# Coupled-channel optical model potential for even-even and odd-A actinides using extended couplings

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# Goal of the project

- Derive optical model potentials describing available experimental data (strength functions, scattering radii, total, reaction XS, elastic and inelastic scattering AD with low-lying collective levels excitations and excitation of isobar-analog states up to 200 MeV nucleon incident energies) even-even and odd-A actinides

- Components:
  - Dispersive Lane-consistent coupled channels optical model with extended couplings
  - Soft rotator model (nuclear structure)
  - OPTMAN and SHEMMAN codes

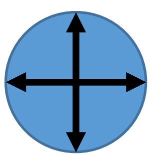
# Introduction

Motivation for extended coupling

# Optical model for soft deformed nuclei

Conventional OMP
$V\big(r, R(\theta', \varphi')\big)$

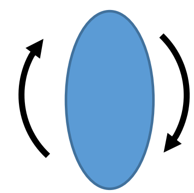
Soft spherical nucleus
(vibrational excitations)



*Taylor expansion near sphere*

Explicit deformations → vibrations
bad convergence for big deformations

Rigid deformed nucleus
(rotational excitations)



*Static multipolar expansion*

Good convergence for big static deformations
no explicit deformations → no vibrations!

**But actinides are both considerably deformed in GS and soft for vibrations**

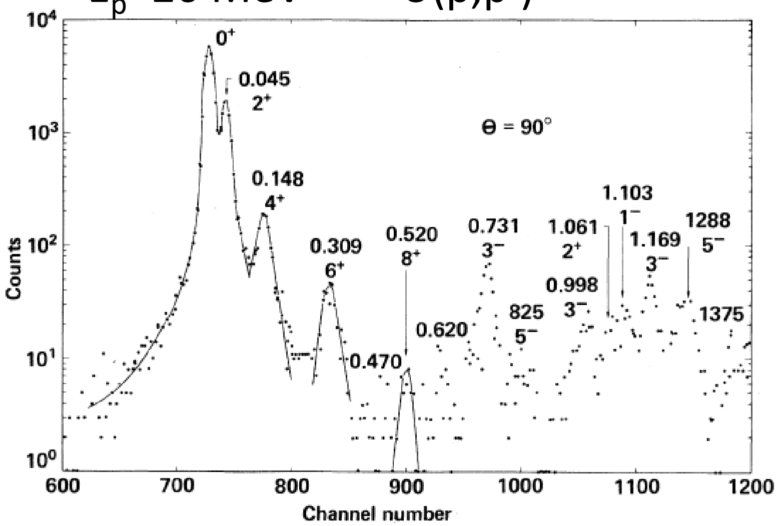
# Are other bands important? (proton inelastic)

No nucleon scattering data for other-than-GS band in EXFOR for actinides

…

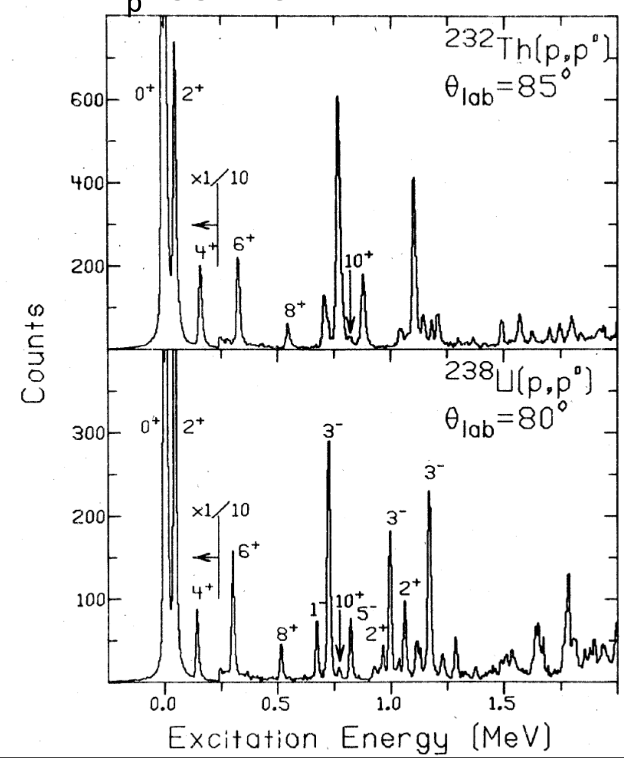
but there are clear evidences of levels from **other bands** in some proton inelastic scattering experimental works

$E_p$=26 MeV $^{238}$U(p,p')



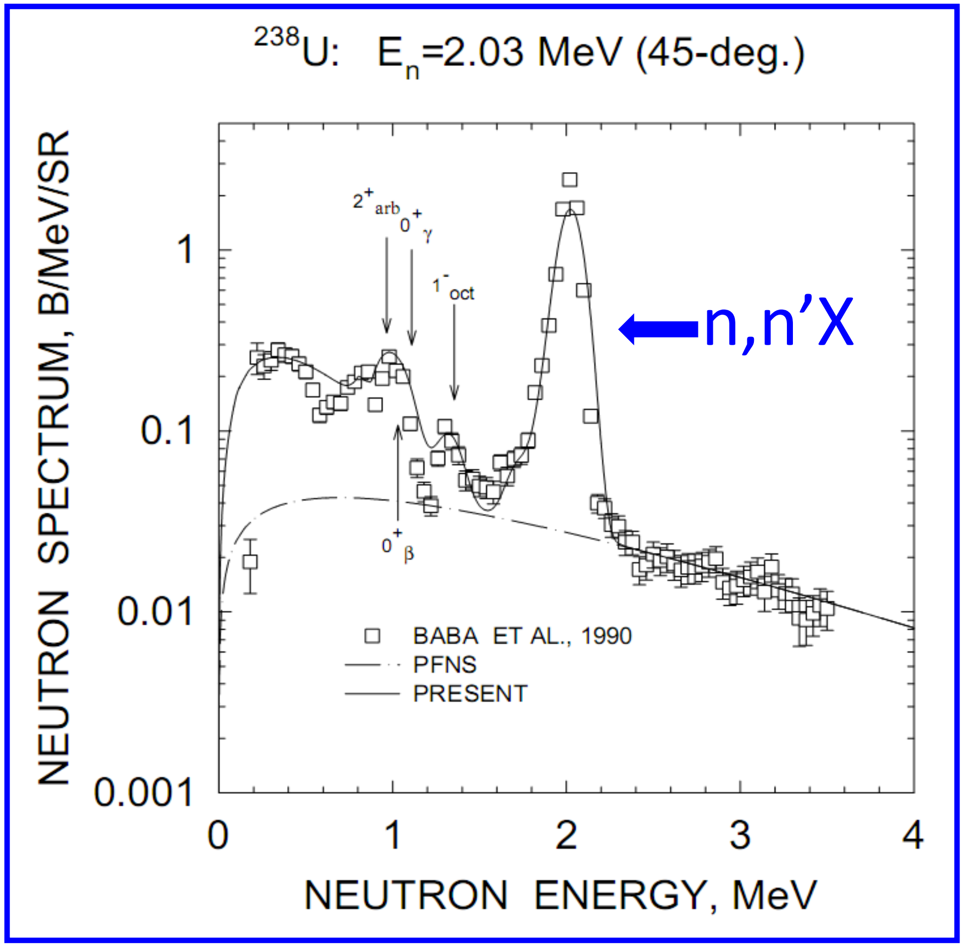

**L. F. Hansen et al, PRC 25 (1982) 189**

$E_p$=35 MeV



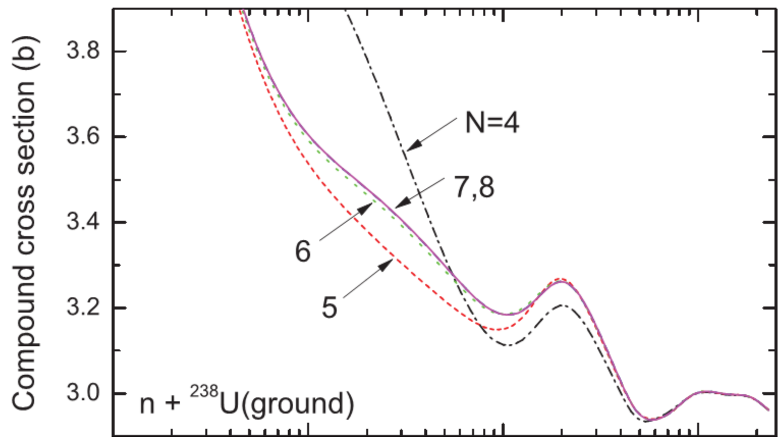

**C. H. King et al, PRC 20 (1979) 2084**

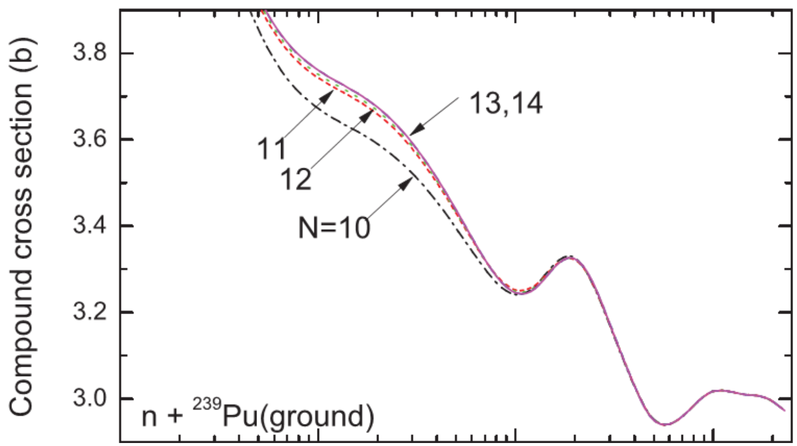
# Are other bands important? ($^{238}U$ neutron emission spectrum)




Also evidence of levels from **other bands**

# Saturation of the coupling scheme




**<u>Saturation</u>** – predicted cross sections do not change upon addition of new levels

Along GS band to saturate we need:

- 6 levels for even-even
- 11 levels for odd

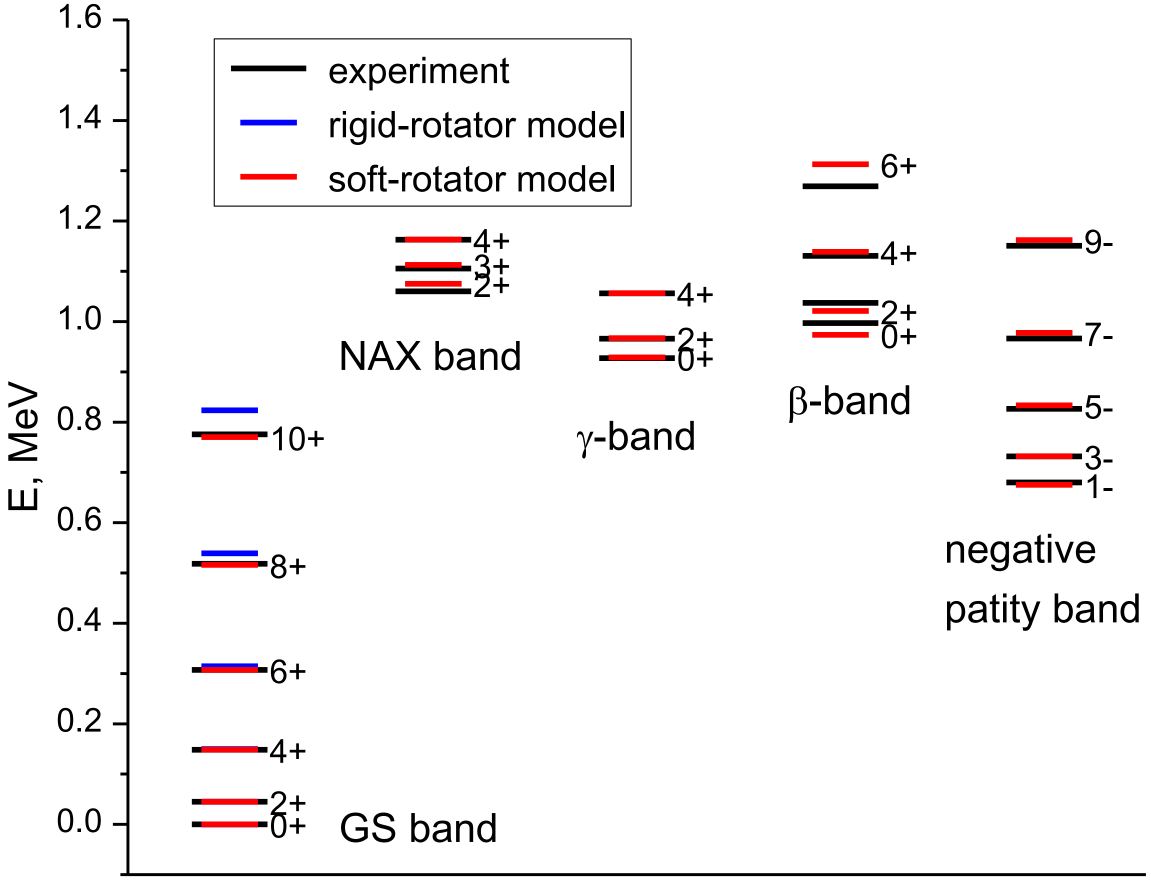
But what about other bands?

F. S. Dietrich et al., Phys. Rev. C 85, 044611 (2012)

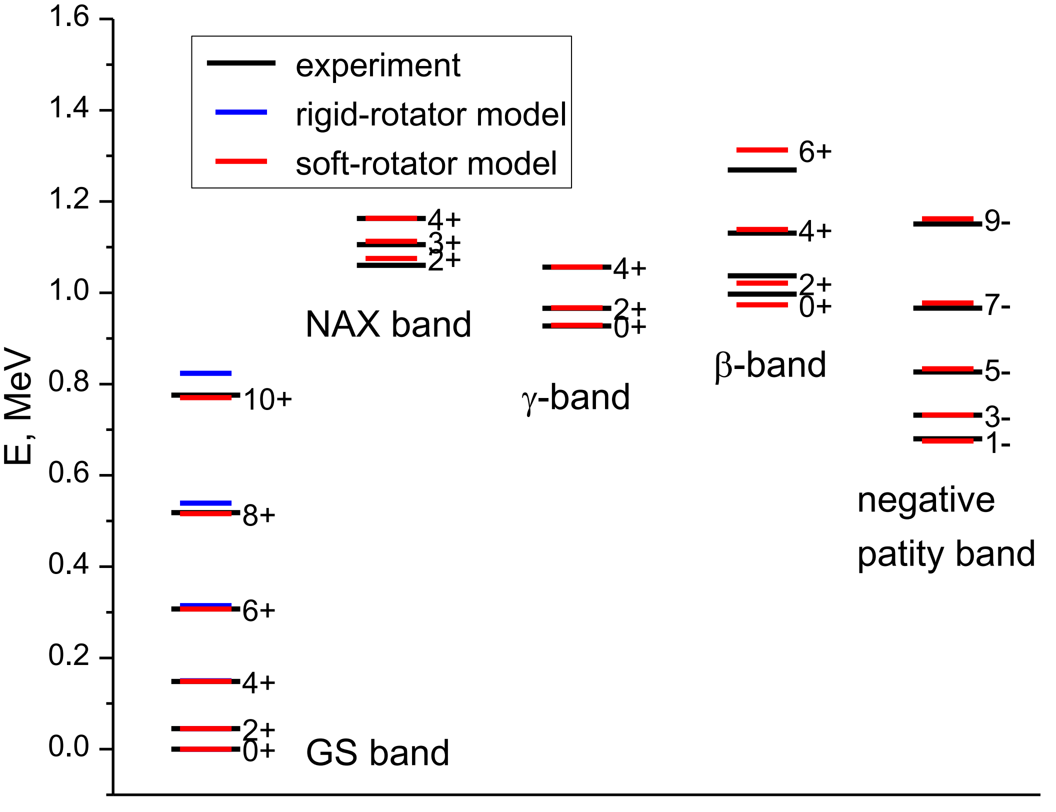
# Is softness important?

GS band levels energies deviate from rigid rotor level sequence for high spins due to nuclear stretching form centrifugal forces.
Soft-rotor model describes experimental energies and other bands as well.

$^{238}$U



# Soft rotator model




$$\hat{H} = \frac{\hbar^2}{2B}\left\{\hat{T}_{\beta_2} + \frac{1}{\beta_2^2}\hat{T}_{\gamma}\right\} + \frac{\hbar^2}{2}\hat{T}_r + \frac{\hbar^2}{2B_3}\hat{T}_{\beta_3} + \frac{\beta_{20}^4}{\beta_2^2}V(\gamma) + V(\beta_2) + V(\beta_3)$$

# Theory

Optical potential for soft deformed nuclei

# Solution: Taylor expansion near axial static form

$$R_i(\theta',\varphi')$$

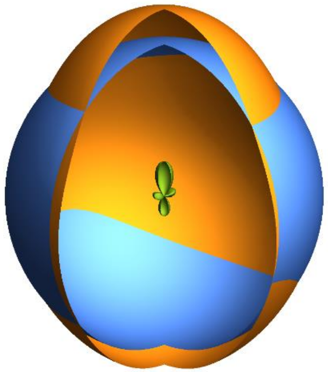
$$= R_{0i}\left\{1 + \sum_{\lambda=2,3;even\ \mu} \beta_{\lambda\mu} Y_{\lambda\mu}(\theta',\varphi')\right.$$

$$= R_i^{zero}(\theta') + \delta R_i(\theta',\varphi';\delta\beta_2,\gamma,\beta_3)$$

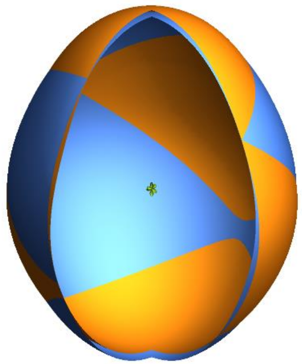
$$\beta_2 = \beta_{20} + \delta\beta_2$$
$$\langle\delta\beta_2\rangle, \langle\beta_{20}\gamma\rangle, \langle\beta_3\rangle \ll \beta_{20}$$

$$= R_{0i}\left\{1 + \sum_{\lambda=2,4,6} \beta_{\lambda 0} Y_{\lambda 0}(\theta')\right\}$$

$$+R_{0i}\left\{\beta_{20}\left[\frac{\delta\beta_2}{\beta_{20}}\cos\gamma + \cos\gamma - 1\right] Y_{20}(\theta') + \frac{(\beta_{20}+\delta\beta_2)\sin\gamma}{\sqrt{2}}\left[Y_{22}(\theta',\varphi') + Y_{2-2}(\theta',\varphi')\right] + \beta_3 Y_{30}(\theta') + \beta_{00}Y_{00} + \beta_{10}Y_{10}\right\}$$



Near sphere



Near axially deformed

# Potential expansion near axially deformed shape

$$V\big(r, R(\theta', \varphi')\big)$$

$$\approx V\big(r, R^{zero}(\theta')\big) + \frac{\partial}{\partial R} V\big(r, R\,(\theta', \varphi')\big)\Big|_{R^{zero}(\theta')} \delta R(\theta', \varphi'; \delta\beta_2, \gamma, \beta_3)$$

$$\approx V\big(r, R^{zero}(\theta')\big) + \frac{\nu_2(r)}{R_0 \beta_{20}} \delta R(\theta', \varphi'; \delta\beta_2, \gamma, \beta_3)$$

Rigid rotor: $V\big(r, R^{zero}(\theta')\big)$

Softness: $\frac{\nu_2(r)}{R_0 \beta_{20}} \delta R(\theta', \varphi'; \delta\beta_2, \gamma, \beta_3)$

$$R_{zero}(\theta') = R_{0i}\left\{1 + \sum_{\lambda=2,4,6} \beta_{\lambda 0} Y_{\lambda 0}(\theta')\right\}$$

$$\nu_2(r) = 2\pi \int_0^{\pi} V\big(r, R^{zero}(\theta')\big) Y_{20}(\theta') \sin\theta' \, d\theta'$$

**E.S. Soukhovitskiĩ et al, PRC 94 (2016) 64605**

# Coupled channels matrix elements

$$\langle i|V(r,\theta,\varphi)|f\rangle$$

$$= \sum_{K}^{I}\sum_{K'}^{I'} A_{K}^{I\tau}A_{K'}^{I'\tau'}\Bigg\{\sum_{\lambda=0,2,4,\ldots} \nu_\lambda(r)\langle IK||D_{;0}^{\lambda}||I'K\rangle A\left(ljI;l'j'I';\lambda J\frac{1}{2}\right)\delta_{KK'}$$

Rigid rotor

$$+\nu_2(r)\left\{\left[[\boldsymbol{\beta}_2]_{eff}+[\boldsymbol{\gamma}_{20}]_{eff}\right]\langle IK||D_{;0}^{2}||I'K\rangle A\left(ljI;l'j'I';2J\frac{1}{2}\right)\delta_{KK'}\right.$$

$\beta$- and $\gamma$-vibrations and stretching

$$+[\boldsymbol{\gamma}_{22}]_{eff}\langle IK||D_{;2}^{2}+D_{;-2}^{2}||I'K\rangle A\left(ljI;l'j'I';2J\frac{1}{2}\right)$$

$K = 2$ band coupling

$$+[\boldsymbol{\beta}_3]_{eff}\langle IK||D_{;0}^{3}||I'K\rangle A\left(ljI;l'j'I';3J\frac{1}{2}\right)\delta_{KK'}$$

Octupole coupling (negative parity band)

$$\left.+[\boldsymbol{\beta}_0]_{eff}\delta_{KK'}\delta_{II'}\delta_{jj'}\delta_{ll'}+[\boldsymbol{\beta}_1]_{eff}\langle IK||D_{;0}^{1}||I'K\rangle A\left(ljI;l'j'I';1J\frac{1}{2}\right)\delta_{KK'}\right\}\Bigg\}$$

Volume and center-of-mass position conservation corrections

# Effective deformations

$$[\boldsymbol{\beta_2}]_{\boldsymbol{eff}} = \left\langle n_i(\beta_2) \left| \frac{\delta\beta_2}{\beta_{20}} \right| n_f(\beta_2) \right\rangle \qquad [\beta_3]_{eff} = \left\langle n_i(\beta_3) \left| \frac{\beta_3}{\beta_{20}} \right| n_f(\beta_3) \right\rangle$$

$$[\gamma_{20}]_{eff} = \langle n_i(\gamma) | \cos\gamma - 1 | n_f(\gamma) \rangle \qquad [\gamma_{22}]_{eff} = \left\langle n_i(\gamma) \left| \frac{\sin\gamma}{\sqrt{2}} \right| n_f(\gamma) \right\rangle$$

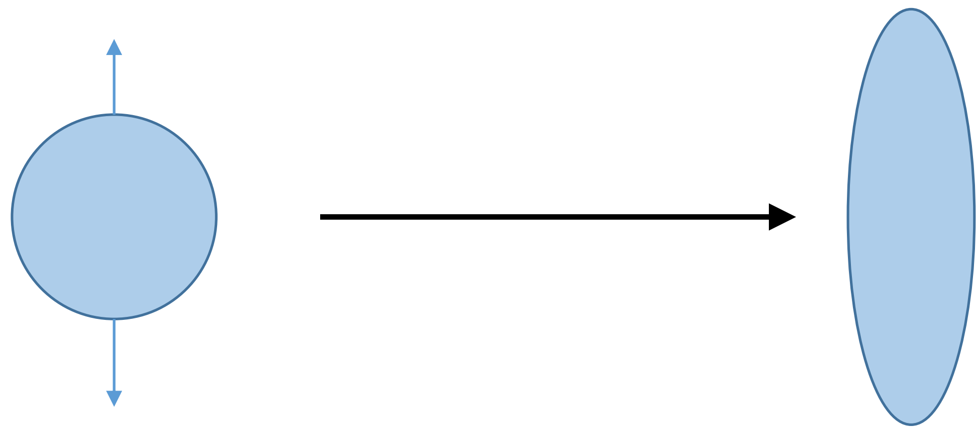
$$[\beta_2^2]_{eff} = \left\langle n_i(\beta_2) \left| \frac{\delta\beta_2^2}{\beta_{20}^2} \right| n_f(\beta_2) \right\rangle \qquad [\beta_3^2]_{eff} = \left\langle n_i(\beta_3) \left| \frac{\beta_3^2}{\beta_{20}^2} \right| n_f(\beta_3) \right\rangle$$

$$[\beta_0]_{eff} = -\frac{\beta_{20}}{\sqrt{4\pi}} \left[ 2[\beta_2]_{eff} + [\beta_2^2]_{eff} + [\beta_3^2]_{eff} \right]$$

$$[\beta_1]_{eff} = -\frac{\beta_{20}}{\sqrt{4\pi}} \sqrt{\frac{3}{7}} [\beta_3]_{eff} \left[ \frac{9}{\sqrt{5}} + \frac{4\beta_{40}}{\beta_{20}} \right]$$

**Effective deformations are defined by collective nuclear wavefunctions**

# Volume conservation term



$$R(\theta,\varphi) = R_0$$

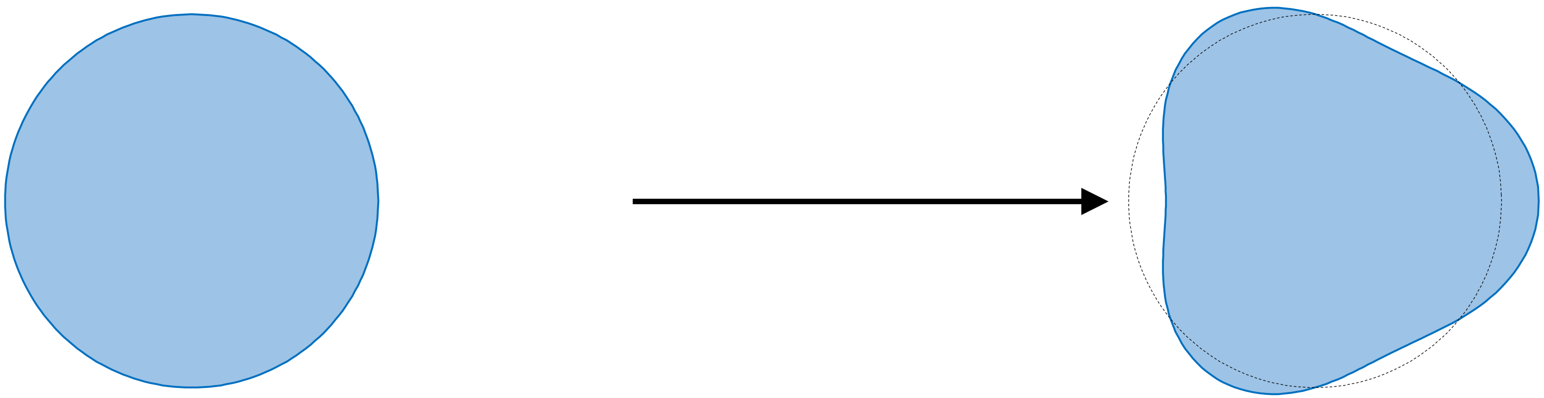
$$R'(\theta,\varphi) = R_0\left\{1 + \beta_{00}Y_{00} + \sum_{\lambda\mu}\beta_{\lambda\mu}Y_{\lambda\mu}(\theta,\varphi)\right\}$$

Compensation term

Incompressible nuclear matter: $V = V'$

$$\beta_{00} = -\frac{\sum\beta_\lambda^2}{\sqrt{4\pi}}$$

# Center-of-mass immobility term



$R(\theta, \varphi) = R_0$

$$R(\theta, \varphi) = R_0 \{1 + \beta_{00} Y_{00} + \beta_{10} Y_{10}(\theta) + \beta_{20} Y_{20}(\theta) + \beta_{22}[Y_{22}(\theta, \varphi) + Y_{2-2}(\theta, \varphi)] + \beta_{30} Y_{30}(\theta)$$

Compensation term

Immobile center of mass: $\vec{r}_{cm} = \vec{r}\,'_{cm}$

$$\beta_{10} = -\frac{1}{\sqrt{4\pi}} \sqrt{\frac{3}{7}} \beta_{30} \left( \frac{9}{\sqrt{5}} \beta_{20}^{eq} + 4\beta_{40} \right)$$

# Approaches to effective deformations

**Effective deformations as fitting parameters**

- Rough model to keep minimal number of parameters, only multiband coupling accounted (rigid rotor coupling within each band)
- Ambiguous description for nuclides with poor experimental data
- No additional knowledge needed

**E.S. Soukhovitskiĩ et al, PRC 94 (2016) 64605**

**Direct calculation**

- Nuclear structure model for soft deformed nuclei is needed
- More consistent result
- Gives all model effects

For even-even nuclides using SRM:

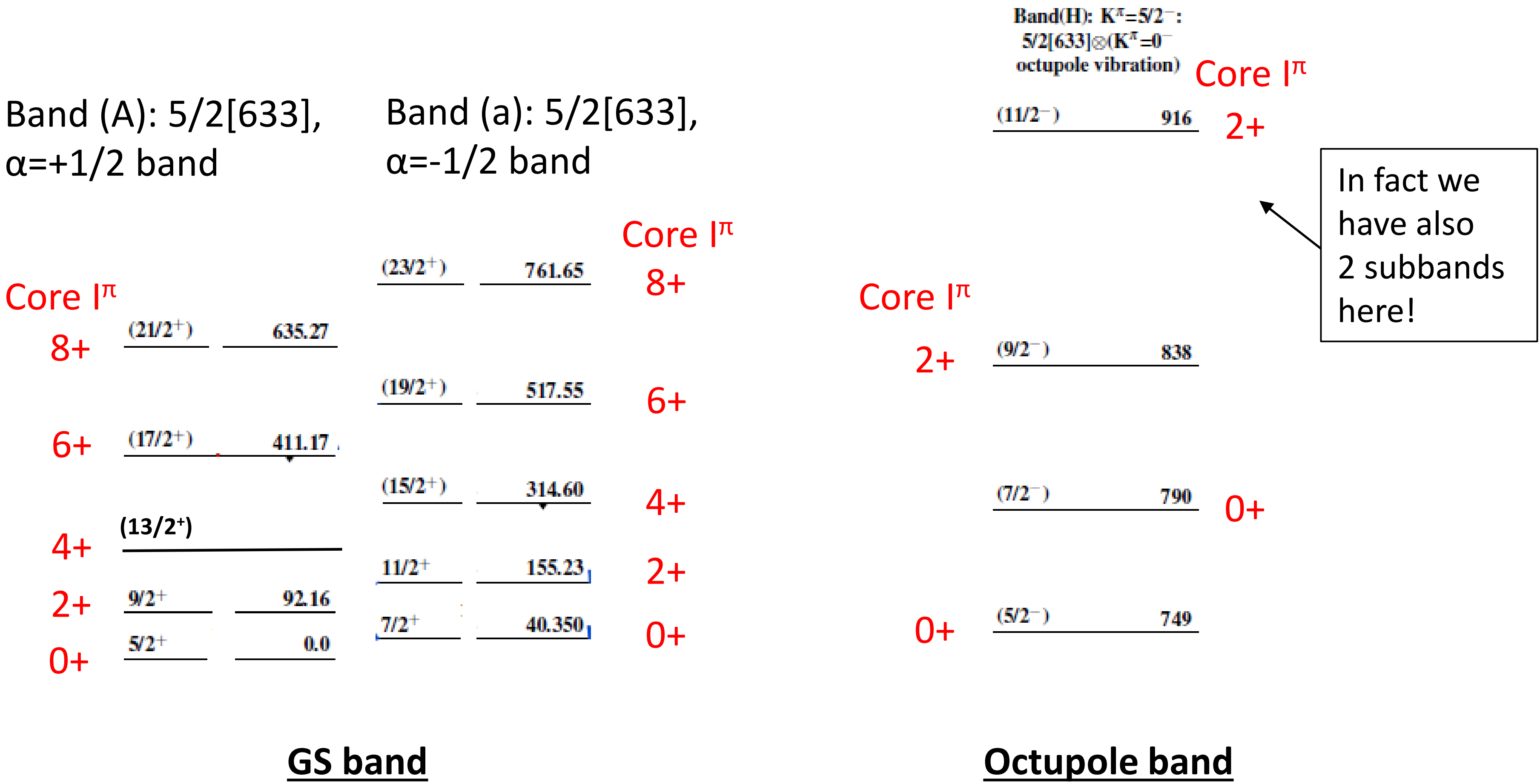
**D. Martyanov et al, EPJ Web Conf. 146 (2017) 12031 (ND2016)**

# Towards odd nuclides

We have soft-rotator model for even-even actinides, but no appropriate nuclear model (describing softness) for odd-A ones…

- Nuclear softness – collective effect, determined mainly by the even-even core, and varies smoothly from nucleus to nucleus
- $\langle \psi_{odd} | \beta | \psi_{odd} \rangle \approx \langle \psi_{core} | \beta | \psi_{core} \rangle$
- We may try to couple levels for bands built on single-particle state same as in GS
- We need to build appropriate core states

# Core states assignment ($^{233}U$ states from ENSDF)




Core state: no vibrational excitation, only rotation

Core state: first octupole excitation, rotation

# Regional potential for actinides

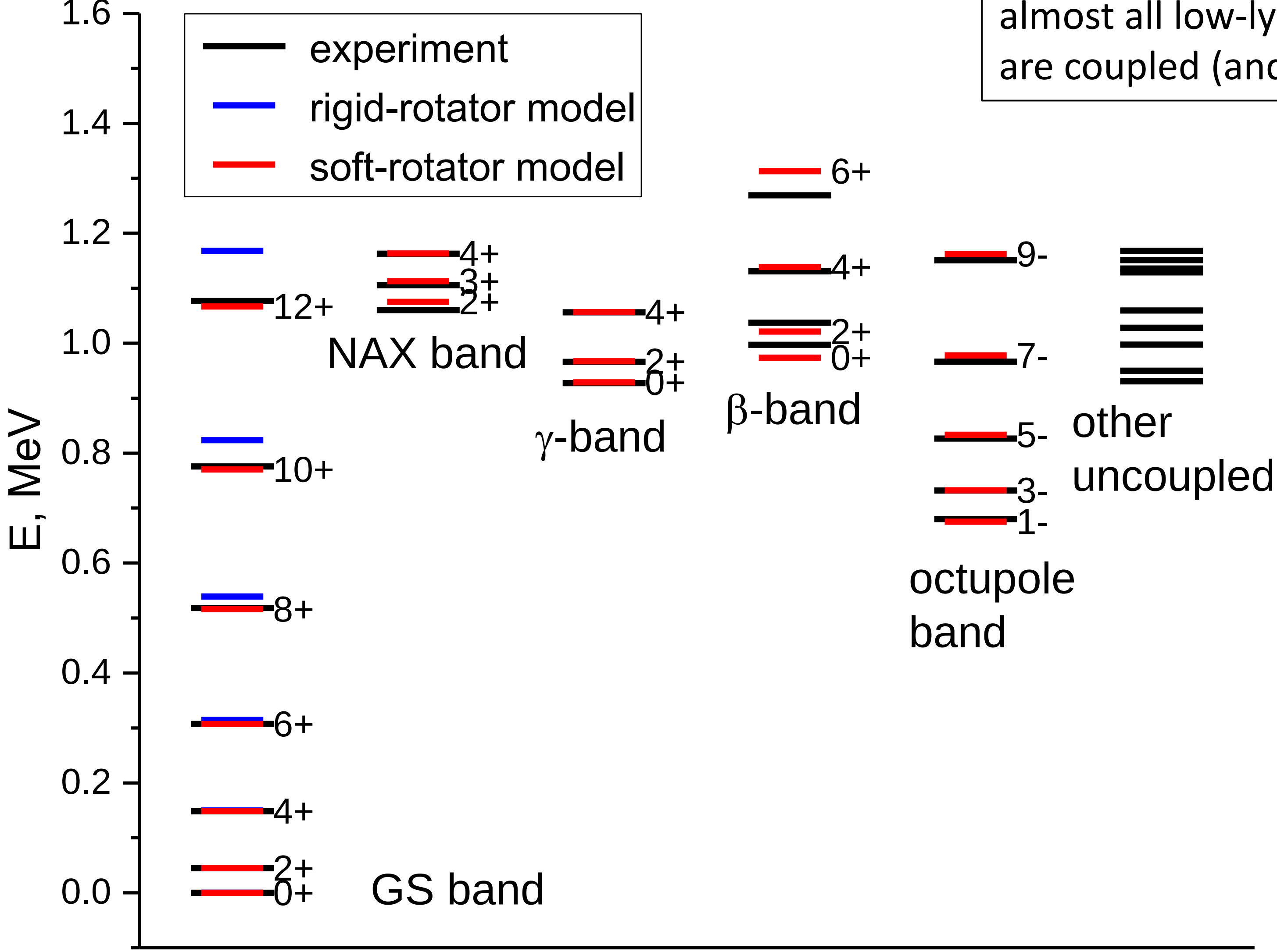
Algorithm,

coupling schemes,

parameters, etc.

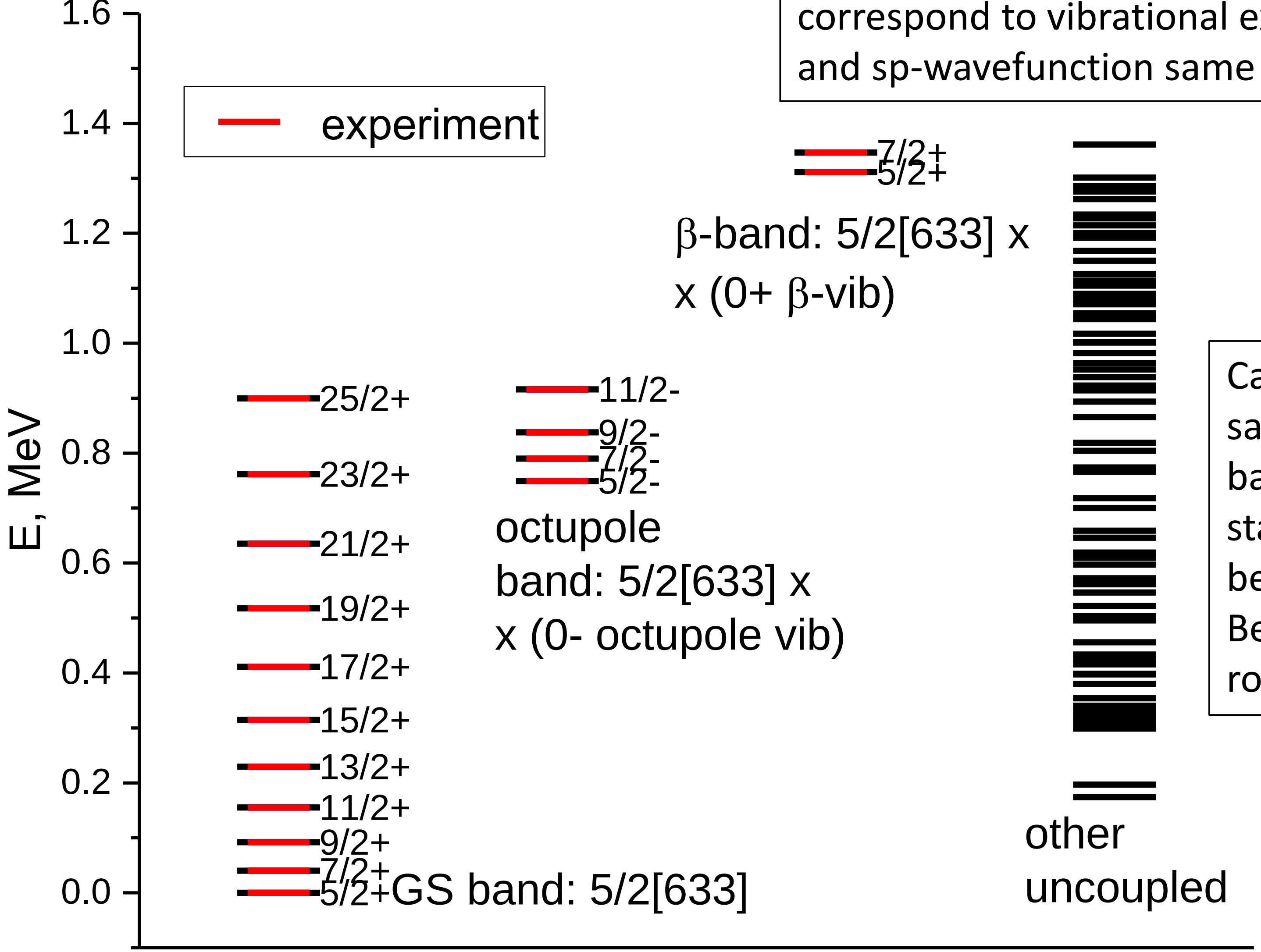
# $^{238}U$ coupling scheme

**<u>Saturated</u>** coupling scheme:
almost all low-lying levels
are coupled (and described by SRM)



# $^{233}$U coupling scheme

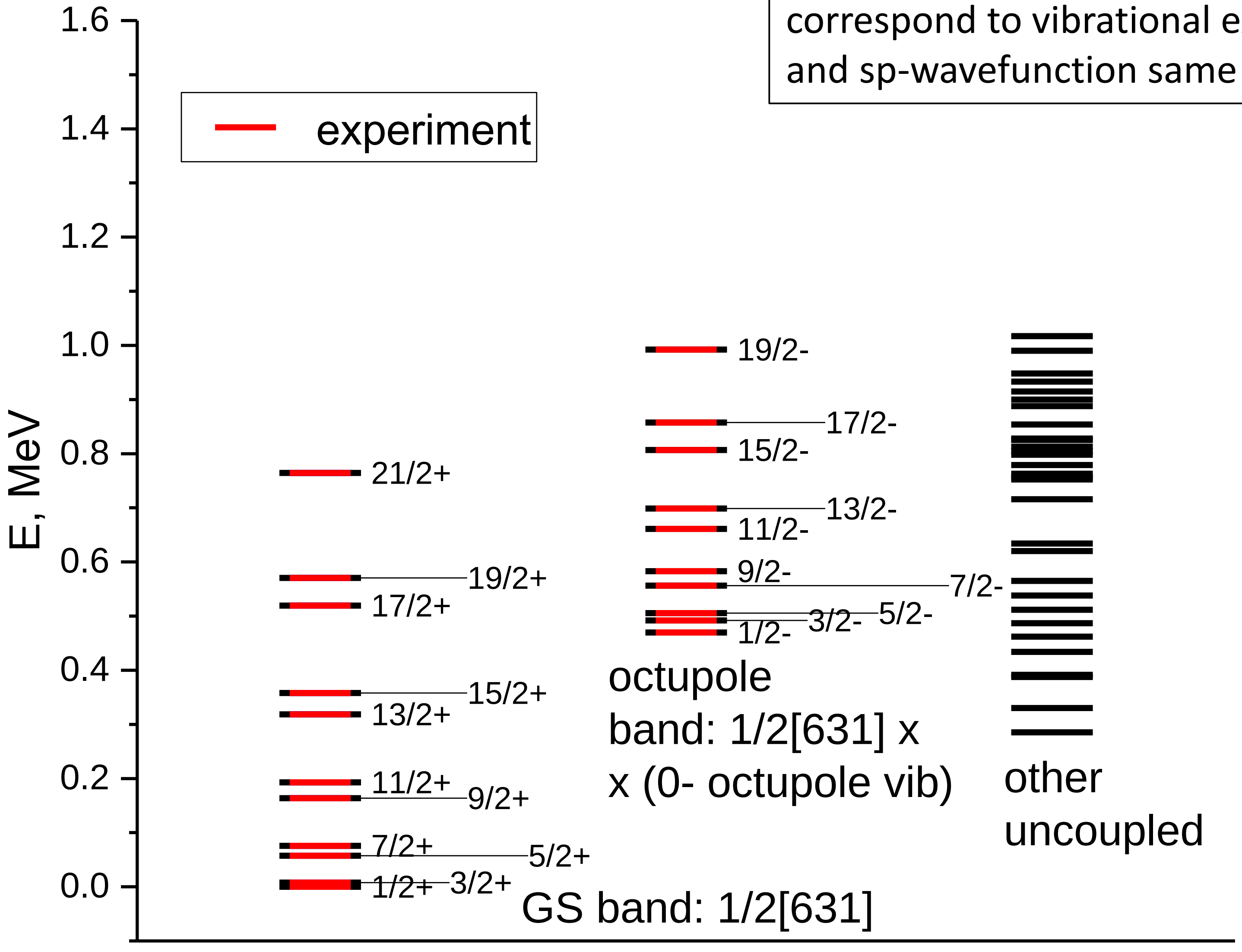
Only a few bands coupled: those that correspond to vibrational excitation of the core and sp-wavefunction same as in GS (ENDSF)



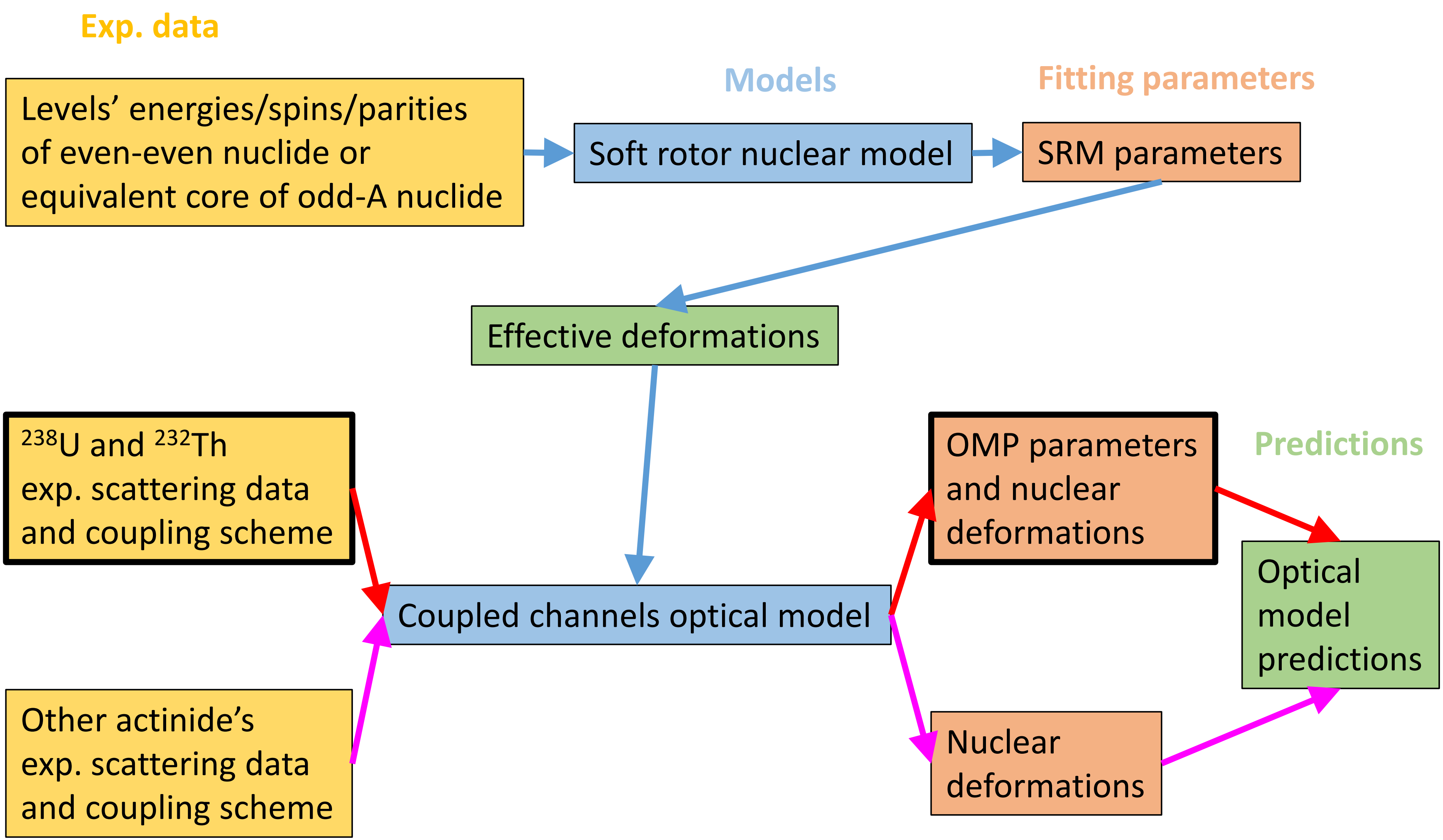

Can not speak about saturation, but bands based on other sp-states are assumed to be weakly coupled. Better than only main rotational band!

# $^{239}Pu$ coupling scheme

Only a few bands coupled: those that correspond to vibrational excitation of the core and sp-wavefunction same as in GS (ENDSF)



# Calculation algorithm



# Fitting parameters

- Nuclear softness and non-axiality (all soft-rotator model parameters) – from level structure, missing levels for coupling can be restored for even-even

- **Many experimental data** for optical model ($^{238}$U and $^{232}$Th) – fit optical potential parameters and deformations
- **Scarce experimental data** ($^{233}$U, $^{240}$Pu…) – fit only deformations ($\beta_{20}, \beta_{30}, \beta_4, \beta_6$) with fixed potential
- **Only strength functions or nothing** available ($^{246}$Cm…) – take deformations from global nuclear mass models, no additional fitting or only $\beta_{20}$ fit to reproduce SF

**WS4** deformations work better than **FRDM2012** for even-even actinides!

# Softness effects

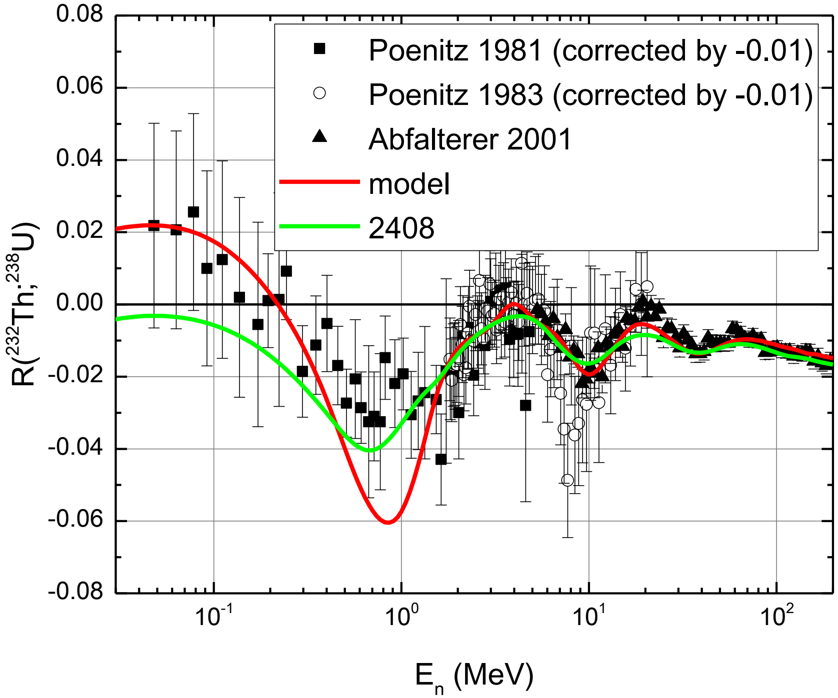
- Multiband coupling (for bands, corresponding to collective excitations)
- Nucleus stretching due to rotation (centrifugal forces)
- Additional monopole coupling due to account of volume conservation in vibrating nucleus

# OMP figure of merit: symmetrized total XS ratio for different nuclei

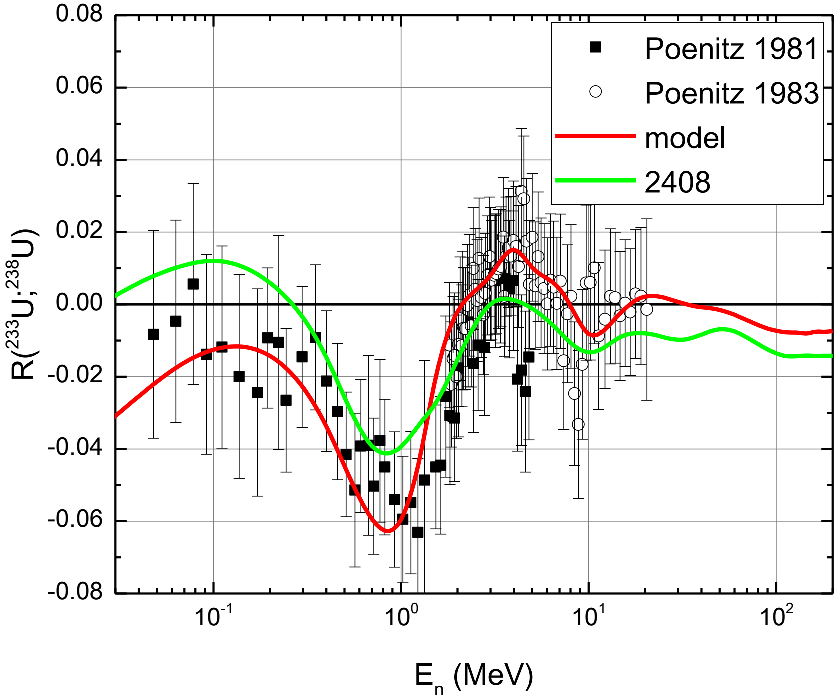
$$R(A,B) = \frac{1}{2}\frac{\sigma_A - \sigma_B}{\sigma_A + \sigma_B}$$

Many other data is fitted: total XS, (in)elastic angular distributions, (p,n), strength functions and scattering radii

**$^{232}$Th to $^{238}$U**



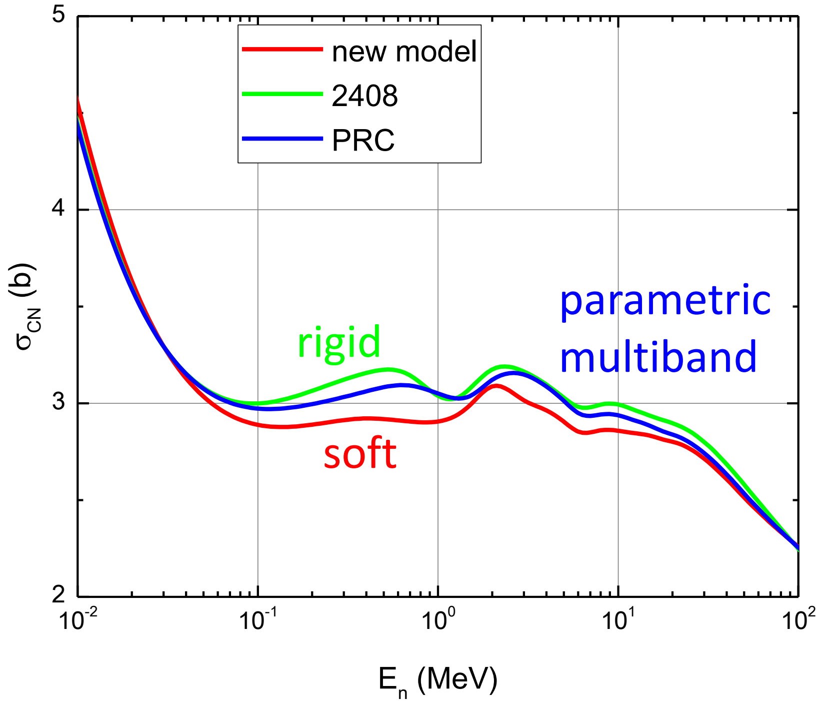

**$^{233}$U to $^{238}$U**



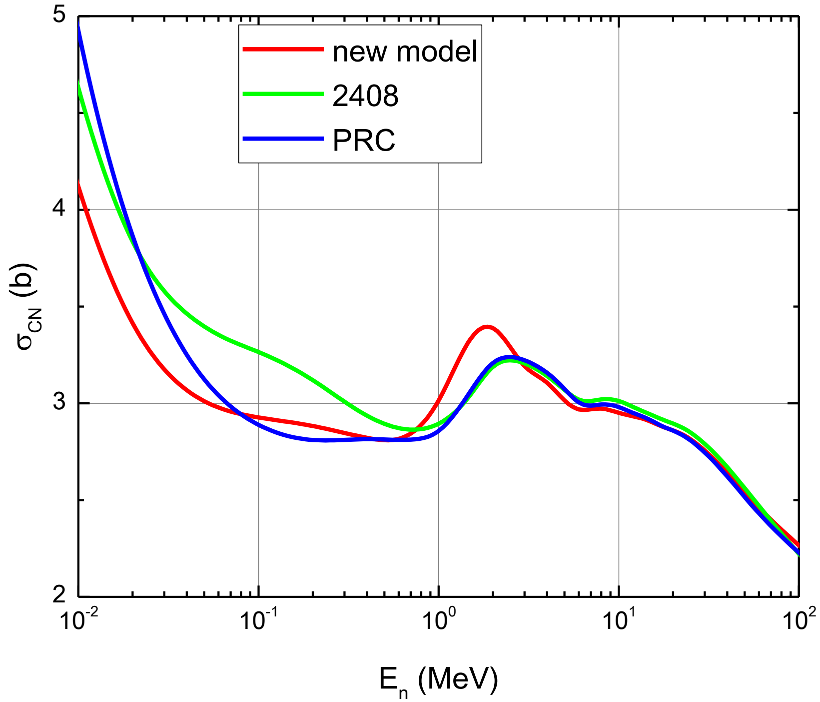
# Comparison with other potentials

**CN XS changes up to 0.3 barn between models fitted to the same data**

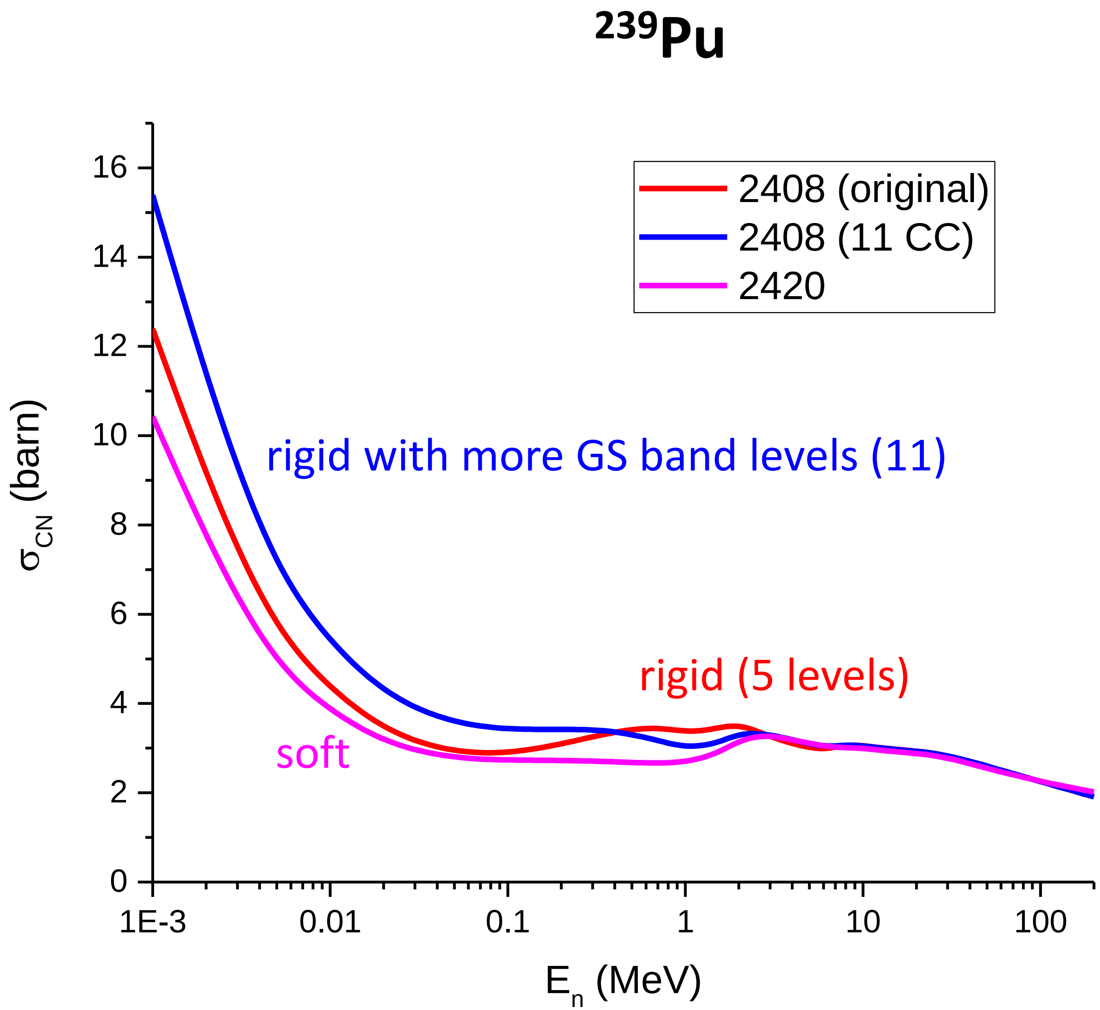
**$^{238}U$**




**$^{233}U$**



# Comparison with other potentials 2

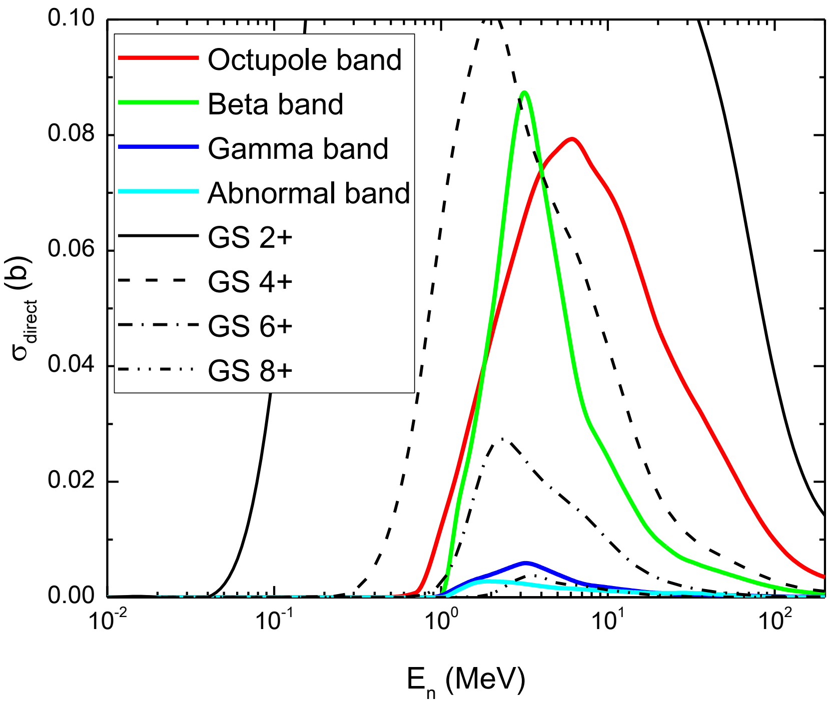



**Simple addition of GS band levels to the coupling scheme is not enough**

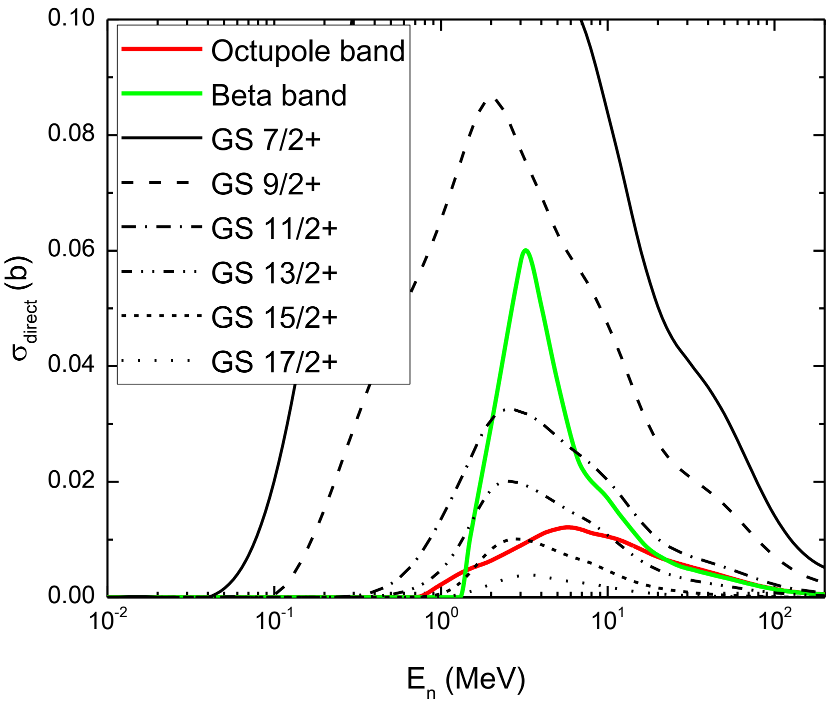
# Multiband coupling: Direct level excitation XS

**Other bands' impact is comparable to one from 2nd/3rd excited GS band level**

**$^{238}U$**



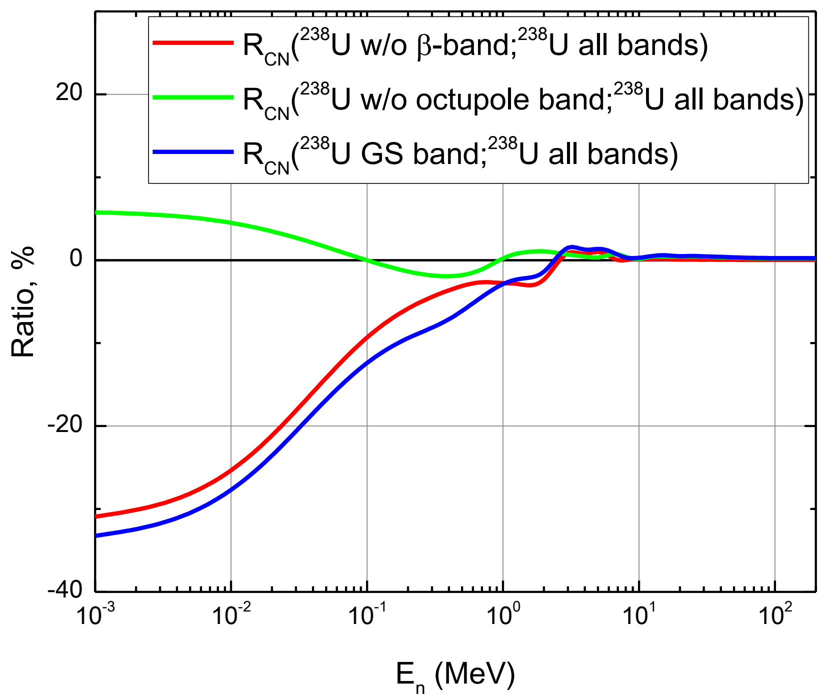

**$^{233}U$**



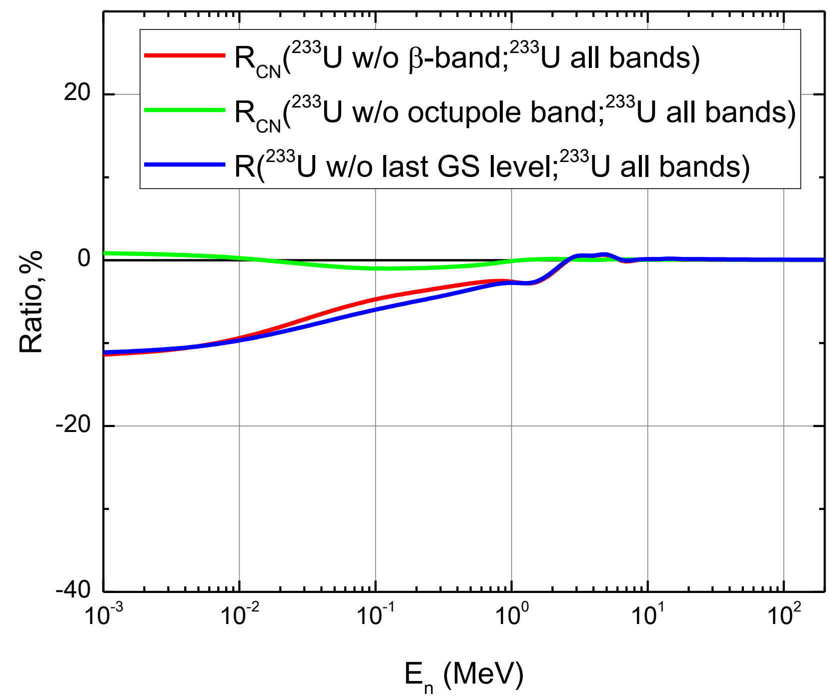
# Multiband coupling:
# CN XS change due to bands removal

**Large impact of *β*-vibrational states in the coupling scheme**

**$^{238}$U**

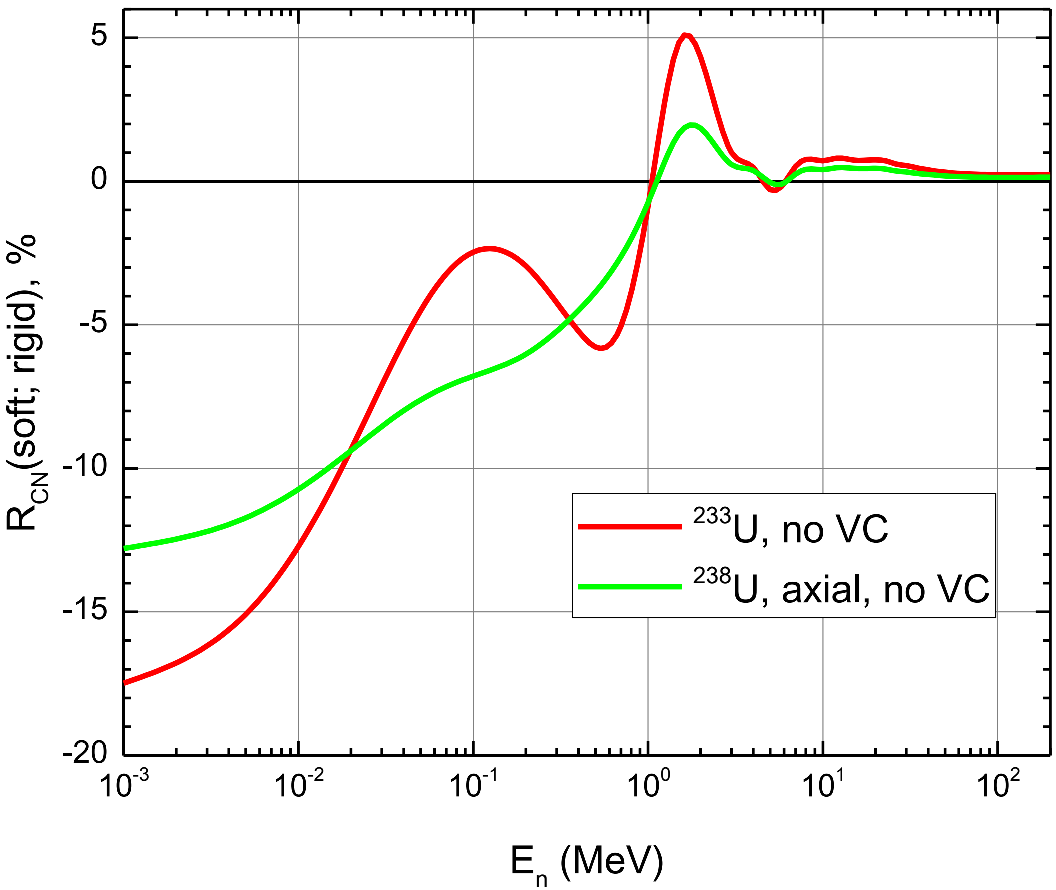



**$^{233}$U**



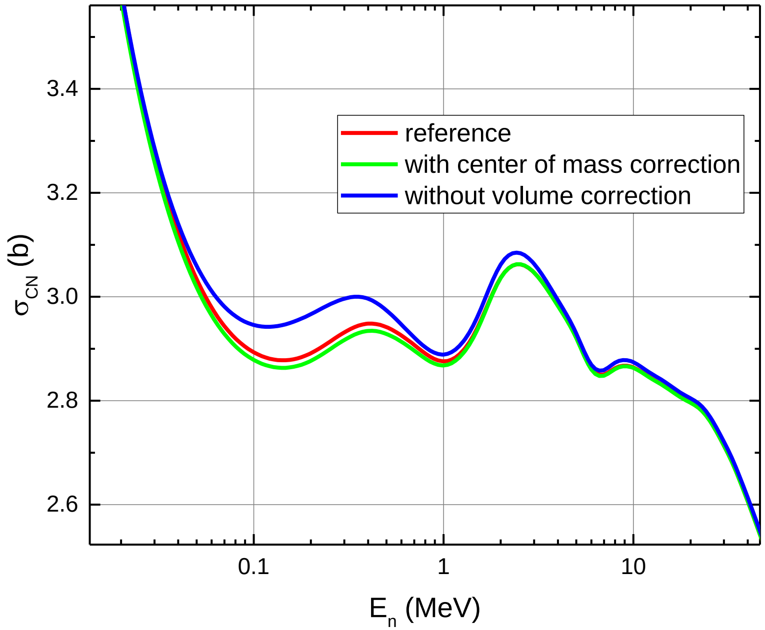
# Nucleus stretching: CN XS change

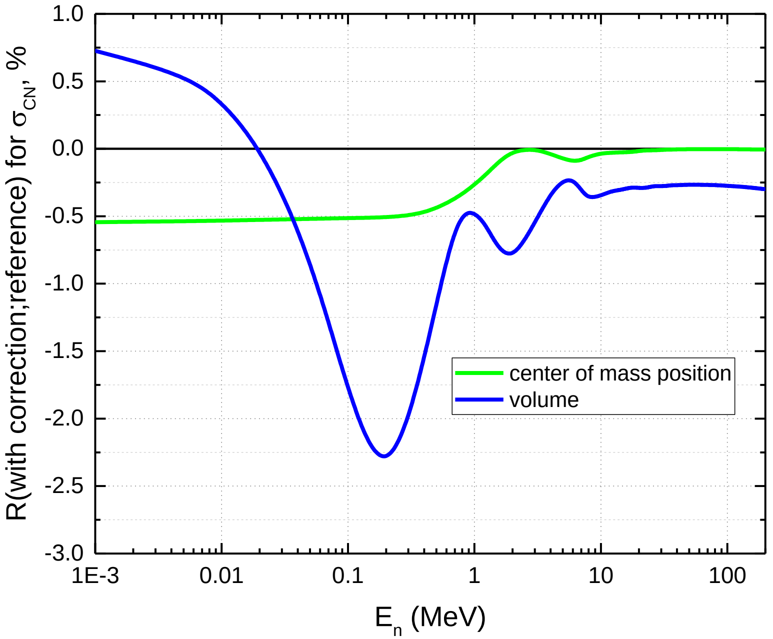
**Nucleus stretching gives large impact even then only GS-band levels are coupled**




Only GS band is coupled here, no non-axiality or volume conservation is accounted

# Volume and center-of-mass position corrections: CN XS change




**Volume conservation may be considered, center-of-mass correction is small**

# Considered nuclei

| | Bands/Levels | SF | Total | Angular |
|---|---|---|---|---|
| 238U | 5/21 | + | + | + |
| 232Th | 5/18(21) | + | + | + |
| 240pu | 5/18(20) | + | + | + |
| 242pu | 3(5)/10(20) | + | + | + |
| 228Th | 5/19(20) | | | |
| 230Th | 4(5)/16(20) | + | | |
| 232U | 5/18(20) | + | | |
| 234U | 5/18(20) | + | | |
| 236U | 4(5)/16(20) | + | | + |
| 238Pu | 5/15(20) | + | | |
| 244Pu | 2(5)/9(20) | + | | |
| 246Cm | 5/16(20) | + | | |
| 248Cm | 4(5)/14(20) | + | | |
| 250Cf | 5/13(20) | | | |
| 233U | 3/17 | + | + | |
| 237Np | 1/10 | + | + | |
| 235U | 1/11 | + | + | + |
| 239Pu | 2/19 | + | + | + |

# Summary

- Extended coupling is important for optical model calculations in even-even and odd-A actinides
- Obtained CCOMP for actinides:
  - Dispersive and Lane-consistent
  - Coupling to levels from multiple bands
  - Softness important even when single band is coupled
  - Saturation for even-even nuclei
  - Account of quadrupole triaxiality, octupole shape, volume and center-of-mass conservation

# Software

All calculations performed by two FORTRAN codes which have been being developed by E. Soukhovitskii and coworkers for many years:

- optical model code **OPTMAN** (optical potential fitting, cross-section calculations) with dispersive corrections as discussed with Quesada, Capote, Chiba et al.
- nuclear structure code **SHEMMAN** (soft-rotator model parameters fitting and levels prediction)

**OPTMAN**

New model implementation is validated by comparison with FRESCO

- recommended to use for SRM potentials compiled in the IAEA reference input parameter library (RIPL-3) for nuclear data evaluation
- used with the EMPIRE nuclear reaction model code for basic research and nuclear data evaluation (e.g. recent Fe-56 CIELO evaluation)

**RIPL-3: Capote, R. et al., Nucl. Data Sheets 110, 3107–3214 (2009)**
**OPTMAN and SHEMMAN: E. Sh. Sukhovitski et al., JAERI-Data/Code 2005-002 (2005)**
**Dispersive corrections: Soukhovitski, E. Sh. et al, JAEA-Data/Code--2008-025 (2008)**
**Soft description of Fe56: W. Sun et al, Nucl. Data Sheets 118, 191-194 (2014)**

# Thank you for the attention!