Microscopic theories of nuclear structure and dynamics (Tsukuba-CSS workshop)
Tsukuba, Japan, December 2018

Nuclear structure studies based on energy density functionals

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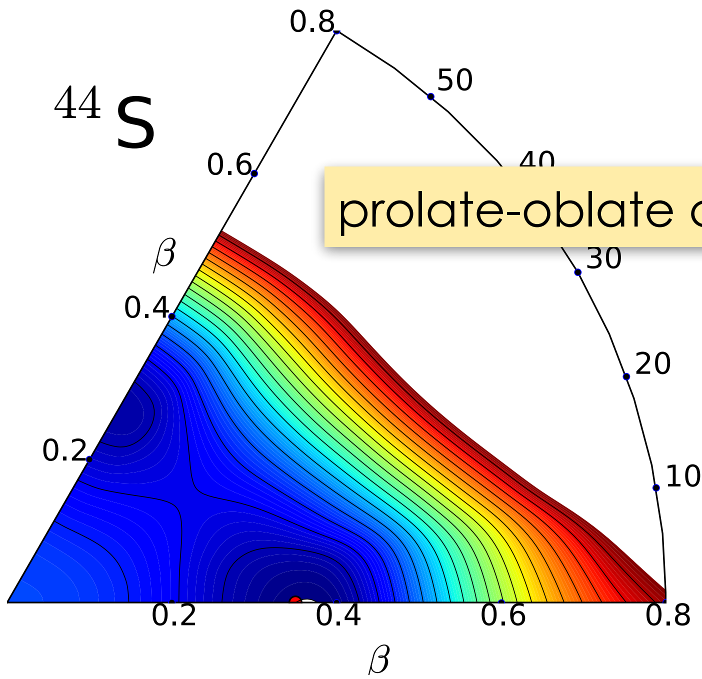
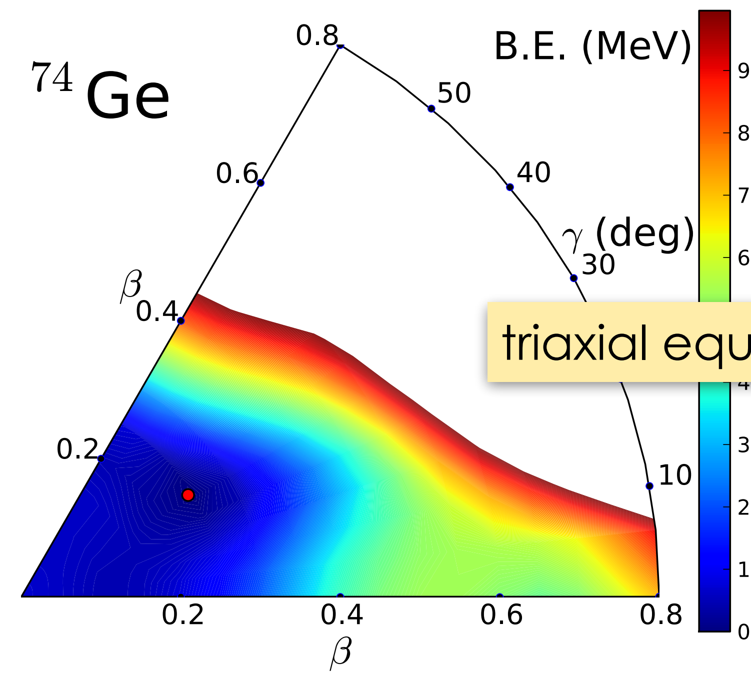
Basic implementation: self-consistent mean-field method

- produces energy surfaces as functions of intrinsic deformation parameters



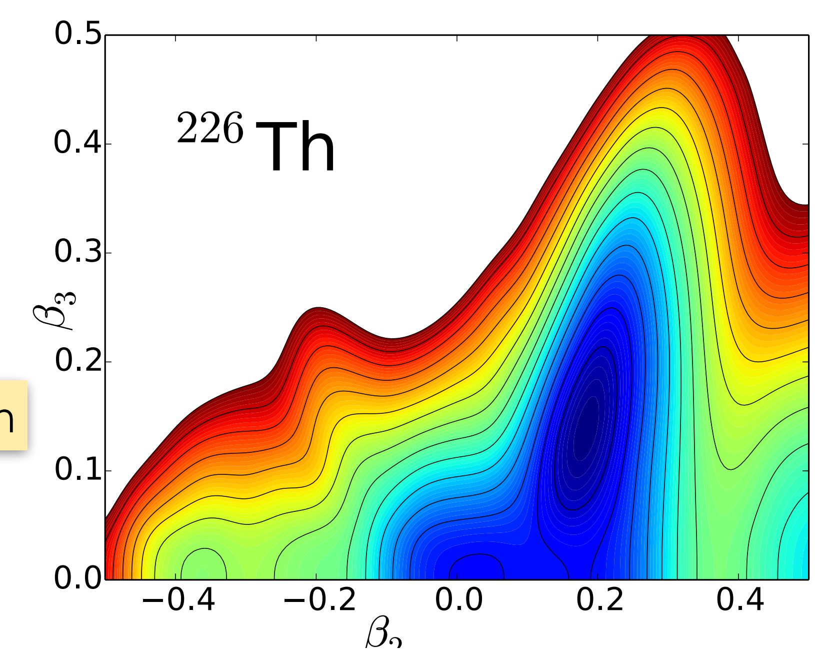
prolate-oblate coexistence



triaxial equilibrium shape

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

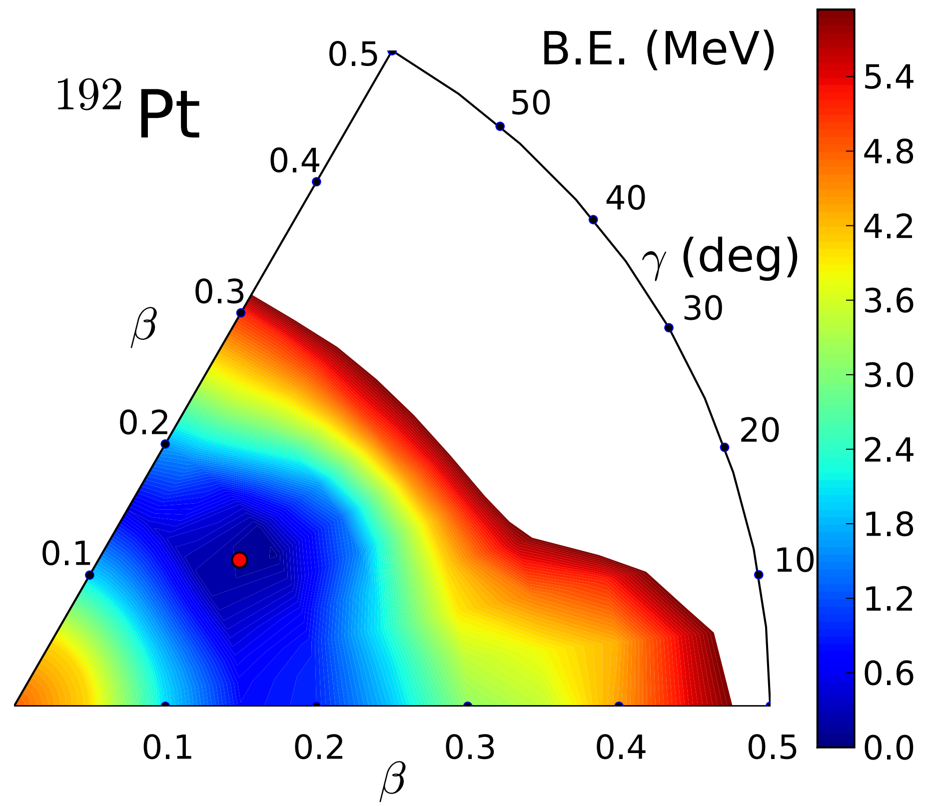
octupole deformation



Beyond mean-field correlations: Collective Hamiltonian

Prog. Part. Nucl. Phys. 66, 519 (2011).
Phys. Rev. C 79, 034303 (2009).

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



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

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

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

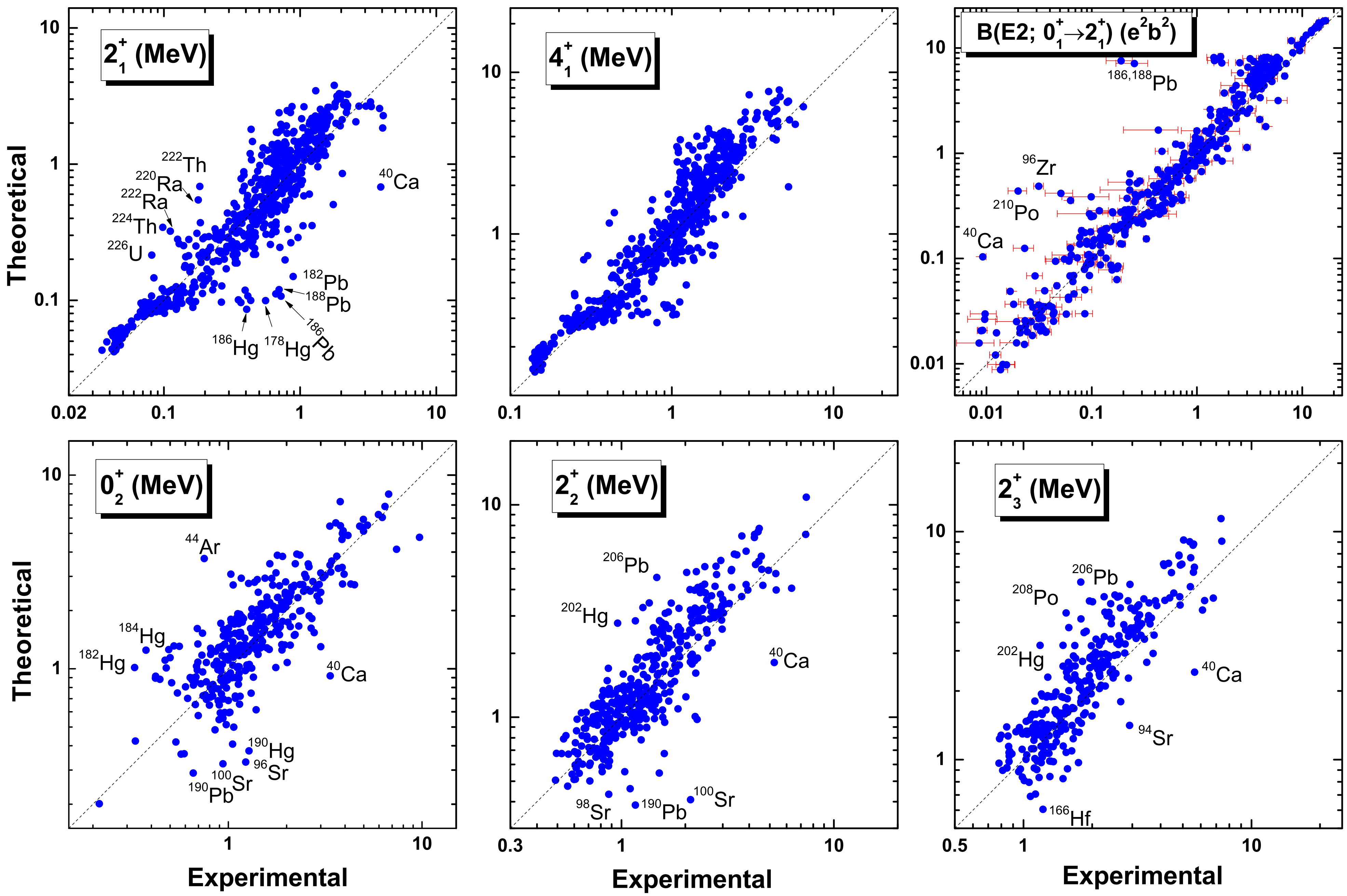
The entire dynamics of the collective Hamiltonian is governed by the seven functions of the intrinsic deformations β and γ: the collective potential, the three mass parameters: $B_{\beta\beta}$, $B_{\beta\gamma}$, $B_{\gamma\gamma}$, and the three moments of inertia I_k.

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

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

Phys. Rev. C 95, 054321 (2017)

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:

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

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

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

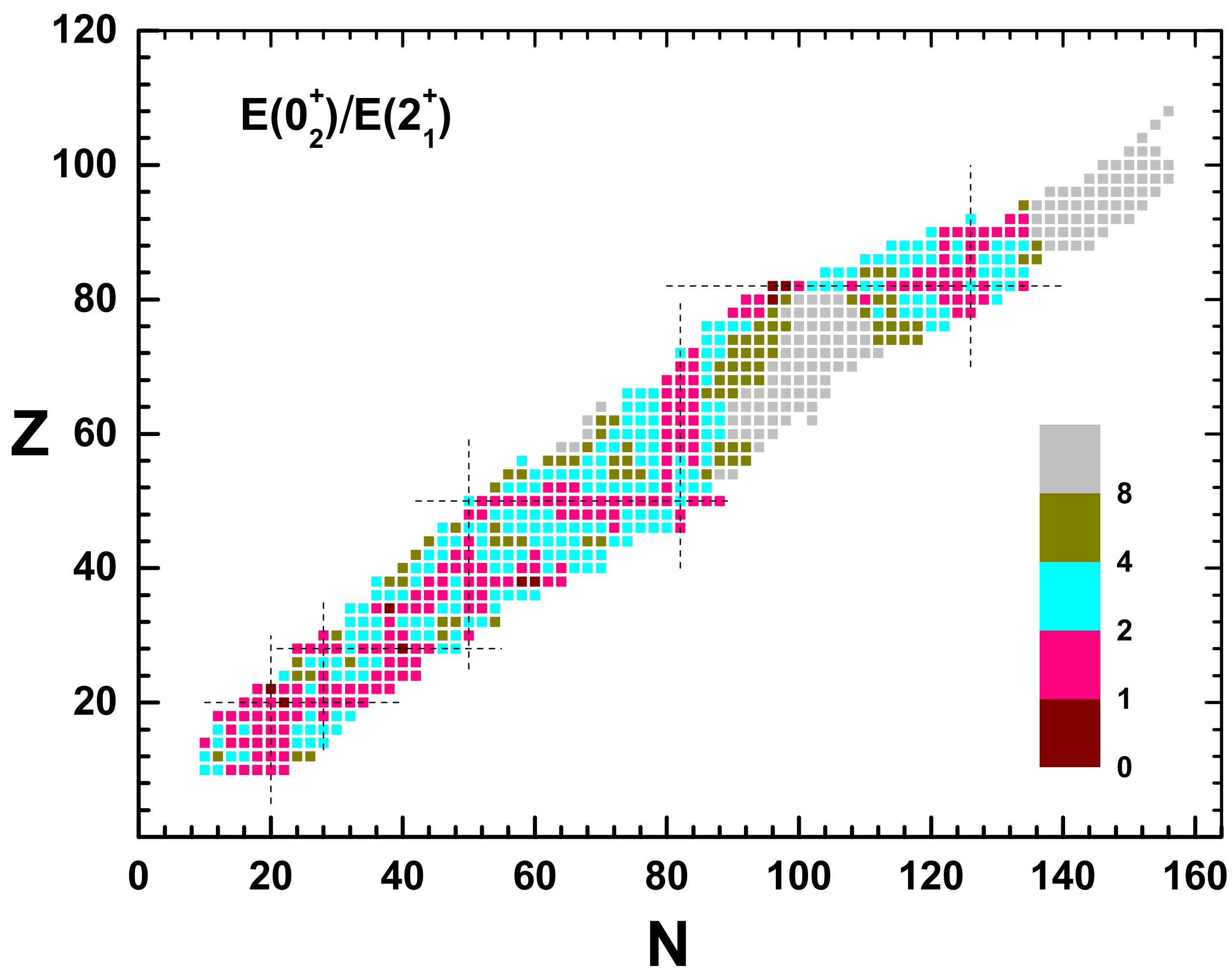
$$\frac{q_3\left(0_i^+\right)}{q_2^{3/2}(0_i^+)} = \frac{\langle \beta^3 \cos 3\gamma \rangle}{\langle \beta^2 \rangle^{3/2}} \equiv \cos 3\gamma_{eff}$$

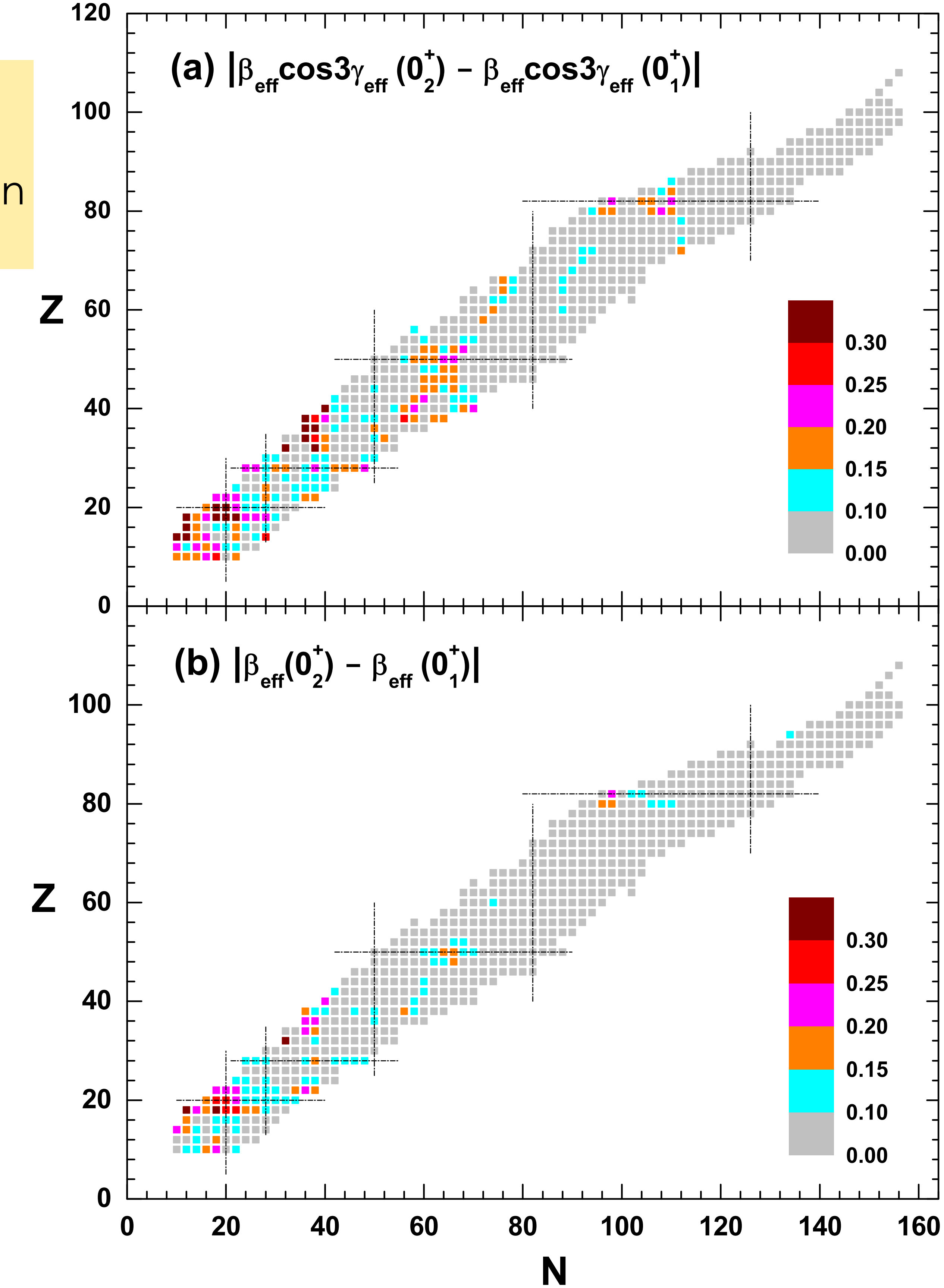
Global analysis of quadrupole shape invariants

Phys. Rev. C 95, 054321 (2017)

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

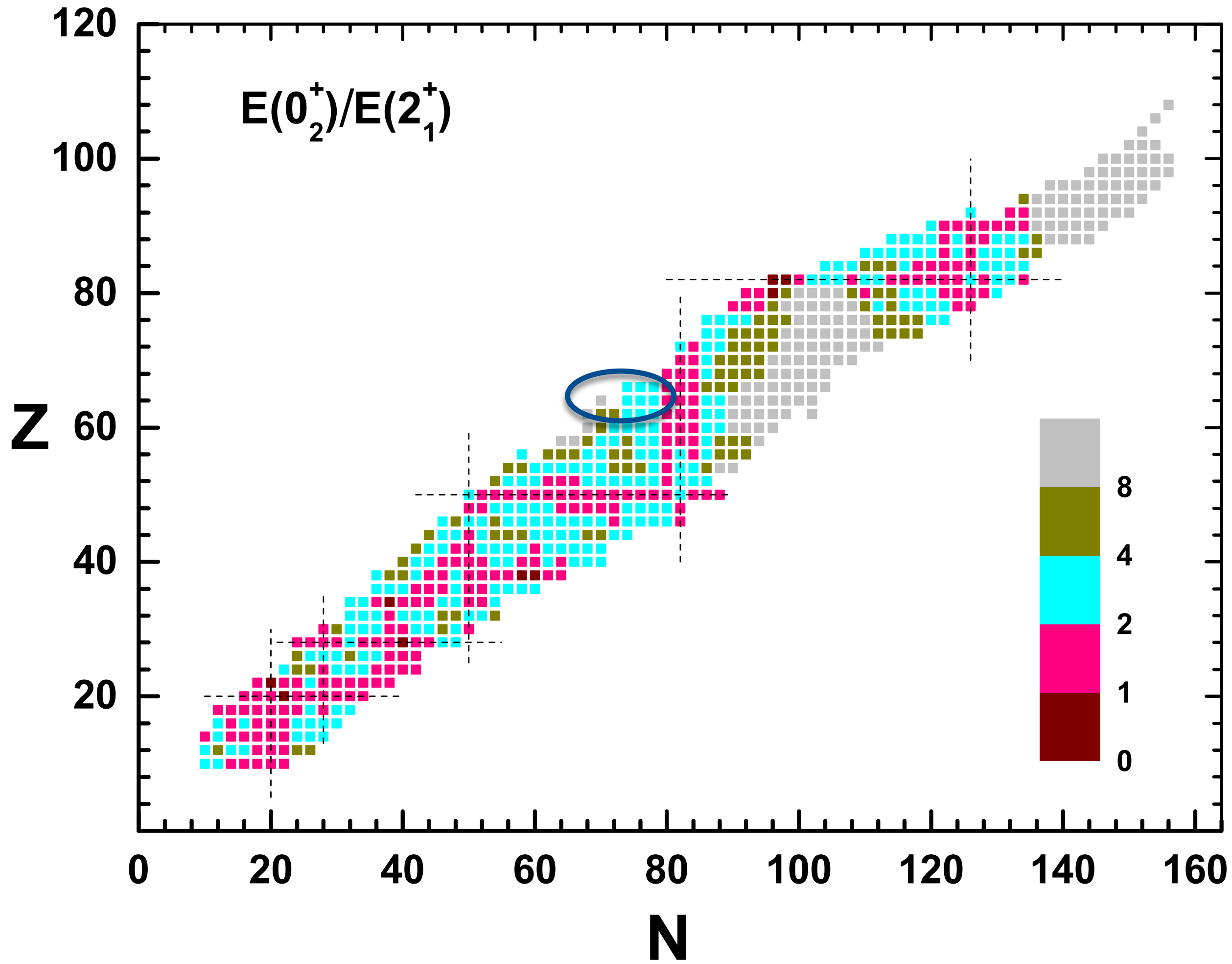


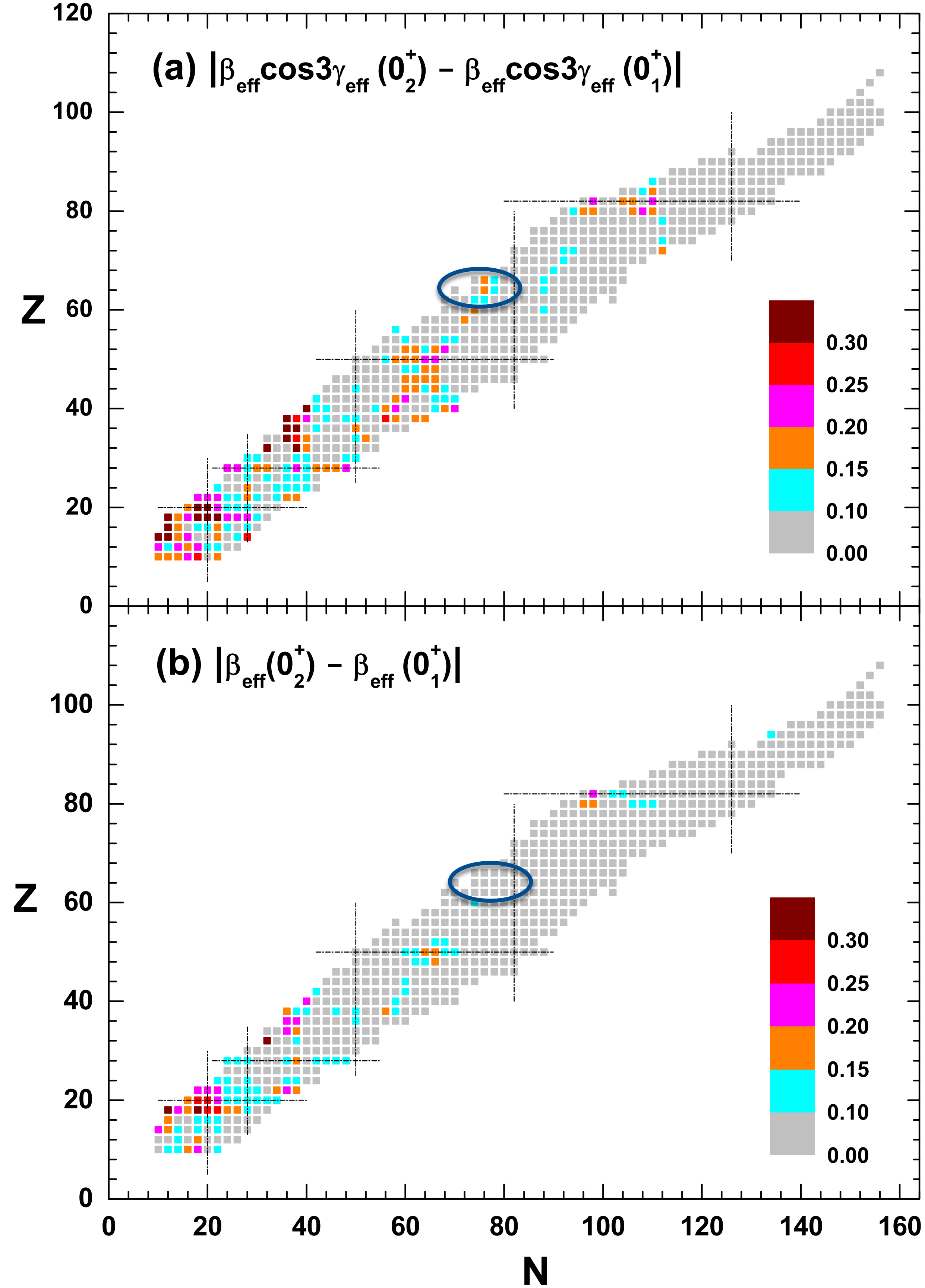


Global analysis of quadrupole shape invariants

Phys. Rev. C 95, 054321 (2017)

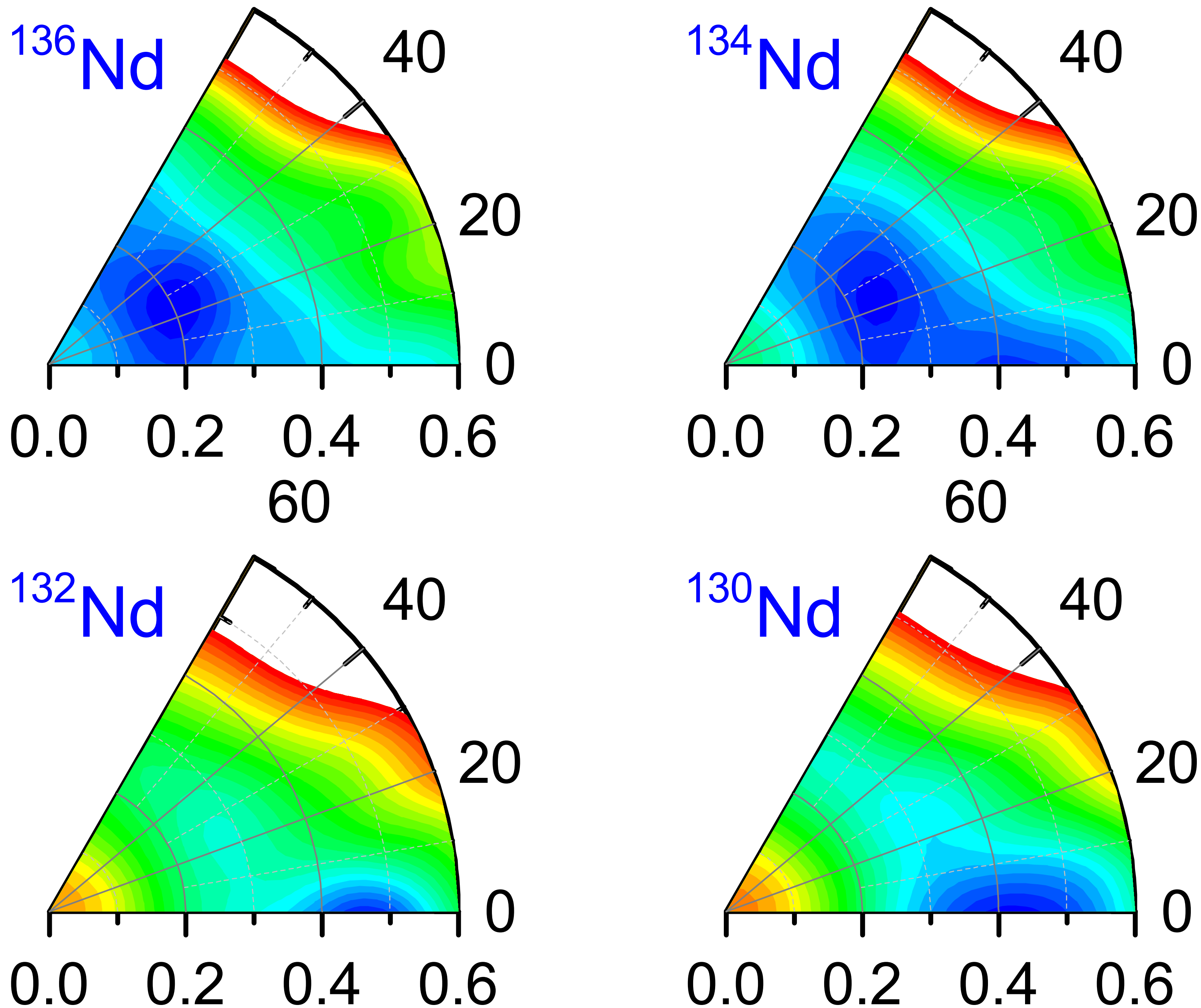
- Z≈64 and N≈76: medium deformed triaxial ground state coexisting with highly deformed prolate excited state





Coexisting shapes in neutron-deficient Nd and Sm isotopes

Phys. Rev. C 98, 054308 (2018)



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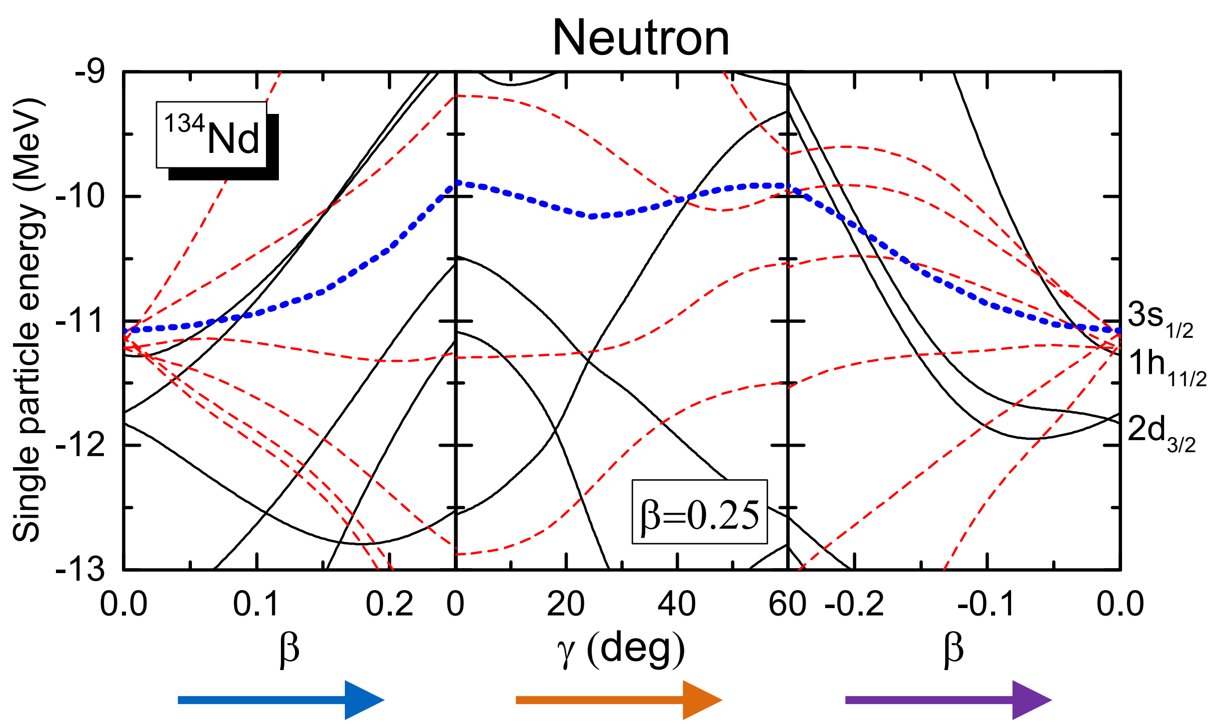

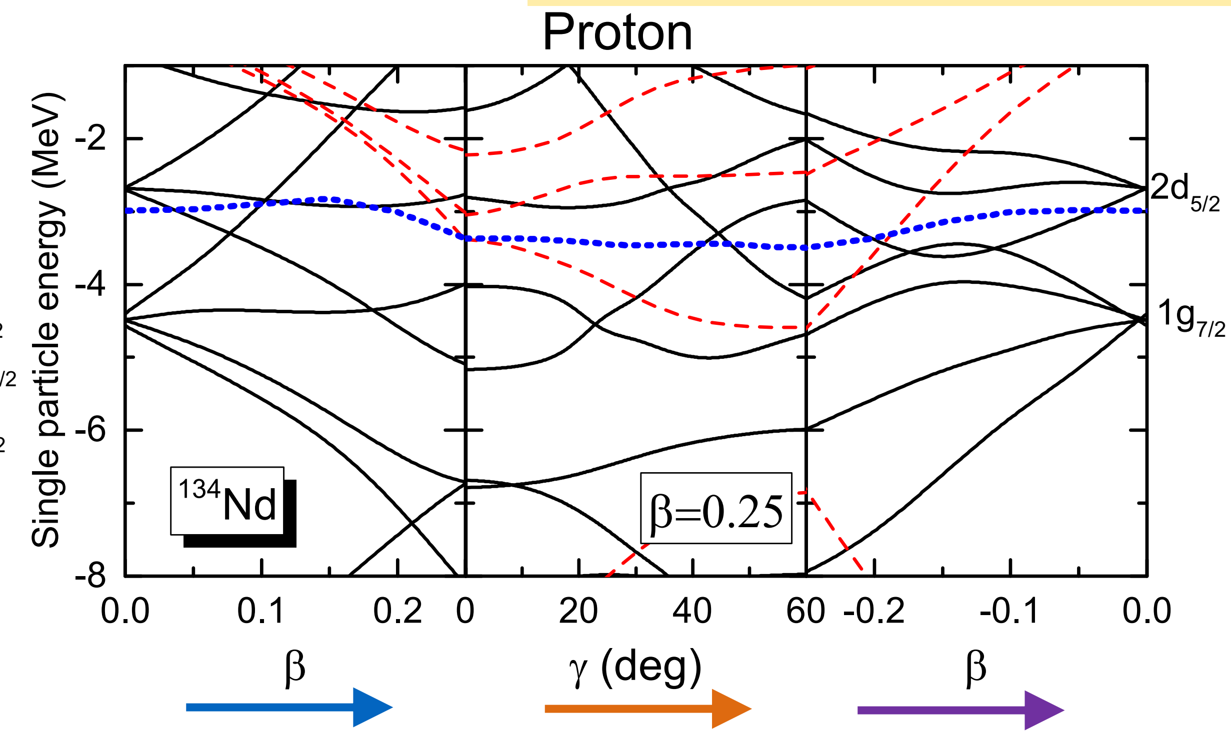

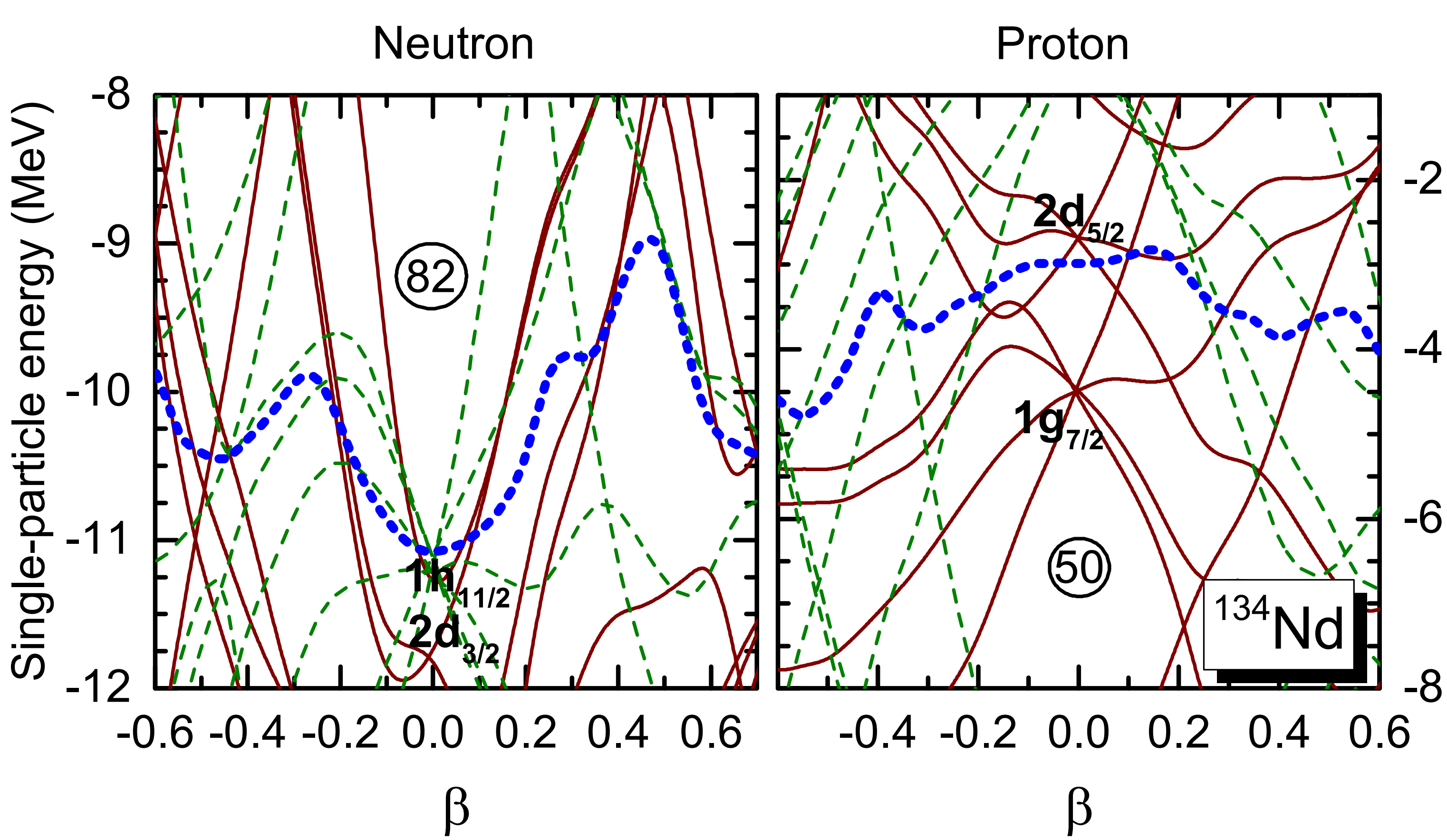

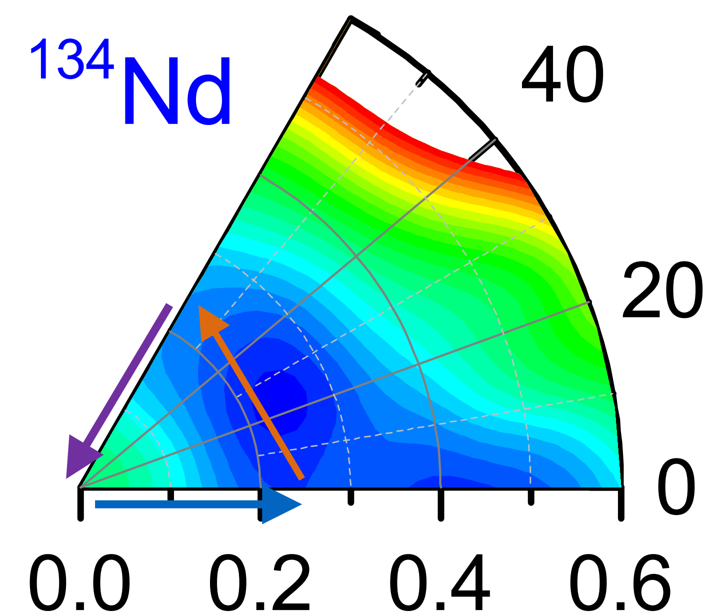

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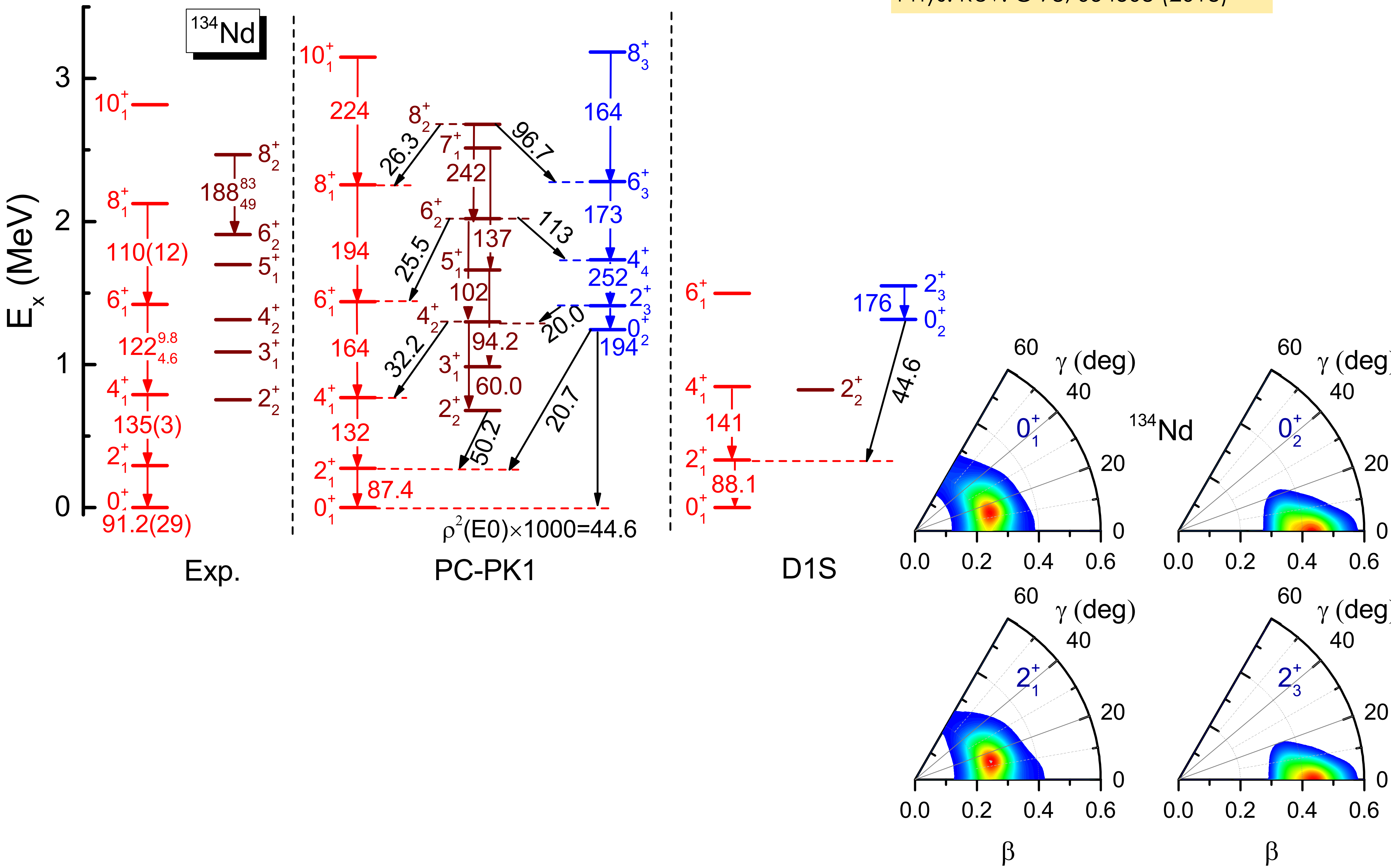


Improving RNEDFs – work in progress

…N data points and the model depends on F dimensionless parameters.

…maximizing the log-likelihood corresponds to minimizing the cost function $\chi^2(\mathbf{p})$:

$$\chi^2(\mathbf{p}) = \sum_{n=1}^{N} r_n(\mathbf{p})^2$$

➙ the residuals:

$$r_n(\mathbf{p}) = \frac{\mathcal{O}_n^{(mod)}(\mathbf{p}) - \mathcal{O}_n}{\Delta\mathcal{O}_n}$$

➙ the ***best*** model: minimum of χ^2 on the model manifold (manifold of predictions embedded in the data space)

$$\left.\frac{\partial\chi^2(\mathbf{p})}{\partial p_\mu}\right|_{\mathbf{p}=\mathbf{p}_0} = 0, \quad \forall\, \mu = 1,\ldots,F$$

In the quadratic approximation of the cost function χ^2 around the best-fit point:

$$\Delta\chi^2(\mathbf{p}) = \chi^2(\mathbf{p}) - \chi^2(\mathbf{p}_0) = \frac{1}{2}\Delta\mathbf{p}^T\hat{\mathcal{M}}\Delta\mathbf{p}$$

$$\Delta\mathbf{p} = \mathbf{p} - \mathbf{p}_0$$

Data could include: nuclear matter properties, properties of finite nuclei (binding energies, charge radii, diffraction radii, surface thickness…)

Improving RNEDFs – work in progress

The symmetric Hessian matrix of second derivatives: $\mathcal{M}_{\mu\nu} = \left. \frac{\partial^2 \chi^2}{\partial p_\mu \partial p_\nu} \right|_{\mathbf{p}=\mathbf{p}_0}$

Diagonalization ⇒ $\Delta\chi^2(\mathbf{p}) = \frac{1}{2}\Delta\mathbf{p}^T \left(\mathcal{A}\mathcal{D}\mathcal{A}^T\right)\Delta\mathbf{p} = \frac{1}{2}\xi^T\mathcal{D}\xi = \frac{1}{2}\sum_{\alpha=1}^{F}\lambda_\alpha\xi_\alpha^2$

Stiff direction ⟹ large eigenvalue λ, χ^2 rapidly worsens away from minimum, the fit places a stringent constraint on this particular linear combination of parameters.

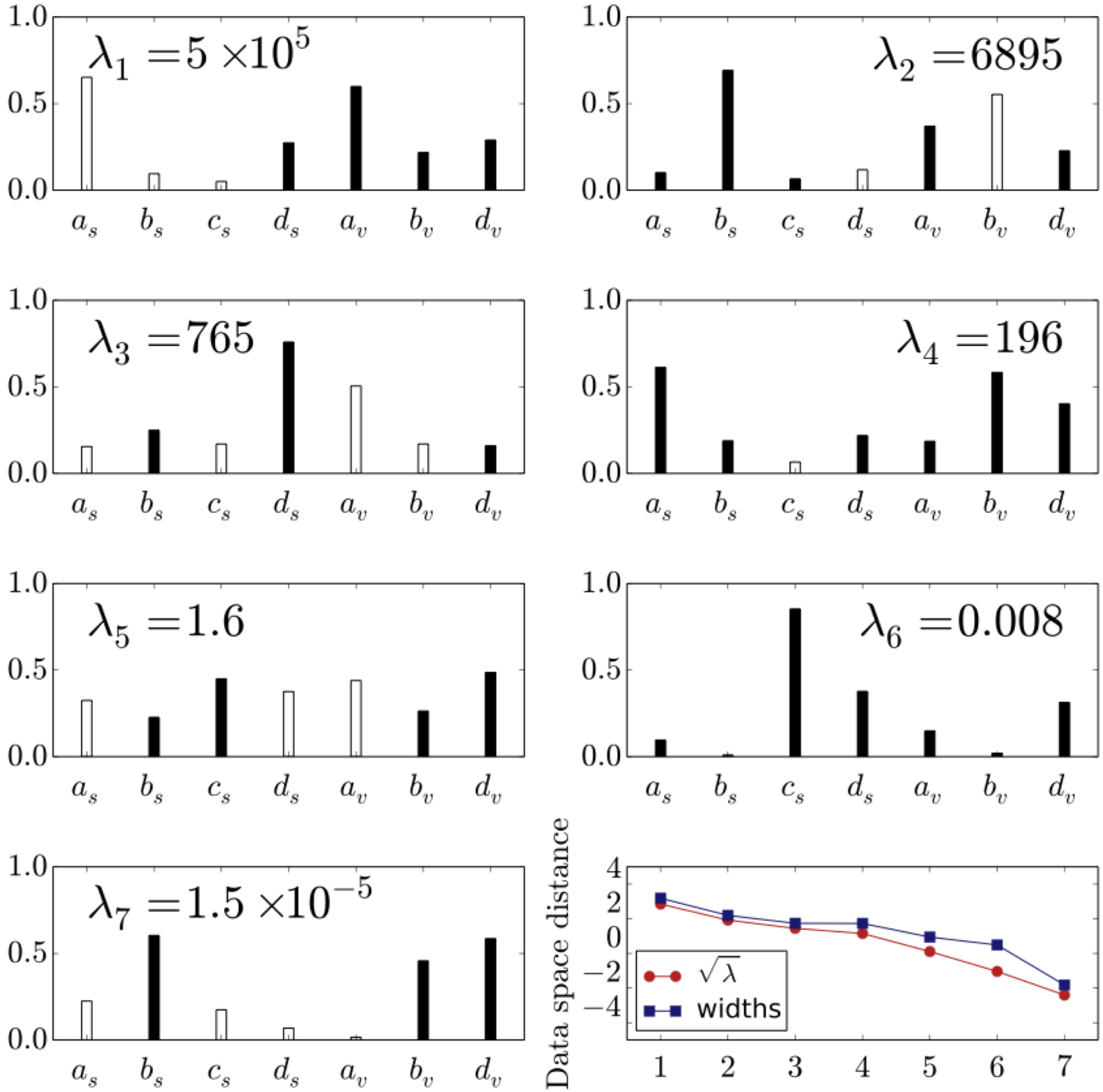
Soft direction ⟹ small eigenvalue λ, little deterioration in χ^2. The corresponding eigenvector ξ involves a particular linear combination of model parameters that is not constrained by the observables included in the fit.

Sloppy models ⟹ some parameters or their combinations are not well constrained by the data

Improving RNEDFs – work in progress

Sloppy models are characterised by an exponential distribution of eigenvalues of the Hessian matrix
→ exponential sensitivity to parameter combinations!

Eigenvectors and eigenvalues of the Hessian matrix $\mathcal{M}$ of second derivatives of $\chi^2(p)$ ➟



...empty and filled bars ⇒ the corresponding amplitudes contribute with opposite signs.

Improving RNEDFs – work in progress

Model manifolds of nonlinear sloppy models have boundaries that can be analysed using geodesics. The geodesic curve in parameter space corresponds to a curve on the model manifold. The arc length of geodesics on the manifold are a measure of the manifold width in each direction.

The parameters corresponding to a geodesic path can be found as the solution of the differential equation:

$$\ddot{p}_\mu + \sum_{\alpha\beta} \Gamma^\mu_{\alpha\beta} \dot{p}_\alpha \dot{p}_\beta = 0$$

➔ initial value problem in the parameter space.

connection coefficients: $$\Gamma^\alpha_{\mu\nu} = \sum_\beta (g^{-1})_{\alpha\beta} \sum_m \frac{\partial r_m}{\partial p_\beta} \frac{\partial^2 r_m}{\partial p_\mu \partial p_\nu}$$

metric tensor: $$g_{\mu\nu} = \sum_m \frac{\partial r_m}{\partial p_\mu} \frac{\partial r_m}{\partial p_\nu}$$

Derivatives with respect to the model parameters →if possible use the automatic differentiation packages (for self-consistent models this is not possible)

The boundary of the manifold is identified by the metric tensor becoming singular.

Improving RNEDFs – work in progress

Phys. Rev. C 95, 054304 (2016)
Phys. Rev. C 94, 024303 (2017)

Manifold boundary approximation method ⟹ systematically reducing the number of model parameters

Transtrum et al., PRL **104**, 060201 (2010)
PRL **113**, 098701 (2014)
J. Chem. Phys. **143**, 010901 (2015)

1. Given a model and a set of parameters, determine the best-fit model, calculate the Hessian and identify the eigendirection with smallest eigenvalue.

2. Integrate the geodesic equation using the best-fit parameter values and the eigendirection with smallest eigenvalue as initial conditions, until the boundary of the model manifold is reached.

3. Evaluate the limit associated with this boundary to produce a new model with one less parameters.

4. Optimise the new model by a least-square fit to the data, and use it as a starting point for the next iteration.

Applications for the nuclear structure models (self-consistent): data set should not be to large

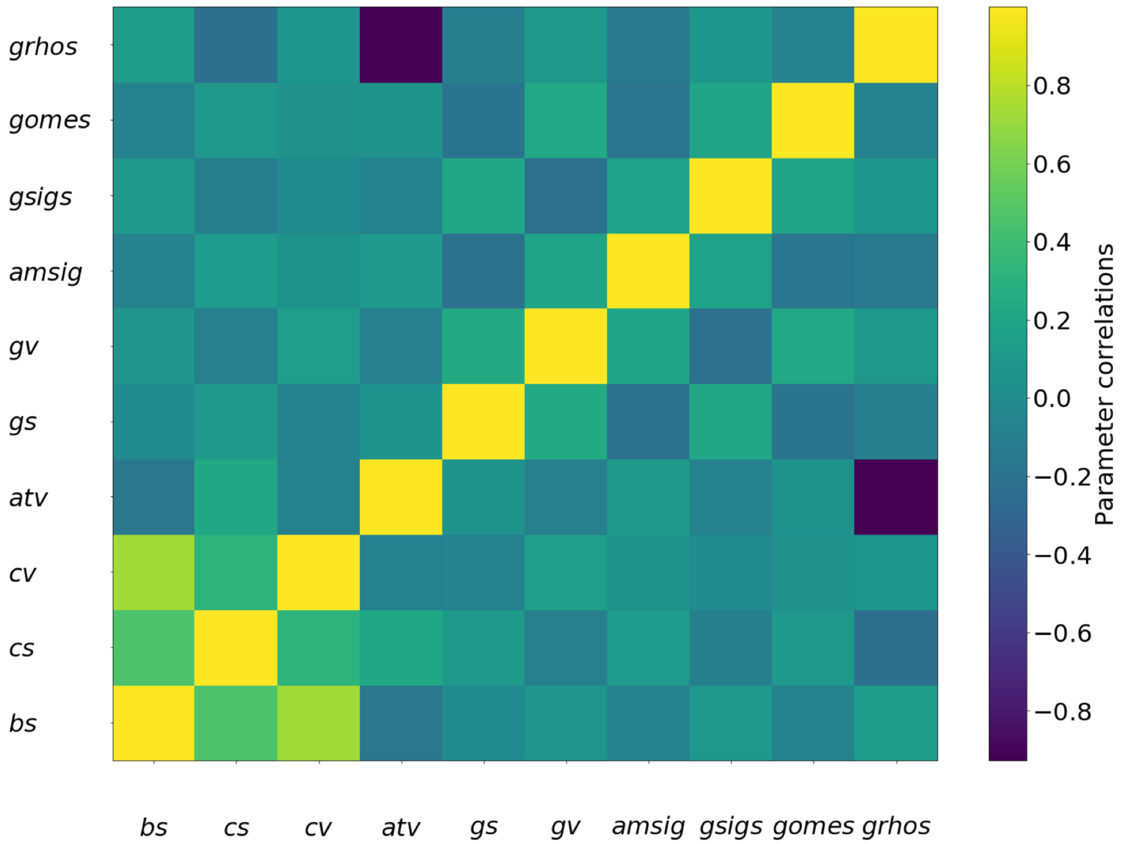
Improving RNEDFs – work in progress

Improving the description of the level densities around the Fermi surface

⟹ possible approach: models with momentum-dependent self-energies

Typel et el., Phys. Rev. C 67, 034002 (2003)
Phys. Rev. C 71, 064301 (2005)

- Develop a point-coupling implementation of the momentum-dependent model
- Fit data – preliminary calculation SV-min data set (PRC 79, 034310 (2009))
- Statistical analysis



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

Collaborators

UniZg: Dario Vretenar, Jie Zhao (China Academy of Engineering Physics, Chengdu), Vaia Prassa (Thessaloniki)

PKU, CAS, Southwest University: Jie Meng, Shan-Gui Zhou, Zhipan Li, Jiangming Yao, Bing-Nan Lu

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https://strukturnifondovi.hr/

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