Gogny energy density functional

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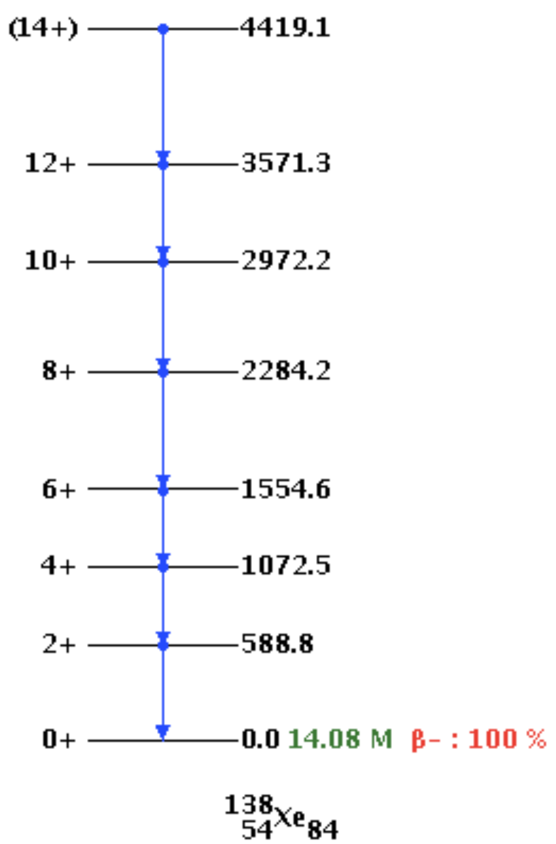
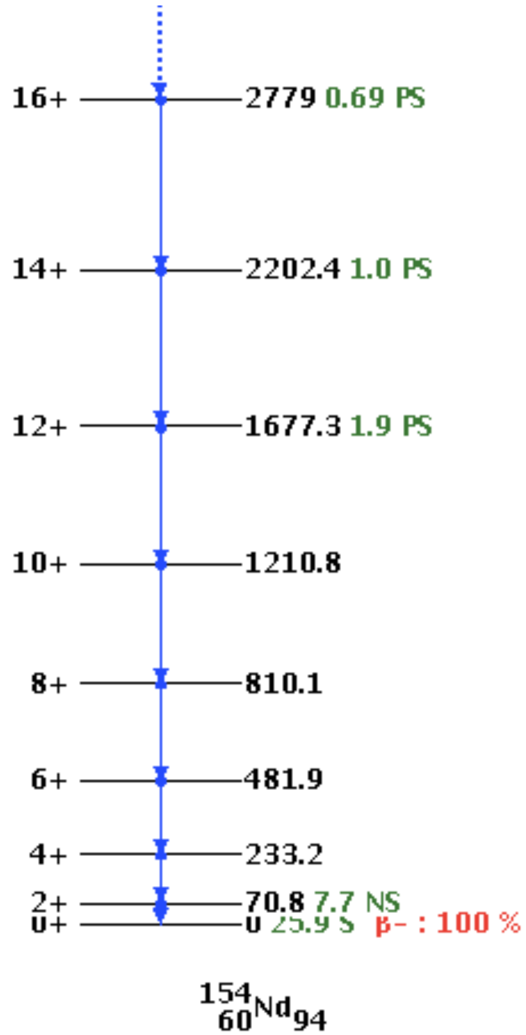
Outline

Introduction

- The **intrinsic shape** of the nuclear states is **not a direct observable**, but...

- Intrinsic nuclear shapes can be inferred from the experimental data (energies and electromagnetic moments and transitions) by comparison with the predictions given by geometrical (simple) models.





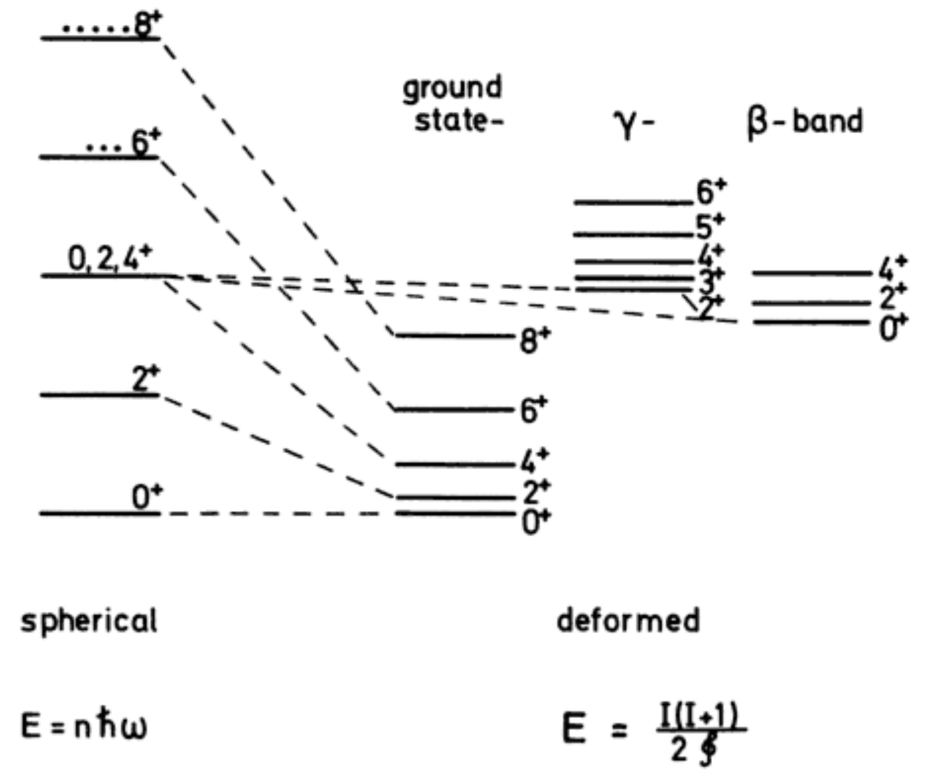


Figure 1.12. Schematic level schemes of spherical and deformed nuclei. (From [SDG 76].)

P. Ring and P. Schuck, *The Nuclear Many-Body Problem*

Introduction

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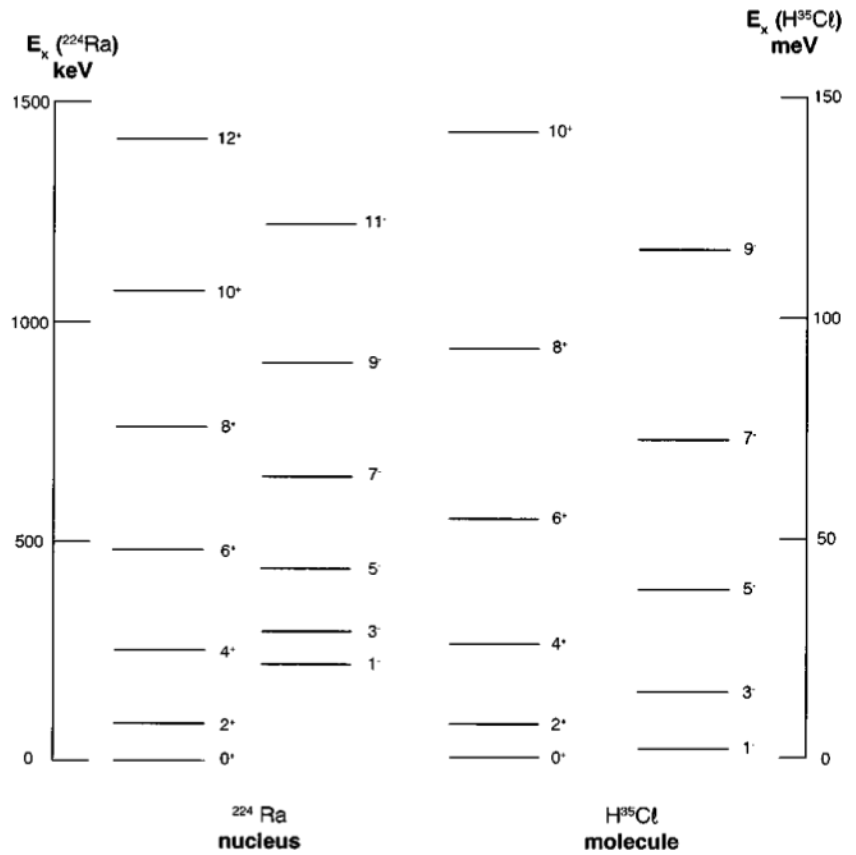


FIG. 1. The low-lying rotational spectra of ^{224}Ra, compared with that of the H^{35}Cl molecule. The spectrum of ^{224}Ra is taken from Poynter *et al.* (1989a). The rotational constants for the H^{35}Cl molecule are taken from Landolt-Börnstein (1974).

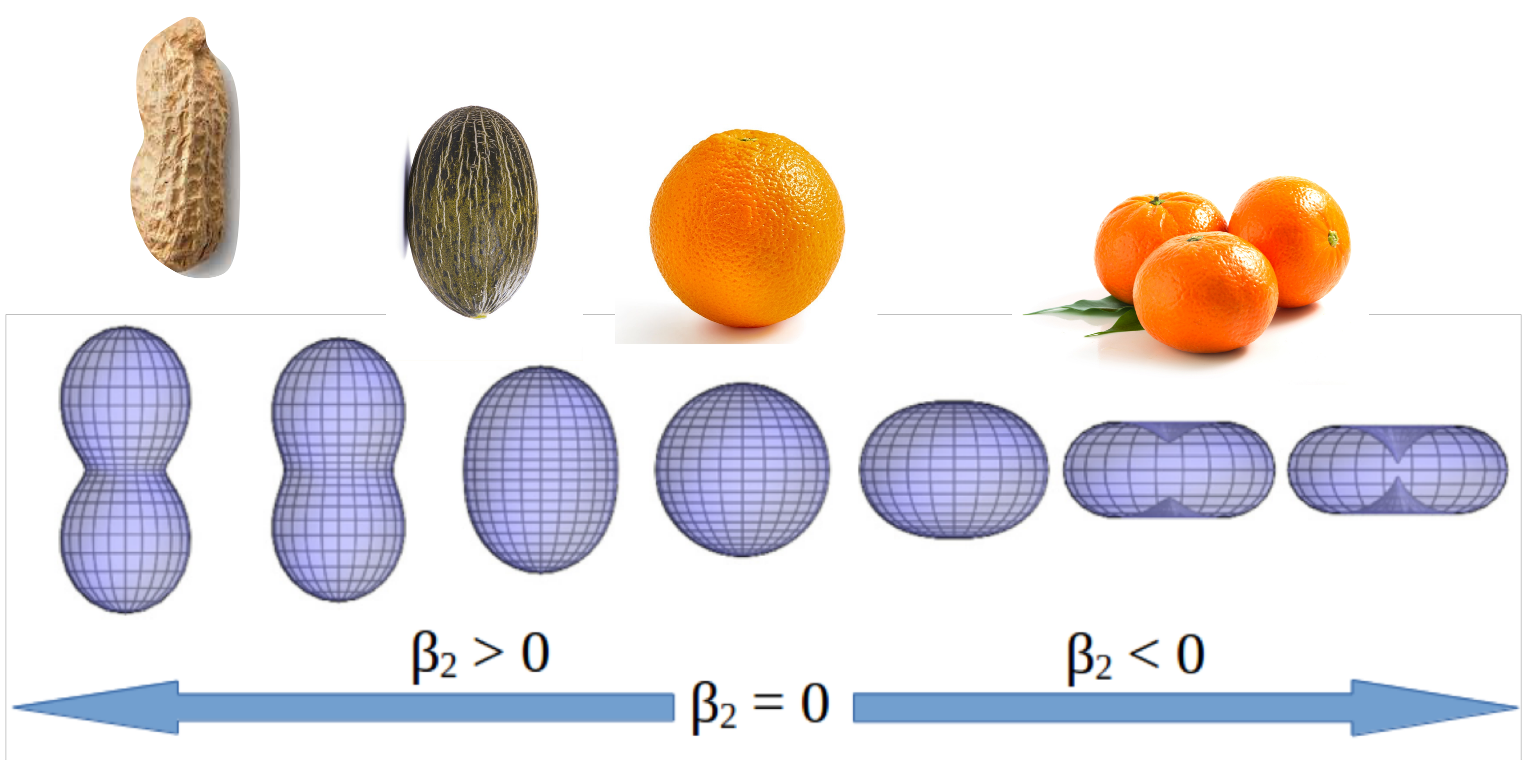
Positive and negative parity interleaved bands as rotational states of octupole shapes

P. A. Butler, W. Nazarewicz, Rev. Mod. Phys. 68, 349 (1996)

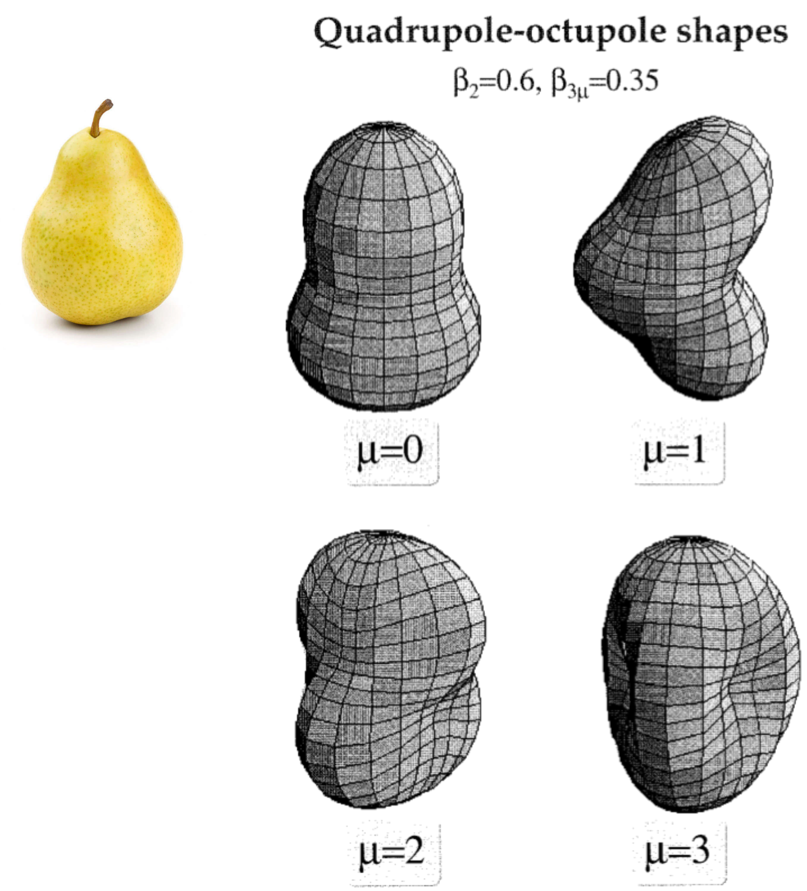
Introduction

- **Collective models** are based on the parametrization of the nuclear radius with a multipole expansion

$$R(\Omega) = c(\alpha)R_0\left[1 + \sum_{\lambda=2}^{\lambda_{\max}} \sum_{\mu=-\lambda}^{+\lambda} \alpha_{\lambda\mu} Y^*_{\lambda\mu}(\Omega)\right]$$

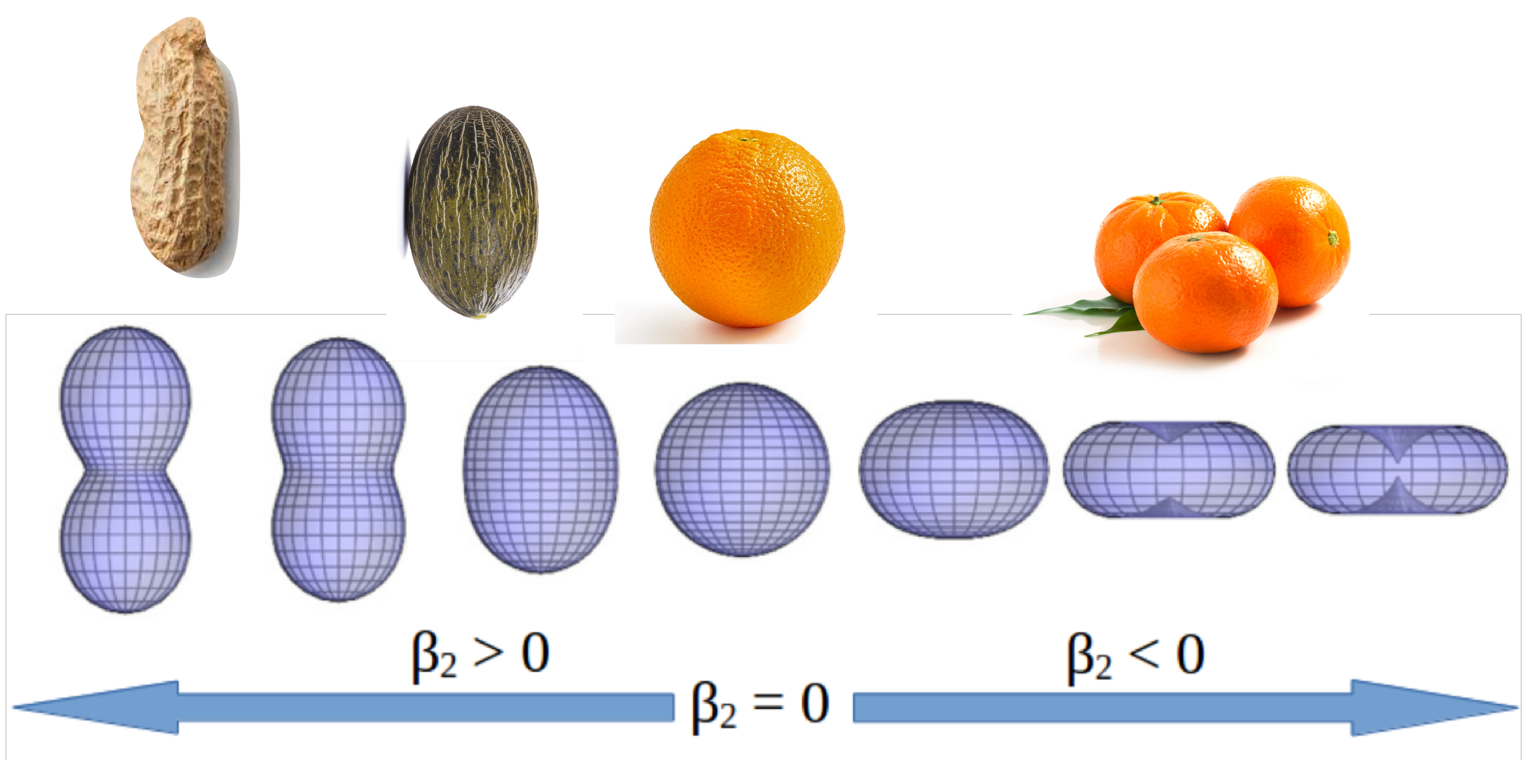


axial quadrupole shapes

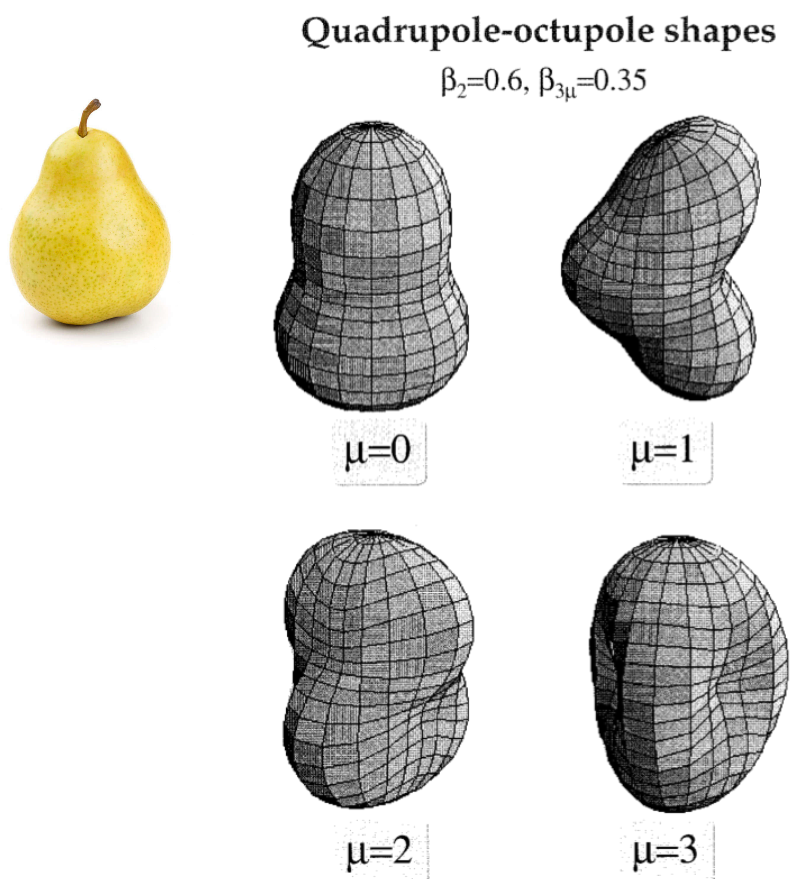


P. A. Butler, W. Nazarewicz, Rev. Mod. Phys. 68, 349 (1996)

Can we provide a **microscopic** description of these collective phenomena?



axial quadrupole shapes



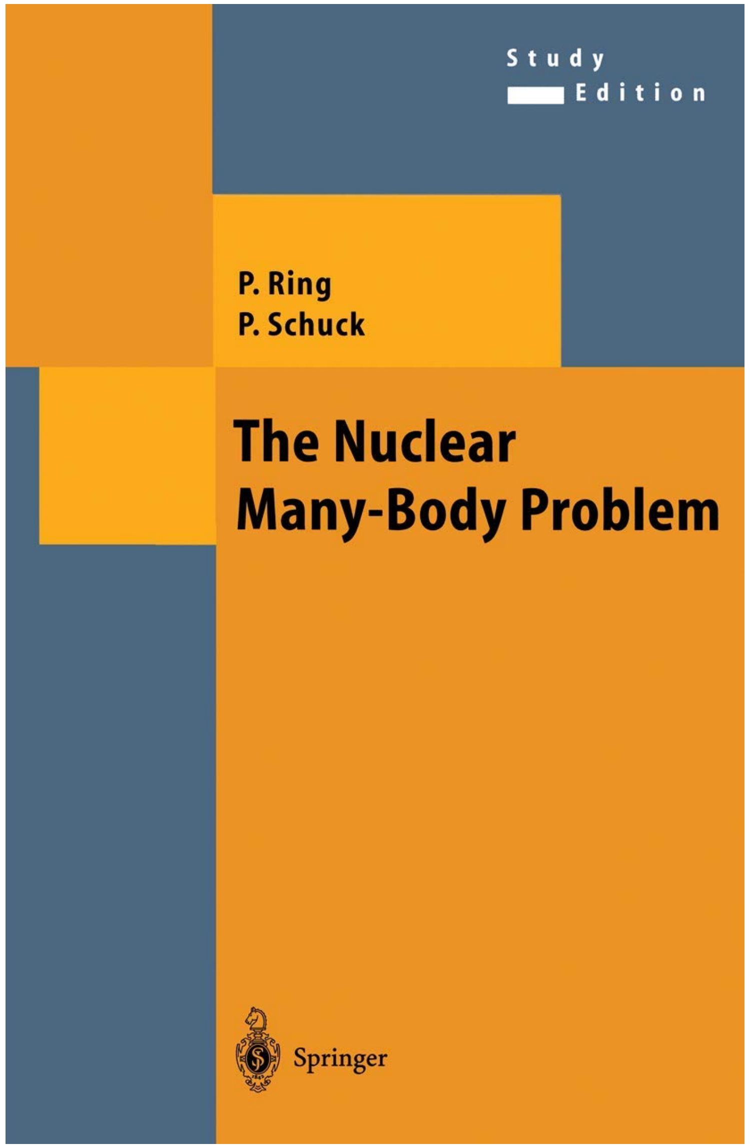
P. A. Butler, W. Nazarewicz, Rev. Mod. Phys. 68, 349 (1996)

The nuclear many-body problem is… a **huge** problem!

- The nuclear interaction is problematic

- The quantum *A*-body system is problematic

We rely on models!



Introduction

Let us assume that *we know* the nuclear interaction. Exact nuclear wave functions and energies cannot be obtained in general because of:

a) the exploding dimensionality of the many-body Hilbert space

b) the huge amount of two-, three- (eventually, *N*-) body matrix elements that are impossible to store

$$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

??

Some of the most widely used *solutions* to attack these problems:

- **Valence-space (Shell Model) calculations** with phenomenological (or normal-ordered, SRG evolved) two-body Hamiltonians
- **Approximate methods (variational)** with phenomenological interactions (or energy density functionals)

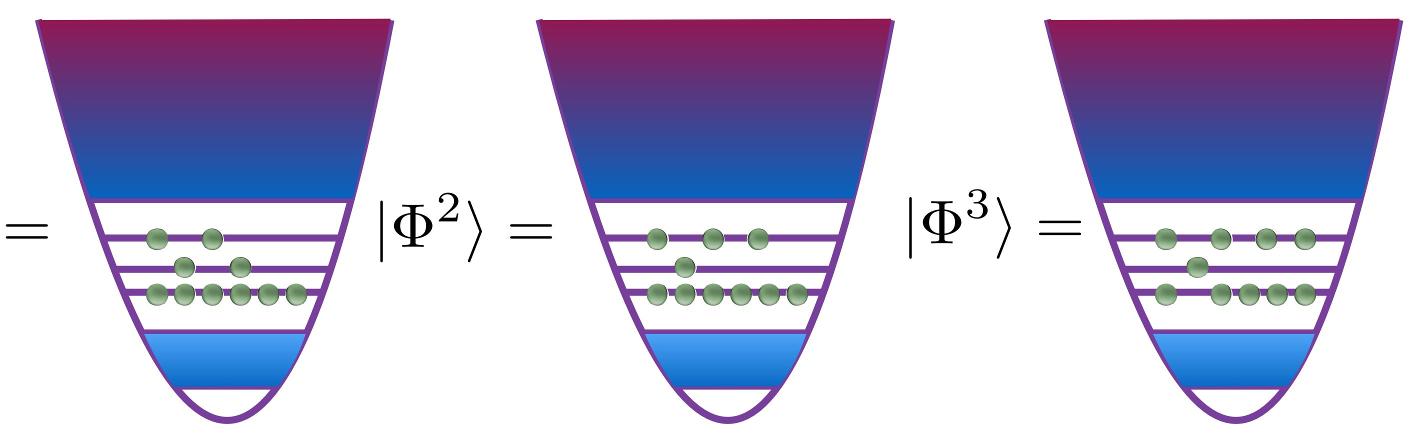
- Valence-space (Shell Model) calculations with phenomenological (or normal-ordered, SRG evolved) two-body Hamiltonians

Full diagonalization of an *adapted* Hamiltonian within a valence space

$$\hat{H}_{v.s.}|\Psi^{n}_{v.s.}\rangle = E_{n}\,|\Psi^{n}_{v.s.}\rangle$$

Nuclear wave functions are linear combinations of Slater determinants written in terms of occupations of spherical orbits

$$|\Psi^{n}_{v.s.}\rangle = \sum_{k\in\, v.s.} C^{n}_{k}|\Phi^{k}\rangle$$



$$|\Phi^1\rangle = \qquad |\Phi^2\rangle = \qquad |\Phi^3\rangle = \qquad \dots$$

Let us assume that *we know* the nuclear interaction. Exact nuclear wave functions and energies cannot be obtained in general because of:

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Some of the most widely used *solutions* to attack these problems:

- **Valence-space (Shell Model) calculations** with phenomenological (or normal-ordered, SRG evolved) two-body Hamiltonians

- **Approximate methods (variational)** with phenomenological interactions (or energy density functionals)

Introduction

Effective nucleon-nucleon interaction: Gogny force (D1S/D1M)

$$V(1,2) = \sum_{i=1}^{2} e^{-(\vec{r}_1-\vec{r}_2)^2/\mu_i^2} \left(W_i + B_i P^\sigma - H_i P^\tau - M_i P^\sigma P^\tau\right)$$

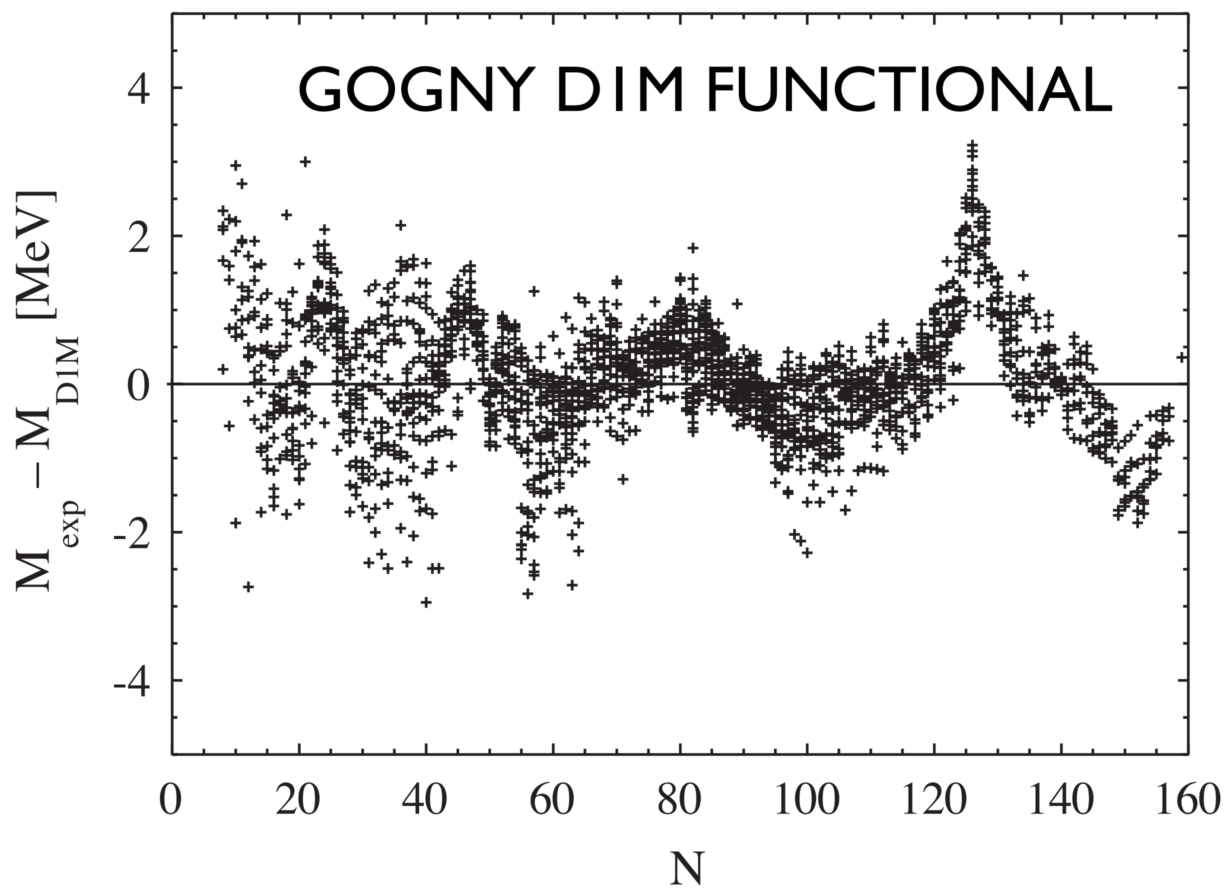
$$+iW_0(\sigma_1+\sigma_2)\vec{k}\times\delta(\vec{r}_1-\vec{r}_2)\vec{k} + V_{\text{Coulomb}}(\vec{r}_1,\vec{r}_2)$$

2-body potential

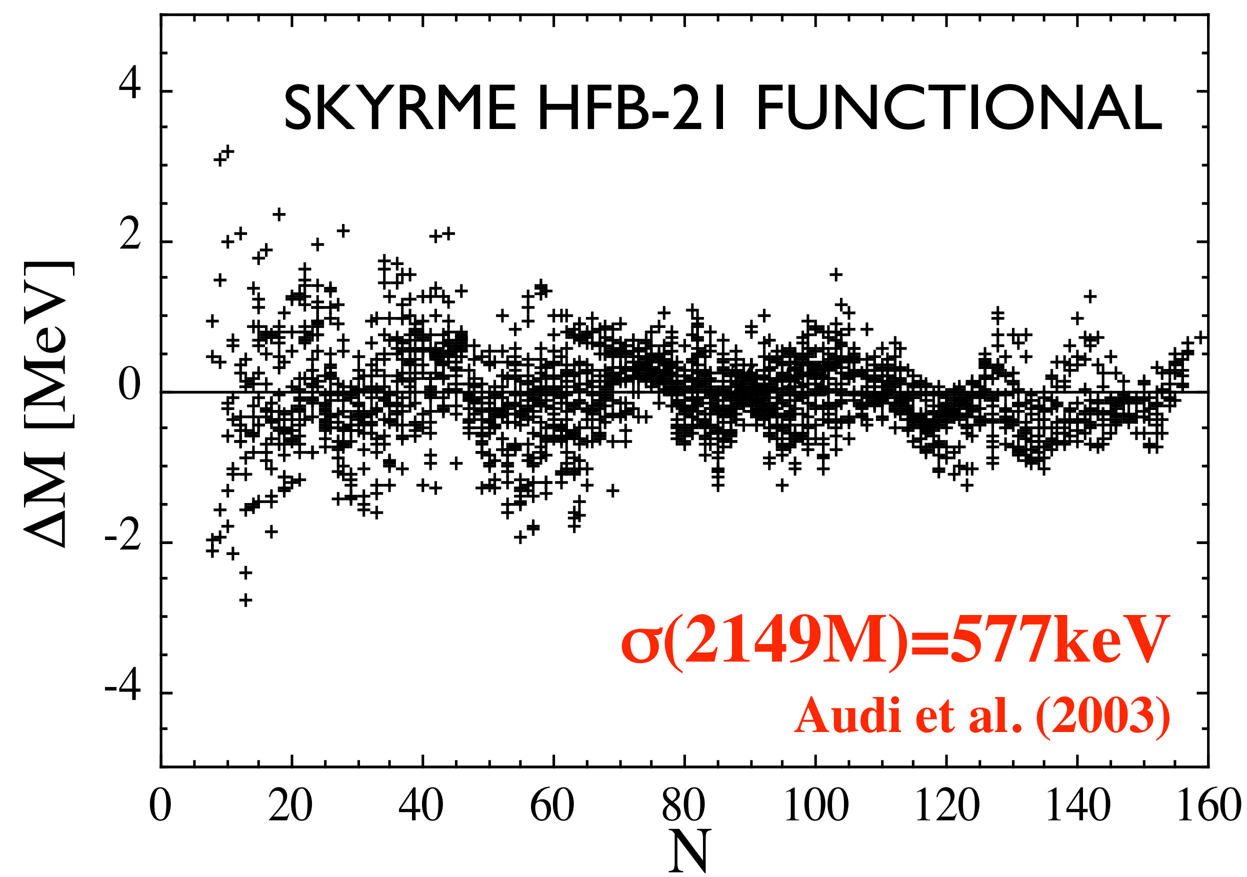
$$+t_3(1+x_0P^\sigma)\delta(\vec{r}_1-\vec{r}_2)\rho^\alpha\left((\vec{r}_1+\vec{r}_2)/2\right)$$

Density dependent term

Introduction



Goriely et al., PRL 102, 242501 (2009)



Goriely et al., PRL 102, 152503 (2009)

Introduction

- Approximate methods (variational) with phenomenological interactions (or energy density functionals)

Variational space of trial wave functions

Hamiltonian machine

$$E_1 = \langle\Psi_1|\hat{H}|\Psi_1\rangle$$

$$E_2 = \langle\Psi_2|\hat{H}|\Psi_2\rangle$$

$$E_{min} = \langle\Psi_{min}|\hat{H}|\Psi_{min}\rangle$$

Variational approach to the exact solution

Introduction

- Approximate methods (variational) with phenomenological interactions (or energy density functionals)

Full Variational space of trial wave functions

Variational spaces

Mean field approach

Hartree-Fock HF-Bogoliubov

Beyond mean field approach

Configuration Mixing

- Nuclear wave functions wave functions: Generator Coordinate Method (GCM) ansatz

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} f_{\sigma;qK}^{JMNZ\pi} P^{J}_{MK} P^{N} P^{Z} P^{\pi} |\Phi(q)\rangle$$

$$\Gamma \equiv (JMNZ\pi)$$

linear combination — coefficients of the linear combination — "basis" states

Theoretical framework

- Nuclear wave functions wave functions: Generator Coordinate Method (GCM) ansatz

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} f_{\sigma;qK}^{JMNZ\pi} P_{MK}^{J} P^{N} P^{Z} P^{\pi} |\Phi(q)\rangle$$

$$\Gamma \equiv (JMNZ\pi)$$

coefficients of the linear combination

The coefficients are obtained by minimizing the expectation value of the Hamiltonian (energy) with those coefficients as the variational parameters:

$$\sum_{q'K'} \left(\mathcal{H}_{qK,q'K'}^{\Gamma} - E_{\sigma}^{\Gamma}\mathcal{N}_{qK,q'K'}^{\Gamma}\right) f_{\sigma;q'K'}^{\Gamma} = 0$$

Hill-Wheeler-Griffin (HWG) equation

$$\mathcal{H}_{qK,q'K'}^{\Gamma} = \langle\Phi(q)|\hat{H} P_{KK'}^{J} P^{N} P^{Z} P^{\pi}|\Phi(q')\rangle,$$

$$\mathcal{N}_{qK;q'K'}^{\Gamma} = \langle\Phi(q)|P_{KK'}^{J} P^{N} P^{Z} P^{\pi}|\Phi(q')\rangle$$

Hamiltonian and norm kernels

- Nuclear wave functions wave functions: Generator Coordinate Method (GCM) ansatz

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} f_{\sigma;qK}^{JMNZ\pi} P_{MK}^{J} P^{N} P^{Z} P^{\pi} |\Phi(q)\rangle$$

$$\Gamma \equiv (JMNZ\pi)$$

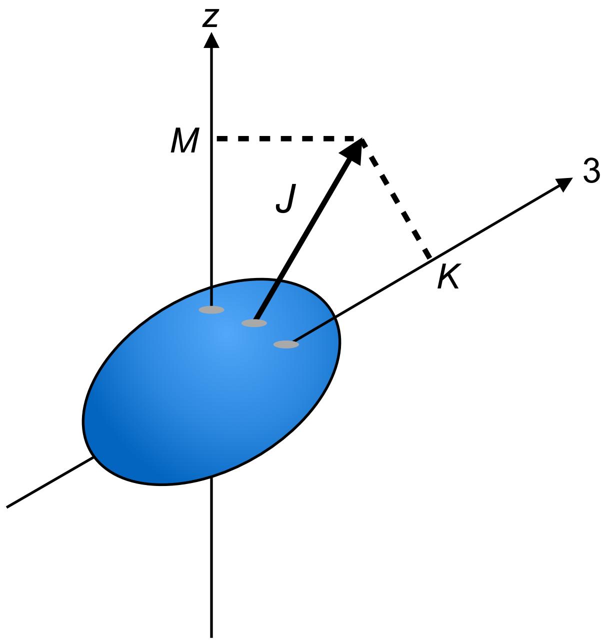
"basis" states

$P_{MK}^{J} \longrightarrow$ angular momentum projector

$P^{N} \longrightarrow$ neutron number projector

$P^{Z} \longrightarrow$ proton number projector

$P^{\pi} \longrightarrow$ spatial parity projector



Theoretical framework

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- Nuclear wave functions wave functions: Generator Coordinate Method (GCM) ansatz

$$|\Psi_{\sigma}^{JMNZ\pi}\rangle = \sum_{qK} f_{\sigma;qK}^{JMNZ\pi} P_{MK}^{J} P^{N} P^{Z} P^{\pi}|\Phi(q)\rangle$$

$$\Gamma \equiv (JMNZ\pi)$$

"basis" states

Intrinsic (HFB-like, Bogoliubov quasiparticle vacuum) state:

$$|\Phi(q)\rangle \rightarrow \beta_b(q)|\Phi(q)\rangle = 0 \quad \forall \quad b \qquad \beta_b^{\dagger}(q) = \sum_a U_{ab}(q)c_a^{\dagger} + V_{ab}(q)c_a$$

We minimize the functionals

$$E'_{\mathrm{HFB}}\left[|\Phi(q)\rangle\right] = \langle\Phi(q)|\hat{H} - \lambda_N\hat{N} - \lambda_Z\hat{Z} - \lambda_q\hat{Q}|\Phi(q)\rangle \text{ or}$$

$$E'_{\mathrm{PNVAP}}\left[|\Phi(q)\rangle\right] = \frac{\langle\Phi(q)|\hat{H}P^{N}P^{Z}|\Phi(q)\rangle}{\langle\Phi(q)|P^{N}P^{Z}|\Phi(q)\rangle} - \langle\Phi(q)|\lambda_q\hat{Q}|\Phi(q)\rangle$$

Constraints $q \longrightarrow$ quadrupole deformations; octupole deformations; pairing fluctuations; intrinsic rotations

Gogny EDF axial

- Initial intrinsic states: PN-VAP M. Anguiano, J. L. Egido, and L. M. Robledo, Nucl. Phys. A 696, 467 (2001).

$$E^{N,Z}[\Phi] = \frac{\langle\Phi|\hat{H}_{2b}\hat{P}^N\hat{P}^Z|\Phi\rangle}{\langle\Phi|\hat{P}^N\hat{P}^Z|\Phi\rangle} + \varepsilon^{N,Z}_{DD}(\Phi) - \lambda_{q_{20}}\langle\Phi|\hat{Q}_{20}|\Phi\rangle$$

- Intermediate Particle Number and Angular Momentum Projected states

$$|I;NZ;\beta_2\rangle = \frac{2I+1}{2}\int_0^\pi d^{I*}_{00}(\beta)e^{-i\beta\hat{J}_y}\hat{P}^N\hat{P}^Z|\Phi\rangle\, d\beta$$

- Final GCM states $|I;NZ;\sigma\rangle = \sum_{\beta_2} f^{I;NZ;\sigma}_{\beta_2}|I;NZ;\beta_2\rangle$

$$\sum_{\beta_2'}\left(\mathcal{H}^{I;NZ}_{\beta_2,\beta_2'} - E^{I;NZ;\sigma}\mathcal{N}^{I;NZ}_{\beta_2,\beta_2'}\right) f^{I;NZ;\sigma}_{\beta_2'} = 0$$

$$\mathcal{N}^{I;NZ}_{\beta_2,\beta_2'} = \langle I;NZ;\beta_2|I;NZ;\beta_2'\rangle$$

$$\mathcal{H}^{I;NZ}_{\beta_2,\beta_2'} = \langle I;NZ;\beta_2|\hat{H}_{2b}|I;NZ;\beta_2'\rangle + \varepsilon^{I;NZ}_{DD}\left(\Phi(\beta_2),\Phi(\beta_2')\right)$$

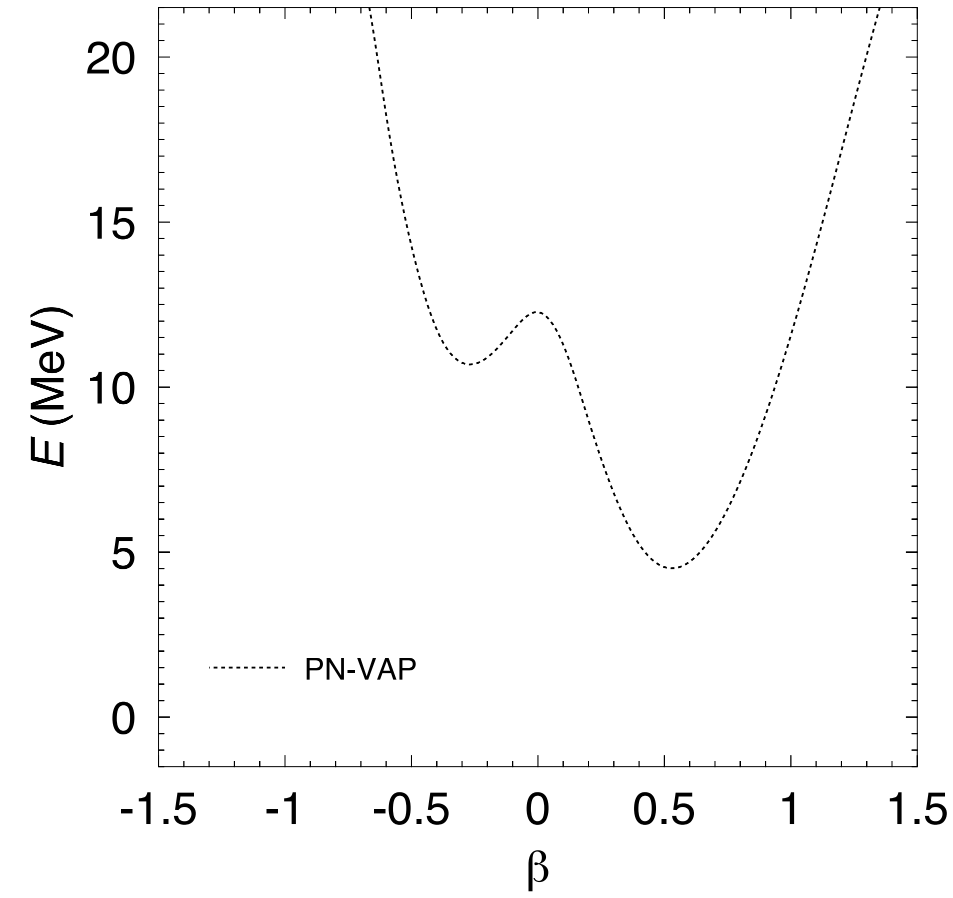
Gogny EDF axial

Axial calculations ^{24}Mg

First step: Particle Number Projection (before the variation) of HFB-type wave functions.

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

Total Energy Surface



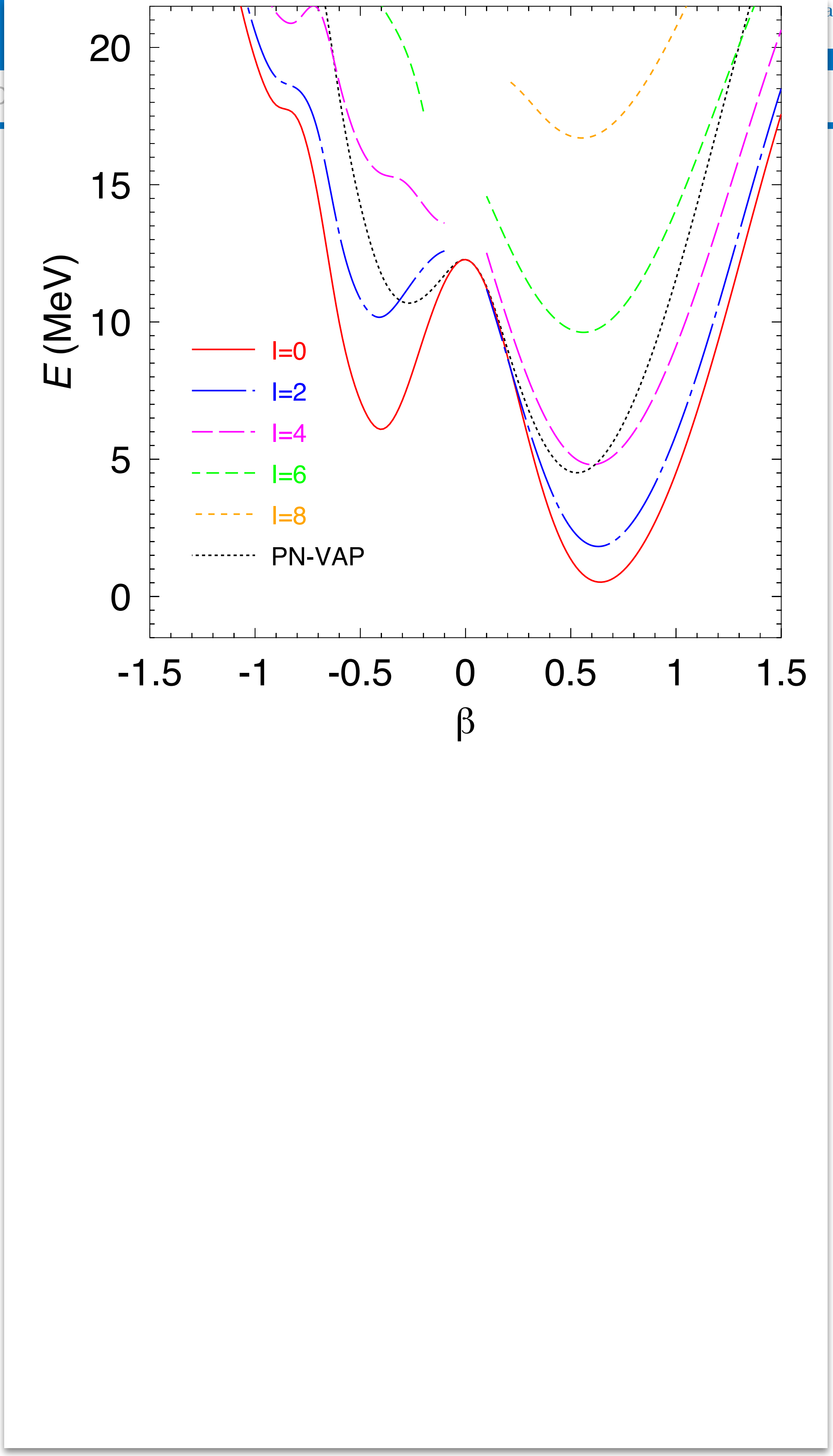
Gogny EDF axial

Axial calculations ^{24}Mg

Second step: Simultaneous **Particle Number and Angular Momentum Projection**

$$|\Phi^{IM;NZ}(\beta)\rangle = P^{I}_{00}P^{N}P^{Z}|\Phi(\beta)\rangle \Rightarrow E^{I,N,Z}(\beta)$$

Total Energy Surface



Gogny EDF axial

Axial calculations ^{24}Mg

Third step: Configuration mixing within the GCM framework

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

Configuration mixing

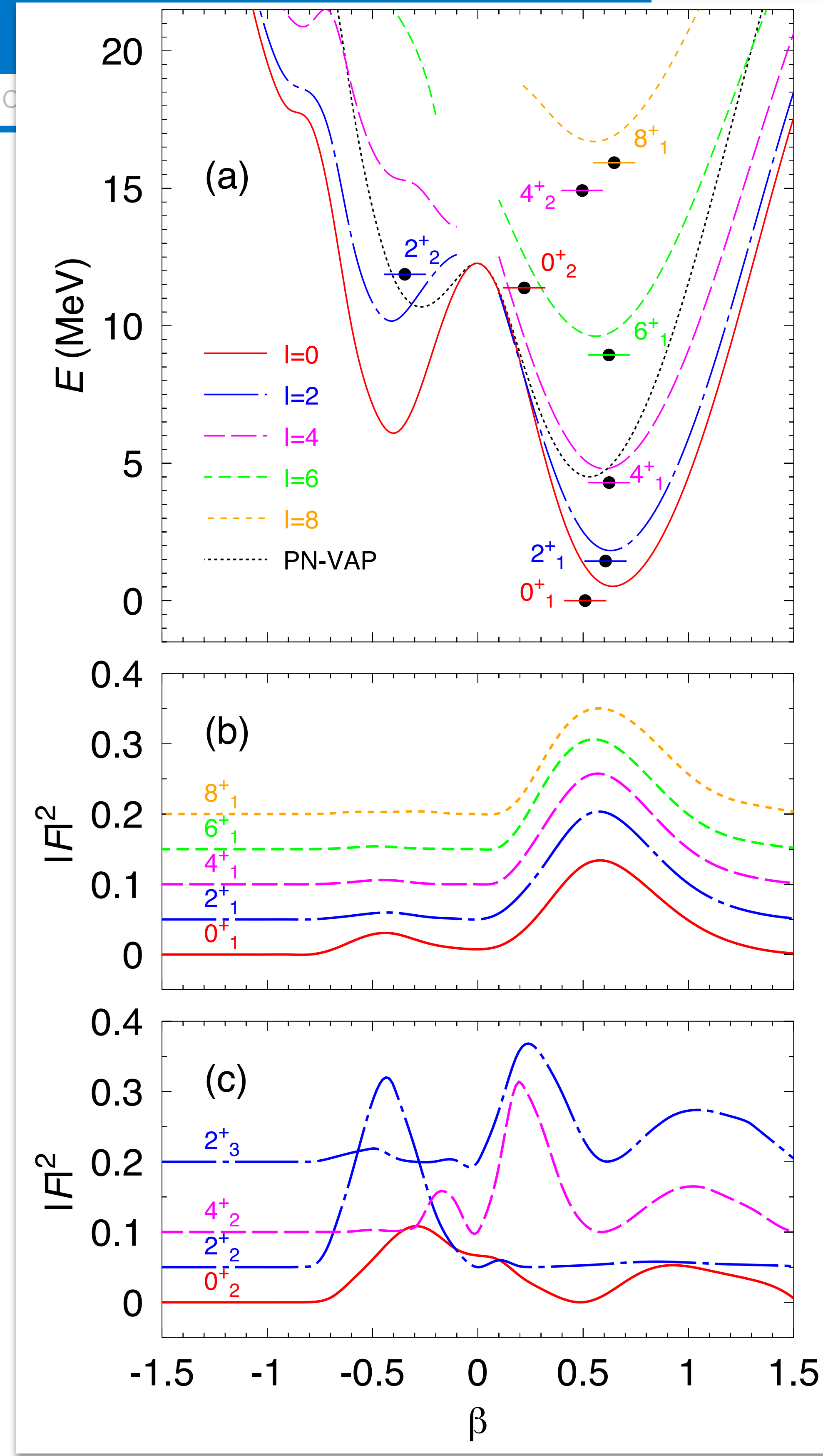
$$\sum_{\beta'} \left(\mathcal{H}^{I;NZ}_{\beta,\beta'} - E^{I;NZ;\sigma}\mathcal{N}_{\beta\beta'}\right) f^{I;NZ;\sigma}_{\beta'} = 0$$

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

$$\mathcal{H}_{\beta\beta'} = \langle\Phi(\beta)|\hat{H}P^{I}_{00}P^{N}P^{Z}|\Phi(\beta)\rangle$$

Hill-Wheeler-Griffin equations

- Energy spectrum
- Observables (mass, radius, B(E2), etc.)
- Distribution of probability for each state (collective w.f.)



Gogny EDF triaxial (TRSC)

- Initial intrinsic states: PN-VAP M. Anguiano, J. L. Egido, and L. M. Robledo, Nucl. Phys. A 696, 467 (2001).

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

- Intermediate Particle Number and Angular Momentum Projected states

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

- Final GCM states

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

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

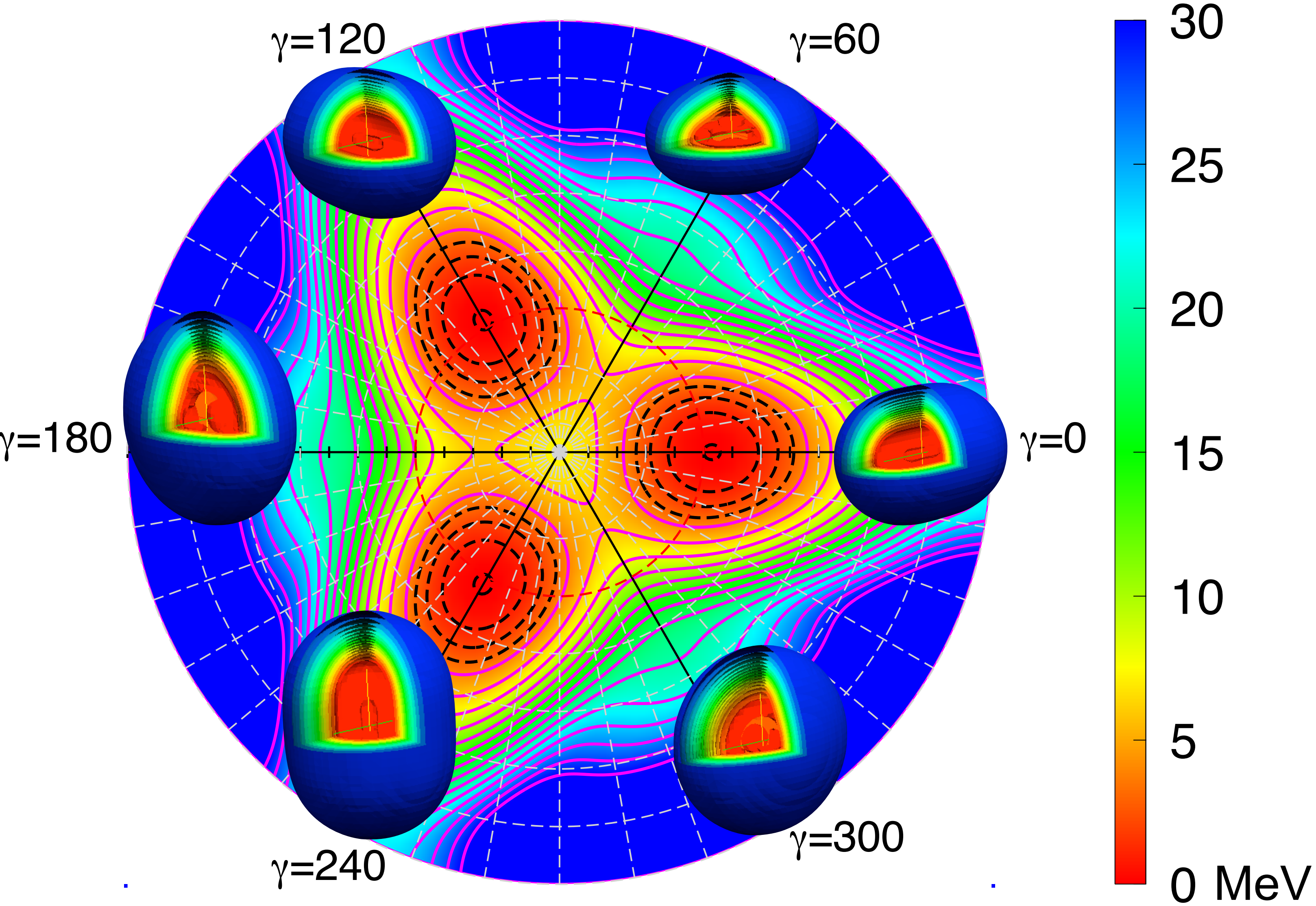
$$\mathcal{N}^{I;NZ}_{K\beta\gamma K'\beta'\gamma'} \equiv \langle IMK;NZ;\beta\gamma|IMK';NZ;\beta'\gamma'\rangle$$

$$\mathcal{H}^{I;NZ}_{K\beta\gamma K'\beta'\gamma'} \equiv \langle IMK;NZ;\beta\gamma|\hat{H}_{2b}|IMK';NZ;\beta'\gamma'\rangle + \varepsilon_{DD}^{IKK';NZ}[\Phi(\beta,\gamma),\Phi'(\beta',\gamma')]$$

Gogny EDF triaxial (TRSC)

Triaxial calculations ^{24}Mg

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



- Symmetry corresponding to the different orientation of the axes
- All configurations are included between γ∈[0º,60º]

T. R. R., J. L. Egido, PRC 81, 064323 (2010)

Triaxial calculations ^{24}Mg

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

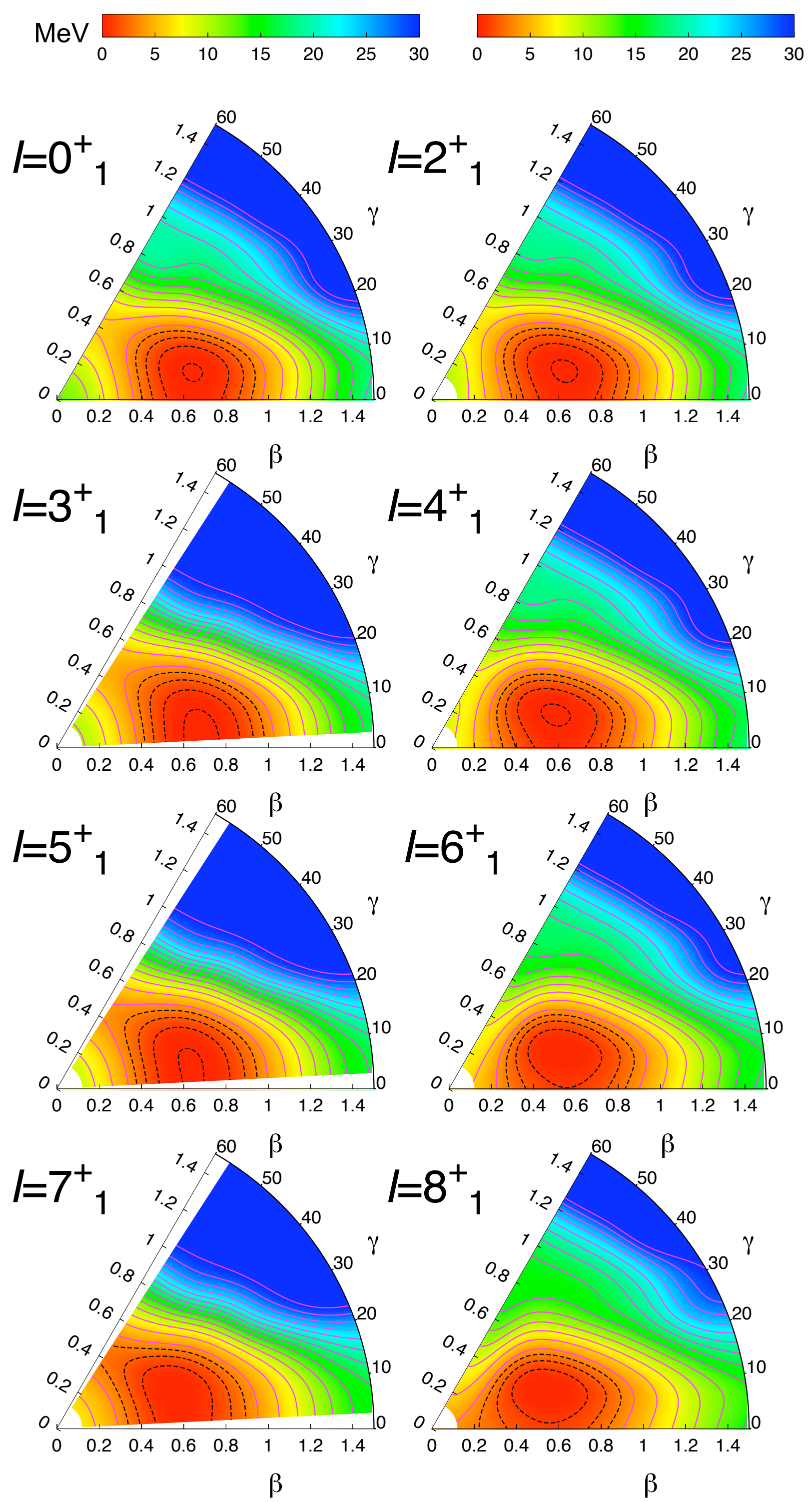
$$|IM;NZ;\beta\gamma\rangle = \sum_K g_K^{IM;NZ;\beta\gamma}|IMK;NZ;\beta\gamma\rangle$$

- 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 ~ 0.7 MeV (0^+)



Triaxial calculations ^{24}Mg

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

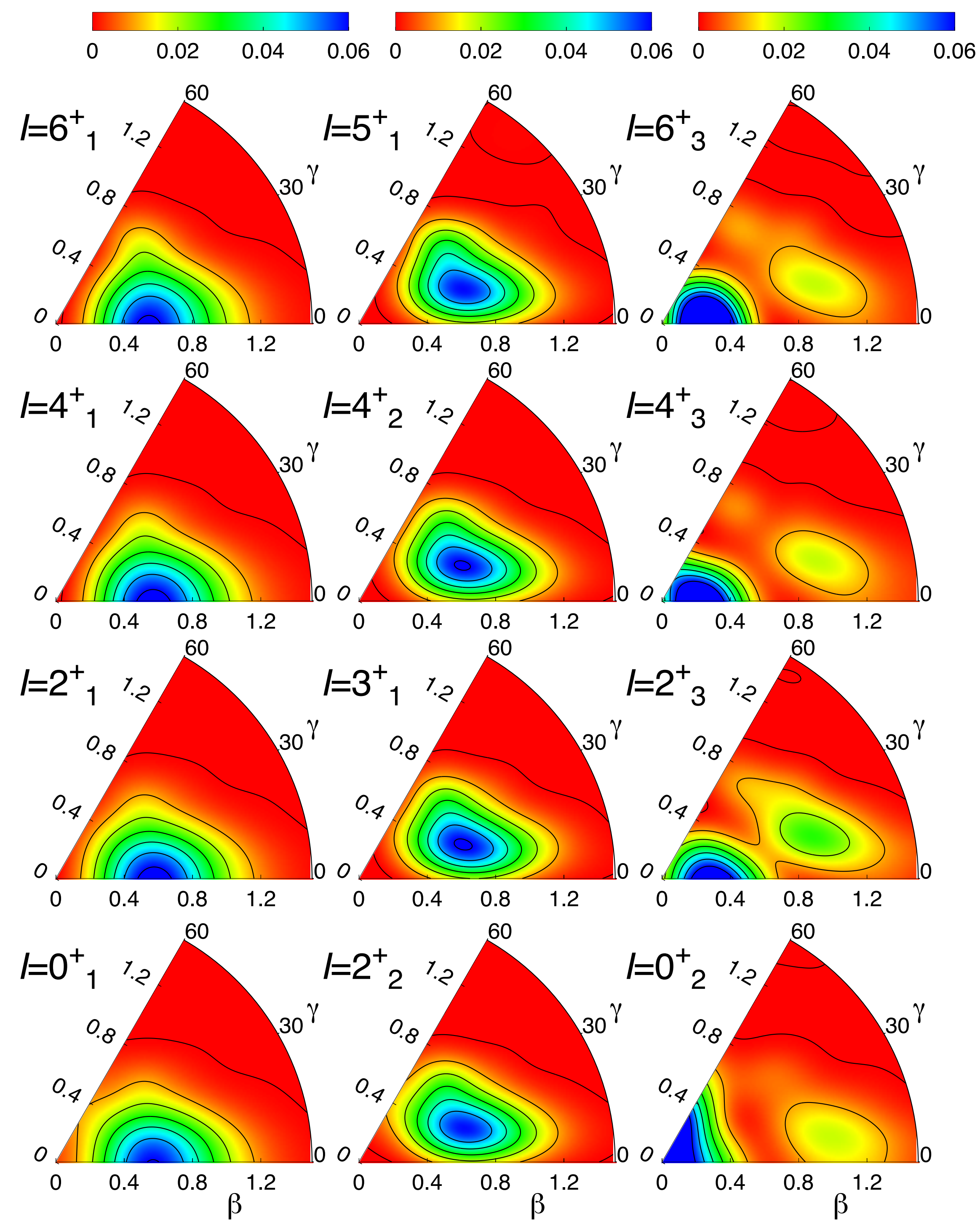
$$|IM;NZ\sigma\rangle = \sum_{K\beta\gamma} f^{I;NZ,\sigma}_{K\beta\gamma}|IMK;NZ;\beta\gamma\rangle$$

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

- Axial ground state rotational band

- Second band associated to a gamma band

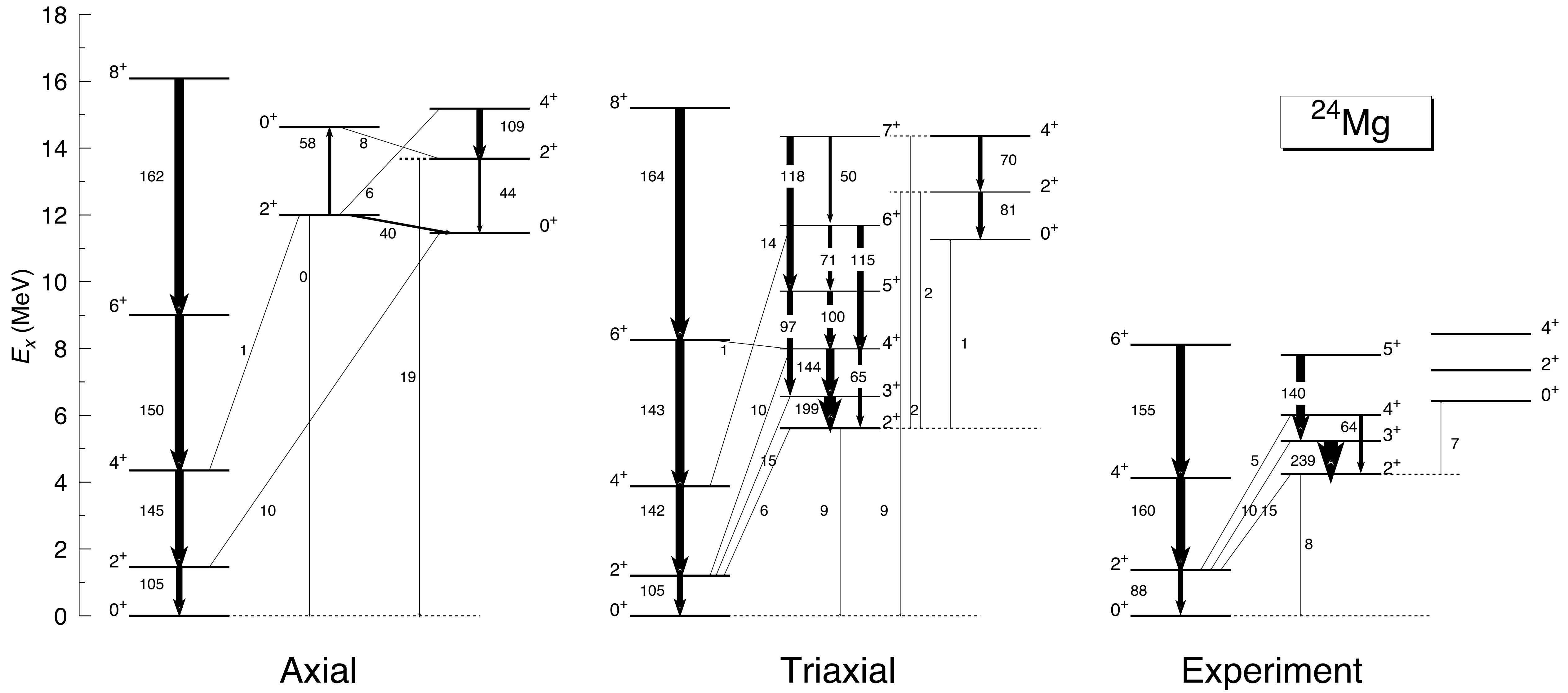
-Third band with shape mixing



Gogny EDF triaxial (TRSC)

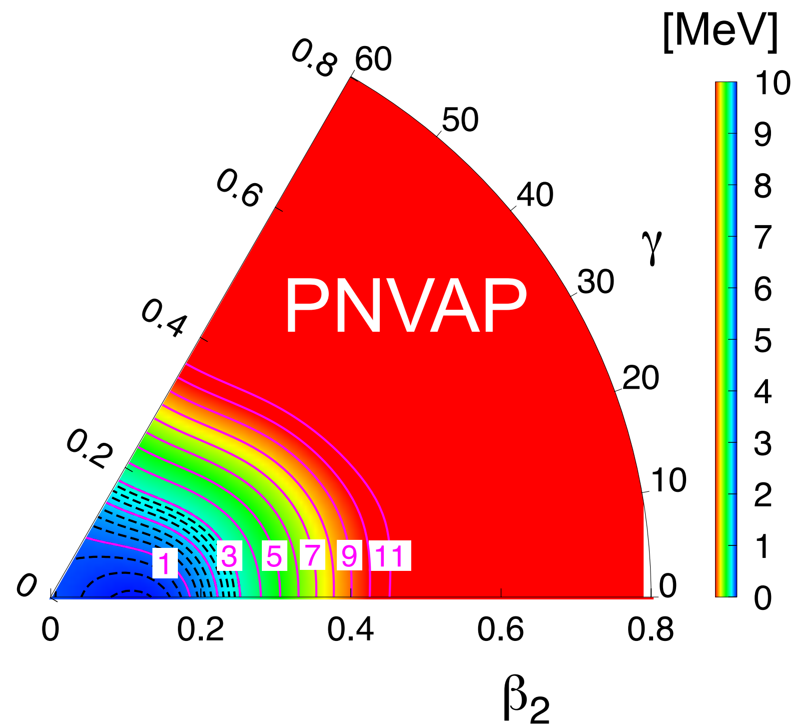
Triaxial calculations ^{24}Mg

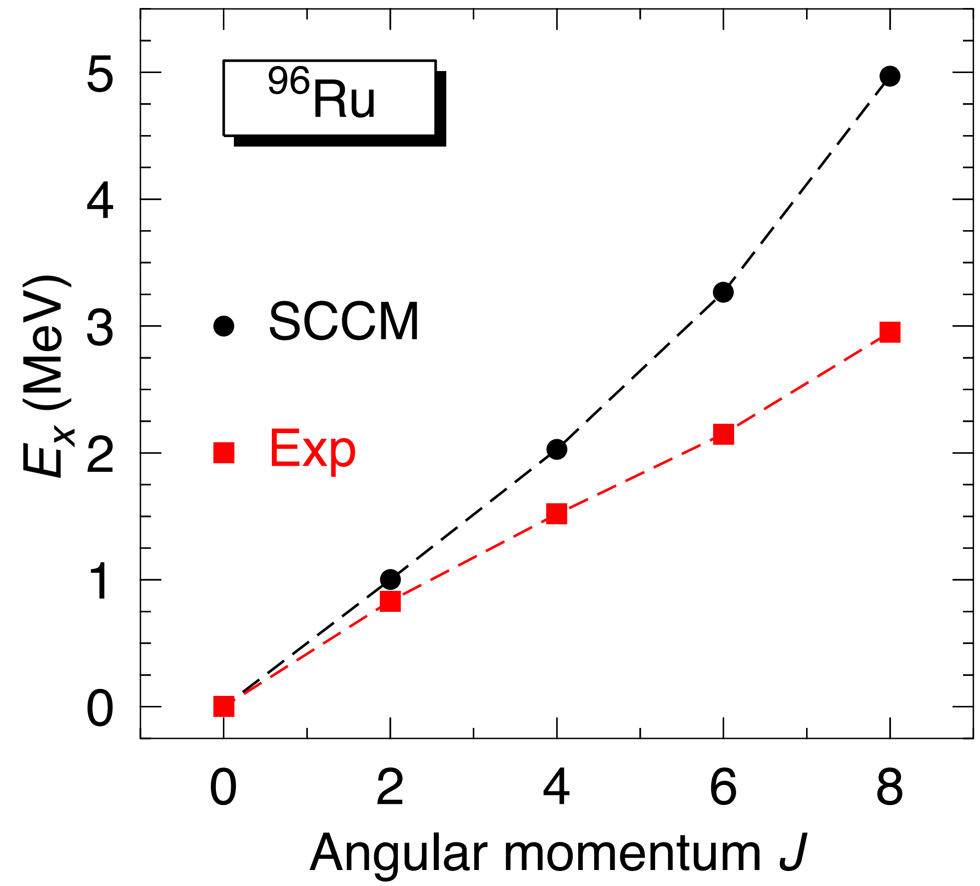
Configuration mixing within the framework of the **Generator Coordinate Method (GCM)**.
***K* and deformation mixing**

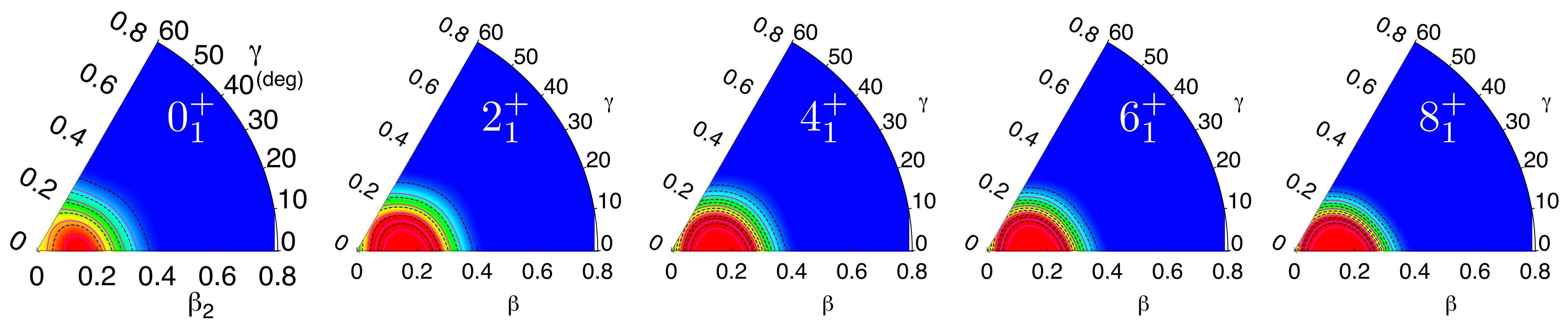


Gogny EDF triaxial (TRSC)

^{96}Ru

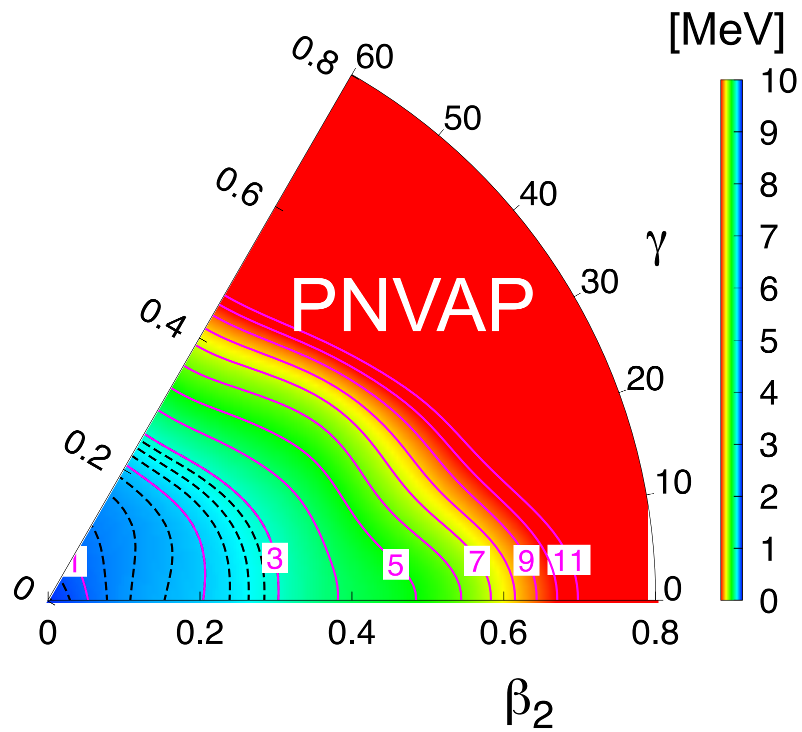


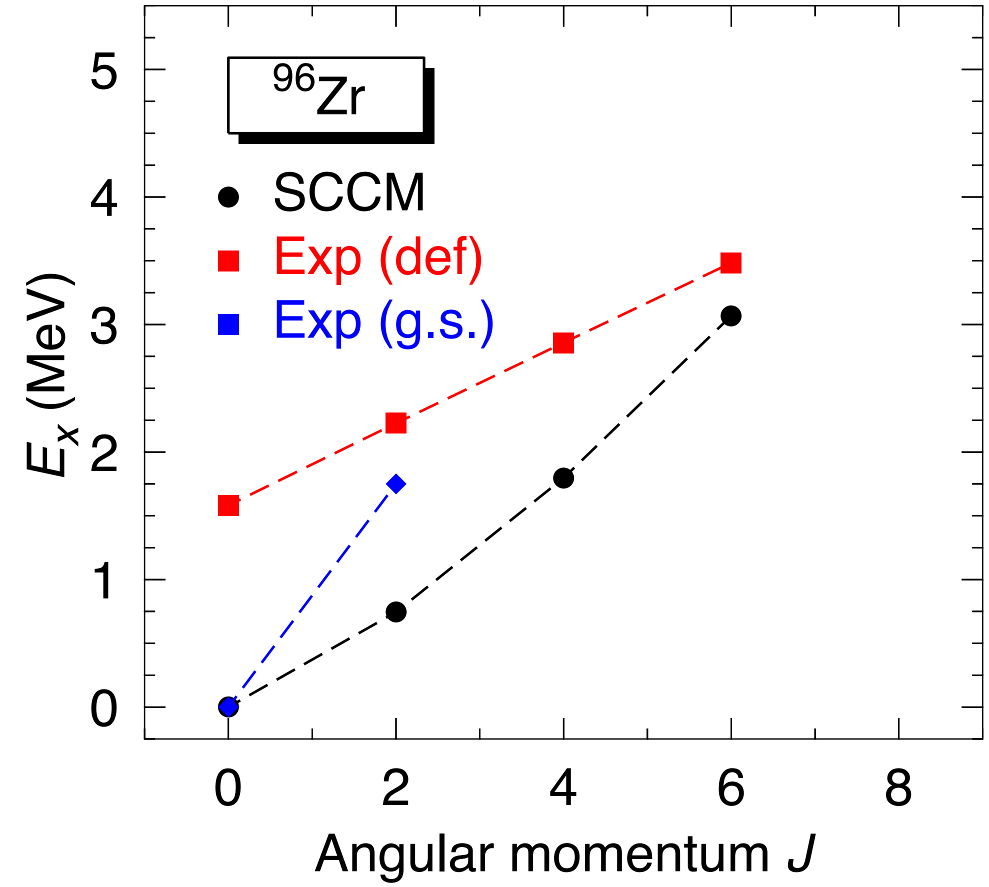


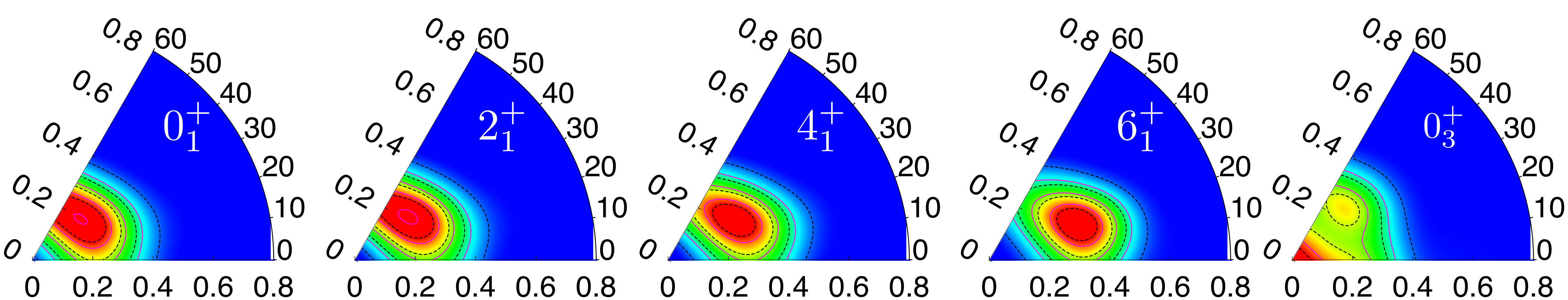


Gogny EDF triaxial (TRSC)

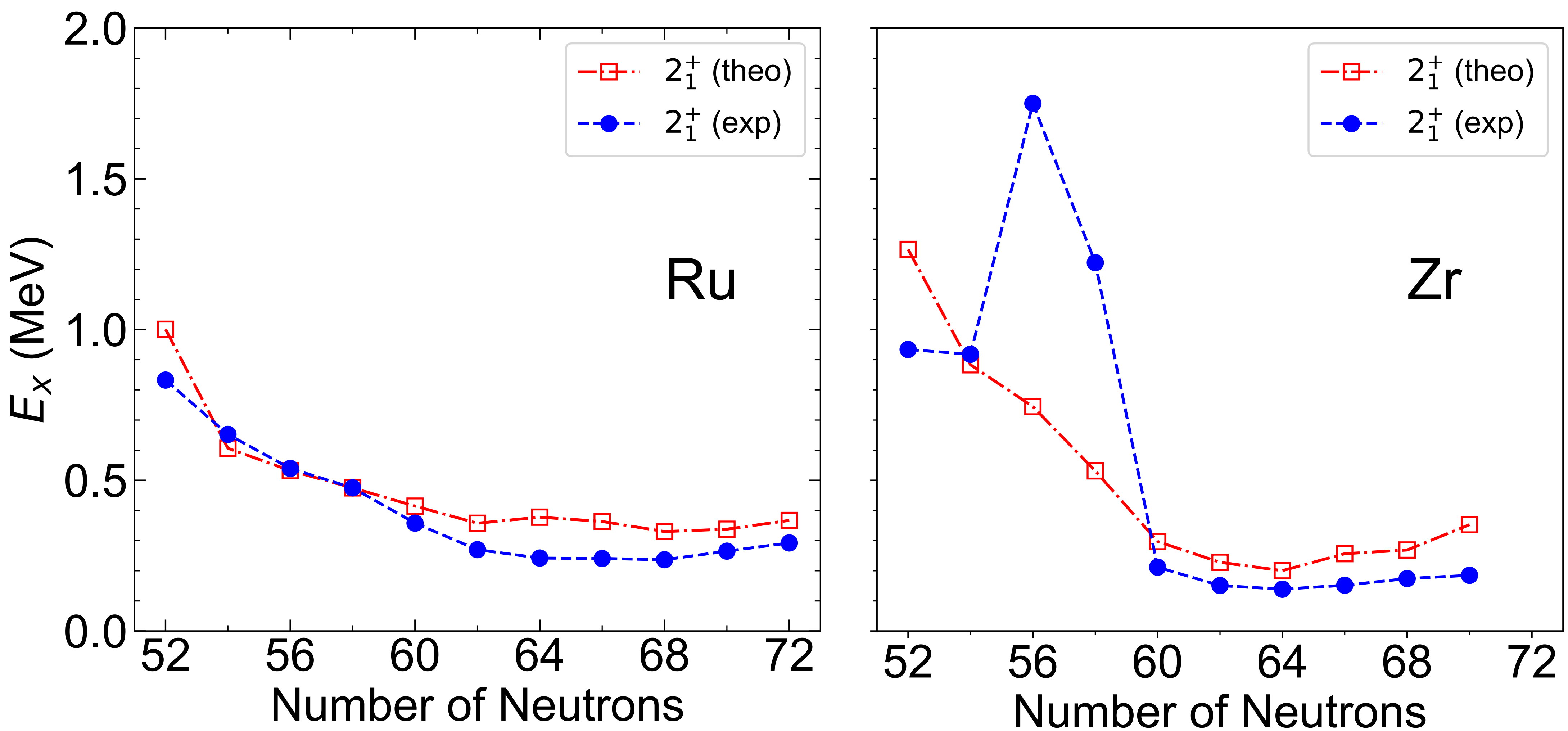
^{96}Zr







Systematics of the 2⁺ excited states

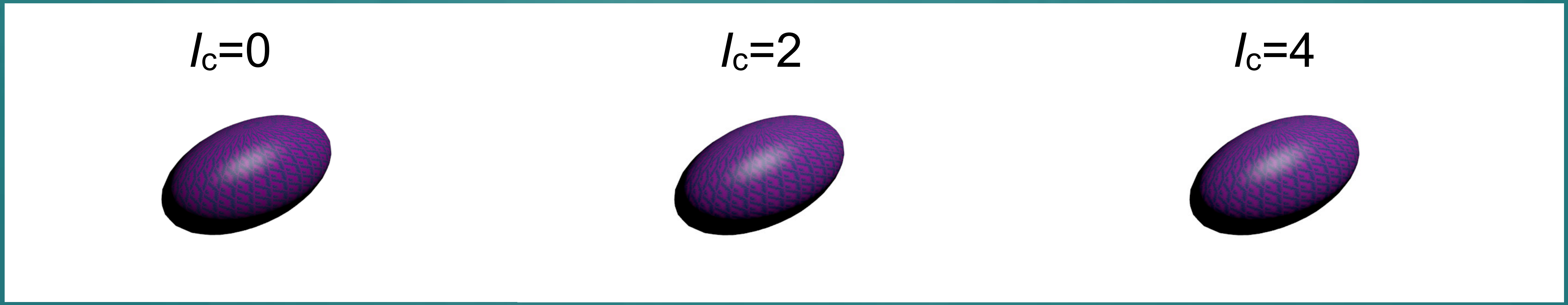


Gogny EDF triaxial (TRSB)

- Initial intrinsic states: PN-VAP

$$E^{N,Z}[\Phi] = \frac{\langle\Phi|\hat{H}_{2b}\hat{P}^N\hat{P}^Z|\Phi\rangle}{\langle\Phi|\hat{P}^N\hat{P}^Z|\Phi\rangle} + \varepsilon_{DD}^{N,Z}(\Phi) - \lambda_{q_{20}}\langle\Phi|\hat{Q}_{20}|\Phi\rangle - \lambda_{q_{22}}\langle\Phi|\hat{Q}_{22}|\Phi\rangle - \omega\langle\Phi|\hat{J}_x|\Phi\rangle$$

cranking term!!



Gogny EDF triaxial (TRSB)

Universidad Autónoma de Madrid

- Initial intrinsic states: PN-VAP

$$E^{N,Z}[\Phi] = \frac{\langle\Phi|\hat{H}_{2b}\hat{P}^N\hat{P}^Z|\Phi\rangle}{\langle\Phi|\hat{P}^N\hat{P}^Z|\Phi\rangle} + \varepsilon_{DD}^{N,Z}(\Phi) - \lambda_{q_{20}}\langle\Phi|\hat{Q}_{20}|\Phi\rangle - \lambda_{q_{22}}\langle\Phi|\hat{Q}_{22}|\Phi\rangle - \omega\langle\Phi|\hat{J}_x|\Phi\rangle$$

- Intermediate Particle Number and Angular Momentum Projected states

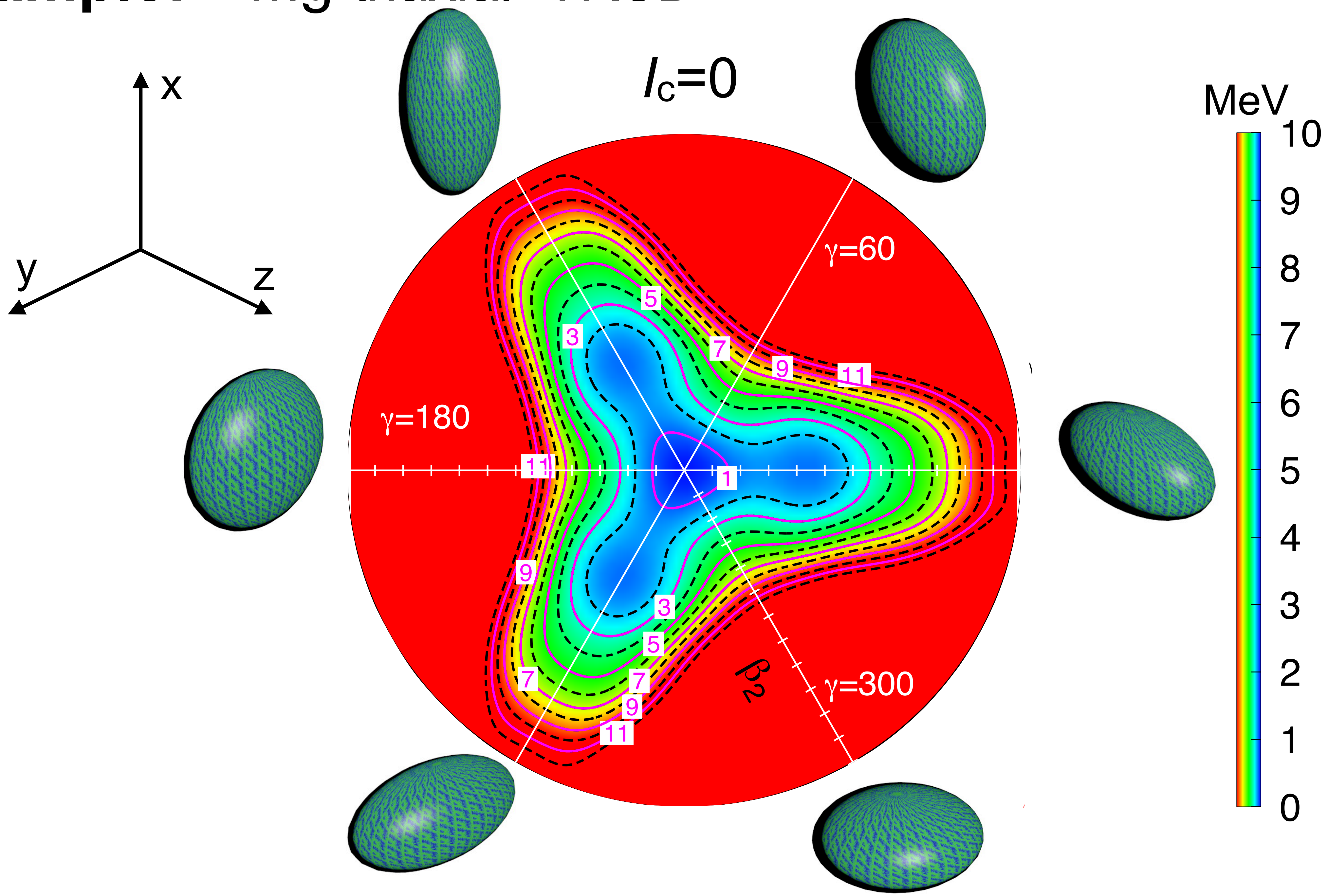
$$|IMK;NZ;\beta\gamma;\omega\rangle = \frac{2I+1}{8\pi^2}\int \mathcal{D}_{KK'}^{I*}(\Omega)\hat{R}(\Omega)\hat{P}^N\hat{P}^Z|\Phi(\beta,\gamma,\omega)\rangle d\Omega$$

- Final GCM states

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

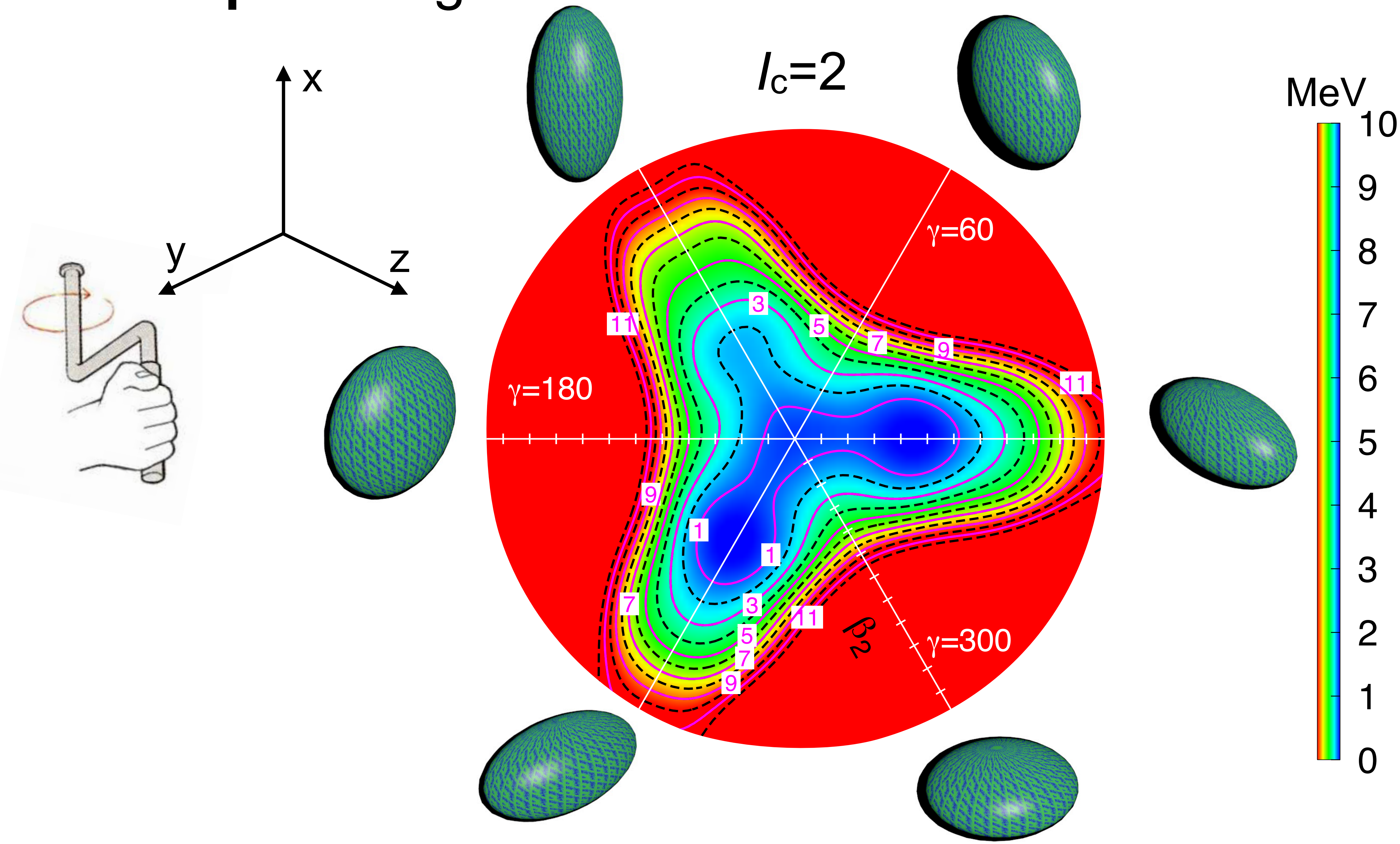
$$\sum_{K'\beta'\gamma'\omega'}\left(\mathcal{H}_{K\beta\gamma\omega;K'\beta'\gamma'\omega'}^{I;NZ} - E^{I;NZ;\sigma}\mathcal{N}_{K\beta\gamma\omega;K'\beta'\gamma'\omega'}^{I;NZ}\right) f_{K'\beta'\gamma'\omega'}^{I;NZ;\sigma} = 0$$

Example: ^{32}Mg triaxial+TRSB



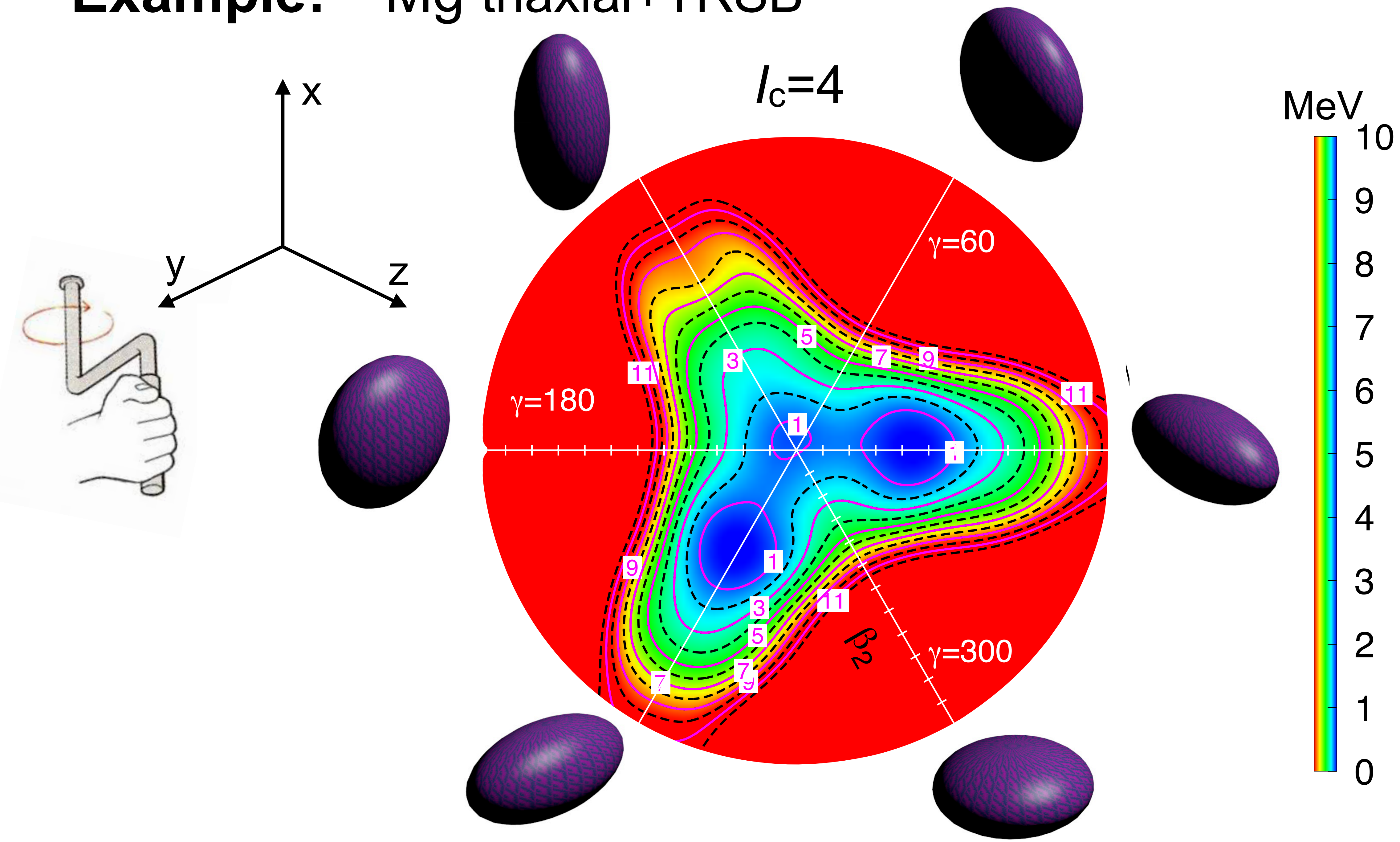
M. Borrajo, T.R.R, J.L. Egido, PLB 746, 341 (2015)

Example: ^{32}Mg triaxial+TRSB



M. Borrajo, T.R.R, J.L. Egido, PLB 746, 341 (2015)

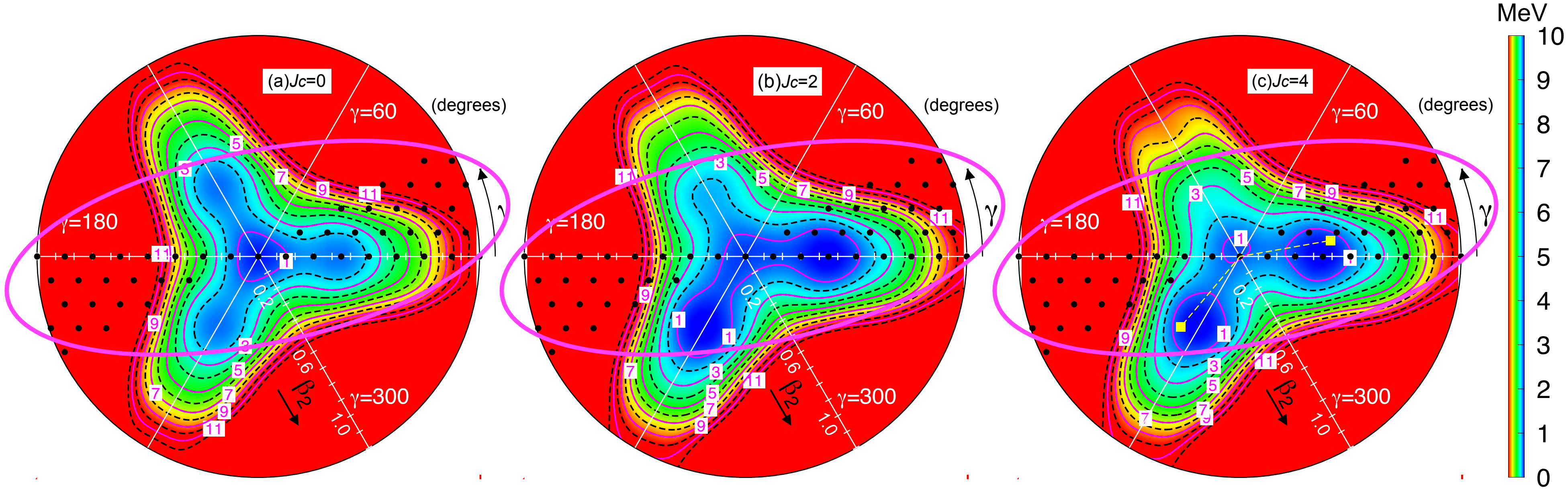
Example: ^{32}Mg triaxial+TRSB

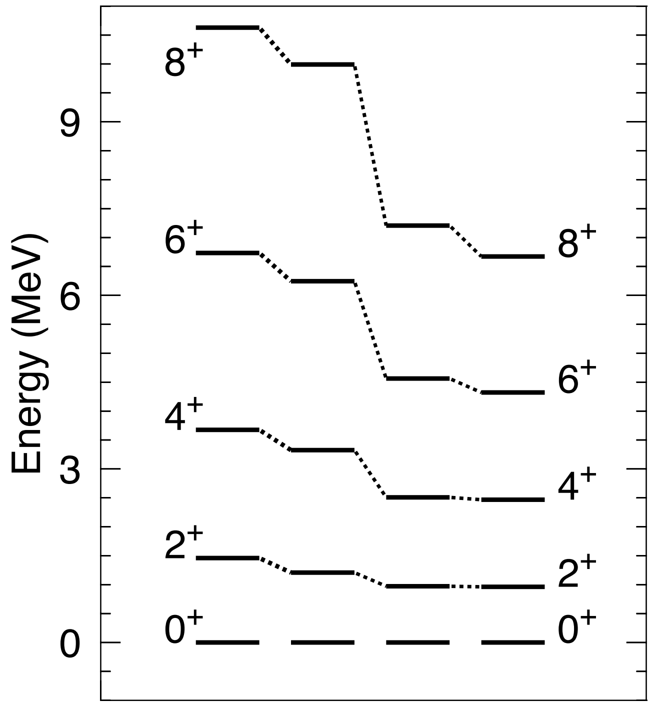


M. Borrajo, T.R.R, J.L. Egido, PLB 746, 341 (2015)

Gogny EDF triaxial (TRSB)

Example: ^{32}Mg; Effect on the excitation energies



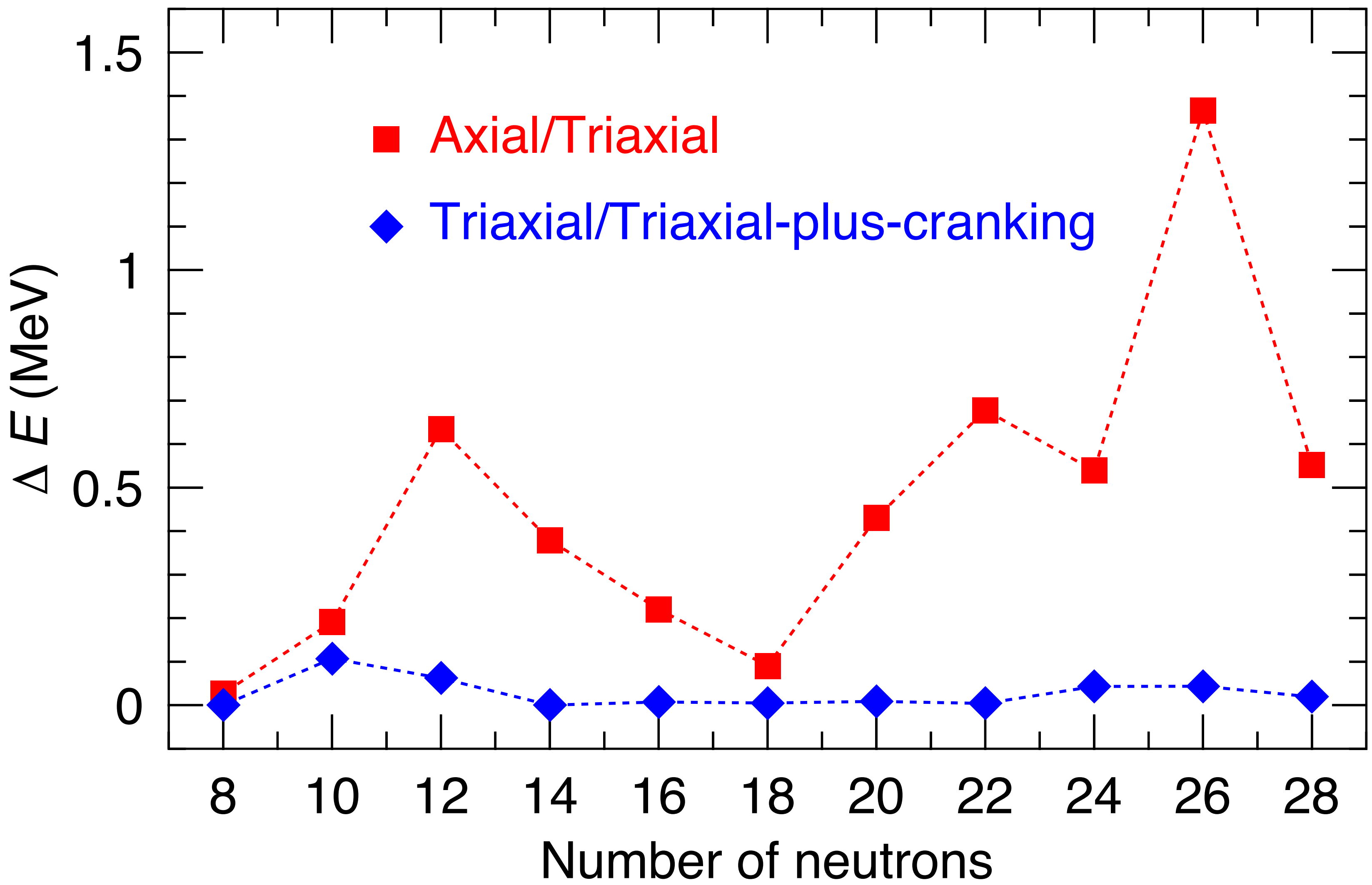


- ✓ Compression of the spectrum is observed.
- ✓ Convergence of the energies of the ground and lowest excited states is obtained.
- ✓ Only one-sextant is included.

E (g.s.)=-253.056,-253.477,-253.486,-253.498 MeV

M. Borrajo, T.R.R, J.L. Egido, PLB 746, 341 (2015)

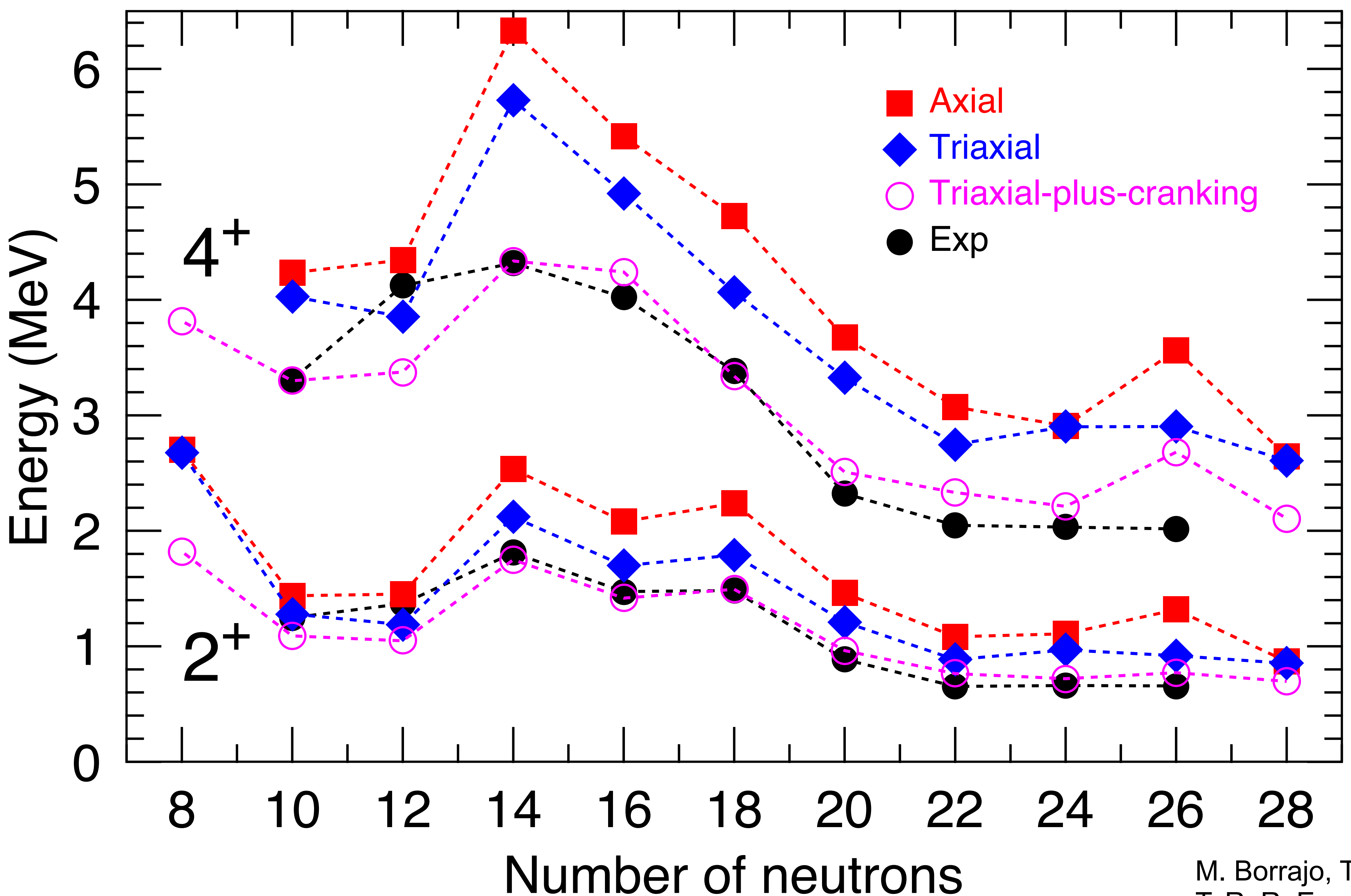
Systematics in the Magnesium isotopic chain



✓ Convergence of the energies of the ground states

T. R. R., Eur. Phys. J. A 52, 190 (2016)

Systematics in the Magnesium isotopic chain



- Trends are rather well described in all approaches.
- *N*=20 and 28 are not good shell closures.
- *N*=8 persists as a magic number.
- Disagreement in *N*=*Z* could indicate the lack of *pn* pairing.

M. Borrajo, T.R.R, J.L. Egido, PLB 746, 341 (2015)
T. R. R. Eur. Phys. J. A 52, 190 (2016).

Gogny EDF axial (PB)

- Initial intrinsic states: PN-VAP

$$E\left[\Phi\right]=\langle\Phi|\hat{H}_{2b}|\Phi\rangle+\varepsilon_{DD}^{N,Z}(\Phi)-\lambda_{N}\langle\Phi|\hat{N}|\Phi\rangle-\lambda_{Z}\langle\Phi|\hat{Z}|\Phi\rangle-\lambda_{q_{20}}\langle\Phi|\hat{Q}_{20}|\Phi\rangle-\lambda_{q_{30}}\langle\Phi|\hat{Q}_{30}|\Phi\rangle$$

- Intermediate Parity, Particle Number and Angular Momentum Projected states

$$|I;NZ;\Pi;\beta_2,\beta_3\rangle=\frac{2I+1}{2}\int_0^{\pi}d_{00}^{I*}(\beta)e^{-i\beta\hat{J}_y}\hat{P}^N\hat{P}^Z\hat{P}^{\Pi}|\Phi\rangle d\beta$$

- Final GCM states

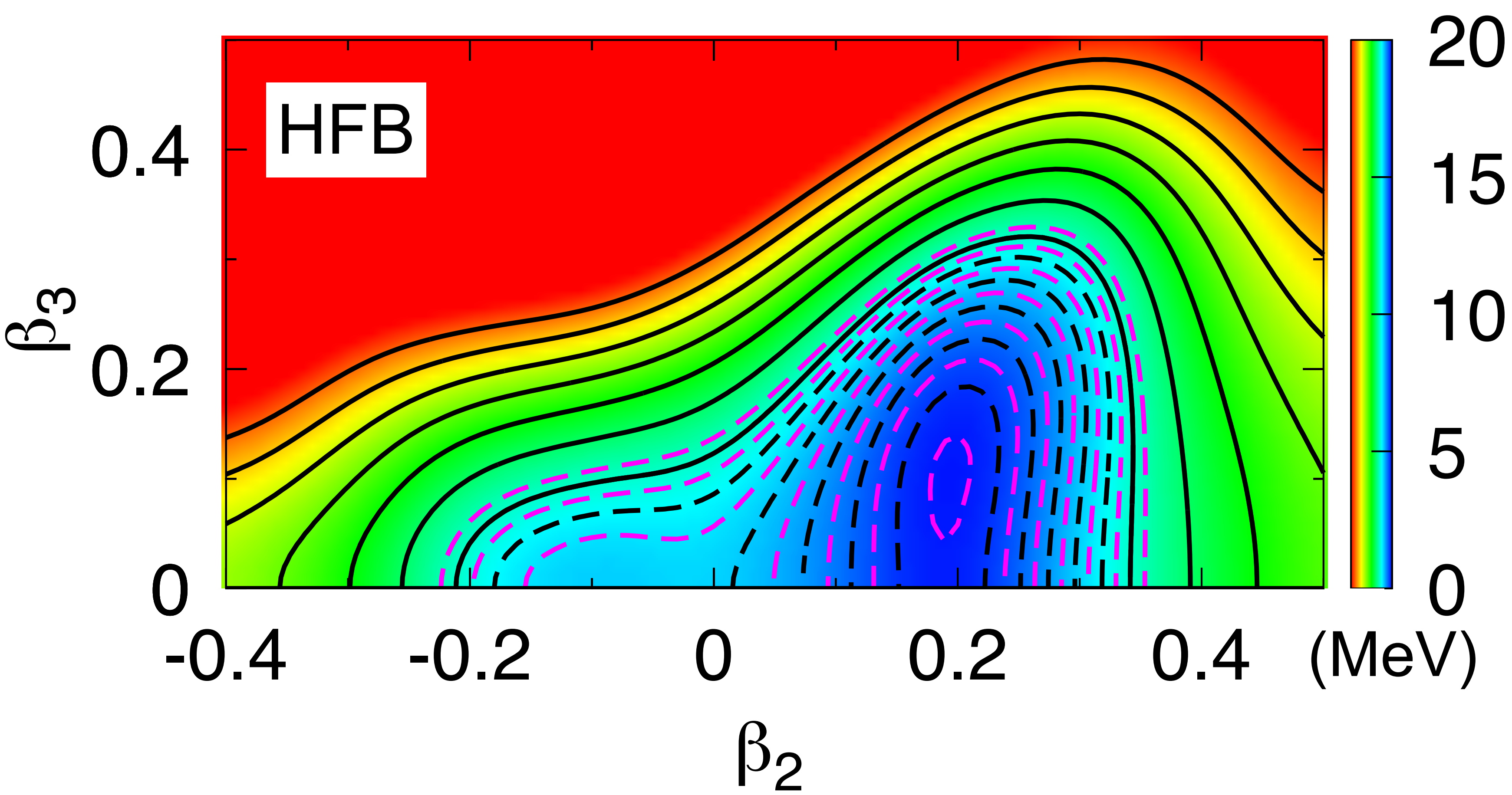
$$|I;NZ;\Pi;\sigma\rangle=\sum_{\beta_2\beta_3}f_{\beta_2\beta_3}^{I;NZ;\Pi;\sigma}|I;NZ;\Pi;\beta_2,\beta_3\rangle$$

$$\sum_{\beta_2'\beta_3'}\left(\mathcal{H}_{\beta_2\beta_3,\beta_2'\beta_3'}^{I;NZ;\Pi}-E^{I;NZ;\Pi;\sigma}\mathcal{N}_{\beta_2\beta_3,\beta_2'\beta_3'}^{I;NZ;\Pi}\right)f_{\beta_2'\beta_3'}^{I;NZ;\Pi;\sigma}=0$$

$$\mathcal{N}_{\beta_2\beta_3,\beta_2'\beta_3'}^{I;NZ;\Pi}=\langle I;NZ;\Pi;\beta_2,\beta_3|I;NZ;\Pi;\beta_2',\beta_3'\rangle$$

$$\mathcal{H}_{\beta_2\beta_3,\beta_2'\beta_3'}^{I;NZ;\Pi}=\langle I;NZ;\Pi;\beta_2,\beta_3|\hat{H}_{2b}|I;NZ;\Pi;\beta_2',\beta_3'\rangle+\varepsilon_{DD}^{I;NZ;\Pi}\left(\Phi(\beta_2,\beta_3),\Phi(\beta_2',\beta_3')\right)$$

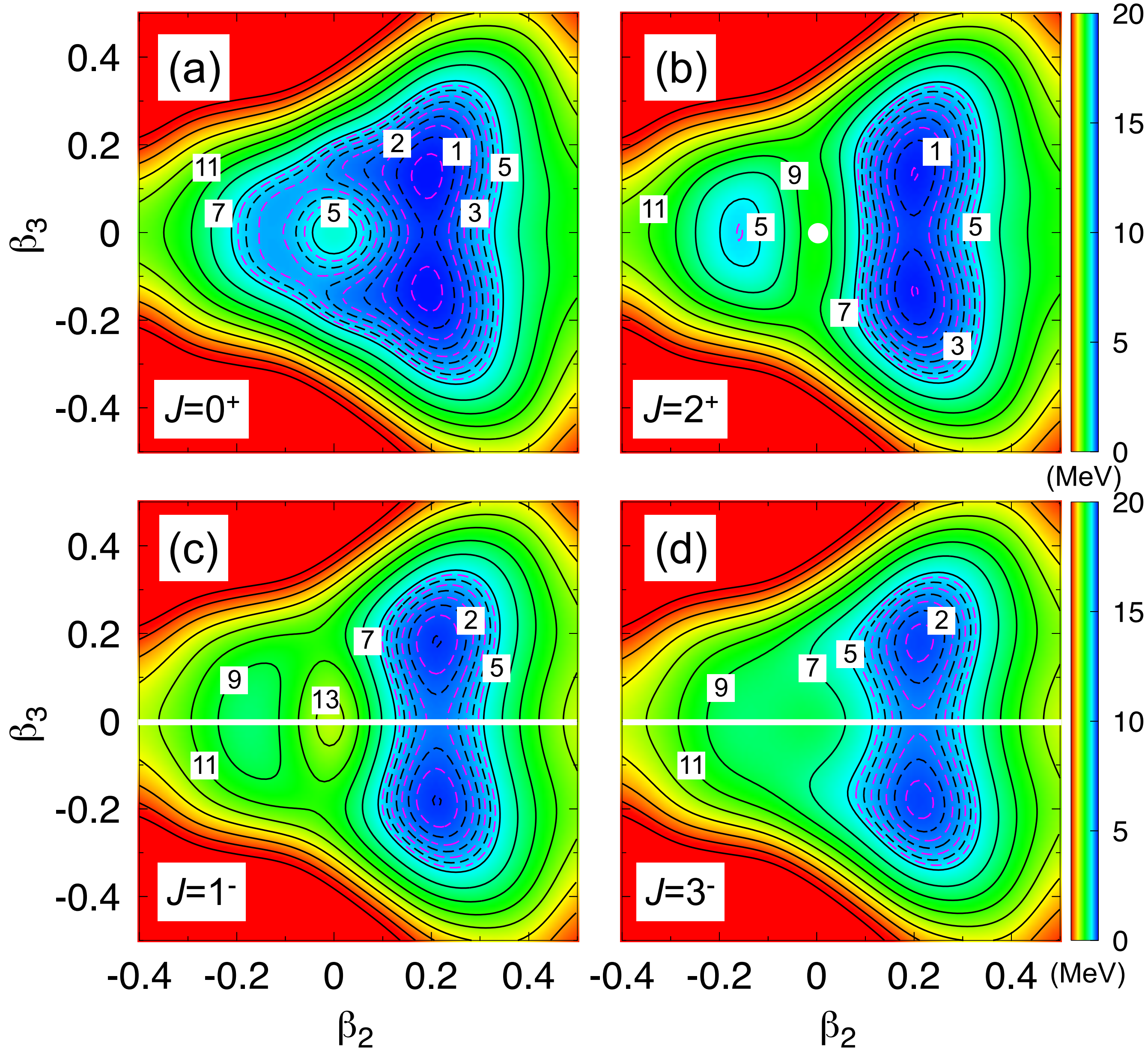
Example: ^{144}Ba axial calculations



R. Bernard, L. M. Robledo, T. R. R., PRC (2016)

Example: ^{144}Ba axial calculations

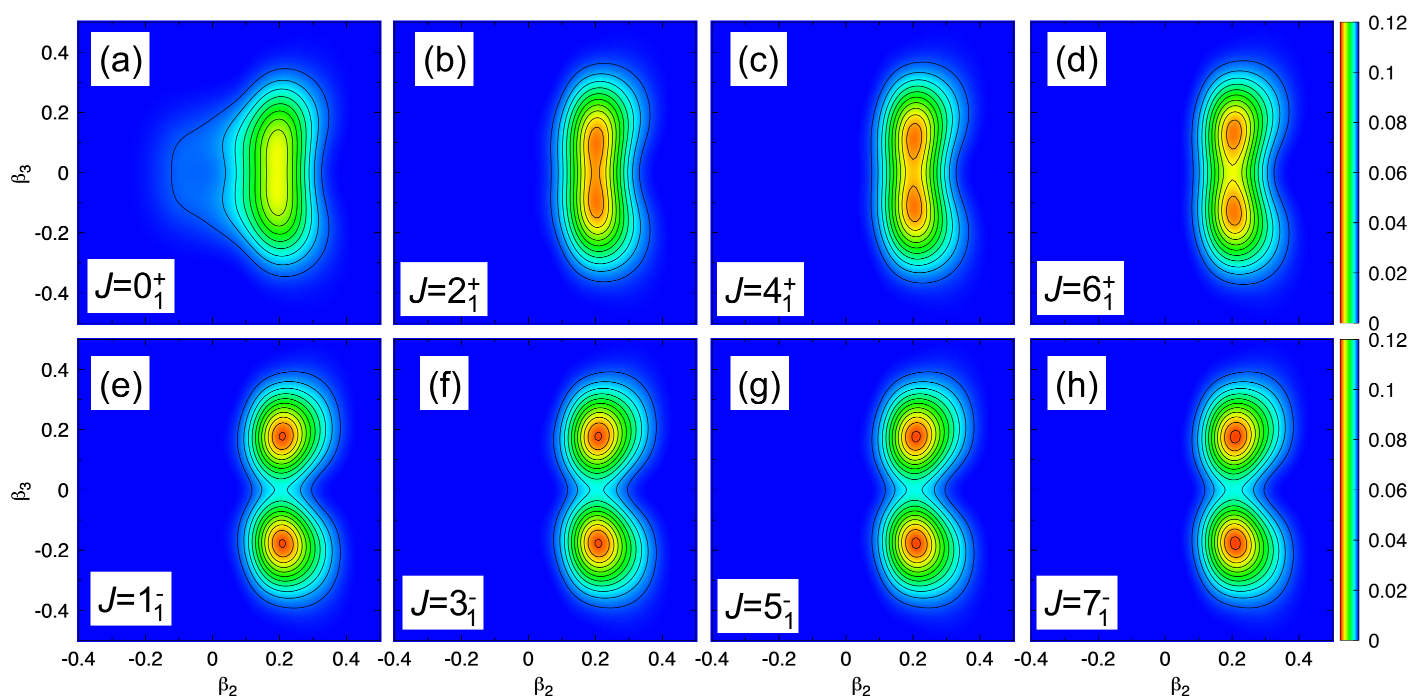
Particle number, angular momentum and parity projected PES

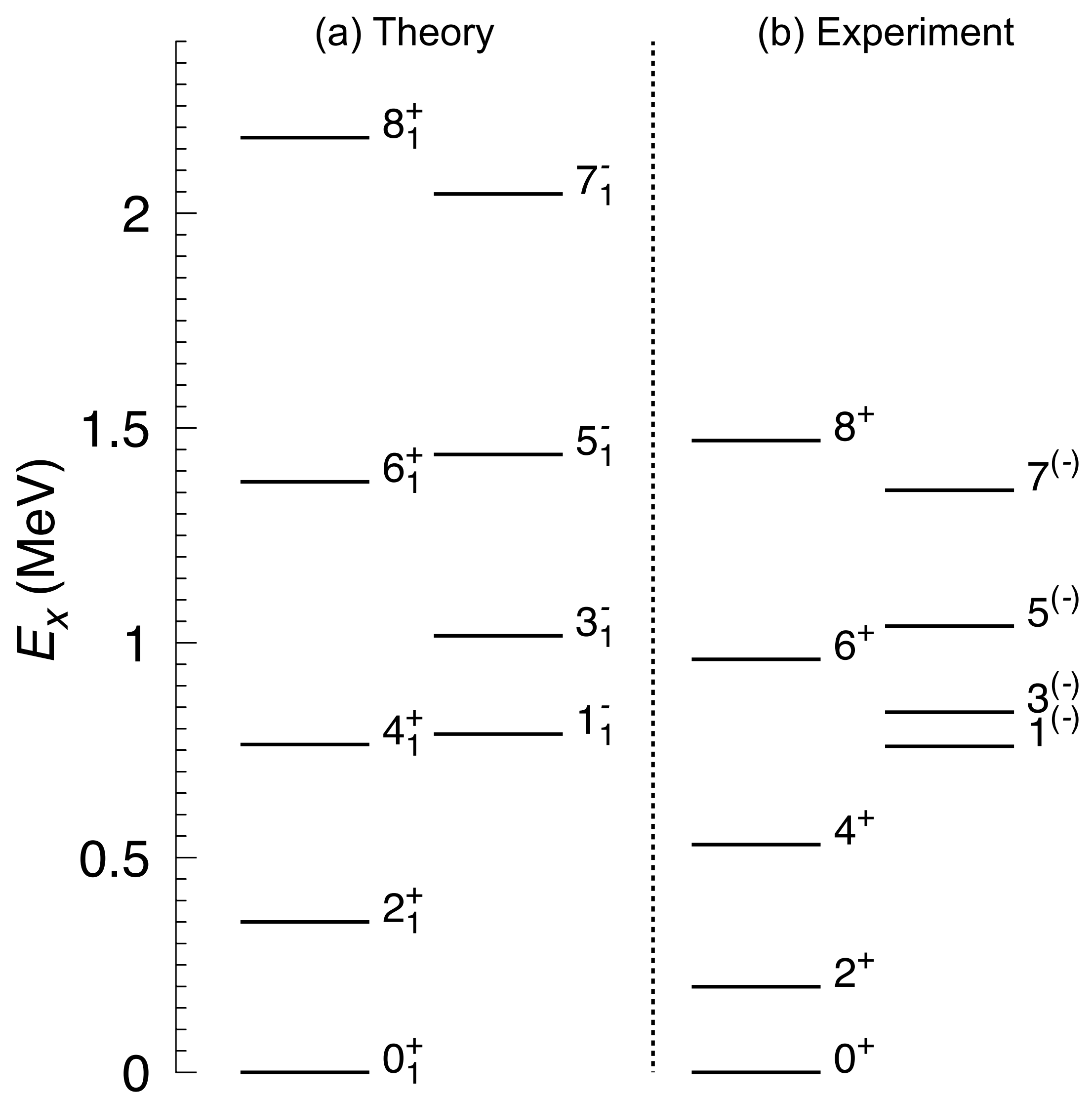


R. Bernard, L. M. Robledo, T. R. R., PRC (2016)

Example: ^{144}Ba axial calculations

Collective wave functions





R. Bernard, L. M. Robledo, T. R. R., PRC (2016)

Results: Transition probabilities.

^{144}Ba

$J_i^\pi \to J_f^\pi$	$E\lambda$	GCM β_2	GCM β_3	GCM $\beta_2-\beta_3$	Exp
$0^+ \to 2^+$	E2	1.148	1.121	1.023	1.042^{+17}_{-22}
$2^+ \to 4^+$	E2	1.865	1.803	1.845	1.860^{+86}_{-81}
$4^+ \to 6^+$	E2	2.371	2.287	2.360	1.78^{+12}_{-10}
$6^+ \to 8^+$	E2	2.800	2.696	2.793	2.04^{+35}_{-23}
$0^+ \to 1^-$	E1	0.007	0.006	0.008	
$1^- \to 2^+$	E1	0.005	0.009	0.006	
$0^+ \to 3^-$	E3	0.450	0.477	0.460	0.65^{+17}_{-23}
$1^- \to 4^+$	E3	0.599	0.635	0.695	
$2^+ \to 5^-$	E3	0.708	0.745	0.810	< 1.2
$3^- \to 6^+$	E3	0.804	0.865	0.810	
$4^+ \to 7^-$	E3	0.887	0.945	1.031	< 1.6

TABLE I. Absolute values of the transition matrix elements $|\langle J_i^\pi||E\lambda||J_f^\pi\rangle|$ (in $eb^{\lambda/2}$) for several transitions of interest. The experimental values are taken from [29].

R. Bernard, L. M. Robledo, T. R. R., PRC 93, 054316 (2016)

^{146}Ba

TABLE I. The experimental $|\langle I_f^\pi\|\hat{M}_\lambda\|I_i^\pi\rangle|$ matrix elements ($e\cdot b^{\lambda/2}$) based on the GOSIA fit along with new symmetry-conserving configuration-mixing calculations (see text and Ref. [23] for details).

$I_i^\pi \to I_f^\pi$	$E\lambda$	Experimental	SCCM
$0^+ \to 1^-$	$E1$	$0.000223\binom{10}{-8}$ [a]	0.00474
$1^- \to 3^-$	$E2$	1.2(5)	1.6
$0^+ \to 2^+$	$E2$	1.17(2) [a]	1.14
$2^+ \to 4^+$	$E2$	1.97(14)	1.90
$4^+ \to 6^+$	$E2$	$2.35\binom{+20}{-24}$	2.43
$6^+ \to 8^+$	$E2$	$2.17\binom{+65}{-33}$	2.90
$0^+ \to 3^-$	$E3$	$0.65\binom{+14}{-20}$	0.54
$2^+ \to 5^-$	$E3$	$1.01\binom{+61}{-20}$	0.87
$4^+ \to 7^-$	$E3$	$1.25\binom{+85}{-34}$	1.11
$6^+ \to 9^-$	$E3$	$1.5\binom{+8}{-12}$	

[a]Primarily determined by previous lifetime and/or branching ratio data [10].

B. Bucher et al., PRL 118, 152504 (2017).

Summary and outlook

- PGCM methods provide a reliable description of nuclear structure observables and they provide the perfect tools to study shape transitions/ mixing/coexistence in nuclei.

- However, it could fail in specific nuclei:
  - Not enough degrees of freedom are explored
  - Some EDF could not be adequate.

- Breaking of:
  - parity allows for a good description of negative parity states.
  - axial symmetry is needed to study properly shape evolution/shape coexistence in many isotopic chains.
  - time-reversal symmetry (cranking states) allows for a quantitative agreement with the experimental energy spectra.