CONFIGURATION MIXING WITH RELATIVISTIC SCMF MODELS

Tamara Nikšić
University of Zagreb

Supported by the Croatian Foundation for Science

Contents

Outline

Relativistic energy density functional

Energy density functional consists of the mean-field and the pairing contribution

$$\mathcal{E} = \mathcal{E}_{RMF}[j_\mu, \rho_s] + \mathcal{E}_{pp}(\kappa, \kappa^*)$$

Elementary building blocks

$$(\bar{\psi}\mathcal{O}_\tau \Gamma \psi) \quad \mathcal{O}_\tau \in \{1, \tau_i\} \quad \Gamma \in \{1, \gamma_\mu, \gamma_5, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\}$$

Isoscalar-scalar density

$$\rho_s(\mathbf{r}) = \sum_k^{occ} \bar{\psi}_k(\mathbf{r})\psi_k(\mathbf{r})$$

Relativistic energy density functional

Energy density functional consists of the mean-field and the pairing contribution

$$\mathcal{E} = \mathcal{E}_{RMF}[j_\mu, \rho_s] + \mathcal{E}_{pp}(\kappa, \kappa^*)$$

Elementary building blocks

$$(\bar{\psi}\mathcal{O}_\tau\Gamma\psi) \quad \mathcal{O}_\tau \in \{1, \tau_i\} \quad \Gamma \in \{1, \gamma_\mu, \gamma_5, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\}$$

Isoscalar-vector current

$$j_\mu(\mathbf{r}) = \sum_k^{occ} \bar{\psi}_k(\mathbf{r})\gamma_\mu\psi_k(\mathbf{r})$$

Relativistic energy density functional

Energy density functional consists of the mean-field and the pairing contribution

$$\mathcal{E} = \mathcal{E}_{RMF}[j_\mu, \rho_s] + \mathcal{E}_{pp}(\kappa, \kappa^*)$$

Elementary building blocks

$$(\bar{\psi}\mathcal{O}_\tau\Gamma\psi) \quad \mathcal{O}_\tau \in \{1, \tau_i\} \quad \Gamma \in \{1, \gamma_\mu, \gamma_5, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\}$$

Isovector-scalar density

$$\vec{\rho}_s(\mathbf{r}) = \sum_k^{occ} \bar{\psi}_k(\mathbf{r})\vec{\tau}\psi_k(\mathbf{r})$$

Relativistic energy density functional

Energy density functional consists of the mean-field and the pairing contribution

$$\mathcal{E} = \mathcal{E}_{RMF}[j_\mu, \rho_s] + \mathcal{E}_{pp}(\kappa, \kappa^*)$$

Elementary building blocks

$$(\bar{\psi}\mathcal{O}_\tau\Gamma\psi) \quad \mathcal{O}_\tau \in \{1, \tau_i\} \quad \Gamma \in \{1, \gamma_\mu, \gamma_5, \gamma_5\gamma_\mu, \sigma_{\mu\nu}\}$$

Isovector-vector current

$$\vec{j}_\mu(\mathbf{r}) = \sum_k^{occ} \bar{\psi}_k(\mathbf{r})\vec{\tau}j_\mu\psi_k(\mathbf{r})$$

Relativistic energy density functional

Energy density functional consists of the mean-field and the pairing contribution

$$\mathcal{E} = \mathcal{E}_{RMF}[j_\mu, \rho_s] + \mathcal{E}_{pp}(\kappa, \kappa^*)$$

Kinetic energy term

$$\mathcal{E}_{kin} = \sum_i v_i^2 \int \bar{\psi}_i(\boldsymbol{r}) \left(-\gamma\boldsymbol{\nabla} + m\right) \psi_i(\boldsymbol{r})$$

Relativistic energy density functional

Energy density functional consists of the mean-field and the pairing contribution

$$\mathcal{E} = \mathcal{E}_{RMF}[j_\mu, \rho_s] + \mathcal{E}_{pp}(\kappa, \kappa^*)$$

Second order terms

$$\mathcal{E}_{2nd} = \frac{1}{2} \int \left[\alpha_v(\rho_v)\rho_v^2 + \alpha_s(\rho_v)\rho_s^2 + \alpha_{tv}(\rho_v)\rho_{tv}^2\right] d\mathbf{r}$$

Relativistic energy density functional

Energy density functional consists of the mean-field and the pairing contribution

$$\mathcal{E} = \mathcal{E}_{RMF}[j_\mu, \rho_s] + \mathcal{E}_{pp}(\kappa, \kappa^*)$$

Derivative terms

$$\mathcal{E}_{der} = \frac{1}{2}\int \delta_s \rho_s \triangle \rho_s d\mathbf{r}$$

Relativistic energy density functional

Energy density functional consists of the mean-field and the pairing contribution

$$\mathcal{E} = \mathcal{E}_{RMF}[j_\mu, \rho_s] + \mathcal{E}_{pp}(\kappa, \kappa^*)$$

Coulomb interaction

$$E_{coul} = \frac{e}{2} \int j^p_\mu A^\mu d\mathbf{r}$$

Relativistic energy density functional

Energy density functional consists of the mean-field and the pairing contribution

$$\mathcal{E} = \mathcal{E}_{RMF}[j_\mu, \rho_s] + \mathcal{E}_{pp}(\kappa, \kappa^*)$$

Pairing interaction: finite range separable pairing

$$V(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}'_1, \boldsymbol{r}'_2) = G\delta(\boldsymbol{R} - \boldsymbol{R}')P(\boldsymbol{r})P(\boldsymbol{r}')\frac{1}{2}(1 - P^\sigma)$$

$$\boldsymbol{R} = \frac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2), \quad \boldsymbol{r} = \boldsymbol{r}_1 - \boldsymbol{r}_2, \quad P(\boldsymbol{r}) = \frac{1}{4\pi a^2} e^{-\frac{r^2}{4a^2}}$$

Parameters a and G are adjusted to reproduce the pairing gap in the symmetric nuclear matter calculated using the Gogny force.

Relativistic energy density functional

Couplings are density-dependent

$$\alpha_i(\rho_v) = a_i + (b_i + c_i x)\, e^{-d_i x}, \quad x = \rho/\rho_{sat}, \quad i \equiv s,\ v,\ tv$$

Model parameters

$$a_s,\ b_s,\ c_s,\ d_s,\ a_v,\ b_v,\ d_v,\ b_{tv},\ d_{tv},\ \delta_s$$

Adjusted to empirical ground-state properties of finite nuclei.

Empirical ground-state properties of finite nuclei can only determine a small set of parameters.

Nuclear many-body correlations

Implicitly included in the EDF

- short-range → hard repulsive core of the NN-interaction
- long-range → mediated by nuclear resonance modes (giant resonances)
- the corresponding corrections vary smoothly with the number of nucleons → absorbed in the model parameters

- heavy deformed systems present best examples of mean-field nuclei
- high density of states reduces the shell effects

Adjusting the model parameters

Empirical mass formula

The calculated masses of finite nuclei are primarily sensitive to three leading terms in the empirical mass formula

$$E_B = a_v A + a_s A^{2/3} + a_4 \frac{(N-Z)^2}{4A} + \cdots$$

Fitting strategy

- generate families of effective interactions that are characterized by different values of a_v, a_s and the symmetry energy $S_2(0.12\text{fm}^{-3})$
- determine which parametrization minimizes the deviation from empirical binding energies of a large set of deformed nuclei

Adjusting the model parameters

Empirical mass formula

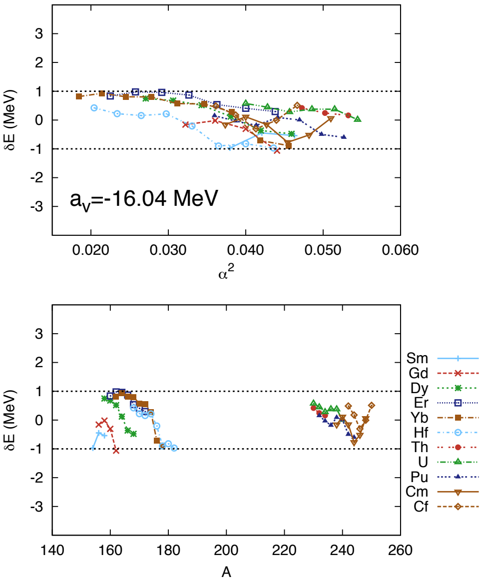
The calculated masses of finite nuclei are primarily sensitive to three leading terms in the empirical mass formula

$$E_B = a_v A + a_s A^{2/3} + a_4 \frac{(N-Z)^2}{4A} + \cdots$$

Fitting strategy

- generate families of effective interactions that are characterized by different values of a_v, a_s and the symmetry energy $S_2(0.12\text{fm}^{-3})$
- determine which parametrization minimizes the deviation from empirical binding energies of a large set of deformed nuclei

Adjusting the model parameters



Rare-earth region

Sm (Z=62), Gd (Z=64), Dy (Z=66), Er (Z=68), Yb (Z=70), Hf (Z=72)

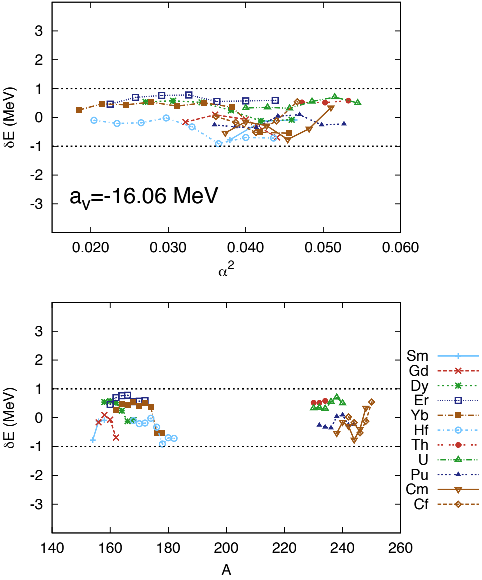
Actinides

Th (Z=90), U (Z=92), Pu (Z=94), Cm (Z=96), Cf (Z=98)

Total

64 isotopes

Adjusting the model parameters



Rare-earth region

Sm (Z=62), Gd (Z=64), Dy (Z=66), Er (Z=68), Yb (Z=70), Hf (Z=72)

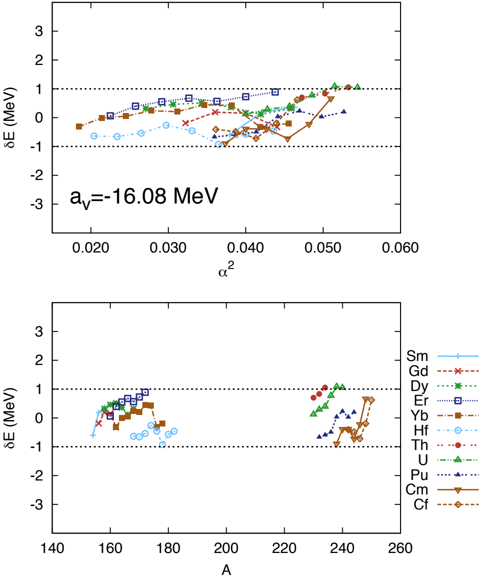
Actinides

Th (Z=90), U (Z=92), Pu (Z=94), Cm (Z=96), Cf (Z=98)

Total

64 isotopes

Adjusting the model parameters



Rare-earth region

Sm (Z=62), Gd (Z=64), Dy (Z=66), Er (Z=68), Yb (Z=70), Hf (Z=72)

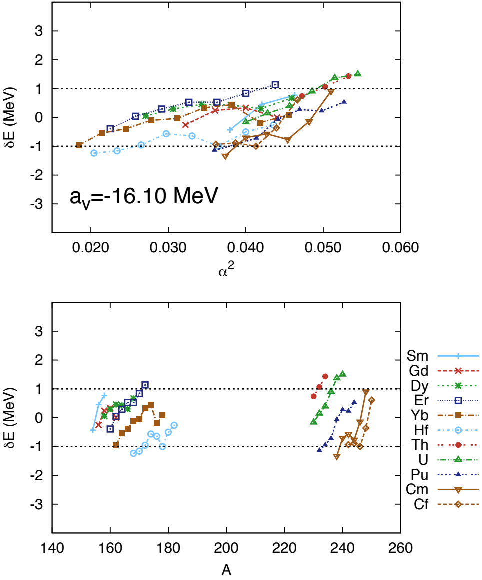
Actinides

Th (Z=90), U (Z=92), Pu (Z=94), Cm (Z=96), Cf (Z=98)

Total

64 isotopes

Adjusting the model parameters



Rare-earth region

Sm (Z=62), Gd (Z=64), Dy (Z=66), Er (Z=68), Yb (Z=70), Hf (Z=72)

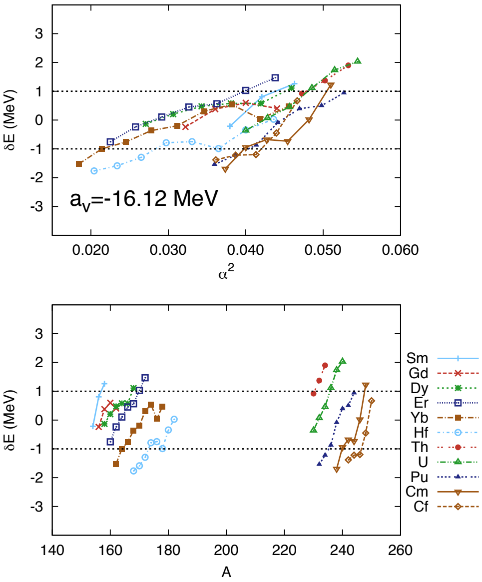
Actinides

Th (Z=90), U (Z=92), Pu (Z=94), Cm (Z=96), Cf (Z=98)

Total

64 isotopes

Adjusting the model parameters



Rare-earth region

Sm (Z=62), Gd (Z=64), Dy (Z=66), Er (Z=68), Yb (Z=70), Hf (Z=72)

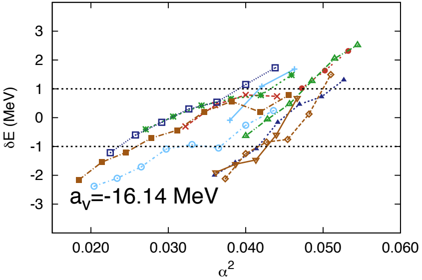
Actinides

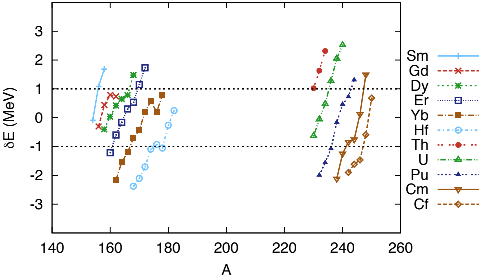
Th (Z=90), U (Z=92), Pu (Z=94), Cm (Z=96), Cf (Z=98)

Total

64 isotopes

Adjusting the model parameters





Rare-earth region

Sm (Z=62), Gd (Z=64), Dy (Z=66), Er (Z=68), Yb (Z=70), Hf (Z=72)

Actinides

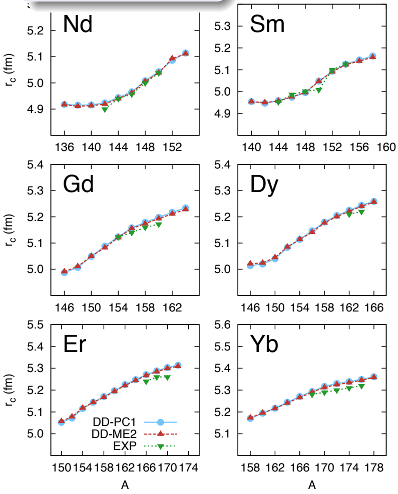
Th (Z=90), U (Z=92), Pu (Z=94), Cm (Z=96), Cf (Z=98)

Total

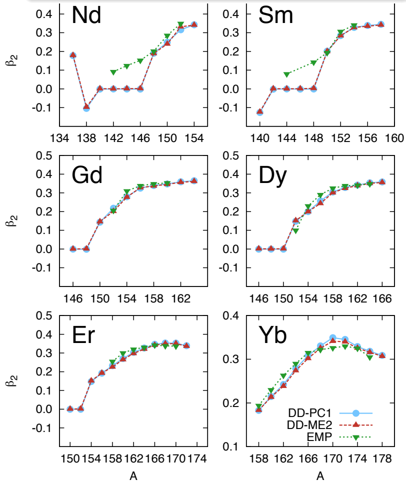
64 isotopes

Ground-state properties

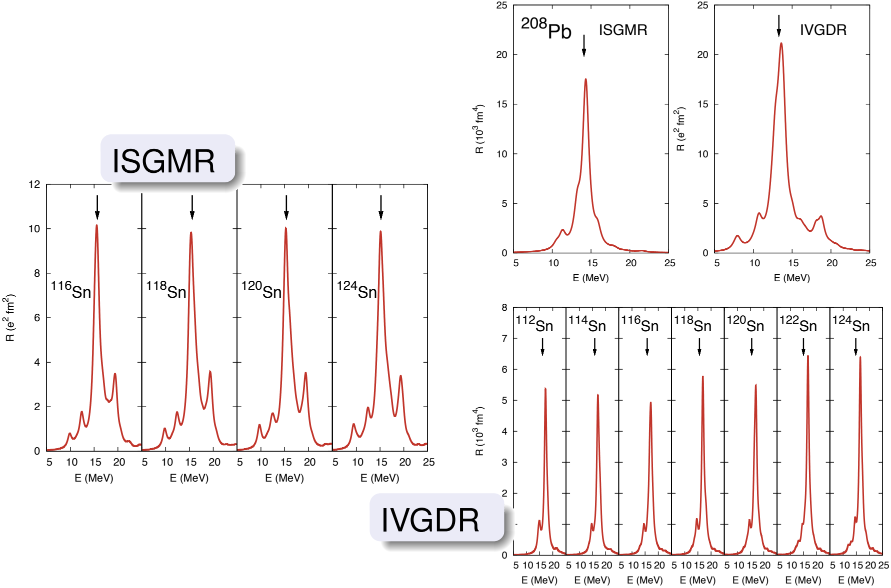
Charge radii



Quadrupole deformations



Excitation energies of collective modes



Implementation of the collective Hamiltonian model based on the SCRMF

Collective Hamiltonian

$$\mathcal{H}_{coll} = \mathcal{T}_{rot} + \mathcal{T}_{vib} + \mathcal{V}_{coll}$$

Rotational energy

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

The moments of inertia are calculated by using the Inglis-Belyaev formula.

Implementation of the collective Hamiltonian model based on the SCRMF

Collective Hamiltonian

$$\mathcal{H}_{coll} = \mathcal{T}_{rot} + \mathcal{T}_{vib} + \mathcal{V}_{coll}$$

Vibrational energy

$$\mathcal{T}_{vib} = -\frac{\hbar^2}{2\beta^4\sqrt{wr}}\left[\partial_\beta\sqrt{\frac{r}{w}}\beta^4 B_{\gamma\gamma}\partial_\beta - \partial_\beta\sqrt{\frac{r}{w}}\beta^3 B_{\beta\gamma}\partial_\gamma\right]$$
$$-\frac{\hbar^2}{\sin 3\gamma\sqrt{wr}}\left[-\frac{1}{\beta^2}\partial_\gamma\sqrt{\frac{r}{w}}\sin 3\gamma B_{\beta\gamma}\partial_\beta + \frac{1}{\beta}\partial_\gamma\sqrt{\frac{r}{w}}\sin 3\gamma B_{\beta\beta}\partial_\gamma\right]$$

The mass parameters are calculated in the cranking approximation .

Implementation of the collective Hamiltonian model based on the SCRMF

Collective Hamiltonian

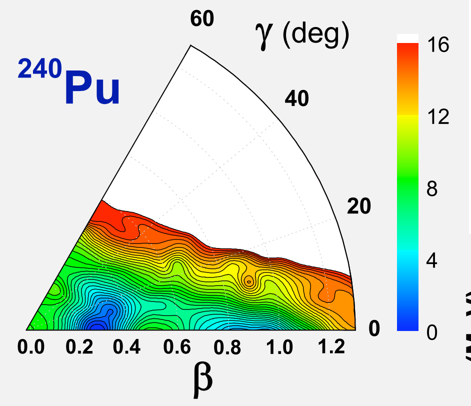
$$\mathcal{H}_{coll} = \mathcal{T}_{rot} + \mathcal{T}_{vib} + \mathcal{V}_{coll}$$

Collective potential

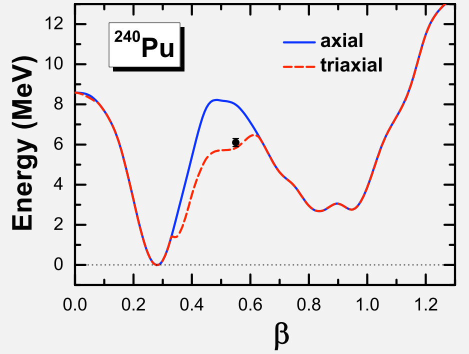
$$\mathcal{V}_{coll}(\beta,\gamma) = E_{tot}(\beta,\gamma) - \Delta V_{vib}(\beta,\gamma) - \Delta V_{rot}(\beta,\gamma)$$

Corresponds to the mean-field potential energy surface with the zero point energy subtracted .

Applications: ^{240}Pu isotope

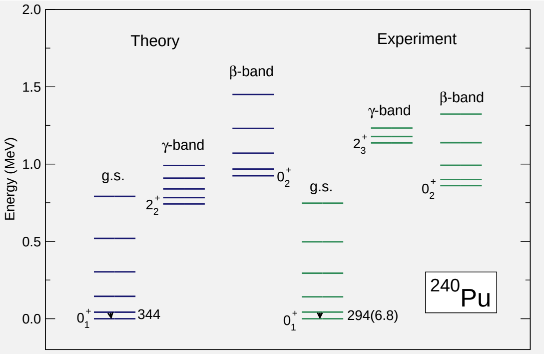


Triaxial effects lower the barrier.



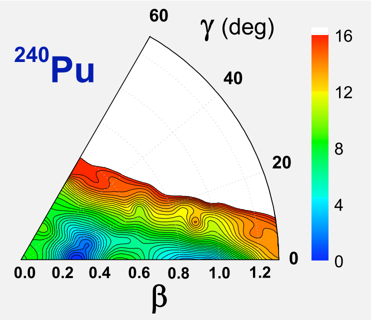
ND and SD minima are separated by the barrier.

Applications: ^{240}Pu isotope



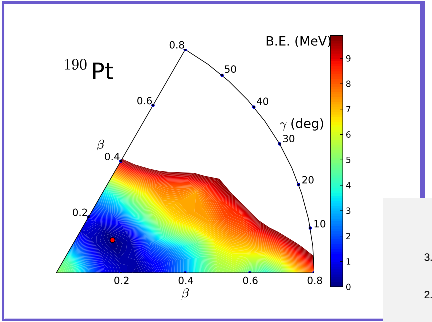
$$E^{th}_{4^+_1} / E^{th}_{2^+_1} = 3.33$$

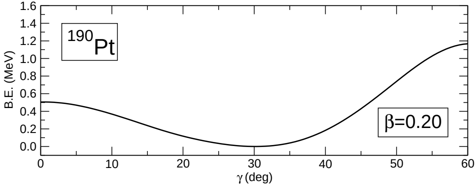
$$E^{exp}_{4^+_1} / E^{exp}_{2^+_1} = 3.31$$

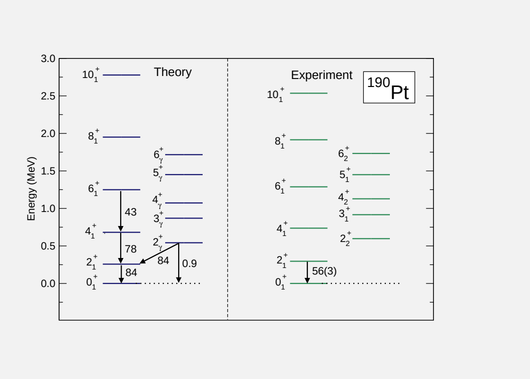


The moments of inertia are renormalized by factor $\approx$ 1.3 to compensate the difference between IB and TV moments of inertia.

Applications: Pt isotopes



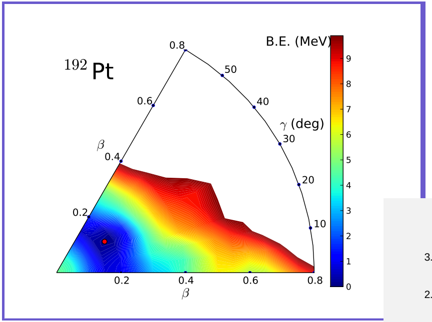


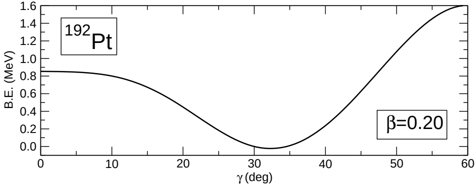


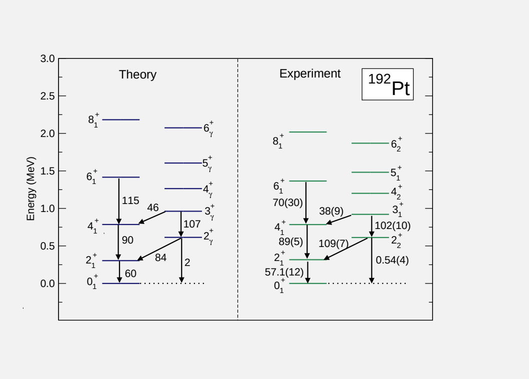
$$E^{th}_{4_1^+} / E^{th}_{2_1^+} = 2.39$$

$$E^{exp}_{4_1^+} / E^{exp}_{2_1^+} = 2.49$$

Applications: Pt isotopes



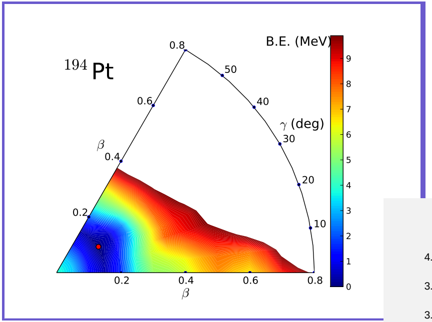


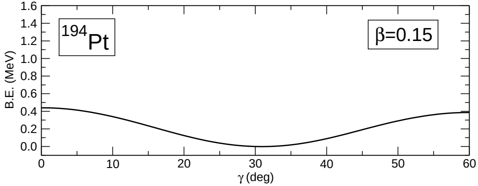


$$E^{th}_{4^+_1} / E^{th}_{2^+_1} = 2.58$$

$$E^{exp}_{4^+_1} / E^{exp}_{2^+_1} = 2.48$$

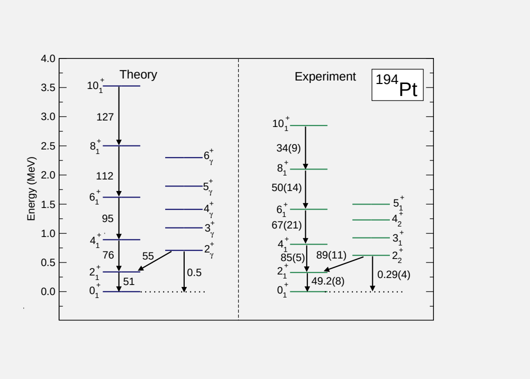
Applications: Pt isotopes



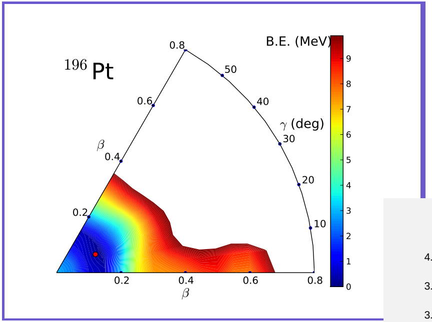


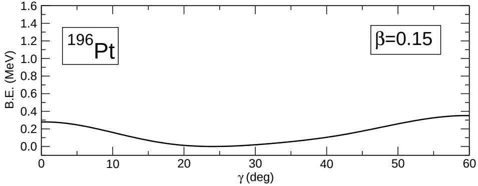
$$E^{th}_{4^+_1} / E^{th}_{2^+_1} = 2.63$$

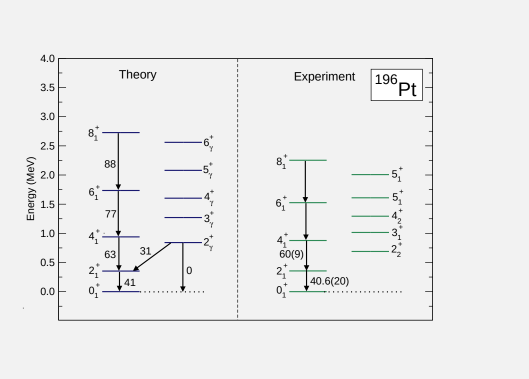
$$E^{exp}_{4^+_1} / E^{exp}_{2^+_1} = 2.47$$



Applications: Pt isotopes



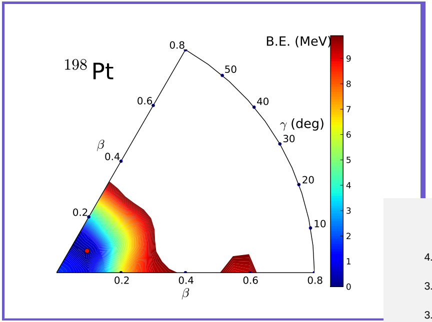


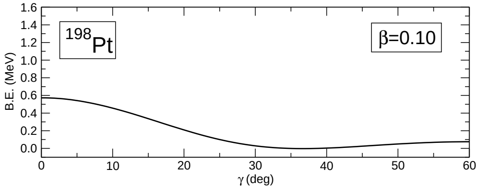


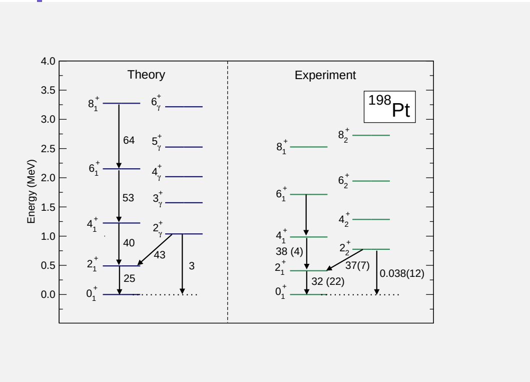
$$E^{th}_{4^+_1} / E^{th}_{2^+_1} = 2.66$$

$$E^{exp}_{4^+_1} / E^{exp}_{2^+_1} = 2.47$$

Applications: Pt isotopes



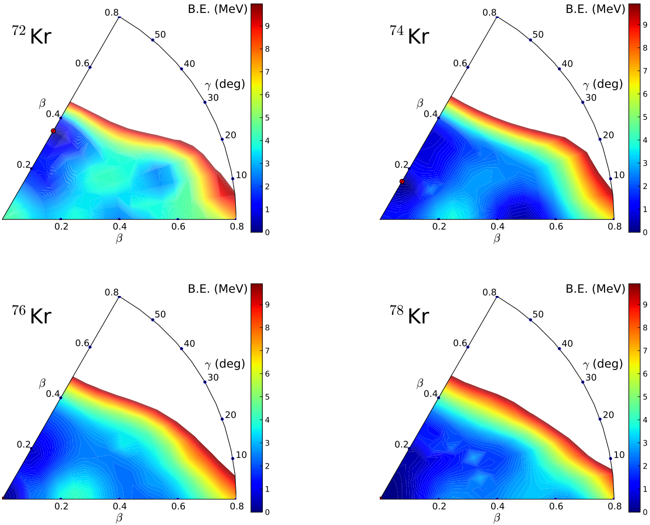




$$E^{th}_{4^+_1} / E^{th}_{2^+_1} = 2.49$$

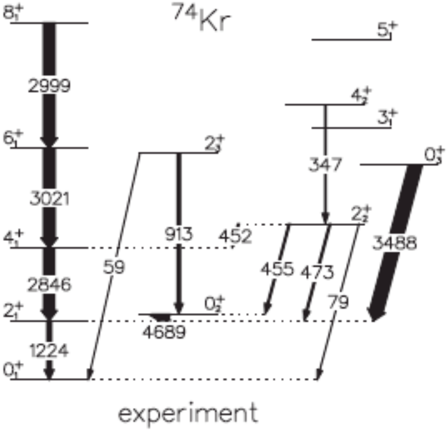
$$E^{exp}_{4^+_1} / E^{exp}_{2^+_1} = 2.42$$

Applications: Kr isotopes



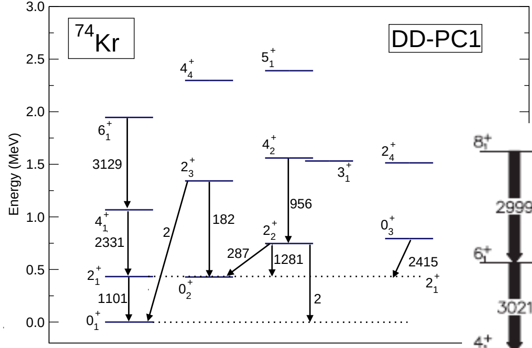
^{74}Kr isotope: level scheme

- g.s. band → predominantely prolate
- 2_2^+ state: γ-vibration
- 0_2^+, 2_3^+ → predominantely oblate
- mixing in the ground state

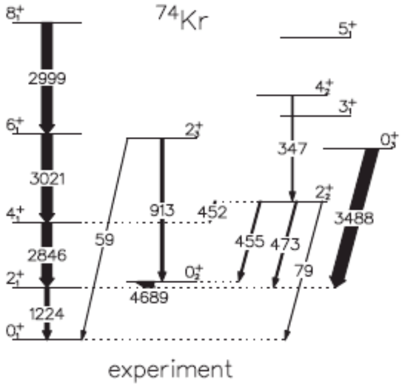


^{74}Kr isotope: level scheme

Collective Hamiltonian+DDPC1

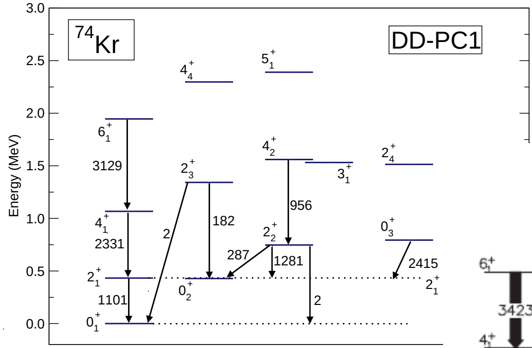


Experiment

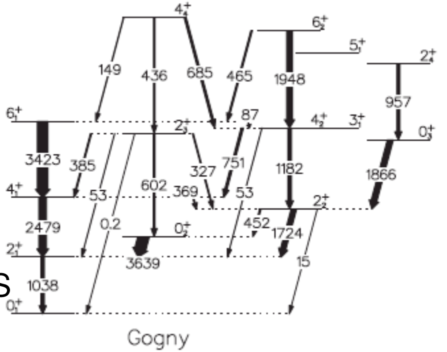


^{74}Kr isotope: level scheme

Collective Hamiltonian+DDPC1

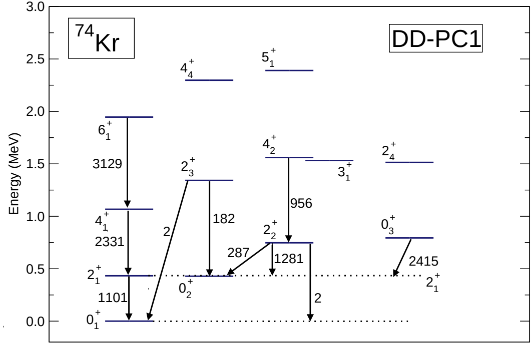


Collective Hamiltonian+Gogny D1S

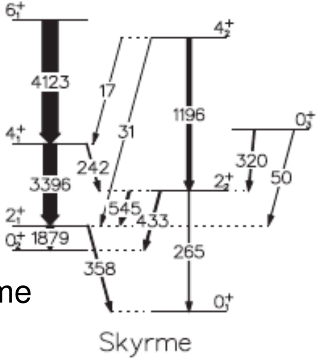


^{74}Kr isotope: level scheme

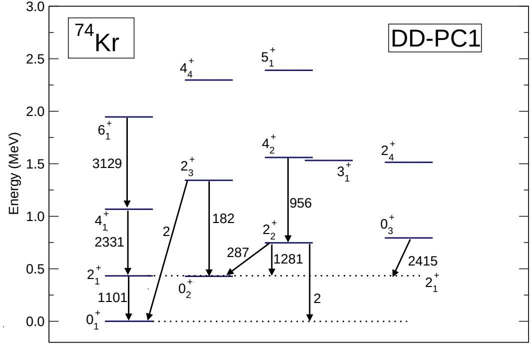
Collective Hamiltonian+DDPC1



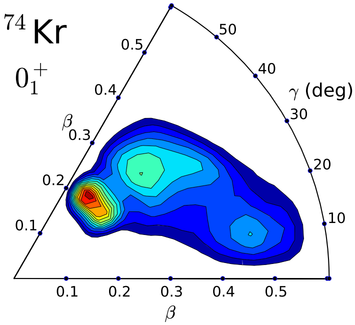
1D AM&PNP Skyrme



^{74}Kr isotope: collective probability



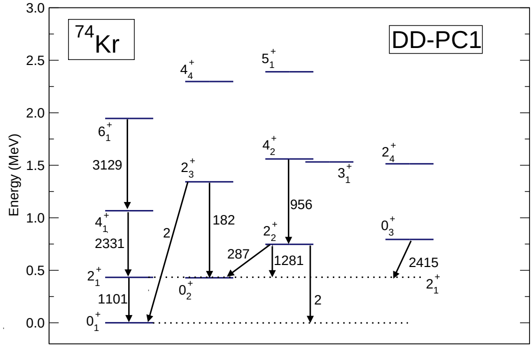
g.s. band



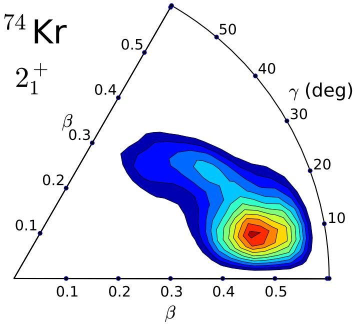
Probability density distribution:

$$\rho_{I\alpha}(\beta,\gamma) = \sum_{K\in\Delta I} |\psi^I_{\alpha K}(\beta,\gamma)|^2 \beta^3 |\sin 3\gamma|$$

^{74}Kr isotope: collective probability



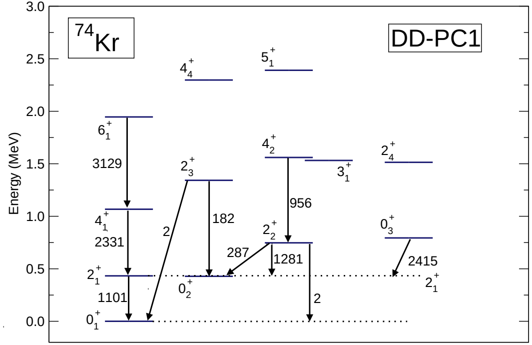
g.s. band



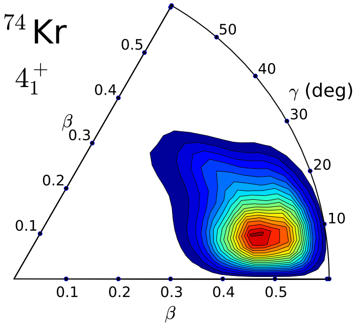
Probability density distribution:

$$\rho_{I\alpha}(\beta,\gamma) = \sum_{K\in\Delta I} |\psi^{I}_{\alpha K}(\beta,\gamma)|^2 \beta^3 \,|\sin 3\gamma|$$

^{74}Kr isotope: collective probability



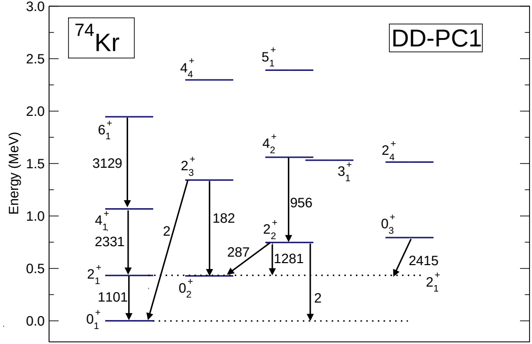
g.s. band



Probability density distribution:

$$\rho_{I\alpha}(\beta,\gamma) = \sum_{K\in\Delta I} |\psi^I_{\alpha K}(\beta,\gamma)|^2 \beta^3 |\sin 3\gamma|$$

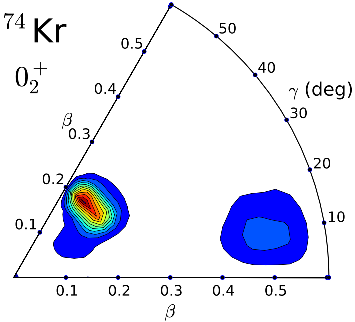
^{74}Kr isotope: collective probability



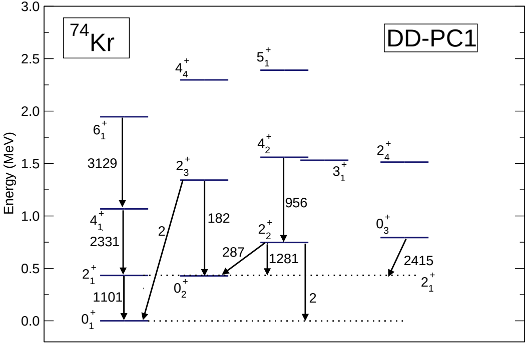
oblate deformed band

Probability density distribution:

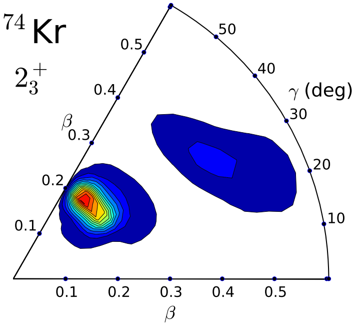
$$\rho_{I\alpha}(\beta,\gamma) = \sum_{K\in\Delta I} |\psi^{I}_{\alpha K}(\beta,\gamma)|^2 \beta^3 \,|\sin 3\gamma|$$



^{74}Kr isotope: collective probability



oblate deformed band

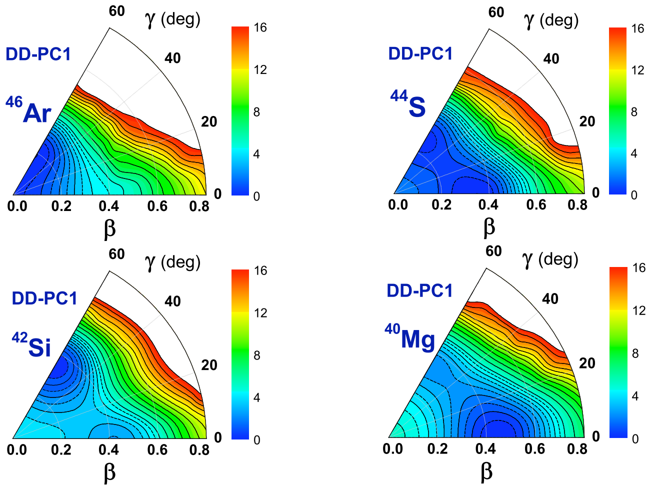


Probability density distribution:

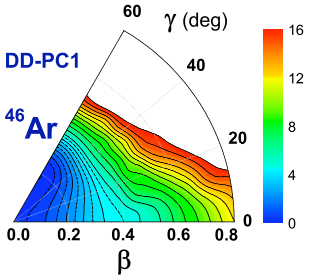
$$\rho_{I\alpha}(\beta,\gamma) = \sum_{K\in\Delta I} |\psi^{I}_{\alpha K}(\beta,\gamma)|^2 \beta^3 \,|\sin 3\gamma|$$

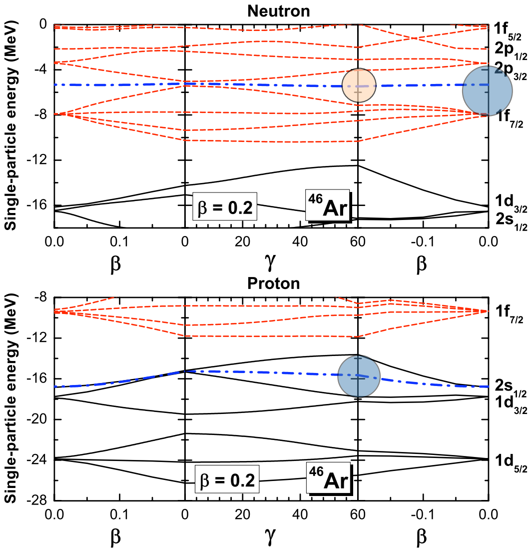
Applications: $N = 28$ isotones

The variation of the mean-field shapes is governed by the evolution of the underlying shell structure of single-nucleon orbitals.

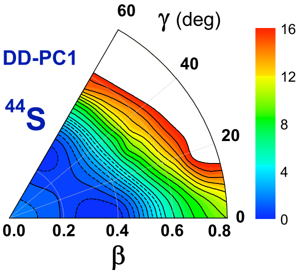


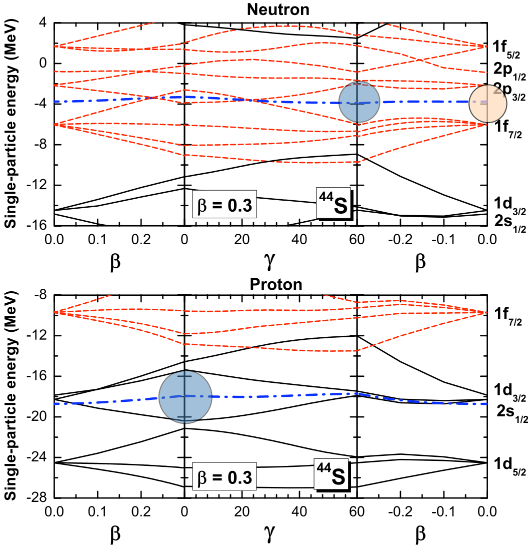
^{46}Ar isotope: single-particle levels



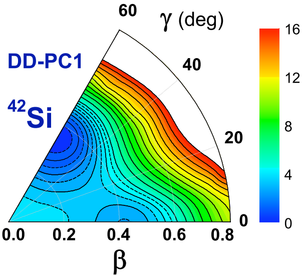


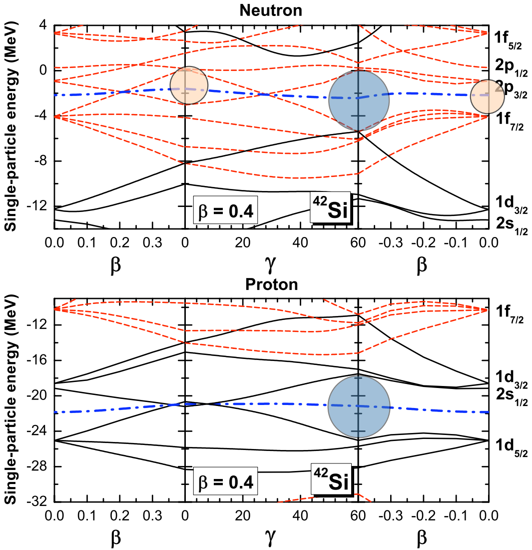
^{44}S isotope: single-particle levels



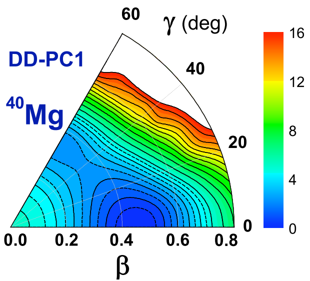


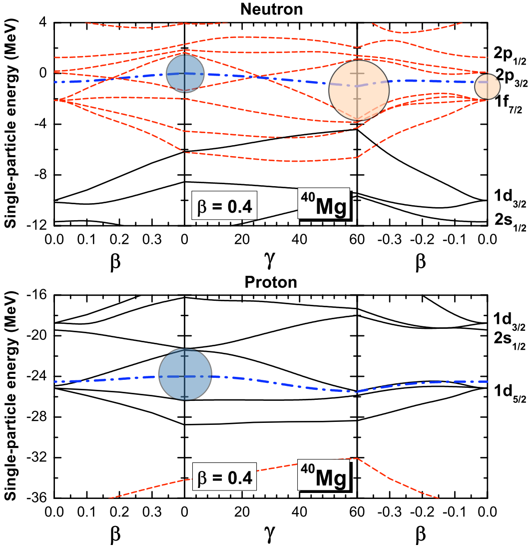
^{42}Si isotope: single-particle levels





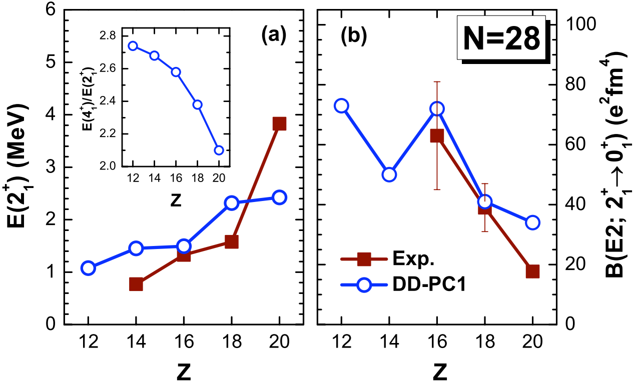
^{40}Mg isotope: single-particle levels



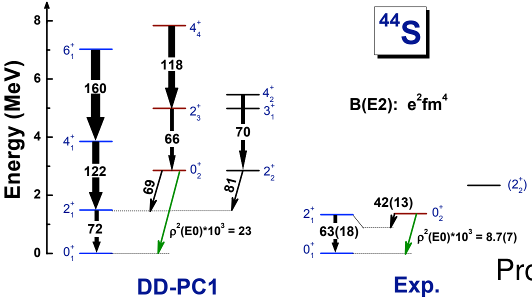


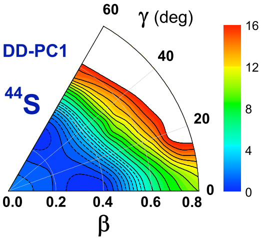
$N \approx 28$ observables

- excitation energies and reduced electric quadrupole transition probabilities
- full configuration space, no need for effective charges



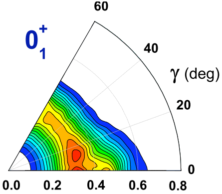
^{44}S isotope: level scheme

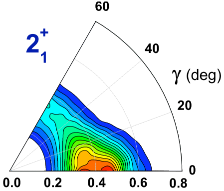


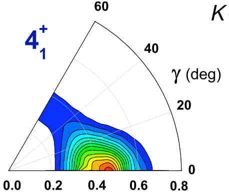


Probability density distribution:

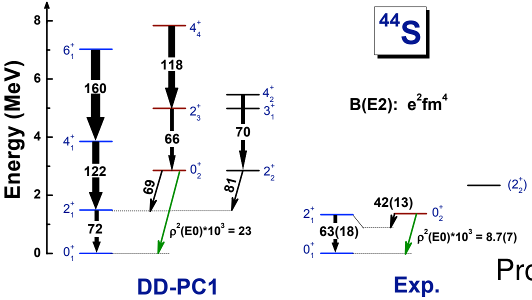
$$\rho_{I\alpha}(\beta,\gamma) = \sum_{K\in\Delta I} |\psi^I_{\alpha K}(\beta,\gamma)|^2 \beta^3$$

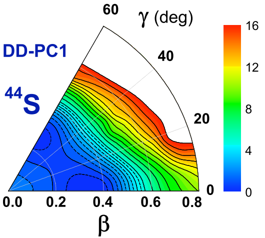






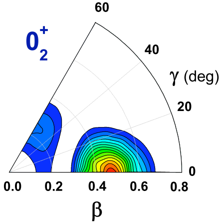
^{44}S isotope: level scheme

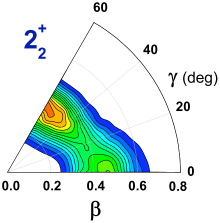


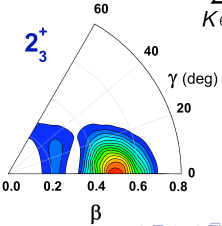


Probability density distribution:

$$\rho_{I\alpha}(\beta,\gamma) = \sum_{K\in\Delta I} |\psi^{I}_{\alpha K}(\beta,\gamma)|^2 \beta^3$$







Summary and outlook

Summary

Unified microscopic description of the structure of stable and nuclei far from stability, and reliable extrapolations toward the drip lines.

Summary

When extended to take into account collective correlations, it describes deformations and shape-coexistence phenomena associated with shell evolution.

Outlook

Further improvements of the model and more systematic calculations.

Summary and outlook

Summary

Unified microscopic description of the structure of stable and nuclei far from stability, and reliable extrapolations toward the drip lines.

Summary

When extended to take into account collective correlations, it describes deformations and shape-coexistence phenomena associated with shell evolution.

Outlook

Further improvements of the model and more systematic calculations.

Summary and outlook

Summary

Unified microscopic description of the structure of stable and nuclei far from stability, and reliable extrapolations toward the drip lines.

Summary

When extended to take into account collective correlations, it describes deformations and shape-coexistence phenomena associated with shell evolution.

Outlook

Further improvements of the model and more systematic calculations.

Collaborators

- Georgios Lalazissis (Aristotle University of Thessaloniki)
- Zhipan Li (Peking University)
- Jie Meng (Peking University)
- Leszek Próchniak (Maria Curie-Sklodowska University, Lublin)
- Peter Ring (Technical University Munich)
- Dario Vretenar (University of Zagreb)