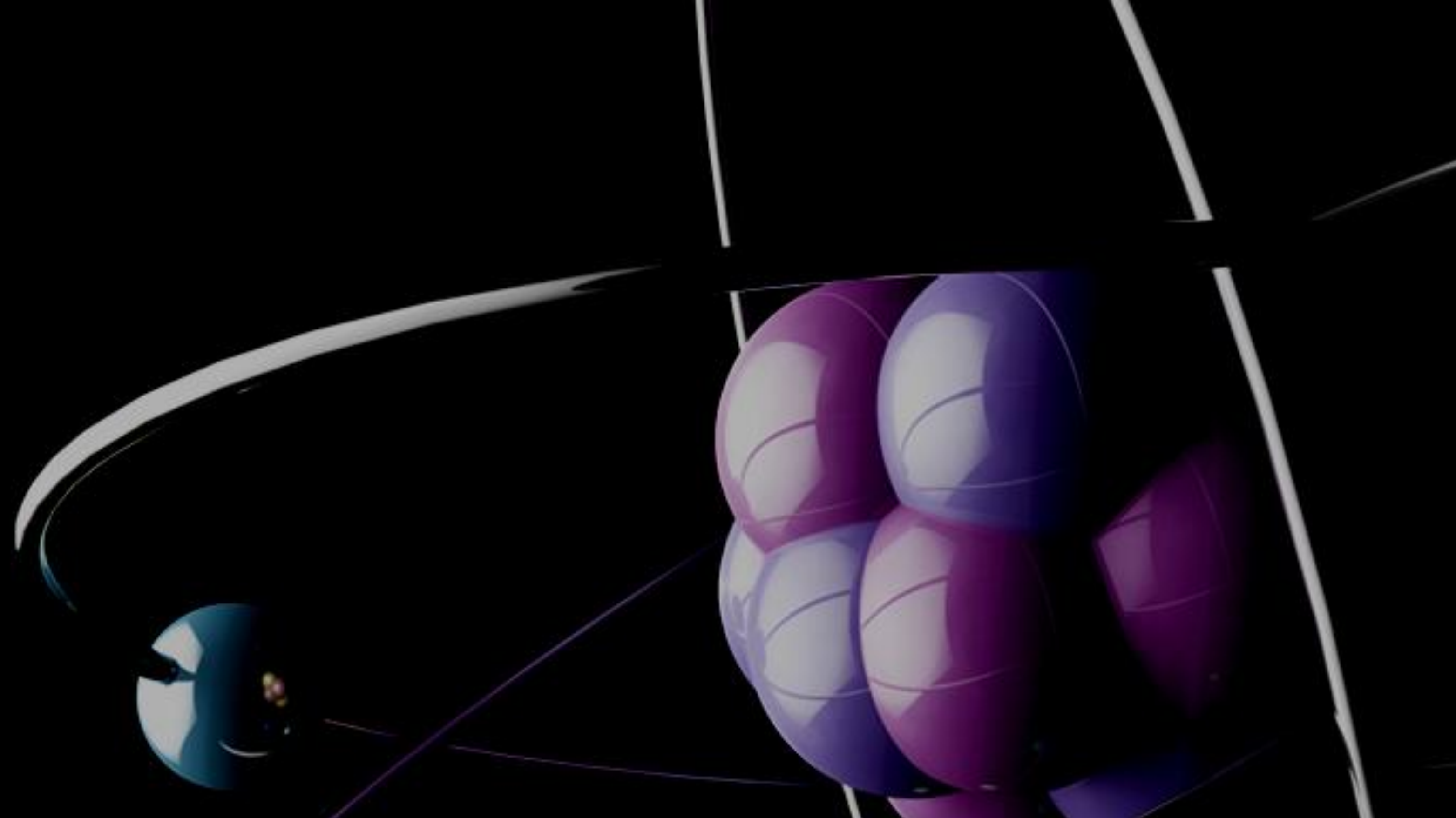


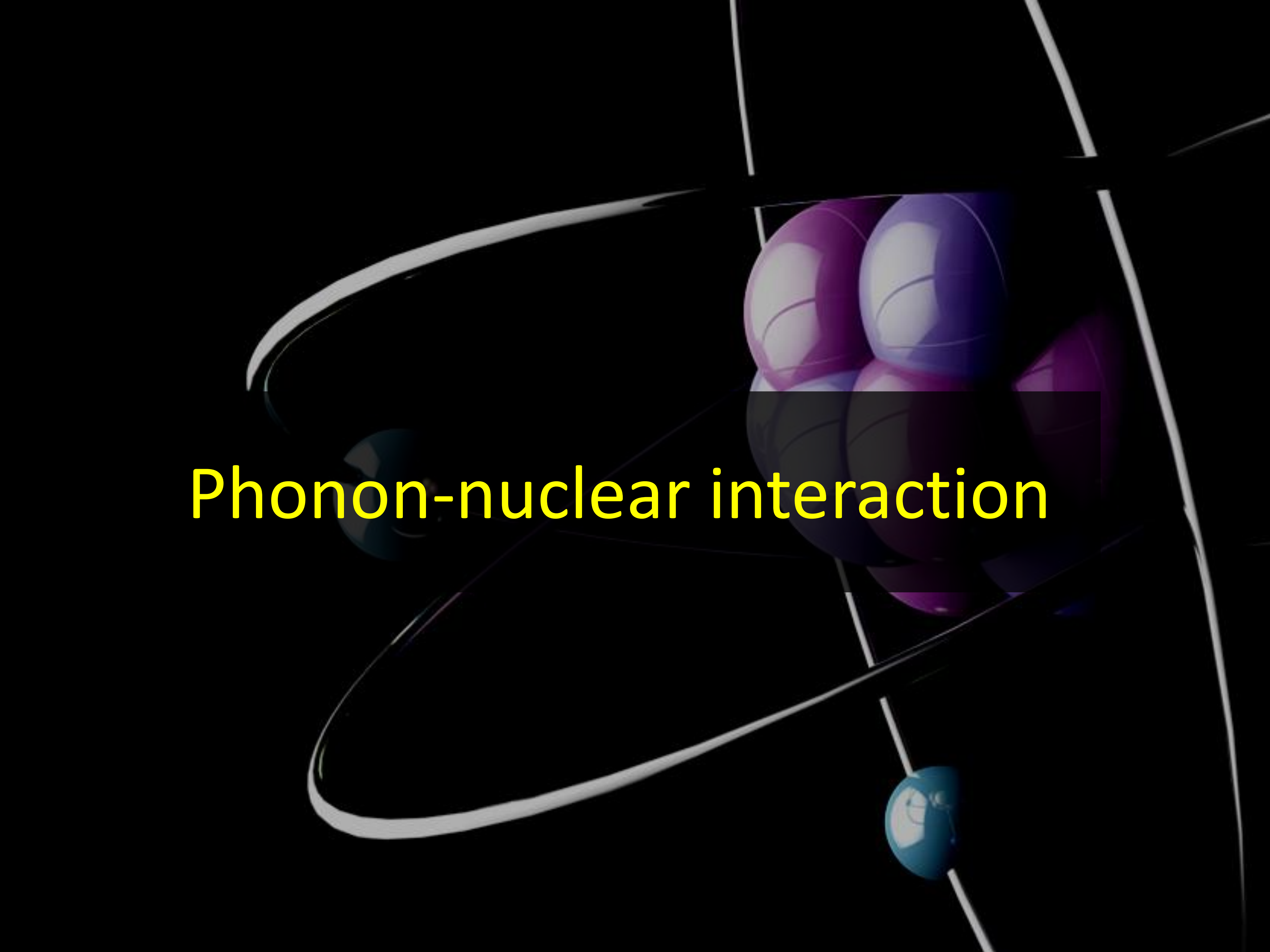
Calculation of the phonon-nuclear coupling matrix element for Ta-181

Peter L Hagelstein
Massachusetts Institute of Technology

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



$$\hat{H} = \sum_j \boldsymbol{\alpha}_j \cdot c\left[\mathbf{p}_j - q_j \mathbf{A}\left(\mathbf{r}_j\right)\right] + \sum_j \beta_j mc^2 + \sum_{j<k} \hat{V}_{jk}\left(\mathbf{r}_k - \mathbf{r}_j\right) + \sum_j q_j \Phi\left(\mathbf{r}_j\right)$$

Partial Foldy-Wouthuysen transformation

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

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

$$\hat{S} = -i\frac{1}{2Mc}\sum_j \beta_j \boldsymbol{\alpha}_j \cdot \left[\hat{\mathbf{P}}_j - Q\mathbf{A}\left(\mathbf{R}\right)\right]$$

nucleus as a particle

$$\hat{H}' = \boxed{\frac{\left|\hat{\mathbf{P}} - Q\mathbf{A}\right|^2}{2M} \frac{1}{N} \sum_j \beta_j + Q\Phi - \frac{\hbar Q}{2M} \frac{1}{N} \sum_j \beta_j \hat{\boldsymbol{\Sigma}}_j \cdot \mathbf{B} - \frac{\hbar^2 Q}{8M^2c^2} \nabla \cdot \mathbf{E} + \frac{\hbar Q}{8M^2c^2} \sum_j \hat{\boldsymbol{\Sigma}}_j \cdot \left[\left(\hat{\mathbf{P}} - Q\mathbf{A}\right) \times \mathbf{E} - \mathbf{E} \times \left(\hat{\mathbf{P}} - Q\mathbf{A}\right) \right]}$$

internal nuclear structure

$$\boxed{+ \sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \hat{V}_{jk}}$$

$$+ \sum_j \left[q_j \Phi\left(\mathbf{R} + \boldsymbol{\xi}_j\right) - \frac{Q}{N} \Phi\left(\mathbf{R}\right) \right] - \sum_j \boldsymbol{\alpha}_j \cdot c \left[q_j \mathbf{A}\left(\mathbf{R} + \boldsymbol{\xi}_j\right) - \frac{Q}{N} \mathbf{A}\left(\mathbf{R}\right) \right]$$

$$+ \sum_j \beta_j \frac{\left(\hat{\mathbf{P}} - Q\mathbf{A}\right) \cdot \hat{\boldsymbol{\pi}}_j}{M} + \frac{1}{2Mc} \sum_{j<k} \left[\left(\beta_j \boldsymbol{\alpha}_j + \beta_k \boldsymbol{\alpha}_k\right) \cdot \left(\hat{\mathbf{P}} - Q\mathbf{A}\right), \hat{V}_{jk} \right]$$

$$+ \cdots$$

kinetic energy of the nucleus

internal nuclear structure

phonon-nuclear coupling

$$\hat{H}' = \boxed{\frac{|\hat{\mathbf{P}}|^2}{2M}} + \boxed{\sum_j \beta_j mc^2 + \sum_j \boldsymbol{\alpha}_j \cdot c\hat{\boldsymbol{\pi}}_j + \sum_{j<k} \hat{V}_{jk}} + \mathbf{a} \cdot c\hat{\mathbf{P}} + \cdots$$

where

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

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

$$\begin{aligned}\hat{H} \; &= \; \beta_1 mc^2 + \boldsymbol{\alpha}_1 \cdot c\hat{\boldsymbol{\pi}}_1 + \beta_2 mc^2 + \boldsymbol{\alpha}_2 \cdot c\hat{\boldsymbol{\pi}}_2 \\ &\quad + \frac{q_1 q_2}{4\pi\varepsilon_0}\left\{\frac{1}{r_{12}} - \frac{1}{2}\left[\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{r_{12}} + \frac{\left(\boldsymbol{\alpha}_1 \cdot c\mathbf{r}_{12}\right)\left(\boldsymbol{\alpha}_2 \cdot c\mathbf{r}_{12}\right)}{r_{12}^3}\right]\right\}\end{aligned}$$

Coulomb and Breit interaction, boosted frame

$$\boldsymbol{\alpha} \;\to\; \frac{\mathbf{v}}{c} \qquad\qquad \text{in rest frame}$$

$$\boldsymbol{\alpha} \;\to\; \frac{\mathbf{v}}{c} + \frac{\mathbf{P}}{Mc} \qquad \text{in moving frame}$$

$$\hat{H} \;\to\; \beta_1 mc^2 + \boldsymbol{\alpha}_1 \cdot c\hat{\boldsymbol{\pi}}_1 + \beta_2 mc^2 + \boldsymbol{\alpha}_2 \cdot c\hat{\boldsymbol{\pi}}_2$$

$$+\frac{q_1 q_2}{4\pi\varepsilon_0}\left\{\frac{1}{r_{12}} - \frac{1}{2}\left[\frac{\left(\boldsymbol{\alpha}_1 + \frac{\hat{\mathbf{P}}}{Mc}\right)\cdot\left(\boldsymbol{\alpha}_2 + \frac{\hat{\mathbf{P}}}{Mc}\right)}{r_{12}} + \frac{\left(\left(\boldsymbol{\alpha}_1 + \frac{\hat{\mathbf{P}}}{Mc}\right)\cdot c\mathbf{r}_{12}\right)\left(\left(\boldsymbol{\alpha}_2 + \frac{\hat{\mathbf{P}}}{Mc}\right)\cdot c\mathbf{r}_{12}\right)}{r_{12}^3}\right]\right\}$$

Keep lowest order terms…

$$
\begin{aligned}
\hat{H} \;\rightarrow\;& \beta_1 mc^2 + \boldsymbol{\alpha}_1 \cdot c\hat{\boldsymbol{\pi}}_1 + \beta_2 mc^2 + \boldsymbol{\alpha}_2 \cdot c\hat{\boldsymbol{\pi}}_2 \\
&+ \frac{q_1 q_2}{4\pi\varepsilon_0} \left\{ \frac{1}{r_{12}} - \frac{1}{2}\left[\frac{\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2}{r_{12}} + \frac{\left(\boldsymbol{\alpha}_1 \cdot c\mathbf{r}_{12}\right)\left(\boldsymbol{\alpha}_2 \cdot c\mathbf{r}_{12}\right)}{r_{12}^3} \right] \right\} \\
&- \frac{1}{2Mc}\frac{q_1 q_2}{4\pi\varepsilon_0} \left[\frac{\hat{\mathbf{P}} \cdot \boldsymbol{\alpha}_1}{r_{12}} + \frac{\hat{\mathbf{P}} \cdot \boldsymbol{\alpha}_2}{r_{12}} + \frac{\left(\hat{\mathbf{P}} \cdot c\mathbf{r}_{12}\right)\left(\boldsymbol{\alpha}_2 \cdot c\mathbf{r}_{12}\right)}{r_{12}^3} + \frac{\left(\boldsymbol{\alpha}_1 \cdot c\mathbf{r}_{12}\right)\left(\hat{\mathbf{P}} \cdot c\mathbf{r}_{12}\right)}{r_{12}^3} \right]
\end{aligned}
$$

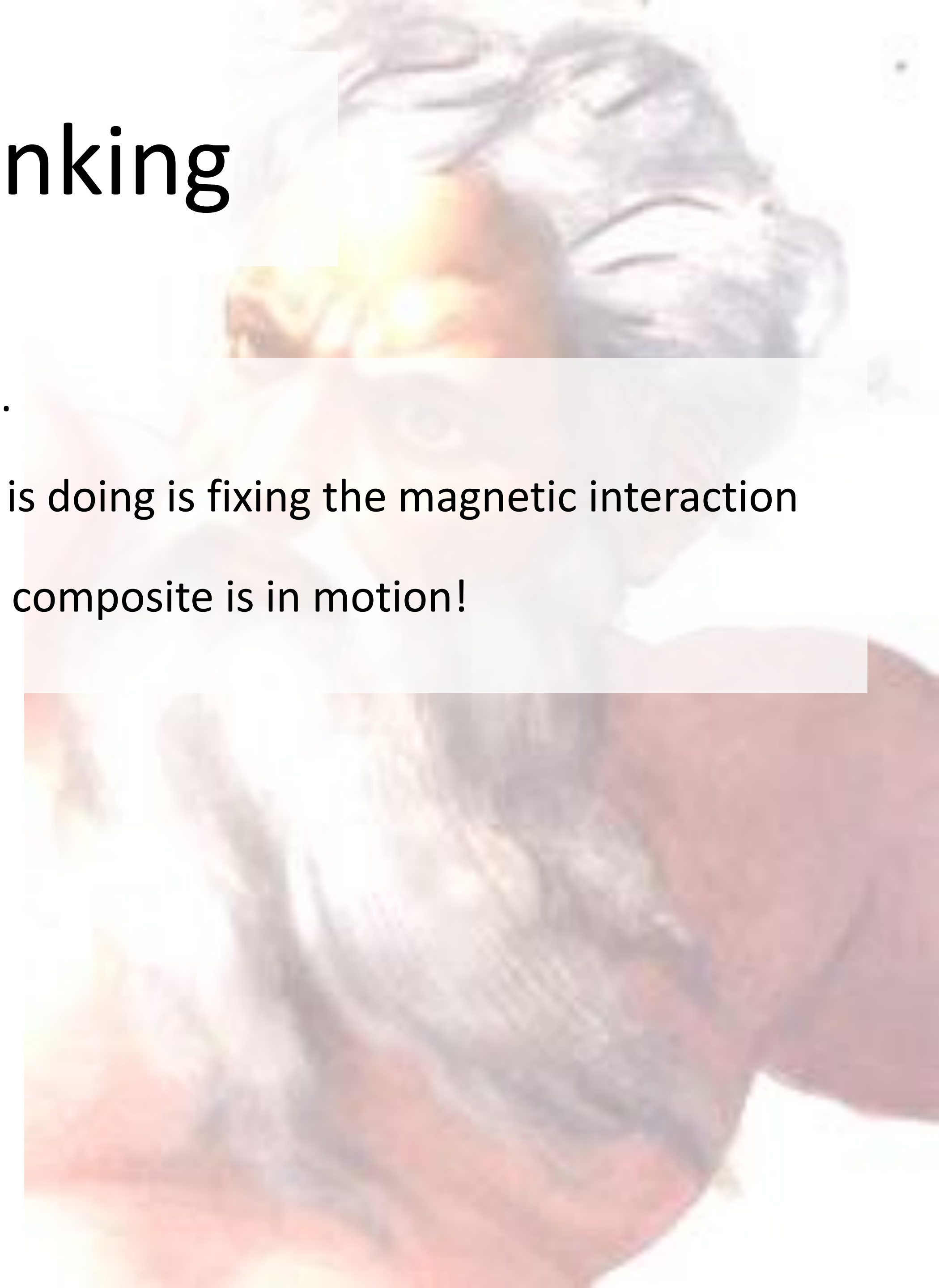
Now evaluate the coupling term

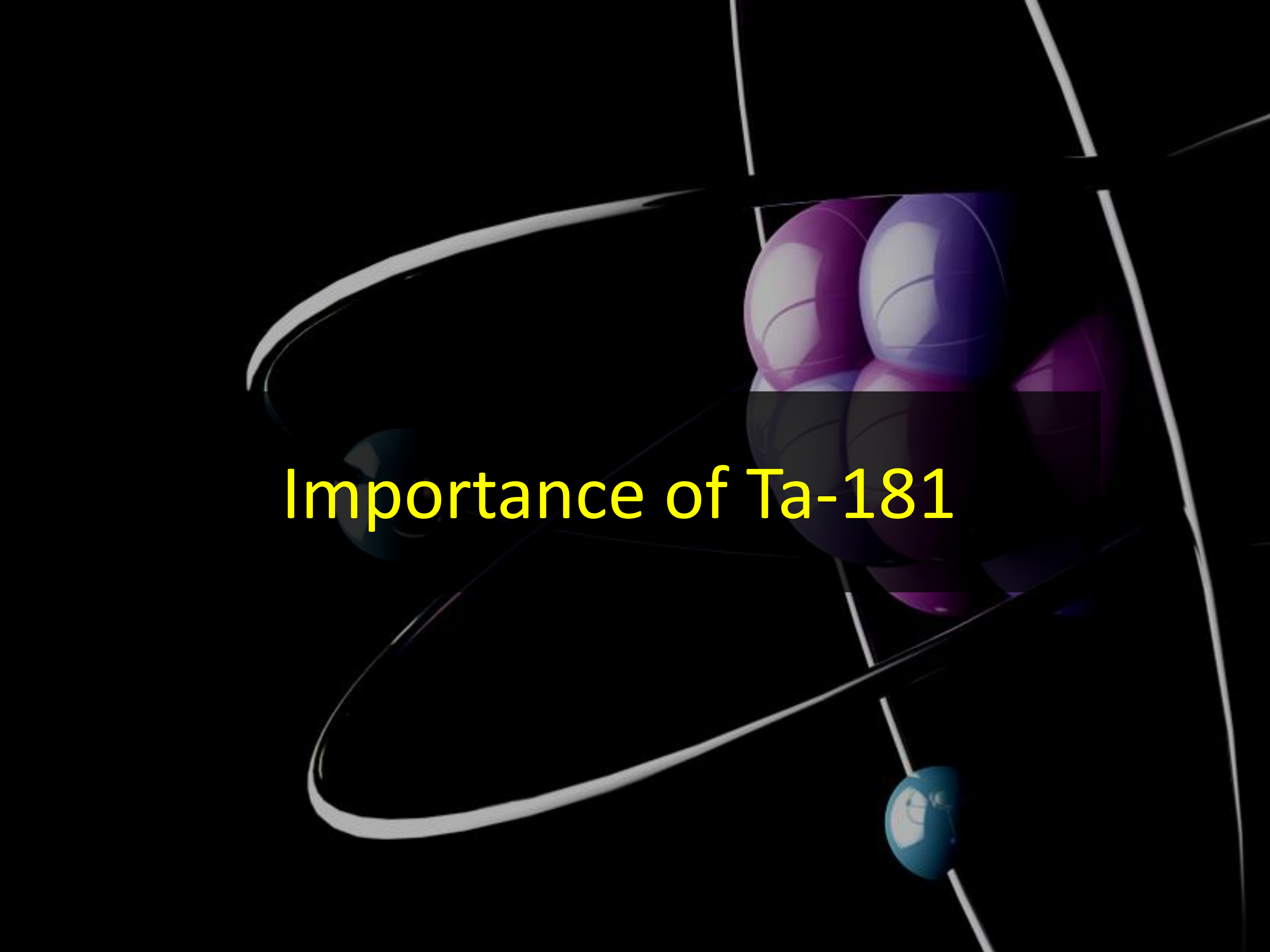
$$\frac{1}{2Mc}\sum_{j<k}\left[\left(\beta_j\boldsymbol{\alpha}_j+\beta_k\boldsymbol{\alpha}_k\right)\cdot\hat{\mathbf{P}},\hat{V}_{jk}\right] =$$

$$-\frac{1}{2Mc}\frac{q_1q_2}{4\pi\varepsilon_0}\left[\frac{\hat{\mathbf{P}}\cdot\boldsymbol{\alpha}_1}{r_{12}}\beta_2+\frac{\hat{\mathbf{P}}\cdot\boldsymbol{\alpha}_2}{r_{12}}\beta_1+\frac{\left(\hat{\mathbf{P}}\cdot c\mathbf{r}_{12}\right)\left(\boldsymbol{\alpha}_2\cdot c\mathbf{r}_{12}\right)}{r_{12}^3}\beta_1+\frac{\left(\boldsymbol{\alpha}_1\cdot c\mathbf{r}_{12}\right)\left(\hat{\mathbf{P}}\cdot c\mathbf{r}_{12}\right)}{r_{12}^3}\beta_2\right]$$

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

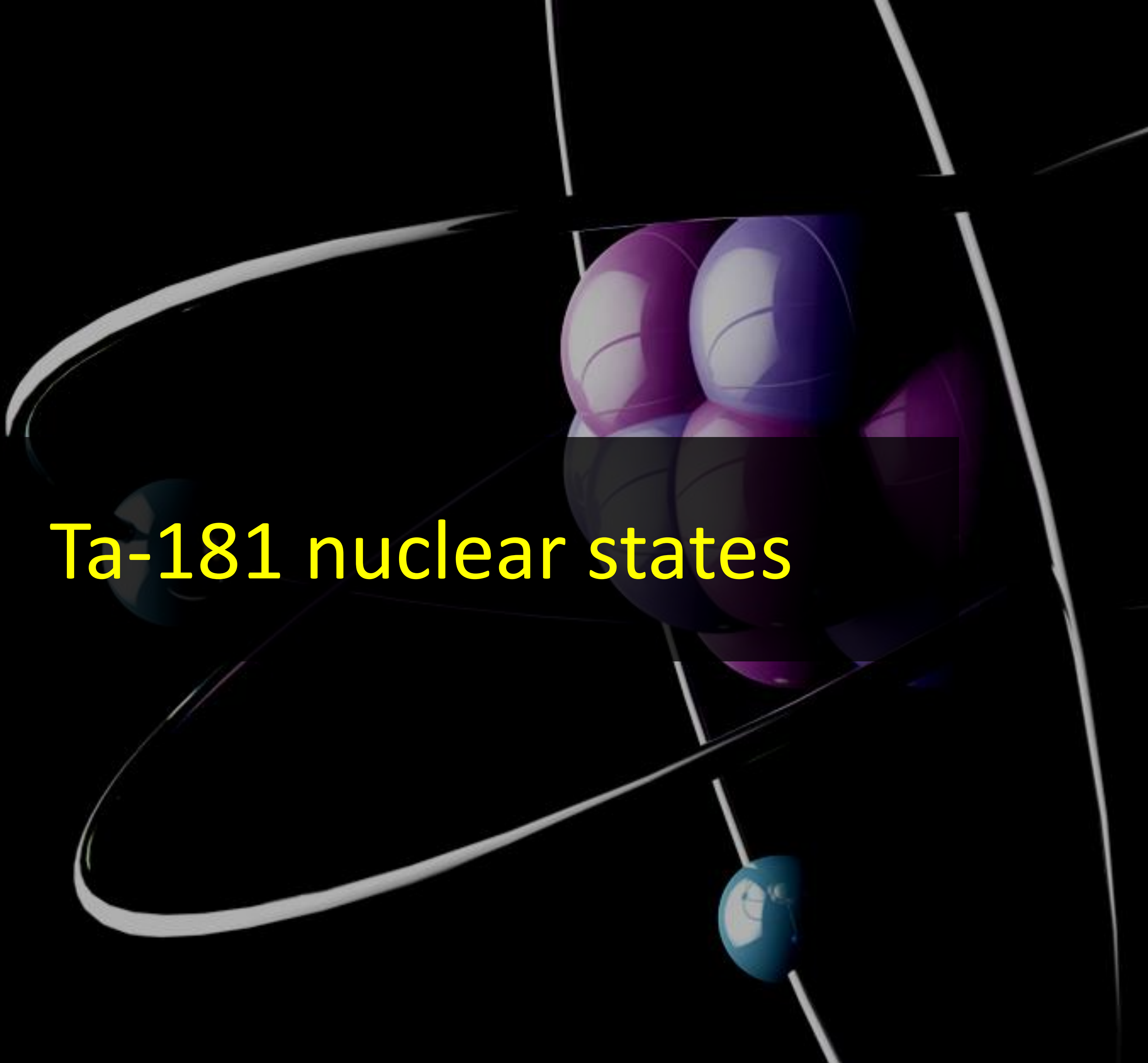
Nucleus	Excited state energy (keV)	half-life	multipolarity
^{201}Hg	1.5648	81 ns	M1+E2
^{181}Ta	6.240	6.05 μs	E1
^{169}Tm	8.41017	4.09 ns	M1+E2
^{83}Kr	9.4051	154.4 ns	M1+E2
^{187}Os	9.75	2.38 ns	M1(+E2)
^{73}Ge	13.2845	2.92 μs	E2
^{57}Fe	14.4129	98.3 ns	M1+E2

Lowest energy E1 transitions

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

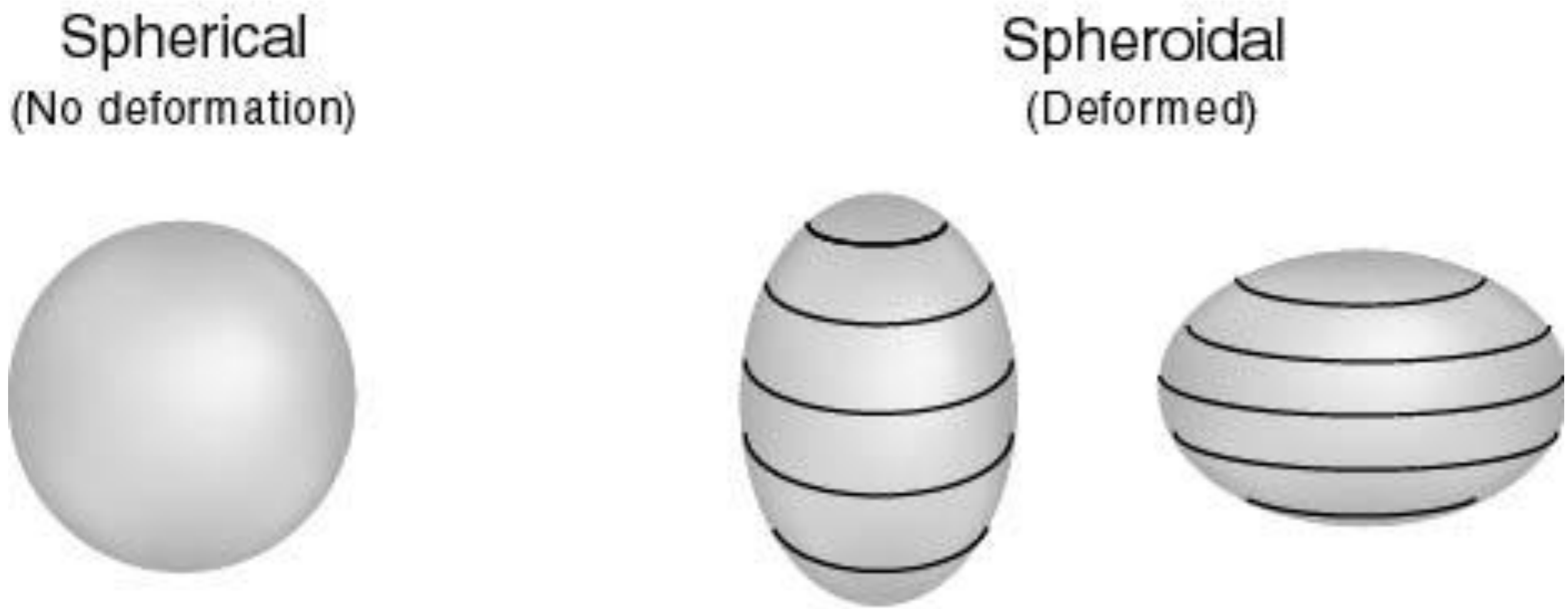
Thinking

- 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



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

kinetic energy

deformed Coulomb potential

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

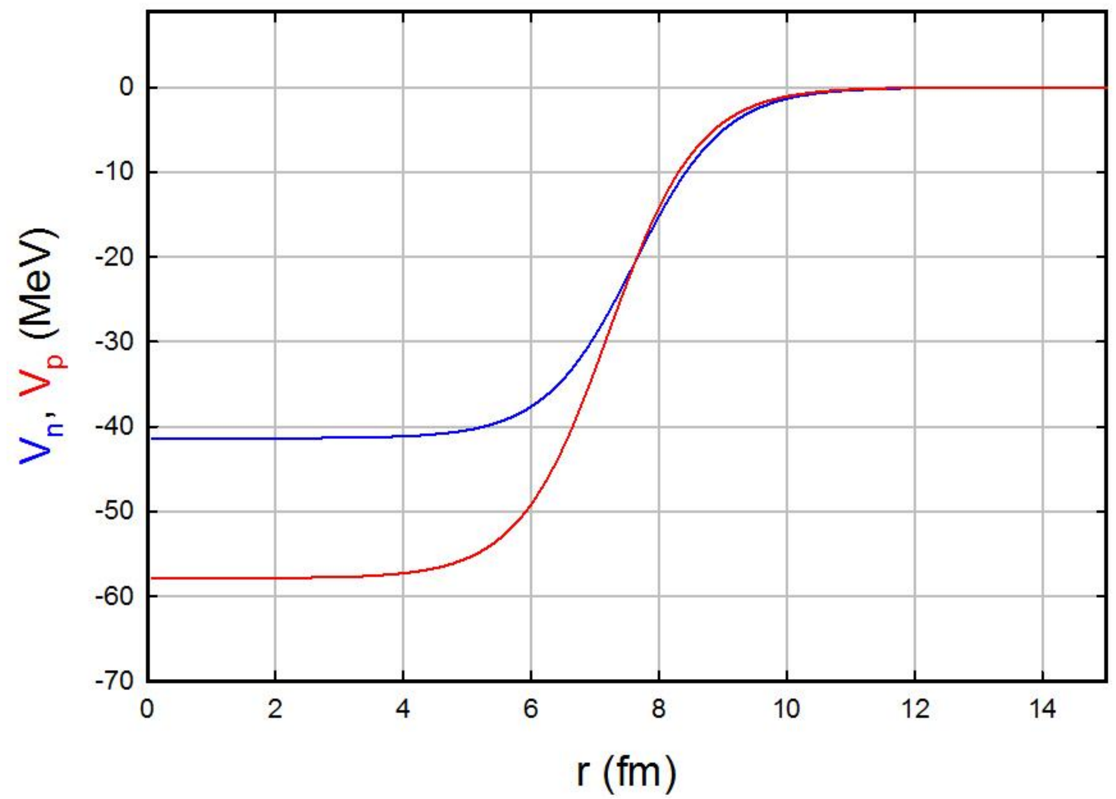
deformed nuclear potential

spin-orbit interaction

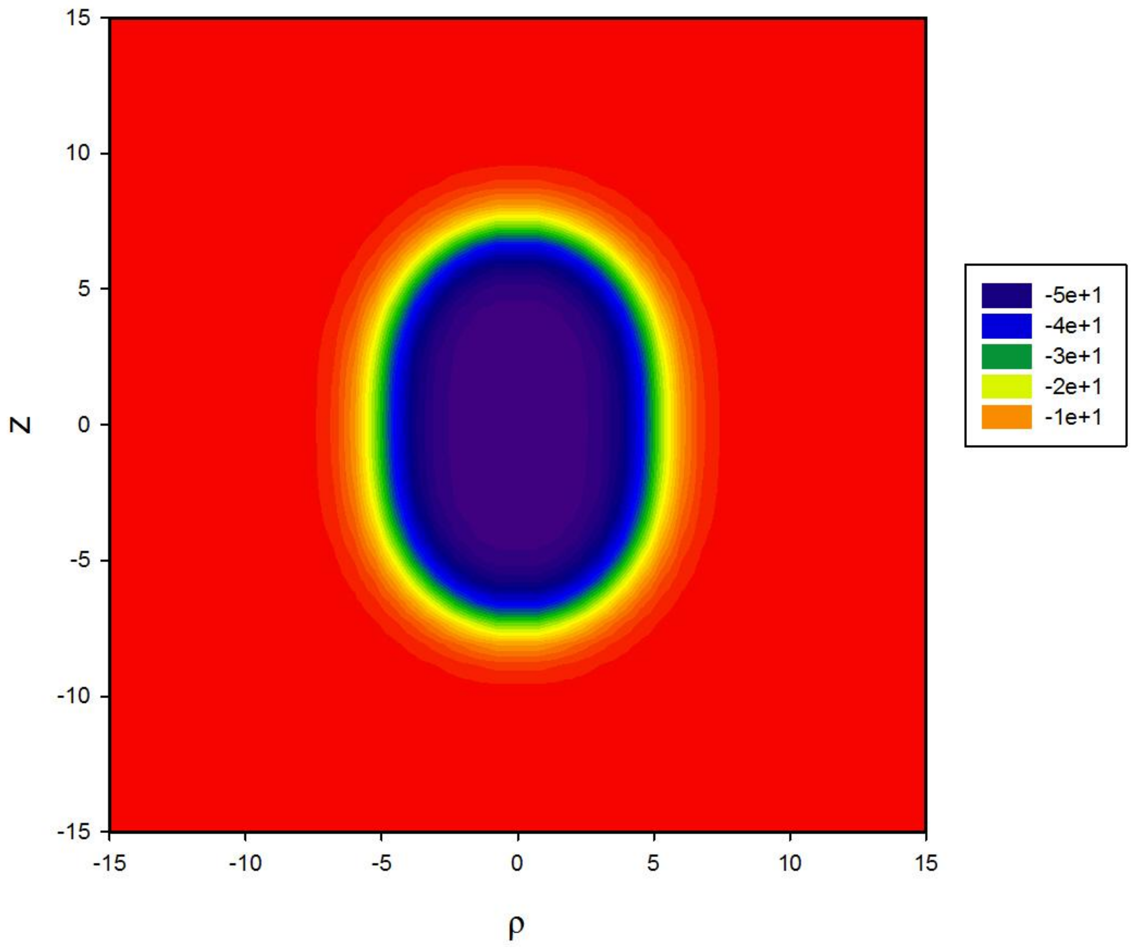
Thinking about the model

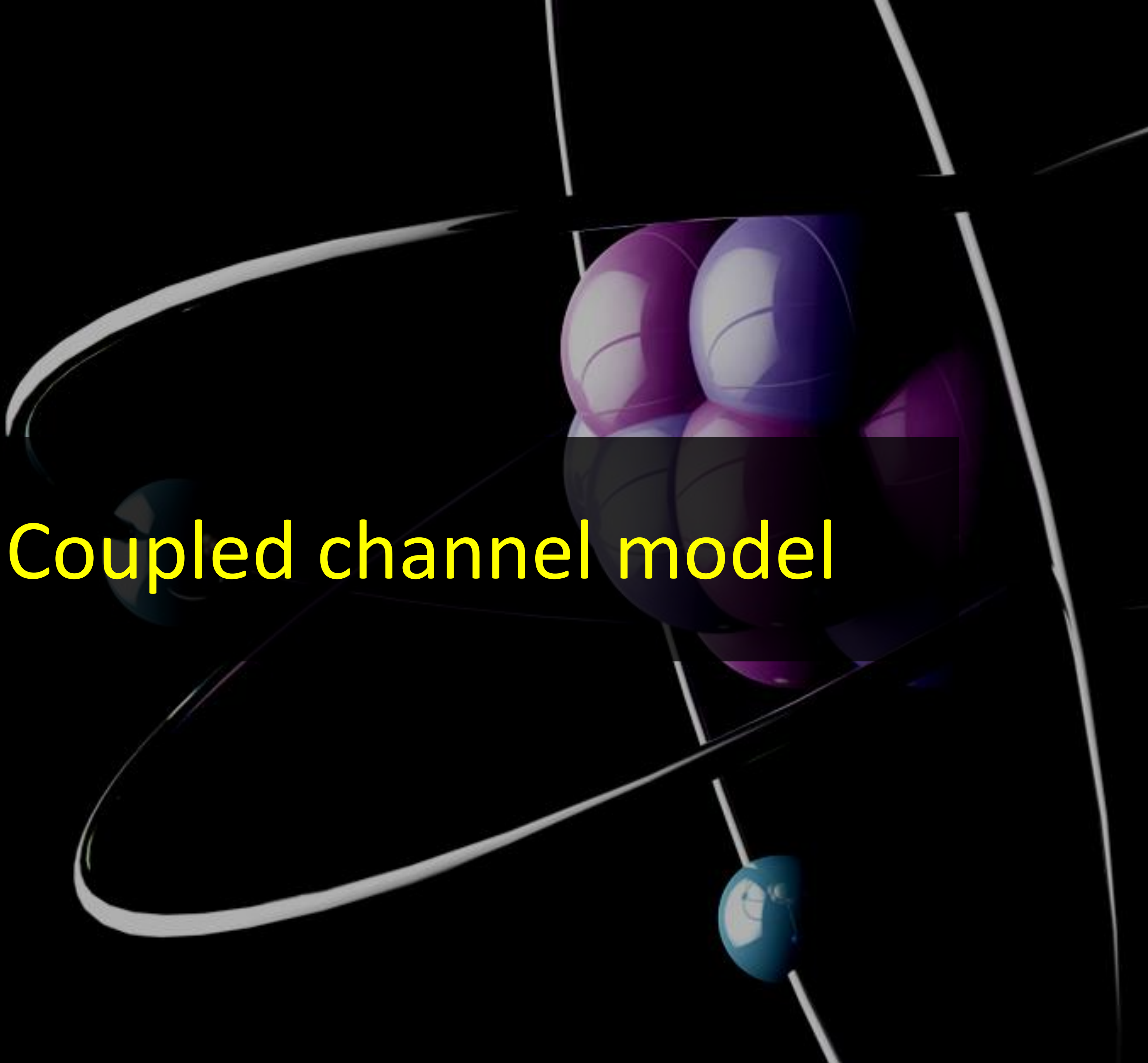
- Model for proton in deformed nucleus is simplest imaginable
- Closely related to earlier spherical models
- Philosophically consistent with electron model in atom
- Deformed nuclear potential models available in the literature
- Deformation models readily available
- Deformed Coulomb interaction easily 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

index	E_{Dudek} (MeV)	$E_{N,100}$ ($R_{max} = 18$)	$E_{N,100}$ ($R_{max} = 16$)	$E_{N,100}$ ($R_{max} = 14$)	$E_{N,100}$ ($R_{max} = 12$)
$1s$	-33.4423	-33.441766	-33.441877	-33.441630	-33.442284
$1d$	-24.5499	-24.549232	-24.548302	-24.547221	-24.546930
$2s$	-22.0258	-22.041675	-22.037155	-22.032858	-22.029881
$1g$	-12.1211	-12.118870	-12.117202	-12.115531	-12.114451
$2d$	-7.9762	-8.002365	-7.994905	-7.988063	-7.981666
$3s$	-6.4807	-6.554117	-6.536953	-6.521485	-6.506343

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

index	E_{Dudek} (MeV)	$E_{N,100}$ ($R_{max}=18$)	$E_{N,100}$ ($R_{max}=16$)	$E_{N,100}$ ($R_{max}=14$)	$E_{N,100}$ ($R_{max}=12$)
$1s_{m=0}$	-33.4405	-33.441232	-33.440791	-33.440187	-33.439678
$1d_{m=0}$	-24.8610	-24.861553	-24.860265	-24.858785	-24.857710
$1d_{m=1}$	-24.6796	-24.679708	-24.678440	-24.677064	-24.675922
$2s_{m=0}$	-21.9604	-21.977080	-21.972089	-21.967546	-21.963552
$1g_{m=0}$	-12.5845	-12.582936	-12.580976	-12.578933	-12.577239
$1g_{m=1}$	-12.5119	-12.510012	-12.508072	-12.506065	-12.504359
$2d_{m=0}$	-8.5715	-8.600592	-8.592264	-8.584514	-8.576888
$2d_{m=1}$	-8.1469	-8.172155	-8.164519	-8.157534	-8.150449

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.

Test for deformed problem

index	E_{Dudek} (MeV)	$E_{N,100}(l_{max} = 6)$ $(R_{max} = 14)$	$E_{N,100}(l_{max} = 8)$ $(R_{max} = 14)$	$E_{N,100}(l_{max} = 10)$ $(R_{max} = 14)$
$1s_{m=0}$	-33.3187	-33.317645	-33.317779	-33.317784
$1d_{m=0}$	-27.8181	-27.814070	-27.817376	-27.817486
$1d_{m=1}$	-25.3873	-25.378282	-25.383892	-25.384111
$2s_{m=0}$	-19.2554	-19.240770	-19.259938	-19.260824
$1g_{m=0}$	-18.0380	-17.948398	-18.035597	-18.039572
$1g_{m=1}$	-16.3821	-16.206008	-16.371370	-16.379615
$2d_{m=0}$	-11.6715	-11.482434	-11.666691	-11.679624
$2d_{m=1}$	-7.2382	-7.046577	-7.219741	-7.239901
$2g_{m=0}$	-5.7574	-4.807565	-5.641637	-5.766948

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

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

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:

$$= -\frac{\lambda}{\hbar}\left(\frac{\hbar}{2Mc}\right)^2 \frac{1}{r}\frac{\partial U}{\partial r}\boldsymbol{\sigma}\cdot\hat{\mathbf{L}}$$

$$+i\lambda\left(\frac{\hbar}{2Mc}\right)^2 \frac{1}{r}\frac{\partial U}{\partial \theta}\left[\sigma_x\left(\sin\phi\frac{\partial}{\partial r}+\frac{\cos\phi}{r}\frac{\partial}{\partial\phi}\right)+\sigma_y\left(-\cos\phi\frac{\partial}{\partial r}+\frac{\sin\phi}{r}\frac{\partial}{\partial\phi}\right)+\sigma_z\frac{\cot\theta}{r}\frac{\partial}{\partial\phi}\right] \quad (22)$$

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…

$$V_{so} \;\rightarrow\; -\frac{\lambda}{\hbar}\left(\frac{\hbar}{2Mc}\right)^2 \frac{1}{r}\frac{\partial U}{\partial r}\boldsymbol{\sigma}\cdot\hat{\mathbf{L}}$$

Test for spherical problem

index	E_{Dudek} (MeV)	$E_{N,100}$ ($R_{max}=18$)	$E_{N,100}$ ($R_{max}=16$)	$E_{N,100}$ ($R_{max}=14$)	$E_{N,100}$ ($R_{max}=12$)
$1s_{1/2}$	-33.4423	-33.441766	-33.441877	-33.441630	-33.442284
$1d_{5/2}$	-24.8964	-24.892350	-24.891437	-24.890375	-24.890089
$1d_{3/2}$	-24.0507	-24.054716	-24.053756	-24.052644	-24.052339
$2s_{1/2}$	-22.0258	-22.041675	-22.037155	-22.032858	-22.029881
$1g_{9/2}$	-13.2043	-13.192241	-13.190589	-13.188941	-13.187862
$1g_{7/2}$	-10.8316	-10.840742	-10.839028	-10.837309	-10.836209
$2d_{5/2}$	-8.4568	-8.478680	-8.471316	-8.464560	-8.458262
$2d_{3/2}$	-7.2581	-7.291413	-7.283792	-7.276802	-7.270245
$3s_{1/2}$	-6.4807	-6.554117	-6.536953	-6.521485	-6.506343

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

index	E_{Dudek} (MeV)	$E_{N,100}(l_{max}=6)$ $(R_{max}=14)$	$E_{N,100}(l_{max}=8)$ $(R_{max}=14)$	$E_{N,100}(l_{max}=10)$ $(R_{max}=14)$
$1s_{m=0}$	-33.3187	-33.324191	-33.324336	-33.324342
$1d_{m=0}$	-27.8562	-27.941897	-27.946091	-27.946233
$1d_{m=1}$	-25.1361	-25.059179	-25.064506	-25.064719
$2s_{m=0}$	-19.2770	-19.280507	-19.315717	-19.317592
$1g_{m=0}$	-18.2630	-18.235448	-18.342173	-18.347647
$1g_{m=1}$	-15.9150	-15.702723	-15.842560	-15.849615
$2d_{m=0}$	-11.7023	-11.516698	-11.710765	-11.726053
$2d_{m=1}$	-6.9487	-6.738900	-6.954404	-7.011201
$2g_{m=0}$	-6.4394	-5.167123	-6.239576	-6.389641

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

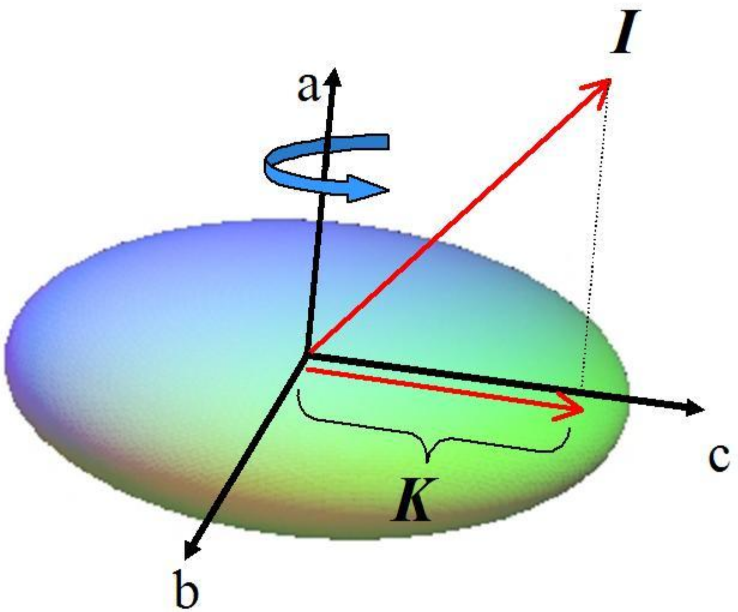
Energy levels from exp’t

energy (keV)	J^π	$[N n_z \Lambda]$	orbital	rotational state
0	$7/2^+$	[404]	$1g_{7/2}$	[404] J=7/2
6.237	$9/2^-$	[514]	$1h_{11/2}$ deformed	[514] J=9/2
136.262	$9/2^+$			[404] J=9/2
158.554	$11/2^-$			[514] J=11/2
301.662	$11/2^+$			[404] J=11/2
337.54	$13/2^-$			[514] J=31/2
482.168	$5/2^+$	[402]	$2d_{5/2}$	[402] J=5/2
495.184	$13/2^+$			[404] J=13/2
542.51	$15/2^-$			[514] J=15/2
590.06	$7/2^+$			[402] J=7/2
615.19	$1/2^+$	[411]	$3s_{1/2}$	[411] J=1/2
618.99	$3/2^+$			[411] J=3/2
716.659	$15/2^+$			[404] J=15/2
727.31	$9/2^+$			[402] J=9/2
772.97	$17/2^-$			[514] J=15/2

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



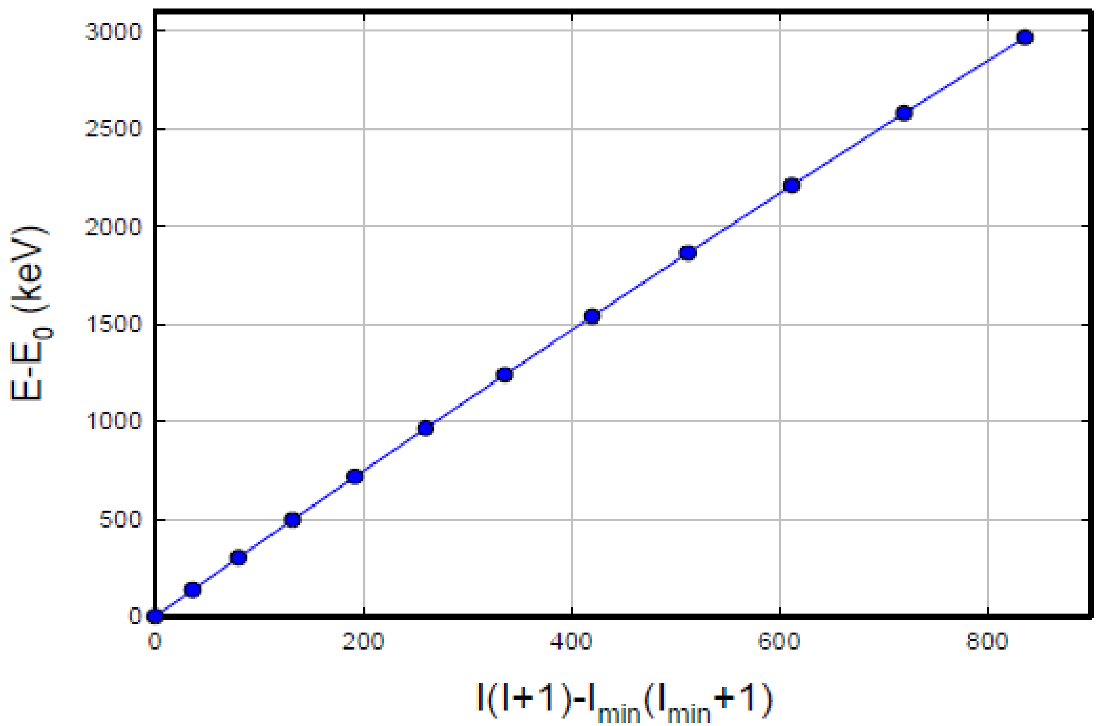
Energy levels from exp't

energy (keV)	J^π	$[N n_z \Lambda]$	orbital	rotational state
0	$7/2^+$	[404]	$1g_{7/2}$	[404] J=7/2
6.237	$9/2^-$	[514]	$1h_{11/2}$ deformed	[514] J=9/2
136.262	$9/2^+$			[404] J=9/2
158.554	$11/2^-$			[514] J=11/2
301.662	$11/2^+$			[404] J=11/2
337.54	$13/2^-$			[514] J=31/2
482.168	$5/2^+$	[402]	$2d_{5/2}$	[402] J=5/2
495.184	$13/2^+$			[404] J=13/2
542.51	$15/2^-$			[514] J=15/2
590.06	$7/2^+$			[402] J=7/2
615.19	$1/2^+$	[411]	$3s_{1/2}$	[411] J=1/2
618.99	$3/2^+$			[411] J=3/2
716.659	$15/2^+$			[404] J=15/2
727.31	$9/2^+$			[402] J=9/2
772.97	$17/2^-$			[514] J=15/2

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

Energy levels due to rotation

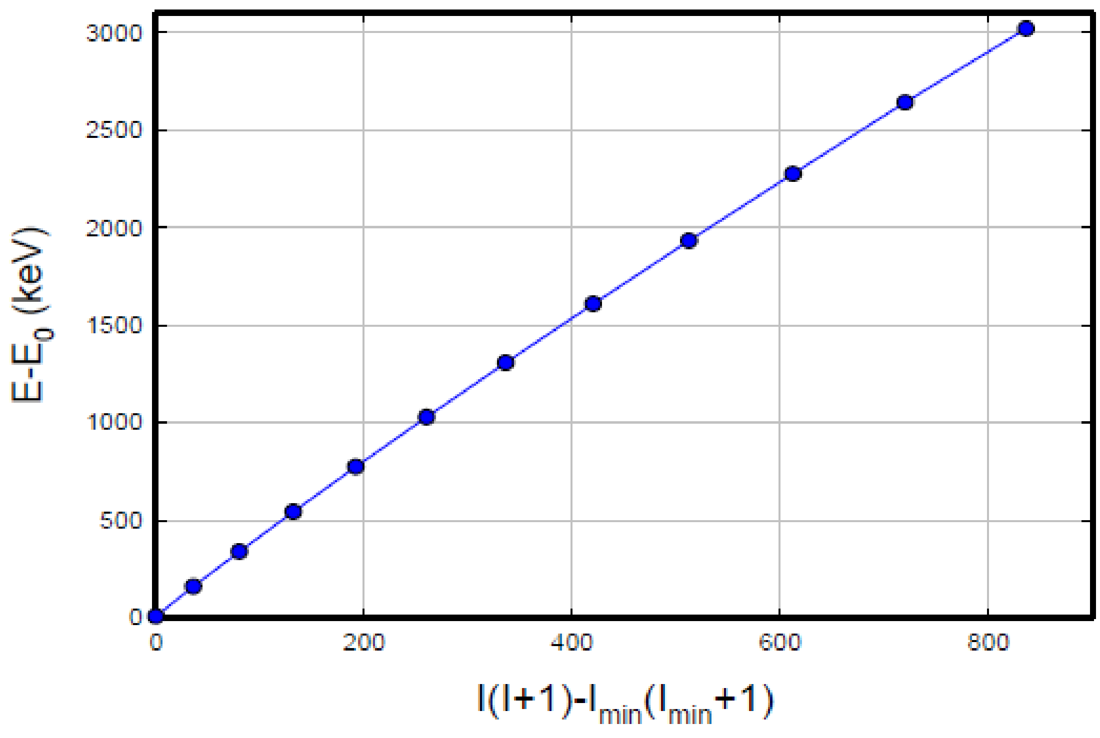
$$T_R = \frac{\hbar^2}{\mathcal{I}}\left[J(J+1) - J_{\min}(J_{\min}+1)\right]$$



Rotational levels in Ta-181 associated with the 7/2+ ground state

Energy levels due to rotation

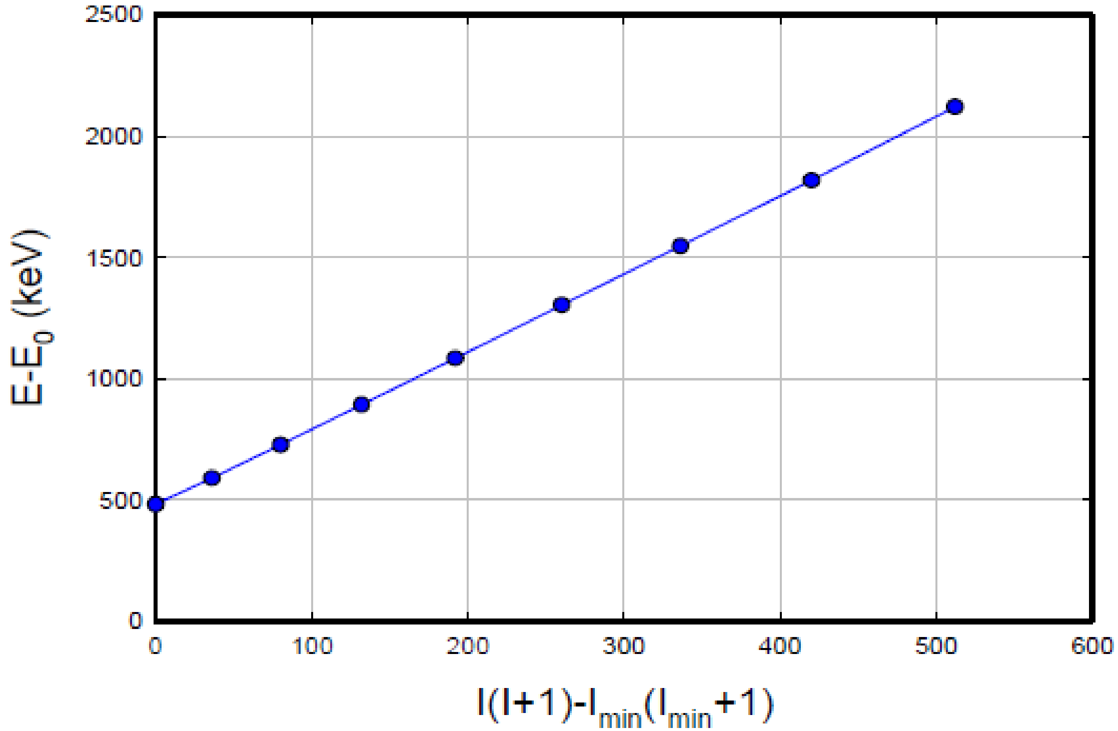
$$T_R = \frac{\hbar^2}{\mathcal{I}}\left[J\left(J+1\right)-J_{\min}\left(J_{\min}+1\right)\right]$$



Rotational levels in Ta-181 associated with the 9/2- first excited state

Energy levels due to rotation

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



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 β_2

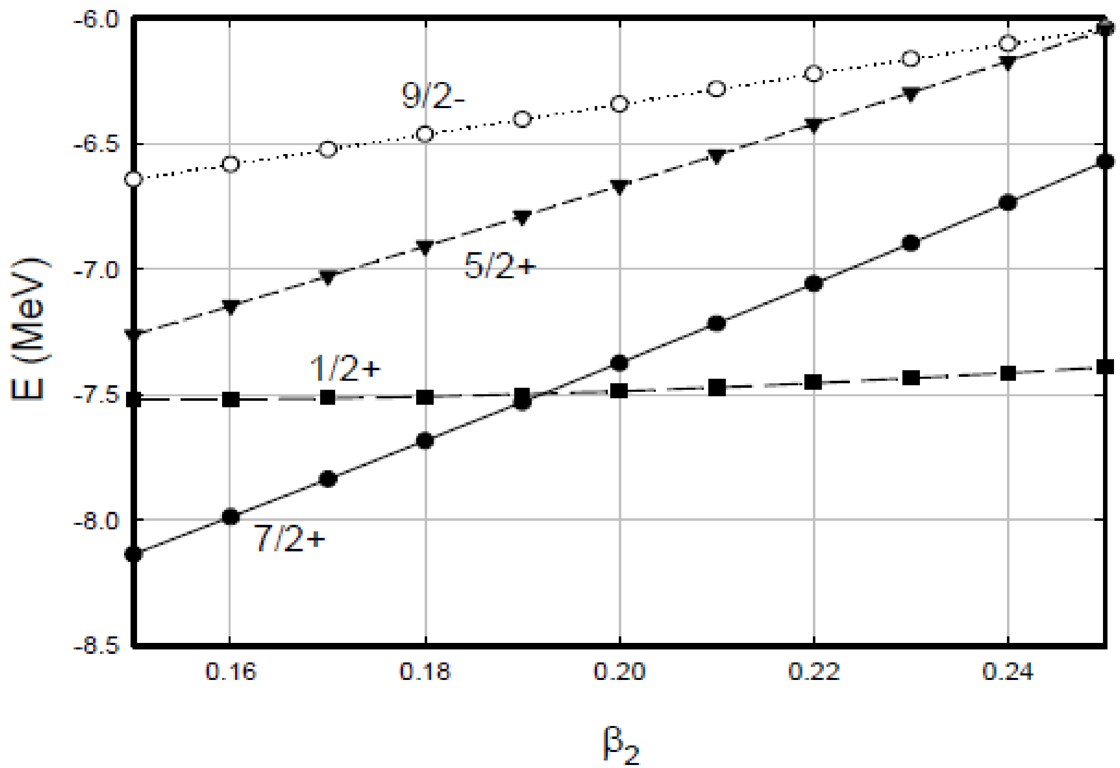
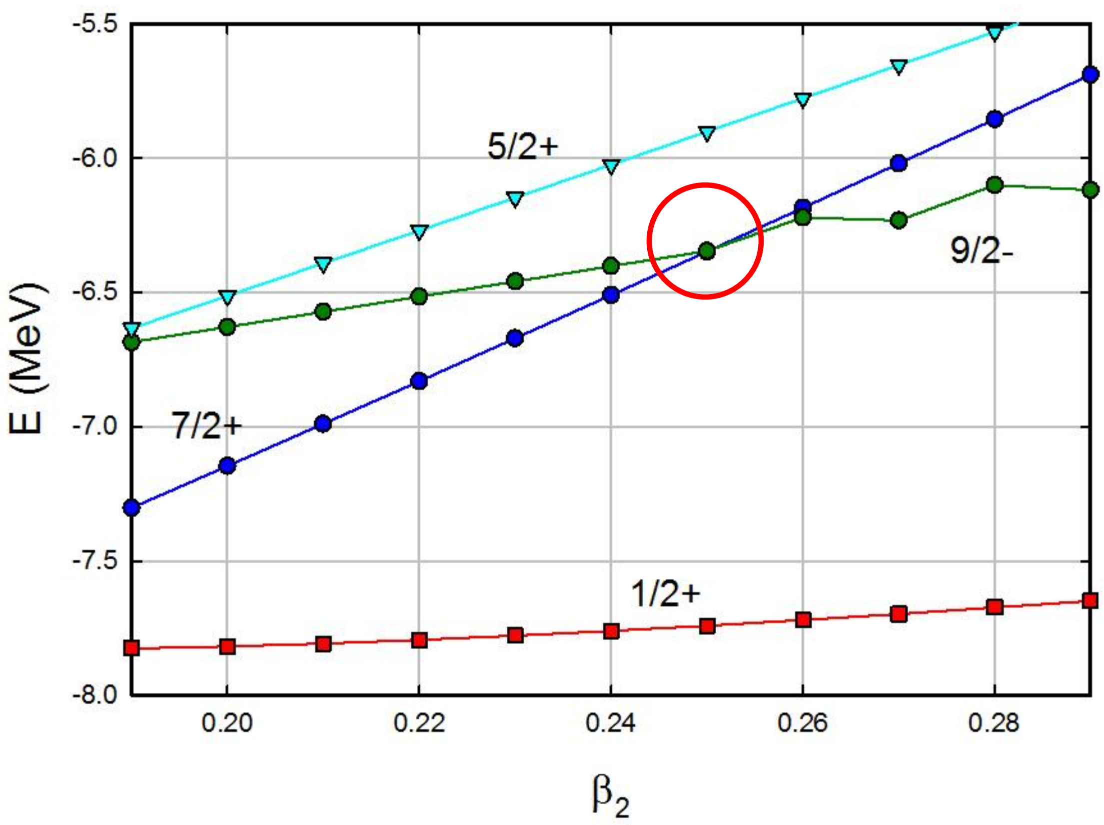


Figure 4. Proton orbital energies as a function of β_2 with $\beta_4 = 0$, for ^{181}Ta, using Dudek's universal model potential parameters.

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 β_2 with β_4 = -0.038



Seems to work

- Now we included β_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 β_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

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

Working on β_2

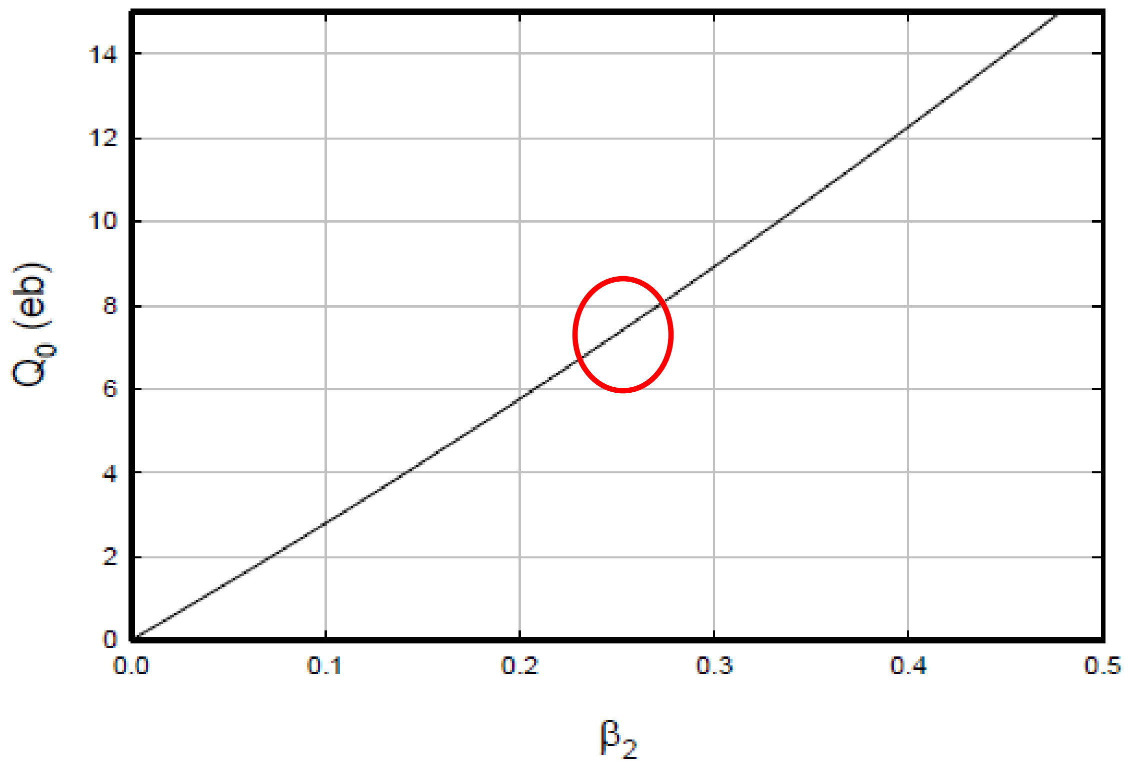
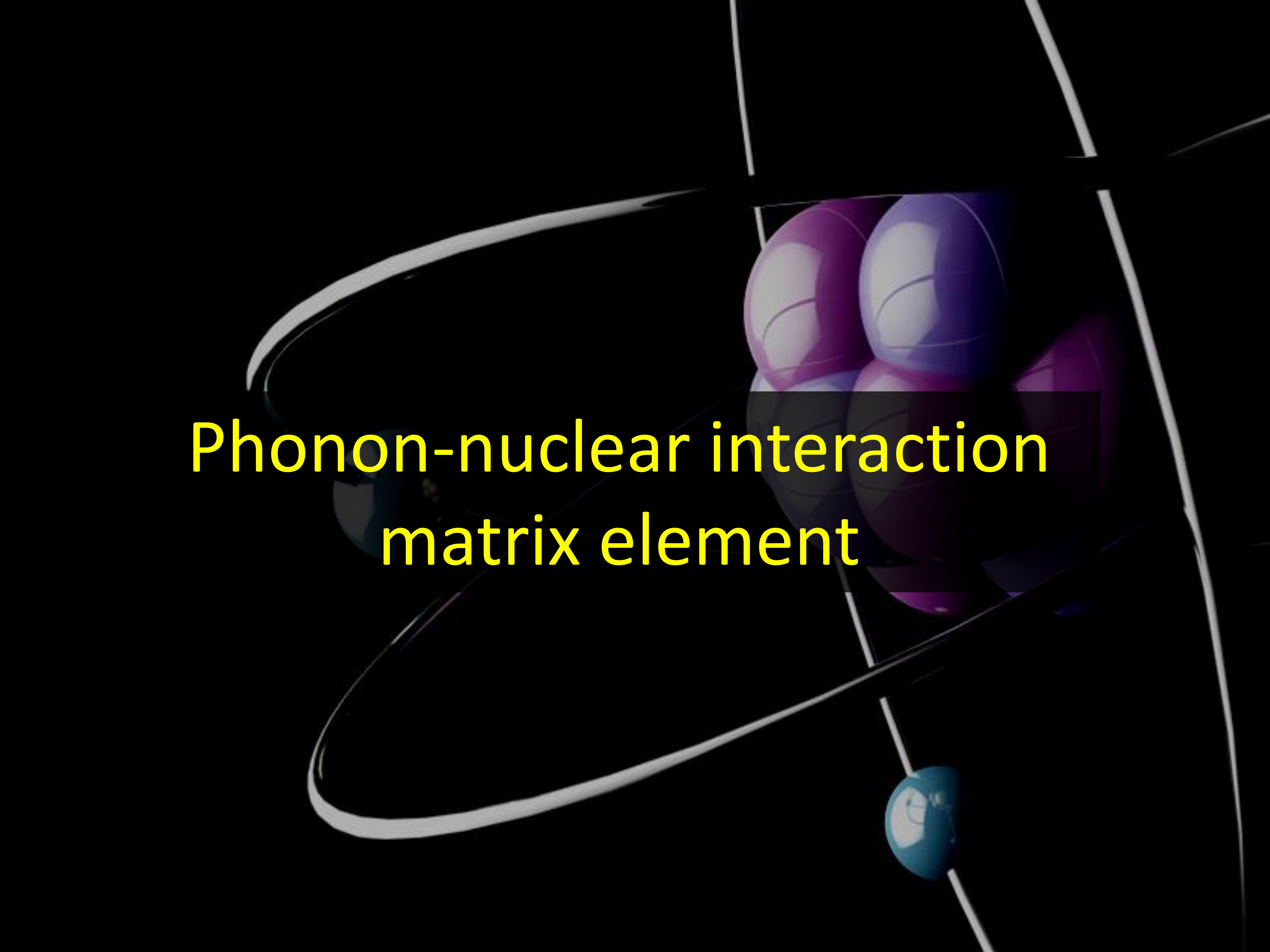


Figure 1. Quadrupole moment as a function of β_2.

Thinking about comparison

- Based on the experimental observation of 7.37 eb, we would expect β_2 = 2.47
- Optimization based on the Dudek code including quadrupole and octupole terms gives a 7/2+ and 9/2- crossing for β_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

$$V_{so} \;=\; \frac{\lambda}{\hbar}\left(\frac{\hbar}{2Mc}\right)^2 \nabla U \cdot \left(\boldsymbol{\sigma}\times\hat{\mathbf{p}}\right)$$

- A boost is implemented using $\qquad \hat{\mathbf{p}} \;\rightarrow\; \hat{\mathbf{p}} + \dfrac{\hat{\mathbf{P}}}{N}$
- This leads to

$$\Delta V_{so} \;=\; \frac{\lambda}{\hbar}\left(\frac{\hbar}{2Mc}\right)^2 \nabla U \cdot \left(\boldsymbol{\sigma}\times\frac{\hat{\mathbf{P}}}{N}\right)$$

Relativistic phonon-nuclear interaction

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

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

- Evaluating the commutators leads to

$$\Delta\hat{V} \rightarrow i\frac{1}{4Mmc^2}[\boldsymbol{\sigma}_k \times (\hat{\boldsymbol{\pi}}_k V_{jk})]\cdot\hat{\mathbf{P}}]$$

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

$$-i\lambda\frac{1}{4Mmc^2}\boldsymbol{\sigma}\cdot[(\hat{\pi}U)\times\mathbf{P}]$$

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

index	E_{Dudek} (MeV)	$E_{N=100}$ $l_{max} = 10$
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

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

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

- with

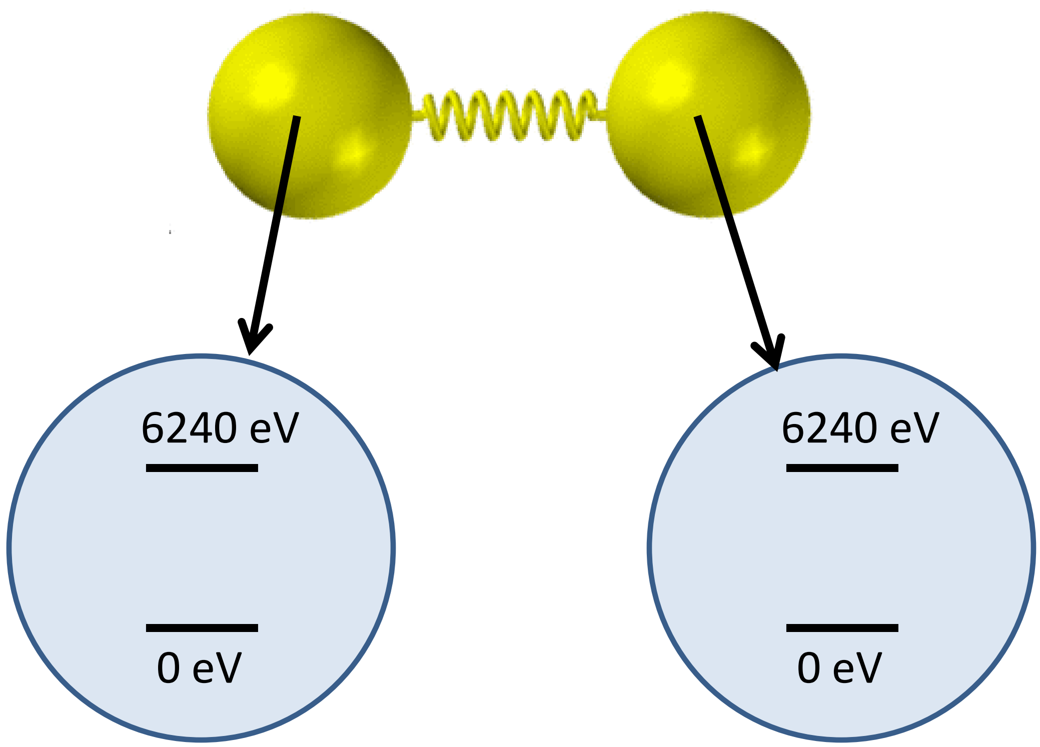
$$\mathbf{a} = -\lambda \frac{\hbar}{4Mmc^3} \boldsymbol{\sigma} \times \left(\nabla U \right)$$

- For this model we estimate

$$\left| \mathbf{a} \right| = 1.29 \times 10^{-6}$$

- 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 Ta2:

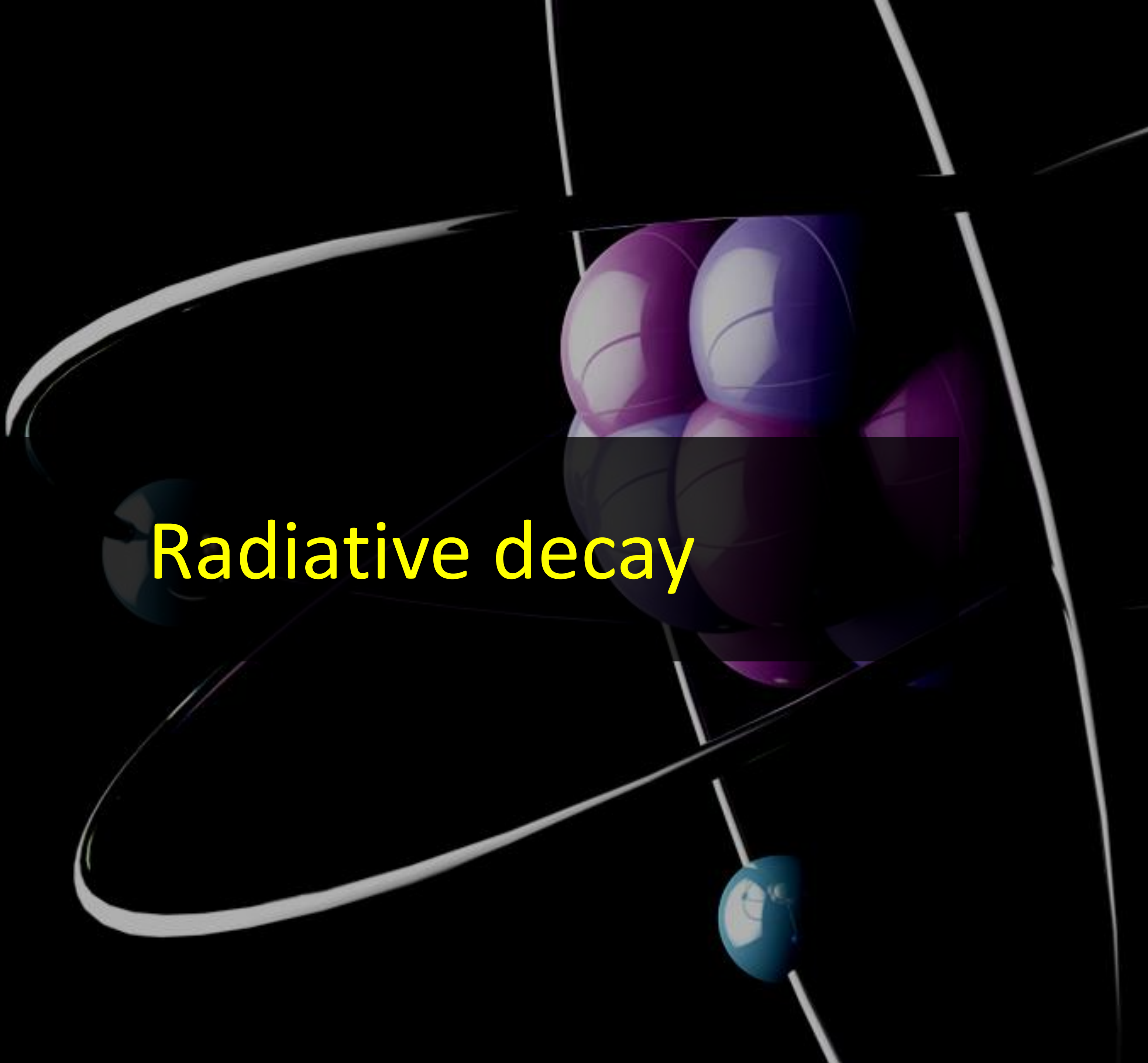
$$\hat{U}_{12} = -\frac{Mc^2\left(\hbar\omega_0\right)^2}{2\left(\Delta E\right)^2}\frac{\left(\mathbf{a}_1\cdot\mathbf{R}_{21}\right)\left(\mathbf{a}_2\cdot\mathbf{R}_{21}\right)}{\left|\mathbf{R}_{21}\right|^2}$$

Plug in numbers:

$$\frac{Mc^2\left(\hbar\omega_0\right)^2}{2\left(\Delta E\right)^2}\left|\mathbf{a}\right|^2 = 6\times10^{-12}\ \text{eV}$$

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

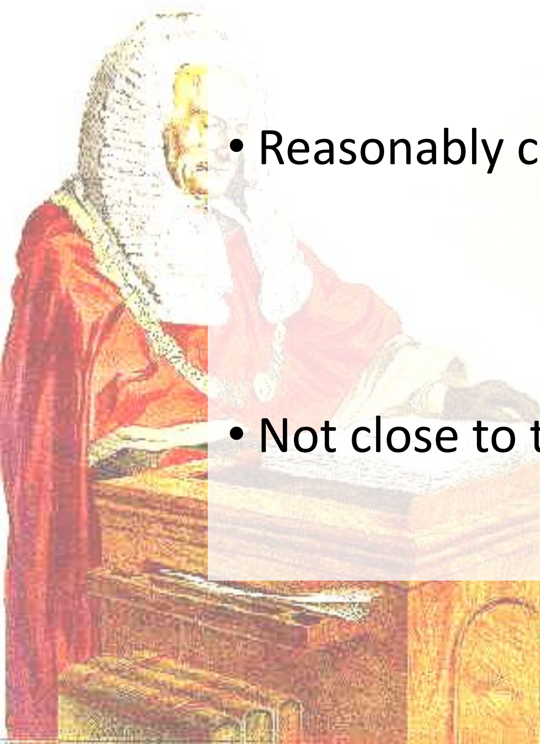
$$\gamma \;=\; \frac{4}{3}\frac{e^2}{4\pi\varepsilon_0}\frac{\omega^3}{\hbar c^3}\left|\left\langle \frac{9}{2}^- \middle| \mathbf{r} \middle| \frac{7}{2}^+ \right\rangle\right|^2 \;=\; 3.89\times 10^8\ \mathrm{sec}^{-1}$$

- Reasonably consistent with the Weisskopf estimate

$$\gamma_W \;=\; 10^{14} A^{2/3} E^3 \;=\; 7.76\times 10^8\ \mathrm{sec}^{-1}$$

- Not close to the experimental value

$$\gamma_{\mathrm{exp't}} \;=\; 2.4\times 10^3\ \mathrm{sec}^{-1}$$



Large discrepancy

- Our simple model gives a fast decay rate of 3.89×10^8, while experiment is probably below 2×10^3
- The ratio of theory to experiment is about 2×10^5
- This indicates a serious problem
- Note that this is not the only transition where there is a disagreement
- Instructive to look at other transitions

Weisskopf vs experiment

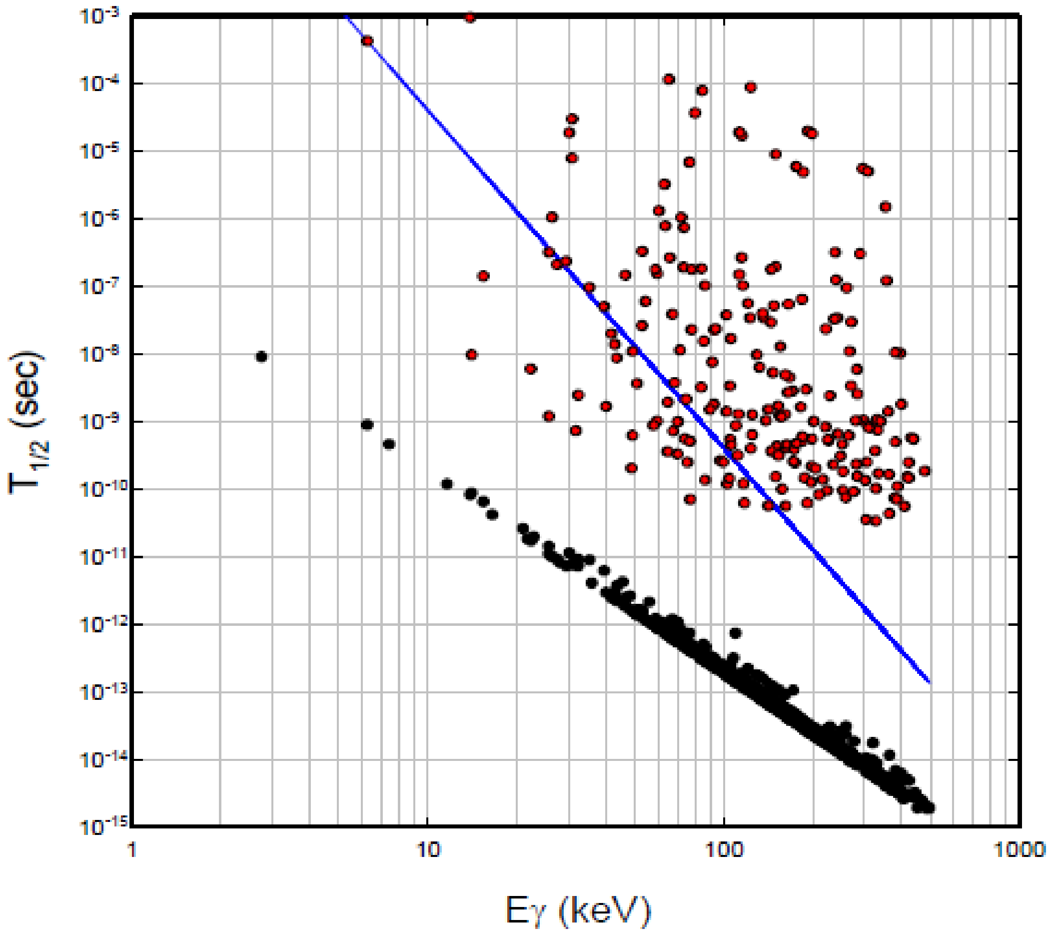


Figure 3. Half-life as a function of the transition energy for odd A nuclei with an even number of neutrons; observed results (red circles); Weisskopf estimate (black circles); scaled estimate assuming $(\Delta E)^5$ scaling (blue line).

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

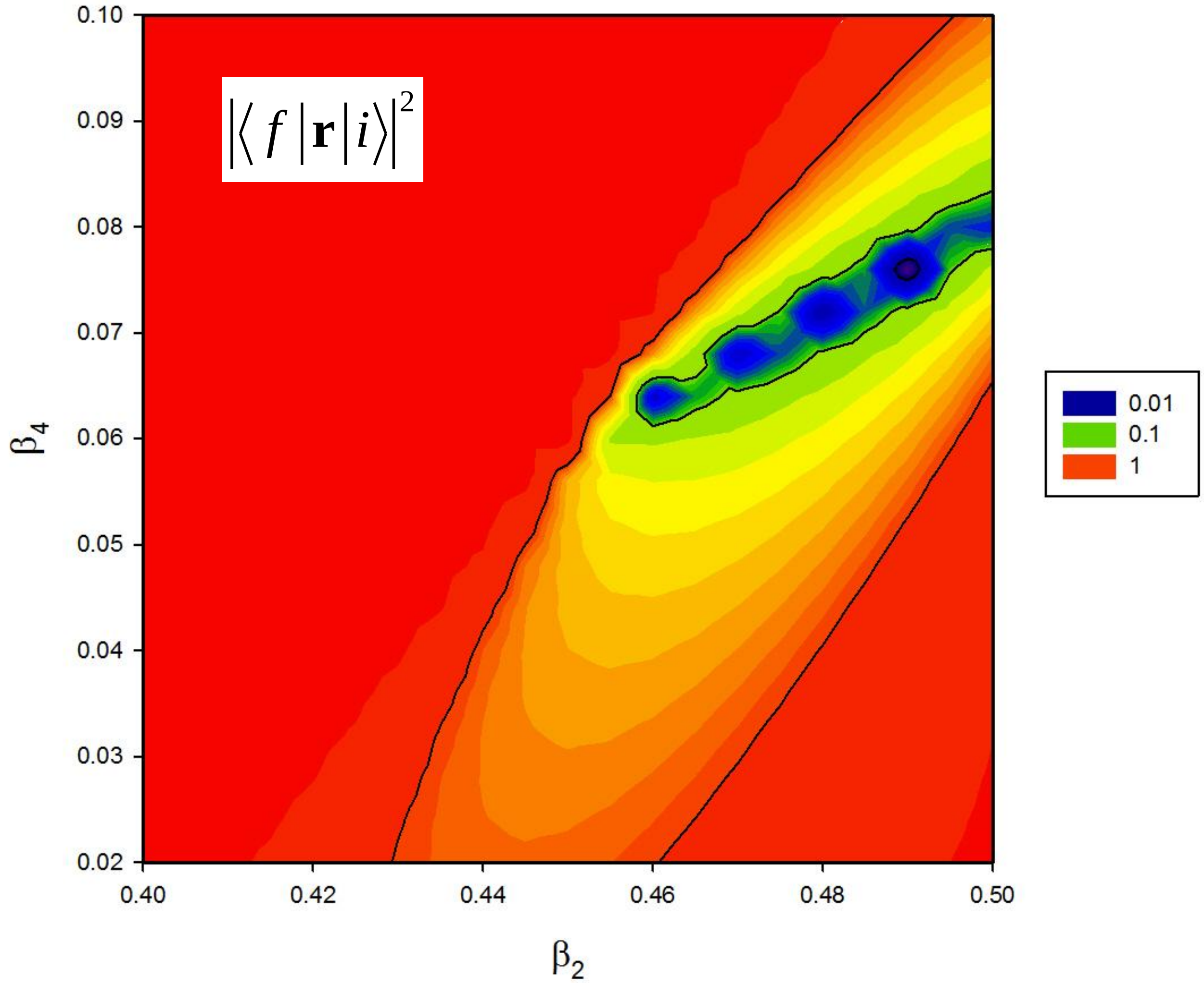
Nilsson and coworkers

- 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



Thinking

- 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|ST model

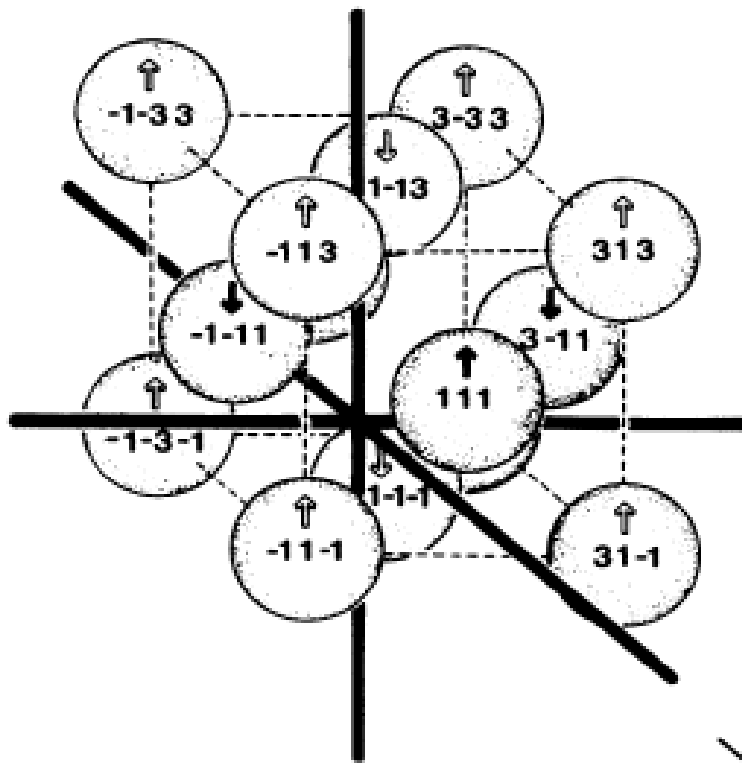
Screening

- 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

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

Then separate according to

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

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

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

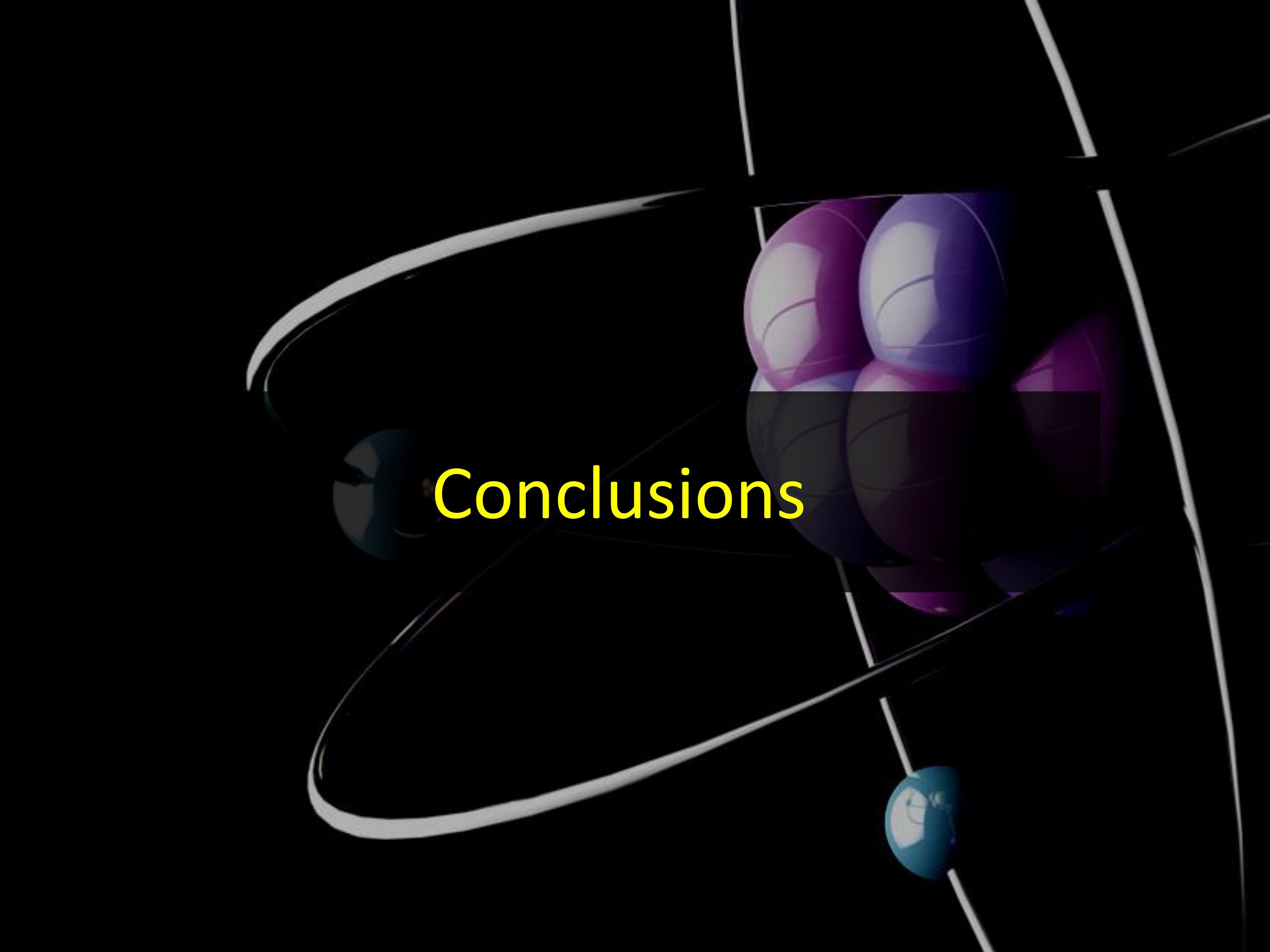
Coherent contribution for central potential

$$
\left\langle \Psi \left| \sum_{\gamma<\delta} (\boldsymbol{\tau}_\gamma \cdot \boldsymbol{\tau}_\delta)(\boldsymbol{\sigma}_\gamma \cdot \boldsymbol{\sigma}_\delta) y_C(r_{\gamma\delta}) \right| \Psi \right\rangle \rightarrow
$$

$$
\begin{aligned}
&\frac{1}{2}\sum_\alpha \sum_\beta c^*(\alpha)c(\beta)\left\langle \left[\frac{1}{2}\sigma_+(\alpha)\sigma_-(\beta) + \frac{1+\sigma_z(\alpha)}{2}\frac{1+\sigma_z(\beta)}{2}\right]\left[\frac{1}{2}\frac{1-\tau_z(\alpha)}{2}\frac{1-\tau_z(\beta)}{2} + \tau_-(\alpha)\tau_+(\beta)\right] y_C(r_{\alpha\beta})\right\rangle \\
&-\frac{1}{2}\sum_\alpha \sum_\beta c^*(\alpha)d(\beta)\left\langle \left[\frac{1+\sigma_z(\alpha)}{2}\frac{1-\sigma_z(\beta)}{2}\right]\left[\frac{1}{2}\frac{1-\tau_z(\alpha)}{2}\frac{1-\tau_z(\beta)}{2} + \tau_-(\alpha)\tau_+(\beta)\right] y_C(r_{\alpha\beta})\right\rangle \\
&-\frac{1}{2}\sum_\alpha \sum_\beta d^*(\alpha)c(\beta)\left\langle \left[\frac{1-\sigma_z(\alpha)}{2}\frac{1+\sigma_z(\beta)}{2}\right]\left[\frac{1}{2}\frac{1-\tau_z(\alpha)}{2}\frac{1-\tau_z(\beta)}{2} + \tau_-(\alpha)\tau_+(\beta)\right] y_C(r_{\alpha\beta})\right\rangle \\
&+\frac{1}{2}\sum_\alpha \sum_\beta d^*(\alpha)d(\beta)\left\langle \left[\frac{1}{2}\sigma_-(\alpha)\sigma_+(\beta) + \frac{1+\sigma_z(\alpha)}{2}\frac{1+\sigma_z(\beta)}{2}\right]\left[\frac{1}{2}\frac{1-\tau_z(\alpha)}{2}\frac{1-\tau_z(\beta)}{2} + \tau_-(\alpha)\tau_+(\beta)\right] y_C(r_{\alpha\beta})\right\rangle
\end{aligned}
\tag{96}
$$

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**.c**P** 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!