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Coexistence of nuclear shapes: mean-field and beyond

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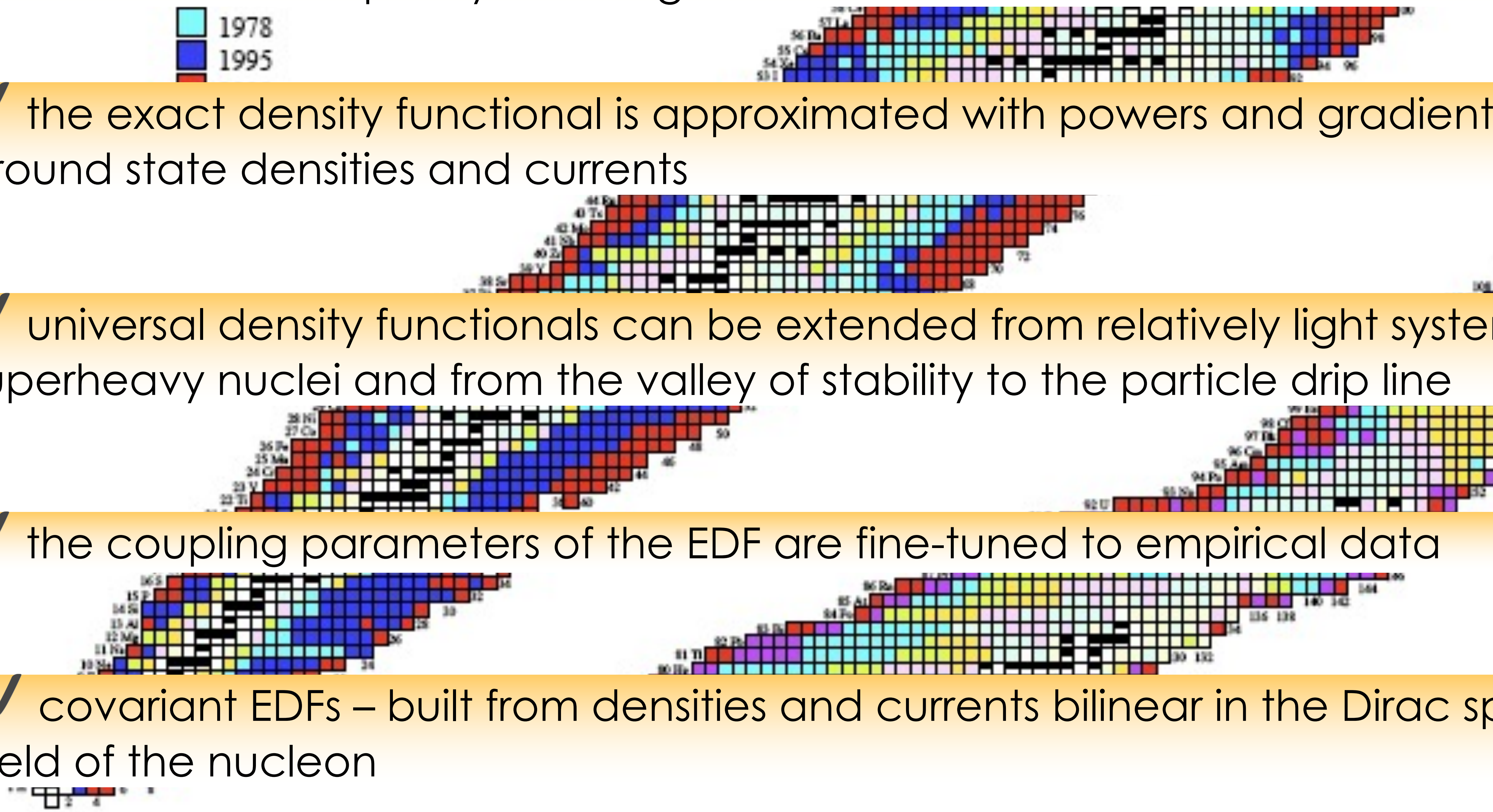
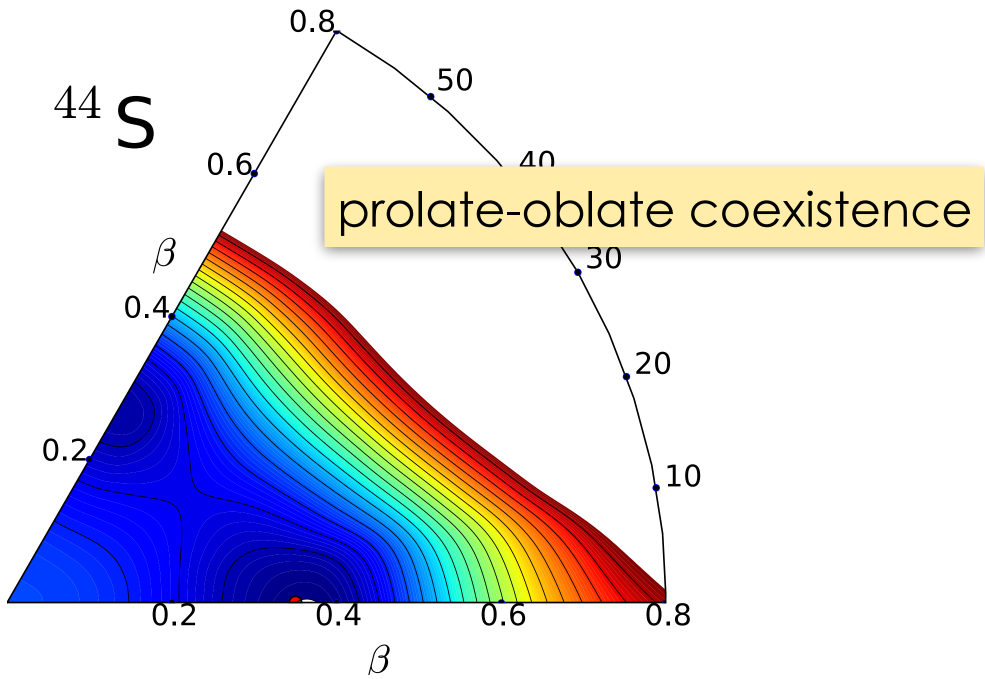
Universal theory framework: Energy Density Functionals

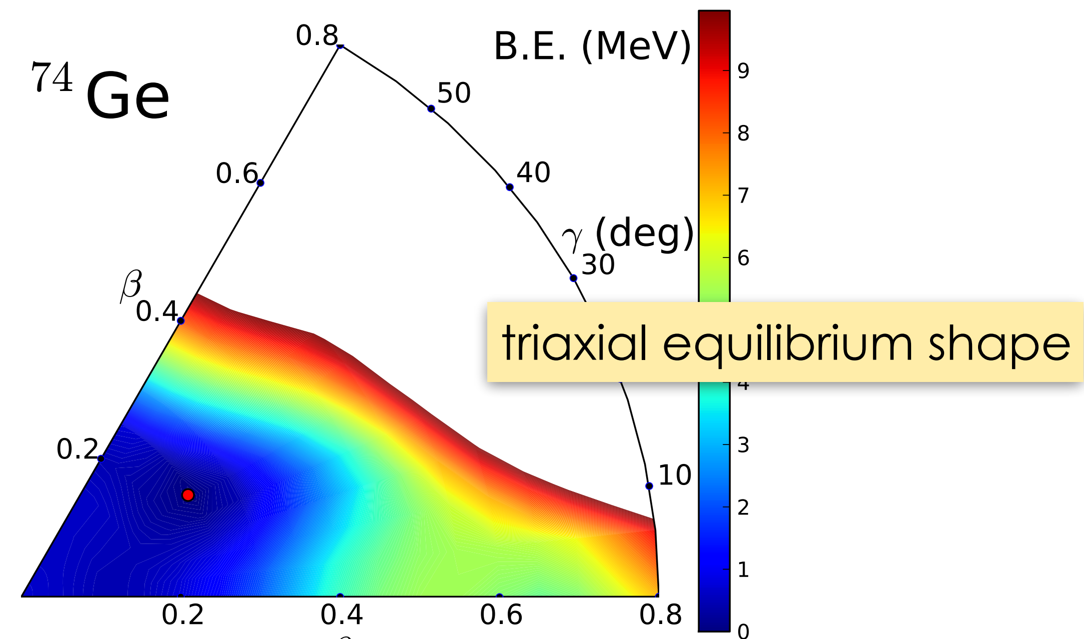


- ✓ the nuclear many-body problem is effectively mapped onto a one-body problem without explicitly involving internucleon interactions
- ✓ the exact density functional is approximated with powers and gradients of ground state densities and currents
- ✓ universal density functionals can be extended from relatively light systems to superheavy nuclei and from the valley of stability to the particle drip line
- ✓ the coupling parameters of the EDF are fine-tuned to empirical data
- ✓ covariant EDFs – built from densities and currents bilinear in the Dirac spinor field of the nucleon

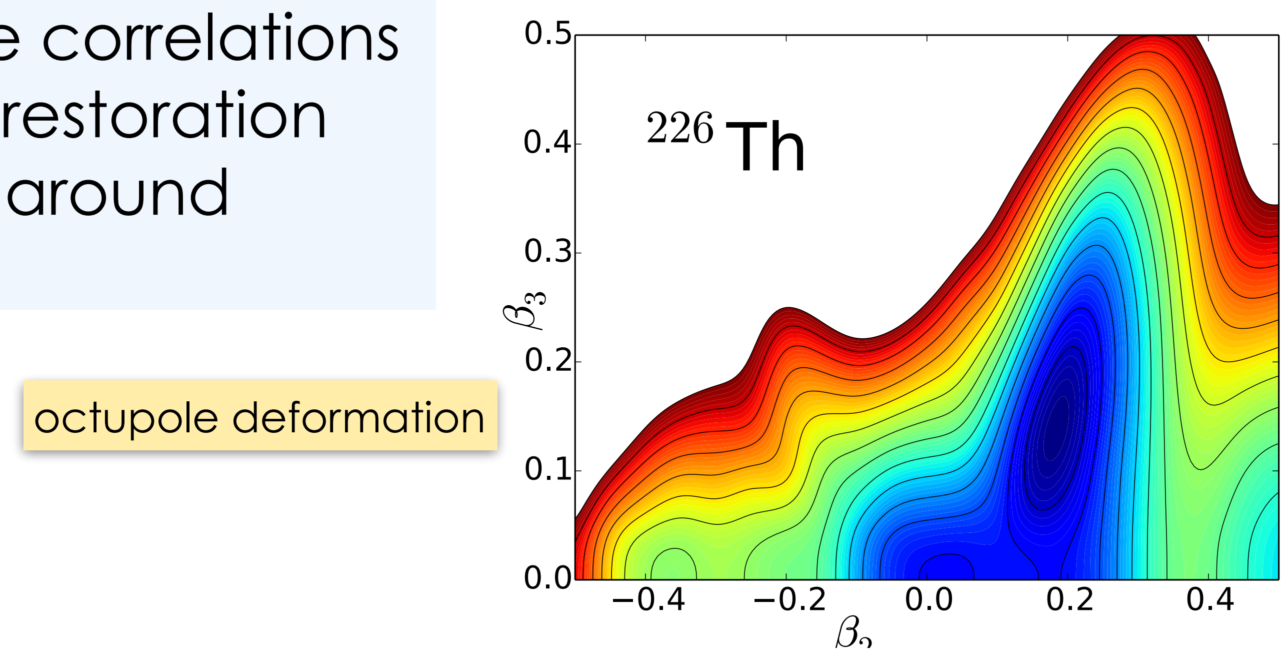
Basic implementation: self-consistent mean-field method

- produces energy surfaces as functions of intrinsic deformation parameters





- includes static correlations: deformations and pairing
- does not include collective correlations originating from symmetry restoration and quantum fluctuations around mean-field minima



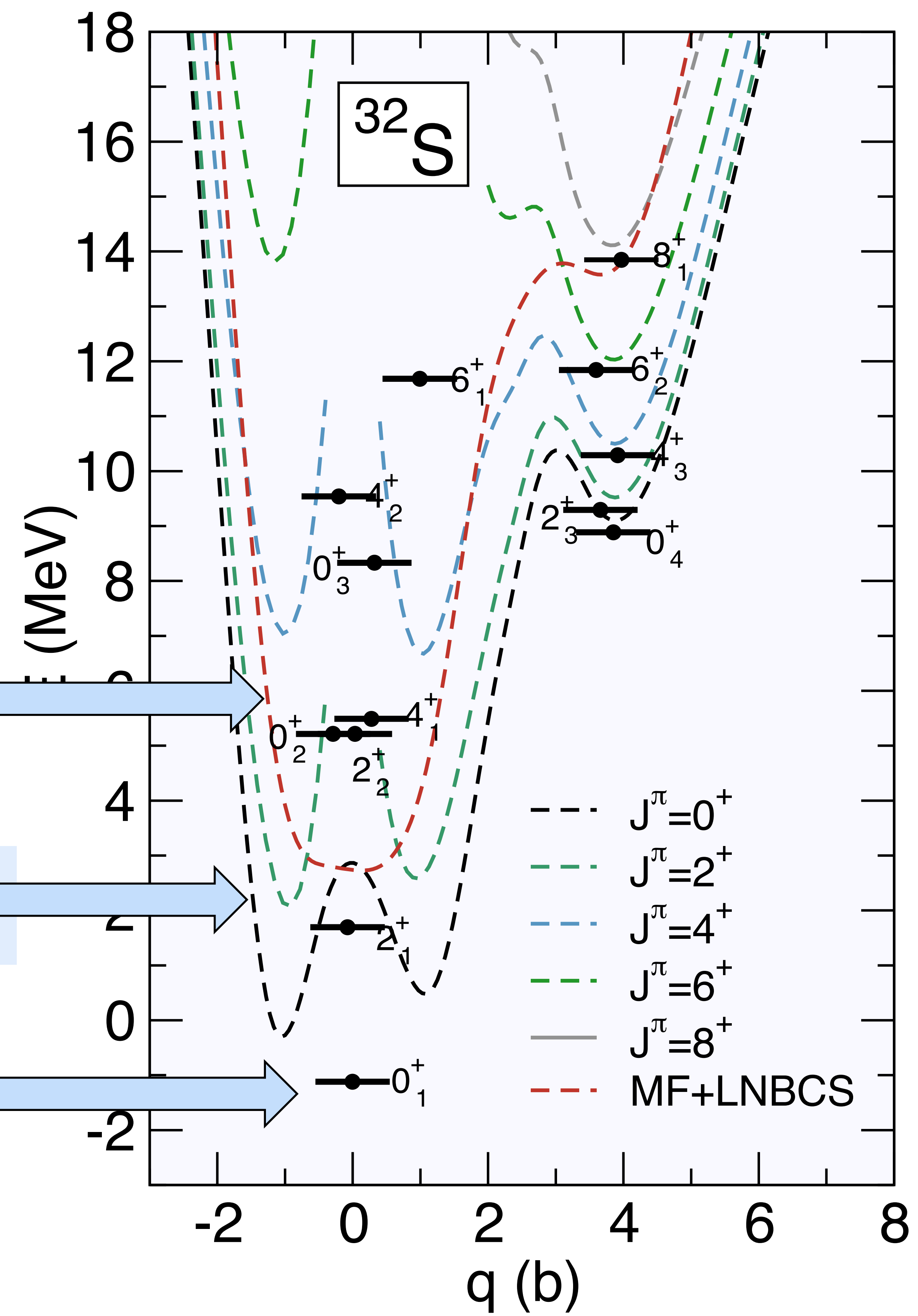
Beyond mean-field correlations: GCM

Restoration of broken symmetries (rotational, parity, particle number) and fluctuations of collective variables (quadrupole deformation)

1. Constraint mean-field calculation

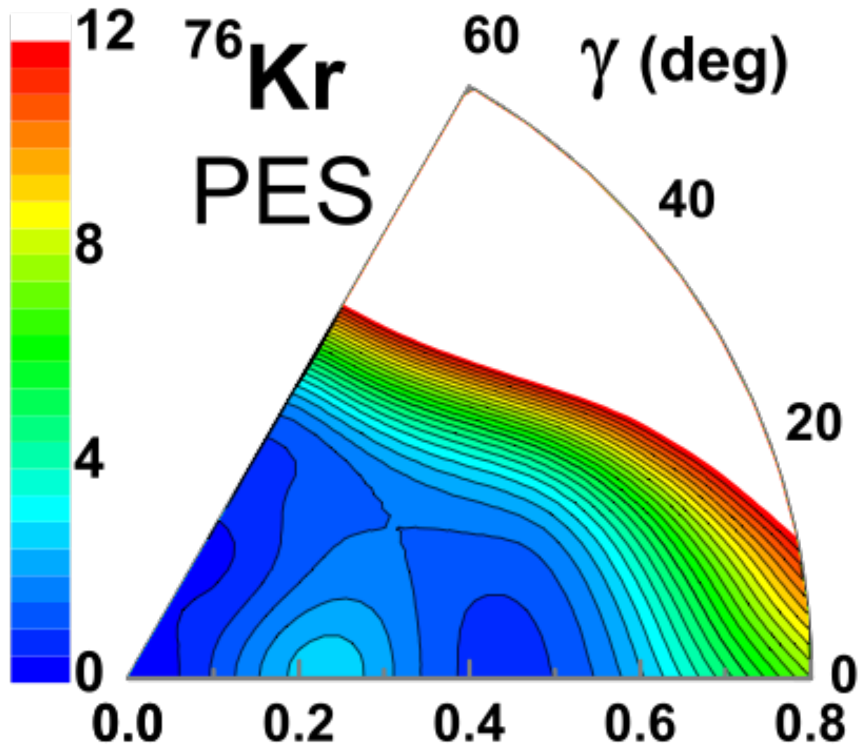
2. Angular momentum, parity and particle number projection

3. Configuration mixing (generator coordinate method)



Beyond mean-field correlations: Collective Hamiltonian

... nuclear excitations determined by quadrupole vibrational and rotational degrees of freedom



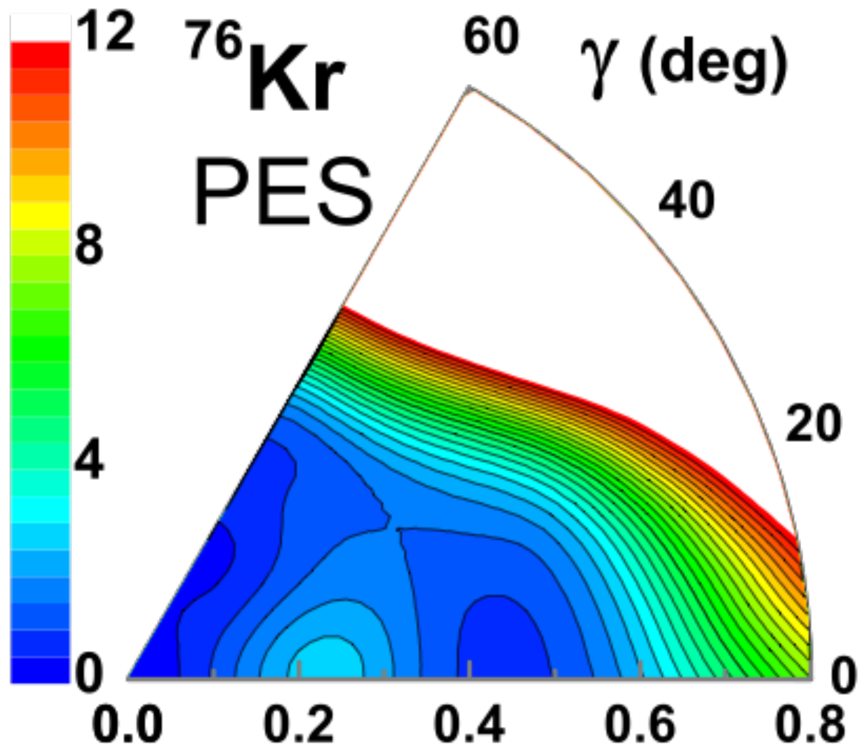
$$H_{\rm coll} = \mathcal{T}_{\rm vib}(\beta,\gamma) + \mathcal{T}_{\rm rot}(\beta,\gamma,\Omega) + \mathcal{V}_{\rm coll}(\beta,\gamma)$$

$$\mathcal{T}_{\rm vib} = \frac{1}{2}B_{\beta\beta}\dot{\beta}^2 + \beta B_{\beta\gamma}\dot{\beta}\dot{\gamma} + \frac{1}{2}\beta^2 B_{\gamma\gamma}\dot{\gamma}^2$$

$$\mathcal{T}_{\rm rot} = \frac{1}{2}\sum_{k=1}^{3}\mathcal{I}_k\omega_k^2$$

The entire dynamics of the collective Hamiltonian is governed by the seven functions of the intrinsic deformations β and γ: the collective potential, the three mass parameters: $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$, and the three moments of inertia I_k.

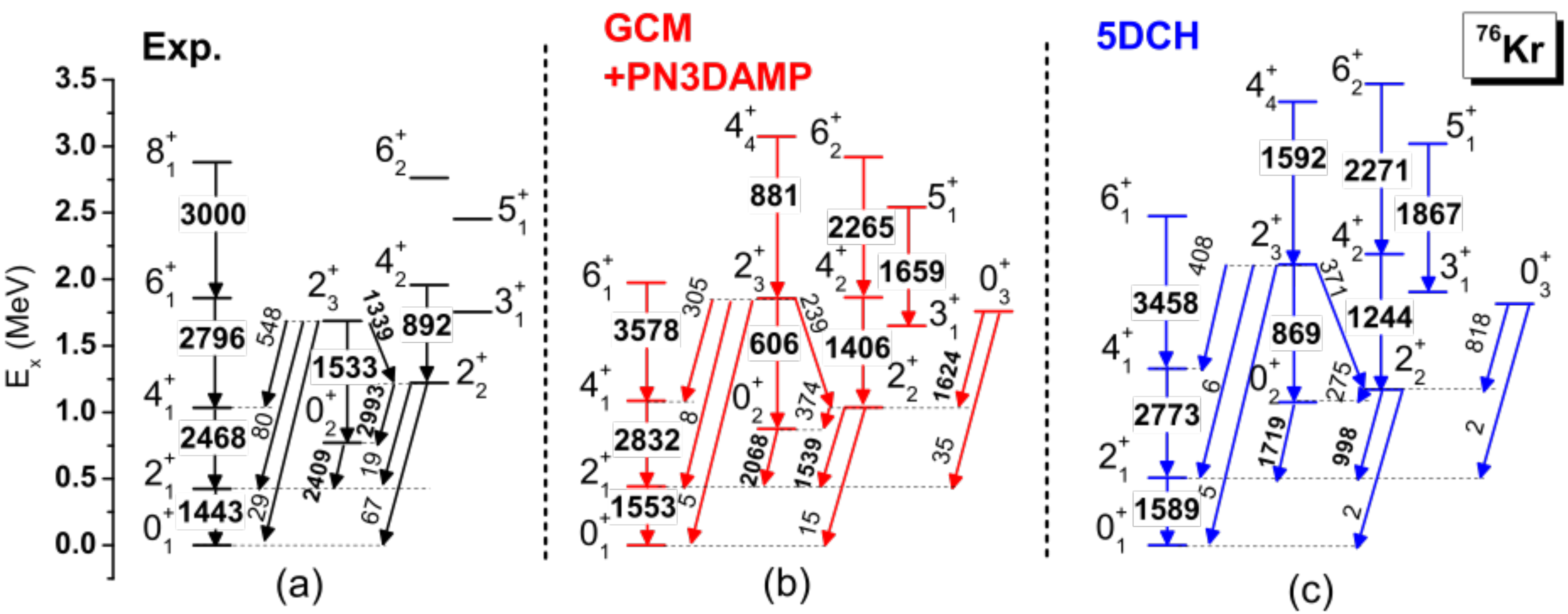
… collective eigenfunction: $\Psi_\alpha^{IM}(\beta,\gamma,\Omega) = \sum_{K\in\Delta I}\psi_{\alpha K}^{I}(\beta,\gamma)\Phi_{MK}^{I}(\Omega)$



✔ an intuitive interpretation of mean-field results in terms of ***intrinsic shapes*** and ***single-particle states***

✔ the ***full model space*** of occupied states can be used; no distinction between core and valence nucleons, ***no need for effective charges!***

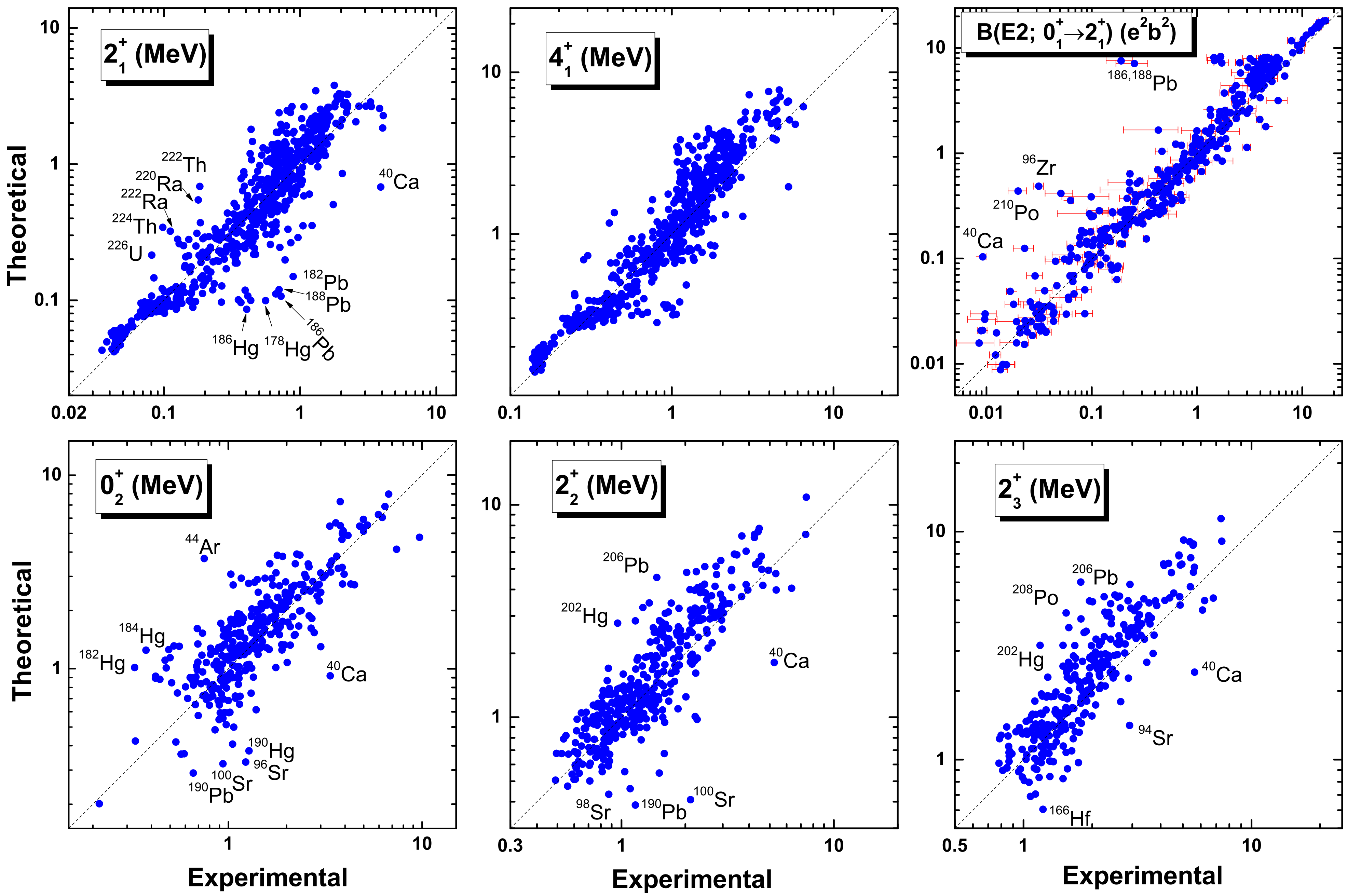
Phys. Rev. C 89, 054306 (2014)



Global analysis of quadrupole shape invariants

Phys. Rev. C 95, 054321 (2017)

- Systematic analysis of characteristic signatures of coexisting shapes in different mass regions
- Calculation includes 621 even-even nuclei with Z,N>10 and for which 2_1^+ state has been determined in experiment



Global analysis of quadrupole shape invariants

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The lowest-order quadrupole invariants:

$$q_2(0_i^+) = \sum_j \langle 0_i^+ || Q || 2_j^+ \rangle \langle 2_j^+ || Q || 0_i^+ \rangle .$$

$$q_3(0_i^+) = \sqrt{\frac{7}{10}} \sum_{jk} \langle 0_i^+ || Q || 2_j^+ \rangle \langle 2_j^+ || Q || 2_k^+ \rangle \langle 2_k^+ || Q || 0_i^+ \rangle .$$

Deformation parameters:

$$q_2(0_i^+) = \left(\frac{3ZeR^2}{4\pi} \right)^2 \langle \beta^2 \rangle \equiv \left(\frac{3ZeR^2}{4\pi} \right)^2 \beta_{eff}^2$$

$$R = r_0 A^{1/3}$$

$$r_0 = 1.2 \text{ fm}$$

$$\frac{q_3\left(0_i^+\right)}{q_2^{3/2}(0_i^+)} = \frac{\langle \beta^3 \cos 3\gamma \rangle}{\langle \beta^2 \rangle^{3/2}} \equiv \cos 3\gamma_{eff}$$

Global analysis of quadrupole shape invariants

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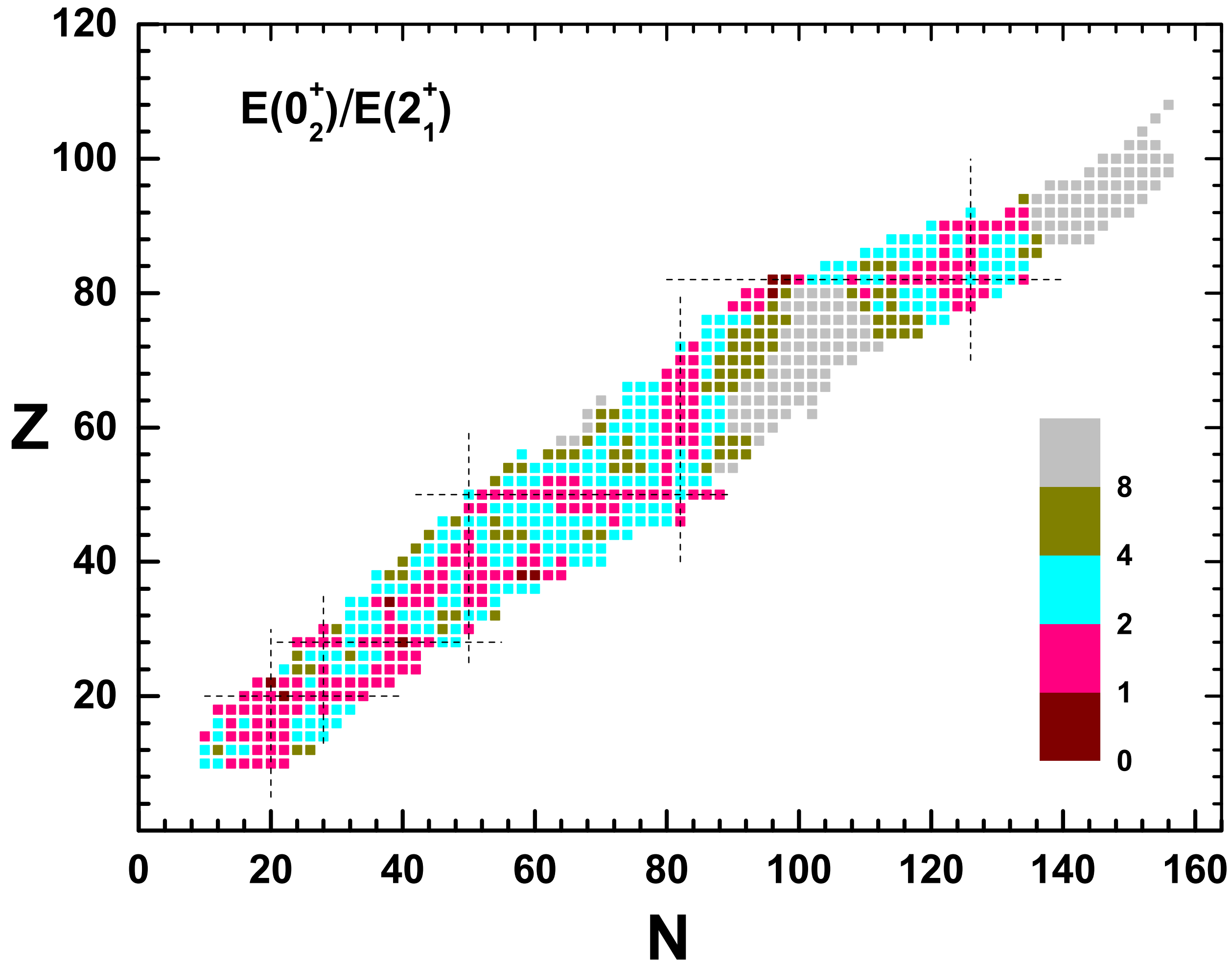
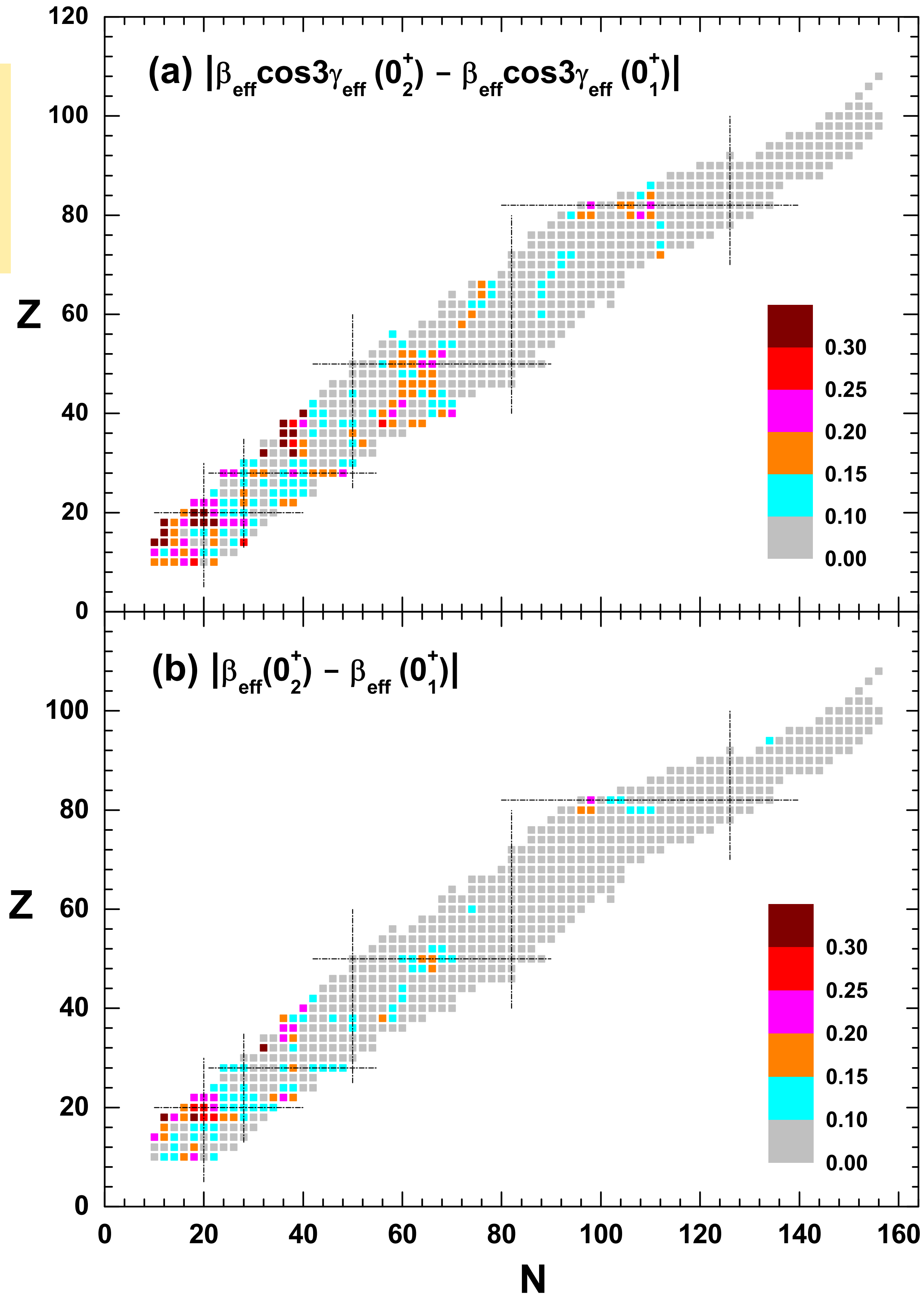
Signatures of shape coexistence:

- The difference between $\beta_{eff}\cos(3\gamma_{eff})$ for the two lowest 0^+ states is large
- The excitation energy of 0_2^+ is low in comparison to the excitation energy of the 2_1^+ state





Global analysis of quadrupole shape invariants

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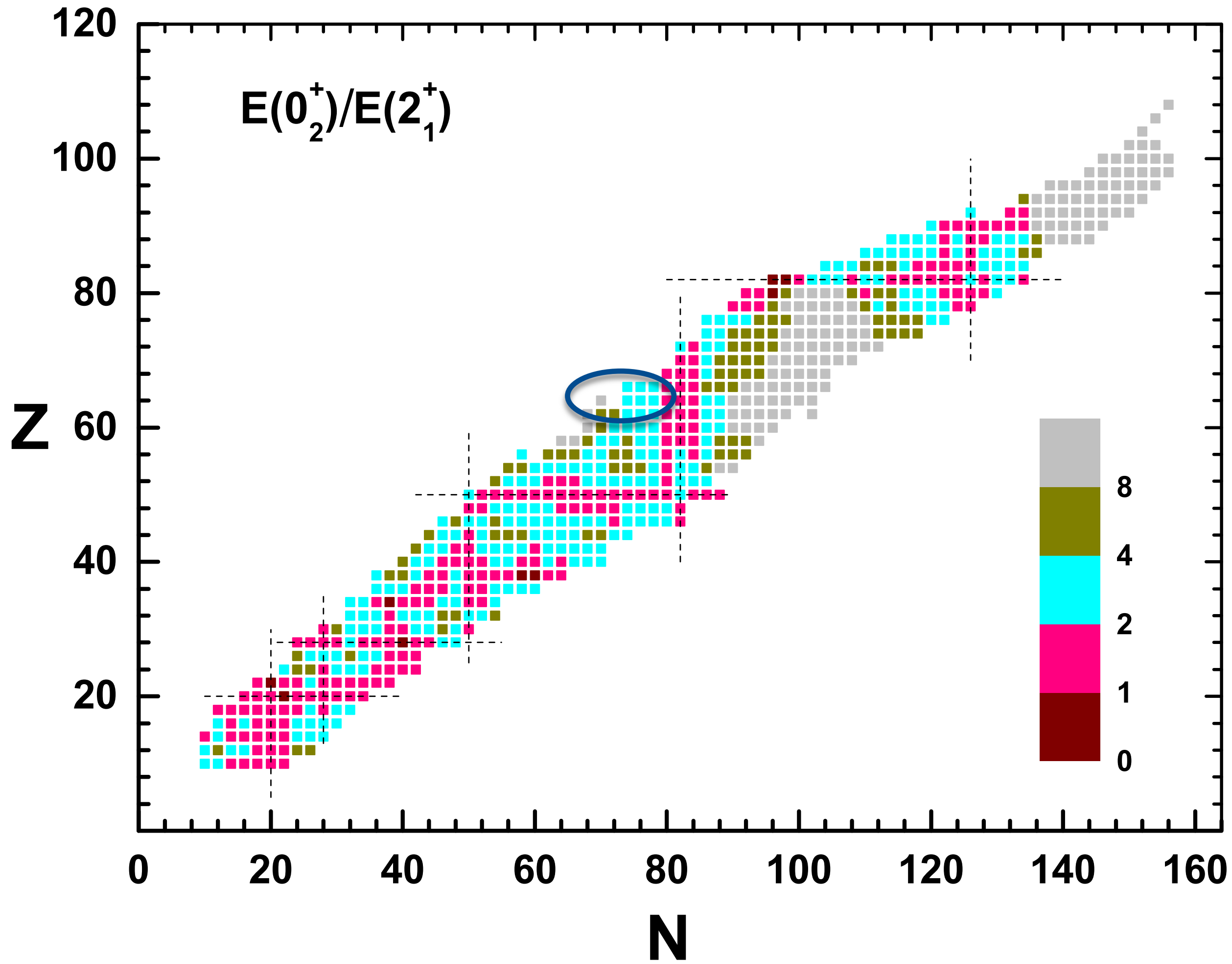
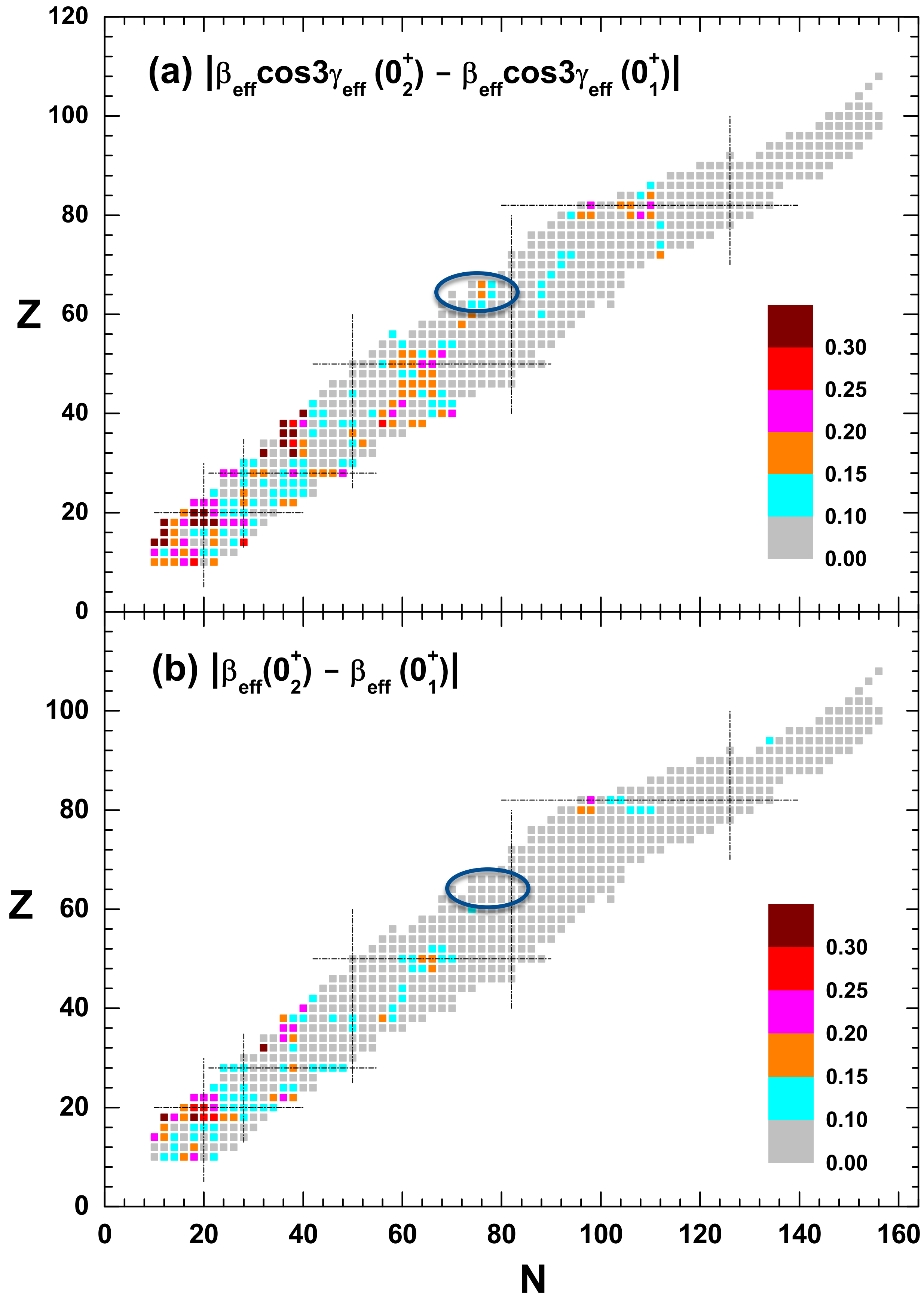
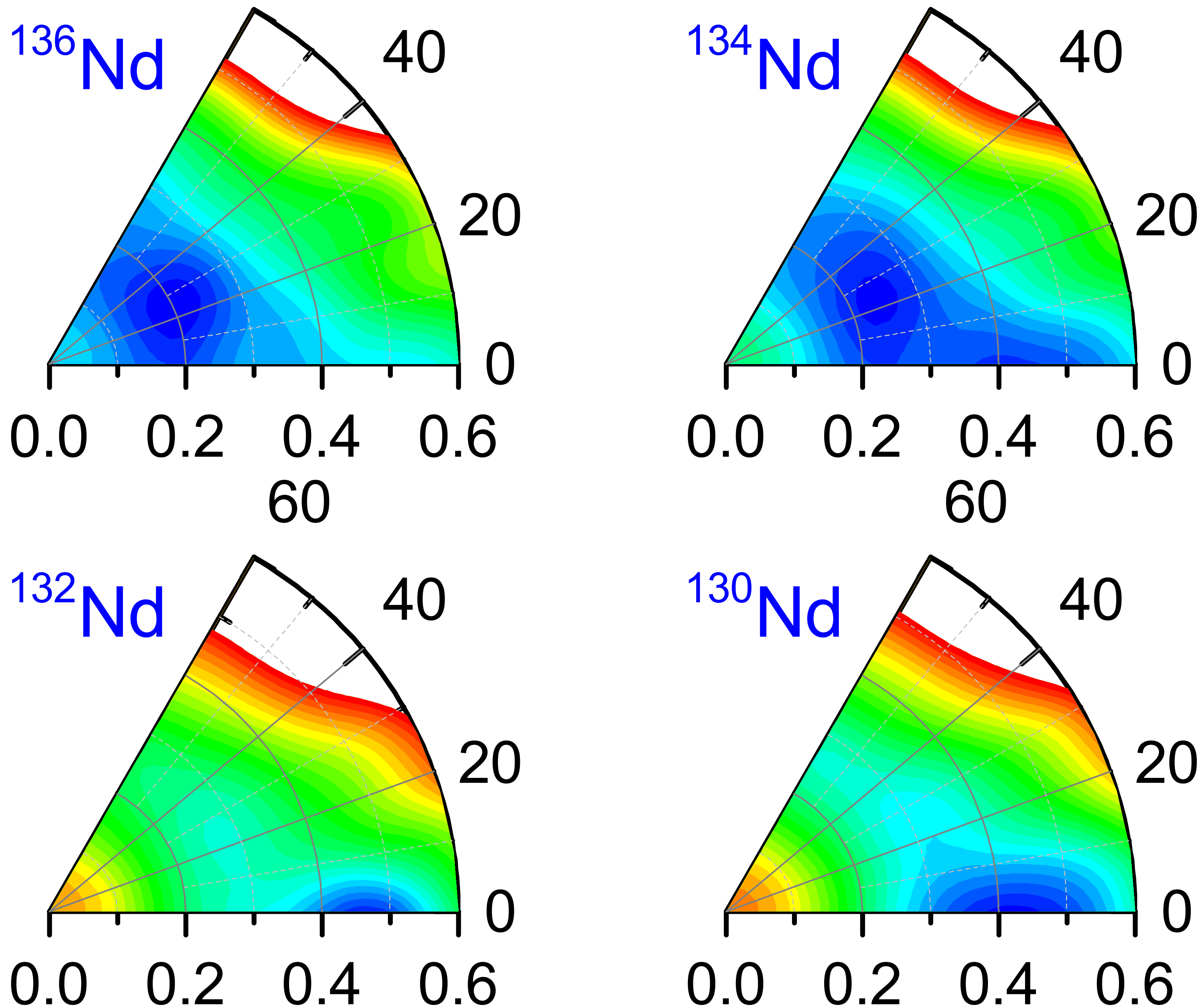
- Z≈64 and N≈76: medium deformed triaxial ground state coexisting with highly deformed prolate excited state





Coexisting shapes in neutron-deficient Nd and Sm isotopes

Phys. Rev. C 98, 054308 (2018)



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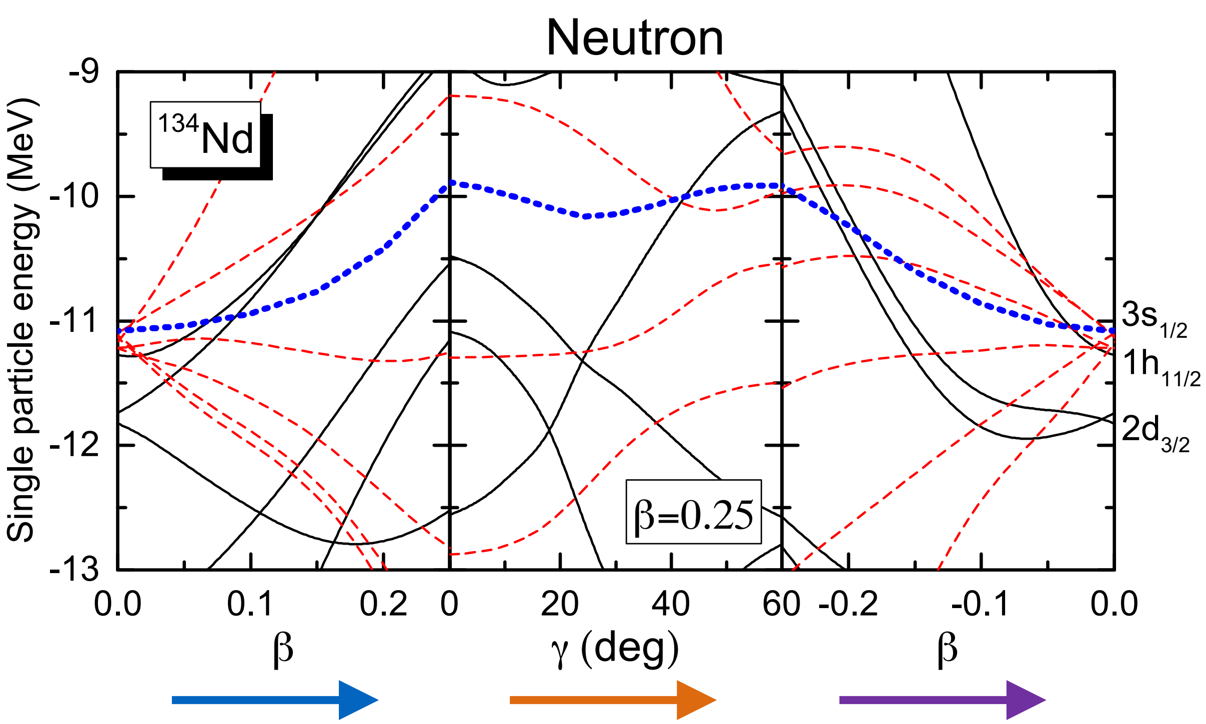

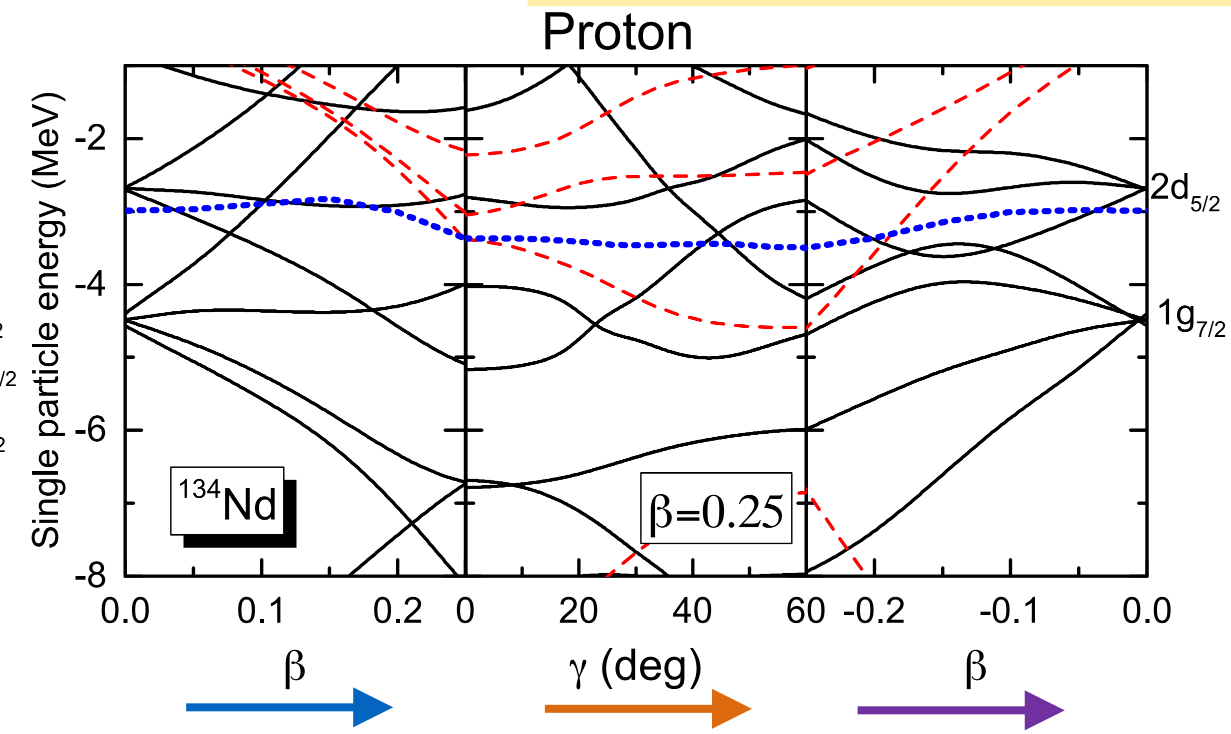

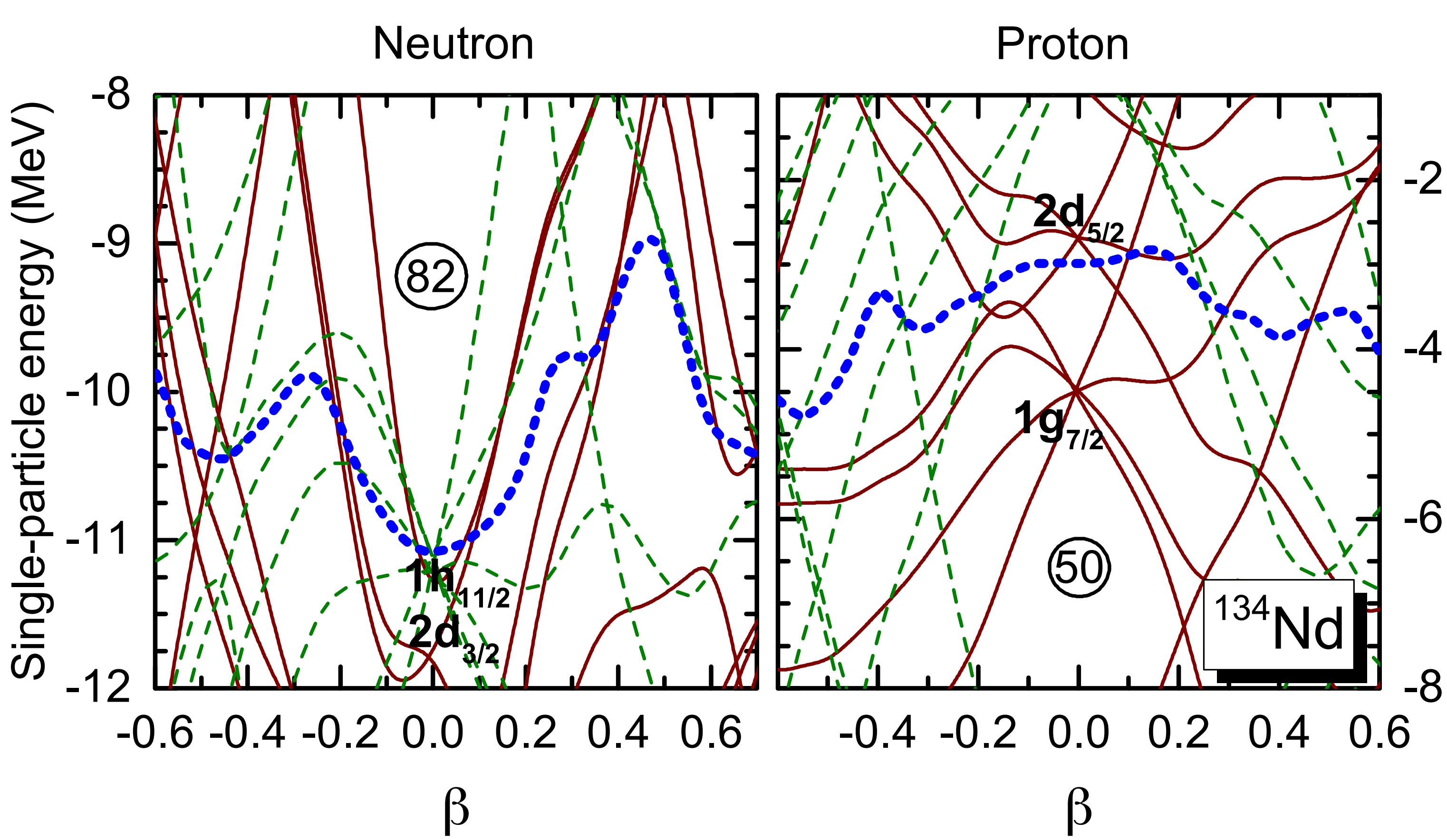

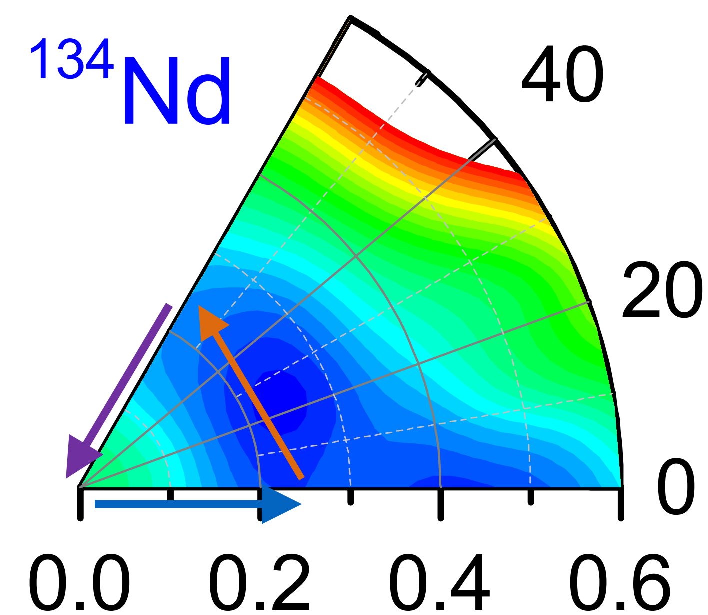

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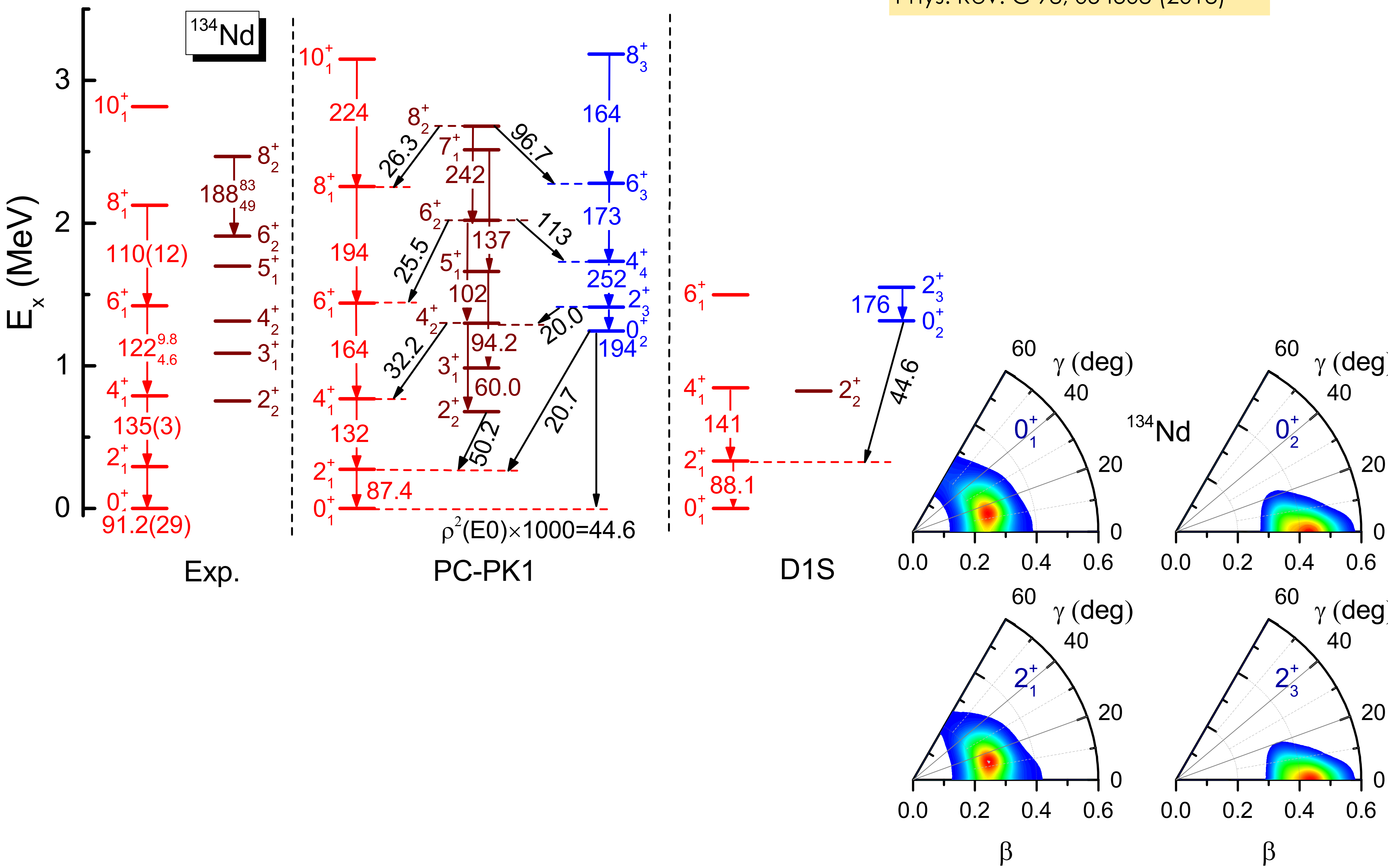
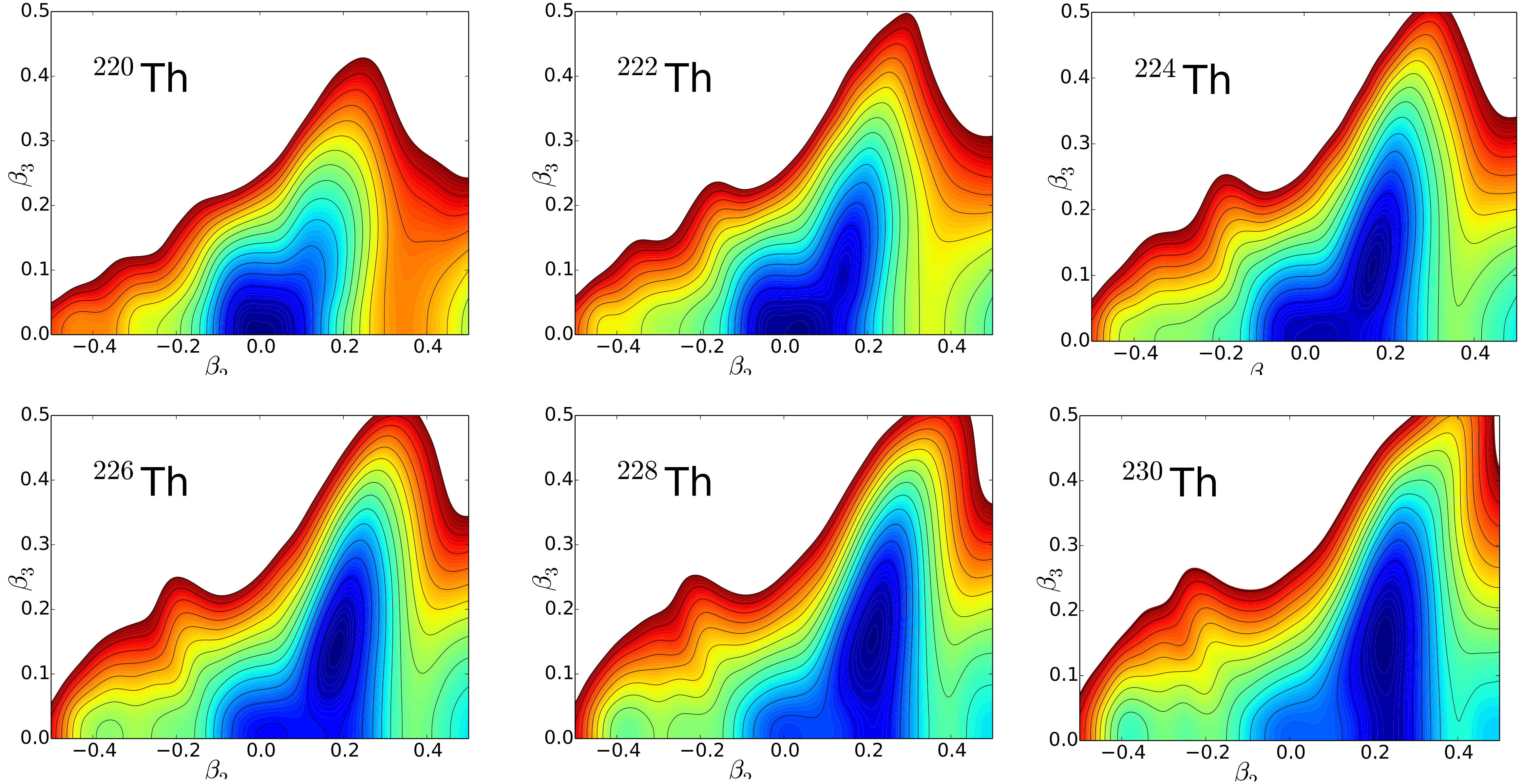


Quadrupole and octupole shape transition in thorium



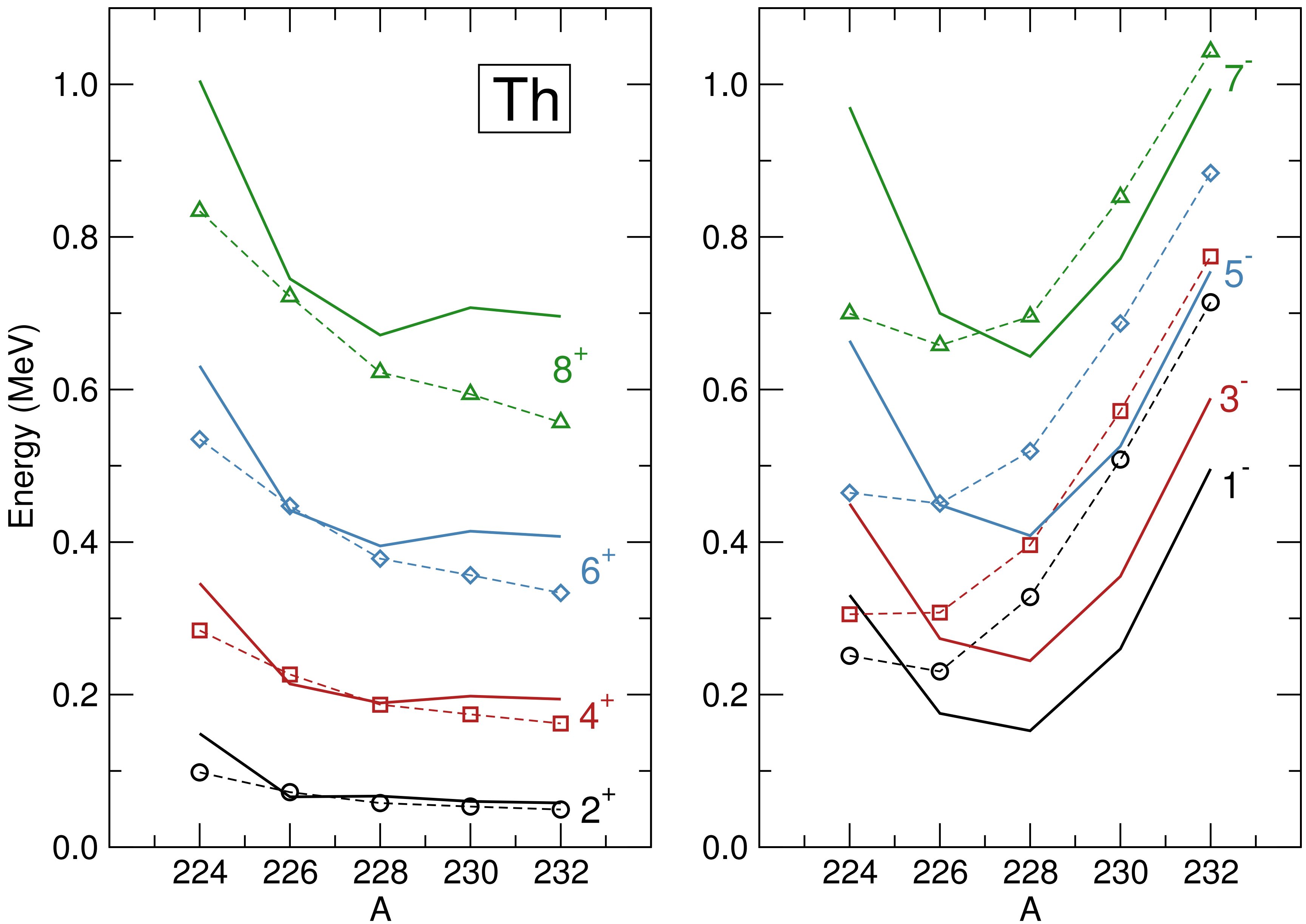
…quadrupole-octupole collective Hamiltonian:

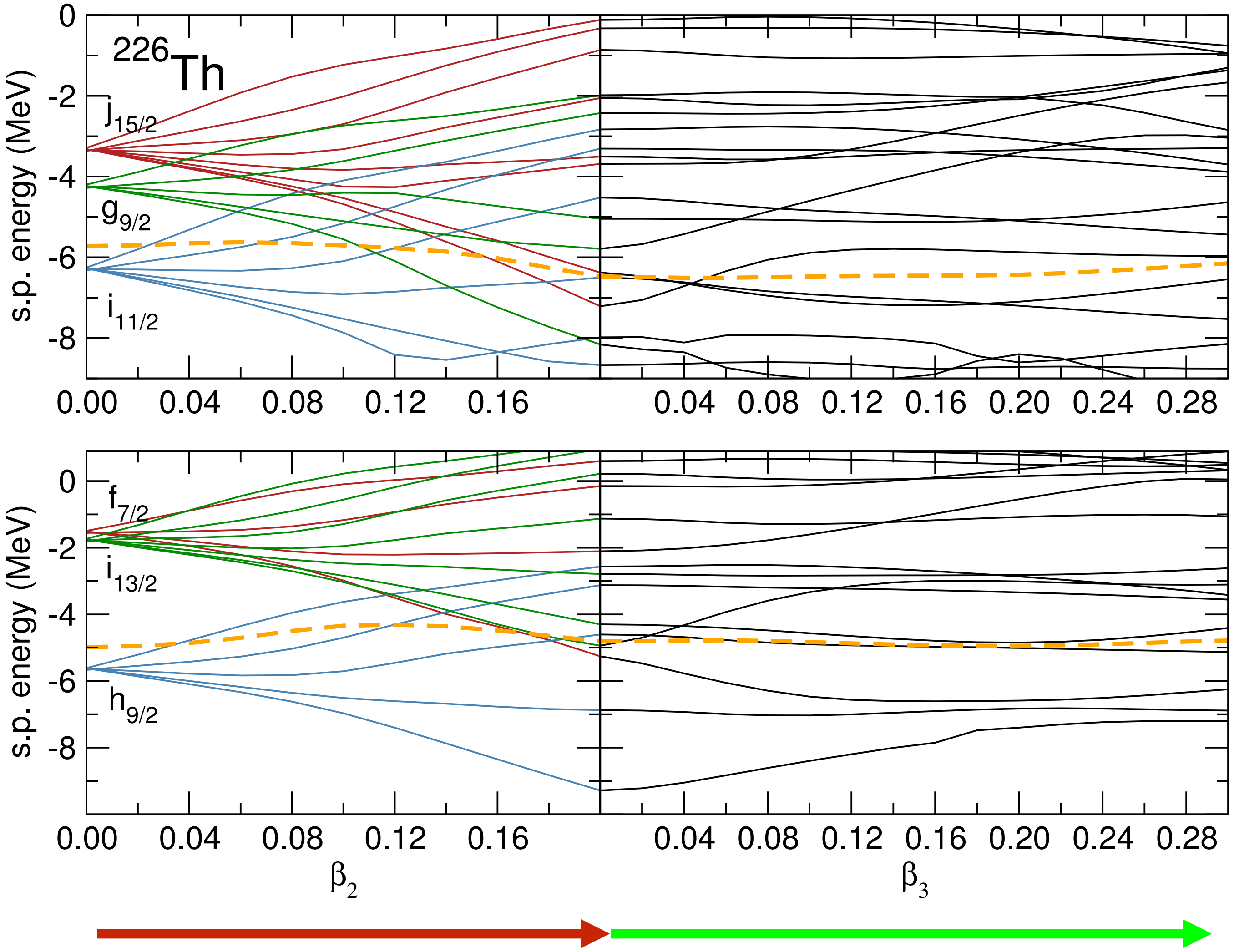
$$H_{coll} = -\frac{\hbar^2}{2\sqrt{w\mathcal{I}}}\left[\frac{\partial}{\partial\beta_2}\sqrt{\frac{\mathcal{I}}{w}}B_{33}\frac{\partial}{\partial\beta_2} - \frac{\partial}{\partial\beta_2}\sqrt{\frac{\mathcal{I}}{w}}B_{23}\frac{\partial}{\partial\beta_3} - \frac{\partial}{\partial\beta_3}\sqrt{\frac{\mathcal{I}}{w}}B_{23}\frac{\partial}{\partial\beta_2} + \frac{\partial}{\partial\beta_3}\sqrt{\frac{\mathcal{I}}{w}}B_{22}\frac{\partial}{\partial\beta_3}\right]$$

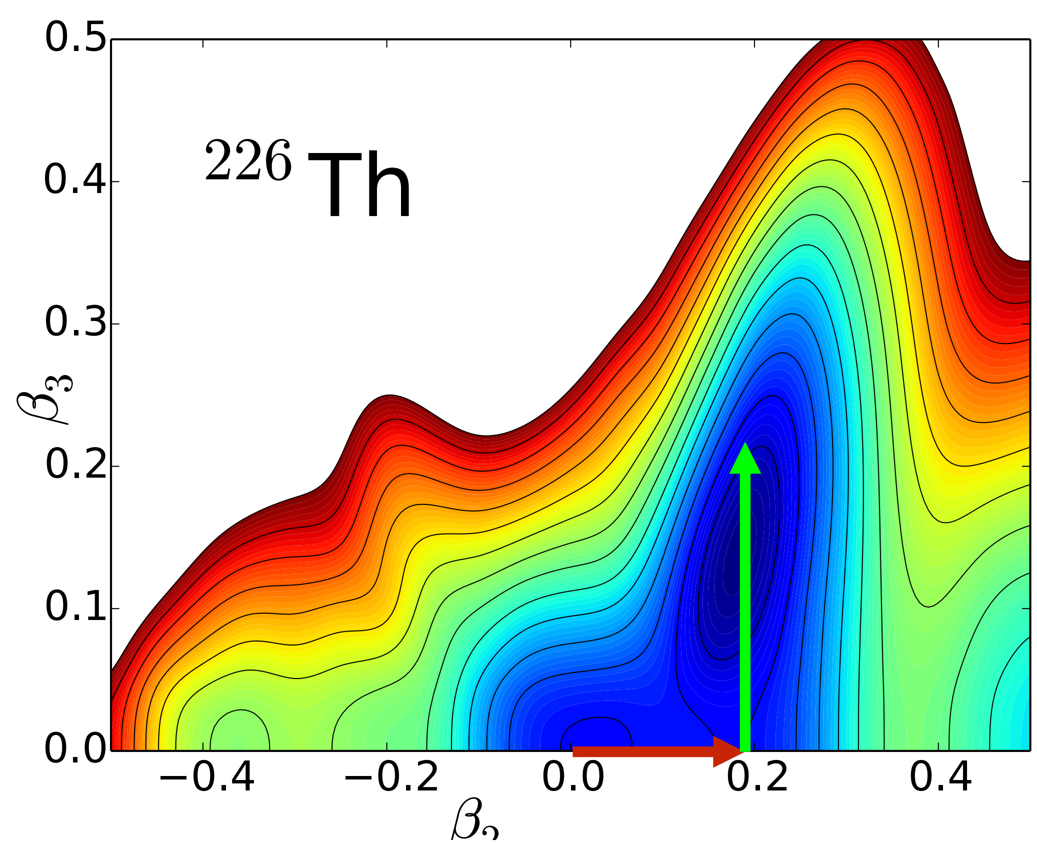
$$+\frac{\hat{J}^2}{2\mathcal{I}} + V(\beta_2, \beta_3)$$

J. Phys. G: Nucl. Part. Phys. 43 (2016) 024005

… systematics of energy spectra of the positive-parity ground- state band ($K^\pi = 0^+$) and the lowest negative-parity ($K^\pi = 0^-$) sequences in $^{224-232}$Th.







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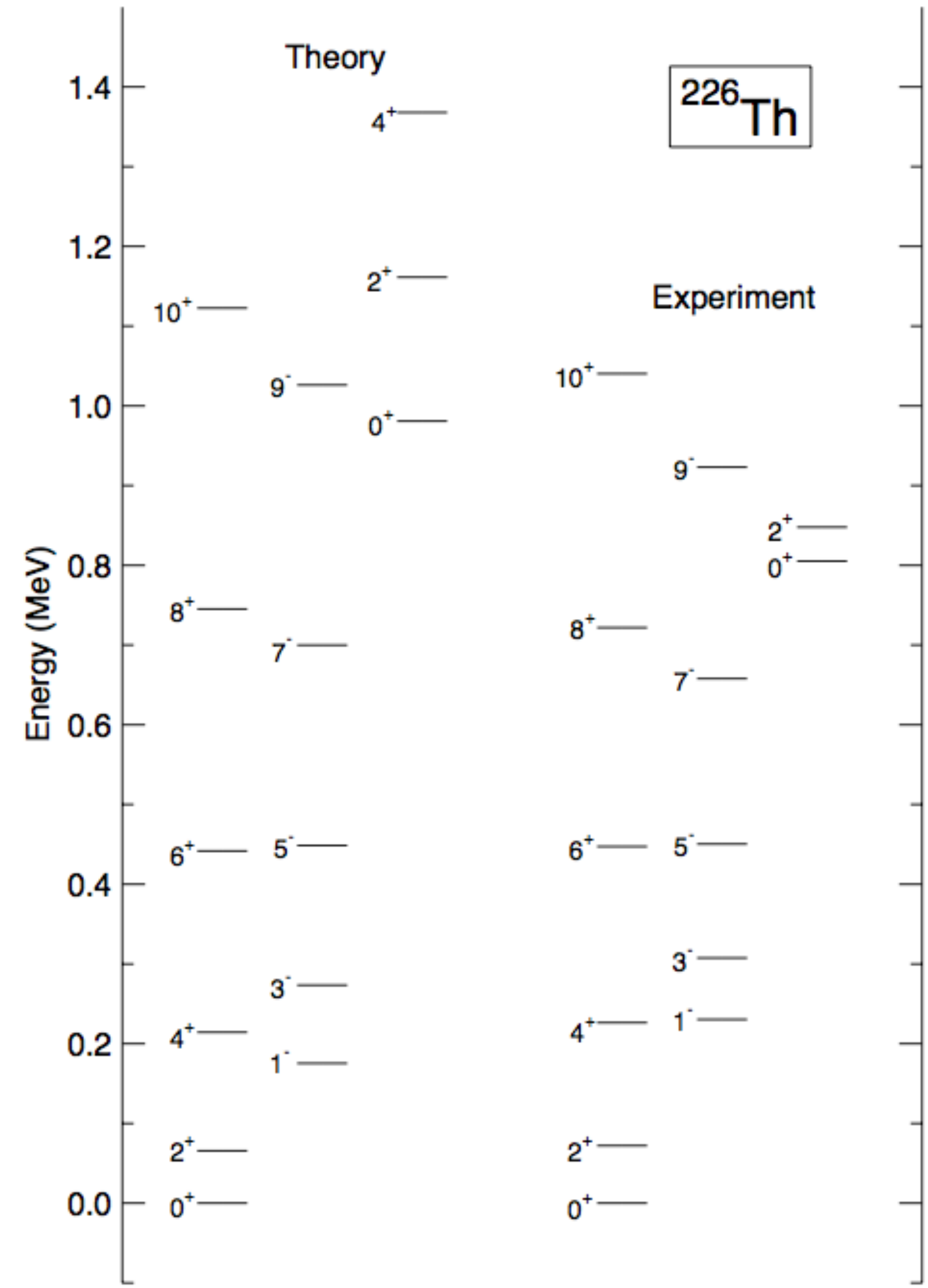

Summary

✓ NEDFs provide an economic, global and accurate microscopic approach to nuclear structure that can be extended from relatively light systems to superheavy nuclei, and from the valley of β-stability to the particle drip-lines.

✓ NEDF-based structure models that take into account collective correlations → microscopic description of low-energy observables: excitation spectra, transition rates, changes in masses, isotope and isomer shifts, related to shell evolution with nuclear deformation, angular momentum, and number of nucleons.

✓ NEDF-based models are applicable to large-scale calculations

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