Nucleon-Nucleus Optical Potentials for Soft Deformed Nuclei

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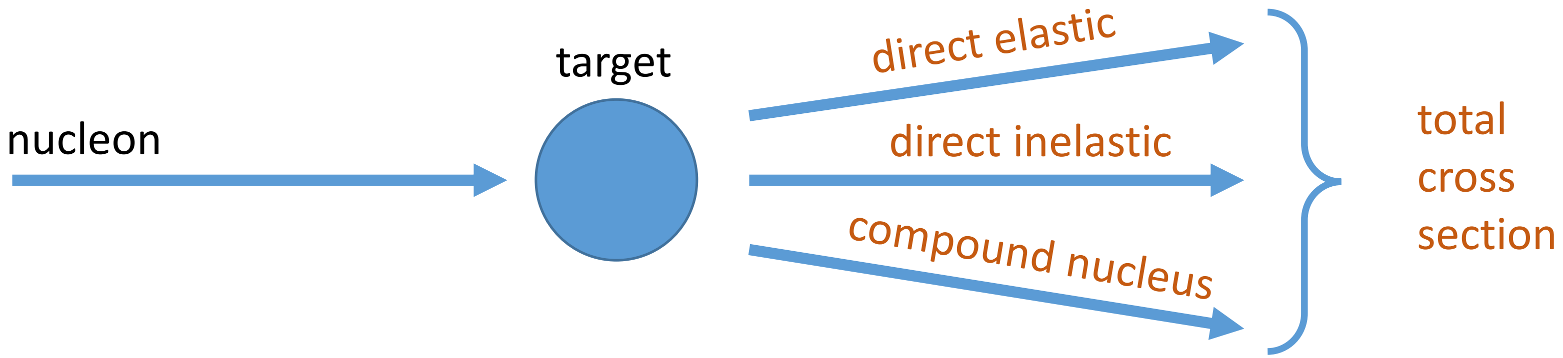
CNR*2024, July 2024, Vienna, IAEA

Coupled channels optical model



- Better target dynamics description → less is left for compound nucleus
- Essential for description of experimental data for deformed nuclides

Model components

- Dispersive Lane-consistent macroscopic potential:
  - Physically realistic
  - Better constrained
  - Describe more experimental data with single parameters set
- Nuclear structure model:
  - Description of low-energy collective excited states of a target – both rotational and vibrational (soft-rotator model)
  - Go beyond main rotational band
- Proper expansion of the deformed optical potential:
  - More details later

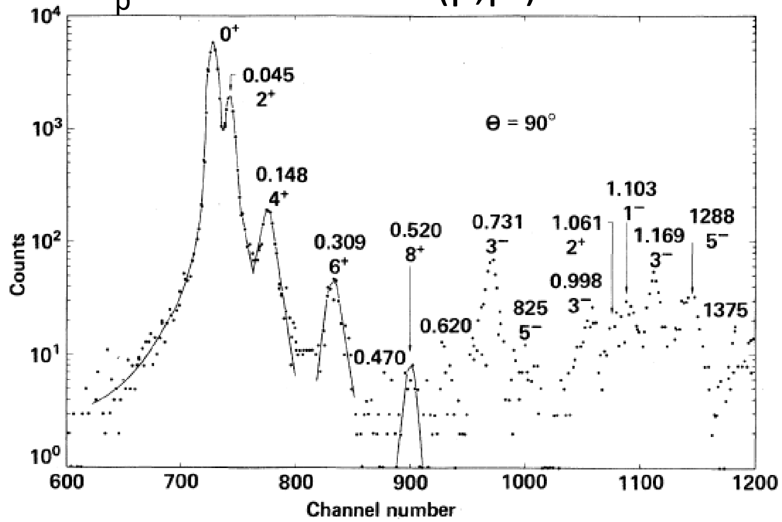
Are other bands important? (proton inelastic)

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

…

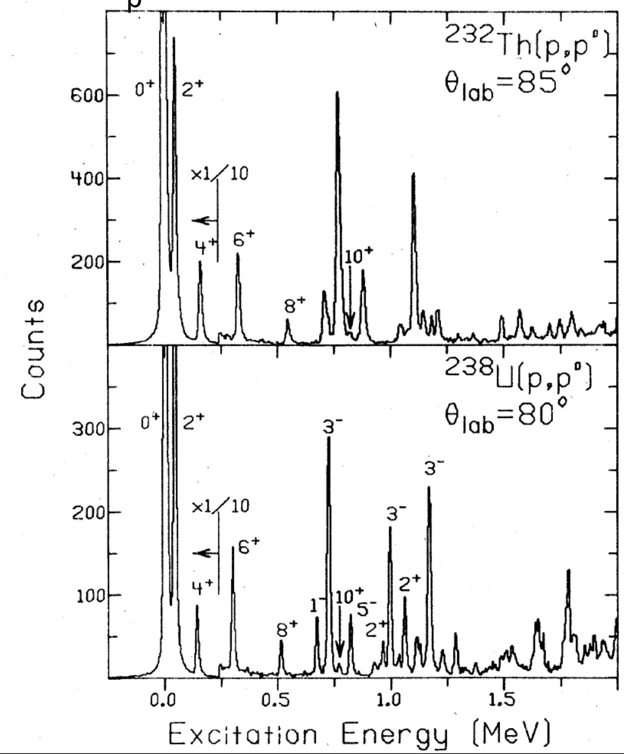
but there are clear evidences of levels from **other bands** in some proton inelastic scattering experimental works

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



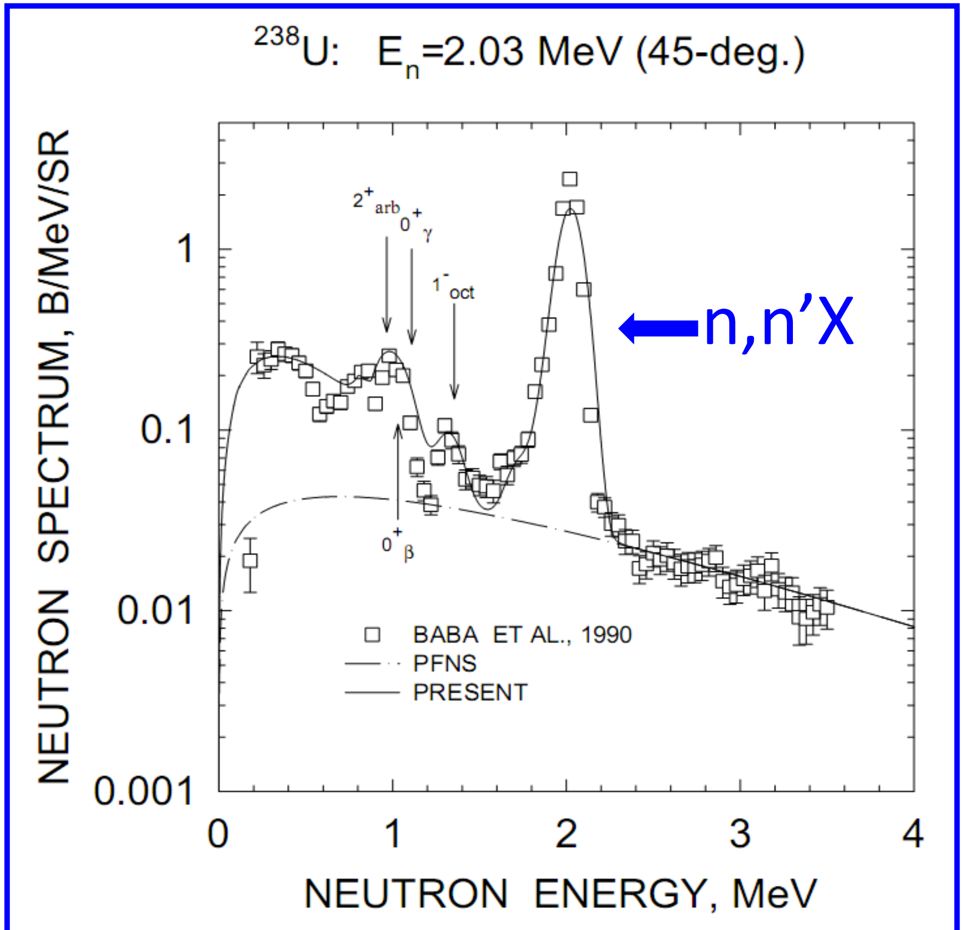
L. F. Hansen et al, PRC 25 (1982) 189

E_p=35 MeV



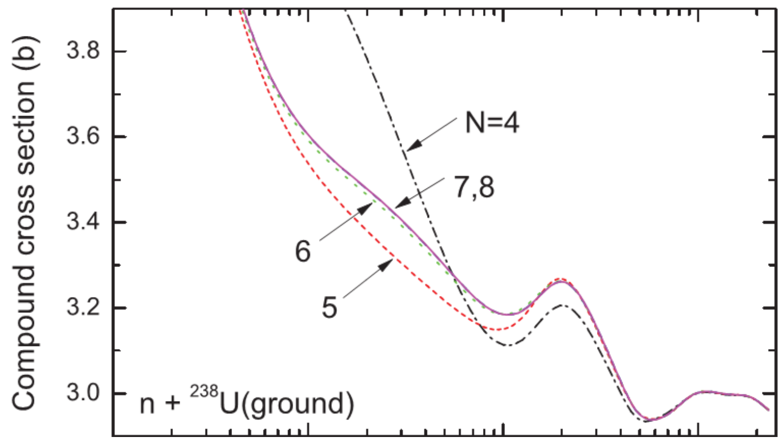
C. H. King et al, PRC 20 (1979) 2084

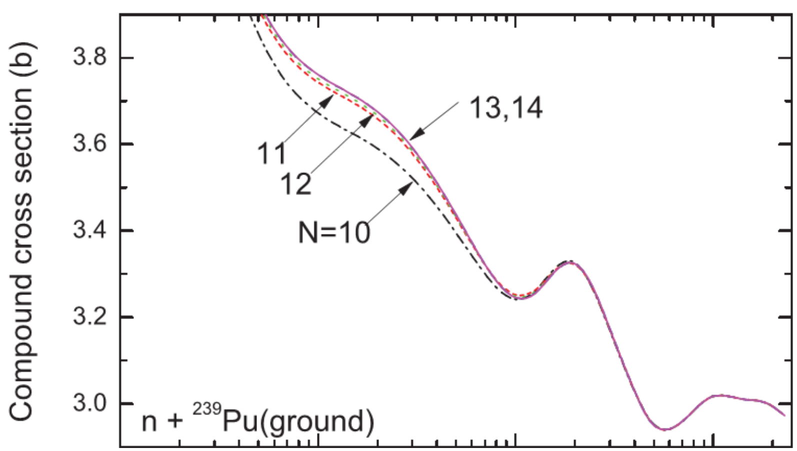
Are other bands important? (^{238}U neutron emission spectrum)



Also evidence of levels from **other bands**

Saturation of the coupling scheme





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

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

Along GS band to saturate we need:

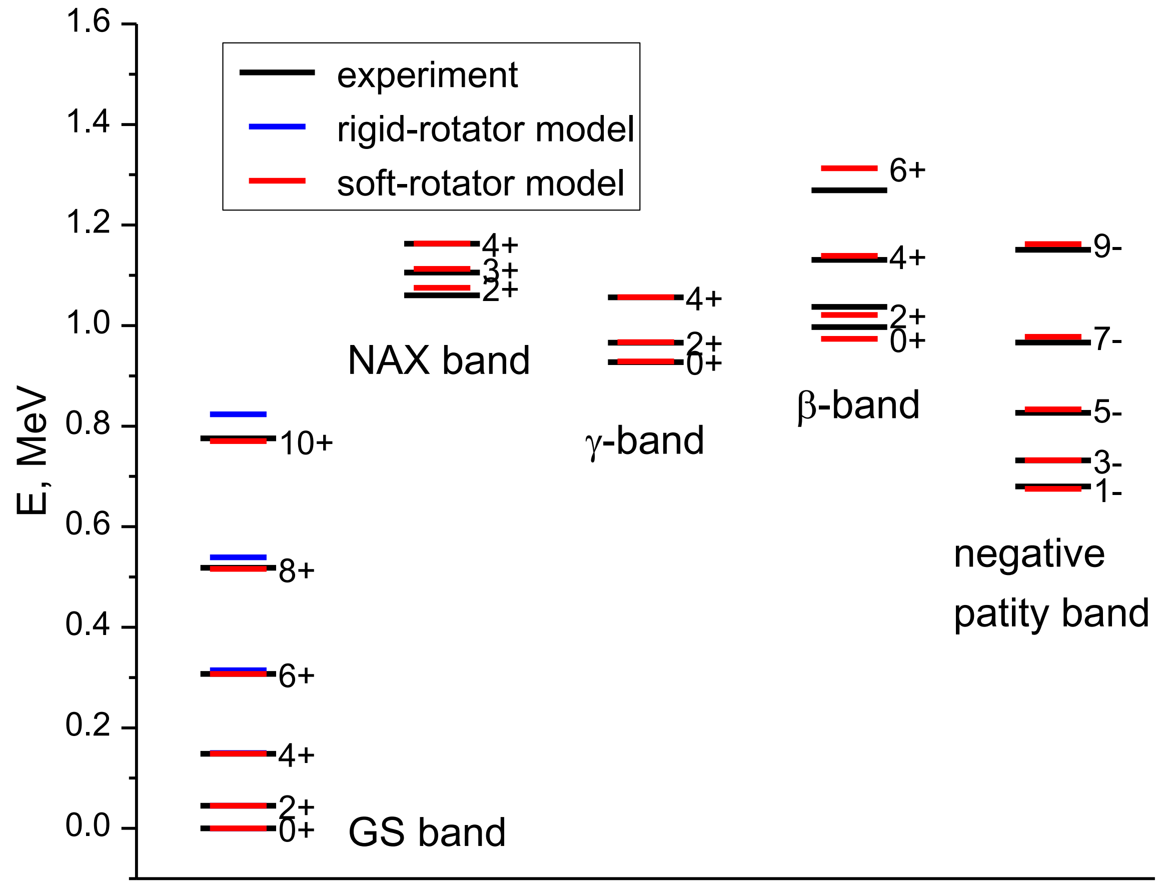
- 6 levels for even-even
- 11 levels for odd

But what about other bands?

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.

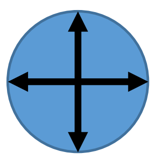
^{238}**U**



Coupled channels for soft deformed nuclei

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

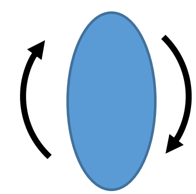
Soft spherical nucleus
(vibrational excitations)



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

Theory

Optical potential for soft deformed nuclei

Solution: Taylor expansion near axial static form

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

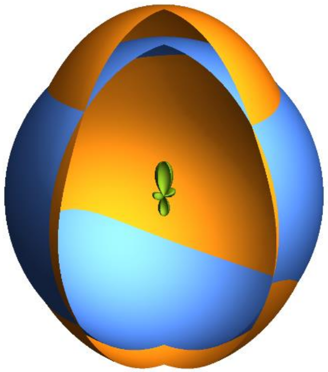
$$= R_{0i}\left\{1 + \sum_{\lambda=2,3;even\ \mu} \beta_{\lambda\mu} Y_{\lambda\mu}(\theta',\varphi')\right.$$

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

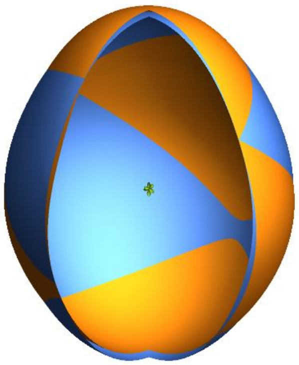
$$\beta_2 = \beta_{20} + \delta\beta_2$$
$$\langle\delta\beta_2\rangle, \langle\beta_{20}\gamma\rangle, \langle\beta_3\rangle \ll \beta_{20}$$

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

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



Near sphere



Near axially deformed

Potential expansion near axially deformed shape

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

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

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

Rigid rotor

Softness

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

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

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

Coupled channels matrix elements

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

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

Rigid rotor

$$+ v_2(r)\Big\{\Big[[\boldsymbol{\beta}_2]_{eff} + [\boldsymbol{\gamma}_{20}]_{eff}\Big]\langle IK||D_{;0}^{2}||I'K\rangle A\left(ljI;l'j'I';2J\frac{1}{2}\right)\delta_{KK'}$$

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)

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

Volume and center-of-mass position conservation corrections

Effective deformations

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

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

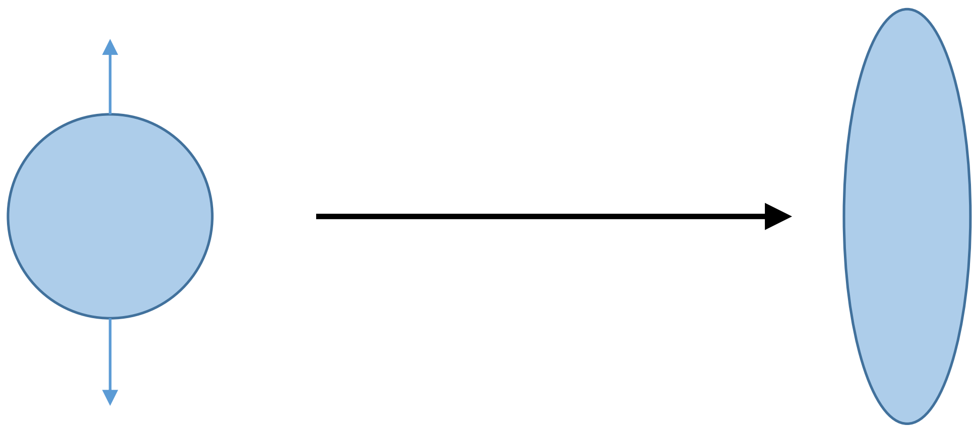
$$[\beta_2^2]_{eff} = \left\langle n_i(\beta_2) \middle| \frac{\delta\beta_2^2}{\beta_{20}^2} \middle| n_f(\beta_2) \right\rangle \qquad [\beta_3^2]_{eff} = \left\langle n_i(\beta_3) \middle| \frac{\beta_3^2}{\beta_{20}^2} \middle| n_f(\beta_3) \right\rangle$$

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

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

Effective deformations are defined by collective nuclear wavefunctions

Volume conservation term



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

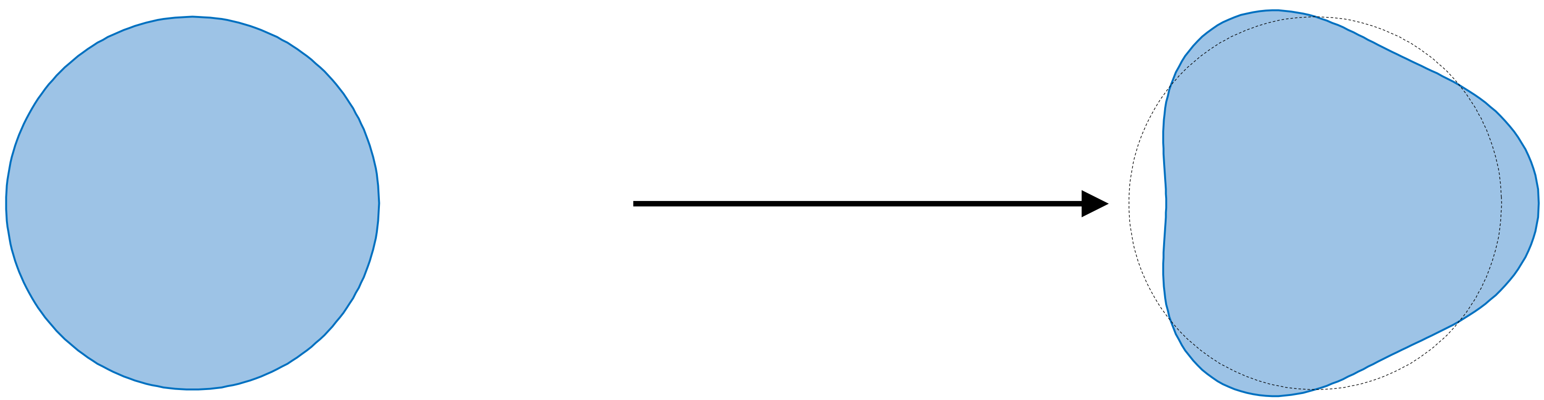
$$R'(\theta,\varphi) = R_0\left\{1 + \boxed{\beta_{00}Y_{00}} + \sum_{\lambda\mu}\beta_{\lambda\mu}Y_{\lambda\mu}(\theta,\varphi)\right\}$$

Compensation term

Incompressible nuclear matter: $V = V'$

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

Center-of-mass immobility term



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

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

Compensation term

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

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

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)
- One coupling param. per band
- Ambiguous description for nuclides with poor experimental data
- No additional knowledge needed

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

Calculation based on structure Hamiltonian

- 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…

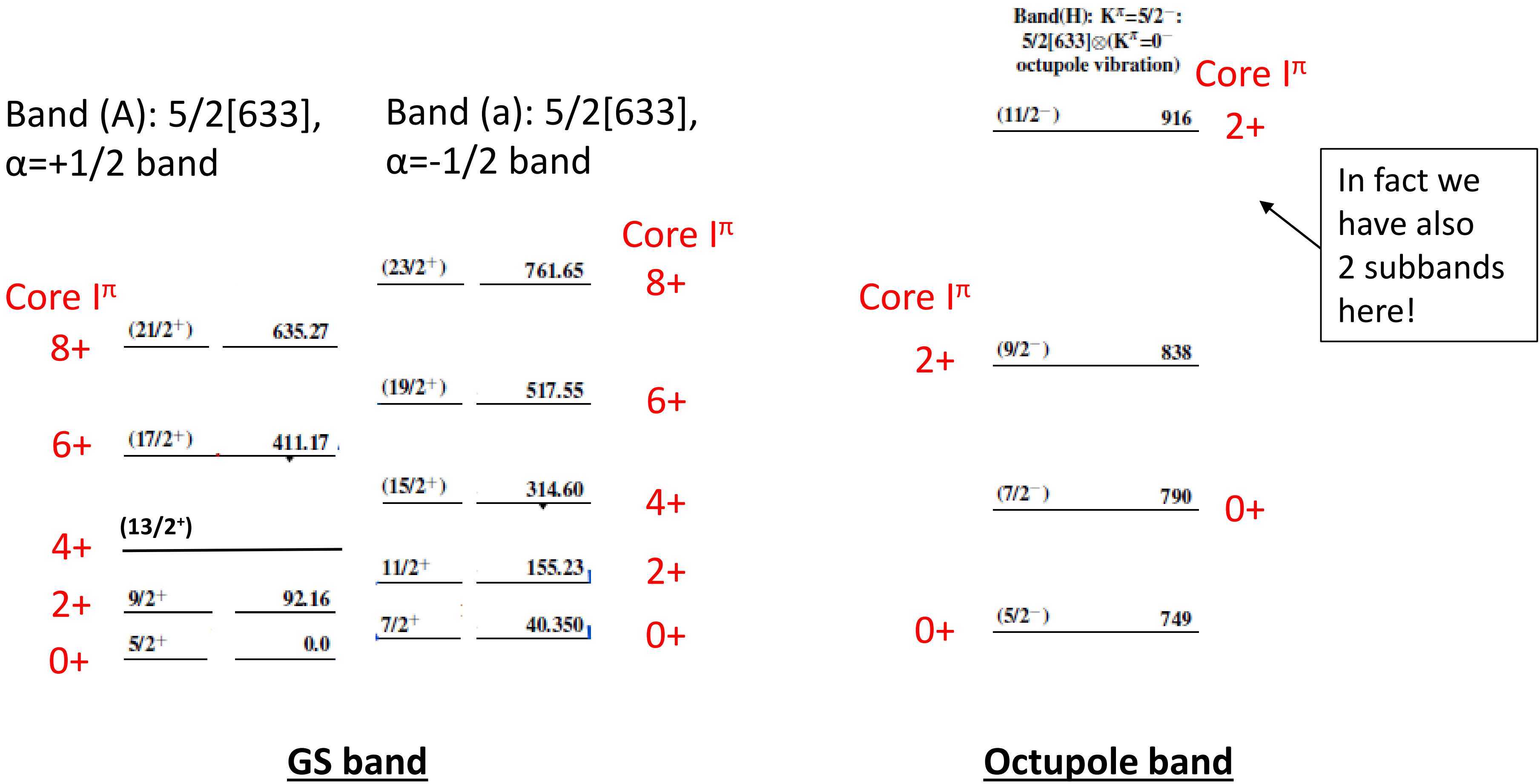
- Nuclear softness – collective effect, determined mainly by the even-even core, and varies smoothly from nucleus to nucleus
- $\langle \psi_{odd} | \beta | \psi_{odd} \rangle \approx \langle \psi_{core} | \beta | \psi_{core} \rangle$
- We may try to couple levels for bands built on single-particle state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

Odd-A matrix elements

- $|\psi_{odd}\rangle \sim \varphi_{sp} |\psi_{even\ core}\rangle$ *no particle-core interaction*

- $\left\langle \psi_{odd} \middle| \beta \middle| \psi'_{odd} \right\rangle \approx \langle \psi_{core} | \beta | \psi'_{core} \rangle$, if $\varphi_{sp} = \varphi'_{sp}$
- $\left\langle \psi_{odd} \middle| \beta \middle| \psi'_{odd} \right\rangle \approx 0$, if $\varphi_{sp} \neq \varphi'_{sp}$

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

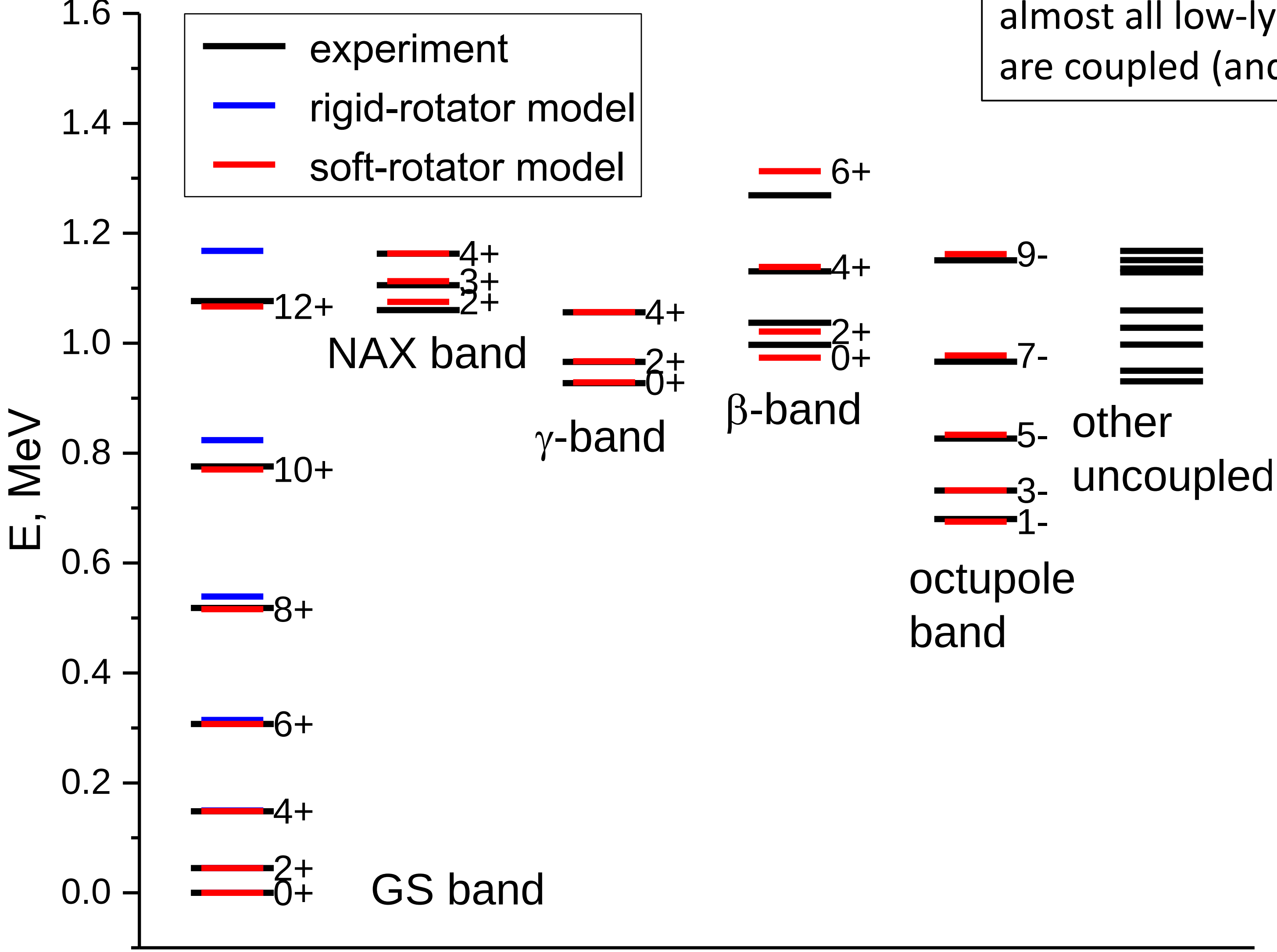
Algorithm,

coupling schemes,

parameters, etc.

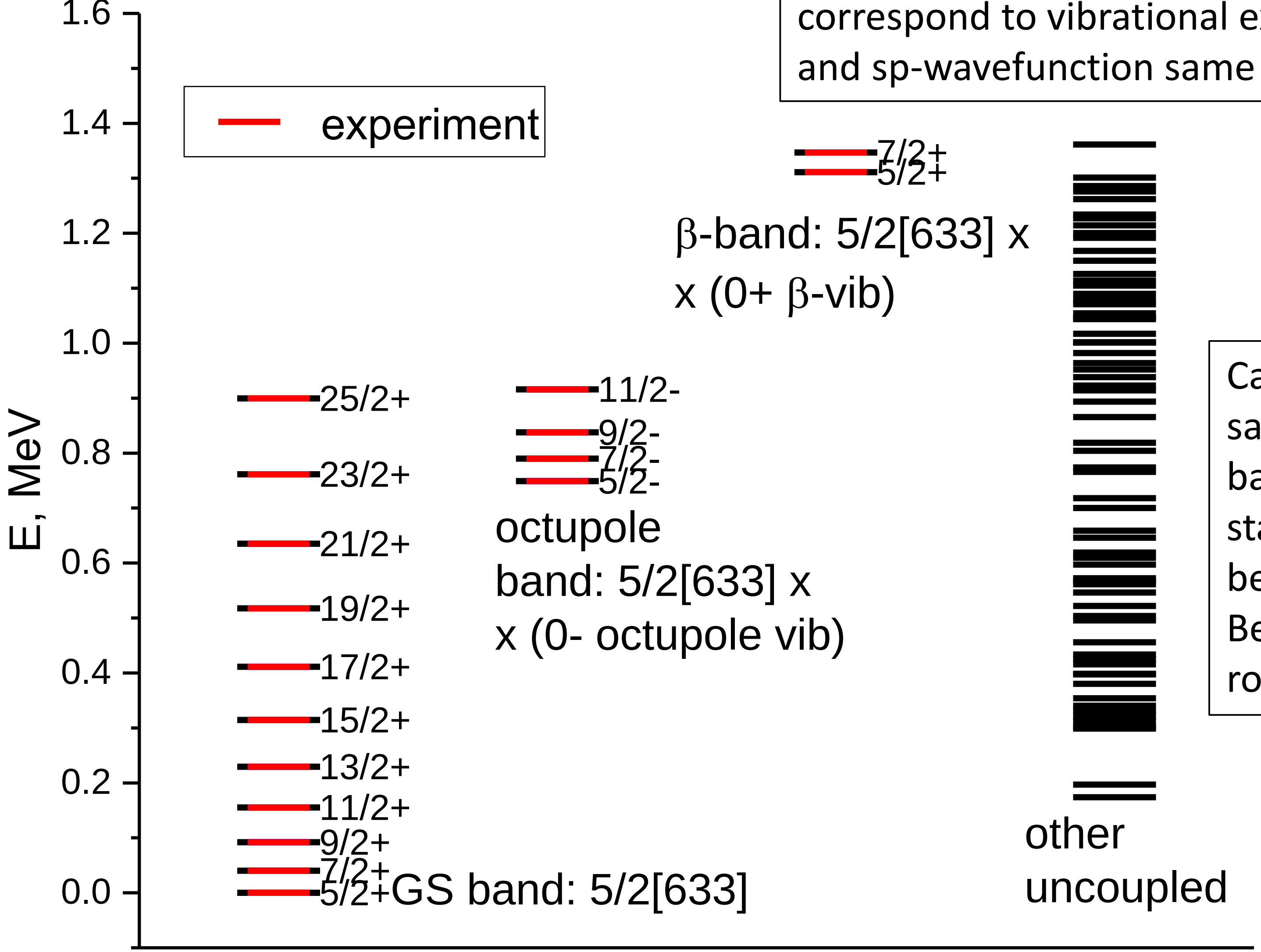
^{238}U coupling scheme

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



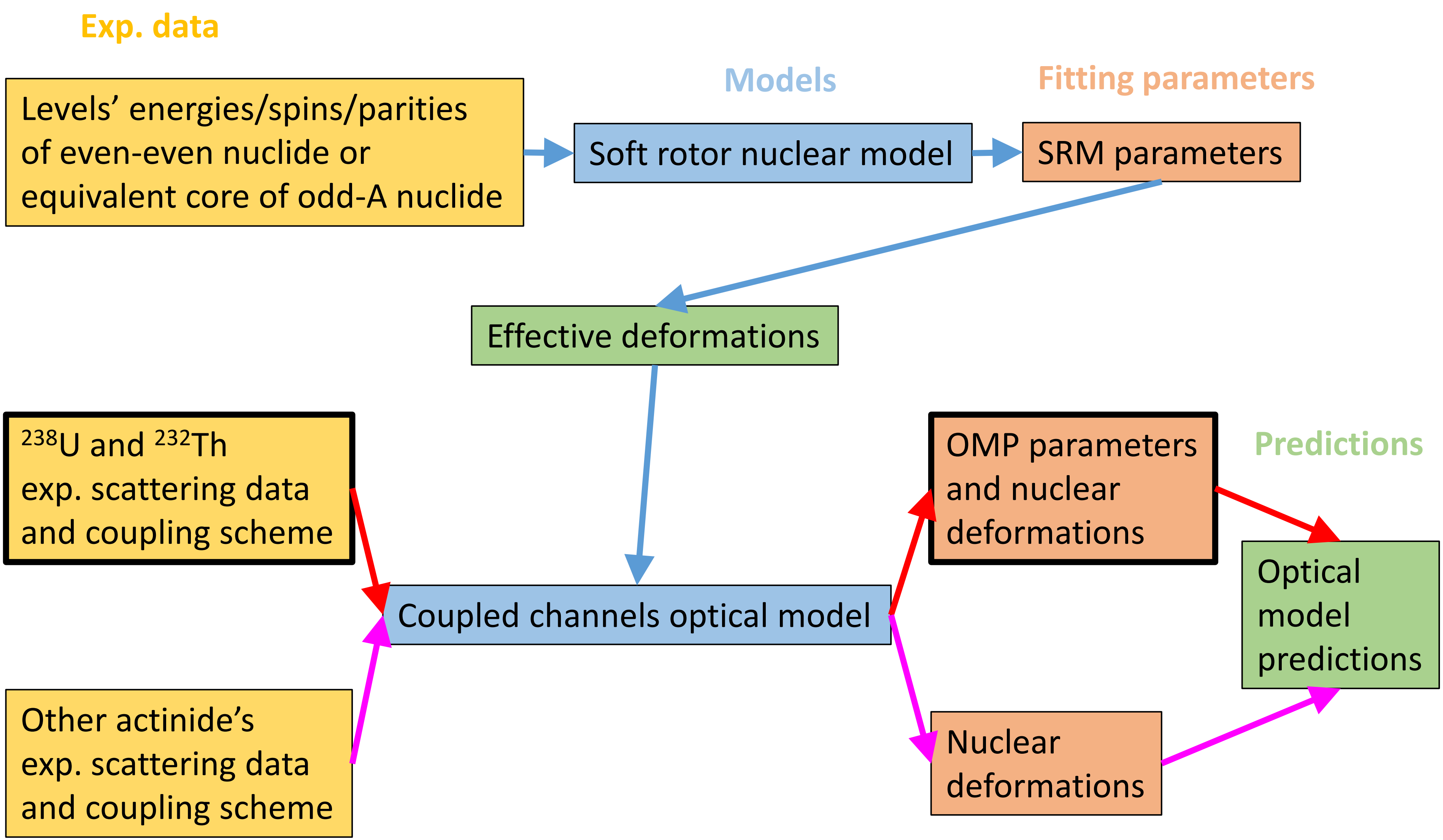
^{233}U coupling scheme

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!

Calculation algorithm



Fitting parameters

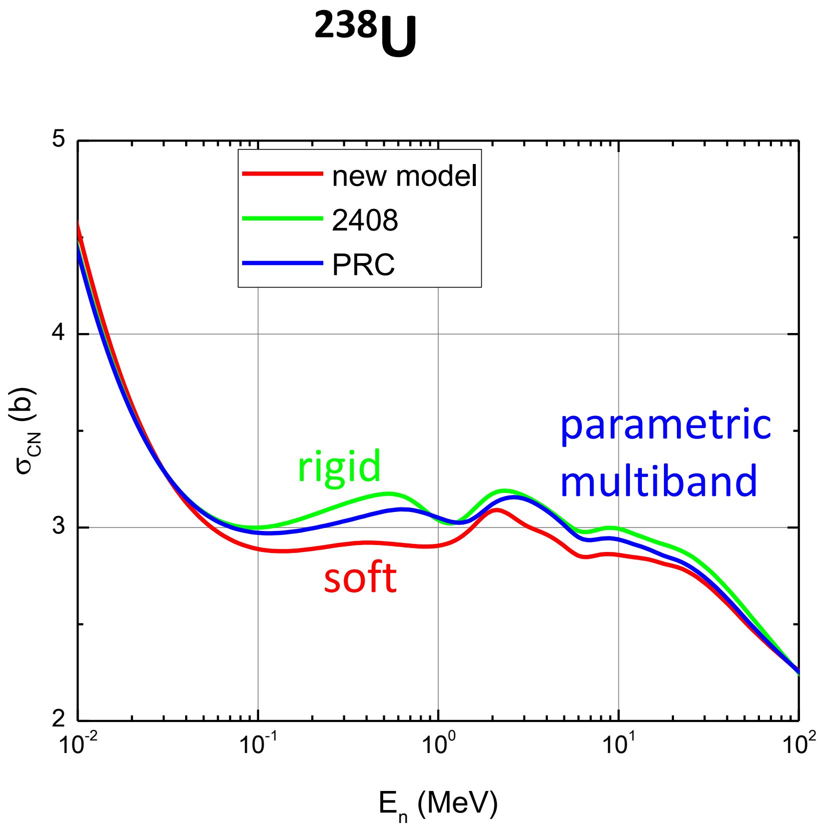
- Nuclear softness and non-axiality (all soft-rotator model parameters) – from level structure, missing levels for coupling can be restored for even-even

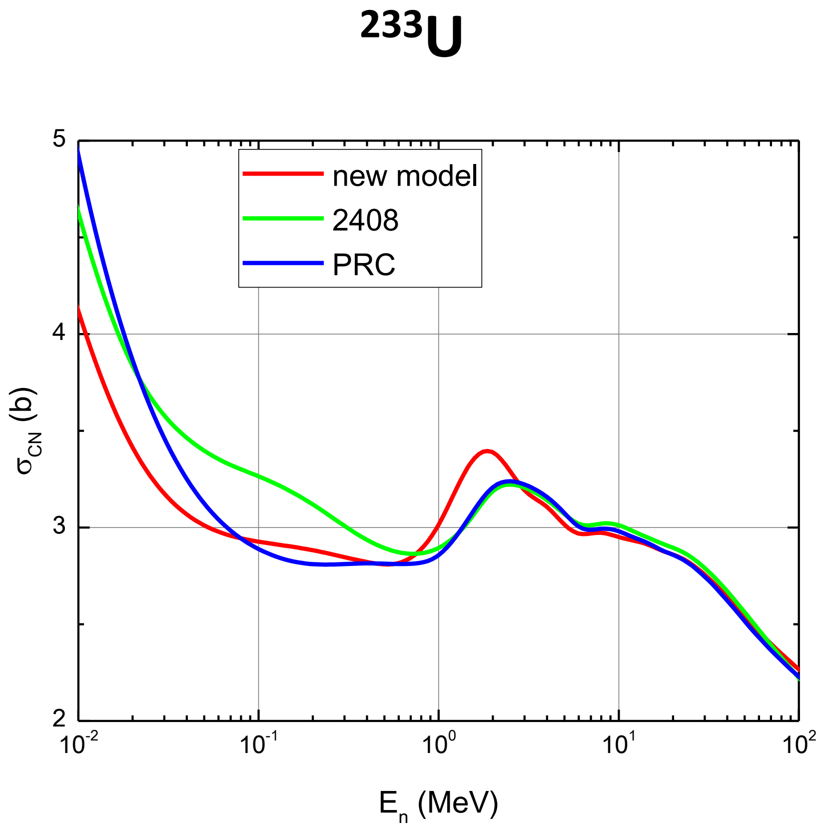
- **Many experimental data** for optical model (^{238}U and ^{232}Th) – fit optical potential parameters and deformations
- **Scarce experimental data** (^{233}U, ^{240}Pu…) – fit only deformations ($\beta_{20}, \beta_{30}, \beta_4, \beta_6$) with fixed potential
- **Only strength functions or nothing**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

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

Comparison with other potentials

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





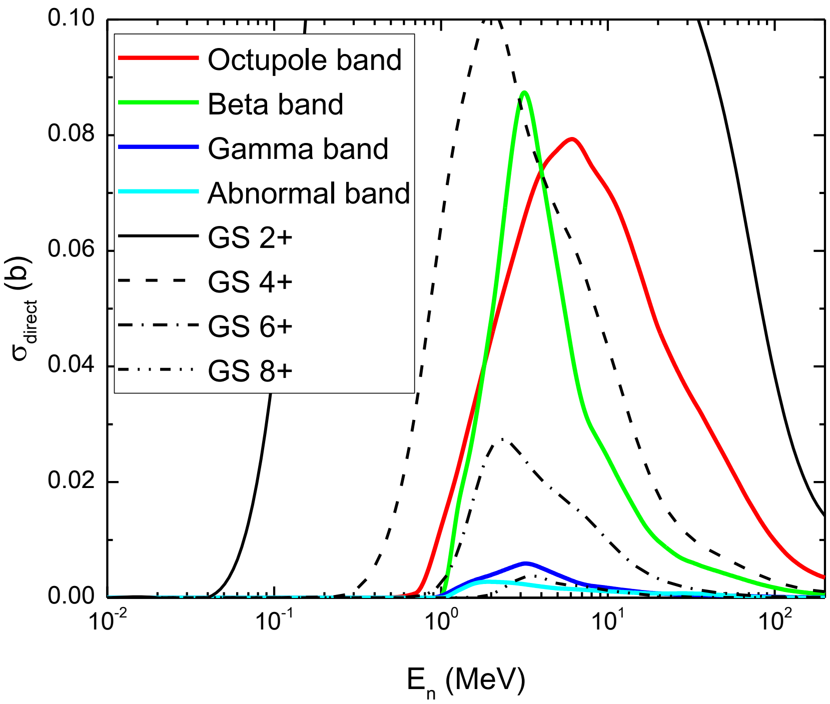
Softness effects

- 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

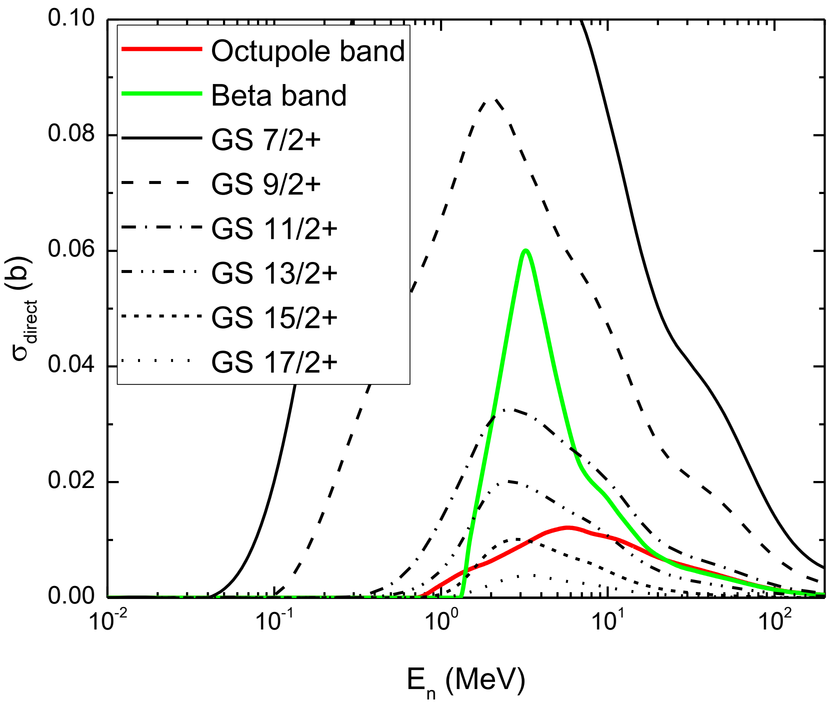
Multiband coupling: Direct level excitation XS

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

^{238}U



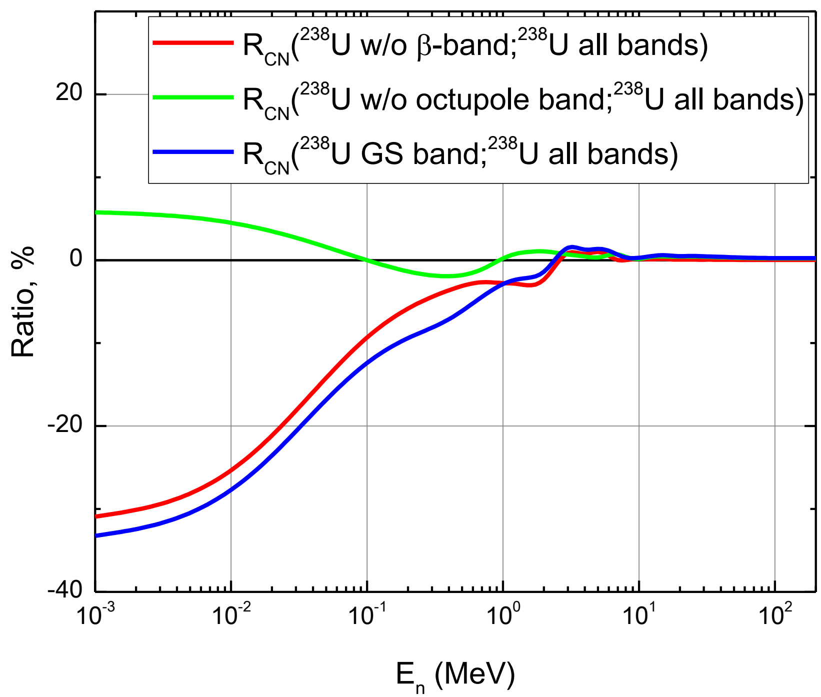
^{233}U



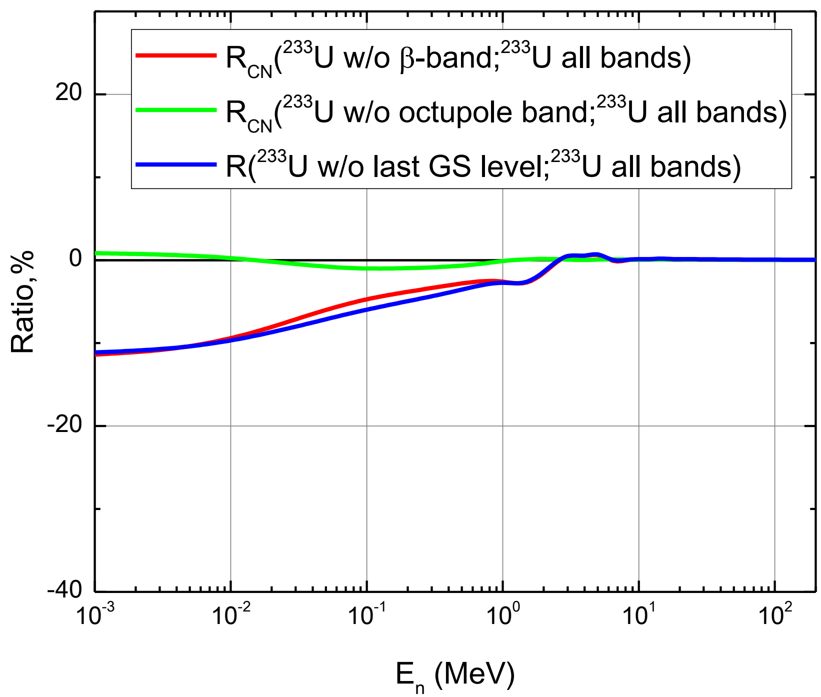
Multiband coupling:
CN XS change due to bands removal

Large impact of β-vibrational states in the coupling scheme

^{238}U

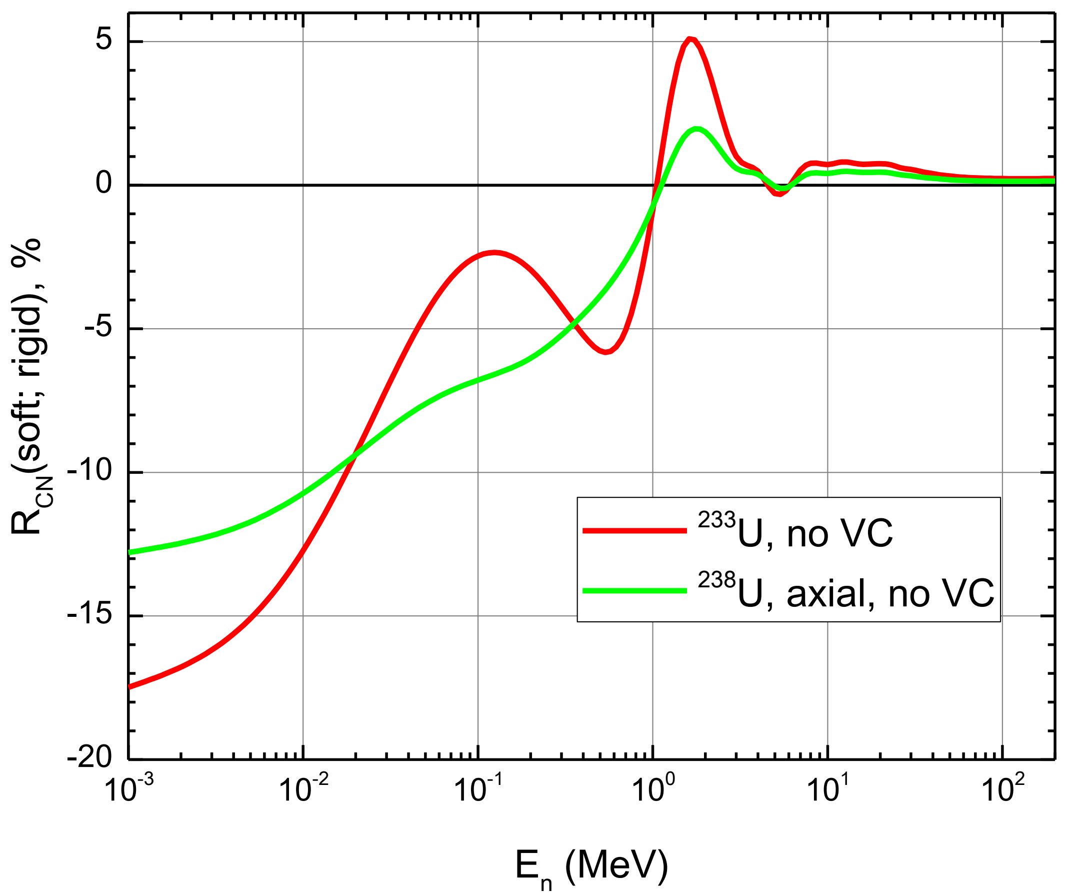


^{233}U



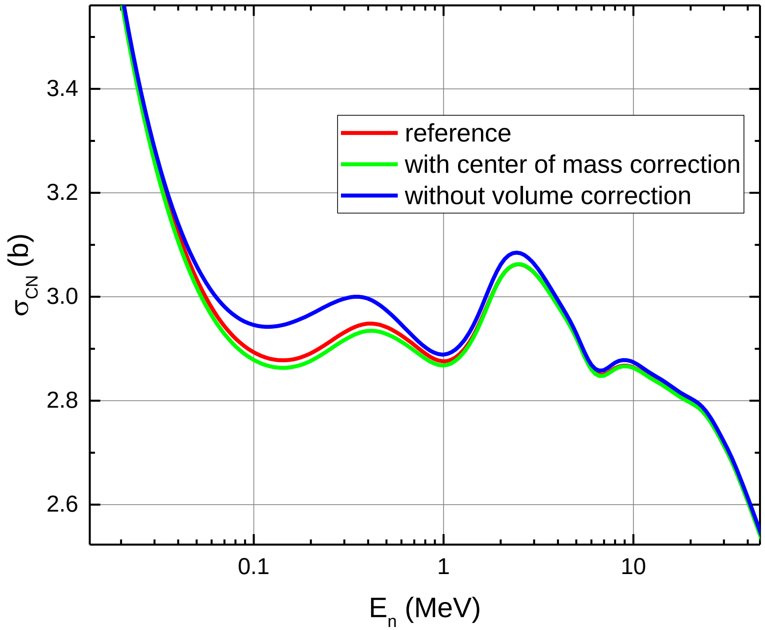
Nucleus stretching: CN XS change

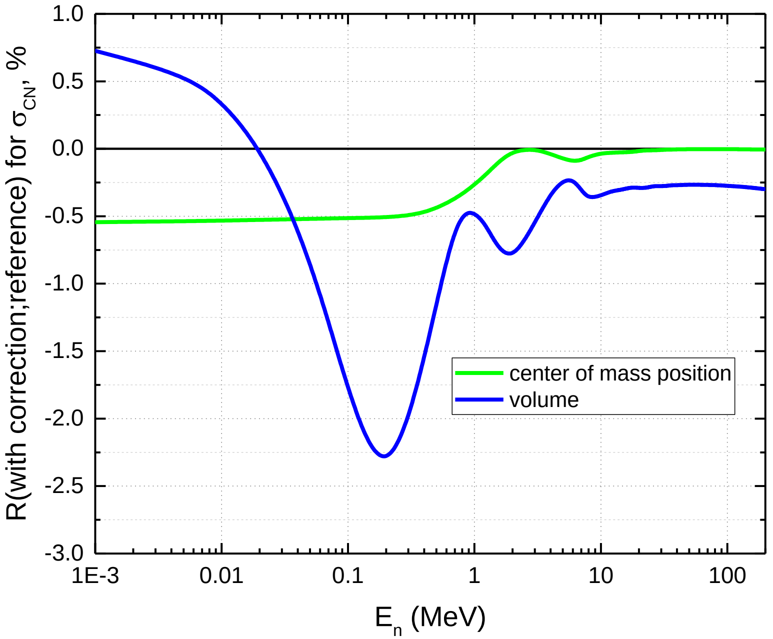
Nucleus stretching gives large impact even then only GS-band levels are coupled



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

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

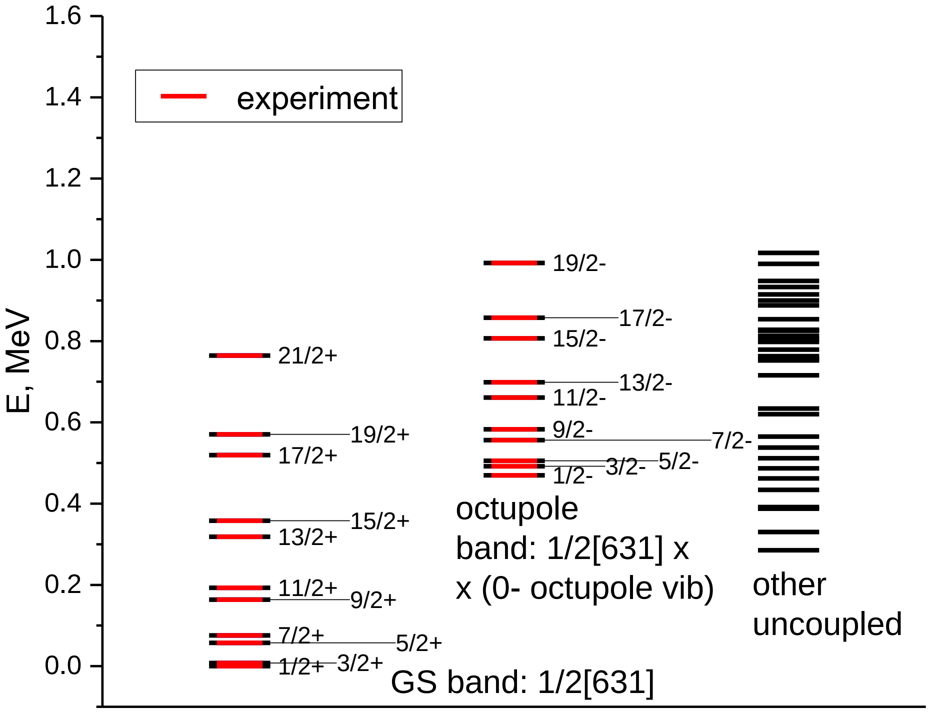


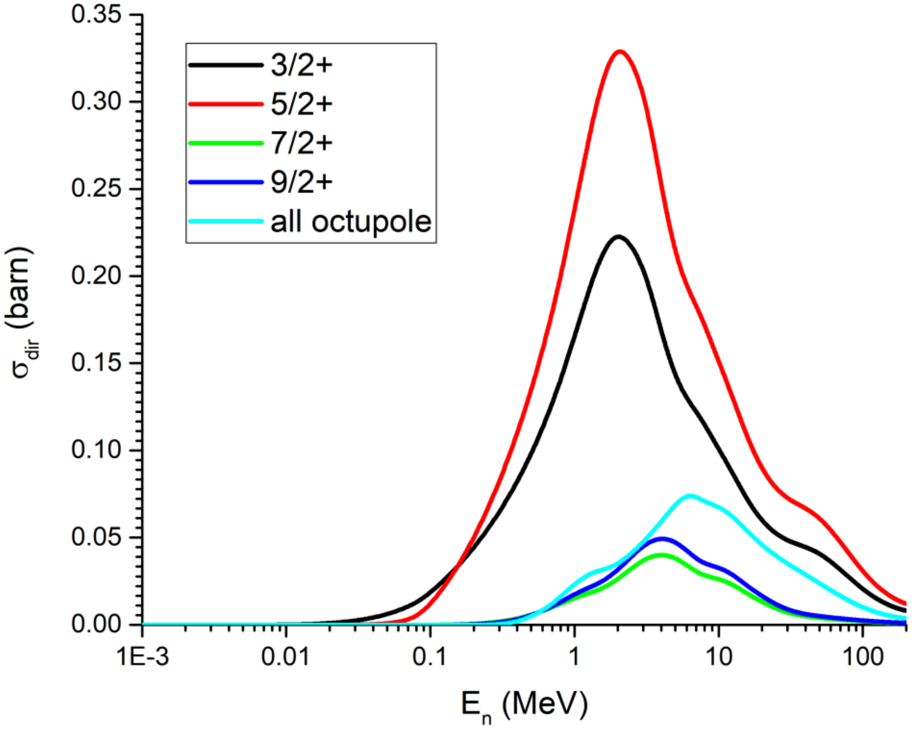


Volume conservation may be considered, center-of-mass correction is small

^{239}Pu: direct level excitation

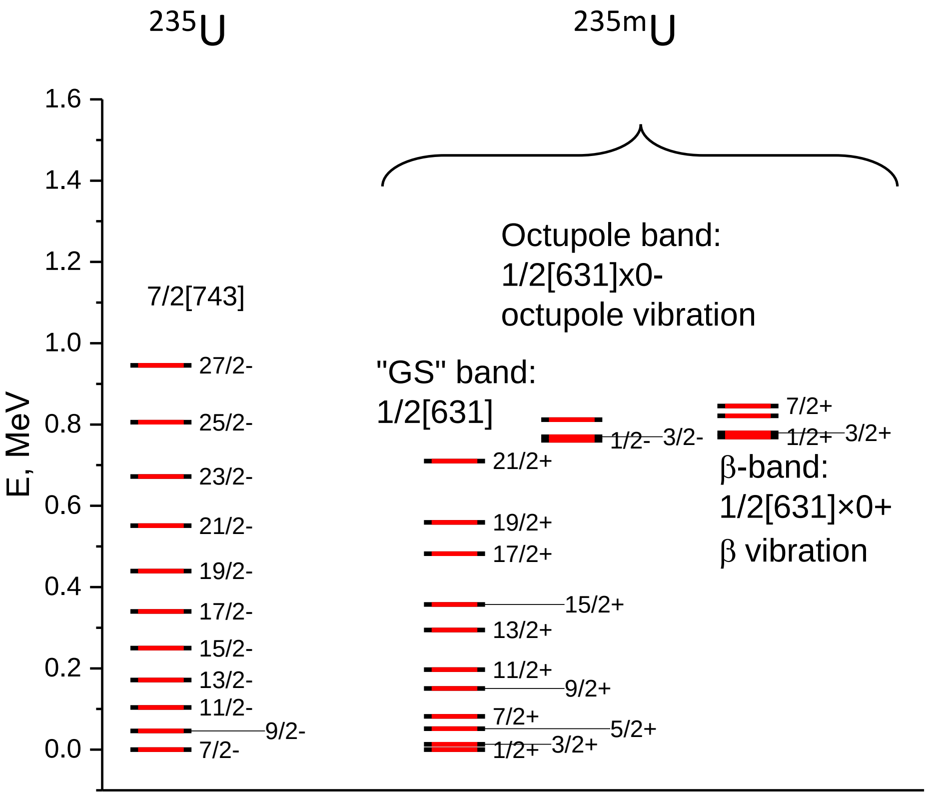
Other bands' impact is comparable to one from 2nd/3rd excited GS band level

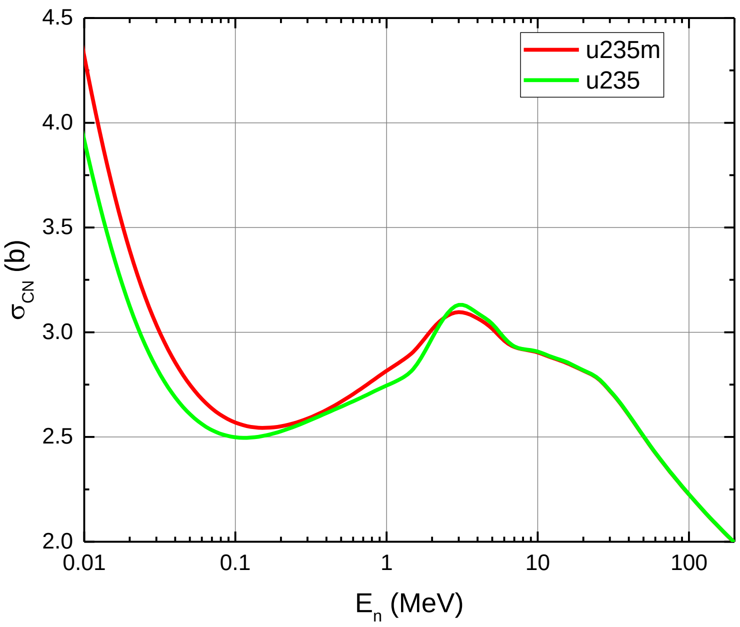




^{235}U and ^{235m}U: change of CN cross section

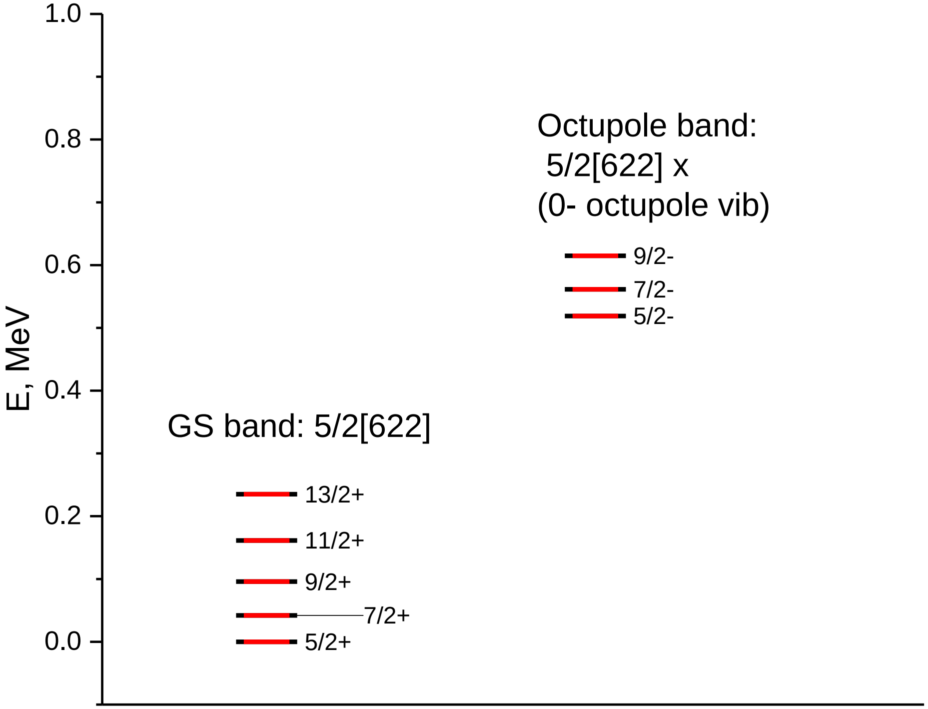
Only one band coupled for ^{235}U but softness is still important
Isomeric state has other coupled levels → cross section changed

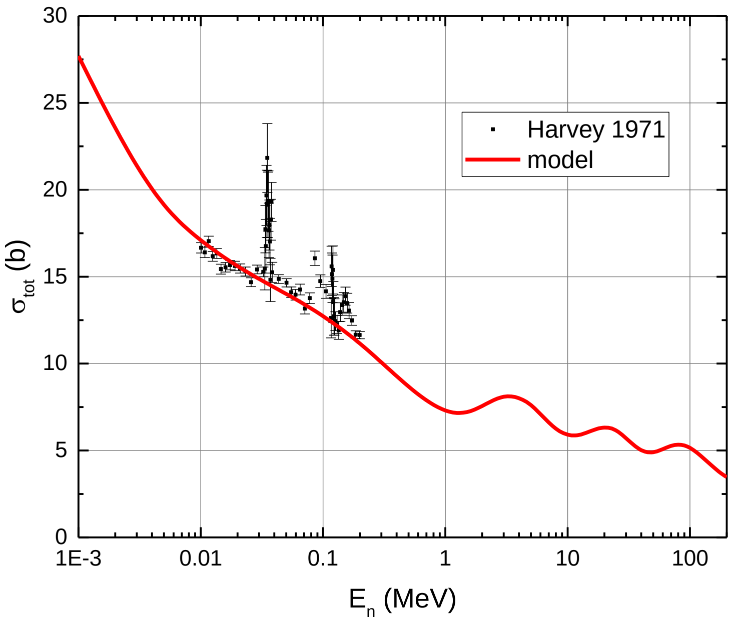




^{241}Pu: total CS

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





Summary

- 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

Thank you for the attention!

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)

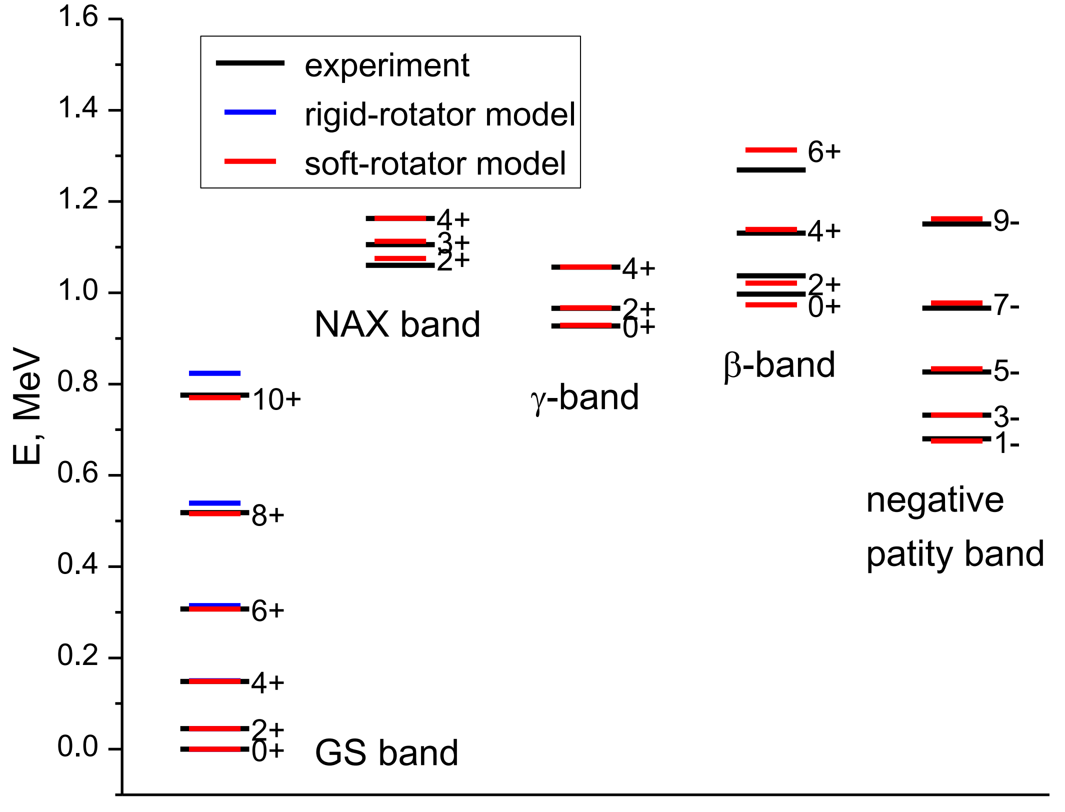
OPTMAN

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)

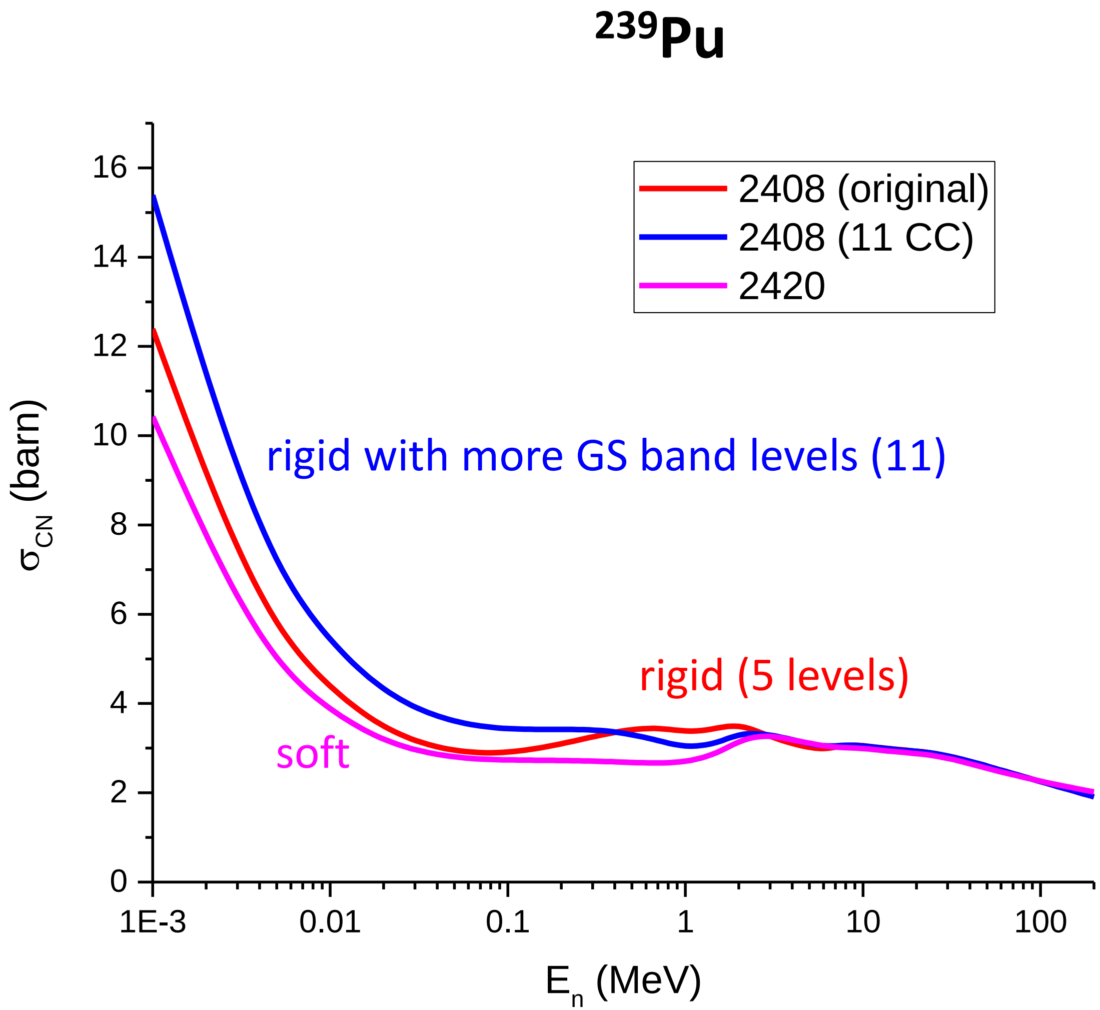
RIPL-3: Capote, R. et al., Nucl. Data Sheets 110, 3107–3214 (2009)
OPTMAN and SHEMMAN: E. Sh. Sukhovitski et al., JAERI-Data/Code 2005-002 (2005)
Dispersive corrections: Soukhovitski, E. Sh. et al, JAEA-Data/Code--2008-025 (2008)
Soft description of Fe56: W. Sun et al, Nucl. Data Sheets 118, 191-194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

Soft rotator model



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

Comparison with other potentials 2



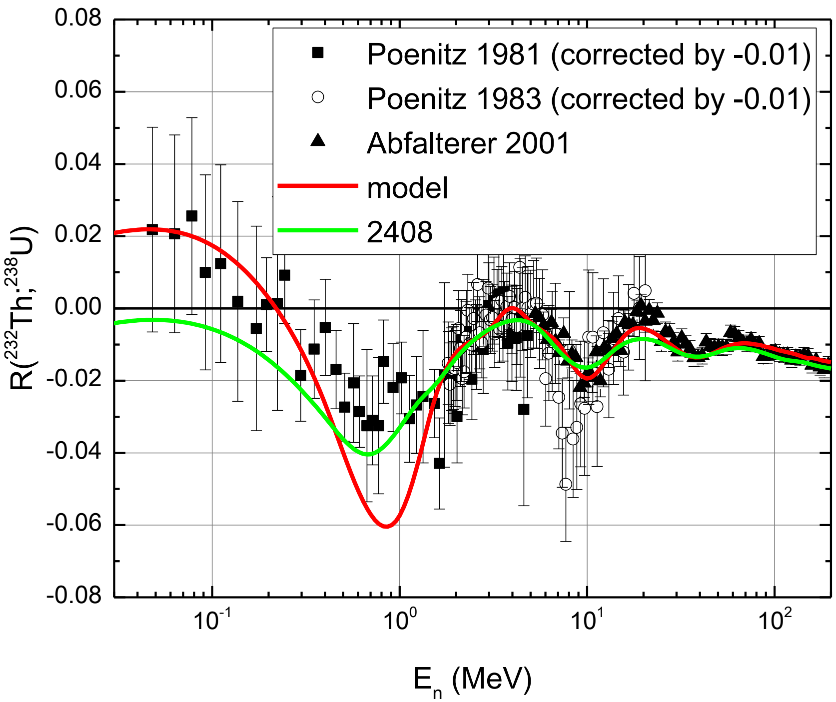
Simple addition of GS band levels to the coupling scheme is not enough

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