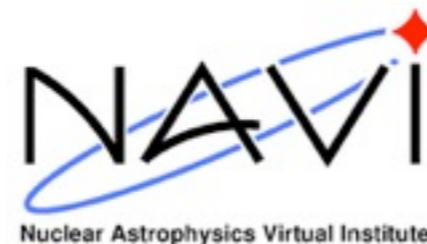


# Energy density functional methods for nuclear structure and neutrinoless double beta decay

**Tomás R. Rodríguez**

**NAVI/JINA Collaboration-Meeting 2012**

**MSU November 2012**



# Outline



TECHNISCHE  
UNIVERSITÄT  
DARMSTADT

**1. Introduction**

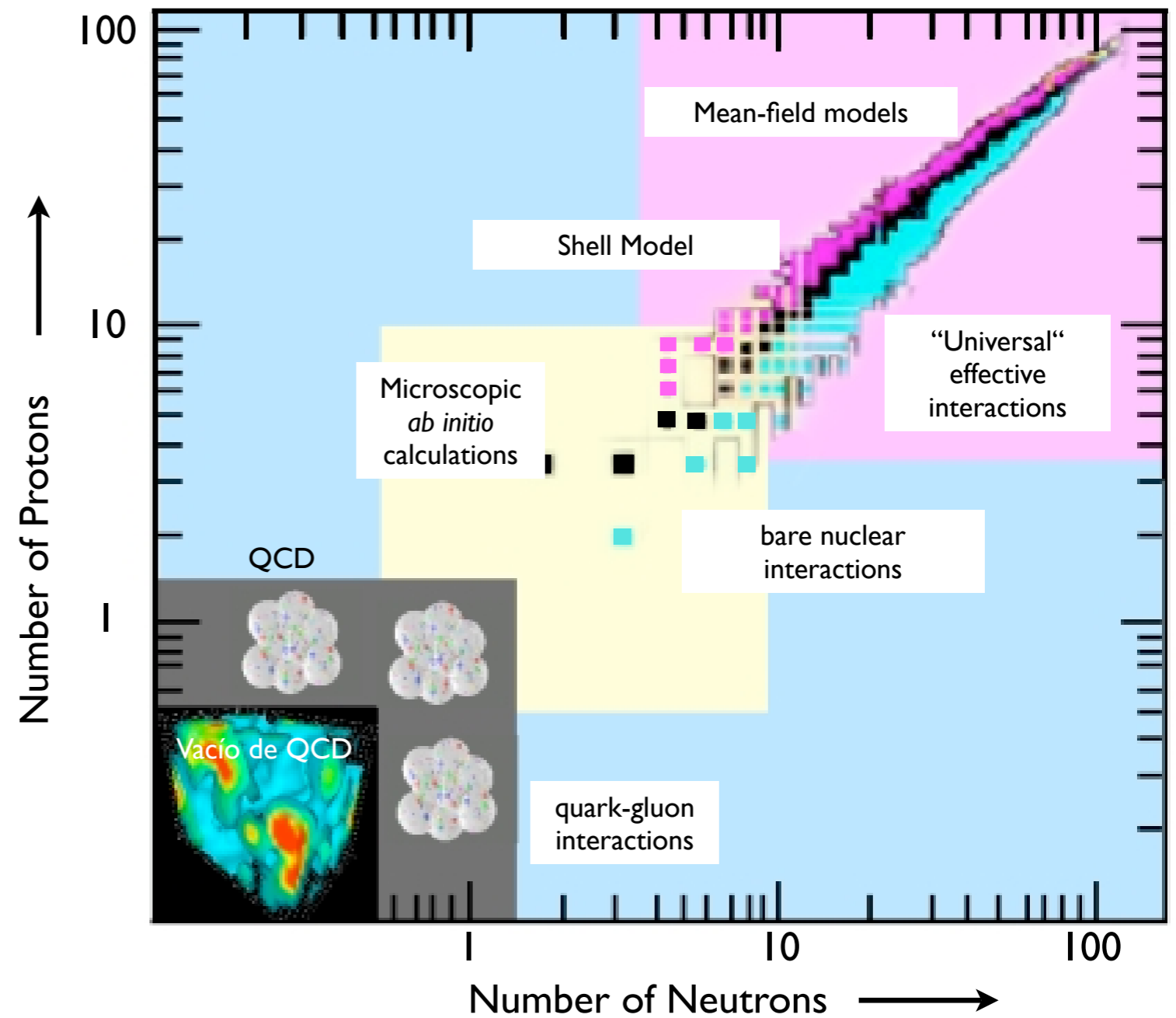
**2. Nuclear structure**

**3. Neutrinoless double beta decay**

**4. Summary and outlook**

# Motivation

Description of the nuclear structure valid for the whole nuclear chart with a single effective interaction.



# Motivation

## I. Introduction

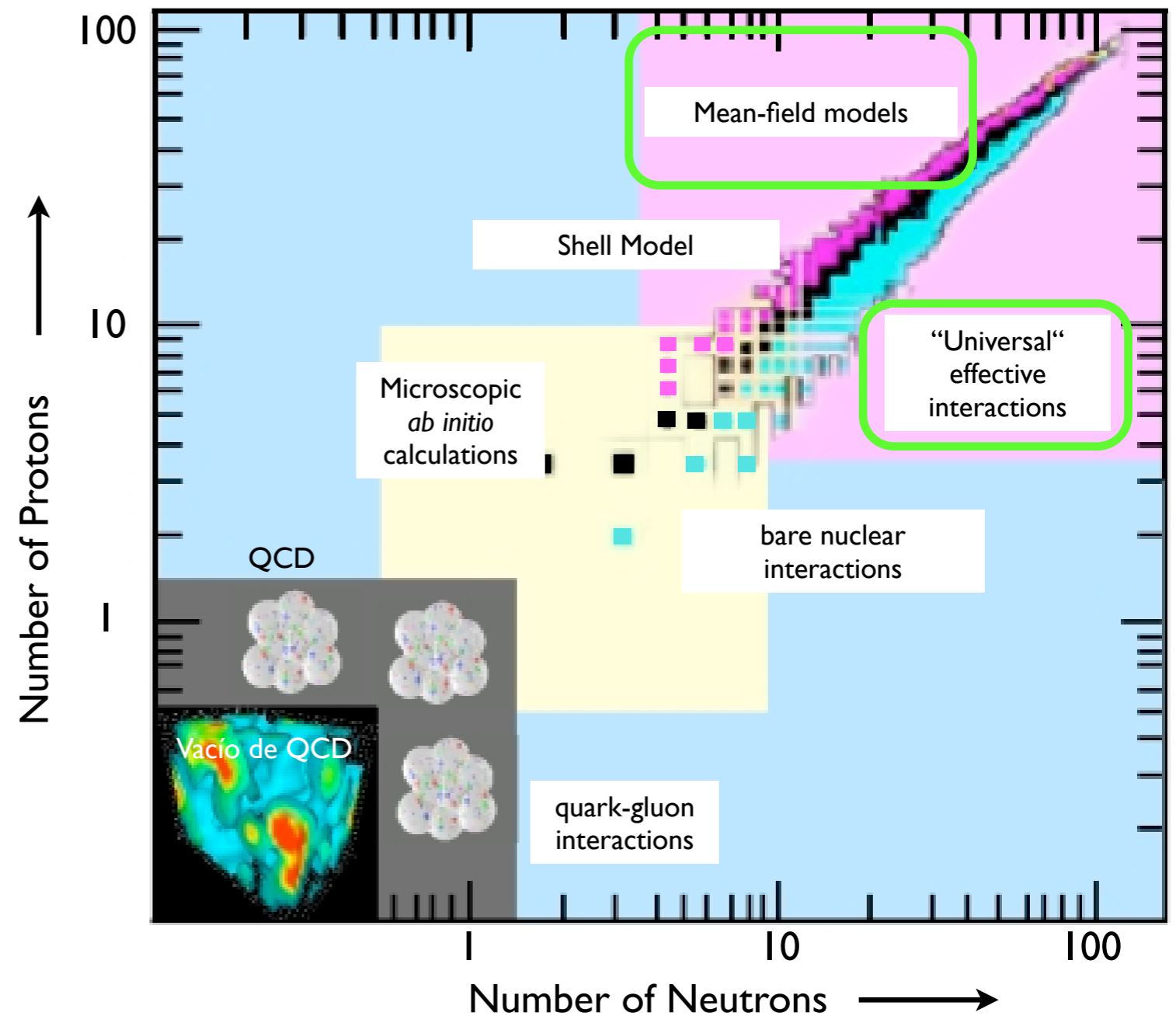
2. Nuclear structure

3.  $0\nu\beta\beta$  decay

4. Summary and outlook

Description of the nuclear structure valid for the whole nuclear chart with a single effective interaction.

- Skyrme functionals
- Gogny functionals
- Relativistic functionals





# Theoretical framework

- **Effective nucleon-nucleon interaction:**

**Gogny force (DIS-DIM)** that is able to describe properly many phenomena along the whole nuclear chart.

$$V(1, 2) = \sum_{i=1}^2 e^{-(\vec{r}_1 - \vec{r}_2)^2 / \mu_i^2} (W_i + B_i P^\sigma - H_i P^\tau - M_i P^\sigma P^\tau) \\ + iW_0(\sigma_1 + \sigma_2) \vec{k} \times \delta(\vec{r}_1 - \vec{r}_2) \vec{k} + t_3(1 + x_0 P^\sigma) \delta(\vec{r}_1 - \vec{r}_2) \rho^\alpha((\vec{r}_1 + \vec{r}_2)/2) \\ + V_{\text{Coulomb}}(\vec{r}_1, \vec{r}_2)$$

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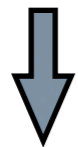
**Second step:** Simultaneous **Particle Number and Angular Momentum Projection** (after the variation).

**Third step:** Configuration mixing within the framework of the **Generator Coordinate Method (GCM)**.

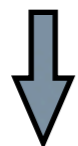
# Particle number projection

## Axial calculations $^{24}\text{Mg}$

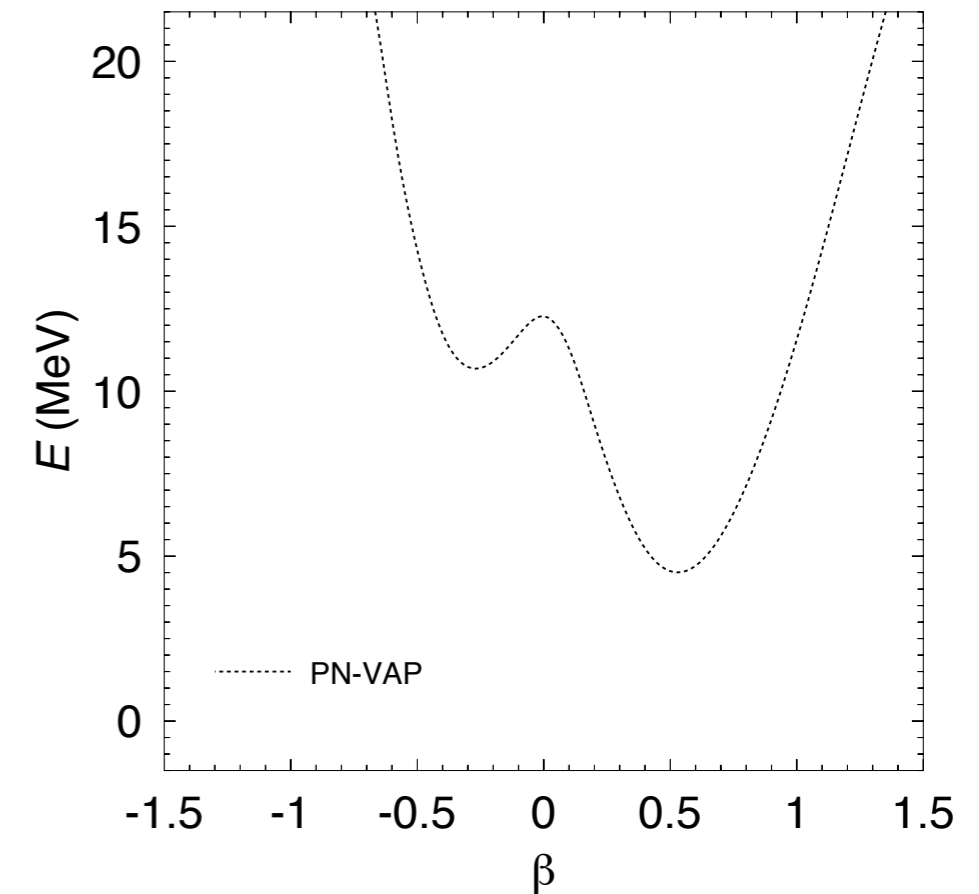
$|\Phi(\beta)\rangle$  product-type many  
body wave function



$$|\Phi^{N,Z}(\beta)\rangle = \hat{P}^N \hat{P}^Z |\Phi(\beta)\rangle$$



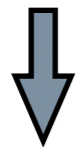
$E^{N,Z}(\beta)$  Potential Energy Surface



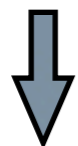
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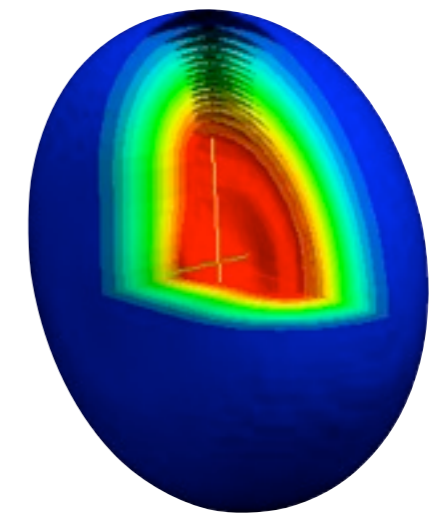
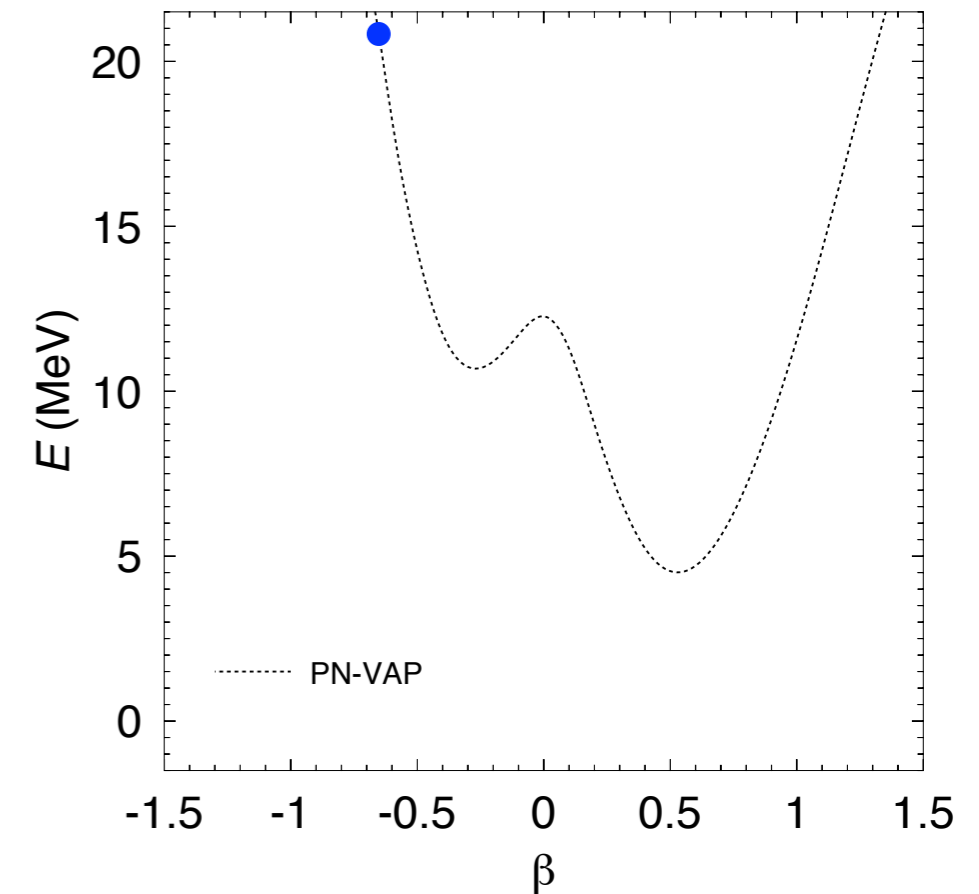
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# Particle number and angular momentum projection

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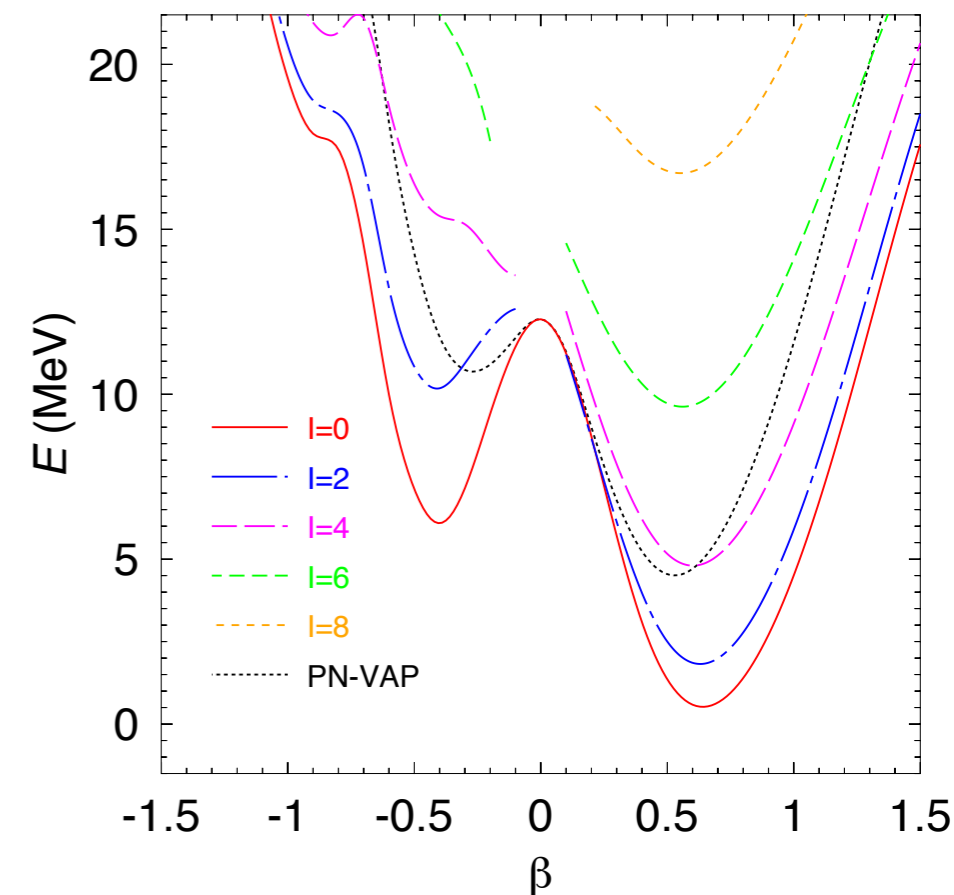
$|\Phi(\beta)\rangle$  product-type many body wave function



$$|\Phi^{I,M;N,Z}(\beta)\rangle = \hat{P}_{00}^I \hat{P}^N \hat{P}^Z |\Phi(\beta)\rangle$$



$E^{I,N,Z}(\beta)$  Projected Potential Energy Surface



# Configuration (shape) mixing

## Axial calculations $^{24}\text{Mg}$

Configuration mixing within the framework of the **Generator Coordinate Method (GCM)**.

$$|\Psi^{I;N,Z;\sigma}\rangle = \sum_{\beta} f^{I;N,Z;\sigma}(\beta) \hat{P}_{00}^I \hat{P}^N \hat{P}^Z |\Phi(\beta)\rangle$$

Configuration mixing

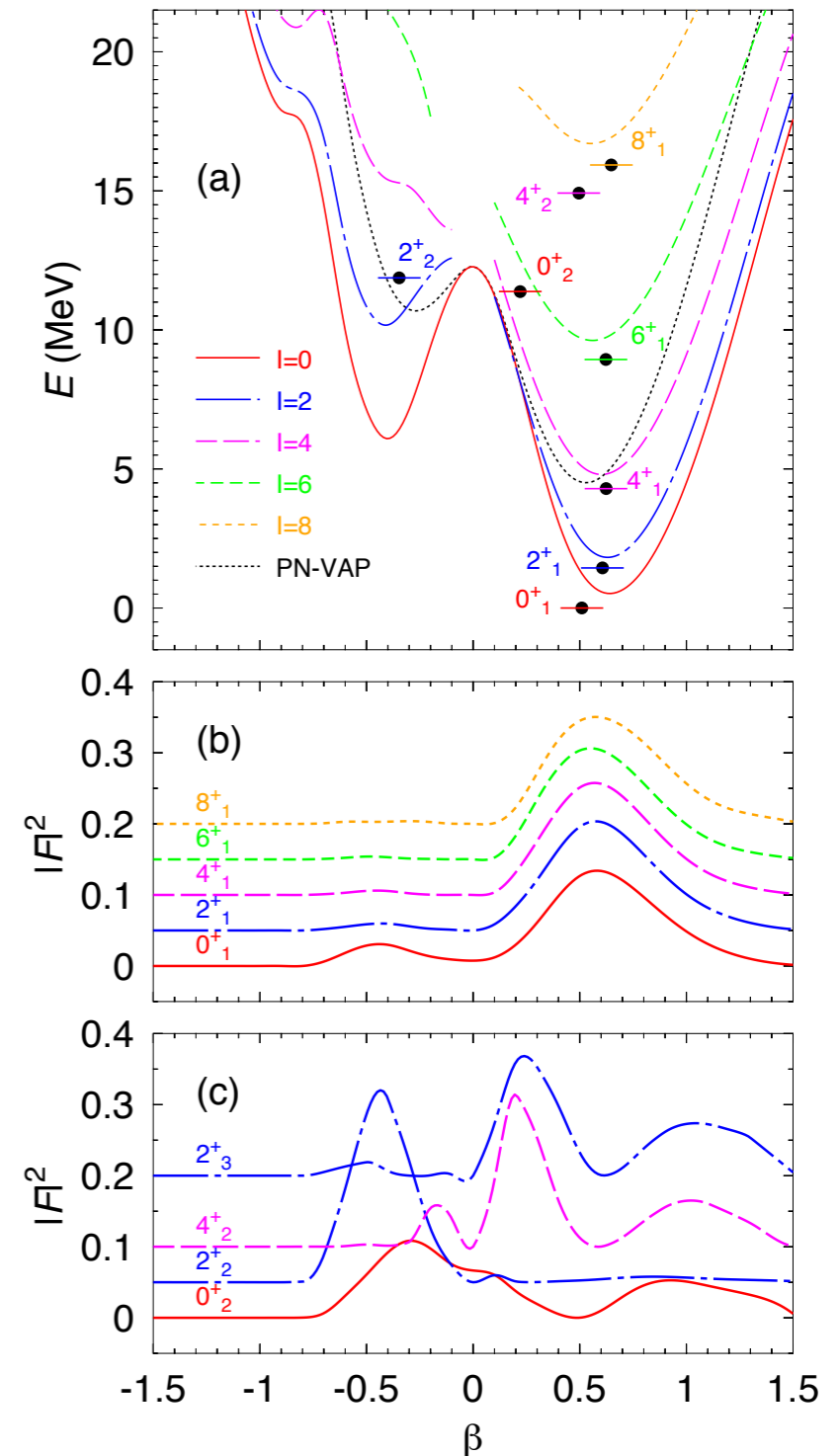
$$\sum_{\beta'} \left( \mathcal{H}_{\beta\beta'}^{I;NZ} - E^{I;NZ;\sigma} \mathcal{N}_{\beta\beta'}^{I;NZ} \right) f_{\beta'}^{I;NZ;\sigma} = 0$$

$$\mathcal{N}_{\beta\beta'}^{I;NZ} \equiv \langle \Phi(\beta) | P_{00}^I P^N P^Z | \Phi(\beta') \rangle$$

$$\mathcal{H}_{\beta\beta'}^{I;NZ} \equiv \langle \Phi(\beta) | \hat{H}_{2b} P_{00}^I P^N P^Z | \Phi(\beta') \rangle + \varepsilon_{DD}^{I;NZ} [\Phi(\beta), \Phi'(\beta')]$$

Hill-Wheeler-Griffin equations

- Energy spectrum
- Observables (mass, radius,  $B(E2)$ , etc.)
- “Collective w.f.”

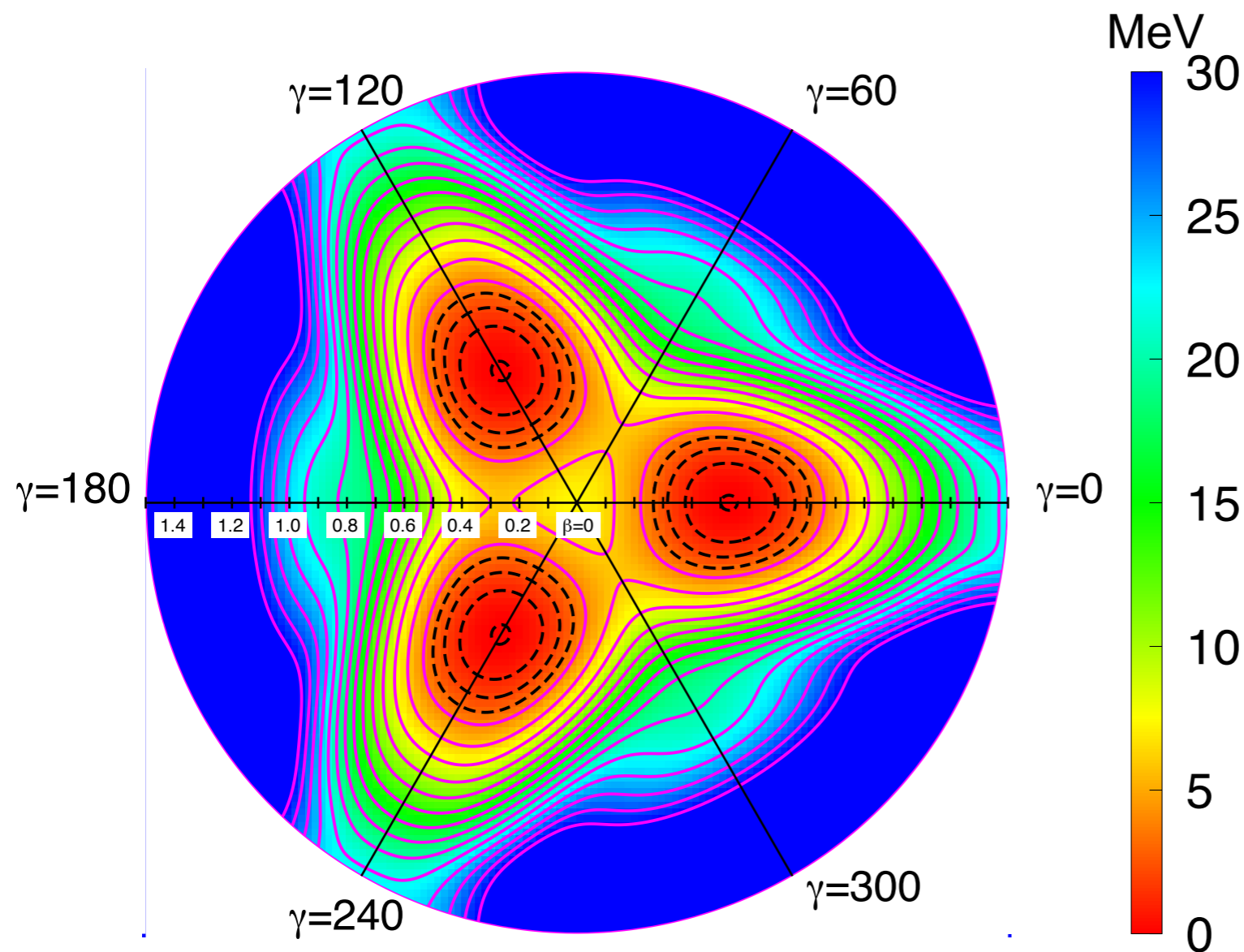




# Particle number projection

## Triaxial calculations $^{24}\text{Mg}$

$$\delta E^{N,Z} [\bar{\Phi}(\beta, \gamma)] \Big|_{\bar{\Phi}=\Phi} = 0 \quad E^{N,Z}[\Phi] = \frac{\langle \Phi | \hat{H}_{2b} \hat{P}^N \hat{P}^Z | \Phi \rangle}{\langle \Phi | \hat{P}^N \hat{P}^Z | \Phi \rangle} + \varepsilon_{DD}^{N,Z}(\Phi) - \lambda_{q_{20}} \langle \Phi | \hat{Q}_{20} | \Phi \rangle - \lambda_{q_{22}} \langle \Phi | \hat{Q}_{22} | \Phi \rangle$$



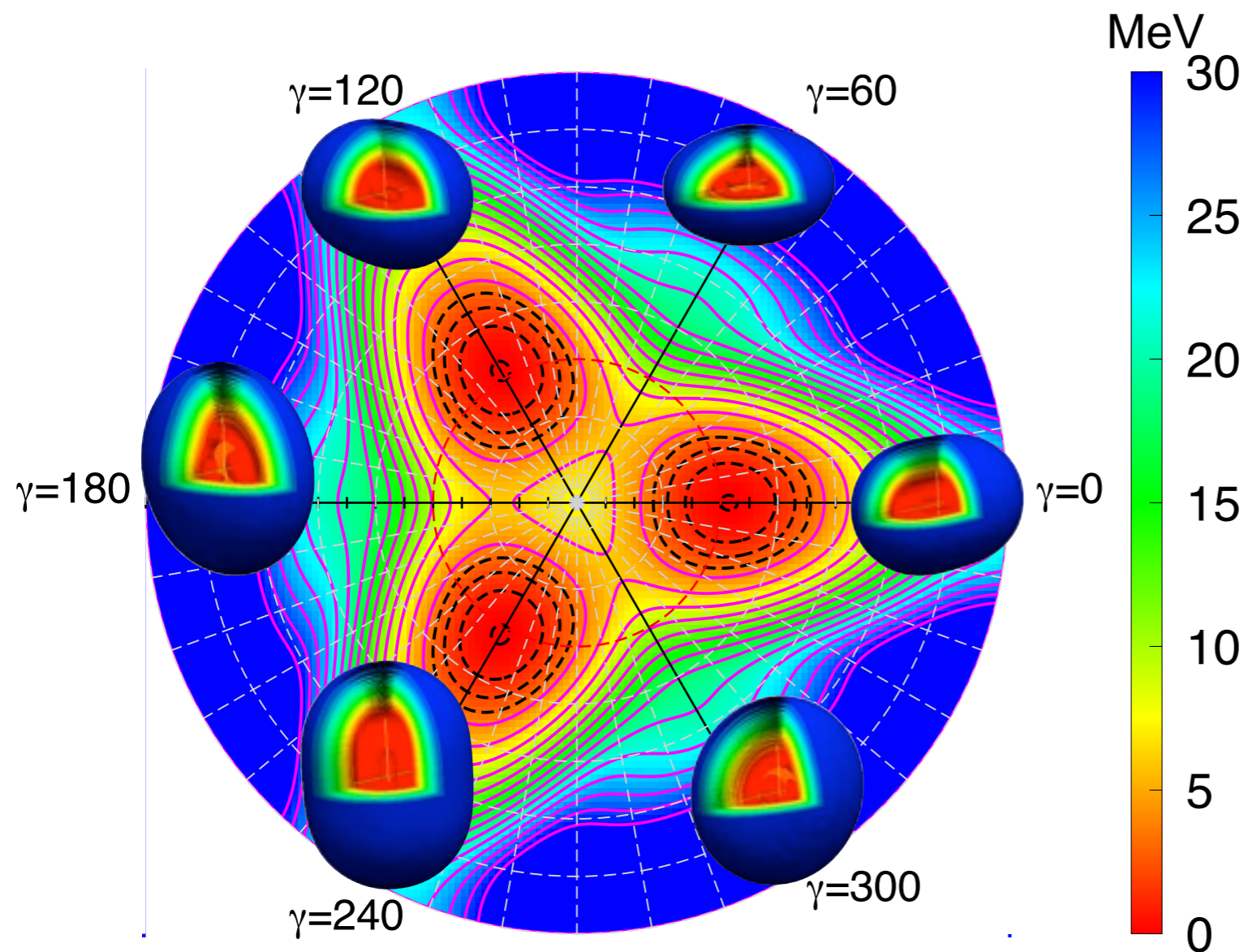
- Symmetry corresponding to the different orientation of the axes
- All configurations are included between  $\gamma \in [0^\circ, 60^\circ]$



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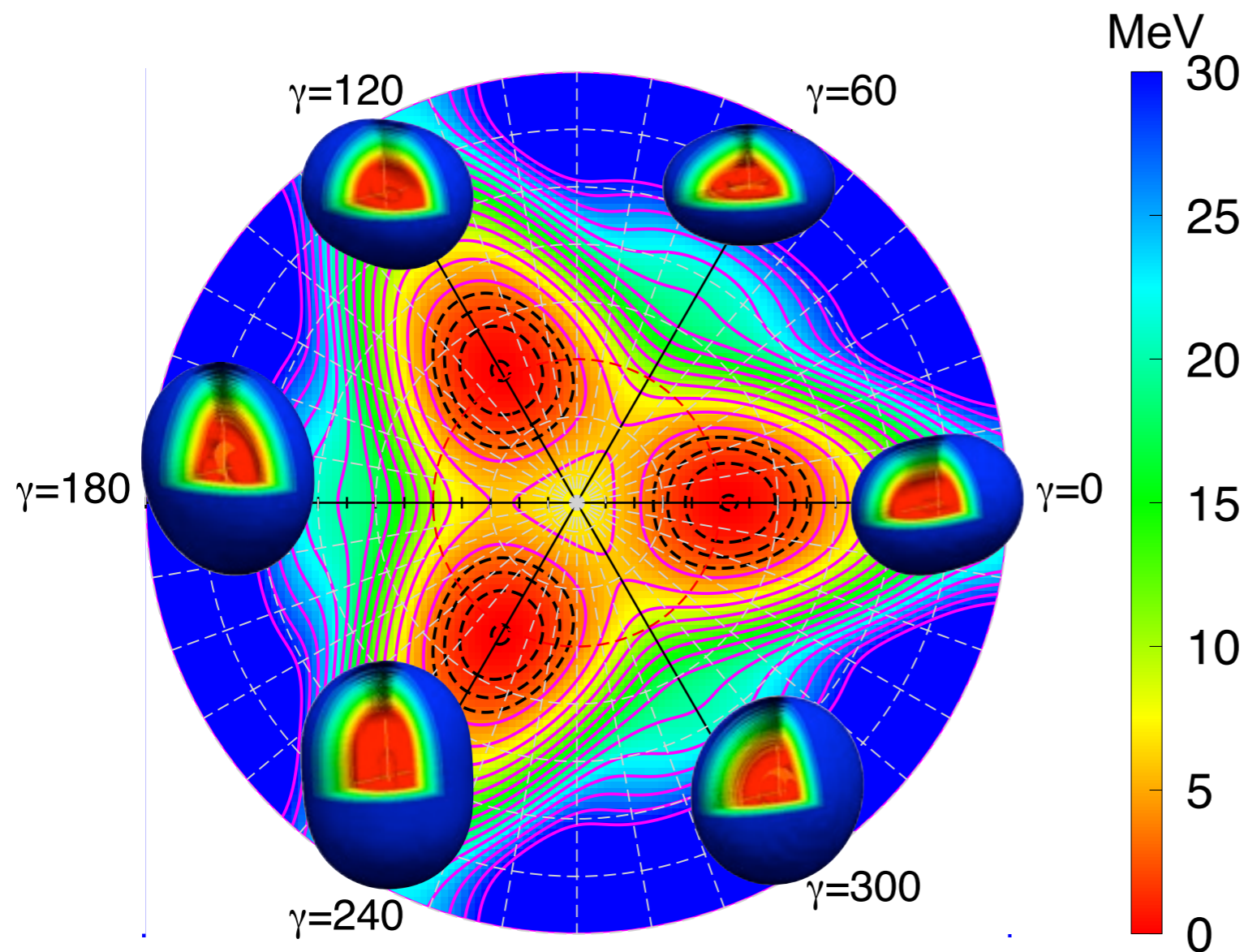


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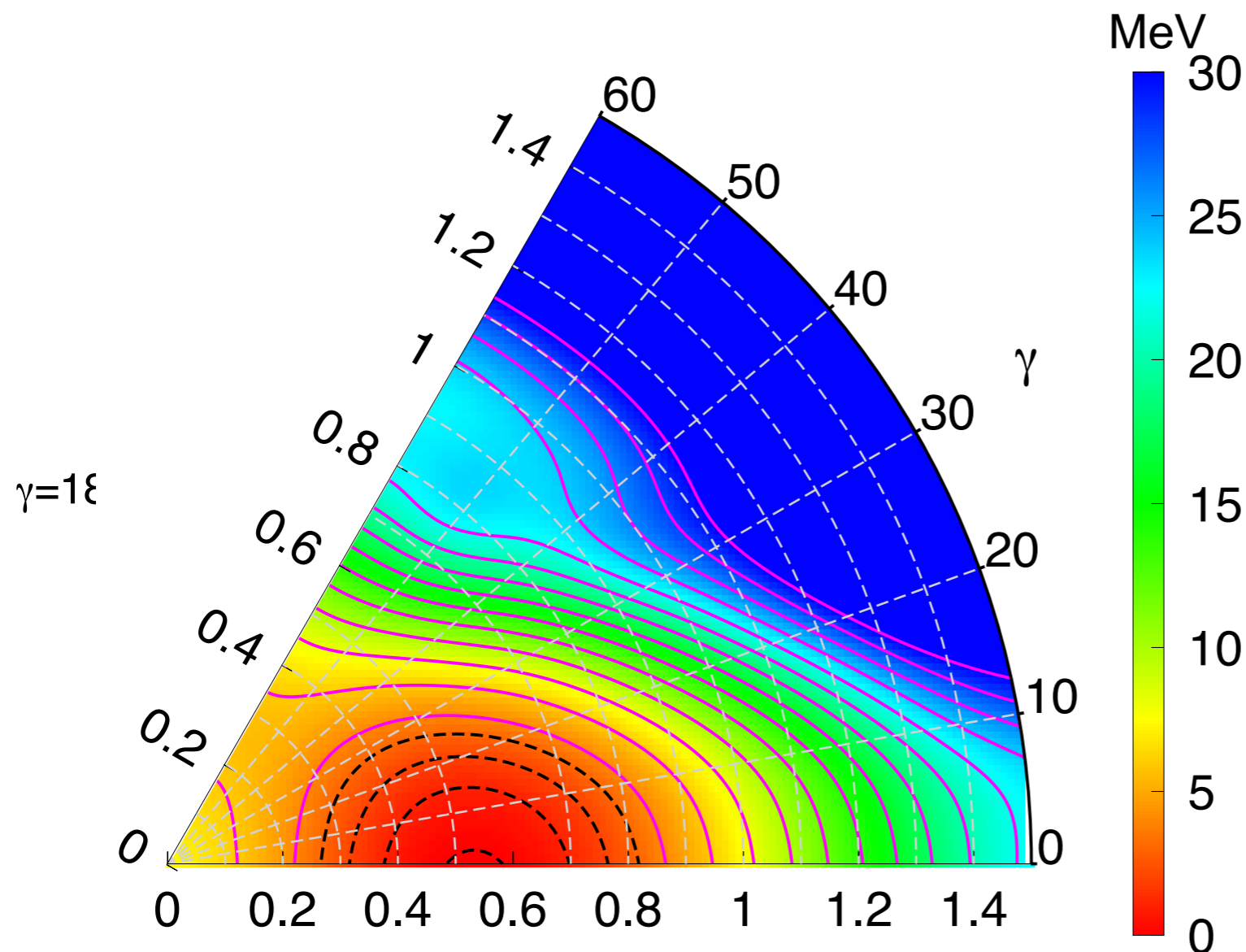


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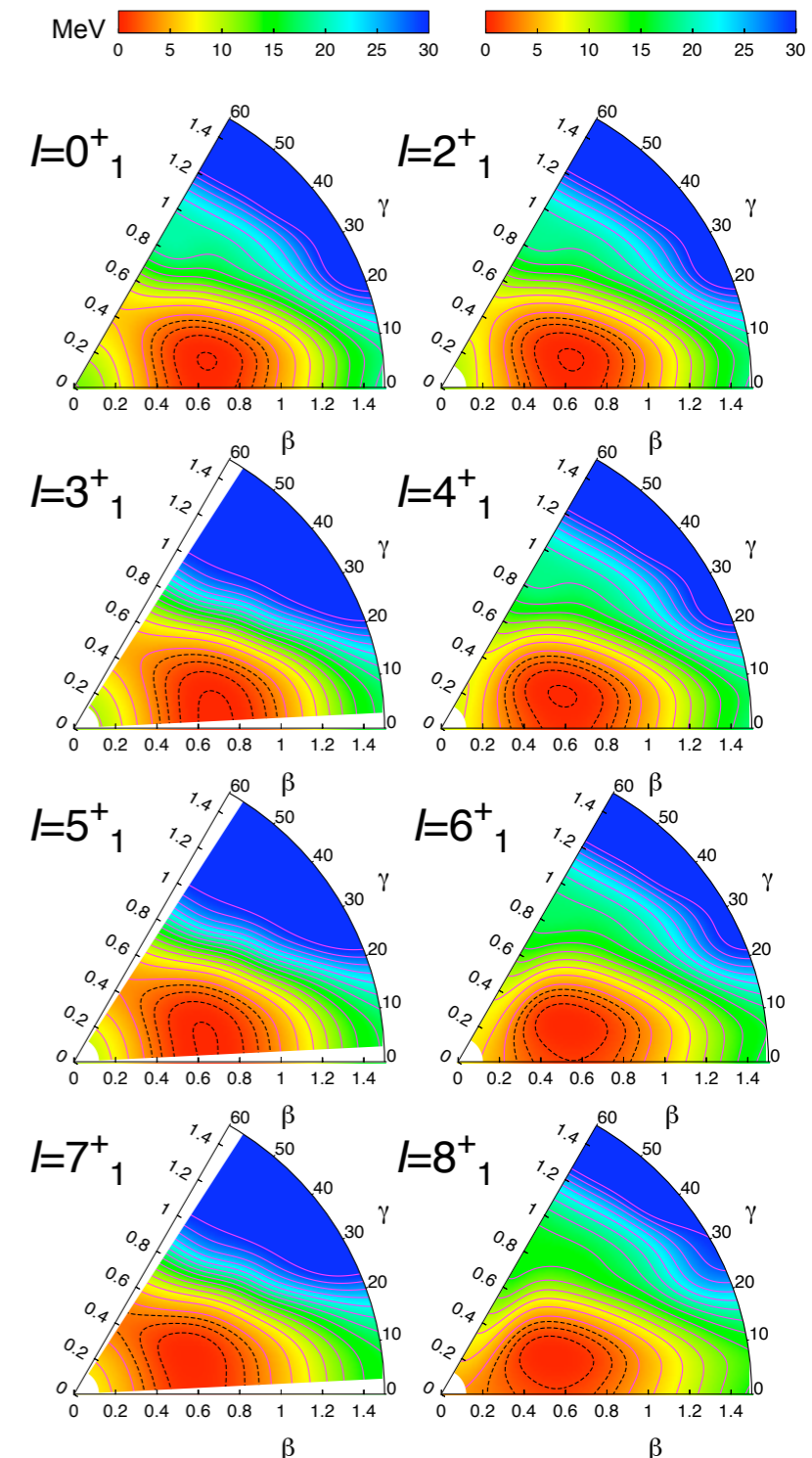
# Particle number and angular momentum projection

## Triaxial calculations $^{24}\text{Mg}$

$$|IMK; NZ; \beta\gamma\rangle = \frac{2I+1}{8\pi^2} \int \mathcal{D}_{MK}^{I*}(\Omega) \hat{R}(\Omega) \hat{P}^N \hat{P}^Z |\Phi(\beta, \gamma)\rangle d\Omega$$

$$|IM; NZ; \beta\gamma\rangle = \sum_K g_K^{IM; NZ; \beta\gamma} |IMK; NZ; \beta\gamma\rangle$$

- Minimum displaced to triaxial shapes.
- Projection onto odd  $I$  angular momentum
- Softening of PES with increasing  $I$ .
- Difference between triaxial minimum and axial saddle point of  $\sim 0.7$  MeV ( $0^+$ )



# Configuration (shape) mixing

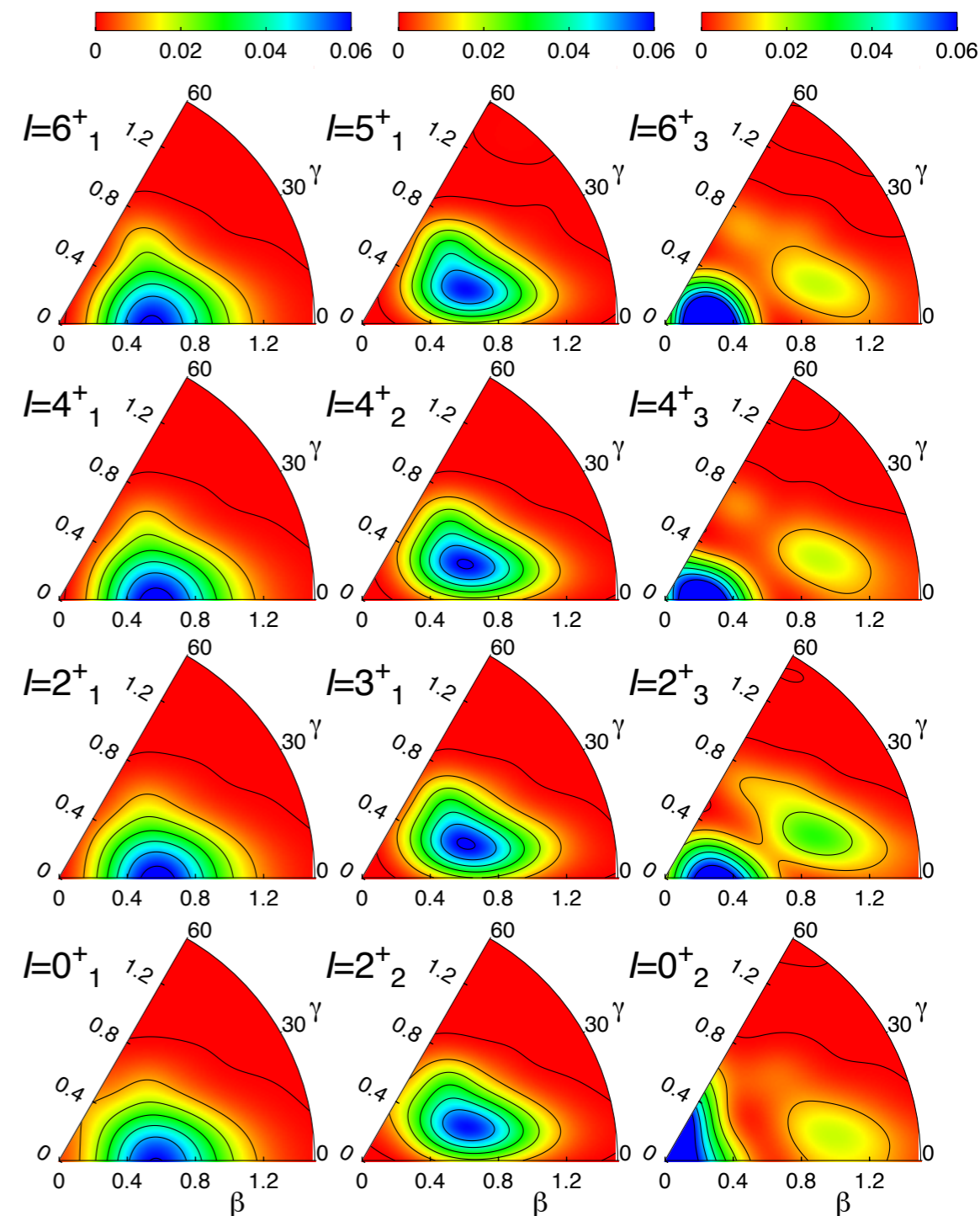
## Triaxial calculations $^{24}\text{Mg}$

Configuration mixing within the framework of the **Generator Coordinate Method (GCM)**.  $K$  and deformation mixing

$$|IM; NZ\sigma\rangle = \sum_{K\beta\gamma} f_{K\beta\gamma}^{I;NZ,\sigma} |IMK; NZ; \beta\gamma\rangle$$

$$\sum_{K'\beta'\gamma'} \left( \mathcal{H}_{K\beta\gamma K'\beta'\gamma'}^{I;NZ} - E^{I;NZ;\sigma} \mathcal{N}_{K\beta\gamma K'\beta'\gamma'}^{I;NZ} \right) f_{K'\beta'\gamma'}^{I;NZ;\sigma} = 0$$

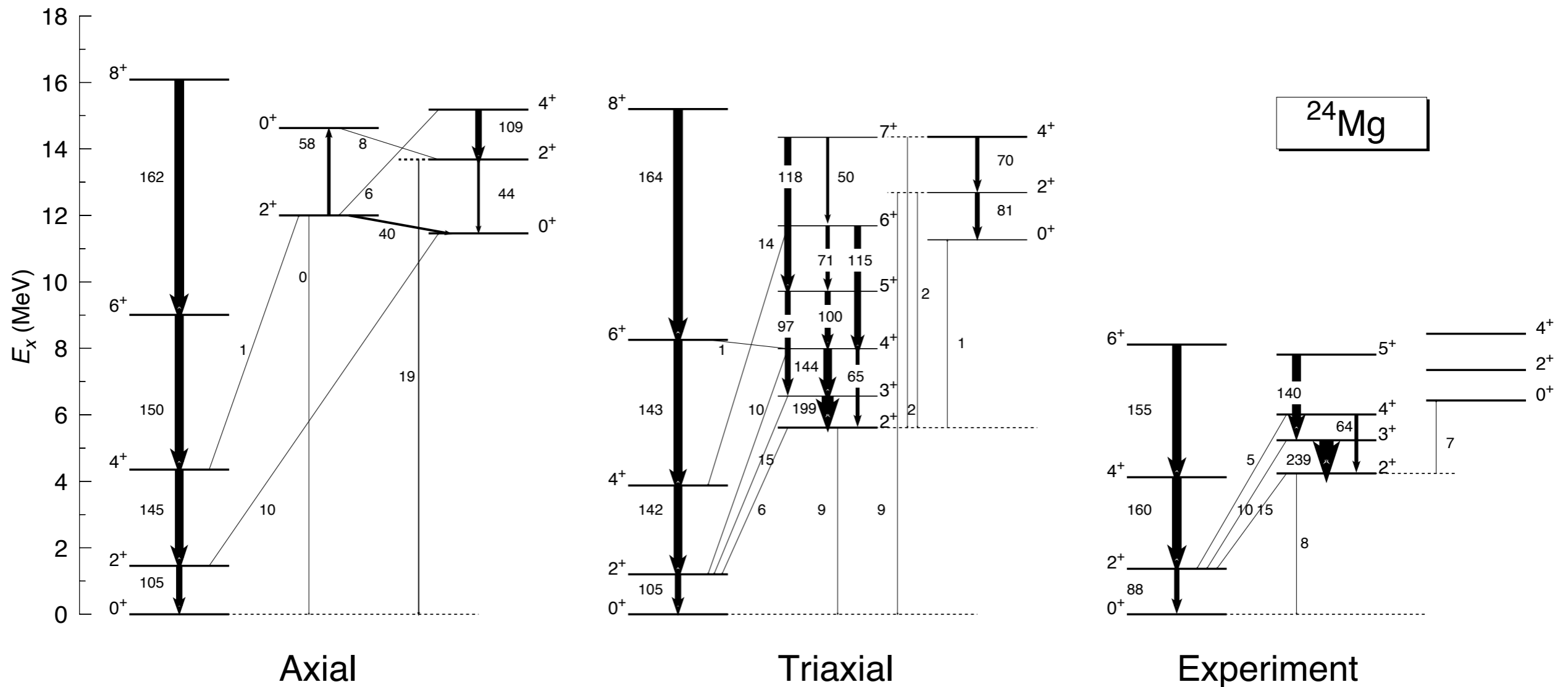
- Axial ground state rotational band
- Second band associated to a gamma band
- Third band with shape mixing



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## Triaxial calculations $^{24}\text{Mg}$

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 **$K$  and deformation mixing**



- **Magic numbers in the valley of the stability**

- ✓ Very stable (high binding energies per nucleon and separation energies).
- ✓ Spherical shape.
- ✓ High excitation energy of the first  $2^+$  state.
- ✓ Small reduced transition probabilities between the first  $2^+$  and ground states.
- ✓ Magic numbers (2, 8, 20, 28, 50, 82, 126) correspond to the shell closures of a harmonic oscillator+spin-orbit single particle potential.

- **Magic numbers in exotic nuclei**

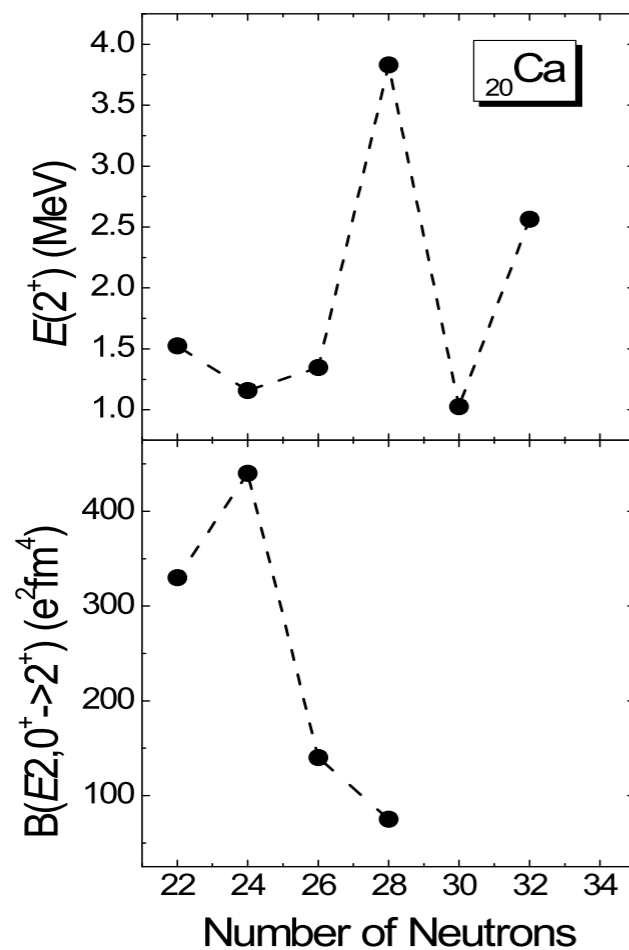
- ✓ Degradation of the traditional shell closures:  $^{32}\text{Mg}$  ( $N=20$ ),  $^{42}\text{Si}$  ( $N=28$ )
- ✓ Appearance of new shell closures:  $N=32$
- ✓ Key relevance in r-process nucleosynthesis (waiting points)
- ✓ Shell quenching in  $N=82$  for Cadmium isotopes?



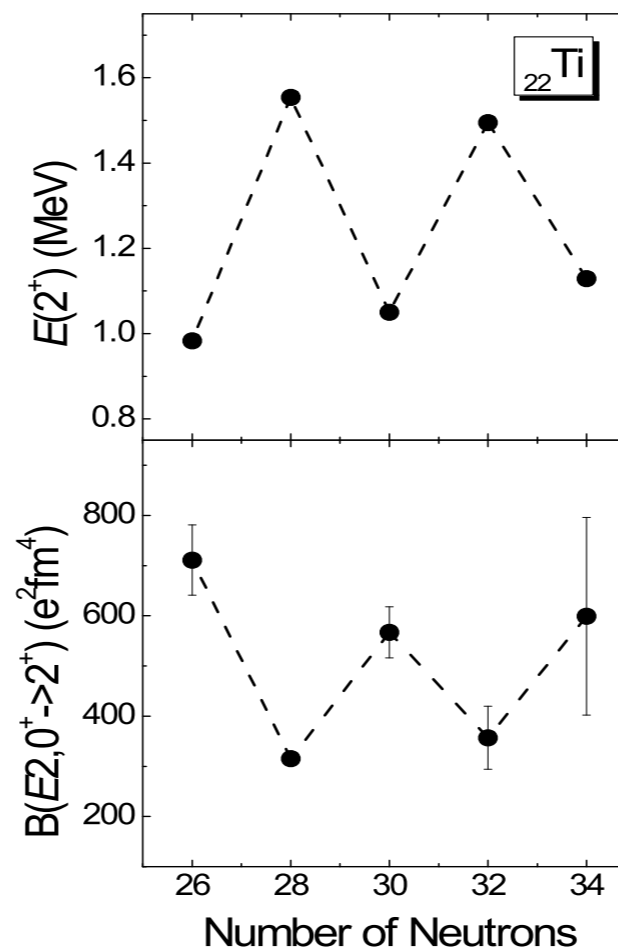
# Shell closures

- $N=32$  and/or  $N=34$  in Ca, Ti and Cr isotopes.

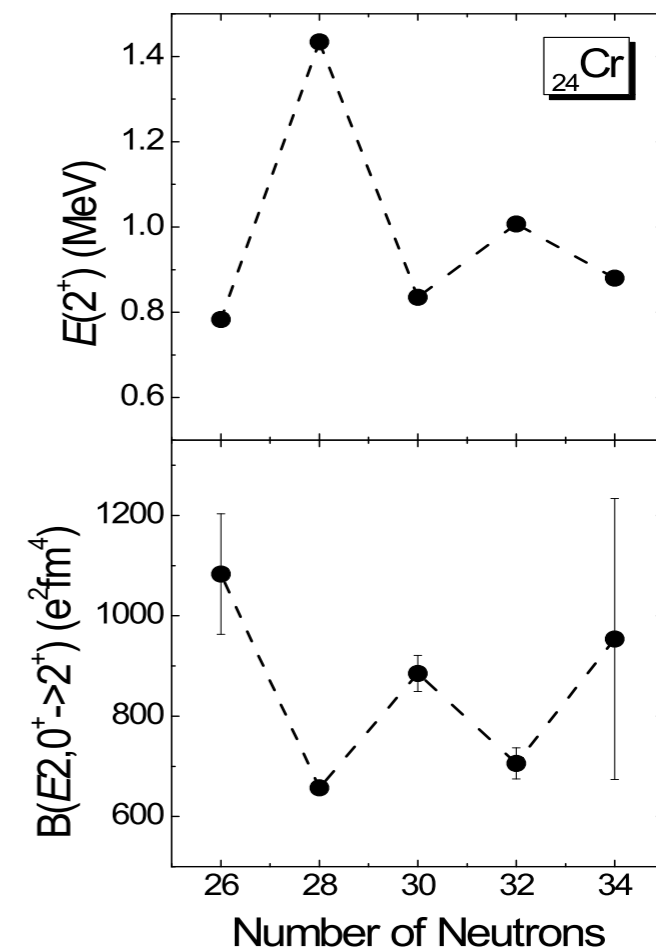
The tendency of the **experimental data** for the excitation energies  $E(2^+)$  and transition probabilities  $B(E2, 0^+ \rightarrow 2^+)$  shows the presence of sub-shell closures.



Schielke *et al* (PL B571, 29(2003))



Dinca *et al* (PR C71,041302(2005))

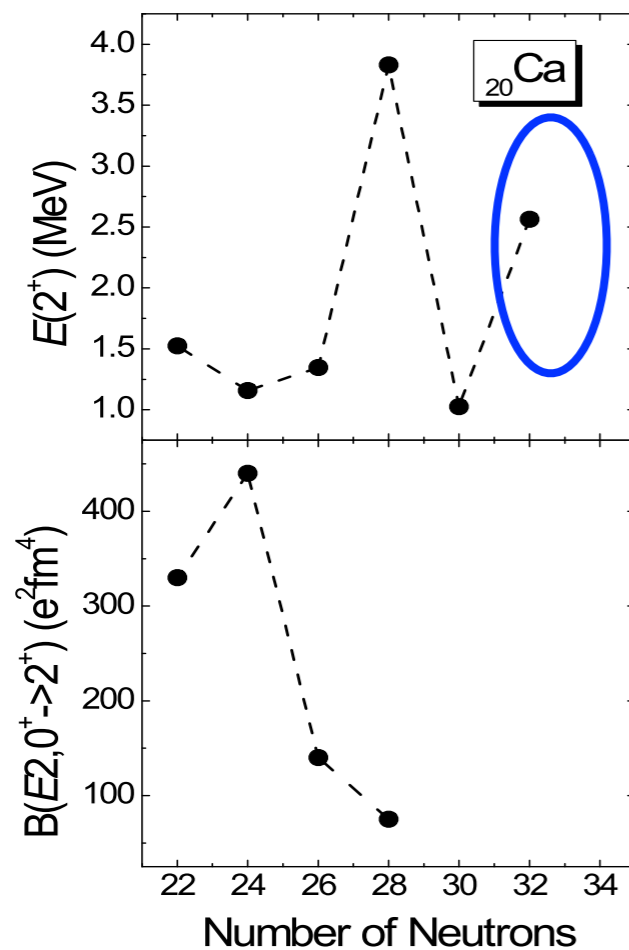


Bürger *et al* (PL B662, 29(2005))

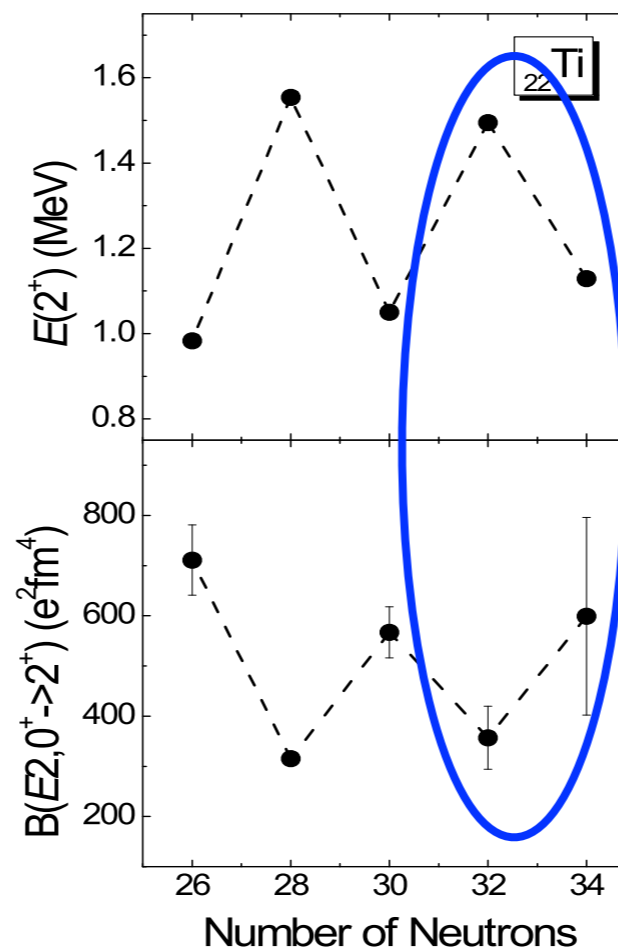
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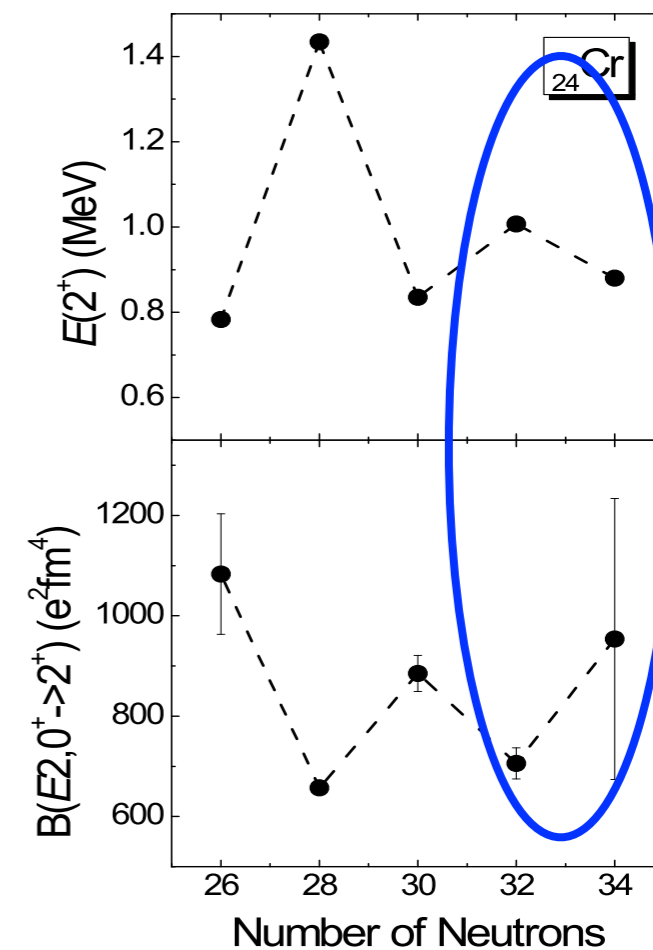
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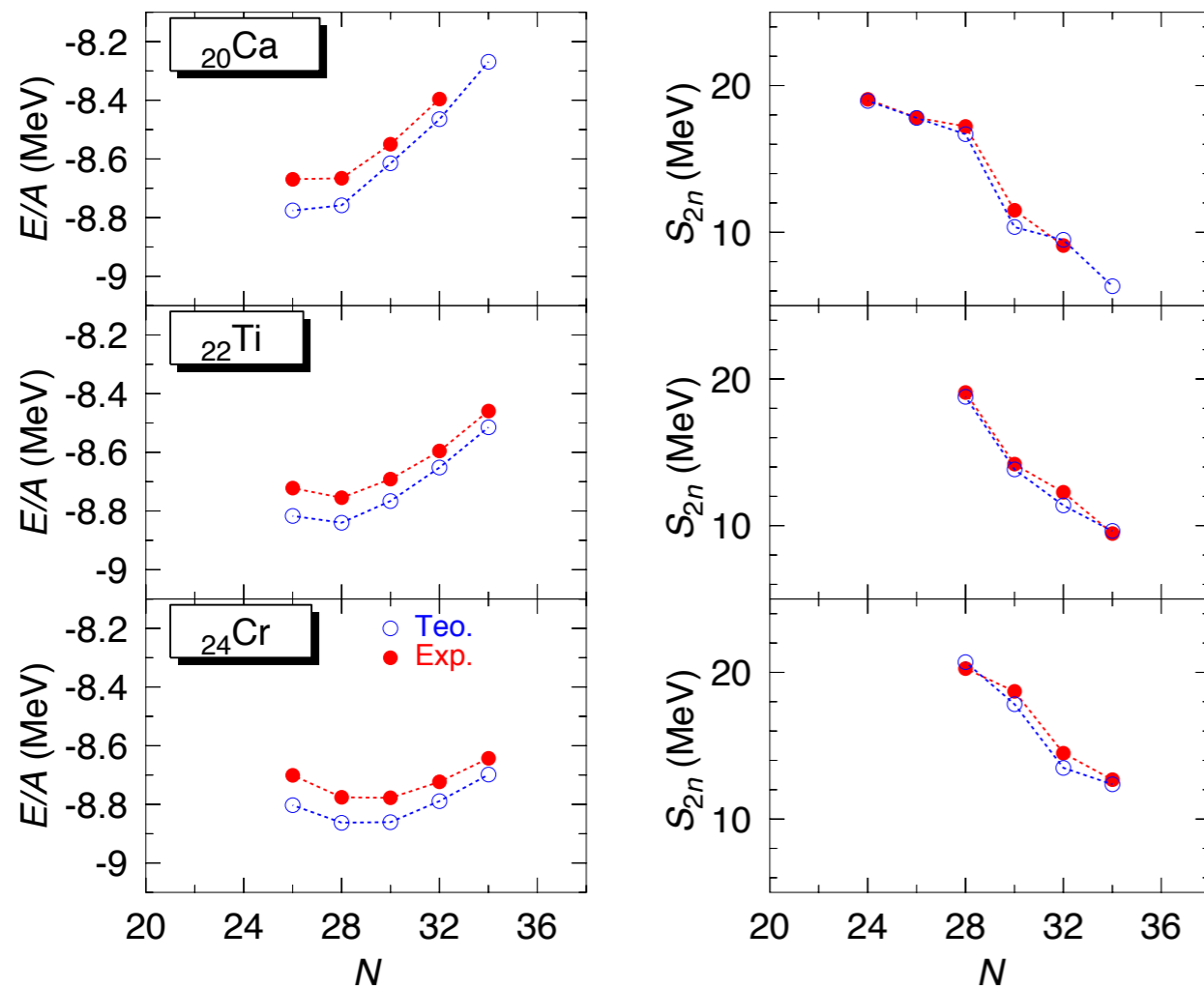
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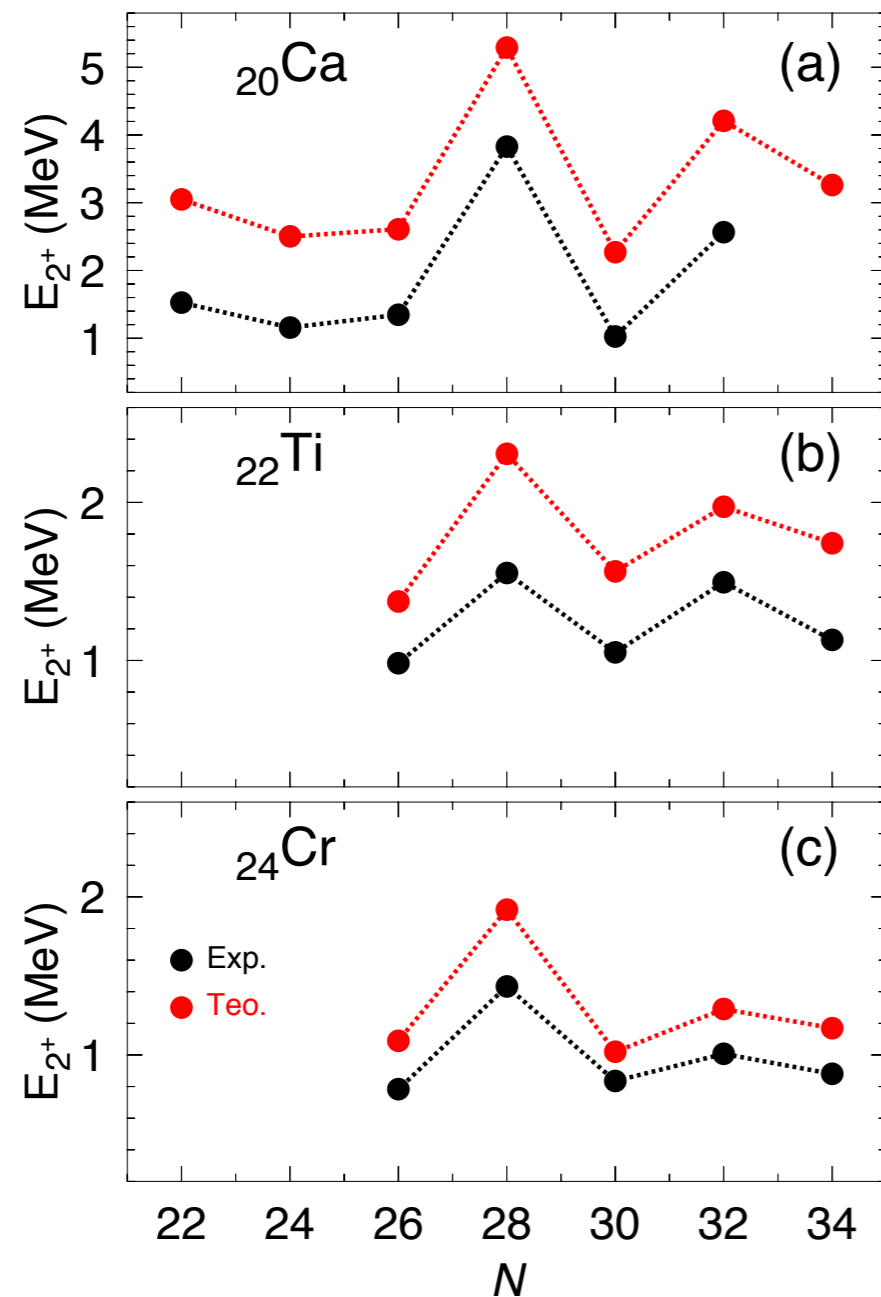


✓ AXIAL calculations

✓ Good agreement in the binding energies and two neutron separation energies.

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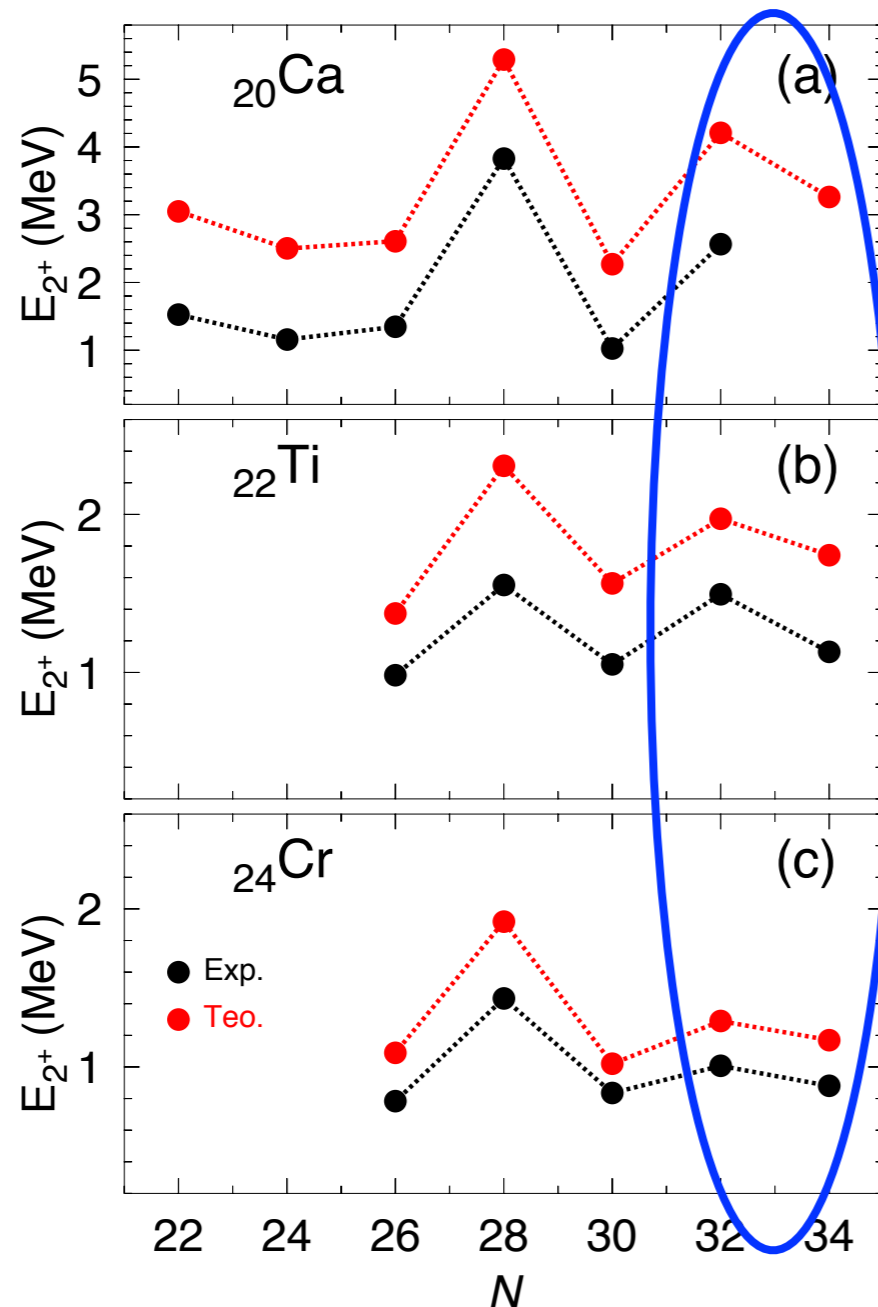
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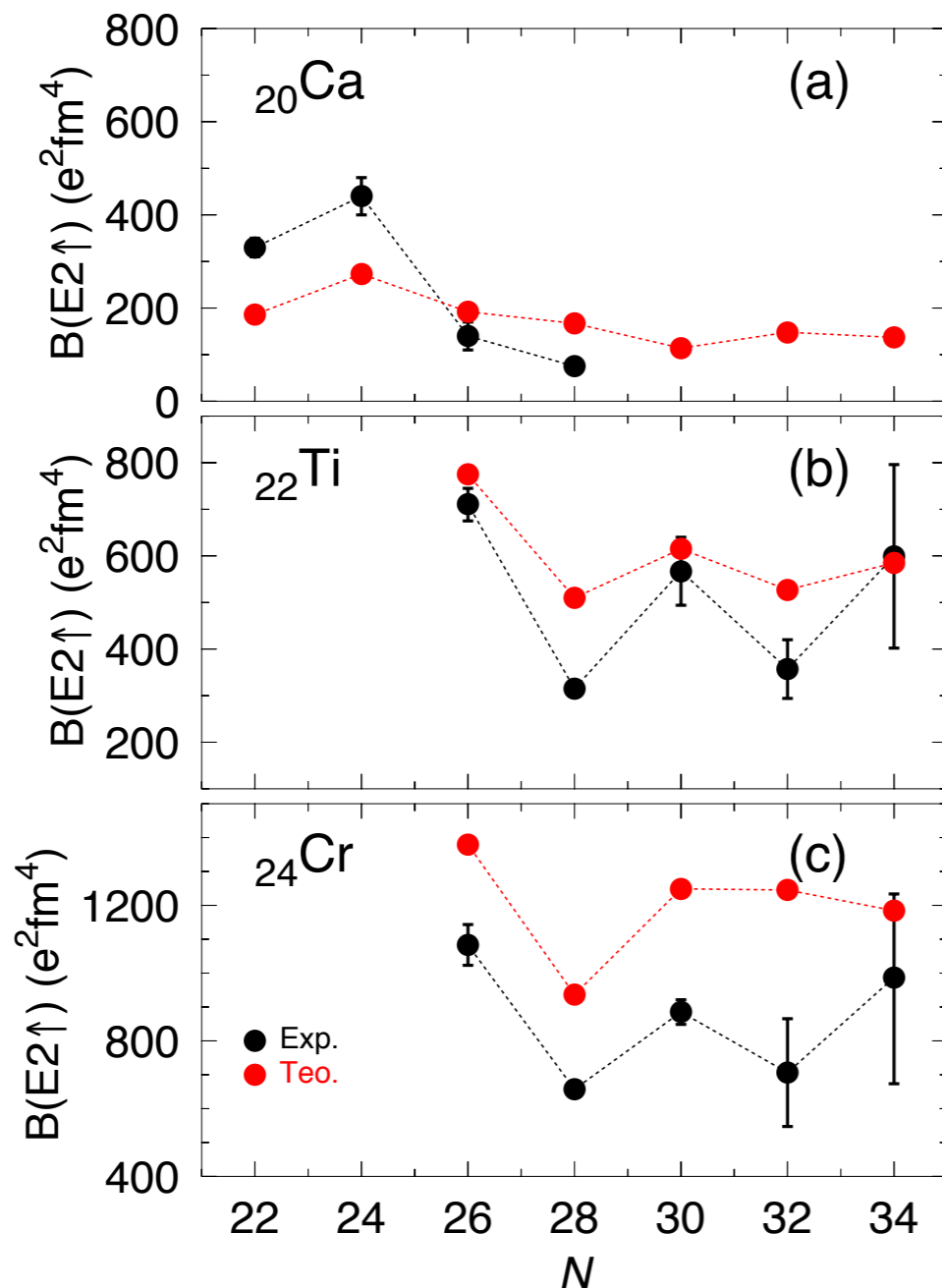
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✓ Staggering of the  $B(E2)$  in Ti isotopes is reproduced without any effective charges

✓ Qualitative agreement in the  $B(E2)$  especially in the lightest isotopes.

T.R.R and J.L. Egido, Phys. Rev. Lett. 99, 06201 (2007)

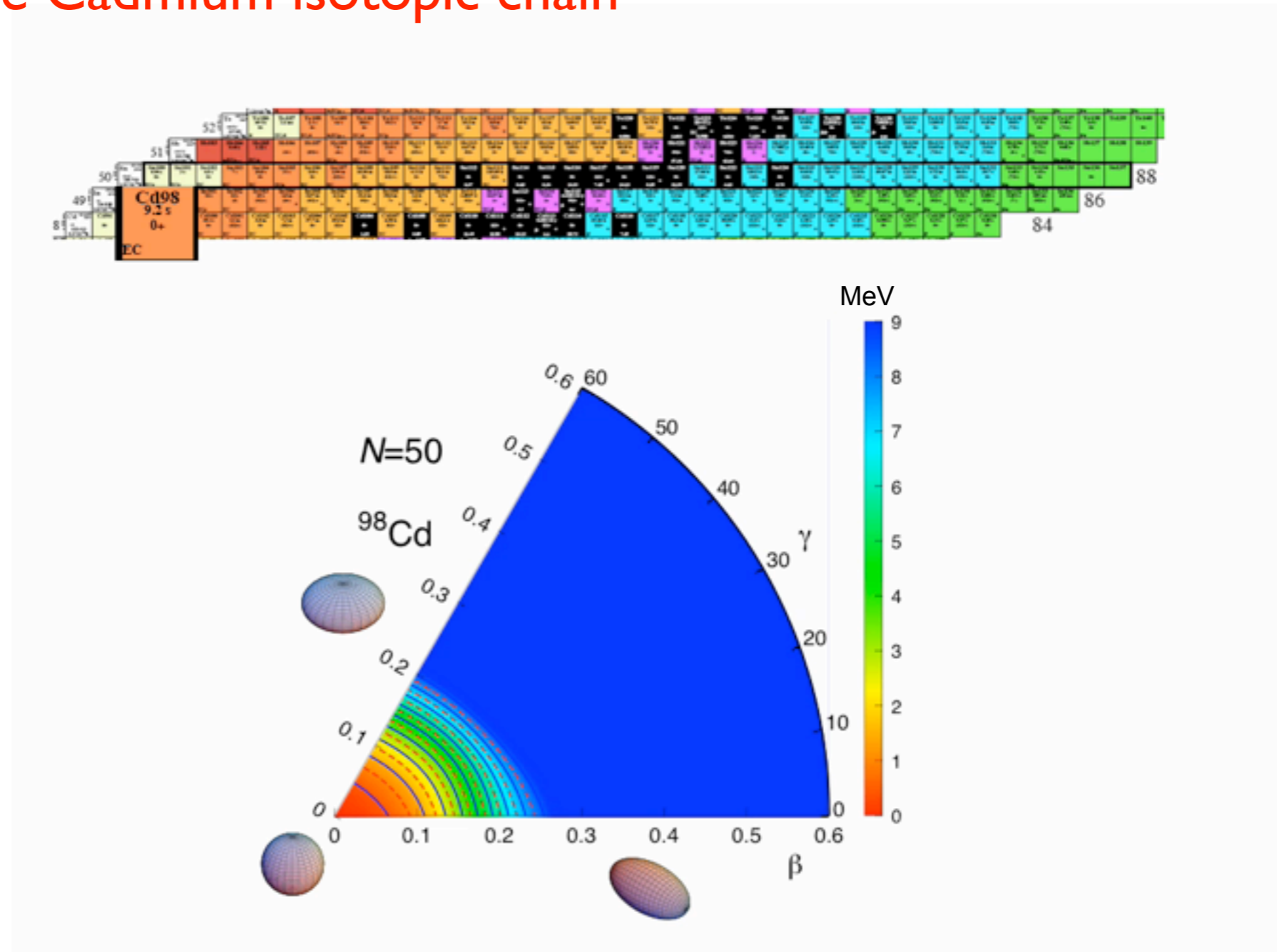
# Shell closures

## Shape evolution in the Cadmium isotopic chain

✓ Shape evolves from  $N=50$  to  $N=82$  magic number through prolate axially symmetric structures

✓ Highest deformation is found in mid-shell nuclei ( $\beta \sim 0.2$ )

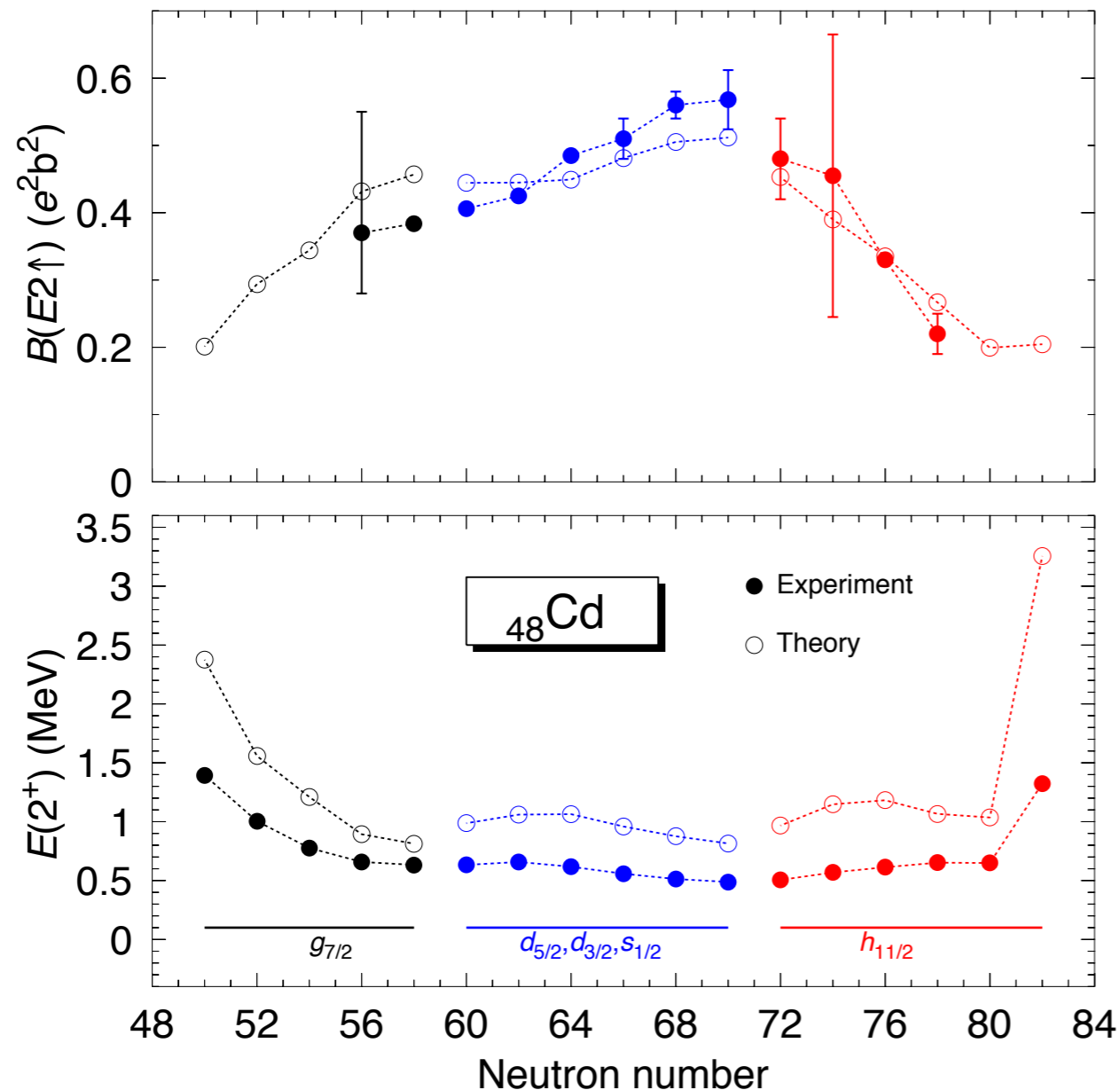
✓ Rest of calculations will assume axial symmetry





# Shell closures

## ● Systematics of the $E(2)$ and $B(E2)$ in Cadmium isotopes



✓ AXIAL calculations

✓ Good qualitative agreement for the  $E(2^+)$  excitation energies and  $B(E2)$  transition probabilities from shell to shell

✓  $N=50-58$  parabolic behavior (filling  $g_{7/2}$  shell)

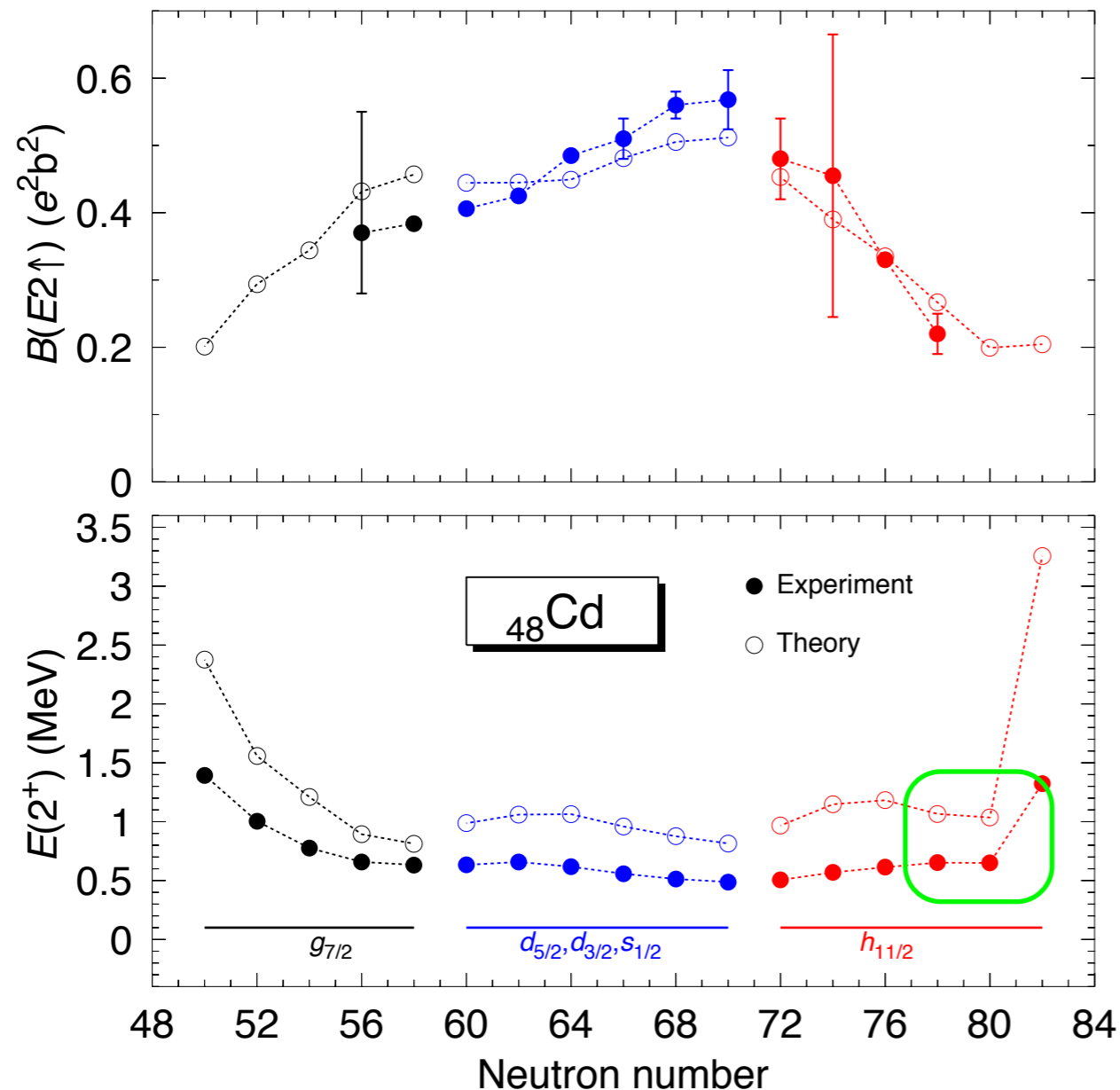
✓  $N=60-70$  flat behavior (filling  $d_{5/2}, d_{3/2}, s_{1/2}$  shells)

✓ Anomalous behavior of  $E(2^+)$  for  $^{128}\text{Cd}$  has been well reproduced

T.R.R., J.L. Egido, A. Jungclaus, Phys. Lett. B 668, 410 (2008)

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# Shape mixing and coexistence

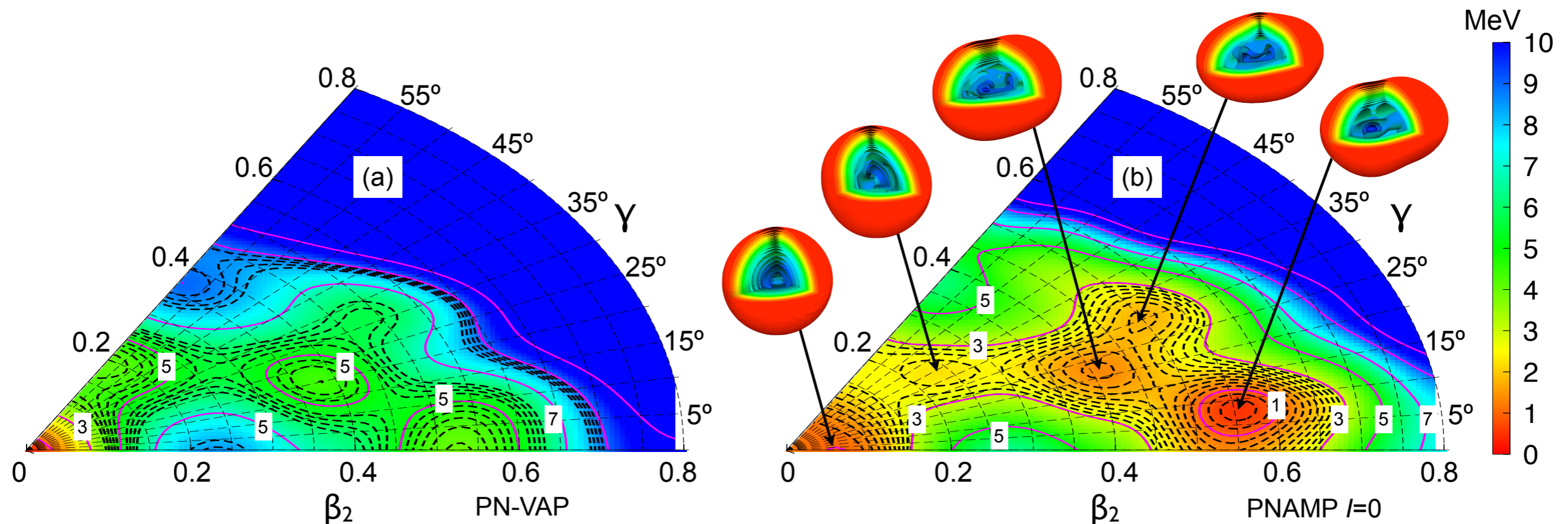
## Triaxial calculations in rp-process waiting point $^{80}\text{Zr}$

- Five minima are closer in energy whenever the rotational invariance is restored.
- Absolute minima corresponds to deformed configuration  $\beta\sim 0.55$
- Barriers between the minima are less than 1 MeV. Mixing?

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T.R.R and J.L. Egido, Phys. Lett. B 705, 255 (2011).

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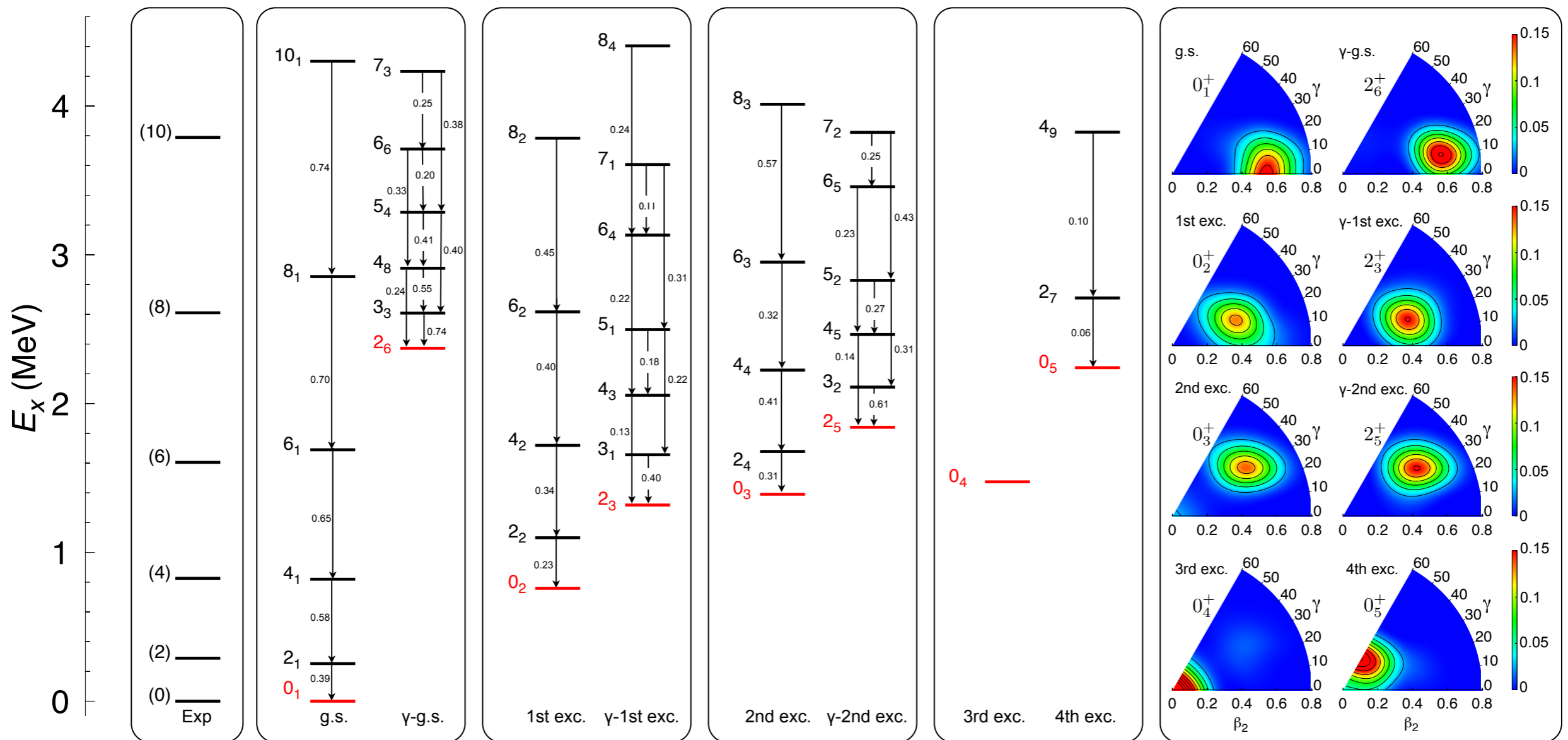
I. Introduction

2. Nuclear structure

3.  $0\nu\beta\beta$  decay

4. Summary and outlook

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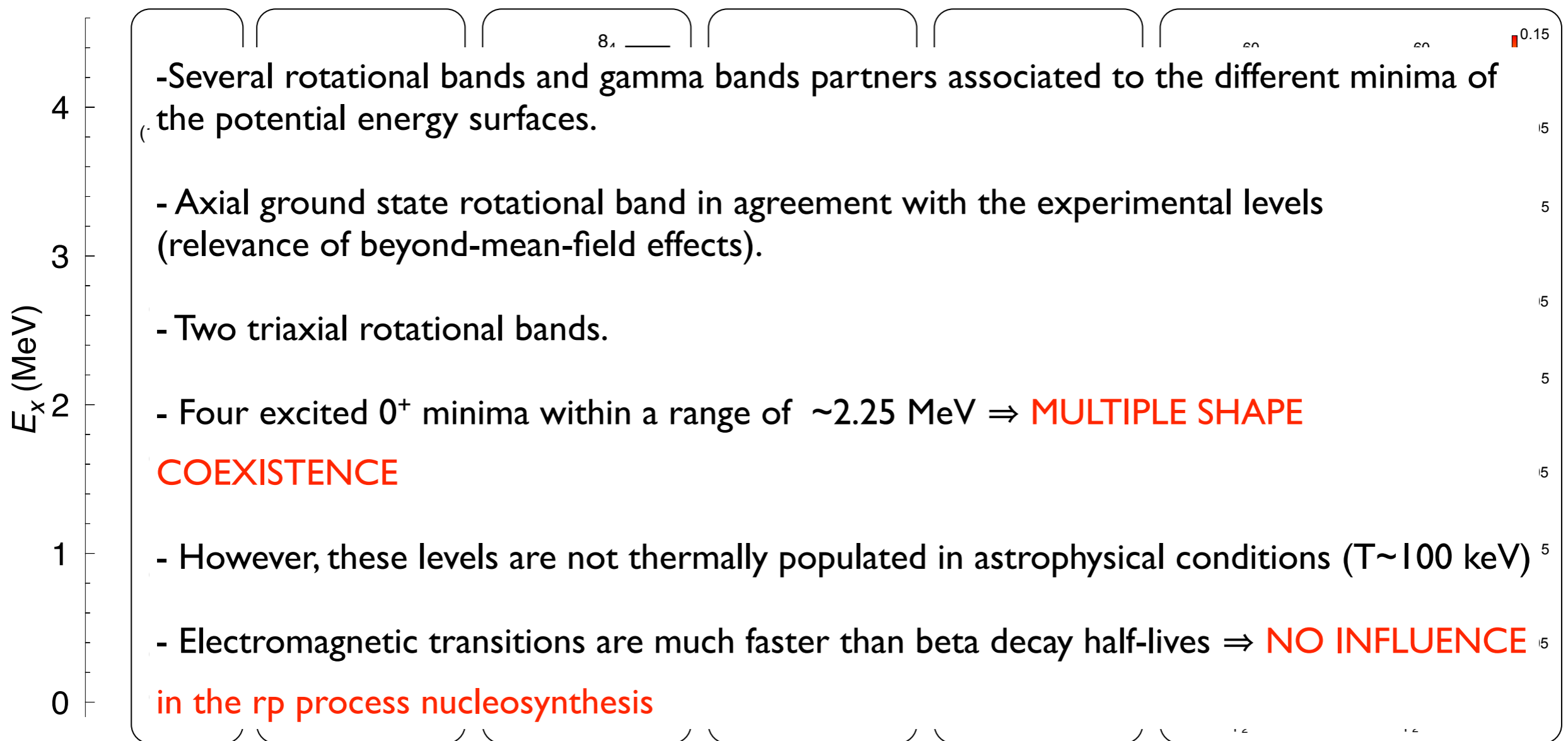


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# Shape mixing and coexistence

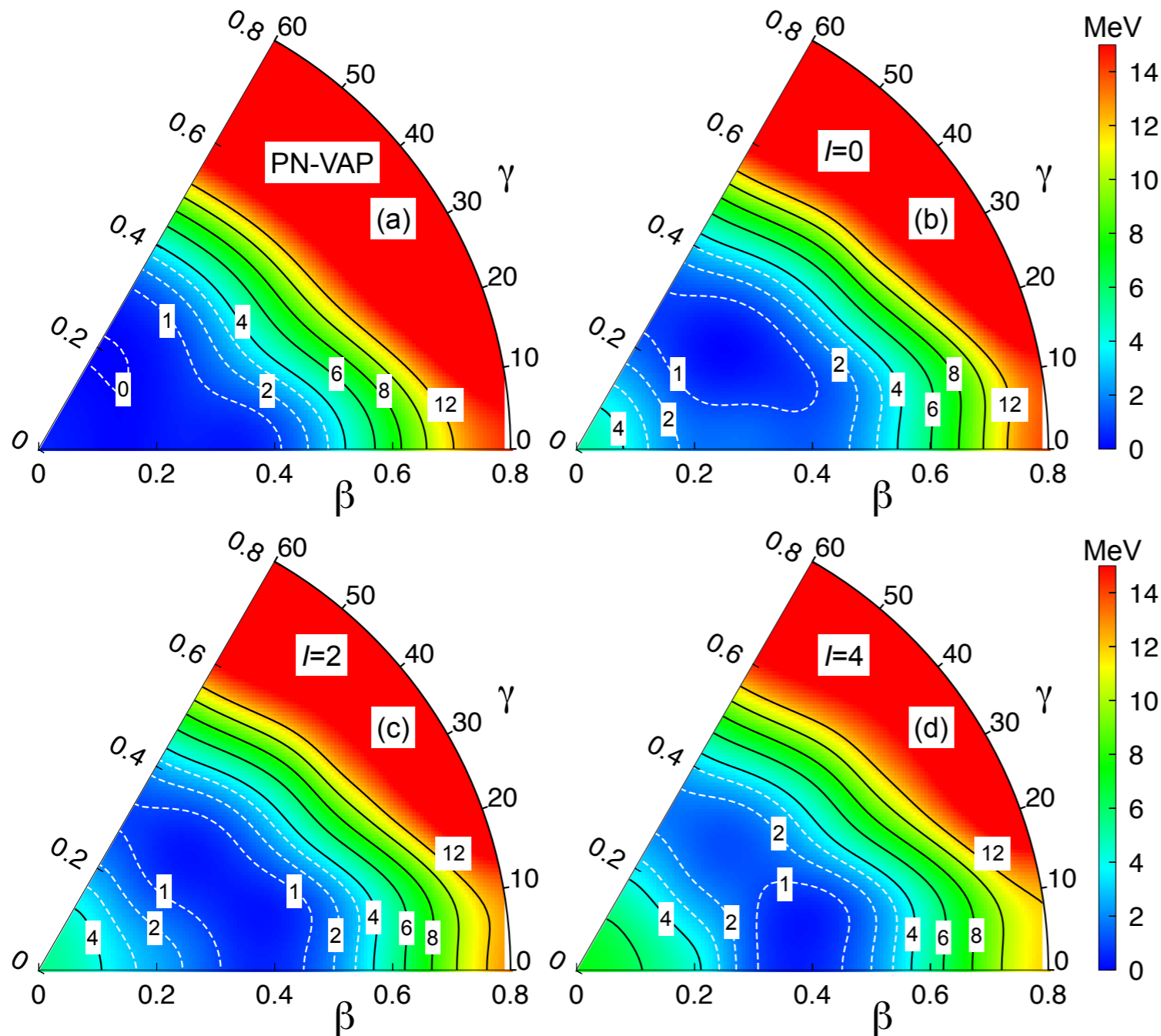
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T.R.R and J.L. Egido, Phys. Lett. B 705, 255 (2011).

# Shape mixing and coexistence

## Triaxial calculations $^{44}\text{S}$



✓  $N=28$  shell closure is already broken at the PN-VAP level

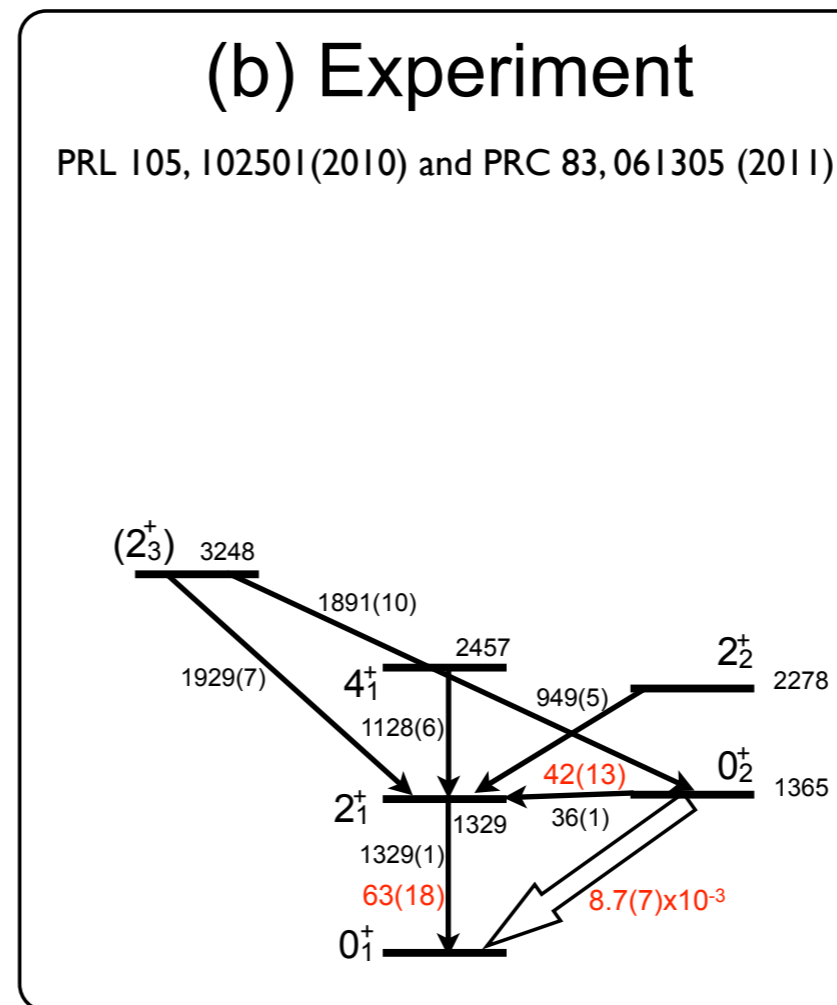
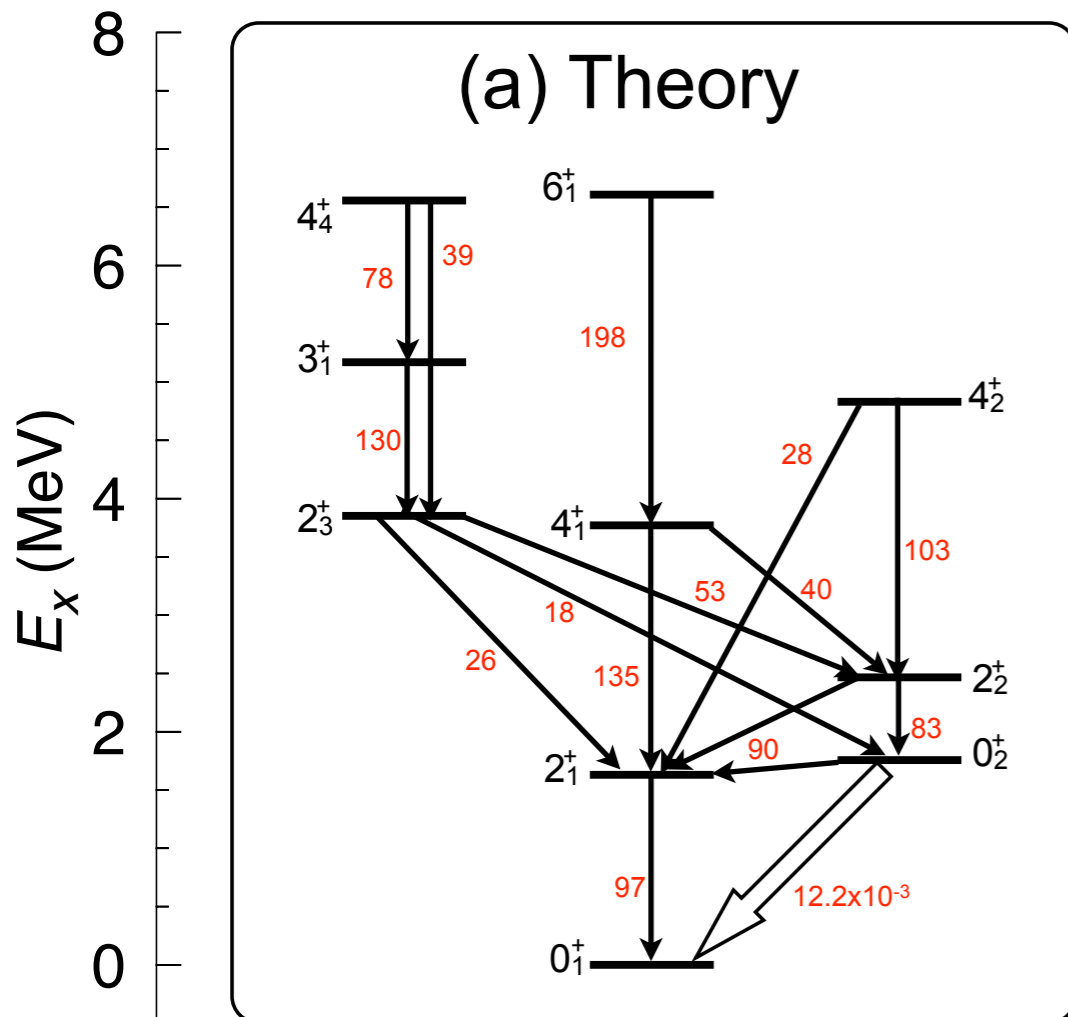
✓ Very flat surface in the gamma direction: Shape mixing rather than shape coexistence

✓ Oblate shapes are a bit lower in energy for  $l=0$  and the contrary for  $l=4$

T.R.R and J.L. Egido, PRC 84, 051307 (2011)

# Shape mixing and coexistence

## Triaxial calculations $^{44}\text{S}$

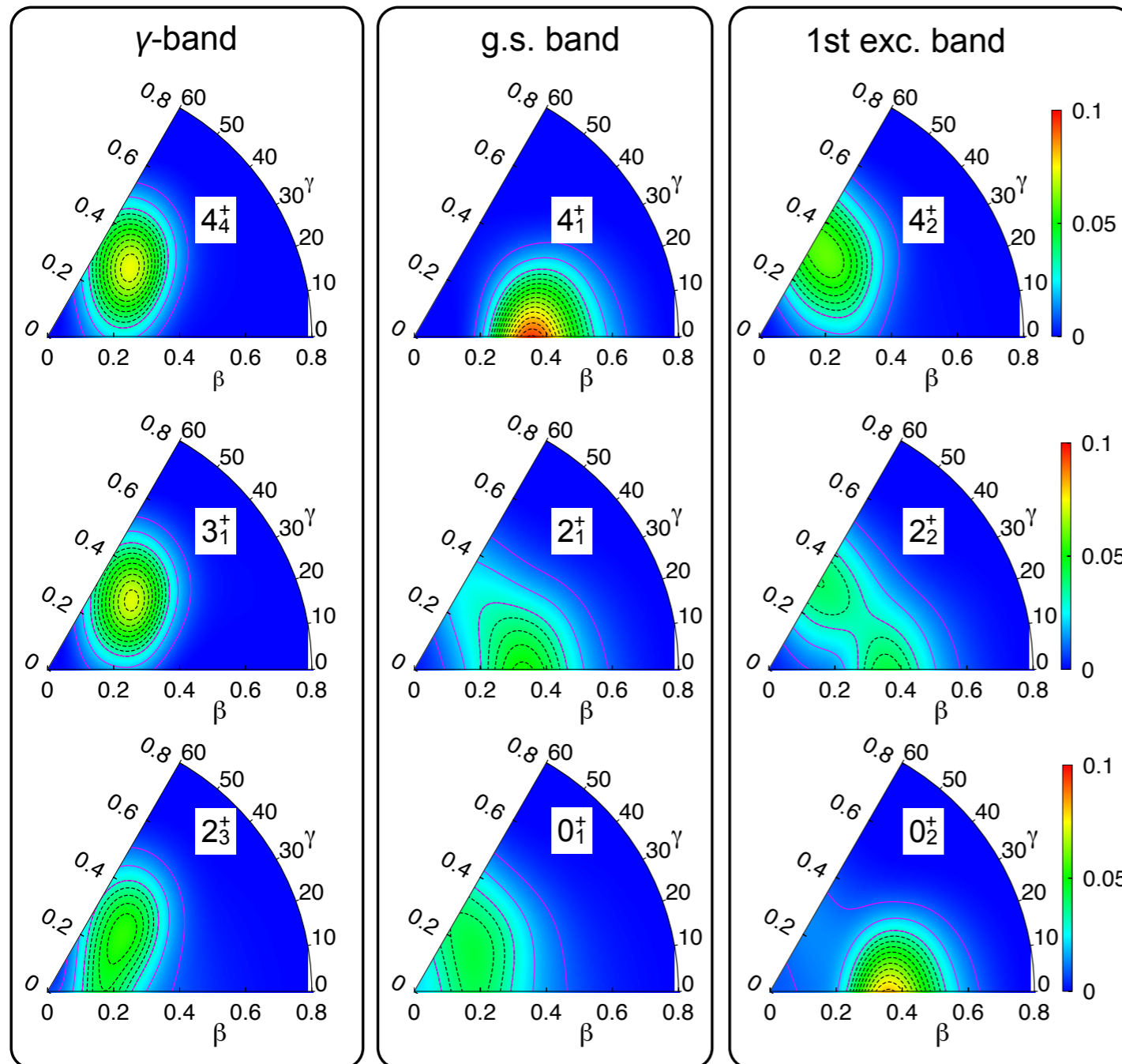


✓ Very good qualitative description of the observed levels and reduced transition probabilities.

✓ We predict three different bands strongly mixed, being the level  $2_3^+$  the band head of a quasi-gamma band.

T.R.R and J.L. Egido, PRC 84, 051307 (2011)

# Shape mixing and coexistence



✓ Deformed ground state with triaxial shape mixing. Weakening of the  $N=28$  magic number.

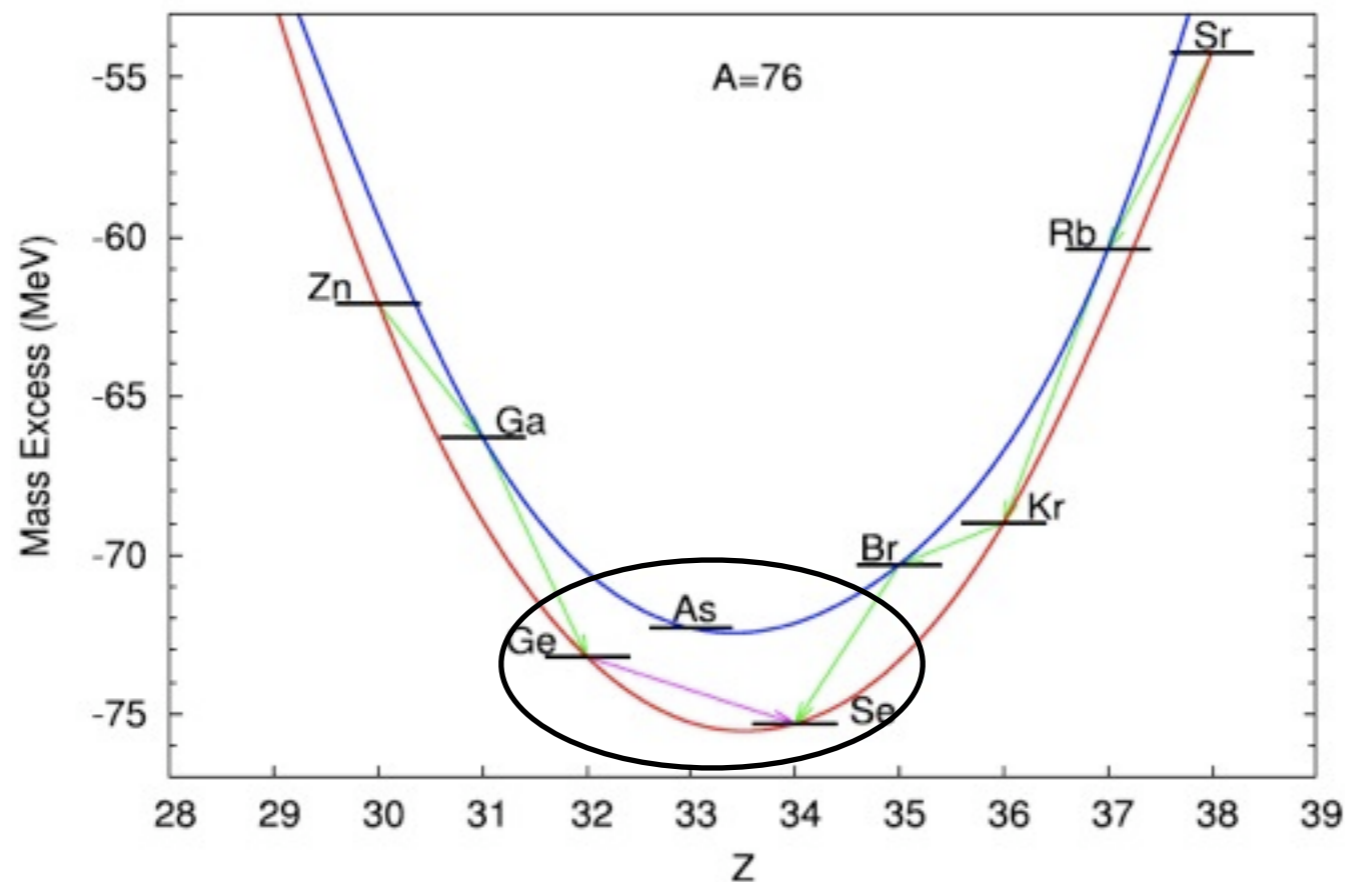
✓ Prolate first  $0^+$  excited state.

✓ There is not a clear signature of rotational structures except for the quasi-gamma band.

✓ We find shape-mixing rather shape coexistence.

# Double beta decay

Process mediated by the weak interaction which occurs in those even-even nuclei where the single beta decay is energetically forbidden.







# Double beta decay

## Half-life neutrinoless double beta decay (Doi et al (1985))

$$\left( T_{1/2}^{0\nu\beta\beta} (0^+ \rightarrow 0^+) \right)^{-1} = G_{01} |M^{0\nu\beta\beta}|^2 \left( \frac{\langle m_\nu \rangle}{m_e} \right)^2$$

light-neutrino exchange mechanism

- Kinematic phase space factor:

$$G_{01} = \frac{(Gg_A(0))^4 m_e^4}{64\pi^5 \ln 2} \int F_0(Z, \varepsilon_1) F_0(Z, \varepsilon_2) \\ \times p_1 p_2 \delta(\varepsilon_1 + \varepsilon_2 - E_f - E_i) d\varepsilon_1 d\varepsilon_2 d(\hat{p}_1 \cdot \hat{p}_2)$$

- Effective neutrino mass:

$$\langle m_\nu \rangle = \sum_j U_{ej}^2 m_j$$

- Nuclear Matrix Element (NME):

$$M^{0\nu\beta\beta} = - \left( \frac{g_V(0)}{g_A(0)} \right)^2 M_F^{0\nu\beta\beta} + M_{GT}^{0\nu\beta\beta} - M_T^{0\nu\beta\beta}$$

Fermi                      Gamow-Teller                      Tensor



# Nuclear Matrix Elements

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- Each term can be written as the expectation value of a transition operator acting on the initial and final states:

$$M_\xi^{0\nu\beta\beta} = \langle 0_f^+ | \hat{O}_\xi^{0\nu\beta\beta} | 0_i^+ \rangle$$

- Nuclear structure methods for calculating these NME:
  - Quasiparticle Random Phase Approximation in different versions: QRPA, RQRPA, SRQRPA. (Tübingen group, Jyväskylä group)
  - Interacting Shell Model -ISM- (Strasbourg-Madrid collaboration, Michigan)
  - Interacting Boson Model -IBM- (Yale group)
  - Projected Hartree-Fock-Bogoliubov -PHFB- (Lucknow-UNAM group)
  - Energy Density Functional

# Nuclear Matrix Elements

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- Nuclear structure methods for calculating these NME:

Different ways to deal with:

- Finding the best initial and final ground states.
- Handling the transition operator (inclusion of most relevant terms, corrections, approximations, etc.).

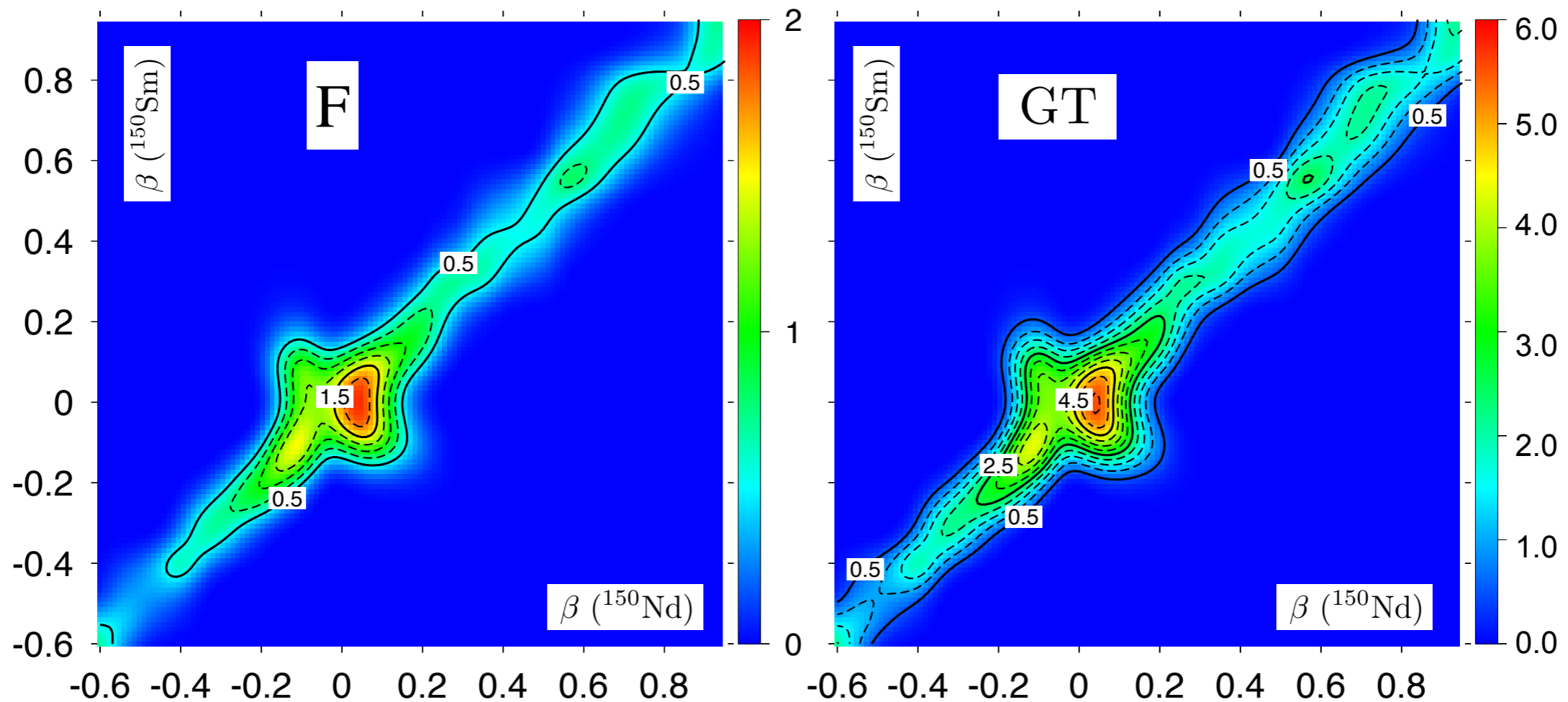
Some remarks about these methods:

- Calculations with limited single particle bases.
- Interactions fitted to the specific region (ISM) or to each nucleus individually (rest).
- Difficulties to include collective degrees of freedom.
- Problems with particle number conservation.

# NME: deformation and mixing

$$\frac{\langle 0; N_f Z_f; q_f | \hat{O}_\xi^{0\nu\beta\beta} | 0; N_i Z_i; q_i \rangle}{\sqrt{\langle 0; N_f Z_f; q_f | 0; N_f Z_f; q_f \rangle \langle 0; N_i Z_i; q_i | 0; N_i Z_i; q_i \rangle}}$$

A=150



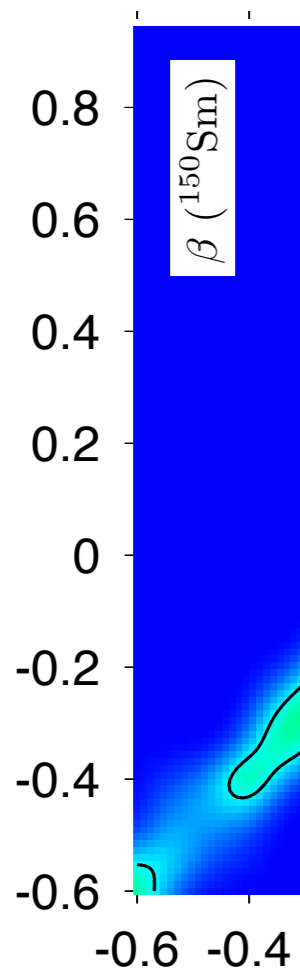
- GT strength greater than Fermi.
- Similar deformation between mother and granddaughter is favored by the transition operators
- Maxima are found close to sphericity although some other local maxima are found



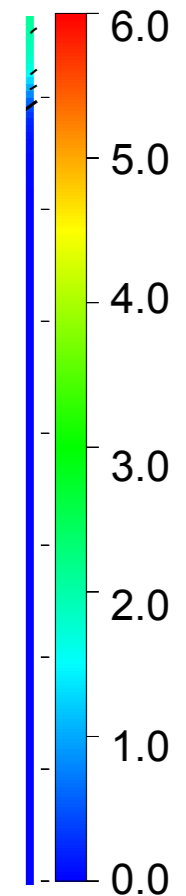
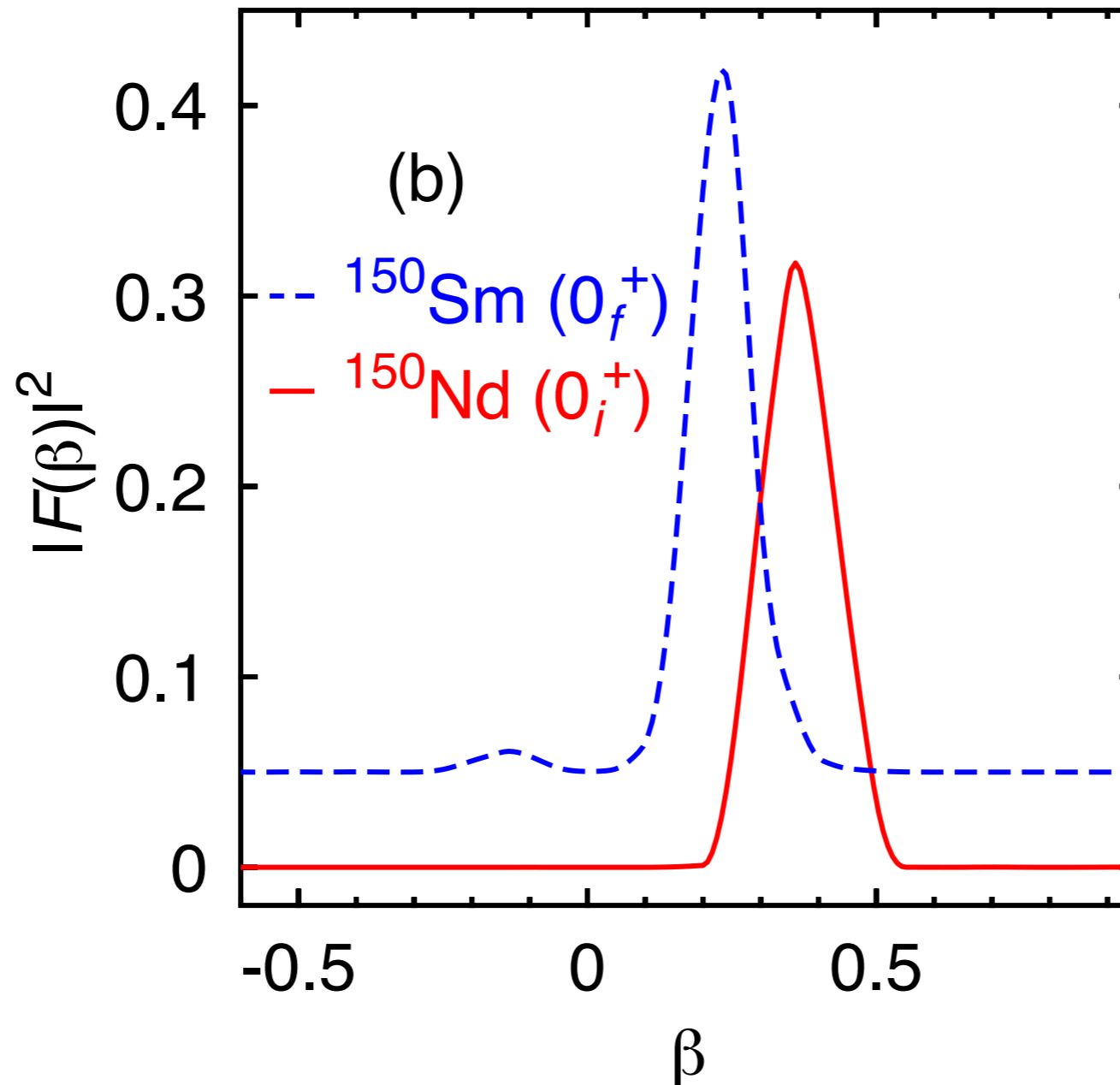
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A=150



- GT stren
- Similar de
- Maxima a
- Final resu
- states with...



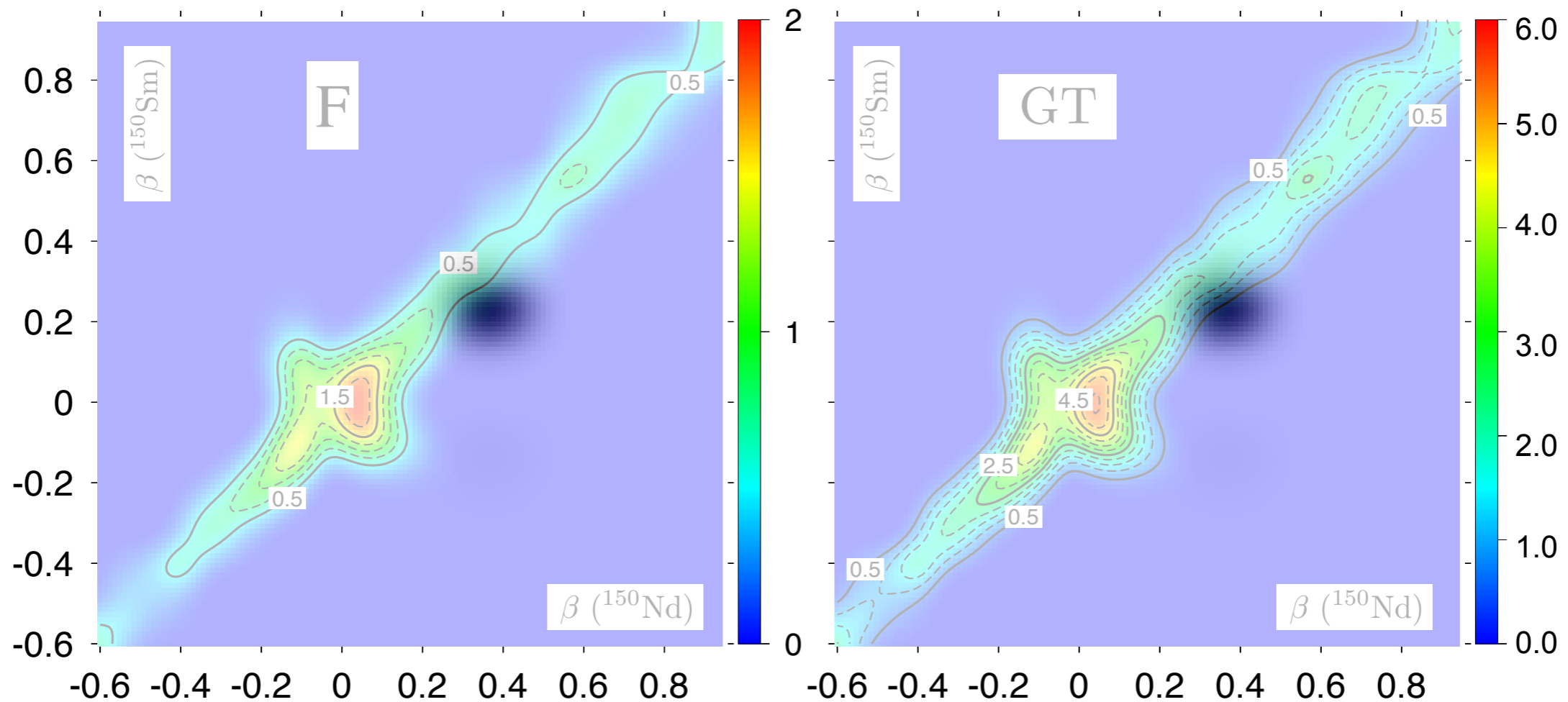
rs

ollective

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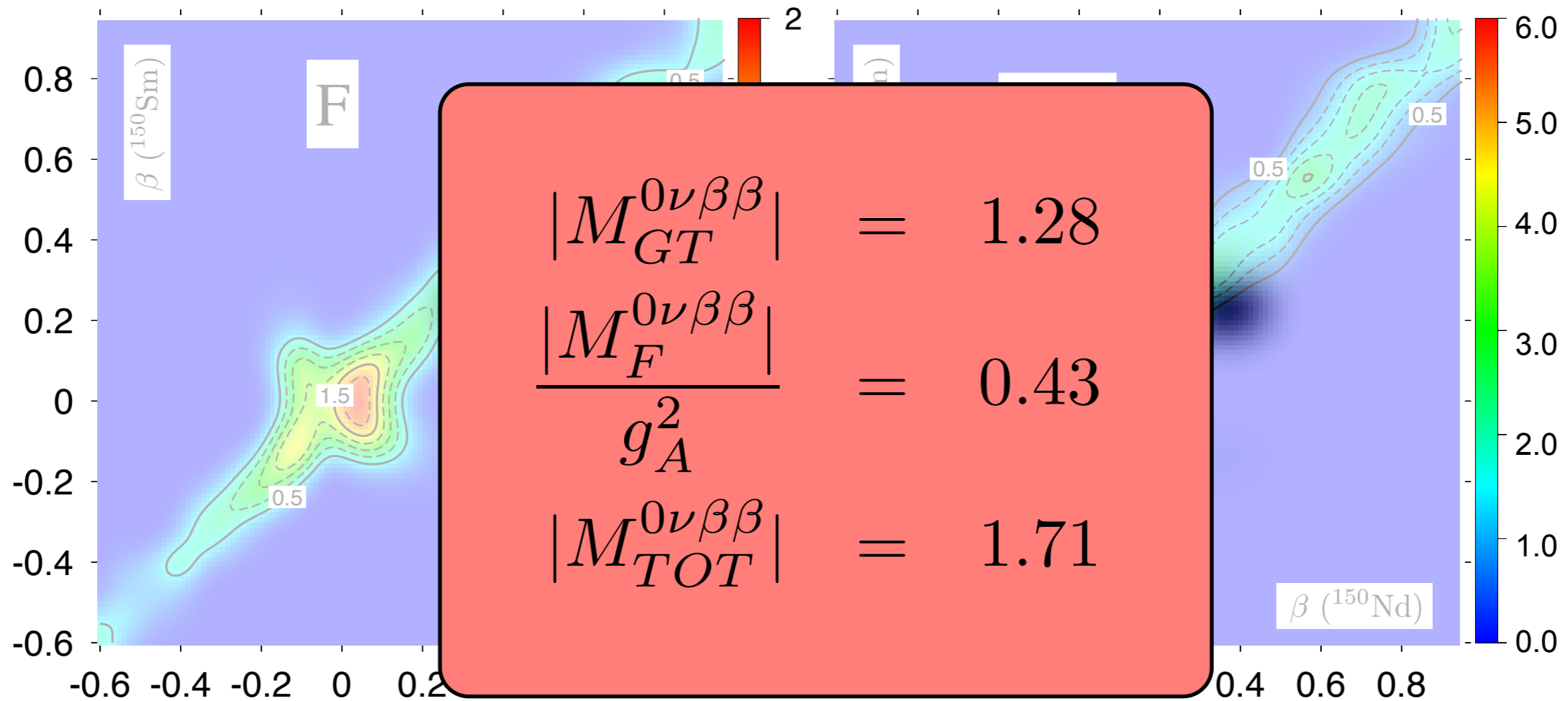


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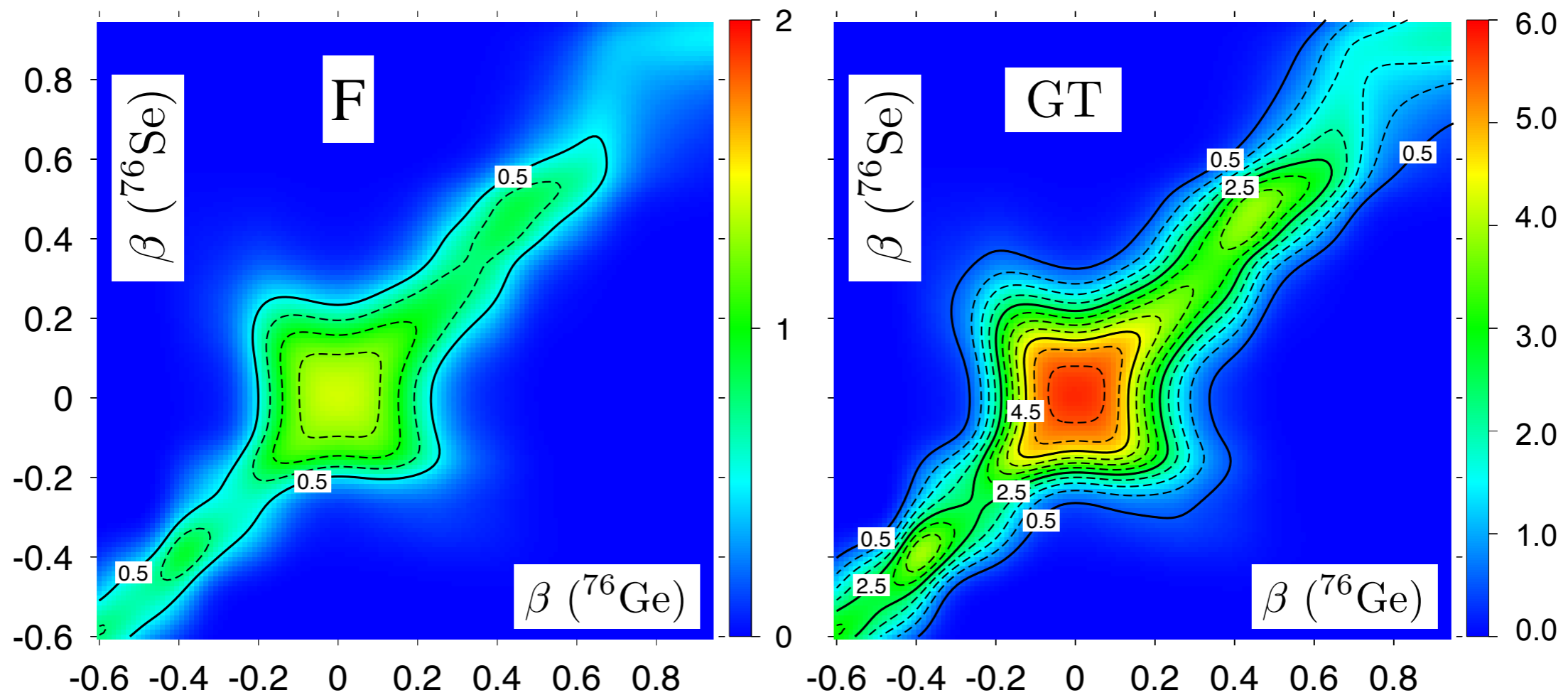


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A=76

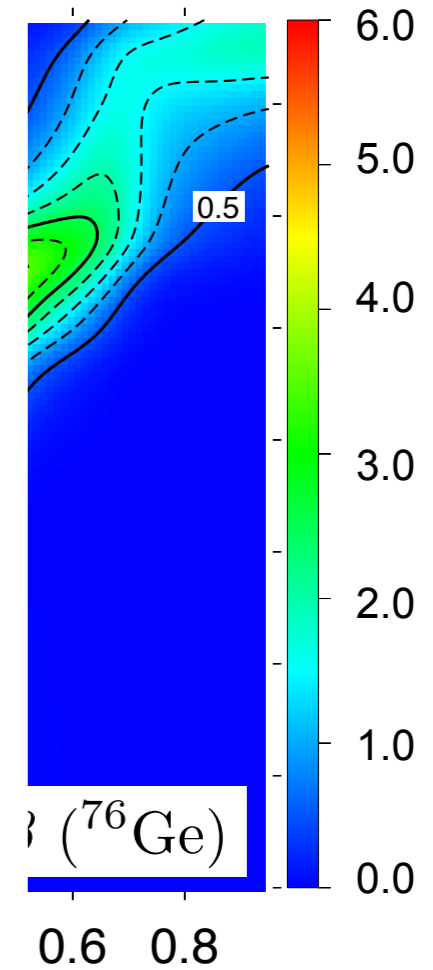
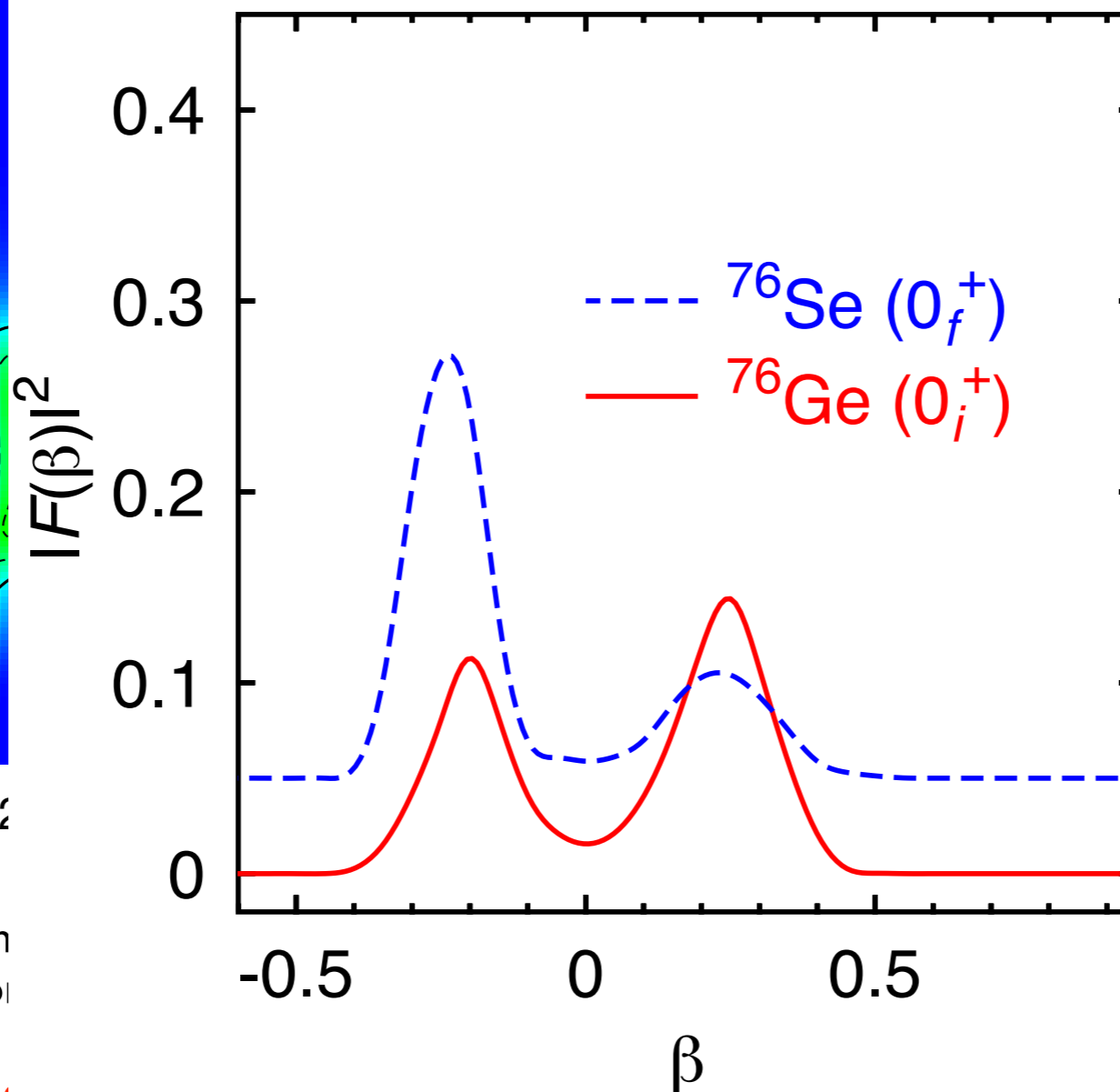
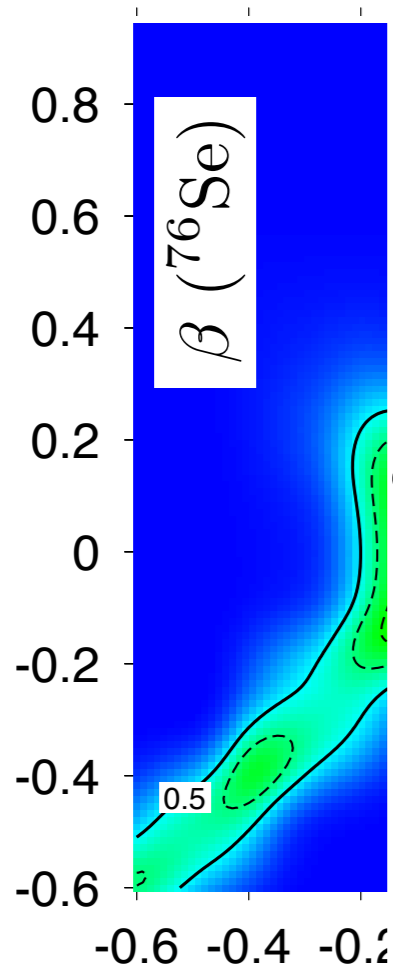


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A=76



- GT strength
- Similar deformation
- Maxima are
- Final result of
- states within

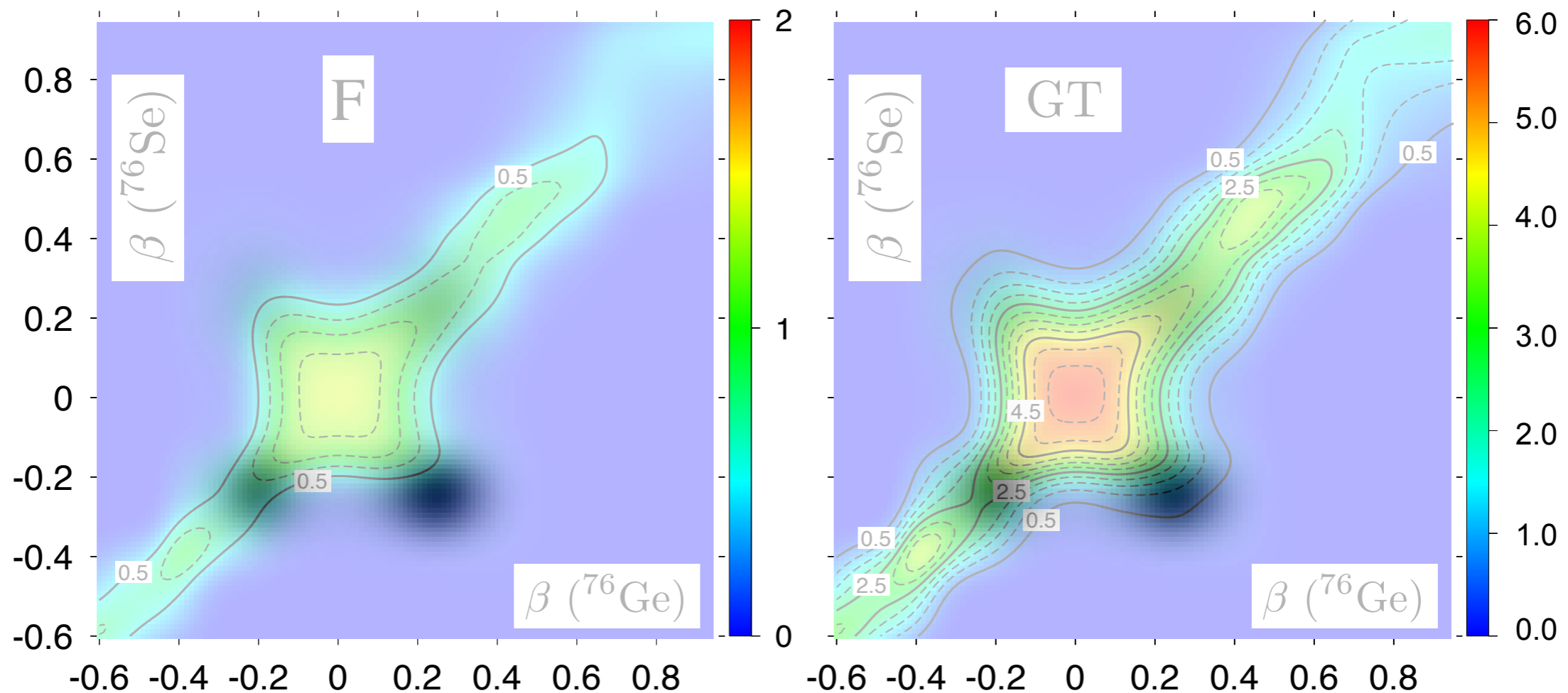
ion operators  
and  
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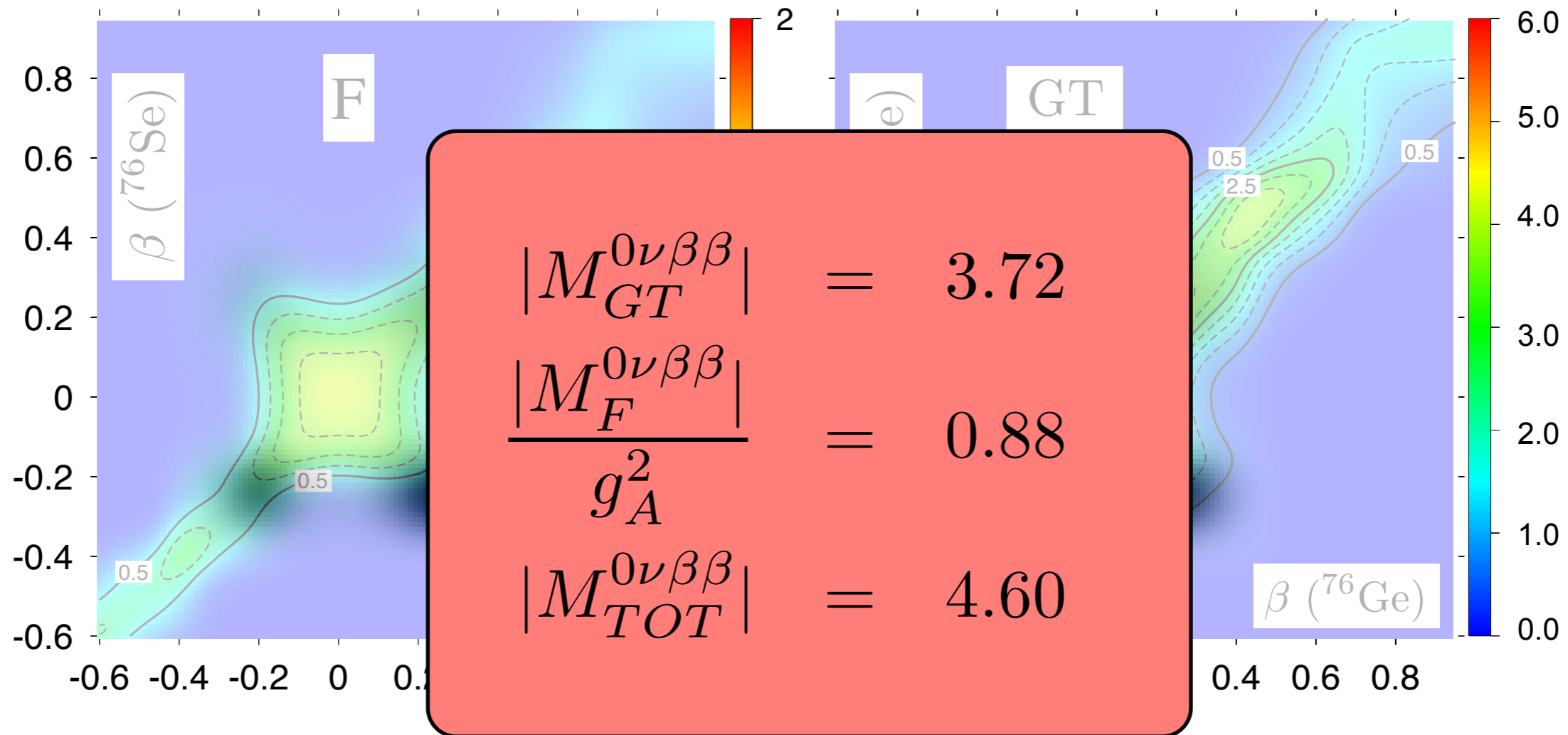


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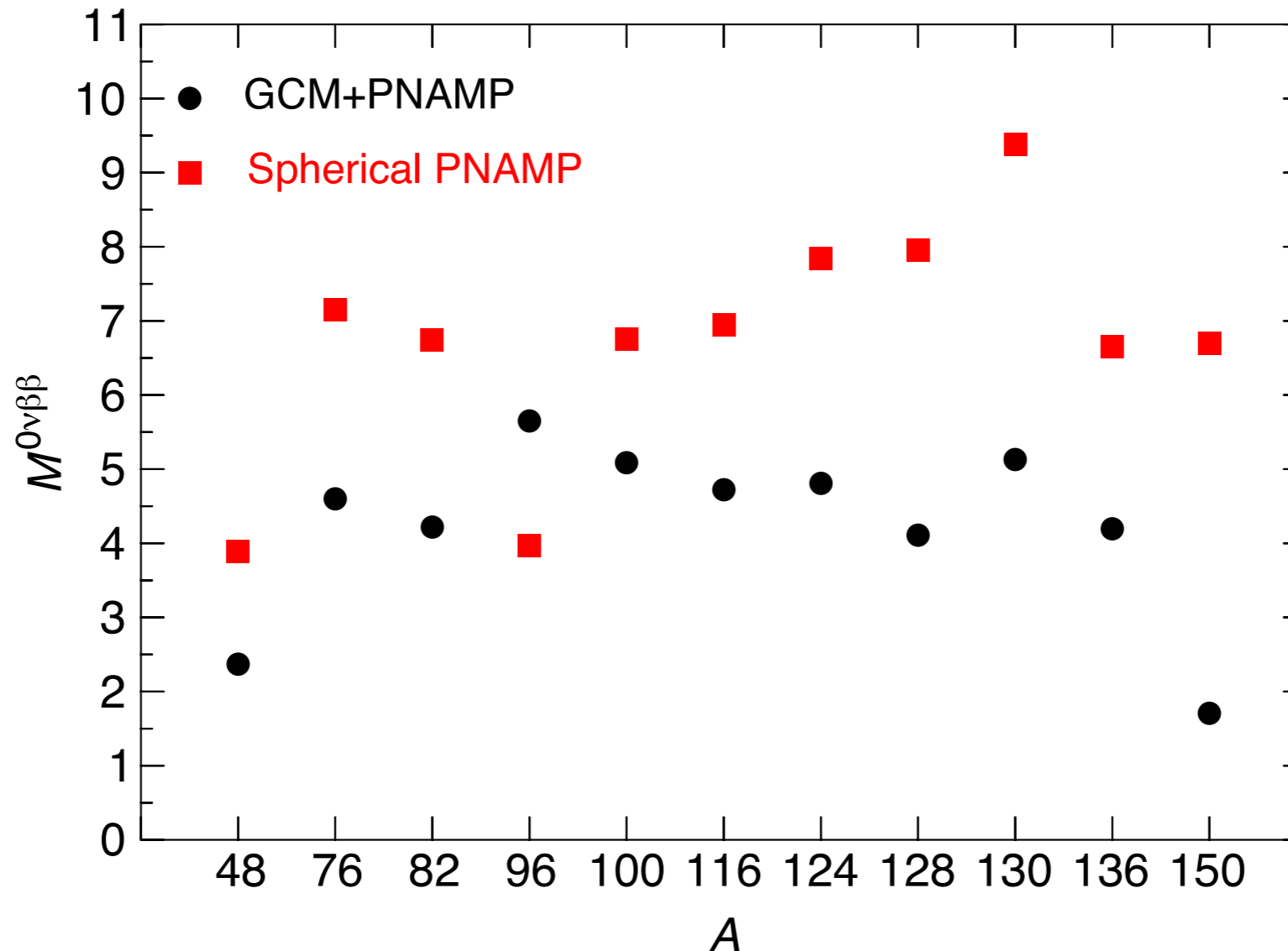
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# NME: deformation and mixing



Noticeable difference in the NME if only intrinsic spherical configurations are considered without configuration mixing.

# NME: Summary of the results

## Gogny DIS parametrization

A	48	76	82	96	100	116	124	128	130	136	150	152	164	180
$M^{0\nu}$	2.37	4.60	4.22	5.65	5.08	4.72	4.81	4.11	5.13	4.20	1.71	1.07	0.64	0.58
$T_{1/2}$ (y)	$28.5 \times 10^{23}$	$76.9 \times 10^{23}$	$20.8 \times 10^{23}$	$5.48 \times 10^{23}$	$8.64 \times 10^{23}$	$9.24 \times 10^{23}$	$16.2 \times 10^{23}$	$343.1 \times 10^{23}$	$8.84 \times 10^{23}$	$12.7 \times 10^{23}$	$16.5 \times 10^{23}$	$4.2 \times 10^{31}$	$1.3 \times 10^{36}$	$1.6 \times 10^{34}$

## Gogny DIM parametrization

A	48	76	82	96	100	116	124	128	130	136	150	152	164	180
$M^{0\nu}$	2.43	4.64	4.28	5.70	5.19	4.83	4.71	3.98	5.07	4.29	1.36	0.89	0.50	0.38
$T_{1/2}$ (y)	$27.1 \times 10^{23}$	$75.6 \times 10^{23}$	$20.2 \times 10^{23}$	$5.38 \times 10^{23}$	$8.28 \times 10^{23}$	$8.82 \times 10^{23}$	$16.9 \times 10^{23}$	$365.8 \times 10^{23}$	$9.05 \times 10^{23}$	$12.2 \times 10^{23}$	$26.1 \times 10^{23}$	$6.2 \times 10^{31}$	$2.1 \times 10^{36}$	$3.8 \times 10^{34}$

double beta decay

double electron capture

# NME: Summary of the results

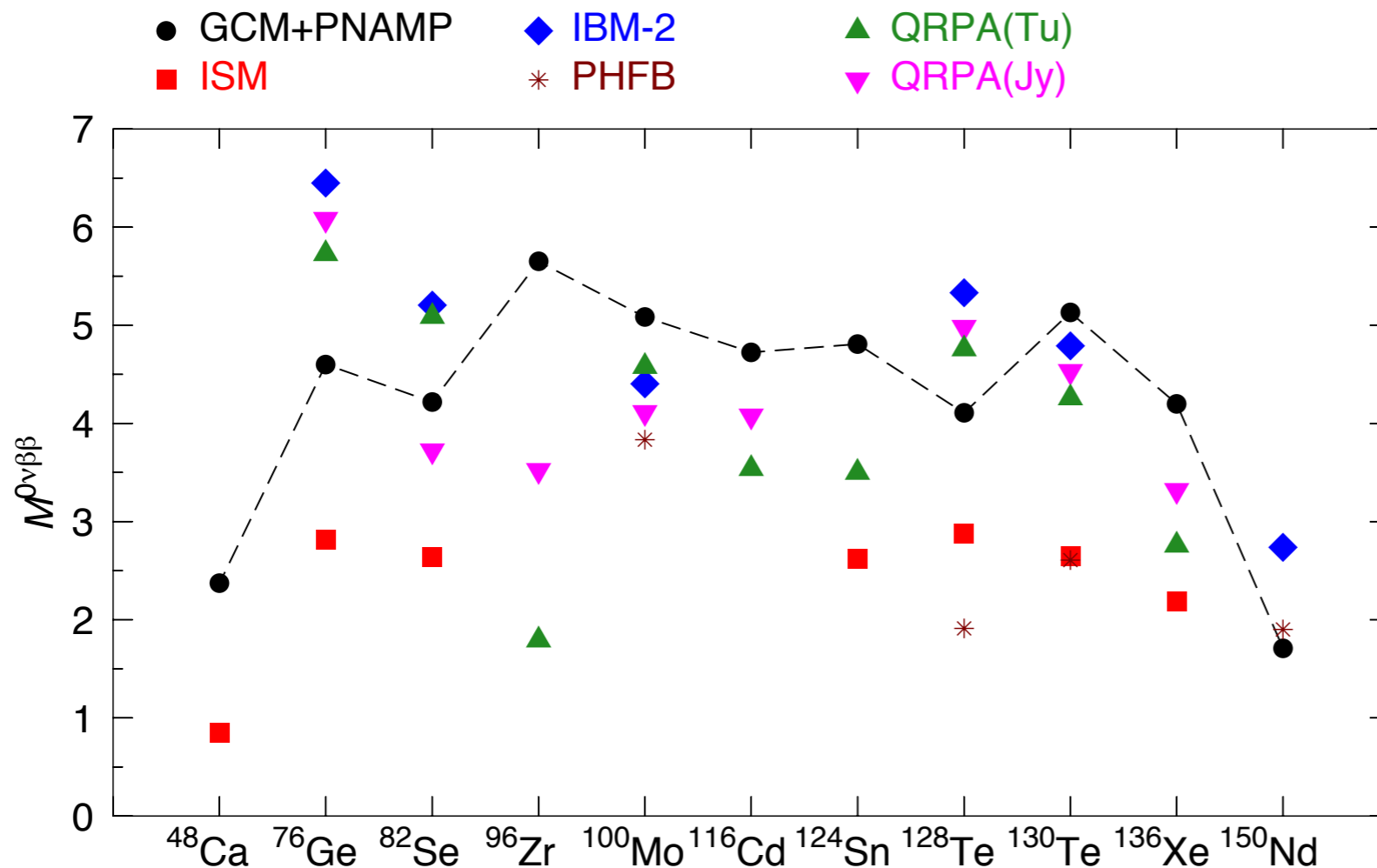
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4. Summary and outlook

T.R.R., Martínez-Pinedo, PRL 2010



QRPA (Jy): J.M. Kortelainen, J. Suhonen, PRC 75, 051303(R) (2007) and PRC 76, 024315 (2007)

QRPA(Tu): F. Simkovic et al., PRC 77, 045503 (2008)

ISM: J. Menendez et al., PRL 100, 52503 (2008)

IBM-2: J. Barea, F. Iachello, PRC 77, 045503 (2008)

PHFB: K. Chaturvedi et al. PRC 78, 054302 (2008)

- Higher values than the ones predicted by ISM calculations (larger valence space, lower seniority components).
- For  $A=76, 82, 128, 150$  we predict smaller values than the ones given by QRPA and/or IBM while for  $A=96, 100, 116, 124, 130, 136$  larger values are obtained.
- Consistent results with the rest of the models. Notice that we are using the same interaction for all the nuclei.
- Further studies are needed to understand what is missing in the different models.



# NME: Summary of the results

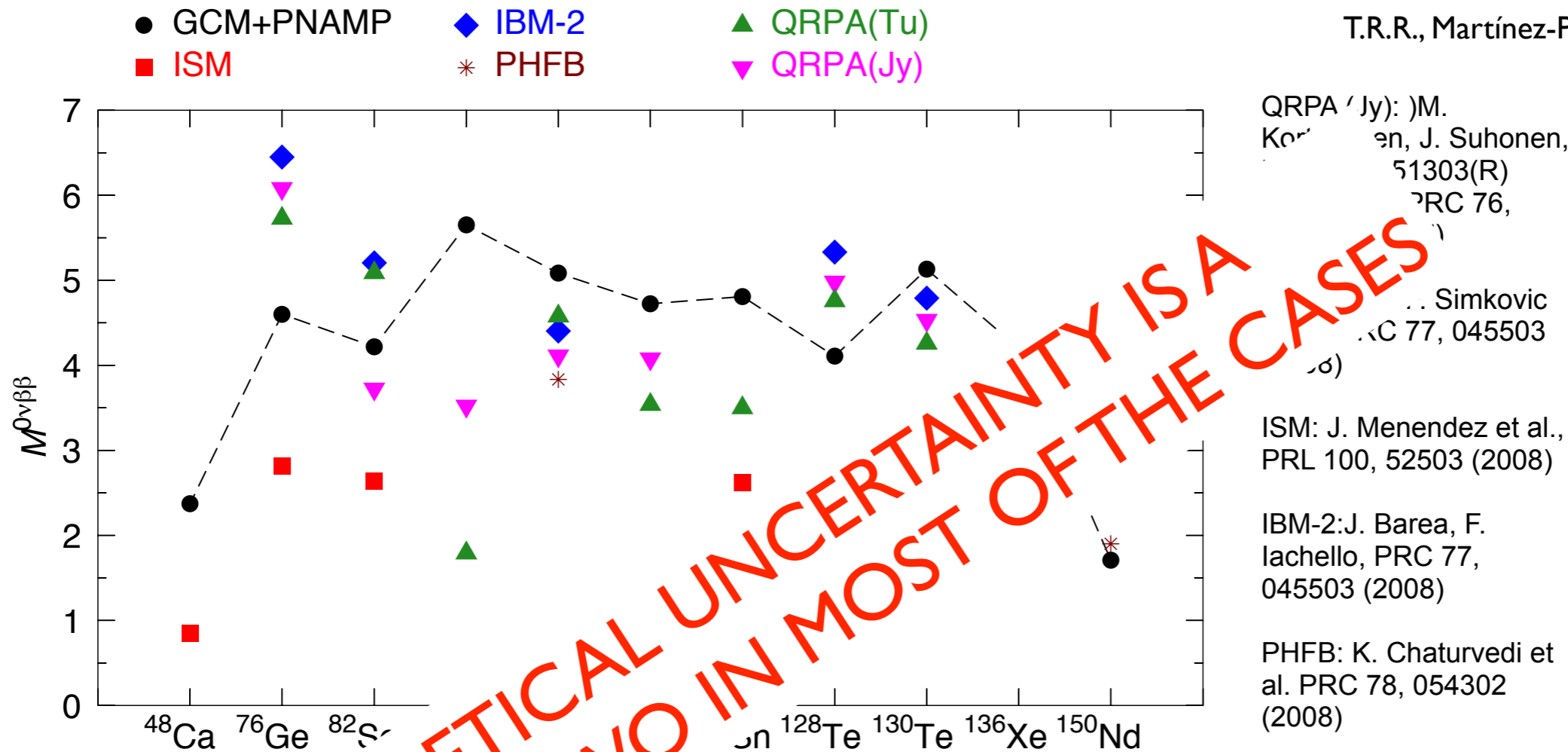
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# Summary and outlook

- Energy density functional methods provide a reliable description of nuclear structure observables and NMEs in lepton number violating processes.
- Other degrees of freedom should be also explored (pairing vibrations, octupole deformations, triaxiality, explicit quasiparticle excitations...)
- Need of energy density functionals adjusted to beyond mean field results.
- Description of odd nuclei at the same level.

# Acknowledgments



**G. Martínez-Pinedo (TU-Darmstadt)**

**K. Langanke (GSI-Darmstadt)**

**J. L. Egido (UAM-Madrid)**

**K. Blaum (U-Heidelberg)**

**C. Smorra (U-Heidelberg)**