

# CONFIGURATION MIXING WITH RELATIVISTIC SCMF MODELS



Tamara Nikšić  
University of Zagreb

---



Supported by the National Foundation for Science, Higher Education and Technological Development of the Republic of Croatia

# Contents

## Outline

- (Relativistic) nuclear energy density functional
  - Adjusting the model parameters
  - Applications: ground-state properties
  - Applications: giant resonances
- collective Hamiltonian model based on the self-consistent RMF
  - Applications:  $^{240}\text{Pu}$  isotope
  - Applications: Pt isotopes
- Summary and outlook

# Contents

## Outline

- (Relativistic) nuclear energy density functional
  - Adjusting the model parameters
  - Applications: ground-state properties
  - Applications: giant resonances
- collective Hamiltonian model based on the self-consistent RMF
  - Applications:  $^{240}\text{Pu}$  isotope
  - Applications: Pt isotopes
- Summary and outlook

# Contents

## Outline

- (Relativistic) nuclear energy density functional
  - Adjusting the model parameters
  - Applications: ground-state properties
  - Applications: giant resonances
- collective Hamiltonian model based on the self-consistent RMF
  - Applications:  $^{240}\text{Pu}$  isotope
  - Applications: Pt isotopes
- Summary and outlook

# 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

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

# Relativistic energy density functional

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

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

## Second order terms

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

# 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

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

# 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

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

# 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

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

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

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

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

## 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

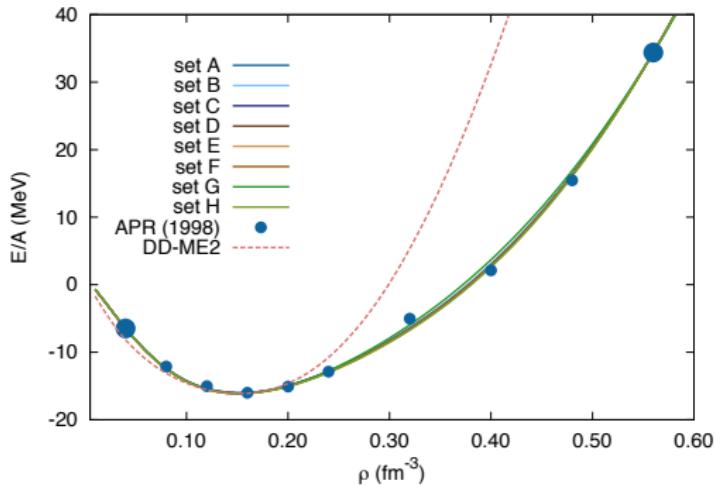
$$E_B = a_v A + a_s A^{2/3} + a_4 \frac{(N - Z)^2}{4A} + \dots$$

## 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

Two points from the microscopic EoS curve of Akmal, Pandharipande and Ravenhall are kept fixed.



$$\rho_{sat} = 0.152 \text{ fm}^{-3}$$

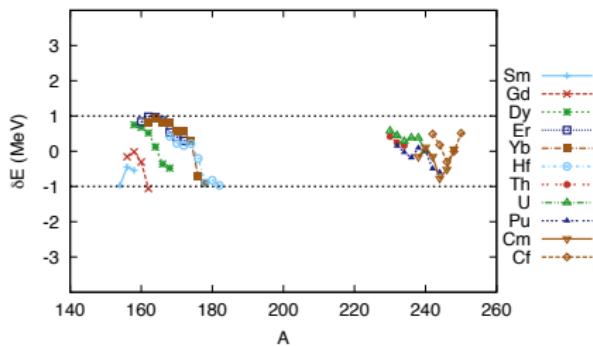
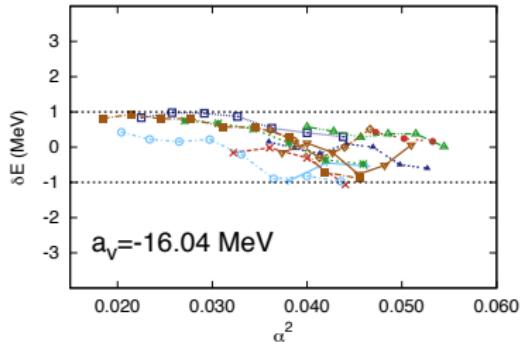
$$m_D = 0.58m$$

$$a_4 = 33 \text{ MeV}$$

$$K_{nm} = 230 \text{ MeV}$$

$$a_v = -16.04 \text{ MeV}, \dots, -16.14 \text{ MeV}$$

# Adjusting the model parameters



## Rare-earth region

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

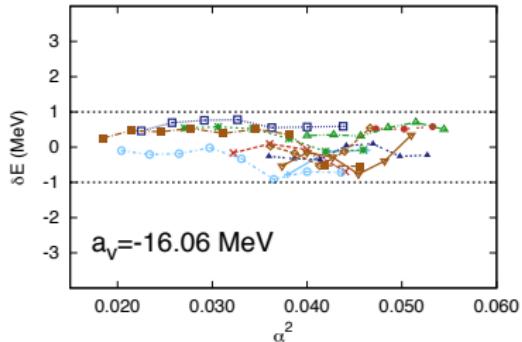
## Actinides

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

## Total

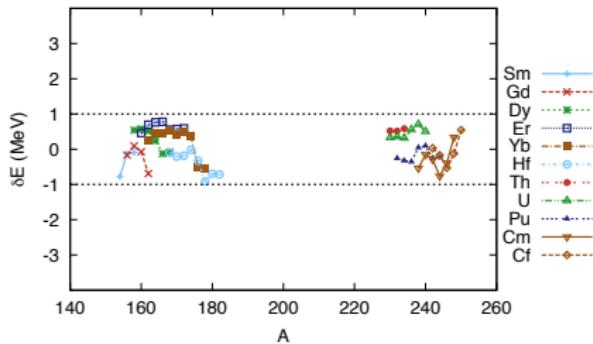
64 isotopes used in the fit

# Adjusting the model parameters



## Rare-earth region

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



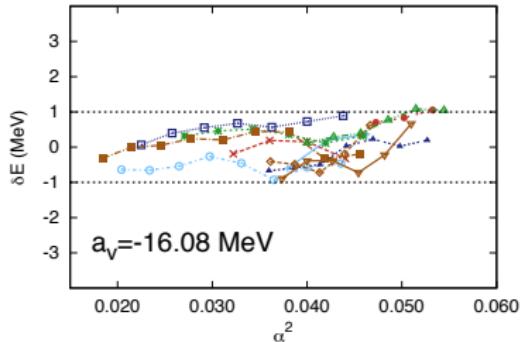
## Actinides

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

## Total

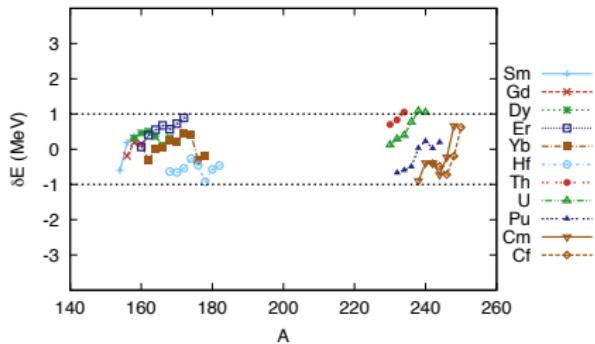
64 isotopes used in the fit

# Adjusting the model parameters



## Rare-earth region

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



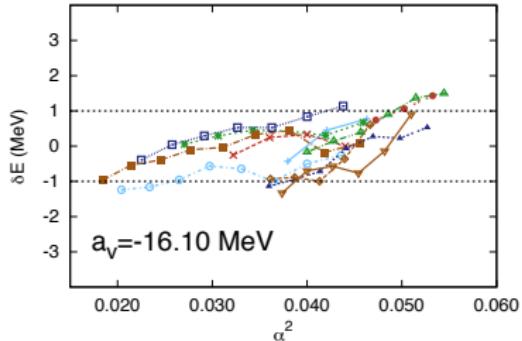
## Actinides

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

## Total

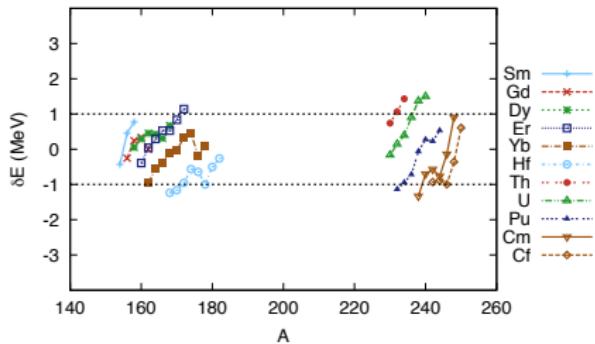
64 isotopes used in the fit

# Adjusting the model parameters



## Rare-earth region

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



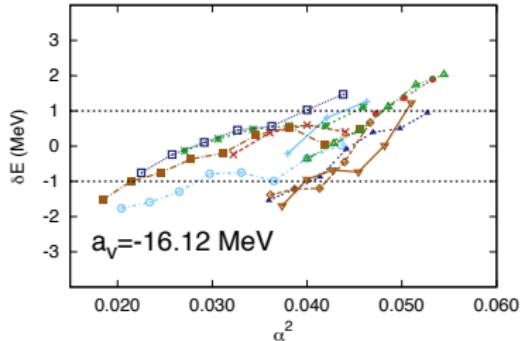
## Actinides

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

## Total

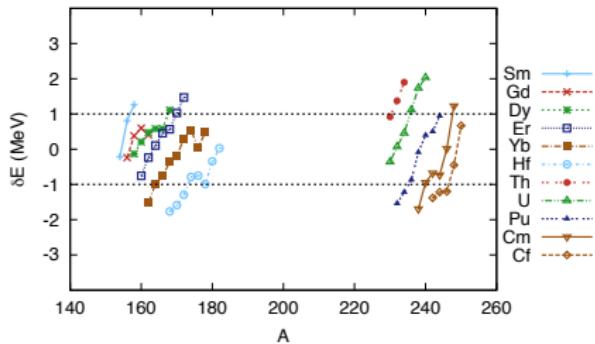
64 isotopes used in the fit

# Adjusting the model parameters



## Rare-earth region

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



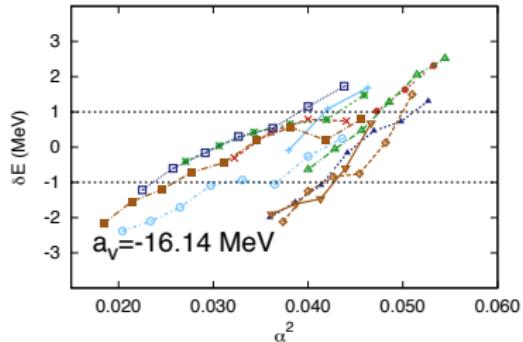
## Actinides

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

## Total

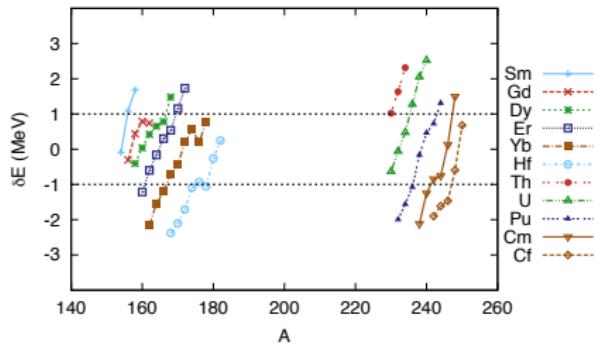
64 isotopes used in the fit

# 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

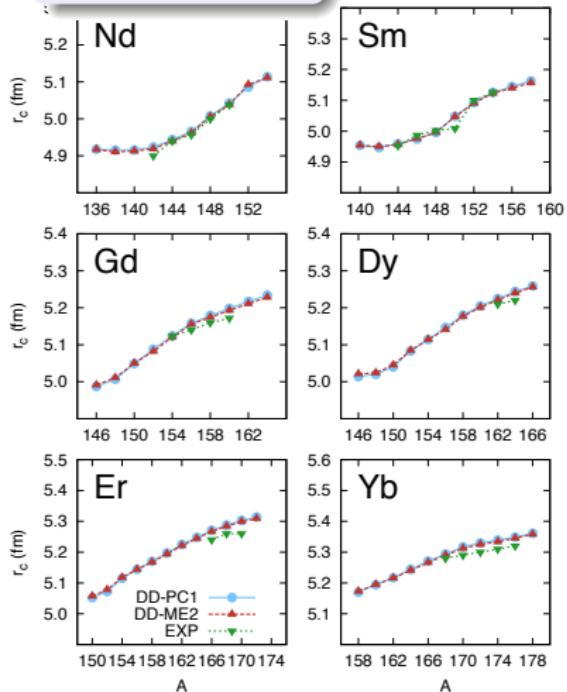
Th ( $Z=90$ ), U ( $Z=92$ ), Pu ( $Z=94$ ), Cm ( $Z=96$ ), Cf ( $Z=98$ )

## Total

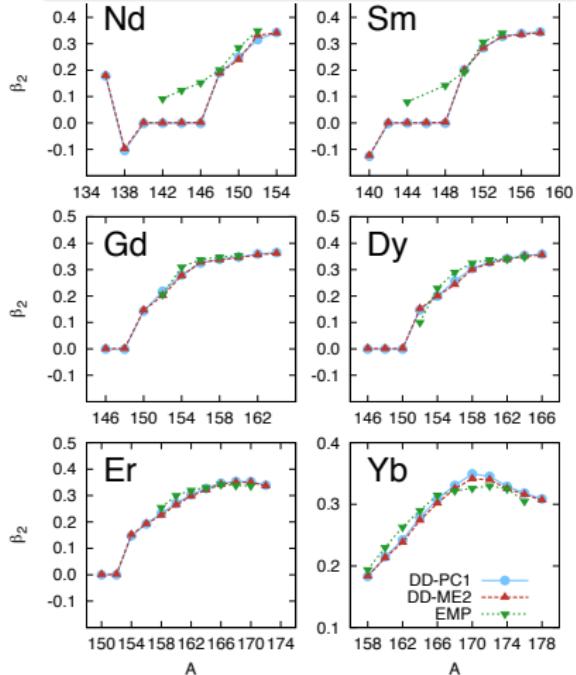
64 isotopes used in the fit

# Ground-state properties

## Charge radii

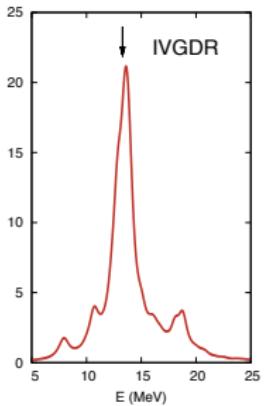
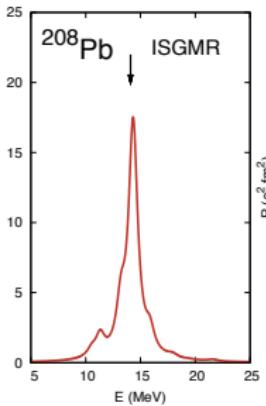
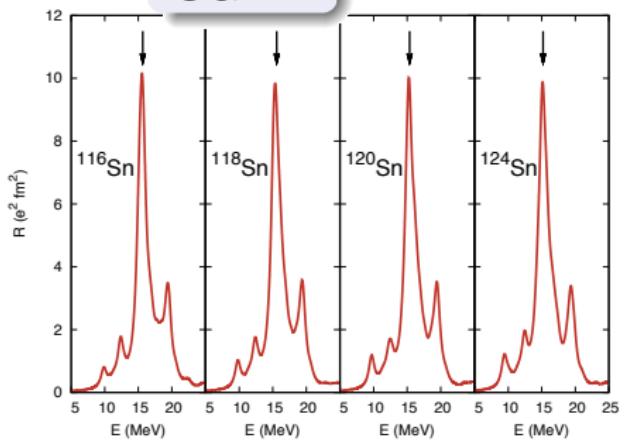


## Quadrupole deformations

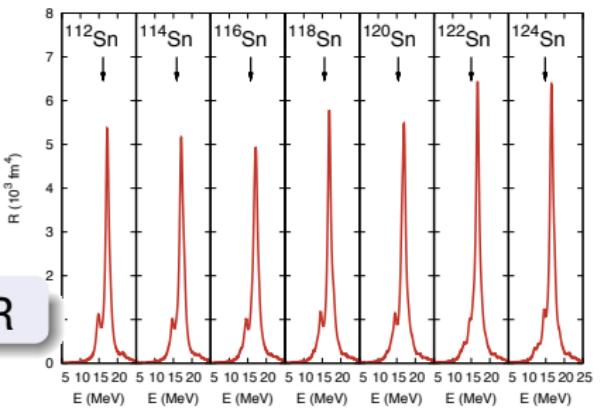


# Excitation energies of collective modes

ISGMR



IVGDR



# 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

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

The mass parameters are calculated in the cranking approximation .

# Implementation of the collective Hamiltonian model based on the SCRMF

## Collective Hamiltonian

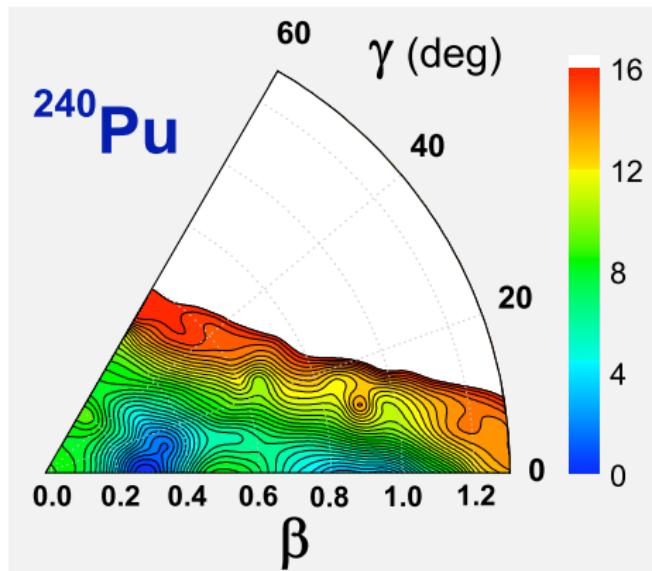
$$\mathcal{H}_{coll} = \mathcal{T}_{rot} + \mathcal{T}_{vib} + \mathcal{V}_{coll}$$

## Collective potential

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

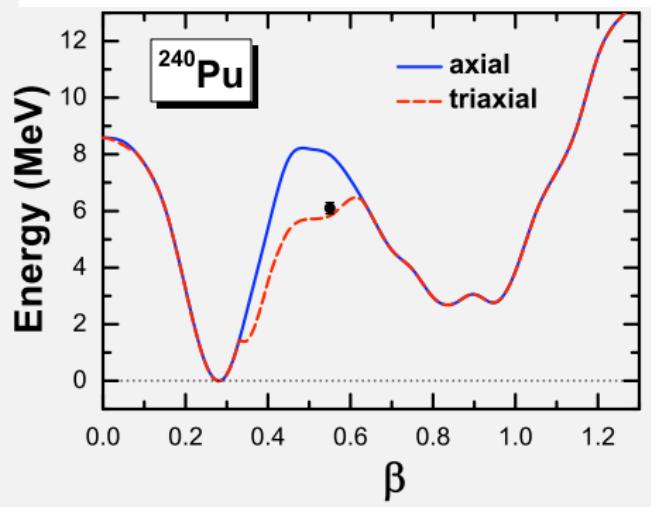
Corresponds to the mean-field potential energy surface with the zero point energy subtracted .

## Applications: $^{240}\text{Pu}$ isotope

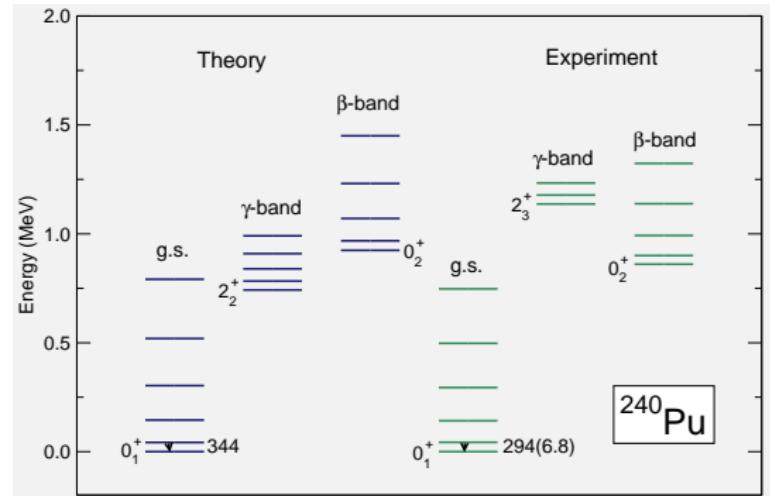


ND and SD minima are separated by the barrier.

Triaxial effects lower the barrier.



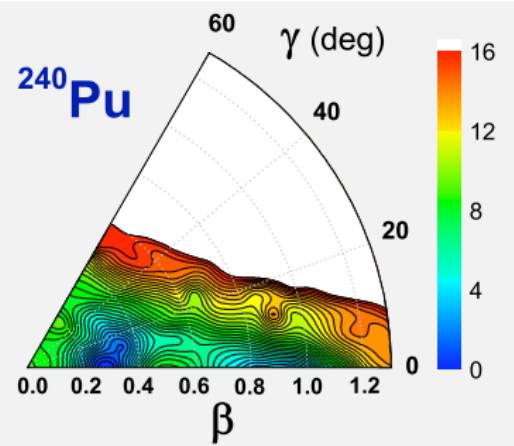
# Applications: $^{240}\text{Pu}$ isotope



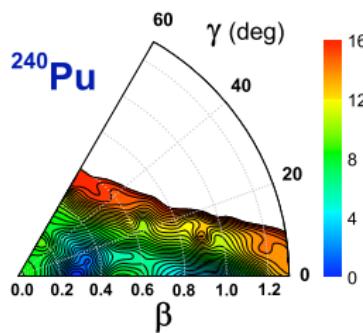
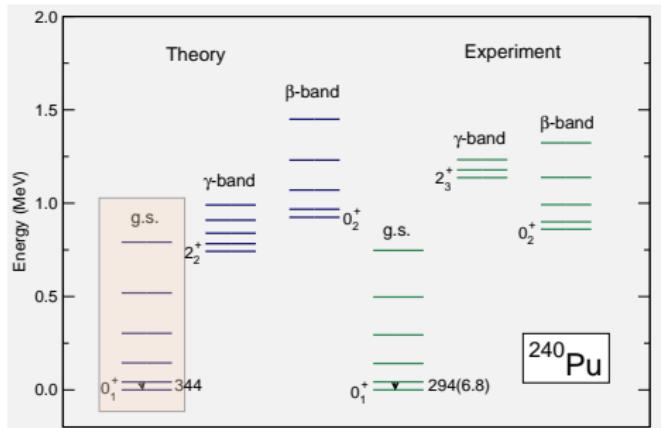
The moments of inertia are renormalized by factor  $\approx 1.3$  to compensate the difference between IB and TV moments of inertia.

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

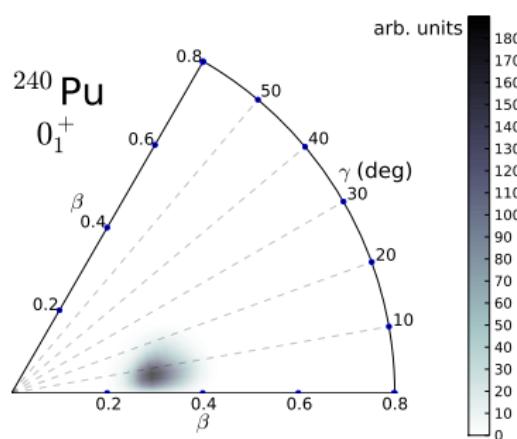
$$E_{4_1^+}^{exp}/E_{2_1^+}^{exp} = 3.31$$



# Applications: $^{240}\text{Pu}$ isotope

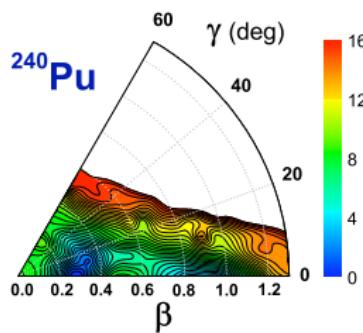
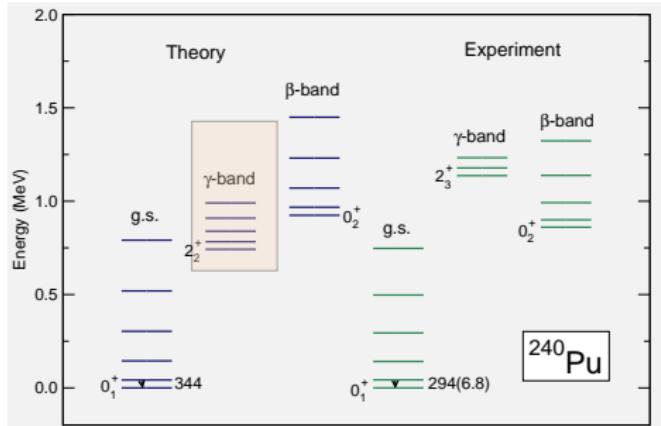


Probability distribution

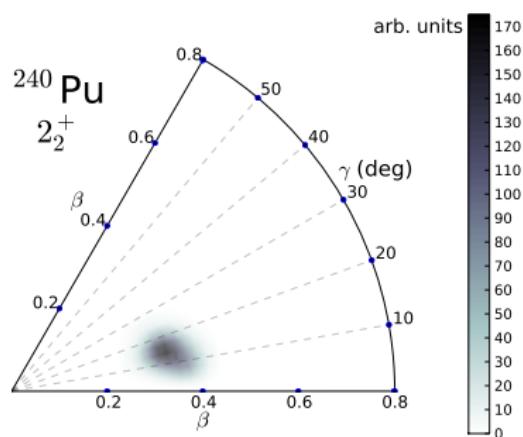


g.s. band head

# Applications: $^{240}\text{Pu}$ isotope

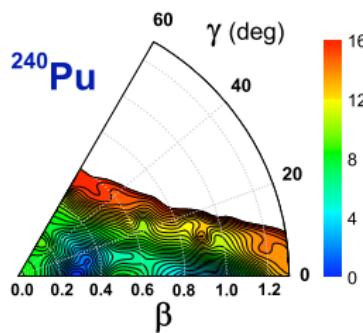
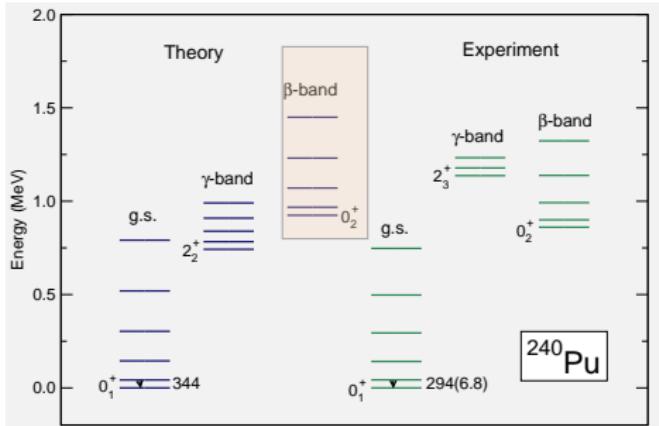


Probability distribution

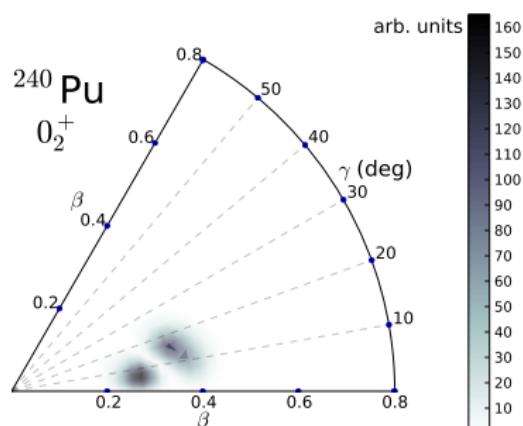


$\gamma$  band head

# Applications: $^{240}\text{Pu}$ isotope

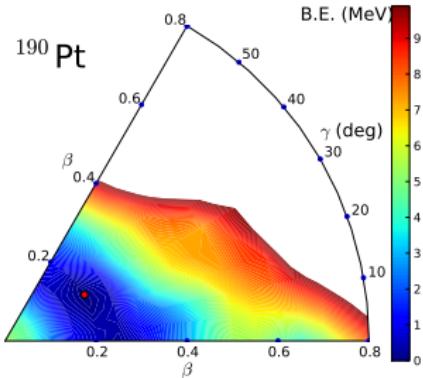


Probability distribution



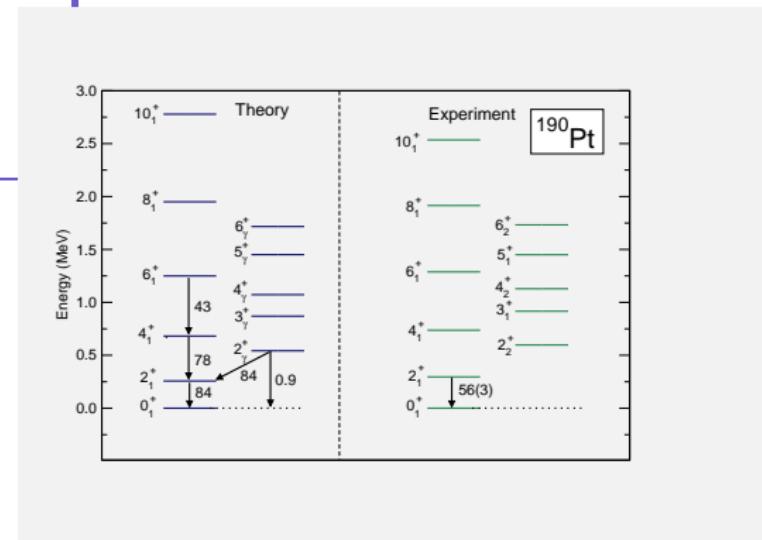
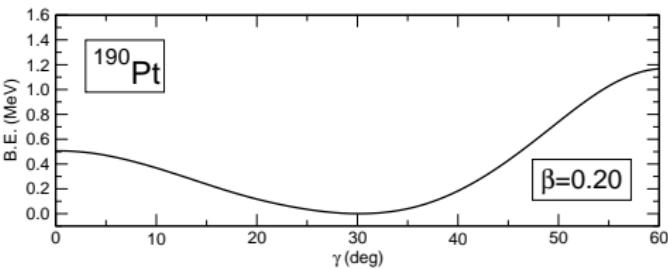
$\beta$  band head

# Applications: Pt isotopes

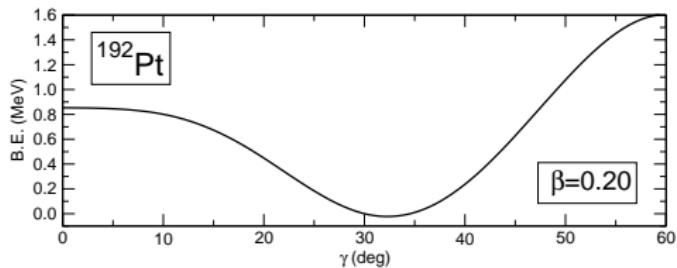
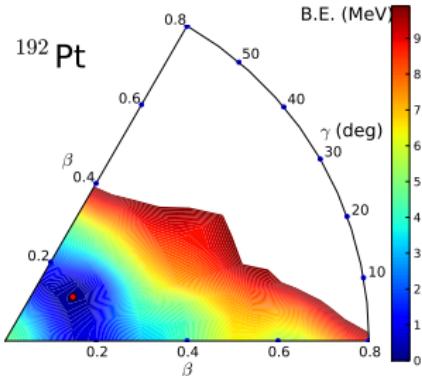


$$E_{4_1^+}^{th}/E_{2_1^+}^{th} = 2.39$$

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

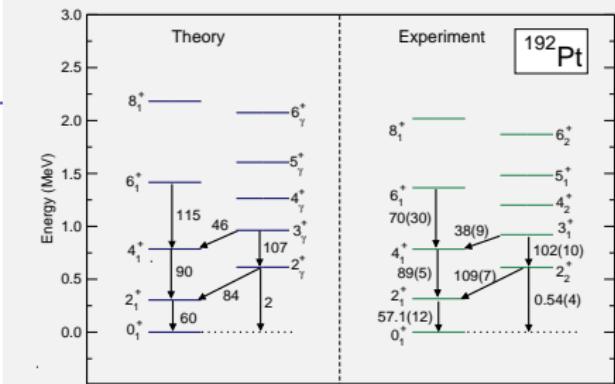


# Applications: Pt isotopes

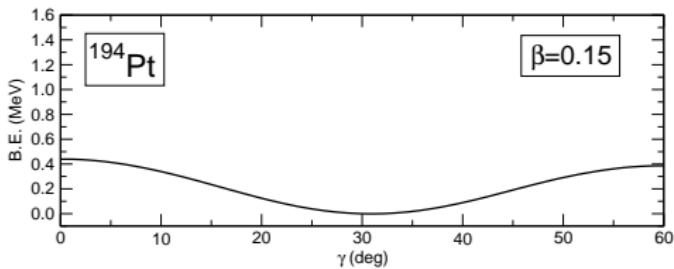
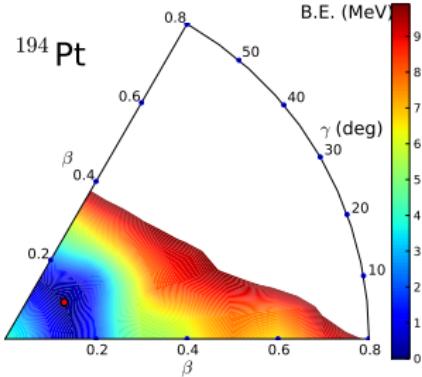


$$E_{4_1^+}^{th}/E_{2_1^+}^{th} = 2.58$$

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

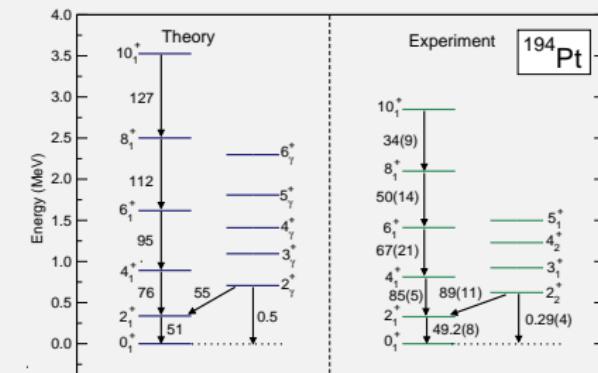


# Applications: Pt isotopes

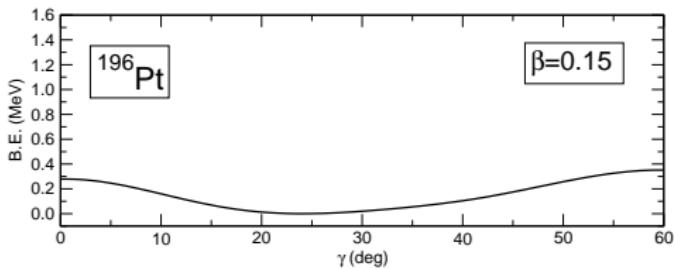
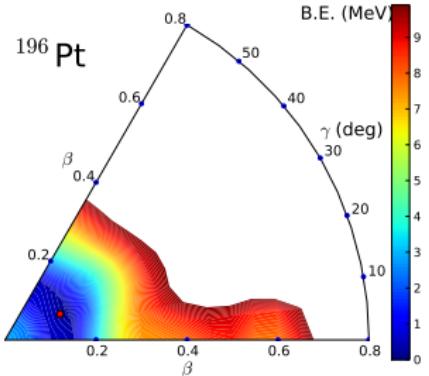


$$E_{4_1^+}^{th}/E_{2_1^+}^{th} = 2.63$$

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

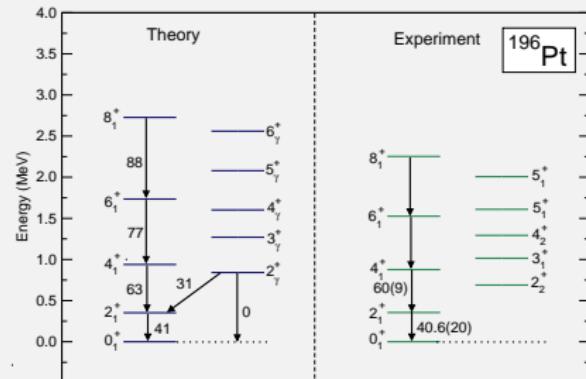


# Applications: Pt isotopes

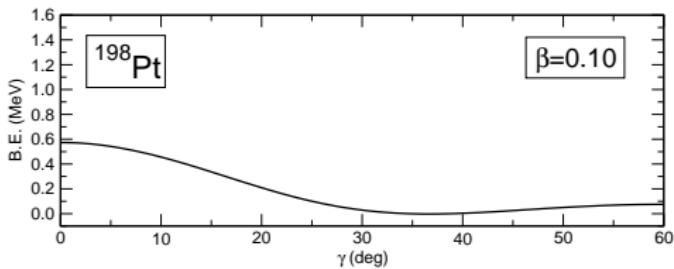
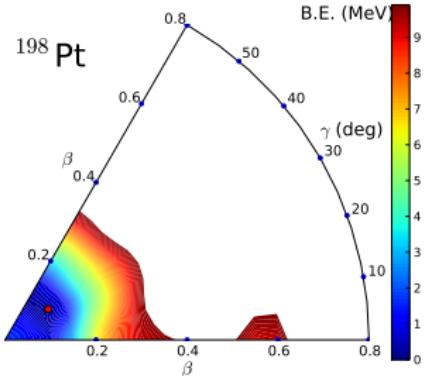


$$E_{4_1^+}^{th}/E_{2_1^+}^{th} = 2.66$$

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

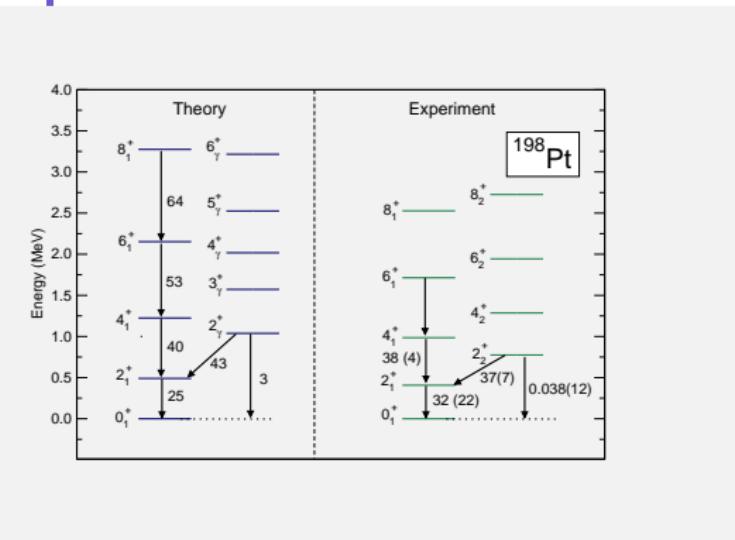


# Applications: Pt isotopes

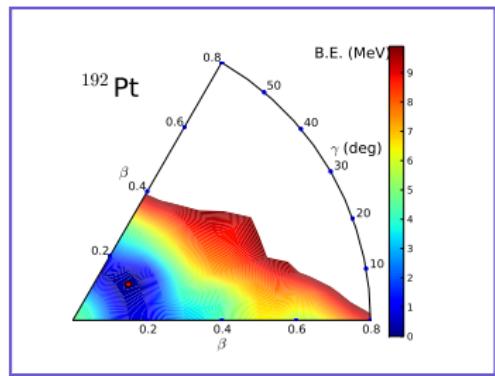
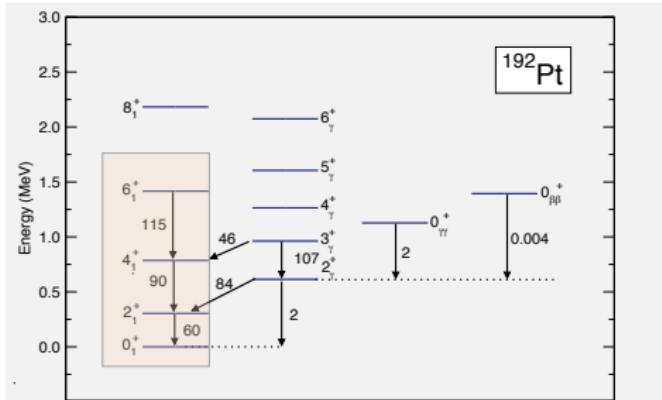


$$E_{4_1^+}^{th}/E_{2_1^+}^{th} = 2.49$$

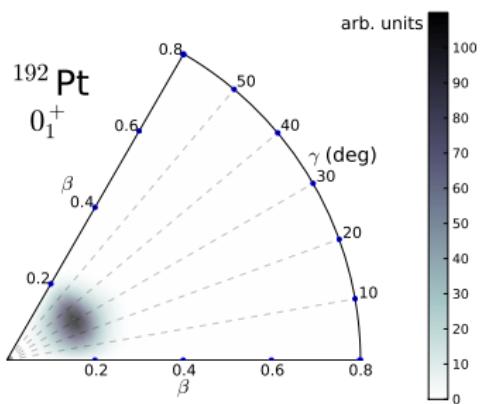
$$E_{4_1^+}^{exp}/E_{2_1^+}^{exp} = 2.42$$



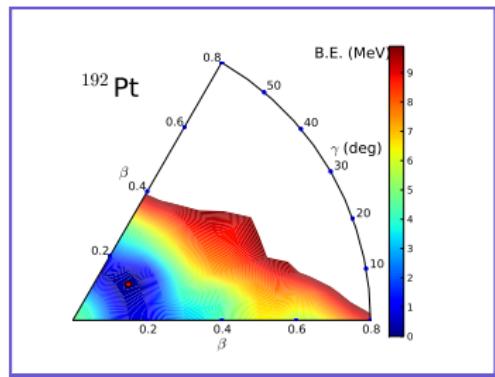
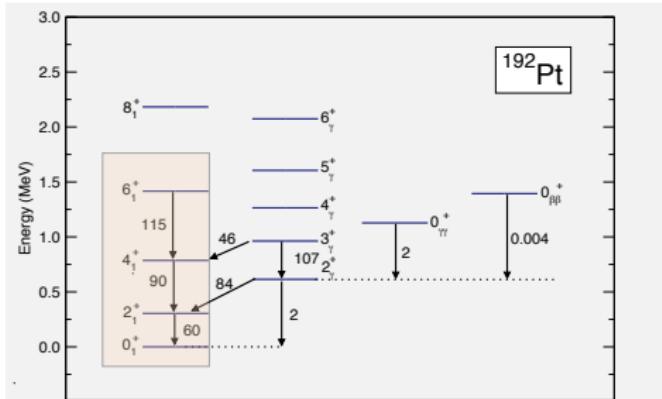
# Applications: $^{192}\text{Pt}$ isotope



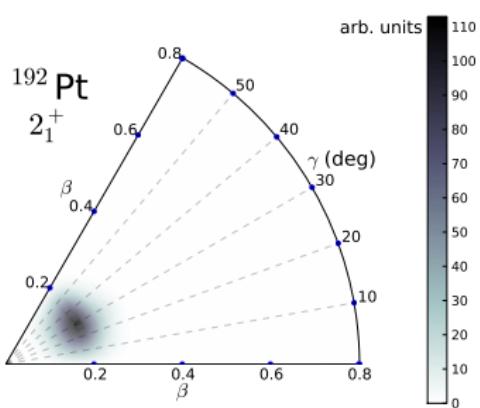
Collective probability



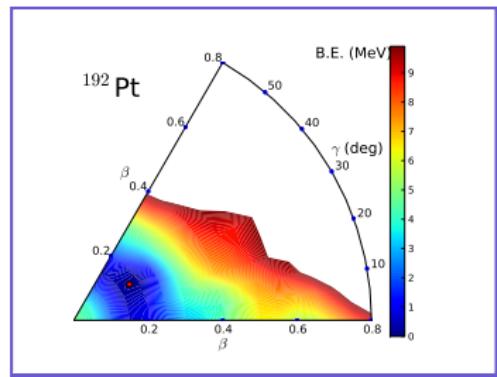
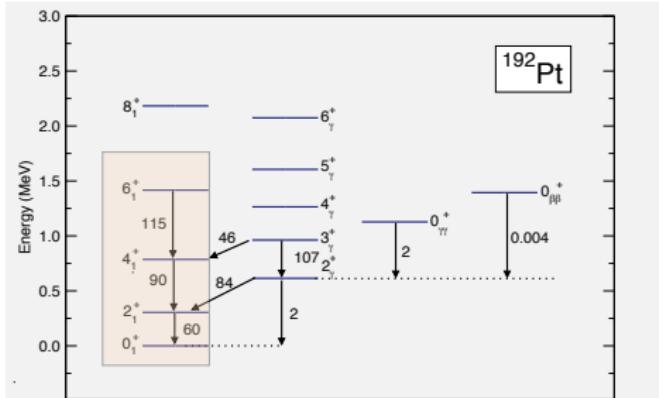
# Applications: $^{192}\text{Pt}$ isotope



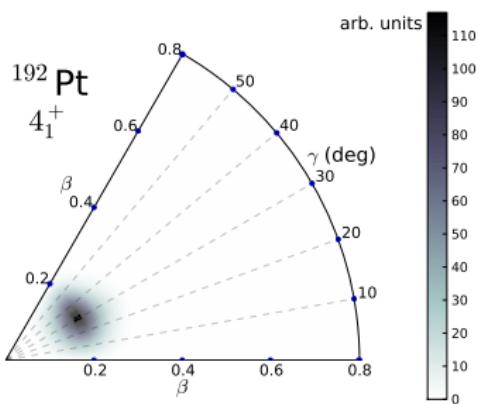
Collective probability



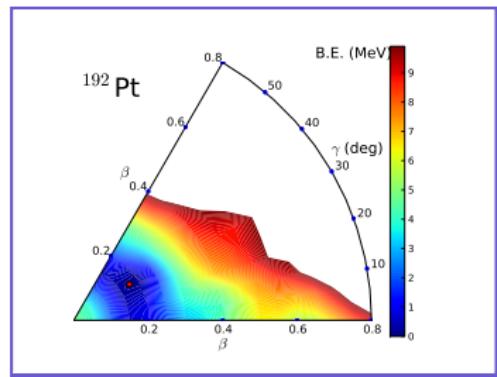
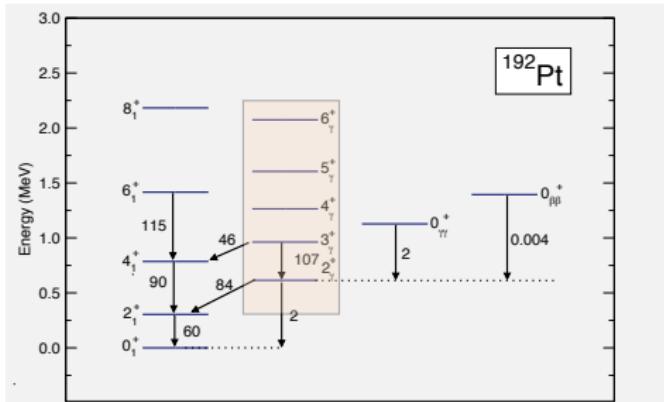
# Applications: $^{192}\text{Pt}$ isotope



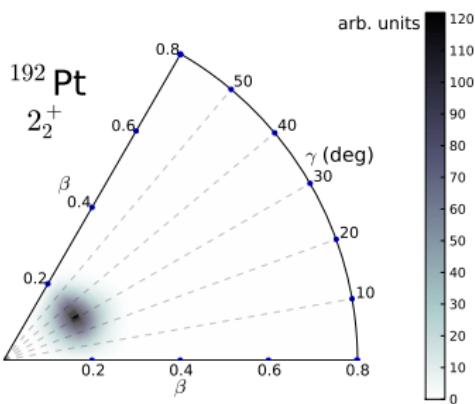
Collective probability



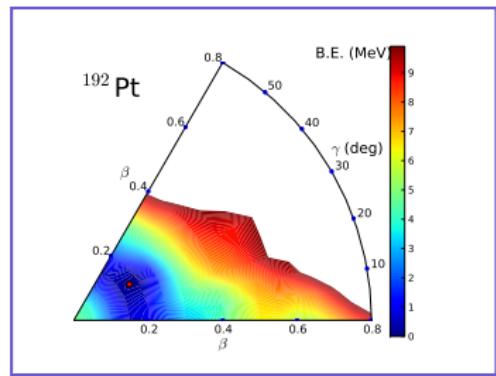
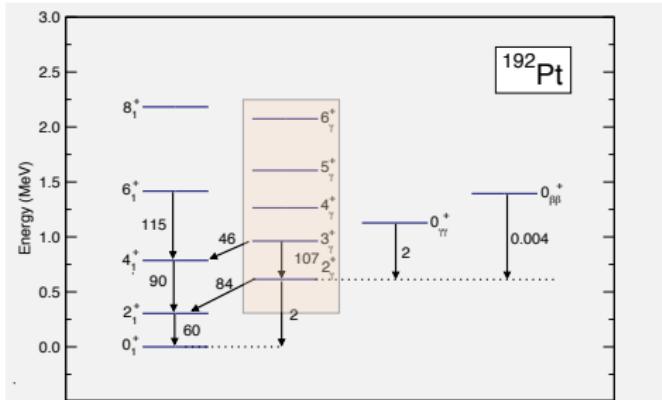
# Applications: $^{192}\text{Pt}$ isotope



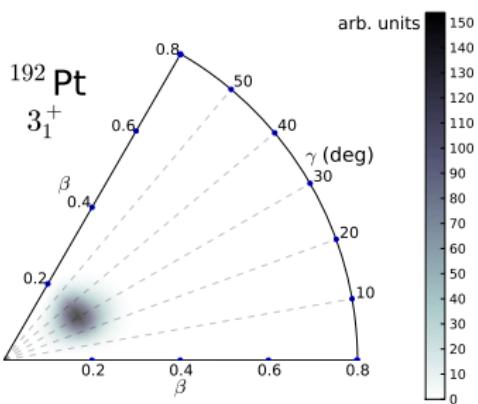
Collective probability



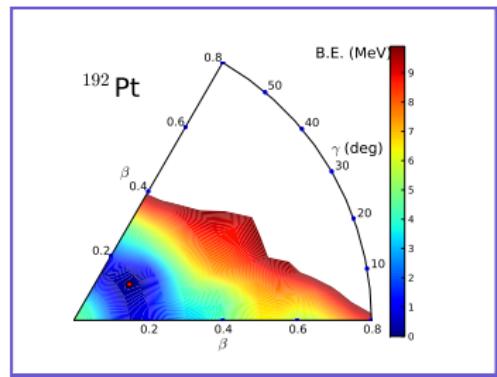
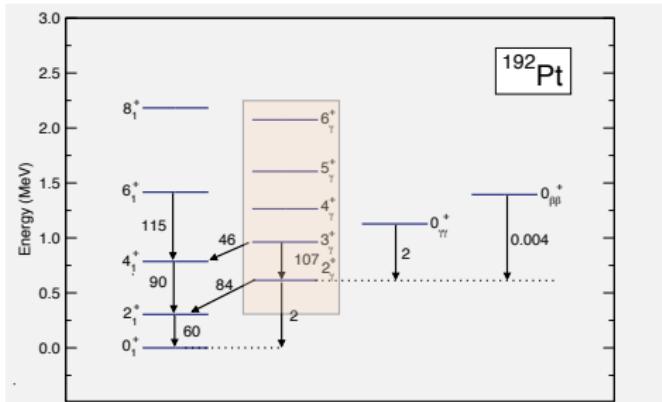
# Applications: $^{192}\text{Pt}$ isotope



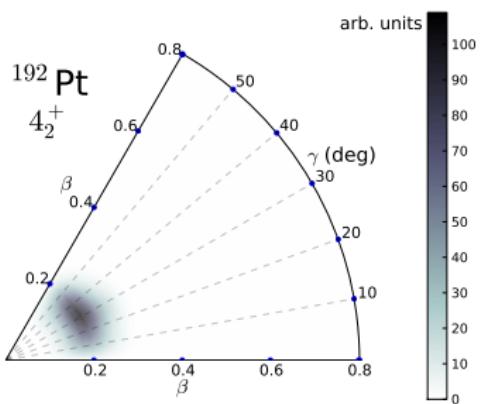
Collective probability



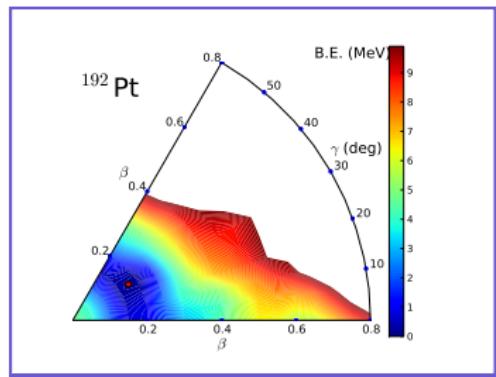
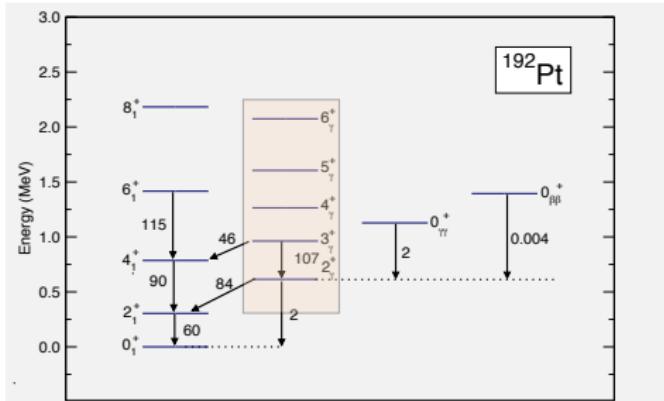
# Applications: $^{192}\text{Pt}$ isotope



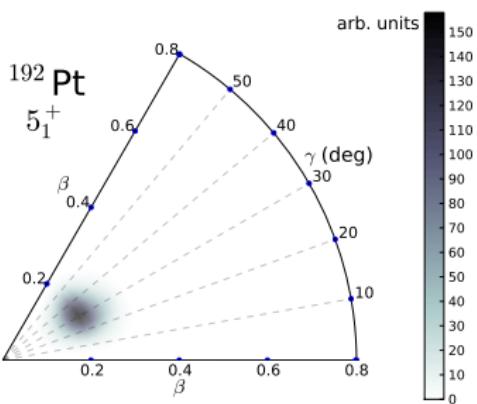
Collective probability



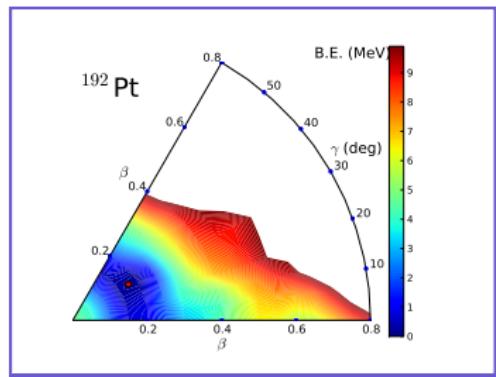
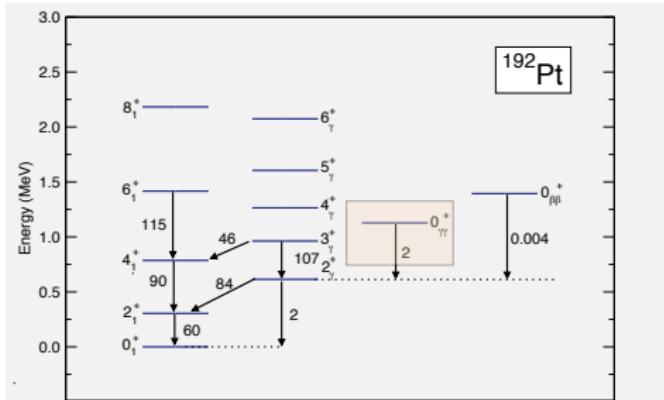
# Applications: $^{192}\text{Pt}$ isotope



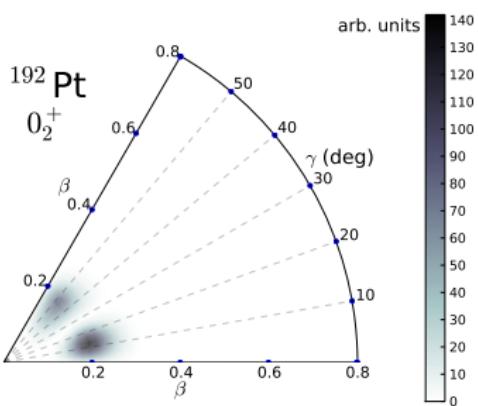
Collective probability



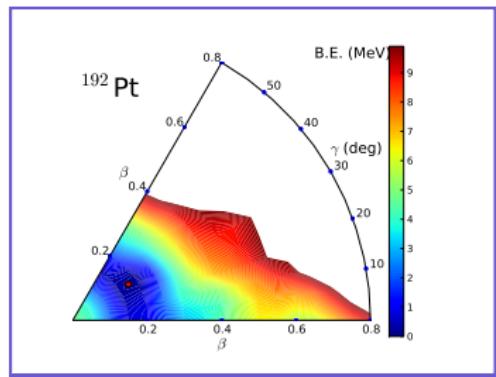
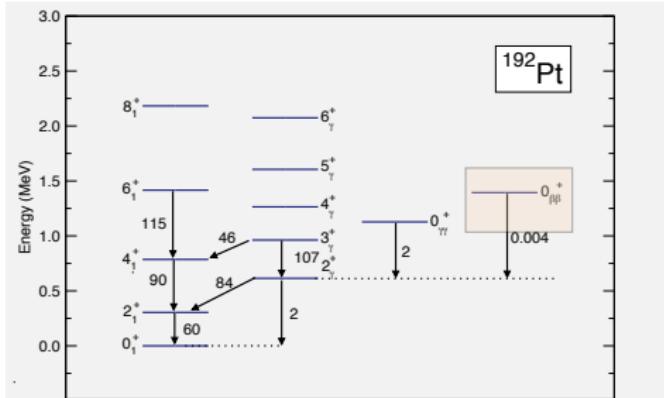
# Applications: $^{192}\text{Pt}$ isotope



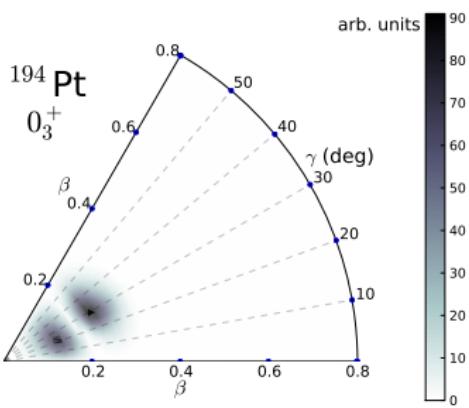
Collective probability



# Applications: $^{192}\text{Pt}$ isotope



Collective probability



# 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)