Calculation of the phonon-nuclear coupling matrix element for Ta-181

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Introduction

• Have been interested in the development of a model for anomalies in condensed matter nuclear science for many years

• One big problem is the coupling between the internal nuclear degrees of freedom and the lattice

• A few years ago we found a relativistic interaction that couples vibrations to the internal nuclear degrees of freedom

• Another big problem concerns energy exchange between the nucleus and the lattice

• 15 years ago we found a mechanism capable of coherent up-conversion and down-conversion for energy exchange
Phonon-nuclear interaction
\[ \hat{H} = \sum_j \alpha_j \cdot c \left[ p_j - q_j A(r_j) \right] + \sum \beta_j mc^2 + \sum_{j < k} \hat{V}_{jk} (r_k - r_j) + \sum q_j \Phi(r_j) \]
Partial Foldy-Wouthuysen transformation

\[ \hat{H}' = e^{i\hat{S}} \left( \hat{H} - i\hbar \frac{\partial}{\partial t} \right) e^{-i\hat{S}} \]

\[ = \hat{H} + i \left[ \hat{S}, \hat{H} \right] - \frac{1}{2} \left[ \hat{S}, \left[ \hat{S}, \hat{H} \right] \right] + \ldots - \hbar \frac{\partial \hat{S}}{\partial t} - i \frac{1}{2} \left[ \hat{S}, \hbar \frac{\partial \hat{S}}{\partial t} \right] + \ldots \]

\[ \hat{S} = -i \frac{1}{2Mc} \sum_j \beta_j \alpha_j \cdot \left[ \hat{P}_j - QA(R) \right] \]
\[
\hat{H}' = \frac{1}{2M} \left| \hat{P} - QA \right|^2 + \frac{1}{N} \sum_j \beta_j + Q \Phi - \frac{\hbar Q}{2M} \frac{1}{N} \sum_j \beta_j \hat{\Sigma}_j \cdot \mathbf{B} - \frac{\hbar^2 Q}{8M^2 c^2} \nabla \cdot \mathbf{E} \\
+ \frac{\hbar Q}{8M^2 c^2} \sum_j \hat{\Sigma}_j \cdot \left[ \left( \hat{P} - QA \right) \times \mathbf{E} - \mathbf{E} \times \left( \hat{P} - QA \right) \right]
\]

\[
+ \sum_j \beta_j mc^2 + \sum_j \alpha_j \cdot c \hat{\pi}_j + \sum_{j<k} \hat{V}_{jk}
\]

\[
+ \sum_j \left[ q_j \Phi \left( \mathbf{R} + \xi_j \right) - \frac{Q}{N} \Phi \left( \mathbf{R} \right) \right] - \sum_j \alpha_j \cdot c \left[ q_j A \left( \mathbf{R} + \xi_j \right) - \frac{Q}{N} A \left( \mathbf{R} \right) \right]
\]

\[
+ \sum_j \beta_j \frac{\left( \hat{P} - QA \right) \cdot \hat{\pi}_j}{M} + \frac{1}{2Mc} \sum_{j<k} \left[ \left( \beta_j \alpha_j + \beta_k \alpha_k \right) \cdot \left( \hat{P} - QA \right), \hat{V}_{jk} \right]
\]

\[
+ \ldots
\]
\[ \hat{H}' = \frac{|\hat{P}|^2}{2M} + \sum_j \beta_j mc^2 + \sum_j \alpha_j \cdot \hat{\pi}_j + \sum_{j<k} \hat{V}_{jk} + \mathbf{a} \cdot \mathbf{c}\hat{\mathbf{P}} + \ldots \]

where

\[ \mathbf{a} \cdot \mathbf{c}\hat{\mathbf{P}} = \left\{ \sum_j \beta_j \frac{\hat{\pi}_j}{M} + \frac{1}{2Mc} \sum_{j<k} \left[ \left( \beta_j \mathbf{a}_j + \beta_k \mathbf{a}_k \right), \hat{V}_{jk} \right] \right\} \cdot \hat{\mathbf{P}} \]
Thinking about the result

- Relativistic model with Dirac phenomenology for protons and neutrons gives phonon-nuclear coupling
- The math is clear, but we would like some intuition
- Dominant coupling is due to boost of nucleon-nucleon interaction
Coulomb and Breit interaction, rest frame

\[
\hat{H} = \beta_1 mc^2 + \alpha_1 \cdot c\hat{\pi}_1 + \beta_2 mc^2 + \alpha_2 \cdot c\hat{\pi}_2 \\
+ \frac{q_1 q_2}{4\pi\varepsilon_0} \left\{ \frac{1}{r_{12}} - \frac{1}{2} \left[ \frac{\alpha_1 \cdot \alpha_2}{r_{12}} + \frac{(\alpha_1 \cdot cr_{12})(\alpha_2 \cdot cr_{12})}{r_{12}^3} \right] \right\}
\]
Coulomb and Breit interaction, boosted frame

\[ \alpha \rightarrow \frac{v}{c} \quad \text{in rest frame} \]

\[ \alpha \rightarrow \frac{v}{c} + \frac{P}{Mc} \quad \text{in moving frame} \]

\[
\hat{H} \rightarrow \beta_1 mc^2 + \alpha_1 \cdot c\hat{\pi}_1 + \beta_2 mc^2 + \alpha_2 \cdot c\hat{\pi}_2 \\
+ \frac{q_1 q_2}{4\pi \varepsilon_0} \left\{ \frac{1}{r_{12}} - \frac{1}{2} \left[ \left( \alpha_1 + \frac{\hat{P}}{Mc} \right) \cdot \left( \alpha_2 + \frac{\hat{P}}{Mc} \right) \right] \right. \\
\left. + \left( \left( \alpha_1 + \frac{\hat{P}}{Mc} \right) \cdot cr_{12} \right) \left( \left( \alpha_2 + \frac{\hat{P}}{Mc} \right) \cdot cr_{12} \right) \right\}
\]
Keep lowest order terms...

\[ \hat{H} \rightarrow \beta_1 mc^2 + \alpha_1 \cdot c \hat{\pi}_1 + \beta_2 mc^2 + \alpha_2 \cdot c \hat{\pi}_2 \]

\[ + \frac{q_1 q_2}{4 \pi \varepsilon_0} \left\{ \frac{1}{r_{12}} - \frac{1}{2} \left[ \frac{\alpha_1 \cdot \alpha_2}{r_{12}^2} + \left( \frac{\alpha_1 \cdot c r_{12}}{r_{12}^3} \right) \left( \frac{\alpha_2 \cdot c r_{12}}{r_{12}^3} \right) \right] \right\} \]

\[ - \frac{1}{2Mc} \frac{q_1 q_2}{4 \pi \varepsilon_0} \left[ \frac{\hat{\mathbf{P}} \cdot \alpha_1}{r_{12}} + \frac{\hat{\mathbf{P}} \cdot \alpha_2}{r_{12}} + \left( \frac{\hat{\mathbf{P}} \cdot c r_{12}}{r_{12}^3} \right) \left( \frac{\alpha_2 \cdot c r_{12}}{r_{12}^3} \right) + \left( \frac{\alpha_1 \cdot c r_{12}}{r_{12}^3} \right) \left( \frac{\hat{\mathbf{P}} \cdot c r_{12}}{r_{12}^3} \right) \right] \]
Now evaluate the coupling term

\[ \frac{1}{2Mc} \sum_{j<k} \left[ (\beta_j \alpha_j + \beta_k \alpha_k) \cdot \hat{P}, \hat{V}_{jk} \right] = \]

\[ - \frac{1}{2Mc} \frac{q_1 q_2}{4\pi \varepsilon_0} \left[ \frac{\hat{P} \cdot \alpha_1}{r_{12}} \beta_2 + \frac{\hat{P} \cdot \alpha_2}{r_{12}} \beta_1 + \frac{(\hat{P} \cdot \mathbf{c}_{r_{12}})(\alpha_2 \cdot \mathbf{c}_{r_{12}})}{r_{12}^3} \beta_1 + \frac{(\alpha_1 \cdot \mathbf{c}_{r_{12}})(\hat{P} \cdot \mathbf{c}_{r_{12}})}{r_{12}^3} \beta_2 \right] \]
Thinking

• Things begin to become clear...
• What the linear coupling term is doing is fixing the magnetic interaction
• ...so that it is correct when the composite is in motion!
Importance of Ta-181
Lowest energy nuclear transitions

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>Excited state energy (keV)</th>
<th>half-life</th>
<th>multipolarity</th>
</tr>
</thead>
<tbody>
<tr>
<td>(^{201}\text{Hg})</td>
<td>1.5648</td>
<td>81 ns</td>
<td>M1+E2</td>
</tr>
<tr>
<td>(^{181}\text{Ta})</td>
<td>6.240</td>
<td>6.05 (\mu\text{s})</td>
<td>E1</td>
</tr>
<tr>
<td>(^{169}\text{Tm})</td>
<td>8.41017</td>
<td>4.09 ns</td>
<td>M1+E2</td>
</tr>
<tr>
<td>(^{83}\text{Kr})</td>
<td>9.4051</td>
<td>154.4 ns</td>
<td>M1+E2</td>
</tr>
<tr>
<td>(^{187}\text{Os})</td>
<td>9.75</td>
<td>2.38 ns</td>
<td>M1(+E2)</td>
</tr>
<tr>
<td>(^{73}\text{Ge})</td>
<td>13.2845</td>
<td>2.92 (\mu\text{s})</td>
<td>E2</td>
</tr>
<tr>
<td>(^{57}\text{Fe})</td>
<td>14.4129</td>
<td>98.3 ns</td>
<td>M1+E2</td>
</tr>
</tbody>
</table>
Lowest energy E1 transitions

<table>
<thead>
<tr>
<th>isotope</th>
<th>$E$(keV)</th>
<th>$T_{1/2}$</th>
<th>multipolarity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ta-181</td>
<td>6.237</td>
<td>6.05 µsec</td>
<td>E1</td>
</tr>
<tr>
<td>Dy-161</td>
<td>25.65135</td>
<td>29.1 ns</td>
<td>E1</td>
</tr>
<tr>
<td>Gd-157</td>
<td>63.929</td>
<td>0.46 µsec</td>
<td>E1</td>
</tr>
<tr>
<td>Dy-161</td>
<td>74.56668</td>
<td>3.14 ns</td>
<td>E1</td>
</tr>
<tr>
<td>Gd-155</td>
<td>86.5479</td>
<td>6.50 ns</td>
<td>E1</td>
</tr>
<tr>
<td>Eu-153</td>
<td>97.43100</td>
<td>0.198 ns</td>
<td>E1</td>
</tr>
<tr>
<td>Dy-161</td>
<td>103.062</td>
<td>0.60 ns</td>
<td>E1</td>
</tr>
<tr>
<td>Gd-155</td>
<td>105.3083</td>
<td>1.16 ns</td>
<td>E1</td>
</tr>
<tr>
<td>F-19</td>
<td>109.9</td>
<td>0.591 ns</td>
<td>E1</td>
</tr>
<tr>
<td>Dy-161</td>
<td>131.8</td>
<td>0.145 ns</td>
<td>[E1]</td>
</tr>
<tr>
<td>Eu-153</td>
<td>151.6245</td>
<td>0.36 ns</td>
<td>E1</td>
</tr>
</tbody>
</table>
Thinking

• Phonon-nuclear interaction has E1 multipolarity (M2, E3, M4... at higher order)

• Ta-181 has the lowest energy E1 transition from ground state of all stable nuclei

• Low energy transitions favored in up-conversion and down-conversion models
Ta-181 nuclear states
Deformed nuclei

Spherical (No deformation)

Spheroidal (Deformed)
What about Ta-181

• Ta-181 nucleus is prolate spheroidal
• Well studied in the early literature
• Nuclear quadrupole deformation can be inferred approximately from (large) quadrupole moment in NMR studies
• Low-lying nuclear states modeled as single proton orbitals in a deformed attractive nuclear core
• Parameterization of the nuclear surface:

\[
R(\theta) = c(\beta_2, \beta_4) R_0 \left[ 1 + \beta_2 Y_{20}(\theta, \phi) + \beta_4 Y_{40}(\theta, \phi) \right]
\]
Model for proton states

\[ \hat{H} = -\frac{\hbar^2 \nabla^2}{2M_p} + V_{nuc}(r, \theta) + V_{Coul}(r, \theta) + \hat{V}_{LS} \]

- kinetic energy
- deformed nuclear potential
- deformed Coulomb potential
- spin-orbit interaction
Thinking about the model

- Model for proton in deformed nucleus is simplest imaginable
- Closely related to earlier spherical models
- Philosophically consistent with electron model in atom
- Deformed nuclear potential models available in the literature
- Deformation models readily available
- Deformed Coulomb interaction easily computed (assume uniform positive background charge density inside nucleus)
- Parameterization available for nuclear spin-orbit interaction
Woods-Saxon potential for Ta-181
Deformed nuclear potential
Coupled channel model
Coupled-channel approach

Write out single-proton wave function in terms of channels

\[ \Psi = \sum_{lm} \sum_{m_s} |l,m\rangle |s,m_s\rangle \frac{P_{lmm_s}(r)}{r} \]

Work with Schrodinger equation

\[ E\Psi = \hat{H}\Psi \]

split into the different channels

\[ E\langle s, m_s; lm |\Psi = \sum_{l,m} \sum_{m_s'} \langle s, m_s; lm | \hat{H} | s, m_s'; l', m' \rangle \langle s, m_s'; l' m' |\Psi \]
Coupled-channel equations

With no spin-orbit interaction can work with

\[
EP_{lm}(r) = \left[ -\frac{\hbar^2}{2M} \frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2Mr^2} + \langle l,m|V|l,m \rangle \right] P_{lm}(r)
\]

\[+ \sum_{l'm'} \langle l,m|V|l',m' \rangle P_{l'm'}(r) \]

We were able to get good results with this
Test for spherical problem

<table>
<thead>
<tr>
<th>index</th>
<th>$E_{Dudek}$ (MeV)</th>
<th>$E_{N,100}$ ($R_{max} = 18$)</th>
<th>$E_{N,100}$ ($R_{max} = 16$)</th>
<th>$E_{N,100}$ ($R_{max} = 14$)</th>
<th>$E_{N,100}$ ($R_{max} = 12$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1s</td>
<td>-33.4423</td>
<td>-33.441766</td>
<td>-33.441877</td>
<td>-33.441630</td>
<td>-33.442284</td>
</tr>
<tr>
<td>1g</td>
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<td>-12.115531</td>
<td>-12.114451</td>
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<td>3s</td>
<td>-6.4807</td>
<td>-6.554117</td>
<td>-6.536953</td>
<td>-6.521485</td>
<td>-6.506343</td>
</tr>
</tbody>
</table>

Table 1. Test of Dudek’s code against the new code in the case of a spherical potential with no spin-orbit interaction. $E_{Dudek}$ are results for the Dudek code; and $E_N$ are numbers we obtained with our code with no spin-orbit coupling, with 100 points and different values for $R_{max}$. 
Test for deformed problem

<table>
<thead>
<tr>
<th>index</th>
<th>$E_{Dudek}$ (MeV)</th>
<th>$E_{N,100}$ ($R_{max} = 18$)</th>
<th>$E_{N,100}$ ($R_{max} = 16$)</th>
<th>$E_{N,100}$ ($R_{max} = 14$)</th>
<th>$E_{N,100}$ ($R_{max} = 12$)</th>
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</thead>
<tbody>
<tr>
<td>$1s_{m=0}$</td>
<td>$-33.4405$</td>
<td>$-33.441232$</td>
<td>$-33.440791$</td>
<td>$-33.440187$</td>
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<td>$1g_{m=0}$</td>
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<tr>
<td>$1g_{m=1}$</td>
<td>$-12.5119$</td>
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<td>$-12.508072$</td>
<td>$-12.506065$</td>
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<tr>
<td>$2d_{m=0}$</td>
<td>$-8.5715$</td>
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<td>$-8.584514$</td>
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<td>$2d_{m=1}$</td>
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<td>$-8.172155$</td>
<td>$-8.164519$</td>
<td>$-8.157534$</td>
<td>$-8.150449$</td>
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</tbody>
</table>

Table 2. Comparison of orbital energies from the Dudek code compared with results from my code for $\beta_2 = 0.05$ with different numbers of radial points, and no spin-orbit interaction.
Table 5. Comparison of orbital energies from the Dudek code compared with results from my code for $\beta_2 = 0.50$ with 100 radial points, no spin-orbit interaction, and different numbers of angular momenta.
Spin-orbit interaction

Basic spin-orbit interaction

\[ \hat{V}_{so} = \frac{\lambda}{\hbar} \left( \frac{\hbar}{2Mc} \right)^2 \nabla U \cdot (\sigma \times \hat{p}) \]

Looks simple enough... But we need to calculate the interaction potentials for the coupled channel equations. So, we have to expand things out in an appropriate form:

\[ \begin{align*}
    &= -\frac{\lambda}{\hbar} \left( \frac{\hbar}{2Mc} \right)^2 \frac{1}{r} \frac{\partial U}{\partial r} \sigma \cdot \hat{L} \\
    &\quad + i\lambda \left( \frac{\hbar}{2Mc} \right)^2 \frac{1}{r} \frac{\partial U}{\partial \theta} \left[ \sigma_x \left( \sin \phi \frac{\partial}{\partial r} + \frac{\cos \phi}{r} \frac{\partial}{\partial \phi} \right) + \sigma_y \left( -\cos \phi \frac{\partial}{\partial r} + \frac{\sin \phi}{r} \frac{\partial}{\partial \phi} \right) + \sigma_z \frac{\cot \theta}{r} \frac{\partial}{\partial \phi} \right]
\end{align*} \]
Approximation

The full spin-orbit interaction is complicated. Since the deformation is not so great, why not work with the simpler part which will be dominant...

\[ V_{so} \rightarrow -\frac{\lambda}{\hbar} \left( \frac{\hbar}{2Mc} \right)^2 \frac{1}{r} \frac{\partial U}{\partial r} \sigma \cdot \hat{L} \]
Test for spherical problem

<table>
<thead>
<tr>
<th>index</th>
<th>$E_{Dudek}$ (MeV)</th>
<th>$E_{N,100}$ ($R_{max} = 18$)</th>
<th>$E_{N,100}$ ($R_{max} = 16$)</th>
<th>$E_{N,100}$ ($R_{max} = 14$)</th>
<th>$E_{N,100}$ ($R_{max} = 12$)</th>
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<tbody>
<tr>
<td>1s_{1/2}</td>
<td>-33.4423</td>
<td>-33.441766</td>
<td>-33.441877</td>
<td>-33.441630</td>
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<td>2s_{1/2}</td>
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<td>2d_{5/2}</td>
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<td>3s_{1/2}</td>
<td>-6.4807</td>
<td>-6.554117</td>
<td>-6.536953</td>
<td>-6.521485</td>
<td>-6.506343</td>
</tr>
</tbody>
</table>

Table 3. Test of the Dudek code against our codes for the spherical version of the problem; these are proton orbital energies focusing on the even states. $E_{Dudek}$ are results with the Dudek code; and for the $E_N$ numbers we used the new code including spin-orbit coupling.
Test for deformed problem

<table>
<thead>
<tr>
<th>index</th>
<th>$E_{Dudek}$ (MeV)</th>
<th>$E_{N,100}(l_{max} = 6)$ ($R_{max} = 14$)</th>
<th>$E_{N,100}(l_{max} = 8)$ ($R_{max} = 14$)</th>
<th>$E_{N,100}(l_{max} = 10)$ ($R_{max} = 14$)</th>
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<td>-33.3187</td>
<td>-33.324191</td>
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Table 6. Comparison of orbital energies from the Dudek code compared with results from my code for $\beta_2 = 0.50$ with 100 radial points, including incomplete spin-orbit interaction, and different numbers of angular momenta.
Thinking

• So, the new code is running

• Gives good answers for spherical problem, with and without spin-orbit interaction

• Gives good answers for deformed problem without spin-orbit interaction

• For deformed problem with spin-orbit interaction we use an incomplete spin-orbit interaction

• Code runs 3x faster, gives answers with minor errors

• Acceptable for what we want to do with it
Ta-181 states
Energy levels from exp’t

<table>
<thead>
<tr>
<th>energy (keV)</th>
<th>J^\pi</th>
<th>[Nn_\Lambda]</th>
<th>orbital</th>
<th>rotational state</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>7/2^+</td>
<td>[404]</td>
<td>1g_{7/2}</td>
<td>[404] J=7/2</td>
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<tr>
<td>136.262</td>
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<td></td>
<td>[404] J=9/2</td>
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<tr>
<td>158.554</td>
<td>11/2^-</td>
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<td>[514] J=11/2</td>
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<td>[404] J=11/2</td>
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<tr>
<td>337.54</td>
<td>13/2^-</td>
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<td></td>
<td>[514] J=31/2</td>
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<tr>
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<td>[402]</td>
<td>2d_{5/2}</td>
<td>[402] J=5/2</td>
</tr>
<tr>
<td>495.184</td>
<td>13/2^+</td>
<td></td>
<td></td>
<td>[404] J=13/2</td>
</tr>
<tr>
<td>542.51</td>
<td>15/2^-</td>
<td></td>
<td></td>
<td>[514] J=15/2</td>
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<tr>
<td>590.06</td>
<td>7/2^+</td>
<td></td>
<td></td>
<td>[402] J=7/2</td>
</tr>
<tr>
<td>615.19</td>
<td>1/2^+</td>
<td>[411]</td>
<td>3s_{1/2}</td>
<td>[411] J=1/2</td>
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<tr>
<td>716.659</td>
<td>15/2^+</td>
<td></td>
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<td>[404] J=15/2</td>
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<tr>
<td>727.31</td>
<td>9/2^+</td>
<td></td>
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<td>[402] J=9/2</td>
</tr>
<tr>
<td>772.97</td>
<td>17/2^-</td>
<td></td>
<td></td>
<td>[514] J=15/2</td>
</tr>
</tbody>
</table>

Table 9. Low-lying energy levels for $^{181}$Ta.
Thinking

• Lots of low-lying states
• Want to understand them
• Some intrinsic states (no rotation)
• Some states which are rotated versions of intrinsic states
Energy levels from exp’t

<table>
<thead>
<tr>
<th>energy (keV)</th>
<th>J$^\pi$</th>
<th>[Nn_L]</th>
<th>orbital</th>
<th>rotational state</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>7/2$^+$</td>
<td>[404]</td>
<td>1g$7/2$</td>
<td>[404] J=7/2</td>
</tr>
<tr>
<td>136.262</td>
<td>9/2$^+$</td>
<td></td>
<td></td>
<td>[404] J=9/2</td>
</tr>
<tr>
<td>158.554</td>
<td>11/2$^-$</td>
<td></td>
<td></td>
<td>[514] J=11/2</td>
</tr>
<tr>
<td>301.662</td>
<td>11/2$^+$</td>
<td></td>
<td></td>
<td>[404] J=11/2</td>
</tr>
<tr>
<td>337.54</td>
<td>13/2$^-$</td>
<td></td>
<td></td>
<td>[514] J=31/2</td>
</tr>
<tr>
<td>482.168</td>
<td>5/2$^+$</td>
<td>[402]</td>
<td>2d$5/2$</td>
<td>[402] J=5/2</td>
</tr>
<tr>
<td>495.184</td>
<td>13/2$^+$</td>
<td></td>
<td></td>
<td>[404] J=13/2</td>
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<td>542.51</td>
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<td>772.97</td>
<td>17/2$^-$</td>
<td></td>
<td></td>
<td>[514] J=15/2</td>
</tr>
</tbody>
</table>

Table 9. Low-lying energy levels for $^{181}$Ta.
Energy levels due to rotation

\[ T_R = \frac{\hbar^2}{I} \left[ J (J+1) - J_{\text{min}} (J_{\text{min}} + 1) \right] \]

Rotational levels in Ta-181 associated with the 7/2+ ground state
Energy levels due to rotation

\[ T_R = \frac{\hbar^2}{I} \left[ J (J + 1) - J_{\text{min}} (J_{\text{min}} + 1) \right] \]

Rotational levels in Ta-181 associated with the 9/2- first excited state
Energy levels due to rotation

\[ T_R = \frac{\hbar^2}{I} \left[ J (J+1) - J_{\text{min}} (J_{\text{min}} + 1) \right] \]

Rotational levels in Ta-181 associated with the [402] excited state
It works!

• Can understand low-lying levels of Ta-181

• See 4 intrinsic states, which correspond to single proton states in a deformed potential

• See lots of rotational states that can be identified as rotating versions of intrinsic states

• Transition we are interested in is between two different single proton intrinsic states
Deformation parameters

• Would like to run the codes to see if we can match the relative state energies
• This has been done before in the literature, so estimates for the parameters are known
• Start with quadrupole deformation
Working on $\beta_2$

Figure 4. Proton orbital energies as a function of $\beta_2$ with $\beta_4 = 0$, for $^{181}$Ta, using Dudek’s universal model potential parameters.
No joy...

• We are getting the ground state 7/2+ state to be close to the 9/2- state
• But energy splitting is one the order of 1 MeV using deformation parameter similar to what is in the literature
• Probably need deformation at next order to do better...
Working on $\beta_2$ with $\beta_4 = -0.038$
Seems to work

• Now we included $\beta_4 = -0.038$ to model a little bit of octupole deformation

• Now we get a crossing of the $7/2^+$ and $9/2^-$ states at a reasonable value of $\beta_2$

• This looks good

• Wonder whether it is consistent with the observed electric quadrupole moment
Electric quadrupole moment

• For Ta-181 there are a number of measurements for the electric quadrupole moment

• Probably the most accurate ones are from measurements of the spectrum of muonic Ta

• From these measurements a value of 7.37 eb has been deduced

• We can check using

\[ Q_0 = \frac{3}{\sqrt{5\pi}} eZ R^2 \beta_2 \left( 1 + \pi^2 \left( \frac{a}{R} \right)^2 + \frac{2}{7} \sqrt{\frac{5}{\pi}} \beta_2 \right) \]
Working on $\beta_2$

Figure 1. Quadrupole moment as a function of $\beta_2$. 
Thinking about comparison

• Based on the experimental observation of 7.37 eb, we would expect $\beta_2 = 2.47$

• Optimization based on the Dudek code including quadrupole and octupole terms gives a $7/2^+$ and $9/2^-$ crossing for $\beta_2 = 2.5$

• The model is consistent

• OK, so this was well known as one of the successes of the Bohr model for deformed nuclei...
Phonon-nuclear interaction matrix element
Boosted spin-orbit interaction

• OK, so let’s consider the boosted spin-orbit interaction, start with the simplest possible argument

• Unboosted spin-orbit interaction is

\[ V_{so} = \frac{\lambda}{\hbar} \left( \frac{\hbar}{2Mc} \right)^2 \nabla U \cdot (\sigma \times \hat{p}) \]

• A boost is implemented using

\[ \hat{p} \rightarrow \hat{p} + \frac{\hat{p}}{N} \]

• This leads to

\[ \Delta V_{so} = \frac{\lambda}{\hbar} \left( \frac{\hbar}{2Mc} \right)^2 \nabla U \cdot \left( \sigma \times \frac{\hat{p}}{N} \right) \]
Relativistic phonon-nuclear interaction

- We would like to compare this with results from the Foldy-Wouthuysen transformation appropriate for a nonrelativistic model

\[ \Delta \hat{V} = -\frac{1}{8Mmc^2} \sum_l \sum_{j<k} \left[ \sigma_l \cdot \hat{P}, \left[ \sigma_l \cdot \hat{\pi}_l, \hat{V}_{jk} \right] \right] - \frac{1}{8Mmc^2} \sum_l \sum_{j<k} \left[ \sigma_l \cdot \hat{\pi}_l, \left[ \sigma_l \cdot \hat{P}, \hat{V}_{jk} \right] \right] \]

- Evaluating the commutators leads to

\[ \Delta \hat{V} \rightarrow i \frac{1}{4Mmc^2} \left[ \sigma_k \times (\hat{\pi}_k V_{jk}) \right] \cdot \hat{P} \]

- This is similar to the boosted version in the previous slide

\[ -i\lambda \frac{1}{4Mmc^2} \sigma \cdot [(\hat{\pi}U) \times \hat{P}] \]
Thinking about the result

• There are lots of issues to consider...

• One is that the FW-transformation is giving a result that is similar in form to the boosted spin-orbit interaction

• Strictly speaking, this result is much smaller than the boosted spin-orbit interaction since it is actually a spin-orbit term rather than a boost of the spin-orbit interaction

• To do it right we would want to go back to the relativistic interaction, and carry out a F-W transformation

• However, for now we are happy since what we are trying to model is a boost of the spin-orbit interaction
Calculating the proton orbitals

• There are some technical issues about the details of the model; however, in the end the results are reasonable

<table>
<table>
<thead>
<tr>
<th>index</th>
<th>$E_{Dudek}$ (MeV)</th>
<th>$E_{N=100 \ l_{max}=10}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>7/2+ (1)</td>
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<td>-13.455392</td>
</tr>
<tr>
<td>7/2+ (2)</td>
<td>-6.3483</td>
<td>-6.289249</td>
</tr>
<tr>
<td>7/2+ (3)</td>
<td>-1.9020</td>
<td>-2.067574</td>
</tr>
<tr>
<td>9/2− (1)</td>
<td>-6.3458</td>
<td>-6.425660</td>
</tr>
<tr>
<td>9/2− (2)</td>
<td>2.9235</td>
<td>2.941132</td>
</tr>
</tbody>
</table>
</table>

Table 10. Orbital energies from the Dudek code compared with results from my code for a deformed version of the problem ($\beta_2 = 0.25$ and $\beta_4 = -0.038$) with a the old spin-orbit potential increased in magnitude to match the universal value.
Magnitude of the matrix element

• The phonon-nuclear coupling matrix element can be written as

\[ \Delta V_{so} = \mathbf{a} \cdot \mathbf{c\hat{P}} \]

• with

\[ \mathbf{a} = -\lambda \frac{\hbar}{4Mmc^3} \mathbf{\sigma} \times (\nabla U) \]

• For this model we estimate

\[ |\mathbf{a}| = 1.29 \times 10^{-6} \]

• This estimate is within the range (but on the low side) of what was expected
Homonuclear diatomic Ta$_2$
To small to see splitting in Ta$_2$

Second-order interaction in Ta$_2$:

$$\hat{U}_{12} = -\frac{Mc^2(\hbar \omega_0)^2}{2(\Delta E)^2} \frac{(a_1 \cdot R_{21})(a_2 \cdot R_{21})}{|R_{21}|^2}$$

Plug in numbers:

$$\frac{Mc^2(\hbar \omega_0)^2}{2(\Delta E)^2}|a|^2 = 6 \times 10^{-12} \text{ eV}$$

Conclude coupling is too small to see in a Mossbauer experiment
Radiative decay
Radiative decay rate

• We can calculate the radiative decay rate for the transition as a test of the nuclear model

• We get

\[
\gamma = \frac{4}{3} \frac{e^2}{4\pi \varepsilon_0} \frac{\omega^3}{\hbar^3} \left| \left\langle \frac{9^-}{2} \right| r \left| \frac{7^+}{2} \right\rangle \right|^2 = 3.89 \times 10^8 \text{ sec}^{-1}
\]

• Reasonably consistent with the Weisskopf estimate

\[
\gamma_W = 10^{14} A^{2/3} E^3 = 7.76 \times 10^8 \text{ sec}^{-1}
\]

• Not close to the experimental value

\[
\gamma_{\text{expt}} = 2.4 \times 10^3 \text{ sec}^{-1}
\]
Large discrepancy

• Our simple model gives a fast decay rate of $3.89 \times 10^8$, while experiment is probably below $2 \times 10^3$

• The ratio of theory to experiment is about $2 \times 10^5$

• This indicates a serious problem

• Note that this is not the only transition where there is a disagreement

• Instructive to look at other transitions
Figure 3. Half-life as a function of the transition energy for odd $A$ nuclei with an even number of neutrons; observed results (red circles); Weisskopf estimate (black circles); scaled estimate assuming $(\Delta E)^5$ scaling (blue line).
Thinking

• All E1 transitions at low energy are much slower than the Weisskopf estimate
• This was noted by Bethe in his 1937 review article
• Bethe noted that not dipolar response is expected for a system composed of particles with identical mass and charge, and that the strong force makes nuclei act this way
• Same problem for M1 and E2 transitions between intrinsic states
• For rotational transitions get fast E2 transition rates that agree with conventional decay rate calculation
Nilsson and coworkers

• In the development of the Bohr and Nilsson deformed nuclear models, an effort was made to resolve this problem
• Low-energy E1 transitions were analyzed within the Nilsson scheme
• Pairing corrections were included
• It was claimed possible to get systematic agreement between theory and experiment for many low-energy E1 radiative decay rates
• We were motivated in our calculations by these papers, hoping that we too could get good agreement
How does it work?

• The early papers started from a direct calculation of the radiative decay rate based on the deformed potential model.

• A very small radiative decay rate (still much faster than experiment) was initially calculated from the deformed models.

• Now, we are using a more sophisticated version of the same model, and we do not see this effect.

• Conclude that reduction in radiative decay rate computed in the 1950s and early 1960s was due to a destructive interference effect.

• In our version of the model the optimum solution is away from where the destructive interference occurs.
Interference effect

\[ |\langle f | r | i \rangle|^2 \]
• We are using models from mid-1980s which do better for connecting with energy levels

• Much work on these models by nuclear theory groups active in 1970s through 1990s

• Can see interference effect which would reduce the radiative decay rate

• But interference effect is in a different region of parameter space than optimum for energy levels

• Nilsson’s explanation is not robust

• We conclude that systematic difference is not due to interference effect
Pairing

• In the 1950s BCS theory emerged to account for superconductivity
• Similar model adopted to describe nuclear energy levels
• Get large amount of configuration interaction
• Pairing model allows one to include some of the configuration interaction in a simple way
• Estimates for pairing correction for radiative decay for Ta-181 transition near 25x reduction in rate
• No modern estimates available
• Pairing cannot account for 5 orders of magnitude
Thinking about a lattice $R \mid ST$ model
Screening

• It would be simplest if screening by the core nucleons could explain the discrepancy

• However, Nilsson model, Hartree-Fock models, and Thomas-Fermi models all predict negligible screening by the core

• If restoring force were Coulombic, then could account for screening

• But if there is a strong force contribution then there is essentially no screening
Quantum gas vs liquid/solid

• No core screening expected at low order in a quantum gas model (Nilsson, Hartree-Fock, Thomas-Fermi...)

• Few (or no) relevant models studied based on quantum liquid or solid formulation

• Could imagine a new formulation where basic liquid or solid structure is determined by the strong force...

• ...and where charge mobility is developed through isospin exchange

• We are beginning to look at such a model

• Crystal lattice model is simplest example
Crystal model from Cook (1987)
R|ST model

Start with

$$\Psi = \psi(\{r\})\Phi(\{\sigma\}, \{\tau\})$$

Then separate according to

$$\lambda_R\psi(\{r\}) = \langle \Phi(\{\sigma\}, \{\tau\})|\hat{H}|\Phi(\{\sigma\}, \{\tau\})\rangle\psi(\{r\})$$

$$\lambda_{ST}\Phi(\{\sigma\}, \{\tau\}) = \langle \psi(\{r\})|\hat{H}|\psi(\{r\})\rangle\Phi(\{\sigma\}, \{\tau\})$$

And make use of a lattice (or liquid) model in space for $\psi(\{r\})$
Make use of R(ST) approach

• Three degrees of freedom in a nuclear model: space, spin and isospin

• Thinking of an approximation which models space through an approximately fixed lattice model

• ...and spin and isospin as dynamical variables

• Simple formulation

• Rigorous derivation possible
Progress so far

- A version of the model has been constructed for the case of a (simple) Hamada-Johnston nuclear potential model
- Can already see features of the model
- Strong force relevant for lattice structure, shape of nucleus
- Spin and isospin exchange within the lattice
- Means that charge is mobile even if the nucleons are approximated fixed in lattice sites
- Clear that derivation of modified Born and Nilsson type of models follow from this approach
Coherent contribution for central potential

\[
\langle \Psi \mid \sum_{\gamma < \delta} (\tau_\gamma \cdot \tau_\delta)(\sigma_\gamma \cdot \sigma_\delta)y_C(r_{\gamma\delta}) \mid \Psi \rangle \rightarrow \\
\frac{1}{2} \sum_{\alpha} \sum_{\beta} c^*(\alpha)c(\beta) \left\langle \left[ \frac{1}{2} \sigma_+ (\alpha)\sigma_- (\beta) + \frac{1 + \sigma_z (\alpha) + \sigma_z (\beta)}{2} \right] \left[ \frac{1 + \tau_z (\alpha) - \tau_z (\beta)}{2} + \tau^- (\alpha)\tau^+ (\beta) \right] y_C(r_{\alpha\beta}) \right\rangle \\
-\frac{1}{2} \sum_{\alpha} \sum_{\beta} c^*(\alpha)d(\beta) \left\langle \left[ \frac{1 + \sigma_z (\alpha) - \sigma_z (\beta)}{2} \right] \left[ \frac{1 + \tau_z (\alpha) - \tau_z (\beta)}{2} + \tau^- (\alpha)\tau^+ (\beta) \right] y_C(r_{\alpha\beta}) \right\rangle \\
-\frac{1}{2} \sum_{\alpha} \sum_{\beta} d^*(\alpha)c(\beta) \left\langle \left[ \frac{1 - \sigma_z (\alpha) + \sigma_z (\beta)}{2} \right] \left[ \frac{1 + \tau_z (\alpha) - \tau_z (\beta)}{2} + \tau^- (\alpha)\tau^+ (\beta) \right] y_C(r_{\alpha\beta}) \right\rangle \\
+\frac{1}{2} \sum_{\alpha} \sum_{\beta} d^*(\alpha)d(\beta) \left\langle \left[ \frac{1}{2} \sigma_- (\alpha)\sigma_+ (\beta) + \frac{1 + \sigma_z (\alpha) + \sigma_z (\beta)}{2} \right] \left[ \frac{1 + \tau_z (\alpha) - \tau_z (\beta)}{2} + \tau^- (\alpha)\tau^+ (\beta) \right] y_C(r_{\alpha\beta}) \right\rangle \\
(96)
\]
Screening and other issues

• This kind of model will show strong screening of electric fields

• Would be consistent with observed hindrance of E1 transitions (no other model is consistent)

• Also leads to larger effective masses for neutrons and protons

• Possible that this approach might give better agreement for intrinsic energy level predictions

• Could be used for electron and charged particle collisions, fusion and fission calculations
Conclusions
Conclusions I

• In our approach, phonon-nuclear interaction provides foundation for understanding CMNS

• In past few years have developed an understanding of how the coupling works

• This calculation is our first for a transition in a heavy nucleus

• Possible now to extend to other transitions

• Ta-181 has lowest energy E1 transition from ground state

• Now have estimate for strength of $a.cP$ interaction

• Within range of what was expected
Conclusions II

• But uncertainties remain, since same model is not accurate for radiative decay
• If discrepancy for radiative decay due to screening, then could develop new model that screens...
  • ...and use it to revisit the phonon-nuclear matrix element
• Still interested in connecting unambiguously with experiment!