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Research Article

Calculation of the Boosted Spin–orbit Contribution to the Phonon–Nuclear Coupling Matrix Element for ^{181}Ta

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Abstract

Modern deformed shell model single–proton wave functions are used to evaluate the boosted spin–orbit contribution to the phonon–nuclear interaction for the 6.237 keV transition in ^{181}Ta. This is the lowest energy E1 transition from the ground state among the stable nuclei, and is important in connection with proposed excitation transfer and up-conversion experiments. The value resulting for the magnitude $|\langle 9/2^-|\hat{\mathbf{a}}|7/2^+\rangle|$ is 1.3×10^{-6}. The wave functions are also used to evaluate the radiative decay rate which is found to be about 2×10^5 higher than the experimental value, which is strongly hindered. The large interference effect found in the Nilsson model for this transition does not occur in the deformed nuclear model we used. One possibility is that the Nilsson model provides a better physical description, and another possibility is that the problem is more fundamental. We speculate about different approaches that might lead to model wave functions relevant to low-energy transition energies, and also for radiative decay rates.

Keywords: Deformed nucleus, E1 radiative decay rate, Phonon–nuclear coupling, Phonon–nuclear matrix element, ^{181}Ta

1. Introduction

After nearly 30 years following the announcement of the Fleischmann–Pons experiment [1,2] there has emerged no consensus as to what microscopic reaction or what physical mechanisms are involved, in spite of the hundreds of theoretical papers that have been put forth over the years. Many in our field are convinced that the origin of the effect is nuclear; however, the absence of energetic nuclear radiation commensurate with the energy produced means that conventional nuclear detectors cannot be used for the determination of a reaction mechanism.

Our efforts in recent years have focused on phonon–nuclear coupling [3], in which the raising or lowering of a nuclear state is coupled to the creation or destruction of a phonon, due to the relativistic boost correction of the nucleon-nucleon interaction in an oscillating nucleus [4]. The boost correction is known in the literature, it is stronger than the coupling derived from external electric and magnetic fields at the nucleus due to the motion of surrounding nuclei, and it has not been considered previously in the literature in connection with the slow oscillations of nuclei in condensed matter. We have interpreted observations of unexpected non-exponential decay of X-ray and gamma lines

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in excitation transfer experiments with a radioactive ^{57}Co source in our lab in terms of excitation transfer mediated by high-frequency phonons as a result of this relativistic boost correction interaction. Models that we have studied for the down-conversion of large energy quanta originating with the D_2/^{4}He transition (followed by subdivision) accomplish the conversion through a great many sequential non-resonant excitation transfer steps which transfer energy from nuclei to phonons while quantum coherence is maintained.

At this point we have a fundamental Hamiltonian, we can make use of perturbation theory to evaluate the indirect coupling associated with excitation transfer [5], and we have some results from models for up-conversion and down-conversion. The models and the results are expressed in terms of the phonon–nuclear coupling matrix elements, which will need to be evaluated explicitly in order to develop quantitative predictions from the theory. We have reported previously some early efforts to evaluate matrix elements of the phonon–nuclear interaction [6,7], which were done prior to the analysis of Ref. [4] and which will need to be done again with the improved version of the interaction.

The phonon–nuclear interaction has selection rules for nuclear transitions consistent with that of an electric dipole, which focused our attention initially on low-energy nuclear electric dipole (E1) transitions. For up-conversion low-energy transitions are favored since fewer quanta are required to produce excitation. For excitation transfer the indirect interaction favors high frequency phonons and low energy nuclear transitions. The lowest energy nuclear E1 transition from a stable ground state of all the nuclei occurs in ^{181}Ta and is listed in the BNL Nudat2 database as involving an excited state at 6.237 keV. We put in some effort to develop an excitation transfer experiment with a ^{181}W source evaporated on a ^{181}Ta plate, but ran into difficulty obtaining radioactive ^{181}W. Nevertheless, this experiment in our view remains a potentially important one (even if we are not able to implement it at this time). In support of this experiment we chose some time ago to focus on a calculation of the phonon–nuclear coupling matrix element. In this report we summarize briefly the associated model, calculation, and result.

2. Nonspherical Potential Model for Proton Orbitals

The ^{181}Ta nucleus is known to be strongly deformed in the ground state and first excited state, based on the large nuclear quadrupole moments [8]. Consequently, the simplest relevant model that we might use is a Nilsson model [9] (see also [10] for earlier work on deformed nuclei).

Prior to the work of Nilsson and collaborators, much progress had been made on shell models for nuclear orbitals in an independent particle model based on spherical potential models. In such models a nonrelativistic Hamiltonian containing the kinetic energy, potential energy, and spin–orbit interaction was used to model proton and neutron orbitals [11,12], which was successful in understanding the shell structure effects in nuclei, and the ordering of the different subshells.

2.1. Deformed models from the Dudek group

Once the model is extended to deformed nuclei, then new issues arise. For example, a deformed nucleus can rotate, which allows for a quantitative explanation of the energy levels of observed rotational levels. From a purely practical perspective, the question of what deformed potential to use must be addressed, along with the parameterization of the spin–orbit potential. Fortunately, there has been much subsequent work on the problem, where models have been optimized to match well with known nuclear levels and quadrupole moments [13–15]. These models have been implemented in a Fortran program that has been made available to the scientific community [16].

It is useful to discuss briefly the difference between the older potential models used by the nuclear physicists of the 1950s, and the more modern potential models of the Dudek group used in since the 1970s. It was not appreciated at the outset of our work the importance of this issue. In the 1950s the focus was largely on models based on deformed harmonic oscillator potentials [9], due in part to the more accessible associated mathematics, and in part from the reasonably good observed agreement with experiment for the resulting single–particle models. The more modern deformed potentials of the Dudek group are essentially deformed Woods–Saxon potentials, which are flat in the interior of the nucleus, and which taper off to zero rapidly at the nuclear boundary. This kind of model is much closer to models long used for nuclear scattering calculations, and would be expected to provide a more realistic description of the interaction of an outer nucleon with the core.

2.2. Deformed potential Hamiltonian

The Hamiltonian for a proton in a deformed potential according to these models is made up of terms accounting (in order) for the proton kinetic energy, strong force potential, Coulomb potential, nuclear spin–orbit interaction, and Coulomb spin–orbit interaction according to

$$\hat{H} = -\frac{\hbar^2\nabla^2}{2M} + U(\rho, z) + V_{\mathrm{C}}(\rho, z) - \lambda\left(\frac{\hbar}{2Mc}\right)^2 \nabla U \cdot \hat{\boldsymbol{\sigma}} \times \hat{\mathbf{p}} + \frac{\hbar}{2M^2c^2}(\nabla V_{\mathrm{C}} \times \hat{\mathbf{p}}) \cdot \hat{\mathbf{s}}, \tag{1}$$

where M is the proton mass; $\hat{\boldsymbol{\sigma}}$ a vector operator made up of Pauli matrices; $\hat{\mathbf{p}}$ the proton momentum operator; $\hat{\mathbf{s}}$ the proton spin operator; V_{C} is the Coulomb potential associated with a uniform charge distribution within the boundary of the nucleus; and c is the speed of light. The scaling parameter λ for the nuclear spin–orbit interaction has been determined empirically by optimizing predicted orbital energies with observed orbital energies. The model strong force potential U is a taken to be a deformed Woods–Saxon potential

$$U = \frac{V_0}{1 + \exp\left[\mathrm{dist}/a\right]} \tag{2}$$

with fitting parameters V_0 and a; where "dist" in this formula is the distance between the position vector and the deformed nuclear surface given by

$$R(\theta) = c' R_0\left[1 + \beta_2 Y_{20}(\theta, \phi) + \beta_4 Y_{40}(\theta, \phi)\right] \tag{3}$$

with Y_{lm} a spherical harmonic function. The deformation parameters R_0, β_2 and β_4 define the shape of the deformed nuclear potential, with c' serving as a normalization constant to preserve the nuclear volume.

2.3. Coupled-channel model

Early in our study we were not aware that any codes were available, so we developed our own numerical models. We began with simple spherical models based on the Woods-Saxon potential and spin–orbit interaction, which very quickly gave us orbital energies in agreement with literature values. The extension of the model to the deformed case involved a great deal of work. After implementing and discarding different numerical implementations (we had high hopes for an elegant iterative coupled channel scheme), we ended up making use of a coupled channel approach that makes use of a brute force sparse matrix eigenvalue solution for the radial equations.

The model assumes a finite basis approximation of the form

$$\Psi = \sum_{m_s}\sum_{l,m} |s, m_s\rangle Y_{lm}(\theta, \phi)\frac{P_{lmsm_s}(r)}{r}, \tag{4}$$

which leads to coupled channel equations that we can write as

$$\begin{aligned} EP_{lmsm_s}(r) \ =& \frac{\hbar^2}{2M}\left[-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}\right]P_{lmsm_s}(r) \\ &+\sum_{l'}\langle lmsm_s|U+V_C|l'msm_s\rangle P_{l'msm_s}(r) \\ &+\sum_{l'm'}\sum_{m_s'}\langle lmsm_s|U_{\rm so}+V_{\rm so}|l'm'sm_s'\rangle P_{l'm'sm_s'}(r), \end{aligned} \tag{5}$$

where $U_{\rm so}$ and $V_{\rm so}$ are the nuclear and Coulomb spin–orbit interactions. The implementation of this model involved a substantial technical effort. In our implementation we approximated the spin–orbit interaction through terms involving radial derivatives and omitted the angular derivatives. This saved much work as well as making the code run faster, for what appears to be a minor loss in accuracy.

3. Phonon–nuclear Coupling Matrix Element

In order to evaluate the phonon–nuclear coupling matrix element, we require a determination of the deformation parameters, as well as a specification of the boost correction.

3.1. Determination of the deformation parameters

The choice of the β_2 parameter can be made by looking for a level crossing (6.237 keV is small compared to the MeV shifts that occur when β_2 is varied between 0.15 and 0.25) between the 7/2$^+$ ground state and the 9/2$^-$ excited state (where the state notation here is I^p, with I the nuclear spin and p the parity). A value of $\beta_4 = -0.038$ was reported for ^{181}Re in Ref. [17], which we adopted for ^{181}Ta. The associated curve crossing occur close to $\beta_2 = 0.250$.

3.2. Quadrupole moment

According to Ref. [18] we can write for the intrinsic quadrupole moment

$$Q_0 = \frac{3}{\sqrt{5\pi}}eZR^2\beta_2\left(1+\pi^2\left(\frac{a}{R}\right)^2+\frac{2}{7}\sqrt{\frac{5}{\pi}}\beta_2\right) \tag{6}$$

with $a = 0.54$ as relevant to the Pb region, and

$$R = 1.2A^{1/3} = 6.788 \text{ fm}. \tag{7}$$

The spectroscopic quadrupole moment $Q_{\rm s}$ is related to the intrinsic quadrupole moment through

$$Q_{\rm s} = \frac{3K^2 - I(I+1)}{(I+1)(2I+3)}Q_0. \tag{8}$$

For the 7/2+ ground state $K = I = 7/2$ and

$$Q_{\rm s} = \frac{7}{15}Q_0. \tag{9}$$

A deformation parameter of $\beta_2 = 0.247$ is consistent with an intrinsic quadrupole moment of 7.37 eb, which is close to the value used in [19], and a bit higher than the spectroscopic values listed in [8].

Note that according to [20] the ratio of the quadrupole moment of the first excited state to the ground state is

$$\frac{Q\left[\frac{9}{2}\right]}{Q\left[\frac{7}{2}\right]} = 1.133 \pm 0.010. \tag{10}$$

3.3. Code comparison

After we had developed preliminary versions of the coupled channel code, we were interested in arranging for tests in order to debug the code. At this point we located the Dudek group code, downloaded it, and got it running on our system. We might have made use of it for matrix element calculations, except that it was not developed for this purpose, and we did not put in sufficient effort to extract the wave functions. Instead we decided to carry out matrix element calculations with our code, which had been developed specifically for this purpose.

Results from the two codes for the $7/2^+$ and $9/2^-$ states are shown in Table 1, including deformation, and with matched underlying spin–orbit models. The agreement is reasonable, with the differences due primarily to the use of an incomplete spin–orbit interaction in the coupled channel code.

3.4. Boosted spin–orbit interaction

The phonon–nuclear interaction in the models we have studied comes about primarily as a boost correction of the nucleon–nucleon interaction. Ideally we would prefer a derivation of the Nilsson model from first principles, and then apply a boost correction systematically to all of the different interactions. However, the Nilsson model is an empirical model, with potential parameters fitted to experimental data. Consequently at present a systematic boosting of all contributing interactions is not possible.

Instead, what is possible is to work with a boosted version of the spin–orbit interaction. This should provide a lower limit within an independent particle picture (the independent particle picture itself will be the focus of some discussion below). The nuclear contribution to the spin–orbit interaction can be written as

$$U_{\text{so}} = -\lambda \left(\frac{\hbar}{2Mc}\right)^2 \nabla U \cdot \boldsymbol{\sigma} \times \hat{\mathbf{p}}. \tag{11}$$

Table 1. Orbital energies from the Dudek code compared with results from the coupled channel code with 100 grid points for a deformed version of the problem ($\beta_2 = 0.25$ and $\beta_4 = -0.038$) and matched spin–orbit models.

Index	E_{Dudek} (MeV)	E_{code} (MeV) $l_{\text{max}} = 10$
$7/2+$ (1)	–13.3163	–13.455392
$7/2+$ (2)	–6.3483	–6.289249
$7/2+$ (3)	–1.9020	–2.067574
$9/2-$ (1)	–6.3458	–6.425660
$9/2-$ (2)	2.9235	2.941132

We can arrange for a boosted momentum according to

$$\hat{\mathbf{p}} \rightarrow \hat{\boldsymbol{\pi}} + \frac{\hat{\mathbf{P}}}{A}, \tag{12}$$

where $\hat{\mathbf{P}}$ is the center of mass momentum and where $\hat{\boldsymbol{\pi}}$ is the relative momentum. For the correction we can write

$$\Delta U_{\text{so}} = -\lambda \left(\frac{\hbar}{2Mc}\right)^2 \nabla U \cdot \boldsymbol{\sigma} \times \frac{\hat{\mathbf{P}}}{A} = \lambda \left(\frac{\hbar}{2Mc}\right)^2 \boldsymbol{\sigma} \times \nabla U \cdot \frac{\hat{\mathbf{P}}}{A} = \hat{\mathbf{a}} \cdot c\hat{\mathbf{P}} \tag{13}$$

with the $\hat{\mathbf{a}}$ operator given by

$$\hat{\mathbf{a}} = \lambda \frac{\hbar^2}{4AM^2c^3} \boldsymbol{\sigma} \times \nabla U. \tag{14}$$

3.5. Matrix element of the $\hat{\mathbf{a}}$ operator

Making use of the proton orbitals discussed above, we calculated the magnitude of the matrix element for the $\hat{\mathbf{a}}$ operator for a one proton transition between the first excited state and the ground state with the result

$$\left| \left\langle \frac{9}{2}^- \middle| \hat{\mathbf{a}} \middle| \frac{7}{2}^+ \right\rangle \right| = 1.3 \times 10^{-6}. \tag{15}$$

4. Radiative Decay

A check on the model can be provided by making use of the deformed model wave functions for the evaluation of the radiative decay rate. While conceptually simple, we will encounter a number of complicated issues as a result.

4.1. Calculation of the single-particle decay rate

For the radiative decay rate we have used the length form according to

$$\gamma = \frac{4}{3}\alpha \left(\frac{N}{A}\right)^2 \frac{\omega^3}{c^2} \left| \left\langle \frac{9}{2}^- \middle| \mathbf{r} \middle| \frac{7}{2}^+ \right\rangle \right|^2, \tag{16}$$

where the electric dipole matrix element was evaluated using the orbitals discussed above. In this formula N is the number of neutrons in the nucleus, and Z is the number of protons. The decay rate that results is

$$\gamma = 3.9 \times 10^8 \text{ s}^{-1}. \tag{17}$$

4.2. Decay rate from experiment

The half-life of the ^{181}Ta 6.237 keV excited state is 6.05 μs according to the Nudat2 database, and the internal conversion coefficient is listed as 70.5. From this we can estimate the radiative decay rate from experiment to be

$$\gamma_{\text{expt}} = \frac{\ln 2}{6.05\ \mu\text{s}} \times \frac{1}{1+70.5} = 1.6 \times 10^3\ \text{s}^{-1}. \tag{18}$$

We see that the deformed shell model estimate for the radiative decay rate is high by more that 2×10^5.

4.3. Discussion

This disagreement between the single–particle theory in general and experiment is of course well known in the literature [21], and occurs at one level or another with all low-energy electric dipole transitions (and also with magnetic dipole transitions, and transitions of other multipolarity). The question is what produces the hindrance.

There is probably agreement that if a sufficiently large set of basis states could be assembled, the it should be possible to make use of (massive) multi-configurational calculations to calculate radiative decay rates accurately (assuming a suitably accurate nuclear potential model). In atomic physics calculations one can do well with generally with a modest number of configurations for simple atoms and ions, largely due to the presence of a strong nuclear potential, goodness of an average potential due to the other electrons, and relatively weak correlation effects. In the nuclear problem there is no dominant central potential, and the nucleon–nucleon interaction is strong, which maximizes correlation effects.

An astonishing advance on the problem of modeling radiative decay rates was reported in the 1950s when Nilsson and coworkers made use of deformed nuclear potential models to compute radiative decay rates for single proton and neutron transitions, where interference effects led to a reduction in the associated matrix elements and correspondingly large reductions in the predicted rates. However, there remained substantial differences between the rates predicted with Nilsson orbitals and experiment to account for. Motivated by the recently developed BCS theory for superconductivity, a similar approach was proposed to account for the residual correlation effects in nuclei. It became possible to account systematically for the decay rates of low-energy nuclear transitions then taking into account deformation and correlation effects [22].

At the beginning of this study we were aware of some of this progress, and the presumption was that by taking advantage of more modern and sophisticated deformed potential models we would have better wave functions and obtain even closer agreement. But as discussed above, the deformation parameters which give the best results for ^{181}Ta do not lead to the same interference associated with the Nilsson model. It is possible to find regions in the associated deformation parameter space where the requisite interference occurs, but this is not particularly close to where our optimization has landed us.

So, the relevant question at this point is how might we interpret the resulting situation?

One possibility is that the Nilsson model is the better physical model, that interference effects occur just as described by the model, and that we are not going to be able to get reliable answers for radiative decay rates from the deformed potential model of Dudek and coworkers. In this case we should not pursue further work with the Dudek model, and instead turn our attention to the Nilsson model with pairing corrections. This could be done, and probably should be done since it would not involve a particularly large investment of effort beyond what has been put in already.

Another possibility is that the problem is more fundamental. As has been pointed out by Cook [23] and others it is hard to see how an independent particle model should apply under conditions where the nucleus is dense, and where the mean free path of an incident nucleon is on the order of a fermi. While a lattice model might be a good approximation for some calculations, the nuclear density is too low for the nucleus to be a solid [24]. Instead, we expect the nucleus to be a Fermi liquid. There has been much development of Fermi liquid theory for nuclei in the literature [25], but this kind of model does not appear to have been used for low-energy E1 transitions in recent years. Other approaches have been successful in modeling E1 transitions over a wide energy range including the low-energy region generally [26,27].

It may be that nucleons do not travel freely throughout the interior of the nucleus, but instead their movement is hindered due to the dense packing of neighboring nuclei. In such a picture, a nucleons is localized some of the time, but tunnels to exchange with a neighboring nuclei. It may be possible to develop an empirical dispersion relation to model this effect, which would have an impact on the energy level spacing for low-lying states. It would be relatively easy to develop and test this kind of single-particle model.

Were we to think of the nucleus from the point of view of a lattice with the frequent coherent exchange of positions, then it would follow that a large reduction of the matrix element for the current should be expected relative to an independent particle picture due to the associated correlation between the nucleons. The question is whether it is possible to develop model many-particle wave functions of this kind, and evaluate matrix elements with them.

5. Summary and Conclusions

Proton wave functions were computed for a proton in a modern deformed nuclear potential to model the boosted spin–orbit contribution to the phonon–nuclear interaction between the ground state and first excited state of ^{181}Ta. The numerical implementation was based on a coupled channel formulation, and we made use of an incomplete spin–orbit interaction to reduce the effort level and run time. The energy eigenvalues are in reasonably good agreement with results from the Dudek group code for this problem and others.

The magnitude of the $\hat{\mathbf{a}}$ matrix element that results is 1.3×10^{-6}, which is on the low end of the range of what we had expected. We might expect boosted versions of the central and tensor interactions to lead to a larger phonon–nuclear interaction; however, at present there is no derivation of the Nilsson or other deformed potential models that we might use to evaluate the associated contributions.

As a check on the model we calculated the radiative decay rate, and found that it was not hindered as in the Nilsson model. That low-energy electric dipole transitions are strongly hindered relative to spherical harmonic oscillator model estimates in nuclei is of course well known. This is modeled in the Nilsson theory through interference effects (which are not present in the Dudek deformed potential model), and also with corrections due to correlation effects. The concern of course is that there may be corresponding reductions in the $\hat{\mathbf{a}}$-matrix element due to interference and correlation effects. It would be worthwhile to make use of an appropriate Nilsson model for the $\hat{\mathbf{a}}$-matrix element calculation, a project of interest to us in the future.

The accurate calculation of phonon-nuclear matrix elements for low-energy transitions is made difficult due to the absence of relevant simple models that a predictive. We are considering a number of possibilities, including Fermi liquid models, an empirical dispersion relation, and the possibility of developing new many-particle models based on a lattice picture with coherent exchange.

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