer reaction. It is known that, under certain conditions, the addition of a single neutron to a lattice can result in significant frequency shifts of three phonon modes. In the case of a perfect crystal initial lattice, the shifted modes are generally local modes; in the case of a lattice with impurities, the shifted modes may be resonance continuum modes. If such a mode is significantly excited prior to a neutron transfer reaction, anomalous energy exchange with the lattice will occur during the reaction as the phonons shift frequency.

II. LINE SHAPES AND PHONON GENERATION

The central issue we are concerned with involves the transfer of energy between a lattice and a nucleus. In our previous works, we analyzed in some detail the lattice effects associated with neutron transfer reactions as they appear in the interaction Hamiltonian, and we obtained explicit operators that describe the coupling. If energy is exchanged between nucleons and the lattice, the effect should manifest itself through modifications in the line shape. Our focus in this section is therefore directed to a brief review of the line shape for the neutron capture process.

The line shape for neutron capture is

$$W(E) \sim \sum_{\alpha}\sum_{\beta} \frac{g(\{\alpha\})|\langle\{\beta\}|\exp[i(\boldsymbol{k}_p - \boldsymbol{k}_n)\cdot\hat{\boldsymbol{R}}_i]\exp(-i\hat{S}_D)|\{\alpha\}\rangle|^2}{[E - E_0 - \Delta E(\alpha,\beta)]^2 + \frac{1}{4}(\hbar\Gamma)^2} , \quad (1)$$

where

$\{\alpha\}$ = set of lattice quantum numbers = initial lattice state

$\{\beta\}$ = final lattice state

$g(\{\alpha\})$ = probability that the lattice is in the initial lattice state

E = emitted gamma energy

E_0 = resonance energy

$\hbar\Gamma$ = homogeneous line width.

As discussed in our earlier technical notes in this series, two distinct effects are accounted for explicitly in this line shape expression. Well known is the primary recoil effect that appears in this formula explicitly through $\exp[i(\boldsymbol{k}_p - \boldsymbol{k}_n)\cdot\hat{\boldsymbol{R}}_i]$. In the following sections, we focus on the limit that $\boldsymbol{k}_p = \boldsymbol{k}_n$ to simplify our analysis of matrix elements of the Duschinsky operator. It is instructive to briefly consider the coupling of energy through recoil before proceeding.

Phonon generation through recoil alone in the absence of the Duschinsky operator in this application corresponds rather well to the non-Mossbauer part of the line shape in conventional resonance emission. For thermal lattices, the phonon generation due to the gamma recoil is quite well known, and the line shape may exhibit identifiable features due to phonon generation. The gamma energy for neutron capture on a proton is 2.225 MeV, which is an order of magnitude greater than for Mossbauer resonance lines, which favors phonon generation. Additionally, the resulting deuteron is relatively light, which also favors phonon generation. Nevertheless, the total energy transfer is on the atomic scale, and the transfer of a mega-electron-volt quantum is precluded by direct calculation: Transferring the energy a few phonons at a time is exponentially inhibited by factors on the order of $(H_{\alpha\beta}/\Delta E)^{2n}$; transferring the energy nonperturbatively by considering high-order terms in the interaction Hamiltonian ultimately leads to the conclusion that the initial proton must have multi-mega-electron-volt initial kinetic energy for substantial energy transfer to occur.

It can be imagined that there might be some way in which the lattice can respond collectively to the recoil operator to be able to accept an anomalously large amount of energy. We investigated this possibility by examining the coupling into a subset of the phonon modes; it can be shown that for a macroscopic lattice, the coupling to any single mode is quite weak, so that the maximum amount of energy that can be coupled nonperturbatively is on the atomic scale. The recoil term could be made to be very strong if the initial neutron momentum is taken to correspond to mega-electron-volt–level kinetic energy. In this case, the transfer of energy to the lattice can be at the mega-electron-volt level, but a very large number of final states result, rendering the overall process irreversible.

As a result, we conclude that the primary recoil operator is simply incapable of mediating the transfer of significant (mega-electron-volt–level) energy to the lattice, in the absence of relative kinetic energy that is on the order of mega-electron-volts. These arguments do not apply to the Duschinsky operator, the analysis of which is the subject of the remainder of this technical note.

The Duschinsky operator is most cleanly studied in the absence of primary recoil effects, and we therefore limit ourselves to the special case of equal photon and neutron momentum ($\boldsymbol{k}_p = \boldsymbol{k}_n$). In this limit, the line shape is

$$W(E) \sim \sum_{\alpha}\sum_{\beta} \frac{g(\{\alpha\})|\langle\{\beta\}|\exp(-i\hat{S}_D)|\{\alpha\}\rangle|^2}{[E - E_0 - \Delta E(\alpha,\beta)]^2 + \frac{1}{4}(\hbar\Gamma)^2} . \quad (2)$$

The Duschinsky operator in general translates and rotates the phonon mode amplitudes[6,7]

$$\exp(-i\hat{S}_D)\Psi(\boldsymbol{q}) = \Psi(\mathbf{A}\cdot\boldsymbol{q} + \boldsymbol{b}) \quad (3)$$

to satisfy the constraint that the nuclear center-of-mass positions remain invariant during a reaction even though the phonon modes are altered.

This model as written is rather general, and there exists considerable literature on line shapes produced with various Duschinsky operators.

In the solid-state literature, the earliest model of phonon generation accompanying an electronic transition in an F-center was the single-configurational-coordinate (SCC) model.[8-10] The electronic transition is assumed to cause a shift in the equilibrium lattice positions while maintaining the phonon mode frequencies. Using the notation of Refs. 8, 9, and 10, the SCC model corresponds mathematically to the Duschinsky transformation in which a single mode is translated

$$\exp(-i\hat{S}_D)\Psi(\boldsymbol{q}) = \Psi(\boldsymbol{q} + \boldsymbol{i}_m \Delta q_m) \ , \tag{4}$$

but where no rotation occurs.

This model was improved by Huang and Rhys,[11] who included translations in a large number of optical phonon modes with identical frequencies; we would write this model as

$$\exp(-i\hat{S}_D)\Psi(\boldsymbol{q}) = \Psi(\boldsymbol{q} + \Delta \boldsymbol{q}_m) \ . \tag{5}$$

This type of model, and the extension to include phonon modes of differing frequencies, has been widely used in the solid-state literature to describe phonon generation for radiative and nonradiative electronic transitions in solids.[12-19]

The inclusion of frequency shifts in the modes would correspond to a Duschinsky operator that translates and scales as

$$\exp(-i\hat{S}_D)\Psi(\boldsymbol{q}) = \Psi(\mathbf{D}\cdot\boldsymbol{q} + \boldsymbol{b}) \ , \tag{6}$$

where $\mathbf{D}$ is a diagonal matrix. In the analysis of multiphonon decay of molecules, a number of analyses have appeared that correspond to this kind of Duschinsky transformation (see Refs. 20 through 24).

To date, we have not found works in the solid-state literature in which both translations and nontrivial rotations have been considered. In the literature on polyatomic molecules, analyses appear that include the full Duschinsky operator with rotation and translation:

$$\exp(-i\hat{S}_D)\Psi(\boldsymbol{q}) = \Psi(\mathbf{A}\cdot\boldsymbol{q} + \boldsymbol{b}) \ . \tag{7}$$

One of the most interesting papers is by Sharp and Rosenstock,[25] who present a generating function method for the evaluation of matrix elements of the Duschinsky operator. There is considerable literature on the computation of such matrix elements (see Refs. 26 through 33), including the application of rather sophisticated operator techniques to the calculation of Duschinsky translated and scaled harmonic oscillator wave functions.[34-37]

Our initial naive proposal[38] for a coupling mechanism in the case of coherent neutron transfer reactions concerned a model analogous to the SCC lattice model mentioned earlier. We argued in Refs. 1 and 2 that no translation occurs to within an excellent approximation since an isotopic change is not expected to modify the electronic configurations significantly; our initial proposal was in error in this aspect. Even if a translation did occur, the model would still be deficient because it is unlikely that a sufficiently large translation to produce mega-electron-volt-level potential energy changes.

The Duschinsky transformation that is correct for neutron transfer reactions is of the form

$$\exp(-i\hat{S}_D)\Psi(\boldsymbol{q}) = \Psi(\mathbf{A}\cdot\boldsymbol{q}) \ , \tag{8}$$

where only a rotation occurs. Although the analysis of matrix elements for such a system constitutes a subset of the general transformations studied in the polyatomic molecule literature, similar analyses in the solid-state literature do not generally appear. An exception to this is in the Mossbauer literature, where discussions of this problem have been given in Refs. 39 through 42. For resonant absorption or emission, the mass shift is quite small; hence, the new effects described in this work do not occur. The Duschinsky transformation matrix associated with an isotope shift in a lattice has been studied and is well known.[43-45] It would seem to be natural to extend the analyses done in other fields to the case of phonon generation associated with neutron capture, but to date, we have not found any papers where this has been done.

III. PROPERTIES OF THE DUSCHINSKY OPERATOR

The line shape for neutron capture in the recoil-free limit is determined by the matrix elements of the Duschinsky operator between different lattice states. Duschinsky matrix elements appear in the computation of oscillator strengths for electronic transitions in polyatomic molecules, and rather sophisticated numerical techniques have been developed to evaluate them. An alternate set of techniques has been developed for the equivalent lattice problem. In Sec. IV, we describe a method for evaluating the Duschinsky matrix element appropriate for a highly nonthermal lattice. The technique relies heavily on properties of the Duschinsky operator, which provides us with motivation to briefly review the Duschinsky operator in this section.

The Duschinsky matrix element we require may be written as follows:

$$M_{fi} = \int \Psi_f^*(\boldsymbol{q}) \exp(-i\hat{S}_D)\Psi_i(\boldsymbol{q})\, d\boldsymbol{q} \ , \tag{9}$$

where the phonon mode amplitudes have been collected together to form a very long vector $\boldsymbol{q} = \sum_m \boldsymbol{i}_m q_m$. We recall that the phonon mode amplitudes describe the center-of-mass positions of the atomic nuclei through

$$\boldsymbol{R}_j = \boldsymbol{R}_j^o + \sum_m \boldsymbol{u}_m(j) q_m \ . \tag{10}$$

Because of the mass change at a lattice site that accompanies a neutron transfer reaction, the initial and final lattice modes are not the same. Although the neutron transfer reaction approximately preserves the center-of-mass locations, the fact that the initial and final lattice modes do not agree implies the presence of a nontrivial transition operator. This is similar to the situation in polyatomic molecules, where an electronic transition alters the force constant, which changes the before and after mode definitions.

The Duschinsky operator satisfies

$$\exp(-i\hat{S}_D)\Psi_i(\boldsymbol{q}) = \Psi_i(\mathbf{A}\cdot\boldsymbol{q} + \boldsymbol{b}) \ , \tag{11}$$

where the matrix $\mathbf{A}$ and the vector $\boldsymbol{b}$ constitute the transformation required to preserve the center-of-mass locations exactly. The individual matrix and vector components can be computed from the displacement vectors $\boldsymbol{u}_m(j)$ and their adjoints. Consider initial and final lattice center-of-mass positions given by

$$\boldsymbol{R}_j = \boldsymbol{R}_j^{o,i} + \sum_m \boldsymbol{u}_m^{(i)}(j) q_m^{(i)} \tag{12}$$

and

$$\boldsymbol{R}_j = \boldsymbol{R}_j^{o,f} + \sum_m \boldsymbol{u}_m^{(f)}(j) q_m^{(f)} \ . \tag{13}$$

The initial-state lattice mode amplitudes $q_m^{(i)}$ can be expressed in terms of the final lattice mode amplitudes $q_m^{(f)}$ through

$$q_m^{(i)} = \sum_j \sum_{m'} [\boldsymbol{v}_m^{(i)}(j)]^T \cdot \boldsymbol{u}_{m'}^{(f)}(j) q_{m'}^{(f)}(j) + \sum_j [\boldsymbol{v}_m^{(i)}(j)]^T \cdot (\boldsymbol{R}_j^{o,f} - \boldsymbol{R}_j^{o,i}) \ , \tag{14}$$

where $\boldsymbol{v}_m(j)$ is the adjoint displacement vector to $\boldsymbol{u}_m(j)$. If we assume that the equilibrium lattice positions do not change following a transfer reaction, then it follows that $\boldsymbol{b} = 0$. The Duschinsky transformation matrix is

$$A_{m,m'} = \sum_j [\boldsymbol{v}_m^{(i)}(j)]^T \cdot \boldsymbol{u}_{m'}^{(f)}(j) \ . \tag{15}$$

The inverse of the Duschinsky transformation matrix can be obtained similarly, starting with

$$q_m^{(f)} = \sum_j \sum_{m'} [\boldsymbol{v}_m^{(f)}(j)]^T \cdot \boldsymbol{u}_{m'}^{(i)}(j) q_{m'}^{(i)}(j) \ , \tag{16}$$

which leads to

$$A_{m,m'}^{-1} = \sum_j [\boldsymbol{v}_m^{(f)}(j)]^T \cdot \boldsymbol{u}_{m'}^{(i)}(j) \ . \tag{17}$$

There exists an intimate relationship between the Duschinsky matrix and its inverse, which is of interest to us in the next section. We have used the biorthogonality of the displacement vectors and their adjoints as

$$\sum_j \boldsymbol{v}_m^T(j) \cdot \boldsymbol{u}_{m'}(j) = \delta_{m,m'} \ . \tag{18}$$

The displacement vectors satisfy

$$\sum_j M_j \boldsymbol{u}_m^T(j) \cdot \boldsymbol{u}_{m'}(j) = M \delta_{m,m'} \ , \tag{19}$$

where M is a mass that is artificially associated with the phonon modes. In the more conventional quantization of the phonons, modes and operators are constructed that do not require the introduction of an artificial mass. We used this approach in our work to be able to use $\boldsymbol{q}$ and $\boldsymbol{p}$ for position and momentum of the quantized oscillators. It follows that the adjoint vectors are related to the displacement vectors by

$$\boldsymbol{v}_m(j) = \frac{M_j}{M} \boldsymbol{u}_m(j) \ . \tag{20}$$

The expressions for the Duschinsky matrix and the transpose of its inverse may be compared and found to be practically equal to each other. The transpose of the inverse is

$$[A^{-1}]_{m,m'}^T = \sum_j [\boldsymbol{v}_{m'}^{(f)}(j)]^T \cdot \boldsymbol{u}_m^{(i)}(j) \ , \tag{21}$$

which may be rewritten as

$$[A^{-1}]_{m,m'}^T = \sum_j \frac{M_j^{(f)}}{M_j^{(i)}} [\boldsymbol{v}_m^{(i)}(j)]^T \cdot \boldsymbol{u}_{m'}^{(f)}(j) \ . \tag{22}$$

The nuclear masses are identical in the initial lattice and the final-state lattice at all sites except where the neutron transfer occurs. As a result, we may recast this as

$$[A^{-1}]_{m,m'}^T = \sum_j [\boldsymbol{v}_m^{(i)}(j)]^T \cdot \boldsymbol{u}_{m'}^{(f)}(j) + \left[\frac{M_j^{(f)}}{M_j^{(i)}} - 1\right] [\boldsymbol{v}_m^{(i)}(0)]^T \cdot \boldsymbol{u}_{m'}^{(f)}(0) \ , \tag{23}$$

where we have identified the site at which the transfer takes place as $m = 0$.

The Duschinsky matrix $\mathbf{A}$ and the transpose of the inverse are seen to differ only by a single term, which is proportional to the square of the displacement vector at the site of the transfer. This term is of order $O(1/N)$ for most continuum modes and is larger only for localized modes and resonance modes.

IV. MATRIX ELEMENTS OF THE DUSCHINSKY OPERATOR

The technique we have used to obtain approximations for the Duschinsky matrix element are most closely related to the generating function method of Sharp and Rosenstock. In our version of the method, we exploit the observation that the Duschinsky operator is essentially a rotation in a high-dimensional space. The transformation of the ground state yields states that are not very much different from the ground state. The explicit evaluation of the transformation of excited states can largely be avoided by bringing the creation operators through the Duschinsky operator; the resulting analysis is then concerned with a study of the algebra associated with the computation of

$$\exp(-i\hat{S}_D) F(\boldsymbol{q},\boldsymbol{p}) \Phi[0] = f(\boldsymbol{q},\boldsymbol{p}) \exp(-i\hat{S}_D) \Phi[0] \ , \tag{24}$$

where $\Phi[0]$ is the phonon ground state. The initial state in this case would be constructed from the ground state by the operation of the creation and annihilation operators included in the operator function $F(\boldsymbol{q},\boldsymbol{p})$:

$$\Psi_i = F(\boldsymbol{q},\boldsymbol{p}) \Phi[0] \ . \tag{25}$$

After passing $F(\boldsymbol{q},\boldsymbol{p})$ through the Duschinsky operator, the transformed version of it, $f(\boldsymbol{q},\boldsymbol{p})$, is produced, ultimately leaving the Duschinsky operator to operate on the ground state.

The Duschinsky matrix element given by

$$M_{fi} = \int \Psi_f^*(\boldsymbol{q}) \exp(-i\hat{S}_D) \Psi_i(\boldsymbol{q}) \, d\boldsymbol{q} \tag{26}$$

can then be evaluated by summing over intermediate states produced by the Duschinsky operator:

$$M_{fi} = \sum_l \int \Psi_f^*(\boldsymbol{q}) f(\boldsymbol{q},\boldsymbol{p}) \Psi_l(\boldsymbol{q}) \, d\boldsymbol{q} \times \int \Psi_l^*(\boldsymbol{q}) \exp(-i\hat{S}_D) \Phi[0] \, d\boldsymbol{q} \ . \tag{27}$$

Since the Duschinsky transformation of the ground state produces only rather weak excitation, the summation over intermediate states Ψ_l will include relatively few terms of low excitation.

The ground state of the lattice is a multidimensional Gaussian, which may be written for the initial state as

$$\Phi_i[0] = \left[\frac{\pi}{\det \mathbf{G}_i}\right]^{M/2} \exp(-\boldsymbol{q}^T \cdot \mathbf{G}_i \cdot \boldsymbol{q}/2) \ . \tag{28}$$

The operation of the Duschinsky operator on the ground state can be computed directly to give

$$\exp(-i\hat{S}_D) \Phi_i[0] = \left[\frac{\pi}{\det \mathbf{G}_i}\right]^{M/2} \exp(-\boldsymbol{q}^T \cdot \mathbf{A}^T \cdot \mathbf{G}_i \cdot \mathbf{A} \cdot \boldsymbol{q}/2) \ . \tag{29}$$

This can be rewritten as

$$\exp(-i\hat{S}_D) \Phi_i[0] = \exp[-\boldsymbol{q}^T \cdot (\mathbf{A}^T \cdot \mathbf{G}_i \cdot \mathbf{A} - \mathbf{G}_i) \cdot \boldsymbol{q}/2] \Phi_i[0] \ . \tag{30}$$

In a real lattice, the Duschinsky operator does not actually do very much to the ground state. The exponential appearing in Eq. (18) will, to lowest order, leave the ground state unperturbed (which will be the case with probability on the order of a half) and generate pairs of phonons to first order.

For the purposes of the discussion to follow, we will be satisfied that little in the way of unexpected anomalies occurs at this step of the analysis.

We next consider the case of an excited initial state. The simplest possible excitation is an initial state in which one phonon has been added to one mode, which can be specified as

$$\Psi_i(\boldsymbol{q}) = \hat{a}_m^\dagger \Phi_i[0] \ , \tag{31}$$

where $\hat{a}_m^\dagger$ is a creation operator for mode m. The Duschinsky operator applied to this initial state requires the evaluation of

$$\exp(-i\hat{S}_D)\Psi_i(\boldsymbol{q}) = \exp(-i\hat{S}_D)\hat{a}_m^\dagger \Phi_i[0] \ . \tag{32}$$

The creation operator $\hat{a}_m^\dagger$ can be expressed in terms of the mode amplitude q_m and the mode momentum p_m through

$$\hat{a}_m^\dagger = \left(\frac{M\omega_m}{2\hbar}\right)^{1/2} q_m - i\left(\frac{1}{2M\hbar\omega_m}\right)^{1/2} p_m \ , \tag{33}$$

where ω_m is the frequency of mode m. The mass M is the mass associated with the phonon mode, which is an artifact of the way in which we have described the phonons as discussed in Sec. III.

It is convenient to recast the creation operator in terms of vectors; we define two vectors

$$\boldsymbol{g} = \boldsymbol{i}_m \left(\frac{M\omega_m}{2\hbar}\right)^{1/2} \tag{34}$$

and

$$\boldsymbol{h} = \boldsymbol{i}_m \left(\frac{1}{2M\hbar\omega_m}\right)^{1/2} \ ; \tag{35}$$

then it follows that

$$\hat{a}_m^\dagger = \boldsymbol{g}\cdot\boldsymbol{q} - i\boldsymbol{h}\cdot\boldsymbol{p} \ . \tag{36}$$

The action of the Duschinsky transformation on the excited initial state can now be expressed algebraically to give

$$\exp(-i\hat{S}_D)\hat{a}_m^\dagger \Phi_i[0] = (\boldsymbol{g}\cdot\mathbf{A}\cdot\boldsymbol{q} - i\boldsymbol{h}\cdot\mathbf{B}\cdot\boldsymbol{p})\exp(-i\hat{S}_D)\Phi_i[0] \ . \tag{37}$$

In this result, we have used the explicit Duschinsky transformation of $\boldsymbol{q}$ as well as the analog transformation of $\boldsymbol{p}$, which scales differently. It may be demonstrated explicitly that

$$\mathbf{B} = [\mathbf{A}^T]^{-1} \ . \tag{38}$$

From the discussion in Sec. III, we note that $\mathbf{B}$ differs from $\mathbf{A}$ by terms that are generally quite small.

It is of interest to examine the Duschinsky transformation of a highly excited lattice state; for the sake of simplicity, we select

$$\Psi_i(\boldsymbol{q}) = (\hat{a}_m^\dagger)^{n_m} \Phi_i[0] \ . \tag{39}$$

Following the previous discussion, the Duschinsky transformation of this state is

$$\exp(-i\hat{S}_D)\Psi_i(\boldsymbol{q}) = (\boldsymbol{g}\cdot\mathbf{A}\cdot\boldsymbol{q} - i\boldsymbol{h}\cdot\mathbf{B}\cdot\boldsymbol{p})^{n_m}\exp(-i\hat{S}_D)\Phi_i[0] \ . \tag{40}$$

Matrix elements of the Duschinsky operator can then be evaluated using

$$M_{if} = \sum_i \int \Psi_f^*(\boldsymbol{q})(\boldsymbol{g}\cdot\mathbf{A}\cdot\boldsymbol{q} - i\boldsymbol{h}\cdot\mathbf{B}\cdot\boldsymbol{p})^{n_m}\Psi_l(\boldsymbol{q})\,d\boldsymbol{q} \times \int \Psi_l^*(\boldsymbol{q})\exp(-i\hat{S}_D)\Phi_i[0]\,d\boldsymbol{q} \ . \tag{41}$$

The first integral in this formula can be recast in terms of creation and annihilation operators to give

$$\int \Psi_f^*(\boldsymbol{q})(\boldsymbol{g}\cdot\mathbf{A}\cdot\boldsymbol{q} - i\boldsymbol{h}\cdot\mathbf{B}\cdot\boldsymbol{p})^{n_m}\Psi_l(\boldsymbol{q})\,d\boldsymbol{q} = \int \Psi_f^*(\boldsymbol{q})\left\{\sum_m \frac{1}{2}\left[\left(\frac{\omega_m}{\omega_{m'}}\right)^{1/2} A_{m,m'} + \left(\frac{\omega_{m'}}{\omega_m}\right)^{1/2} B_{m,m'}\right]\hat{a}_{m'}^\dagger + \frac{1}{2}\left[\left(\frac{\omega_m}{\omega_{m'}}\right)^{1/2} A_{m,m'} - \left(\frac{\omega_{m'}}{\omega_m}\right)^{1/2} B_{m,m'}\right]\hat{a}_{m'}\right\}^{n_m} \times \Psi_l(\boldsymbol{q})\,d\boldsymbol{q} \ . \tag{42}$$

If the number of modes were small and if n_m were also small, then it would be practical to simply multiply out the creation and annihilation operators and obtain an evaluation of the individual final-state matrix elements by simply picking off the associated expansion coefficients.

There is an interesting feature to be noted from this formula: The initial n_m phonon state Duschinsky-transforms to create final states with n_m or fewer phonons distributed over a potentially large number of modes. The Duschinsky operator can generate only a relatively small number of phonons due completely to the contribution of the second integral in Eq. (41); much more important is the ability of the operator to take phonons that are initially present and to exchange them for final-state phonons of different energies. Considerable leverage is potentially available in the event that initial-state modes can be found that Duschinsky-transform to form modes with disparate final-state energies.

V. SHIFTED GAUSSIAN LINE SHAPE MODEL

The detailed analysis of the neutron capture line shape that results from the model is, in general, a complicated matter. Under normal circumstances, the Duschinsky operator contributes a small amount of broadening and a small net shift to the line profile. The transformation between initial lattice modes and final lattice modes conserves energy to $O(1/N)$ for nearly all modes, and the spread in energy of the final-state modes to which a single initial-state mode couples is generally on the order of $O(1/\sqrt{N})$.

We argued in Sec. IV that an initial lattice in the ground state leads to no anomalies in the neutron capture line shape. This argument ultimately leads to the conclusion that no anomalies occur for a thermal initial state either. It is possible to obtain accurate low-temperature shift and width parameters for a thermal lattice directly from the phonon-mode displacement vectors in the special case where either the initial state or final state is a perfect crystal; we describe the results of such a calculation elsewhere. It is also possible to use moment methods developed for the calculation of the second-order Doppler shift of Mossbauer lines for the neutron capture problem.

Since neither ground state nor thermal lattices yield anomalies in the neutron capture line shape and since we are interested in this work specifically in lattice conditions that might result in anomalies, we defer a detailed analysis of ground state and thermal systems until later. Instead, we focus on highly excited nonthermal lattice states to establish that anomalies are possible, at least mathematically.

An initial lattice phonon mode that Duschinsky-transforms to final lattice modes of significantly different mode frequency is of particular interest in this discussion. For example, a PdD lattice that contains a single tritium substituted for a deuteron (at which site the neutron ionization is assumed to take place) possesses three local modes with a frequency lower than that of all optical continuum modes. If the neutron is ionized from the tritium nucleus, the local modes disappear. Whatever phonons were initially in the local modes become transformed into continuum modes at a higher frequency, with an associated net change in energy on the order of $n\hbar\Delta\omega$, where n is the number of high-frequency initial phonons and where $\Delta\omega$ is the average frequency shift. The frequency shift for this particular example has been computed and is equal to 3.1×10^{11} Hz (the shift for high-frequency localized modes in the vicinity of a proton is much smaller, $<10^9$ Hz).

It might be possible to begin arranging for an anomaly by putting a large number of phonons into the localized mode and then watching the capture line shift as high-frequency localized phonons are exchanged for lower frequency continuum phonons. The net shift will be proportional to the number of phonons initially present in the localized mode; unfortunately, the maximum number of phonons that can be put into a localized mode before the mode goes nonlinear is relatively small. It does not seem likely that a shift of more than a few electron-volts could be arranged in this manner.

We conclude from this discussion that it is not possible to couple significant energy either to or from a lattice in which either the initial or final state is a perfect PdD crystal and no net recoil is present. The continuum modes can hold a very large number of phonons, but the associated frequency shifts on a neutron transfer are small. The localized modes have a large frequency shift but cannot be excited sufficiently strongly to produce much of an effect.

It is possible to arrange for continuum phonon modes to exist that have the property that the frequency shift of the transformed modes is large; such modes would give rise to very substantial anomalies if highly excited. If a PdD lattice were loaded with a small number of tritium nuclei, then an impurity band would form near the frequency of the localized modes. When a neutron transfer occurs, three of the modes jump the gap between the deuterium modes and the tritium modes. These modes are proper continuum modes (with a localized component) and can be excited to contain a very large number of phonons.

The existence of such modes was noted previously[46-49] and is the source of interesting spectral features. That the effect is sensible can be seen through the consideration of an idealized example. Consider a moderately heavy metal lattice with a low concentration of interstitial hydrogen and deuterium; the frequency distribution of the phonons will include an acoustical branch as well as two optical branches centered around the hydrogen and deuterium resonant frequencies [$\omega_H = (K/M_H)^{1/2}$ and $\omega_D = (K/M_D)^{1/2}$]. The number of modes in the hydrogen branch will be $3N_H$, and the number of modes in the deuterium branch will be $3N_D$. If a neutron transfer reaction causes a deuterium to turn into a hydrogen, then it is clear that three phonon modes must jump the gap to accommodate the change. This is the essence of the phonon-mode "gap jumps" of interest here.

Under these assumptions, the line shape can be crudely approximated by a shifted Gaussian. In the case of recoil-free neutron capture onto a proton embedded in a lattice with a very highly excited gap-jumping mode, and with all other modes in the ground state, the line shape is

$$W(E) \sim \exp[-(E - E_0 - \Delta E)^2/2(\delta E)^2] \ , \qquad (43)$$

where ΔE is the total line shift, which is due to n phonons in a mode that jumps the gap:

$$\Delta E = n\Delta\epsilon \ , \qquad (44)$$

where $\epsilon = \hbar\Delta\omega$ is the average jump energy. The width of the line is due to the spread in mode energy of the final lattice modes, where the contribution of each Duschinsky-transformed phonon adds, in quadrature,

$$(\delta E)^2 = n(\delta\epsilon)^2 \ . \qquad (45)$$

The analysis of Sec. IV may be used to demonstrate this. In the limit discussed earlier, the line shape is dominated by phonon transfer rather than by phonon generation due to the Duschinsky operator transforming the ground state. If we choose to neglect all effects of the latter type, then an approximation can be arranged in which it is assumed that

$$\int \Psi_l^*(\boldsymbol{q}) \exp(-i\hat{S}_D)\Phi[0]\, d\boldsymbol{q} \to \delta_{l,0} \ . \qquad (46)$$

In this approximation, the matrix element of the Duschinsky operator is approximately

$$M_{if} = \int \Psi_f^*(\boldsymbol{q}) \left\{ \sum_m \frac{1}{2}\left[\left(\frac{\omega_m}{\omega_{m'}}\right)^{1/2} A_{m,m'} + \left(\frac{\omega_{m'}}{\omega_m}\right)^{1/2} B_{m,m'}\right]\hat{a}_{m'}^\dagger \times \frac{1}{2}\left[\left(\frac{\omega_m}{\omega_{m'}}\right)^{1/2} A_{m,m'} - \left(\frac{\omega_{m'}}{\omega_m}\right)^{1/2} B_{m,m'}\right]\hat{a}_{m'} \right\}^{n_m} \times \Phi_f[0]\, d\boldsymbol{q} \ . \qquad (47)$$

In the limit where the number of phonons n_m in mode m is much less than the number of atoms in the lattice, it will almost never be the case that the annihilation operators in Eq. (47) will find a phonon to destroy. In this limit, the matrix element M_{if} simplifies to

$$M_{if} = \int \Psi_f^*(\boldsymbol{q}) \left\{ \sum_m \frac{1}{2}\left[\left(\frac{\omega_m}{\omega_{m'}}\right)^{1/2} A_{m,m'} + \left(\frac{\omega_{m'}}{\omega_m}\right)^{1/2} B_{m,m'}\right]\hat{a}_{m'}^\dagger \right\}^{n_m} \Phi_f[0]\, d\boldsymbol{q} \ . \qquad (48)$$

The line shape for this idealized model is

$$W(E) \sim \sum_f \frac{|M_{if}|^2}{[E - E_0 - \Delta E(i,f)]^2 + \frac{1}{4}(\hbar\Gamma)^2} \ . \qquad (49)$$

If the Lorentzian is replaced by its Fourier representation

$$\int_{-\infty}^{\infty} \exp\{-i[E - E_0 - \Delta E(i,f)]t/\hbar\}\exp(-\Gamma|t|/2)\, dt = \frac{\hbar^2\Gamma}{[E - E_0 - \Delta E(i,f)]^2 + \frac{1}{4}(\hbar\Gamma)^2} \ , \qquad (50)$$

then the line shape may be rewritten as

$$W(E) \sim \int_{-\infty}^{\infty} \exp[-i(E - E_0)t/\hbar]\exp(-\Gamma|t|/2)w(t)\, dt \ , \qquad (51)$$

where

$$w(t) = \sum_f |M_{if}|^2 \exp[i(E_f - E_i)t/\hbar] \ . \qquad (52)$$

Since we have assumed that the number of phonons in mode m is much less than the number of atoms in the lattice, it follows that the creation operators in Eq. (48) will likely operate only once on the vacuum. In this limit, there are so many more modes than phonons that having two phonons be in a single mode will occur only infrequently. As a result, the final states will include nearly exclusively n_m phonon states, and the Fourier transform $w(t)$ may be written approximately as

$$w(t) = \sum_{m_1} \sum_{m_2} \cdots \sum_{m_{n_m}} |C_{m,m_1}|^2 |C_{m,m_2}|^2 \cdots |C_{m,n_m}|^2 \times \exp[i(E_{m_1} + E_{m_2} + \ldots E_{m_{n_m}} - E_i)t/\hbar] \ , \quad (53)$$

where the coefficients $C_{m,m'}$ are defined as

$$C_{m,m'} = \frac{1}{2}\left[\left(\frac{\omega_m}{\omega_{m'}}\right)^{1/2} A_{m,m'} + \left(\frac{\omega_{m'}}{\omega_m}\right)^{1/2} B_{m,m'}\right] \ . \quad (54)$$

This result [Eq. (53)] is approximate in that it does not correctly include contributions from states where more than one phonon is present in a single mode. The summations in Eq. (52) can be recast as

$$w(t) = \left\{\sum_{m'} |C_{m,m'}|^2 \exp[i(E_{m'} - E_i/n_m)t/\hbar]\right\}^{n_m} \ . \quad (55)$$

The salient time dependence of $w(t)$ can be obtained by expanding the exponential to second order to give

$$w(t) = \left\{\sum_{m'} |C_{m,m'}|^2 \left[1 + i(E_{m'} - E_i/n_m)t/\hbar - \frac{1}{2}(E_{m'} - E_i/n_m)^2 t^2/\hbar^2 + \ldots\right]\right\}^{n_m} \ . \quad (56)$$

The average energy shift per phonon is defined to be

$$\Delta\epsilon = \frac{\sum_{m'} |C_{m,m'}|^2 (E_{m'} - E_i/n_m)}{\sum_{m'} |C_{m,m'}|^2} \ . \quad (57)$$

We also define a second moment to be

$$(\delta\epsilon)^2 = \frac{\sum_{m'} |C_{m,m'}|^2 (E_{m'} - E_i/n_m - \Delta\epsilon)^2}{\sum_{m'} |C_{m,m'}|^2} \ . \quad (58)$$

In terms of these parameters, the Fourier transform $w(t)$ is

$$w(t) \approx \left(\sum_{m'} |C_{m,m'}|^2\right)^{n_m} \times \{\exp(i\Delta\epsilon t/\hbar)\exp[-(\delta\epsilon)t^2/2\hbar^2]\}^{n_m} \ . \quad (59)$$

After transforming to obtain $W(E)$ and taking the limit as $\Gamma \to 0$, we recover

$$W(E) \sim \exp[-(E - E_0 - n_m\Delta\epsilon)^2/2n_m(\delta\epsilon)^2] \ , \quad (60)$$

which agrees with our simple estimates given earlier.

The example described here constitutes the simplest and perhaps cleanest example of anomalous energy exchange with the lattice in the case of ostensibly recoil-free (since the neutron and gamma momentum are assumed to be matched) neutron capture. In this case, the final lattice energy is less than the initial lattice energy, which implies that the gamma is emitted at an energy that is anomalously high. The coherent neutron transfer reactions that we wish to describe require capture energy to be ultimately taken up by the lattice, which means that we would like to study examples in which the emitted gamma energy is reduced rather than raised. The example discussed here is useful in its simplicity but shifts in the wrong direction relative to what we seek. Nevertheless, this example is perhaps the first theoretical demonstration of the ability of the Duschinsky operator to transfer an anomalous amount of energy during a neutron capture reaction.

VI. SUMMARY AND CONCLUSIONS

In this technical note, we continued our examination of energy transfer between nucleons and a lattice during a neutron transfer reaction. Of the possible interaction mechanisms, we identified the Duschinsky operator over recoil as having the best chance of transferring significant amounts of energy between the nucleons and the lattice. As a result, we focused on an idealized reaction in which the gamma and neutron momenta coincide to eliminate the primary recoil term.

If energy transfer does occur, it must be reflected by modifications in the associated gamma line shape; our discussion in this work therefore centered on the computation of the line profile, in search of anomalously large shifts or widths that would be a signature of anomalous coupling.

We developed a variant of the Sharp and Rosenstock method to analyze the matrix elements of the Duschinsky operator for lattice states that are highly excited in a single mode. Thermal lattices are not expected to show any significant anomalies in the Duschinsky matrix elements since most of the lattice energy is in modes that do not shift their energies appreciably under a Duschinsky transformation.

The basic new effect that we found is the presence of anomalously large energy transfer in the case of a neutron transfer reaction, which causes a very highly excited phonon mode to shift its energy significantly under the Duschinsky transformation. Highly excited localized modes that are embedded in a continuum are predicted to show the effect. The total energy transfer for such a reaction is on the order of $n\hbar\Delta\omega$, where n is the number of phonons present in the mode and where $\Delta\omega$ is the frequency shift of the mode that occurs as a result of the neutron transfer reaction.

In our original proposal of the coherent neutron transfer model, we speculated that the lattice could cause neutron ionization by coupling lattice energy into a neutron ionization reaction. Although the mechanism described here can couple a very significant amount of energy to or from the lattice when a neutron transfer reaction occurs, the sign of the energy transfer does not allow the proposed effect. For example, neutron ionization is endothermic; the shift in mode frequencies is positive since the resulting nucleus is lighter, and, by the present mechanism, the lattice is capable of increasing its energy during such a reaction. We have not yet found a way to reduce the lattice energy during neutron ionization using this mechanism.

Neutron transfer reactions could, in principle, still be viable if the present mechanism were used to balance the total energy in the case of a second-order process where two neutron transfer reactions occurred, one of them a capture and one an ionization. In this case, if the capture occurs first and energy is taken from the lattice, then the nuclear/lattice system is off the mass shell; a subsequent neutron ionization with an associated energy input to the lattice could then bring the coupled system back into energy balance. The price to be paid for this off-resonant route is a factor on the order of $|H|/\Delta E$. In future works, we shall explore this mechanism further to see whether it can account for the reported anomalies.

EDITOR'S NOTE: "Coherent and Semicoherent Neutron Transfer Reactions II: Transition Operators" (Ref. 2) will be published in a future issue of *Fusion Technology*.

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