Soft rotator multiband optical model parameters for fissile actinides

<u>D.Martyanov</u>, R.Capote, J.M.Quesada Molina, S.Chiba

Outline

- Model overview
  - Dispersive Lane-consistent multiband coupled channels optical model for soft deformed nuclides
- Optical potential building routine
- Results
  - ^{239}Pu and ^{233}U (multiband, many data to fit)
  - ^{235}U and ^{235m}U (isomeric state)
  - Pu241 (scarce experimental data)

Model feature 1: Dispersive relation

Casuality → Kramers–Kronig relations:

- Energy-dependent imaginary part of the potential yields additional (polarization) term to the real part:

$$\Delta V(E) = \frac{1}{\pi}\mathcal{P}\int_{-\infty}^{\infty}\frac{W(E')}{E'-E}dE'$$

- Physically realistic and constraint energy dependence of the potential
- Used energy dependence allows analytical expressions for $\Delta V(E)$
- **Result - better constrained model!**

Model feature 2: Lane consistency

Isospin-symmetric form of optical potential (only nuclear part without Coulomb):

- $V_{pp} = V_0 + \frac{N-Z}{4A} V_1,$
- $V_{nn} = V_0 - \frac{N-Z}{4A} V_1$
- $V_{pn} = \frac{\sqrt{N-Z}}{2A} V_1$

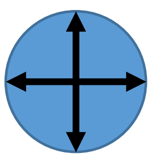
Allows same parameterization for direct neutron, proton scattering and (p,n)-reactions

Model feature 3: Extended coupling for soft deformed targets

Optical model for soft deformed nuclei

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

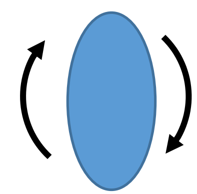
Soft spherical nucleus
(vibrational excitations)



Taylor expansion near sphere

Explicit deformations → vibrations
bad convergence for big deformations

Rigid deformed nucleus
(rotational excitations)



Static multipolar expansion

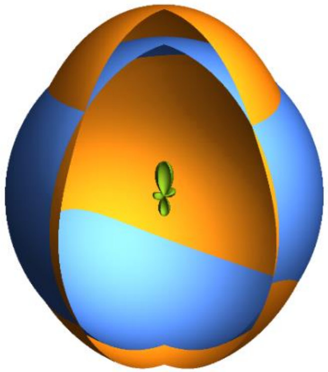
Good convergence for big static deformations
no explicit deformations → no vibrations!

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

Solution: Taylor expansion near axial static form

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

$$= R_{0i}\left\{1 + \sum_{\lambda=2,3;even\,\mu} \beta_{\lambda\mu} Y_{\lambda\mu}(\theta',\varphi') + \sum_{\lambda=4,6} \beta_{\lambda 0} Y_{\lambda 0}(\theta')\right\}$$



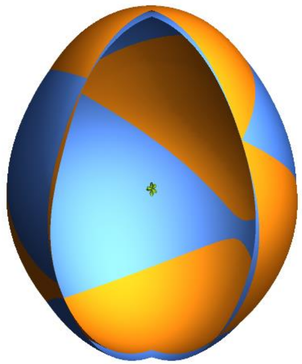
Near sphere

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

$$\beta_2 = \beta_{20} + \delta\beta_2$$
$$\langle\delta\beta_2\rangle, \langle\beta_{20}\gamma\rangle, \langle\beta_3\rangle, \langle\beta_{00}\rangle \ll \beta_{20}$$

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

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



Near axially deformed

Potential expansion near axially deformed shape

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

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

$$\approx \boxed{V\big(r, R^{zero}(\theta')\big)} + \boxed{\frac{v_2(r)}{R_0\beta_{20}} \delta R(\theta', \varphi'; \delta\beta_2, \gamma, \beta_3)}$$

Rigid rotor

Softness

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

$$v_2(r) = 2\pi \int_0^{\pi} V\big(r, R^{zero}(\theta')\big) Y_{20}(\theta') \sin\theta' \, d\theta'$$

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Coupled channels matrix elements

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

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

Rigid rotor

$$+ v_2(r)\left\{\left[[\boldsymbol{\beta_2}]_{eff} + [\boldsymbol{\gamma_{20}}]_{eff}\right]\langle IK||D_{;0}^{2}||I'K\rangle A\left(ljI;l'j'I';2J\frac{1}{2}\right)\delta_{KK'}\right.$$

β- and γ-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)

$$\left. + [\boldsymbol{\beta_0}]_{eff}\delta_{KK'}\delta_{II'}\delta_{jj'}\delta_{ll'}\right\}\Bigg\}$$

Volume conservation correction

Effective deformations

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

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

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

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

Effective deformations are defined by collective nuclear wavefunctions
Soft rotator model (nuclear structure) is needed here!

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” (spin)

Major implications of extended couplings

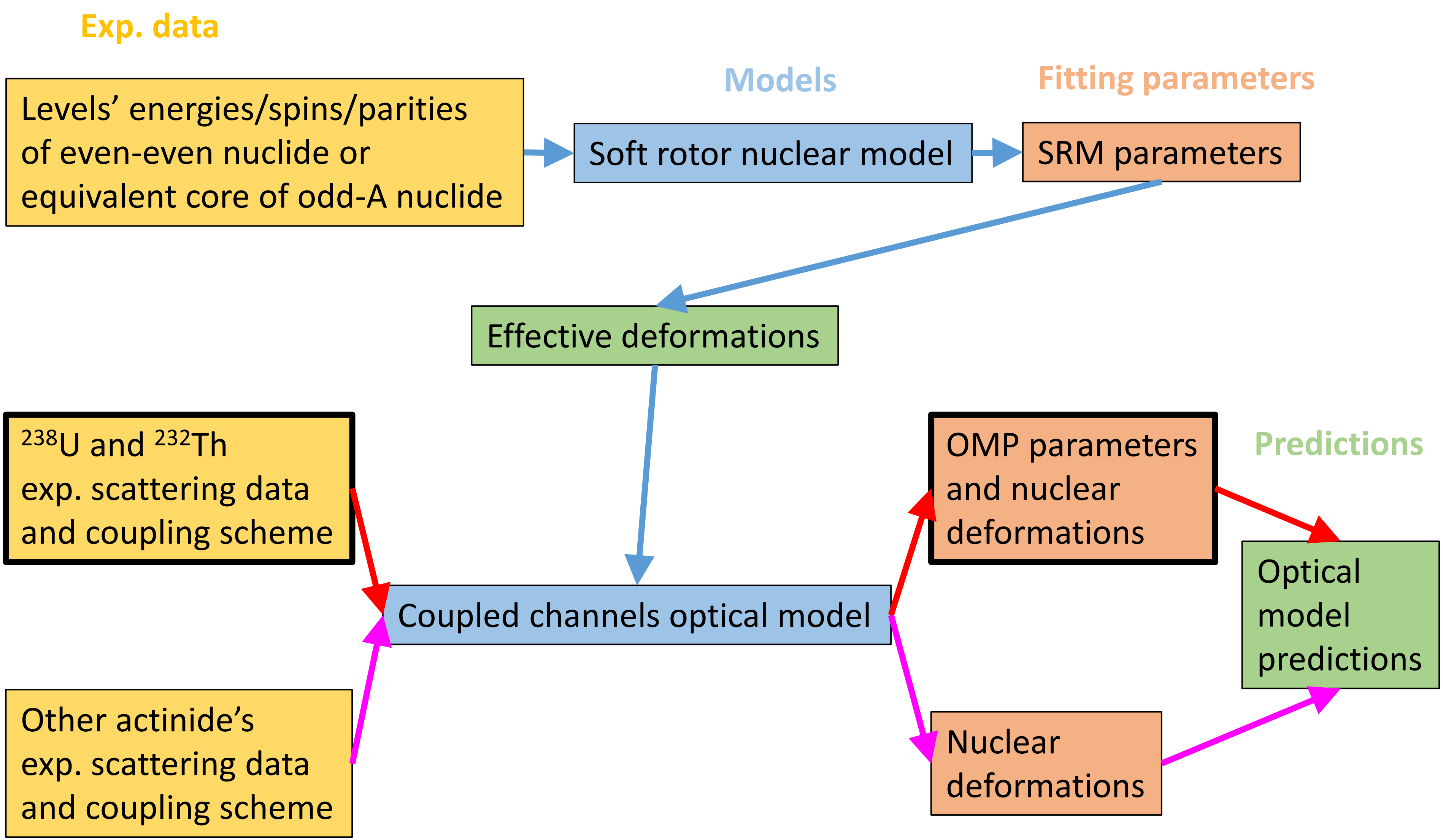
- **Saturated coupling (at least for even-even nuclides)**

- **Multiband coupling (for bands, corresponding to collective excitations)** → impact comparable to one from 2nd or 3rd levels from main rotational band

- **Nucleus stretching due to rotation (centrifugal forces)** → alter predictions even when only levels from main rotational band are coupled

- **Additional monopole coupling due to account of volume conservation in vibrating nucleus** → additional changes of predicted cross sections

Regional potential for actinides: calculation algorithm



Fitting parameters

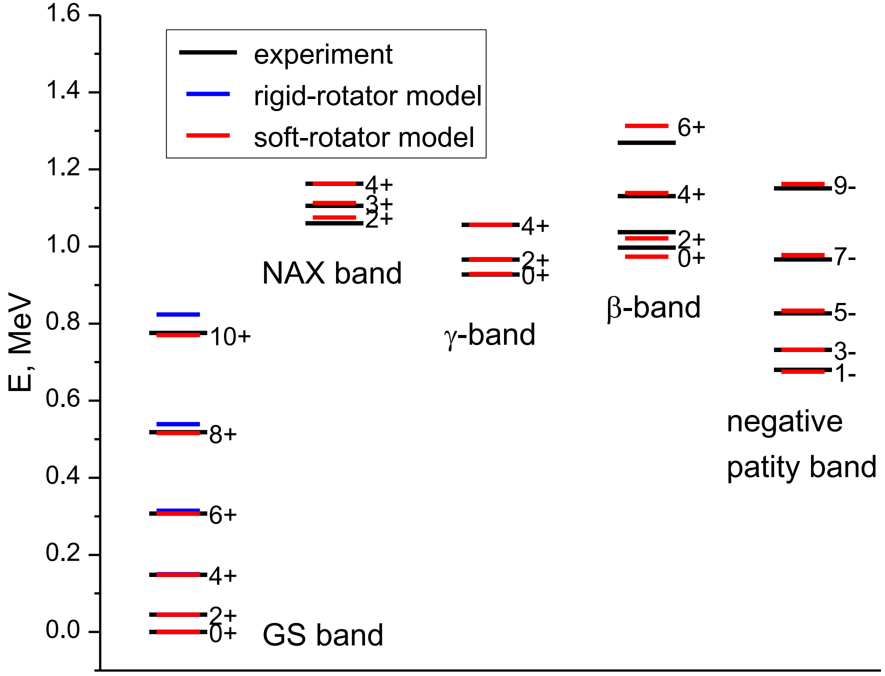
- Nuclear softness and non-axiality (all soft-rotator model parameters) – from level structure, missing levels for coupling can be restored for even-even

- **Many experimental data** for optical model (^{238}U and ^{232}Th) – fit optical potential parameters and deformations
- **Scarce experimental data** (^{233}U, ^{239}Pu…) – fit only deformations ($\beta_{20}, \beta_{30}, \beta_4, \beta_6$) with fixed potential
- **Only strength functions or nothing** available (^{241}Pu…) – take deformations from global nuclear mass models, no additional fitting or only β_{20} fit to reproduce SF

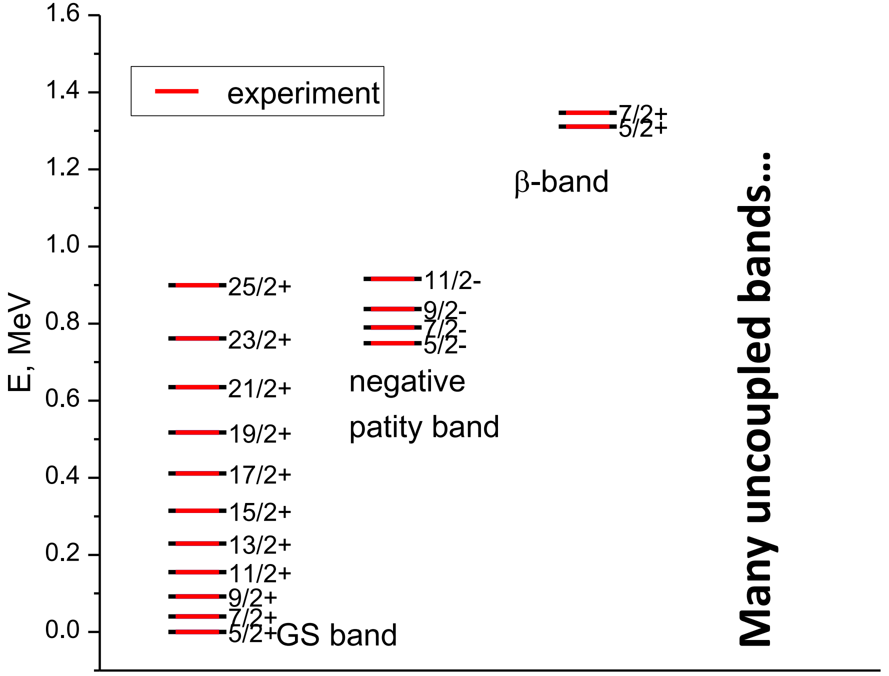
WS4 deformations work better than **FRDM2012** for even-even actinides!

Coupling scheme

^{238}U



^{233}U



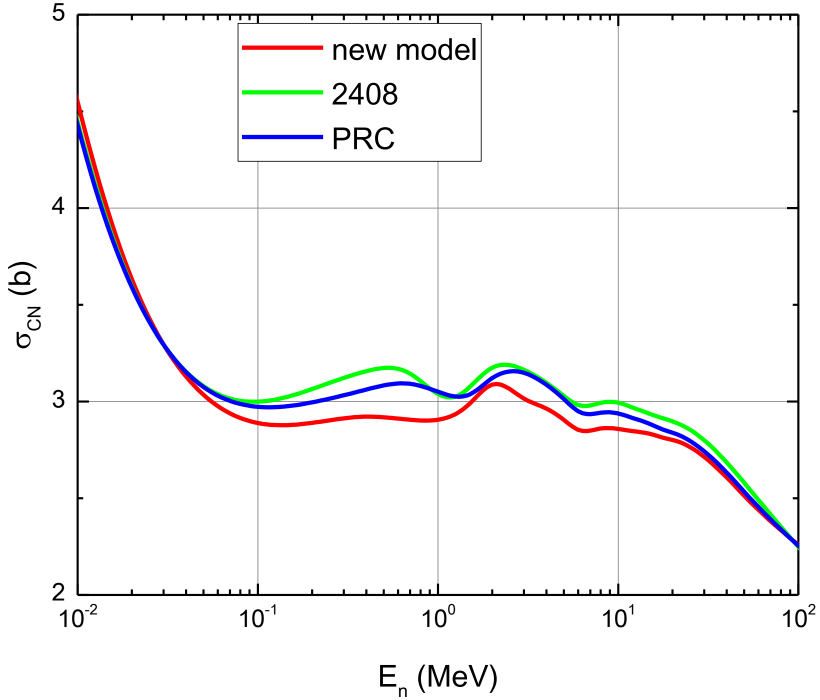
Saturated coupling scheme:
almost all low-lying levels
are coupled (and described by SRM)

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

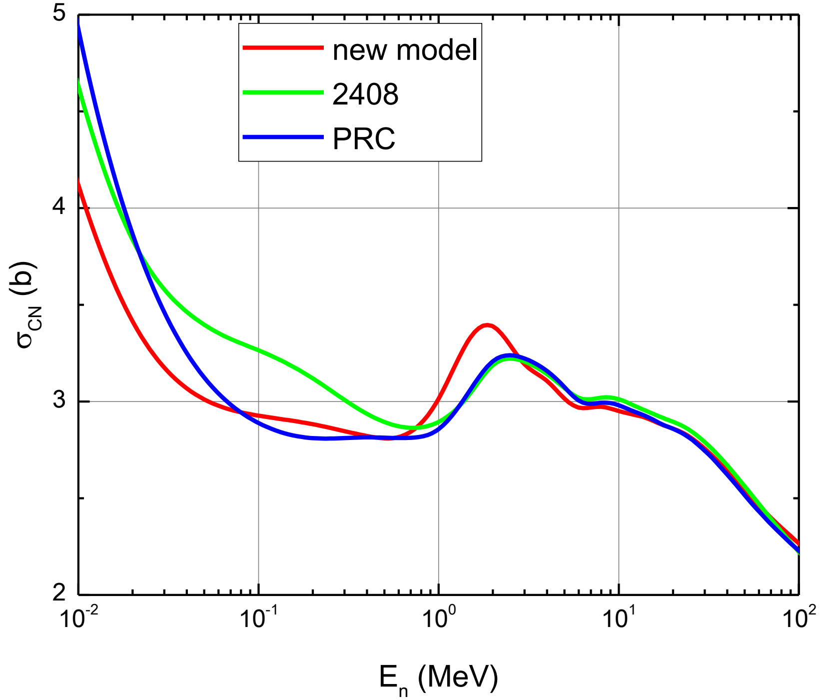
Comparison with other potentials

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

^{238}U

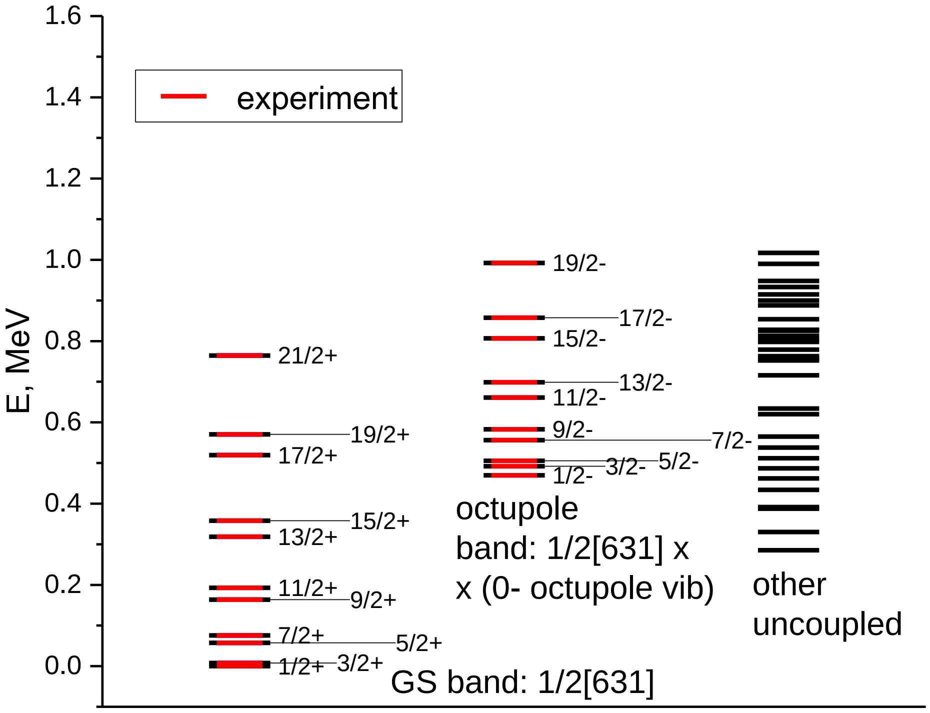


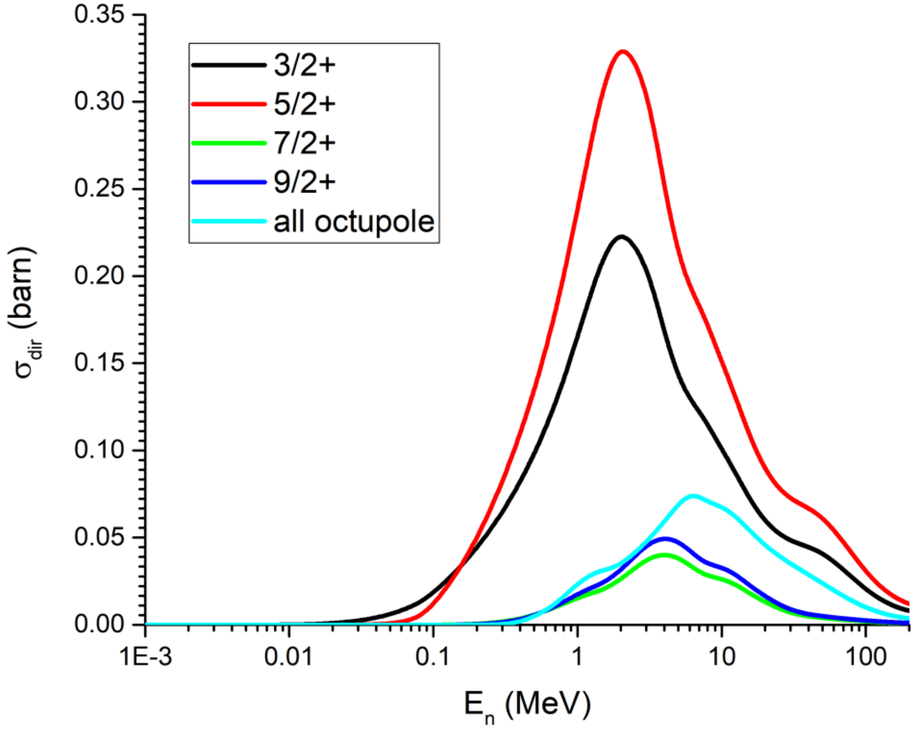
^{233}U



^{239}Pu: direct level excitation

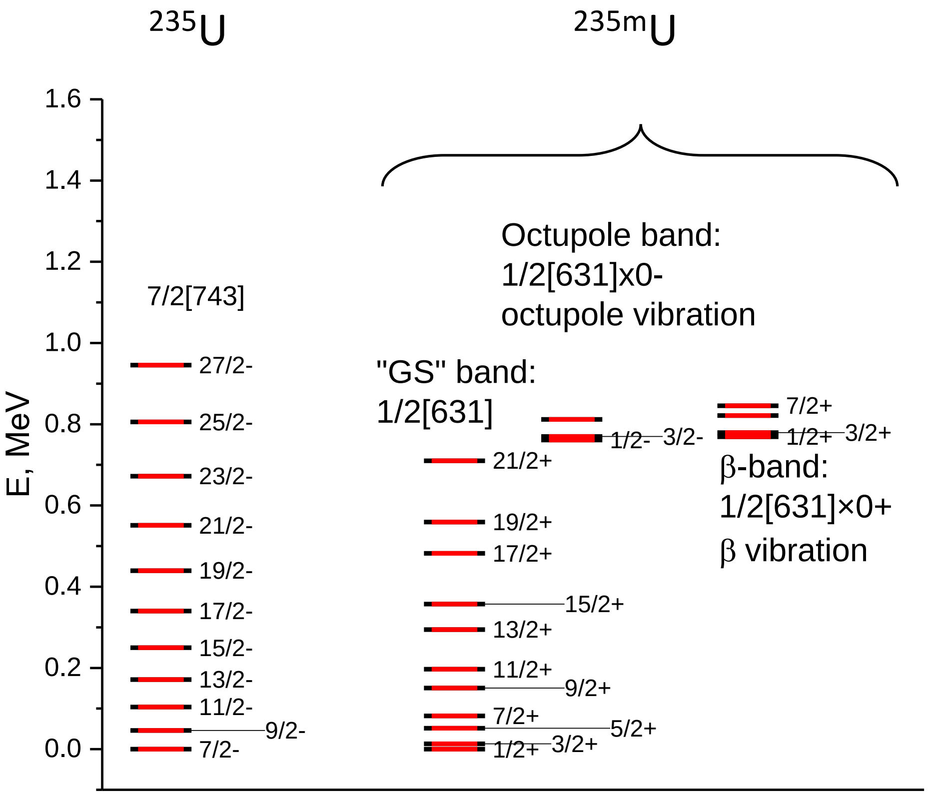
Other bands' impact is comparable to one from 2nd/3rd excited GS band level

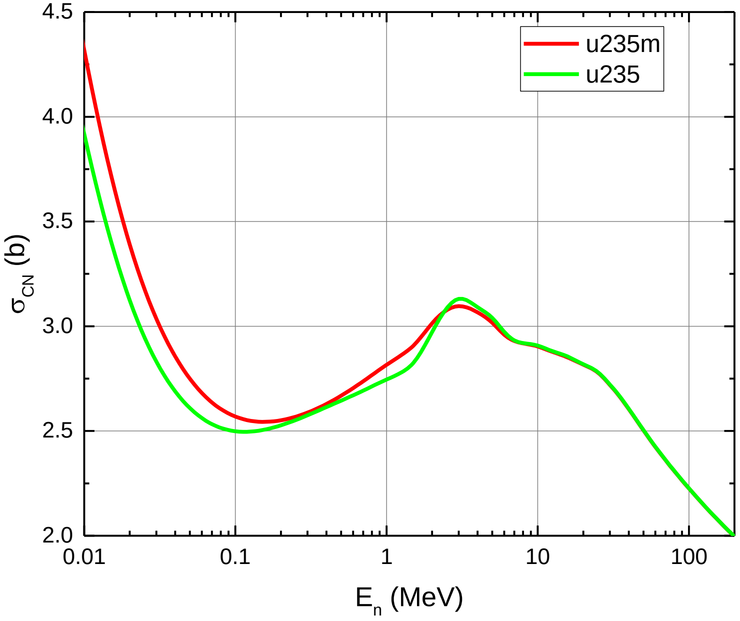




^{235}U and ^{235m}U: change of CN cross section

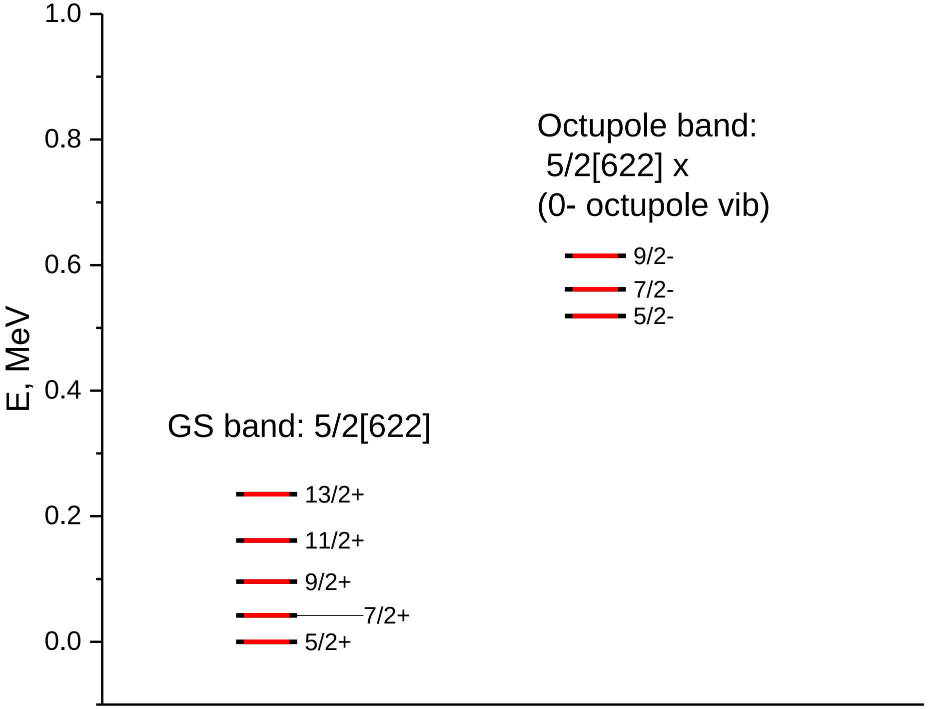
Only one band coupled for ^{235}U but softness is still important
Isomeric state has other coupled levels → cross section changed

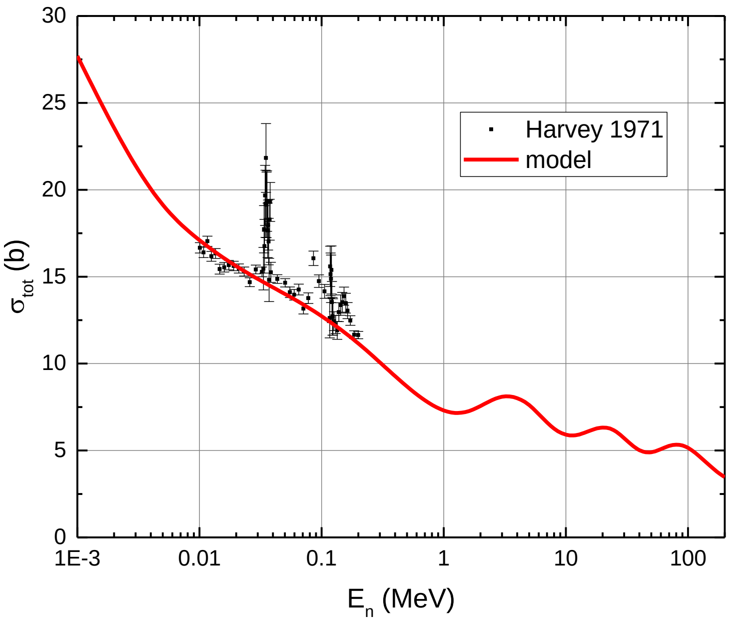




^{241}Pu: total CS

We fit only β_2 to reproduce S_0 value, but scarce URR total CS is fairly reproduced





Summary

- Dispersive Lane-consistent coupled channels optical model with extended couplings is described
- Softness and multiband coupling are important to reach accurate calculations results for both even-even and odd-A nuclides
- Suggested method to calculate optical model predictions for odd-A, poorly investigated nuclei or isomeric states is demonstrated on $^{233,235,235m}U$ and $^{239,241}Pu$

Thank you for your attention!

Backup slides

Software

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

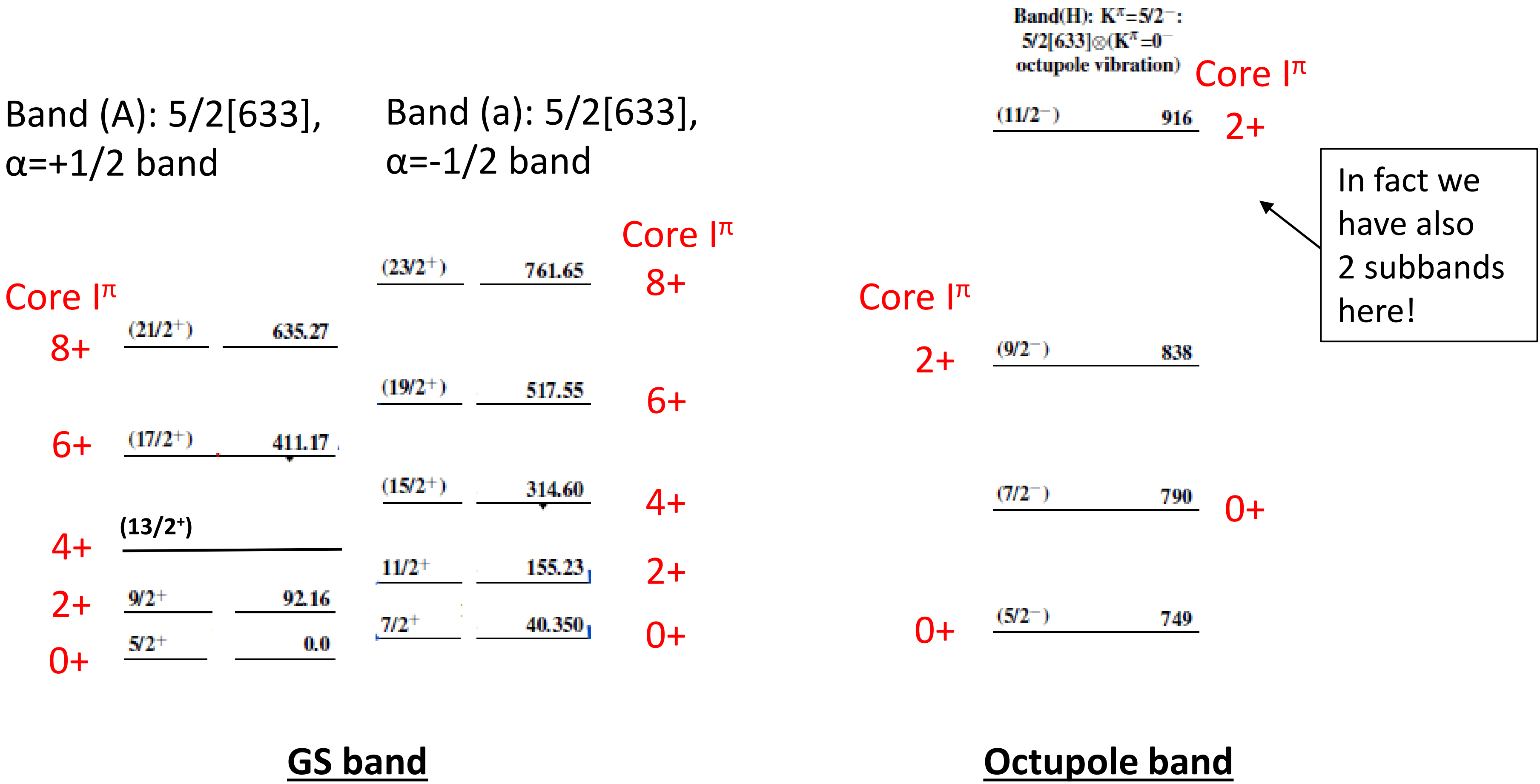
- optical model code **OPTMAN** (optical potential fitting, cross-section calculations) with dispersive corrections as discussed with Quesada, Capote, Chiba et al.
- nuclear structure code **SHEMMAN** (soft-rotator model parameters fitting and levels prediction)

OPTMAN

- 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)

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



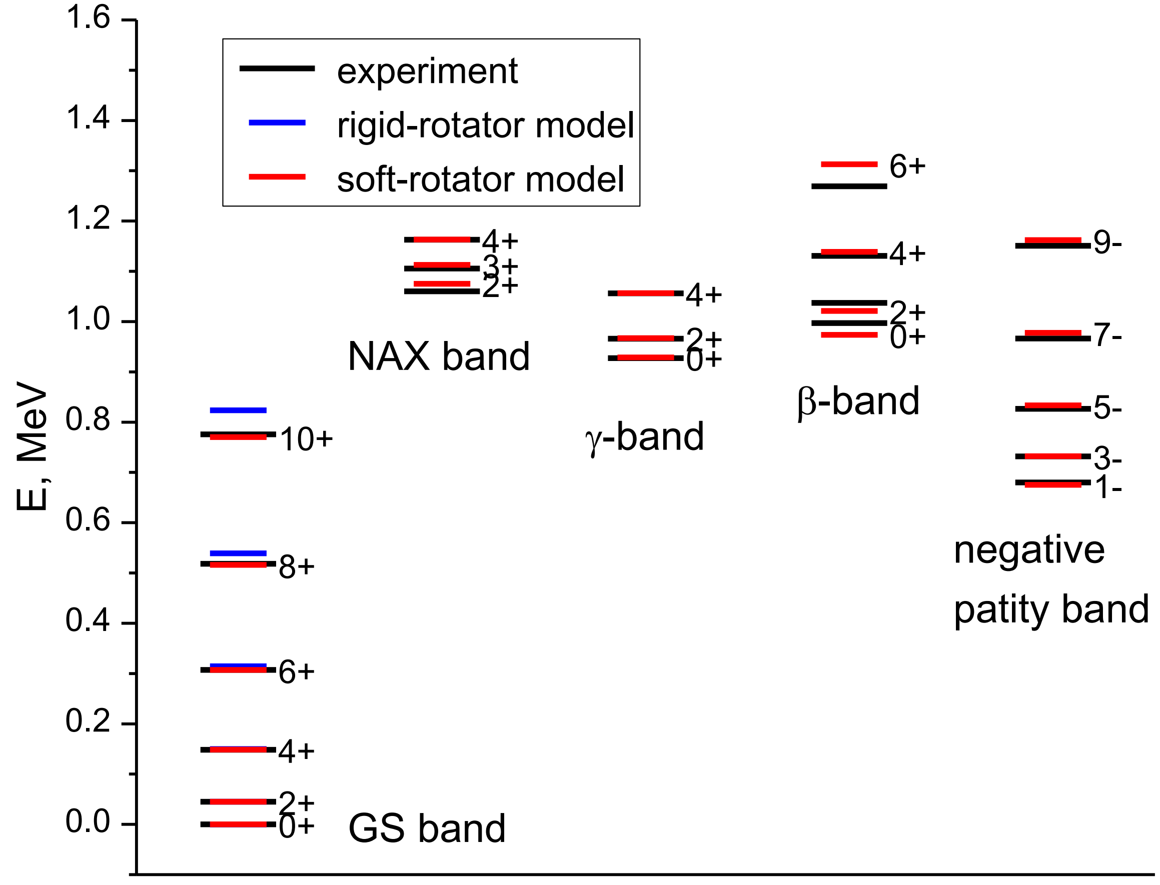
Core state: no vibrational excitation, only rotation

Core state: first octupole excitation, rotation

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.

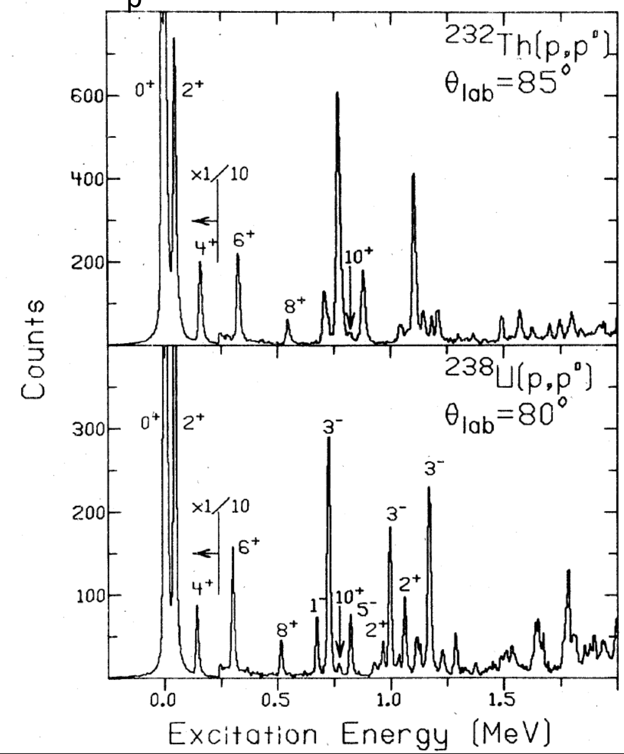
^{238}U



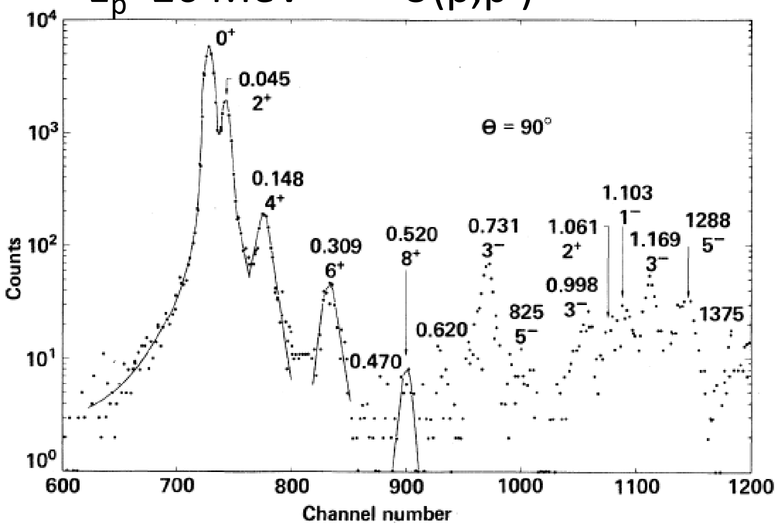
Are other bands important?

No nucleon scattering data for other-than-GS band in EXFOR for actinides
…
but there are clear evidences of levels from **<u>other bands</u>** in some proton inelastic scattering experimental works

E_p=35 MeV



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



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

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

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)

Recent dispersive OMP development

Dispersive Lane-consistent OMP for deformed nuclei (actinides):

- **2008** – rigid rotor regional potential (RIPL 2408)
- **2015** – parametric multiband coupling, rigid intra-band coupling; good description of even-even, but only sp-excitations were used for odd-A nuclides (PRC 2016)
- **2016** – soft rotor description of even-even nuclei (ND 2016)
- **2019** – approach to soft odd-A nuclides: collective excitation of the core, not sp-states; detailed analysis of softness effects (ND 2019)

Towards other odd-A actinides

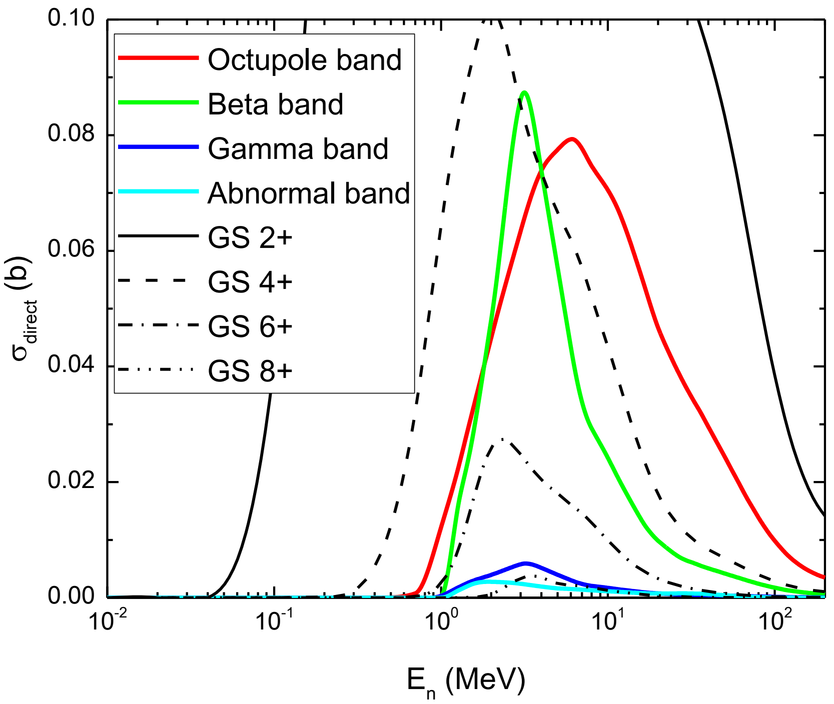
How to evaluate many important nuclides with no identified bands built on **only** vibrational excitation of the core (e.g. ^{235}U)?

- Make calculation with only GS band levels coupled, but using soft model – results should be more reliable than for rigid rotor (primary calculations are done for ^{235}U and ^{239}Pu)
- Use more sophisticated nuclear structure models to identify corresponding states
- Construct these states using evaluations of the core (corresponding even-even nucleus) excitations and correct level/spin sequence for an odd-A nuclide

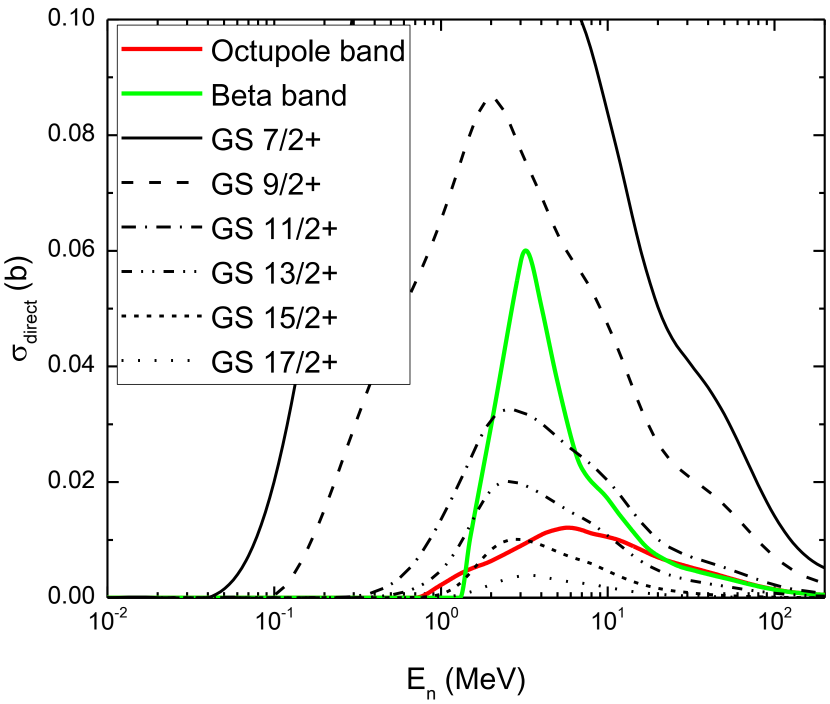
Multiband coupling 1: Direct level excitation XS

Other bands' impact is comparable to one from $2^{nd}/3^{rd}$ excited GS band level

^{238}U



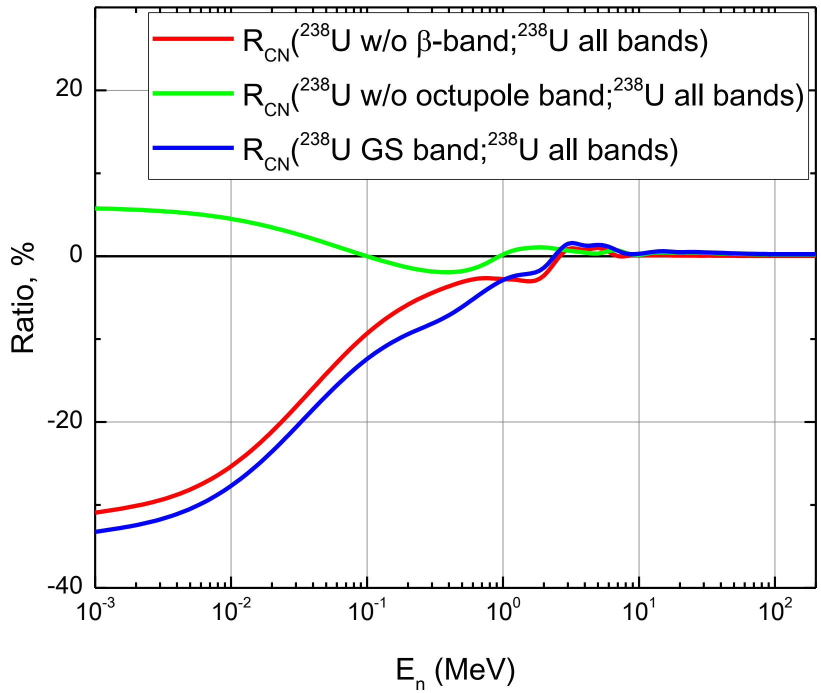
^{233}U



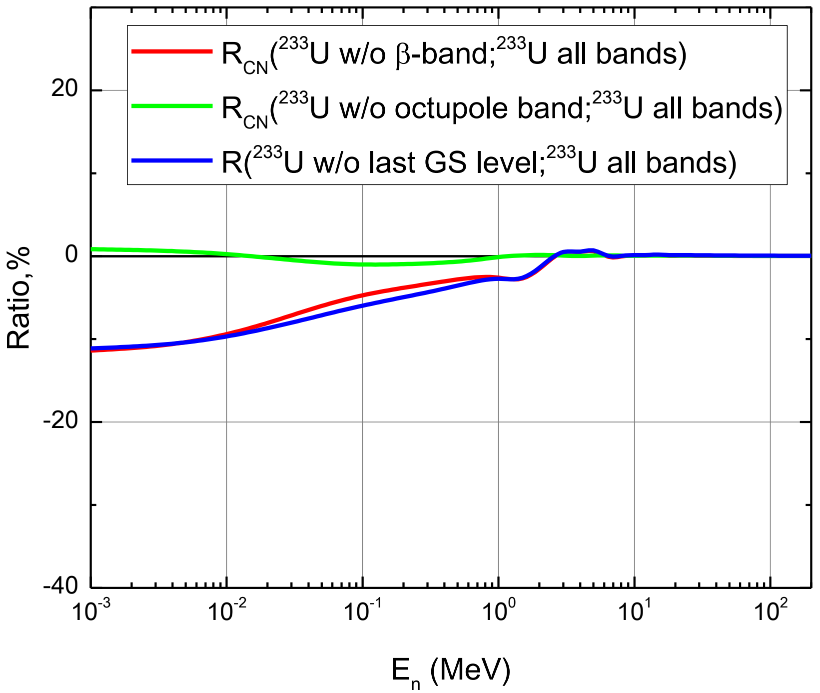
Multiband coupling 2: CN XS change due to bands removal

Large impact of β-vibrational states in the coupling scheme

^{238}U

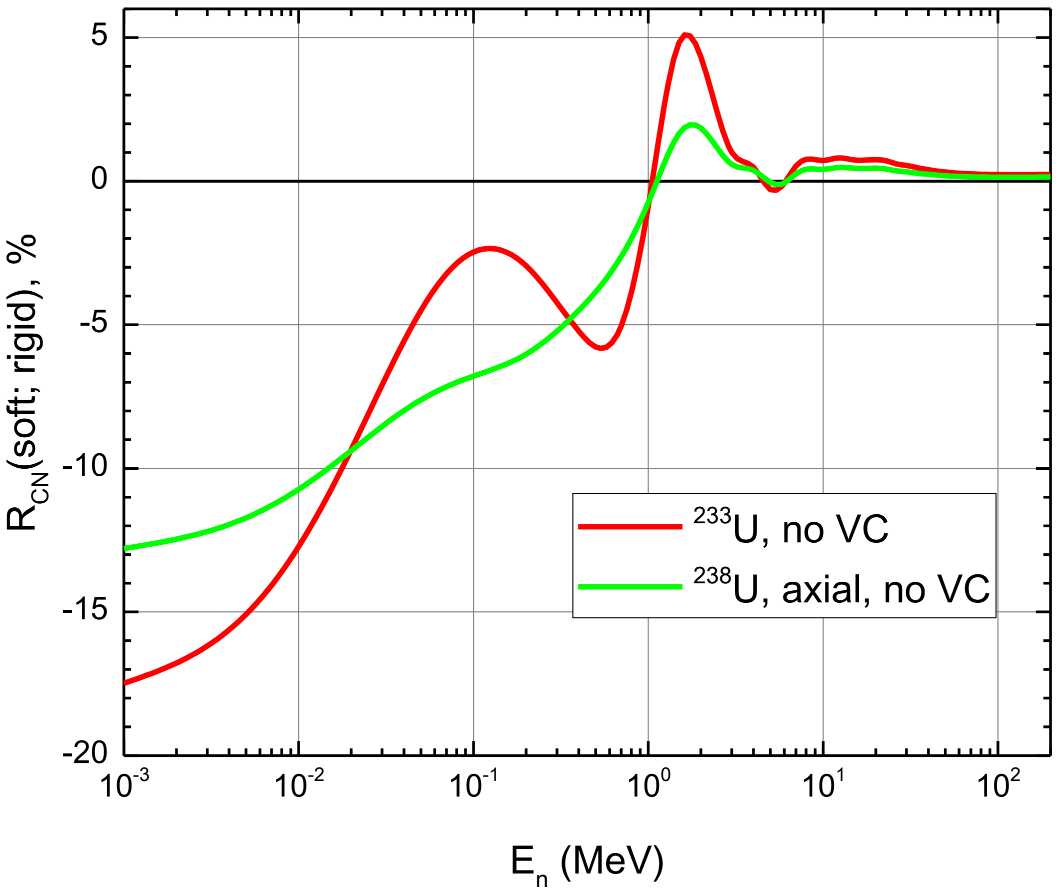


^{233}U



Nucleus stretching: CN XS change

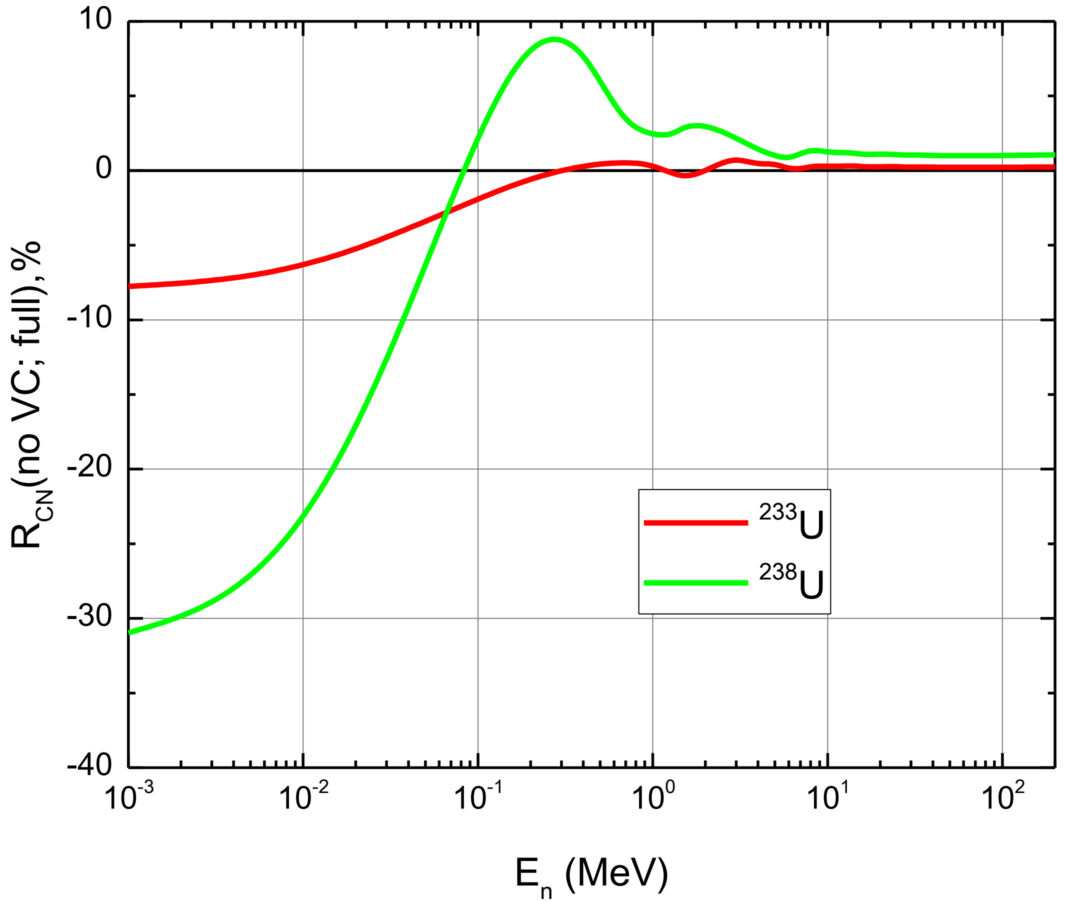
Nucleus stretching gives large impact even then only GS-band levels are coupled



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

Volume conservation: CN XS change

Volume conservation effect is also important but static deformations also contribute here



Optical potential

Energy and other — *Radial profile* — *Nucleus shape*

$$V(r,R(\theta,\varphi),E) = -V_{HF}(E) f_{WS}\big(r, R_{HF}(\theta,\varphi)\big)$$ Main real part

$$-[\boldsymbol{\Delta V_v(E)} + iW_v(E)] f_{WS}\big(r, R_v(\theta,\varphi)\big)$$ Volume

$$-[\boldsymbol{\Delta V_s(E)} + iW_s(E)] g_{WS}\big(r, R_s(\theta,\varphi)\big)$$ Surface

$$+V_{Coul}\big(r, R_c(\theta,\varphi)\big)$$ Coulomb

$$+\left(\frac{\hbar}{m_\pi c}\right)^2 [V_{so}(E) + \boldsymbol{\Delta V_{so}(E)} + iW_{so}(E)] \times \frac{1}{r}\frac{d}{dr} f_{WS}(r, R_{so})(\hat{\boldsymbol{l}} \cdot \hat{\boldsymbol{\sigma}})$$ Spin-orbit

$$f_{WS}(r,R) = \frac{1}{1+\exp\left(\frac{r-R}{a}\right)}$$

Coulomb correction (allows Lane consistency):

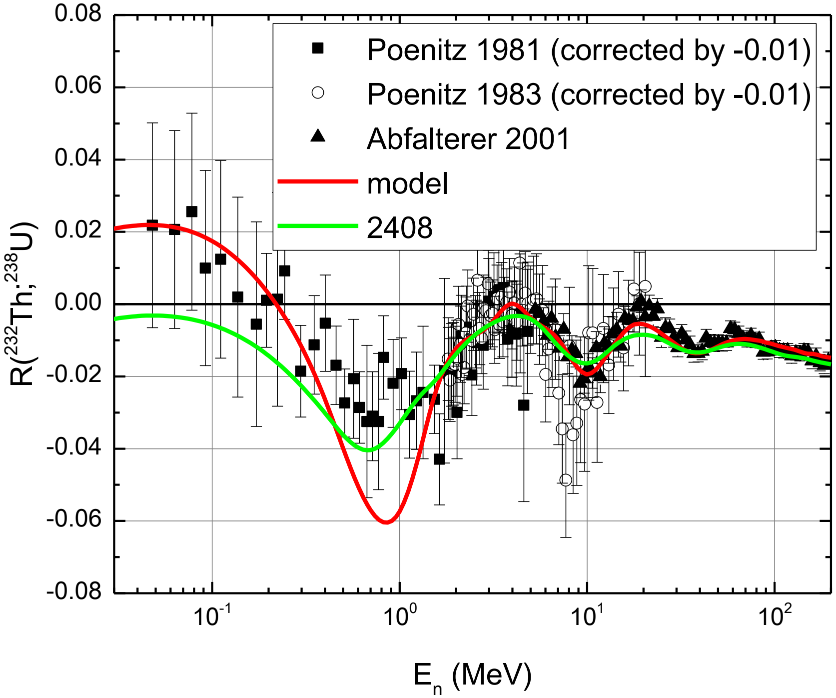
$$E = E_{inc} - E_{Coul}$$

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

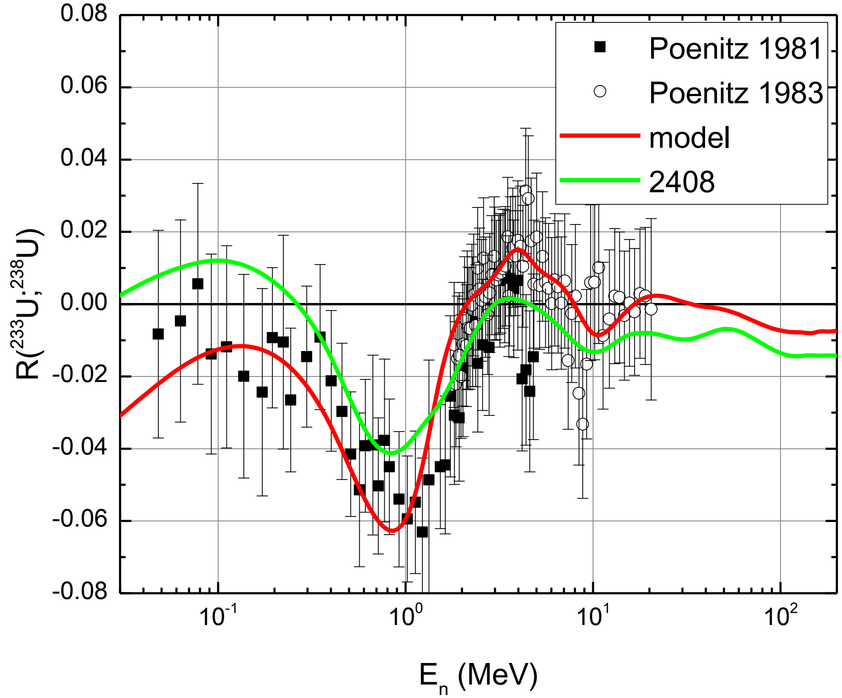
$$R(A,B) = \frac{1}{2}\frac{\sigma_A - \sigma_B}{\sigma_A + \sigma_B}$$

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

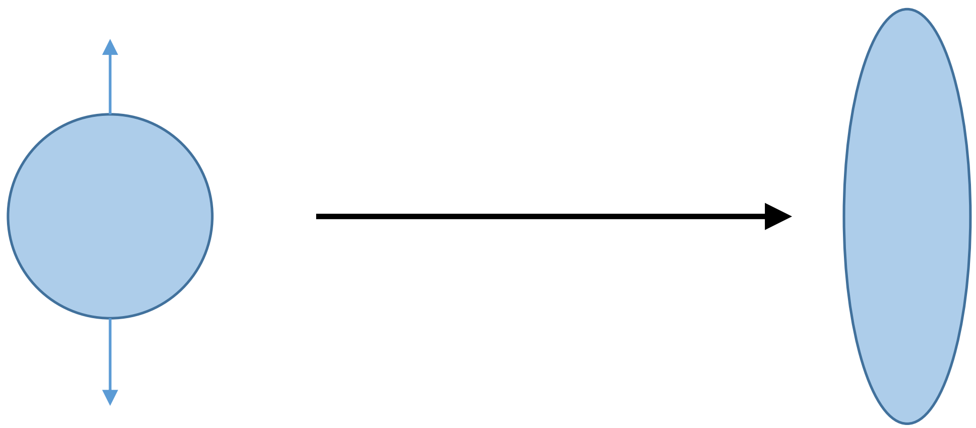
^{232}Th to ^{238}U



^{233}U to ^{238}U



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: $V = V'$

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