

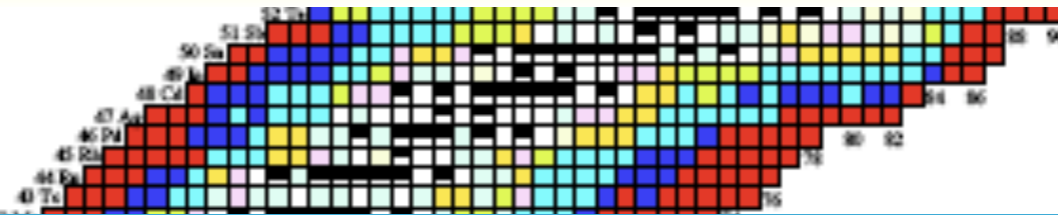
Relativistic Nuclear Energy Density Functionals: Masses and Ground-State Correlations

Dario Vretenar
University of Zagreb



Energy Density Functionals

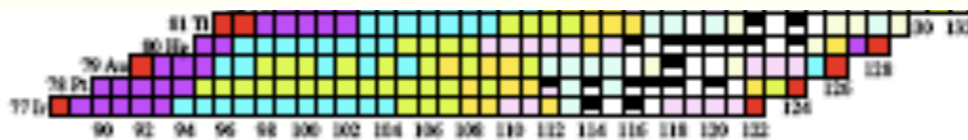
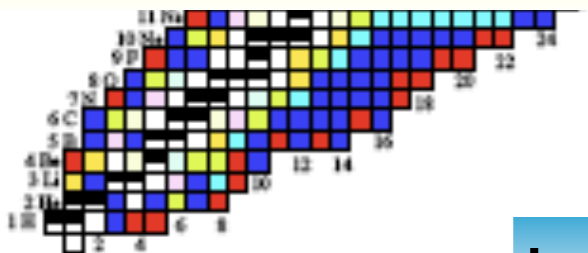
✓ the quantum many-body problem is mapped onto a **one-body problem** without explicitly involving inter-particle interactions!



✓ the exact density functional is approximated with **powers and gradients of ground-state densities and currents.**



✓ **universal density functionals** can be applied to all nuclei throughout the chart of nuclides.



Important for extrapolations to regions far from stability!

Kohn-Sham DFT

For any interacting system, there exists a local single-particle (Kohn-Sham) potential, such that the exact ground-state density equals the ground-state density of a non-interacting system:

$$n(\mathbf{r}) = n_s(\mathbf{r}) \equiv \sum_i^{occ} |\phi_i(\mathbf{r})|^2$$

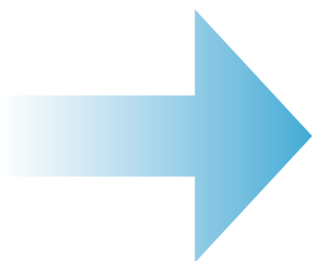
The single-particle orbitals are solutions of the Kohn-Sham equations:

$$\left[-\nabla^2/2 + v_s(\mathbf{r}) \right] \phi_i(\mathbf{r}) = \varepsilon_i \phi_i(\mathbf{r})$$

$$v_s[n(\mathbf{r})] = v(\mathbf{r}) + \int d^3r' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + v_{xc}[n(\mathbf{r})]$$

the **exchange-correlation potential** is defined by:

$$v_{xc}[n(\mathbf{r})] = \frac{\delta E_{xc}[n]}{\delta n(\mathbf{r})}$$

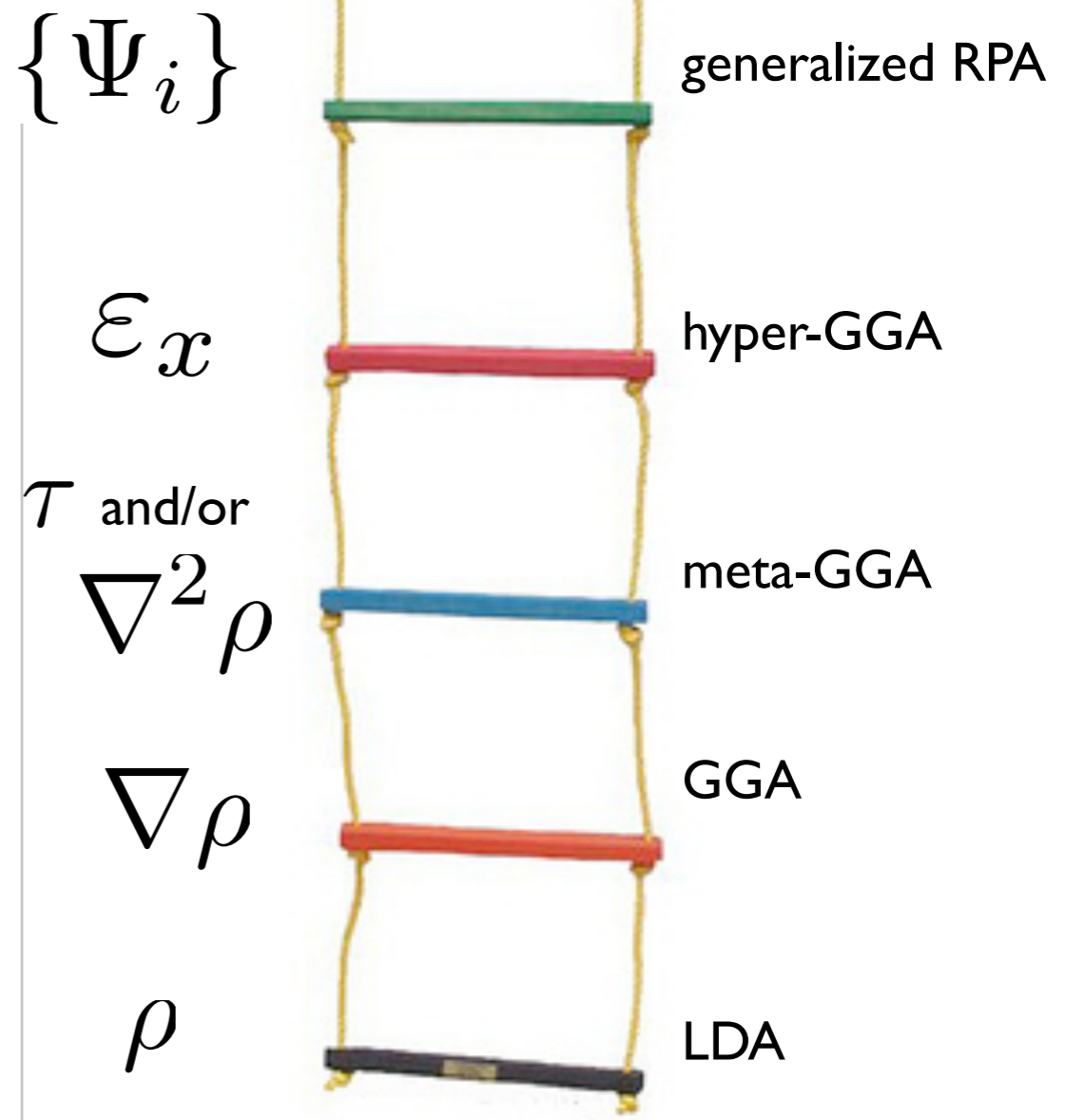
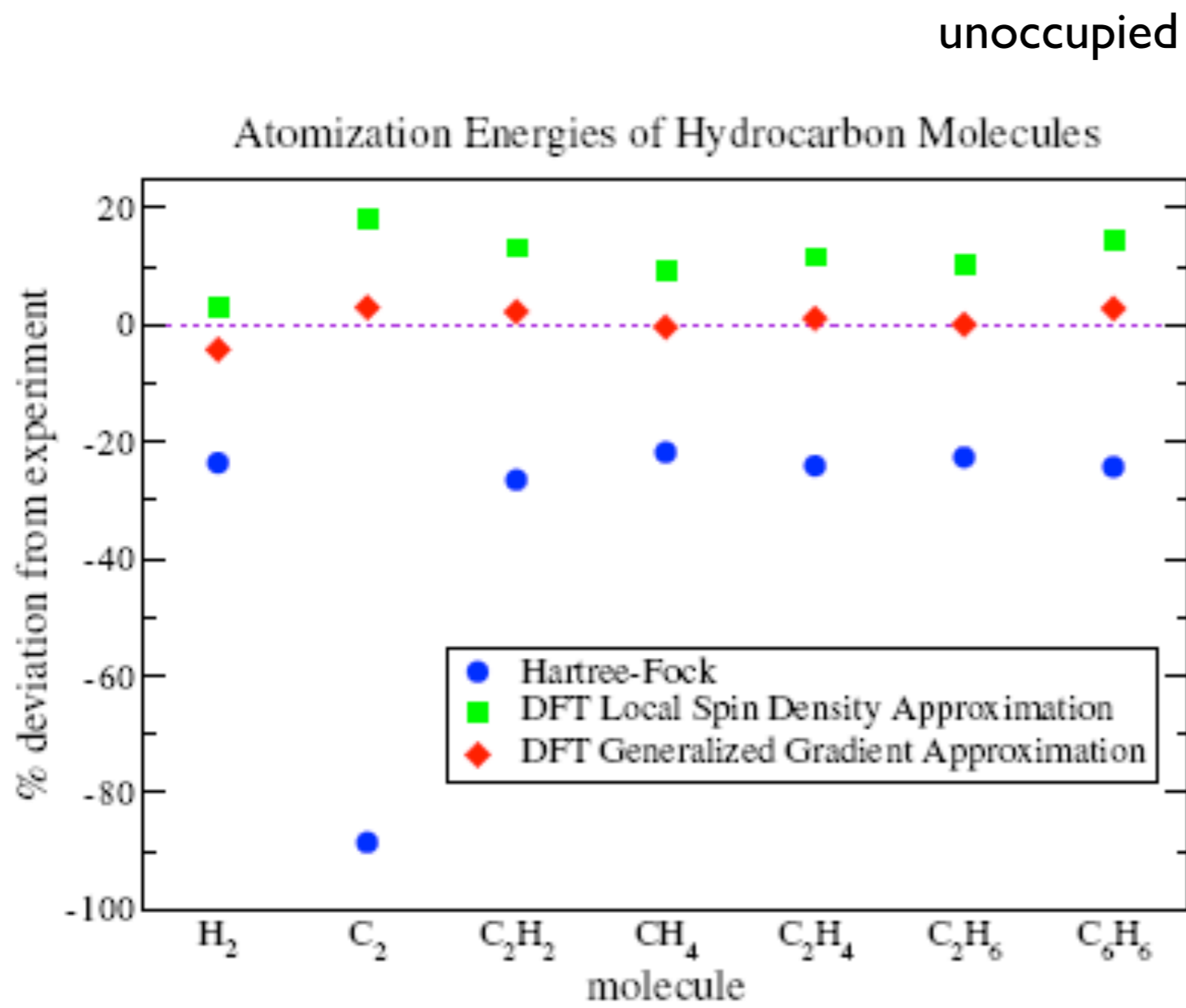


self-consistent Kohn-Sham DFT: includes correlations and therefore goes beyond the HF. It has the advantage of being a **local scheme**.

The practical usefulness of the Kohn-Sham scheme depends entirely on whether accurate approximations for E_{xc} can be found!

Exchange-correlation functional:

Heaven of chemical accuracy



Hartree world

Jacob's ladder of DFT approximations for E_{xc}

TABLE I. Atomization energies of molecules, in kcal/mol (1 eV = 23.06 kcal/mol). E_{XC} has been evaluated on self-consistent densities at experimental geometries [33]. Nonspherical densities and Kohn-Sham potentials have been used for open-shell atoms [34]. The calculations are performed with a modified version of the CADPAC program [35]. The experimental values for ΔE (with zero point vibration removed) are taken from Ref. [36]. PBE is the simplified GGA proposed here. UHF is unrestricted Hartree-Fock, for comparison.

System	ΔE^{UHF}	ΔE^{LSD}	ΔE^{PW91}	ΔE^{PBE}	ΔE^{expt}
H ₂	84	113	105	105	109
LiH	33	60	53	52	58
CH ₄	328	462	421	420	419
NH ₃	201	337	303	302	297
OH	68	124	110	110	107
H ₂ O	155	267	235	234	232
HF	97	162	143	142	141
Li ₂	3	23	20	19	24
LiF	89	153	137	136	139
Be ₂	-7	13	10	10	3
C ₂ H ₂	294	460	415	415	405
C ₂ H ₄	428	633	573	571	563
HCN	199	361	326	326	312
CO	174	299	269	269	259
N ₂	115	267	242	243	229
NO	53	199	171	172	153
O ₂	33	175	143	144	121
F ₂	-37	78	54	53	39
P ₂	36	142	120	120	117
Cl ₂	17	81	64	63	58
Mean abs. error	71.2	31.4	8.0	7.9	...

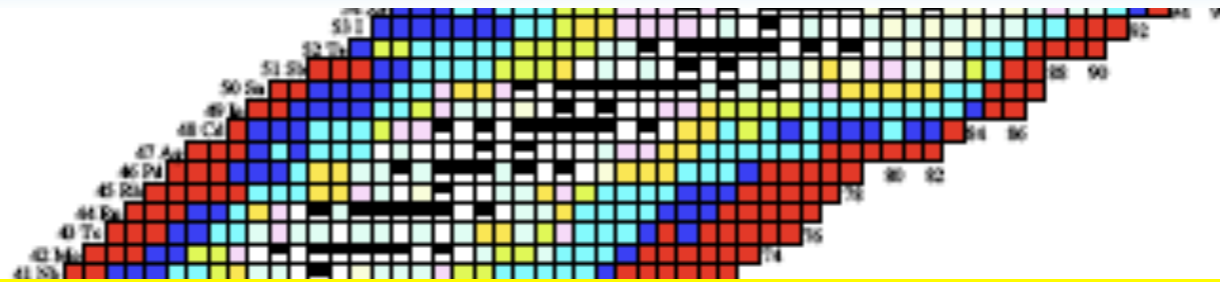
Mean absolute error of the atomization energies for 20 molecules, evaluated using various approximations:

Approximation	Mean abs. error (eV)
Unrestricted Hartree-Fock	3.1 (underbinding)
LDA	1.3 (overbinding)
GGA	0.3 (mostly overbinding)
Desired “chemical accuracy”	0.05

⇒ Multiply by **10⁶** and compare with the nuclear case!

Relativistic Energy Density Functionals

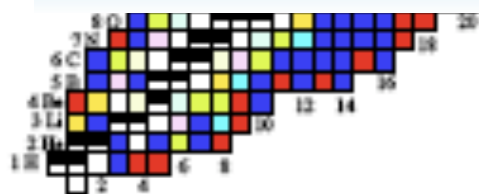
✓ natural inclusion of the **spin degree of freedom** (spin-orbit potential with empirical strength)



✓ unique parameterization of **time-odd components** (currents) of the nuclear mean-field



✓ the distinction between scalar and vector self-energies leads to a natural **saturation mechanism for nuclear matter**



Relativistic energy density functionals:

The elementary building blocks are two-fermion terms of the general type:

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

... isoscalar and isovector four-currents and scalar densities:

$$\begin{aligned} j_\mu &= \langle \phi_0 | \bar{\psi} \gamma_\mu \psi | \phi_0 \rangle = \sum_k \bar{\psi}_k \gamma_\mu \psi_k , \\ \vec{j}_\mu &= \langle \phi_0 | \bar{\psi} \gamma_\mu \vec{\tau} \psi | \phi_0 \rangle = \sum_k \bar{\psi}_k \gamma_\mu \vec{\tau} \psi_k , \\ \rho_S &= \langle \phi_0 | \bar{\psi} \psi | \phi_0 \rangle = \sum_k \bar{\psi}_k \psi_k , \\ \vec{\rho}_S &= \langle \phi_0 | \bar{\psi} \vec{\tau} \psi | \phi_0 \rangle = \sum_k \bar{\psi}_k \vec{\tau} \psi_k \end{aligned}$$

where $|\phi_0\rangle$ is the nuclear ground state.

Four-fermion (contact) interaction terms in the various isospace-space channels:

isoscalar-scalar:	$(\bar{\psi}\psi)^2$
isoscalar-vector:	$(\bar{\psi}\gamma_\mu\psi)(\bar{\psi}\gamma^\mu\psi)$
isovector-scalar:	$(\bar{\psi}\vec{\tau}\psi) \cdot (\bar{\psi}\vec{\tau}\psi)$
isovector-vector:	$(\bar{\psi}\vec{\tau}\gamma_\mu\psi) \cdot (\bar{\psi}\vec{\tau}\gamma^\mu\psi)$

Empirical ground-state properties of finite nuclei can only determine a small set of parameters in the expansion of an effective Lagrangian in powers of fields and their derivatives.

Already at lowest order one finds more parameters than can be uniquely determined from data.

Effective Lagrangian:

$$\begin{aligned}\mathcal{L} = & \bar{\psi}(i\gamma \cdot \partial - m)\psi \\ & - \frac{1}{2}\alpha_S(\hat{\rho})(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\hat{\rho})(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi) \\ & - \frac{1}{2}\alpha_{TV}(\hat{\rho})(\bar{\psi}\vec{\tau}\gamma^\mu\psi)(\bar{\psi}\vec{\tau}\gamma_\mu\psi) \\ & - \frac{1}{2}\delta_S(\partial_\nu\bar{\psi}\psi)(\partial^\nu\bar{\psi}\psi) - e\bar{\psi}\gamma \cdot A\frac{(1-\tau_3)}{2}\psi\end{aligned}$$

$$\alpha_i(\rho) = a_i + (b_i + c_i x)e^{-d_i x} \quad (i \equiv S, V, TV) \quad x = \rho/\rho_{sat}$$

Hartree

correlations

Only one isovector term and one derivative term can be constrained by data.

Microscopic functionals

... universal exchange-correlation functional $E_{xc}[\rho]$

1st step: **Local Density Approximation**

$$E_{xc}^{LDA} \equiv \int \varepsilon^{ChPT}[\rho(\mathbf{r})] \rho(\mathbf{r}) d^3r$$

2nd step: **second-order gradient correction to the LDA**

EFT calculations for inhomogeneous nuclear matter:

$$\mathcal{E}(\rho, \nabla\rho) = \rho \bar{E}(k_f) + (\nabla\rho)^2 F_{\nabla}(k_f) + \dots$$

Semi-phenomenological functionals

Infinite nuclear matter cannot determine the density functional on the level of accuracy that is needed for a quantitative description of structure phenomena in finite nuclei.

... start from a favorite microscopic nuclear matter EOS

... the parameters of the functional are fine-tuned to data of finite nuclei

DD-PC1

... starts from microscopic nucleon self-energies in nuclear matter.

... parameters adjusted in self-consistent mean-field calculations of masses of **64** axially deformed nuclei in the mass regions $A \sim 150-180$ and $A \sim 230-250$.

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

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

... generate families of effective interactions characterized by different values of a_v , a_s and a_4 , and determine which parametrization minimizes the deviation from the empirical binding energies of a large set of deformed nuclei.

Nikšić, Vretenar, and Ring, Phys. Rev. C **78**, 034318 (2008)

The nuclear matter saturation density, compression modulus, and Dirac mass are kept fixed:

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

$$m_D^* = m + \Sigma_S = 0.58m$$

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

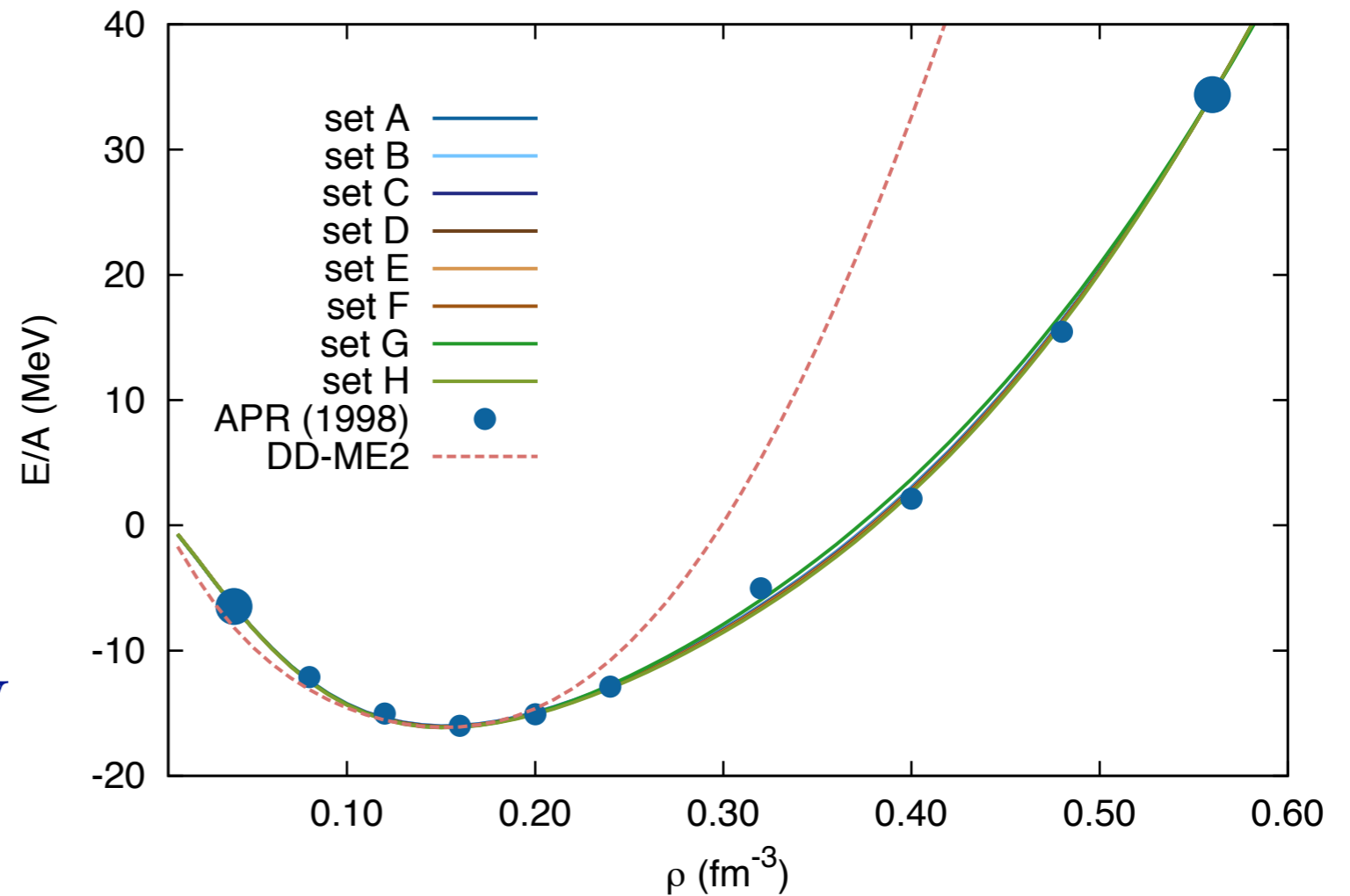
DD-ME1, DD-ME2

data on GMR

... plus two additional points on the microscopic EoS curve of Akmal, Pandharipande and Ravenhall:

$$\rho = 0.56 \text{ fm}^{-3} \quad E = 34.39 \text{ MeV}$$

$$\rho = 0.04 \text{ fm}^{-3} \quad E = -6.48 \text{ MeV}$$



$a_v = -16.02$ (A), -16.04 (B), -16.06 (C), ..., -16.14 (H) MeV

Isovector channel:
$$S_2(\rho) = a_4 + \frac{p_0}{\rho_{sat}^2} (\rho - \rho_{sat}) + \frac{\Delta K_0}{18\rho_{sat}^2} (\rho - \rho_{sat})^2 + \dots$$

... fix $a_4 = 33$ MeV and vary $S_2(\rho = 0.12 \text{ fm}^{-3})$

Deformed nuclei

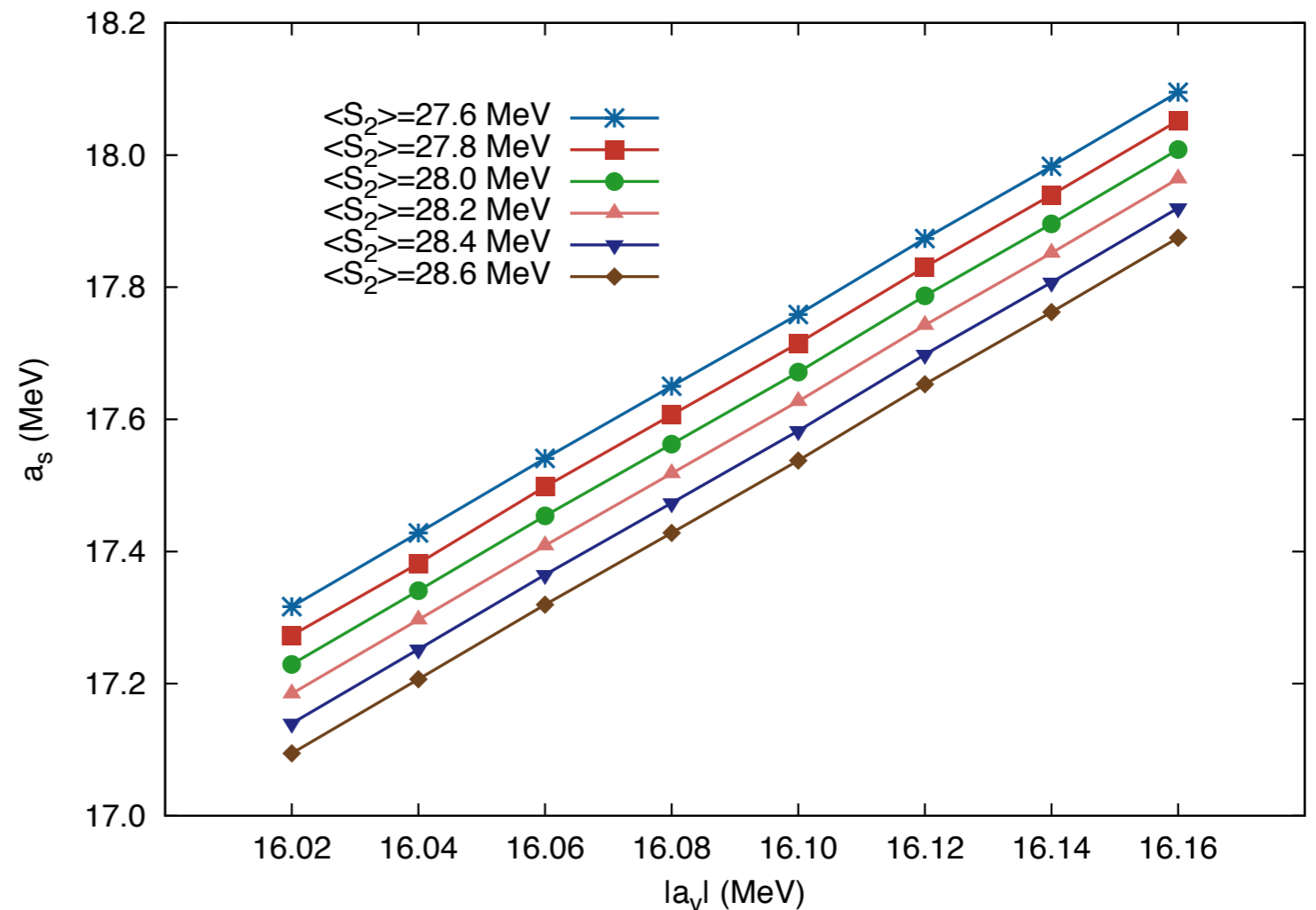
Binding energies used to adjust the parameters of the functional:

Z	62	64	66	68	70	72	90	92	94	96	98
N_{min}	92	92	92	92	92	72	140	138	138	142	144
N_{max}	96	98	102	104	108	110	144	148	150	152	152

Pairing correlations:
BCS with empirical pairing gaps.

Surface energies of semi-infinite nuclear matter that minimize the deviation of the calculated binding energies from data.

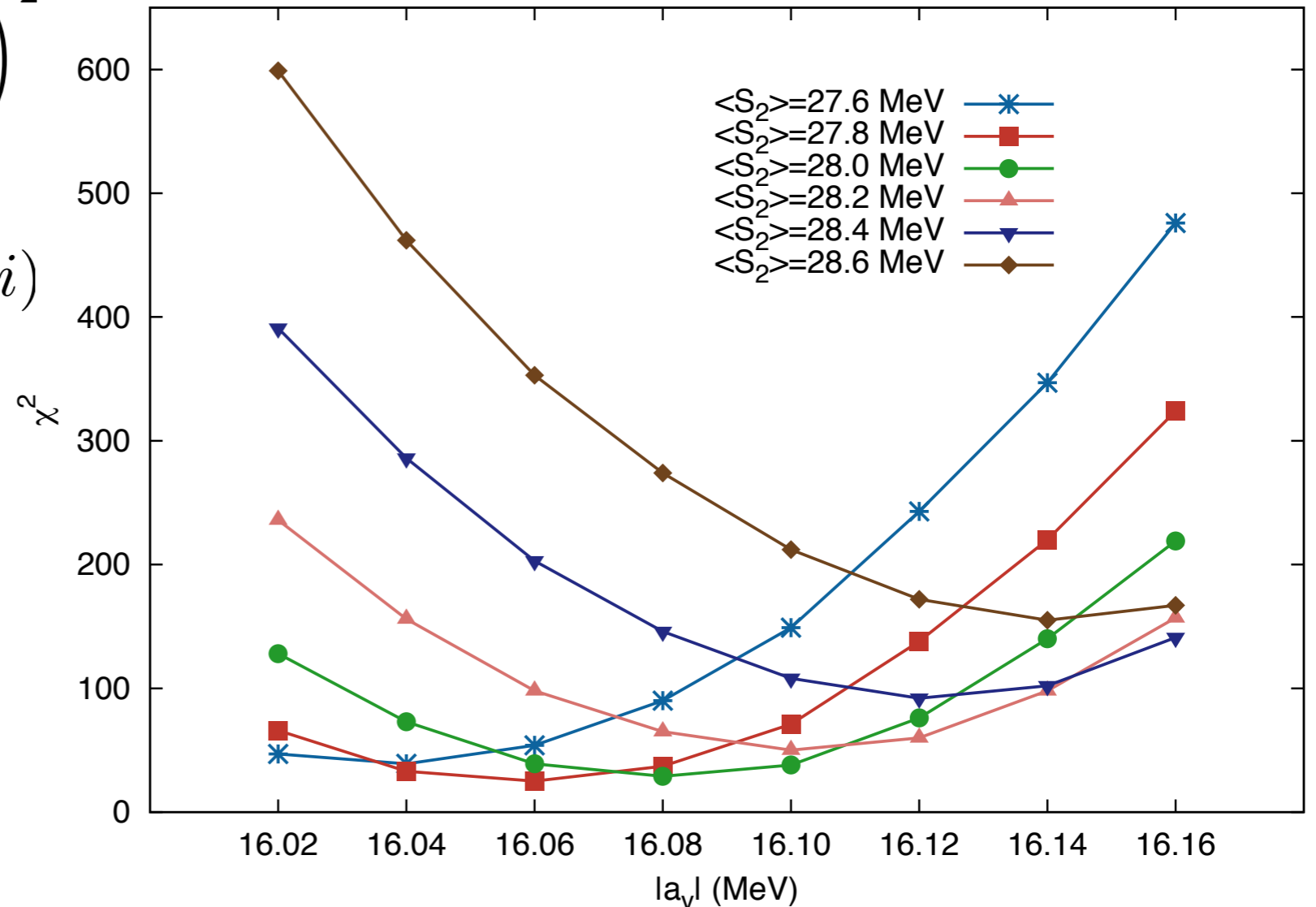
Required accuracy **0.05%** \Rightarrow absolute error of ± 1 MeV for the total binding energy



... 48 parameterizations of the energy density functional:

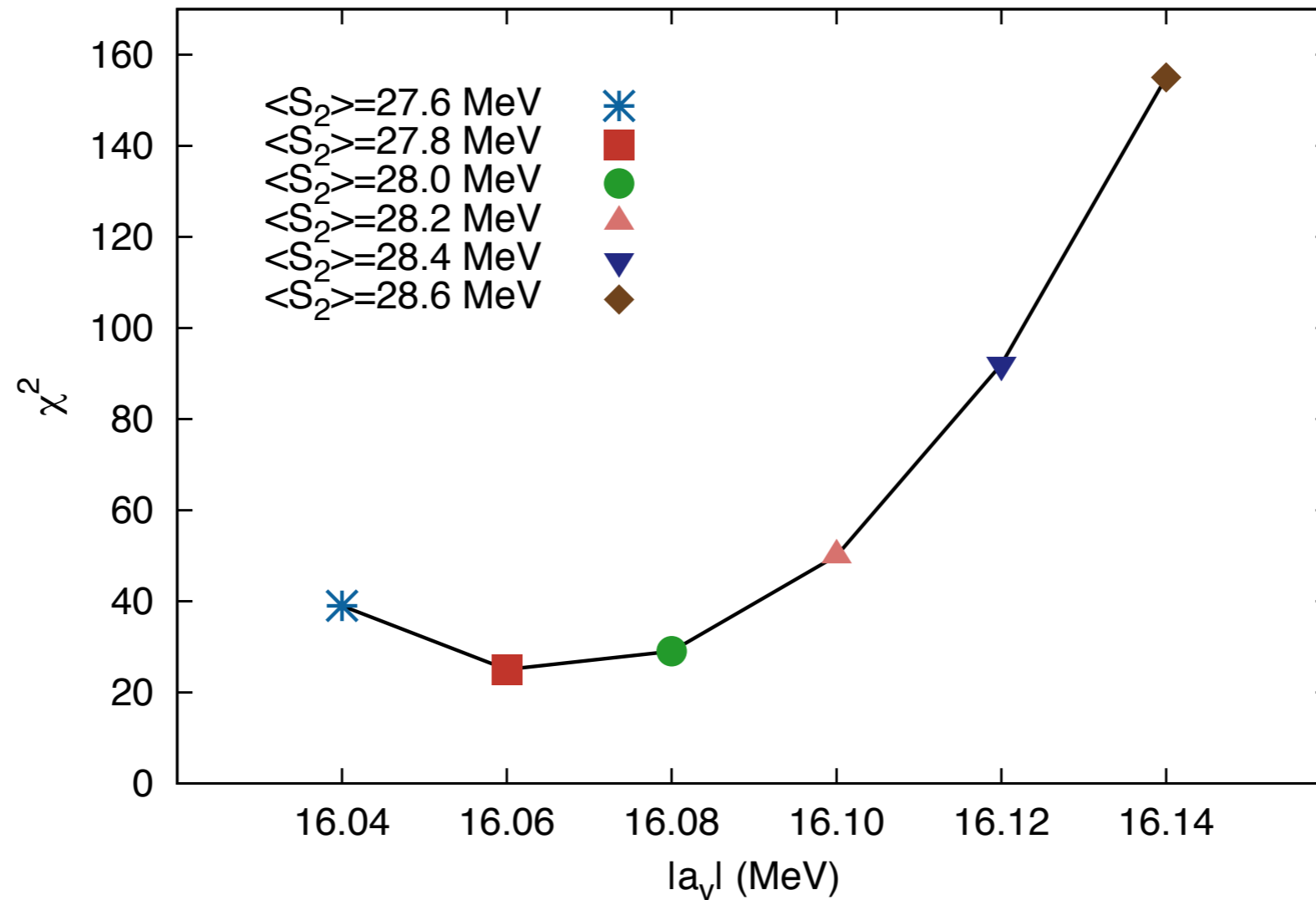
$$\chi^2 = \sum_i \left(\frac{E_B^{th}(i) - E_B^{exp}(i)}{\Delta E_B^{exp}(i)} \right)^2$$

$$\Delta E_B^{exp}(i) = 0.0005 E_B^{exp}(i)$$



For each value $\langle S_2 \rangle$ of the symmetry energy, there is a unique combination of volume and surface energies that minimizes χ^2 .

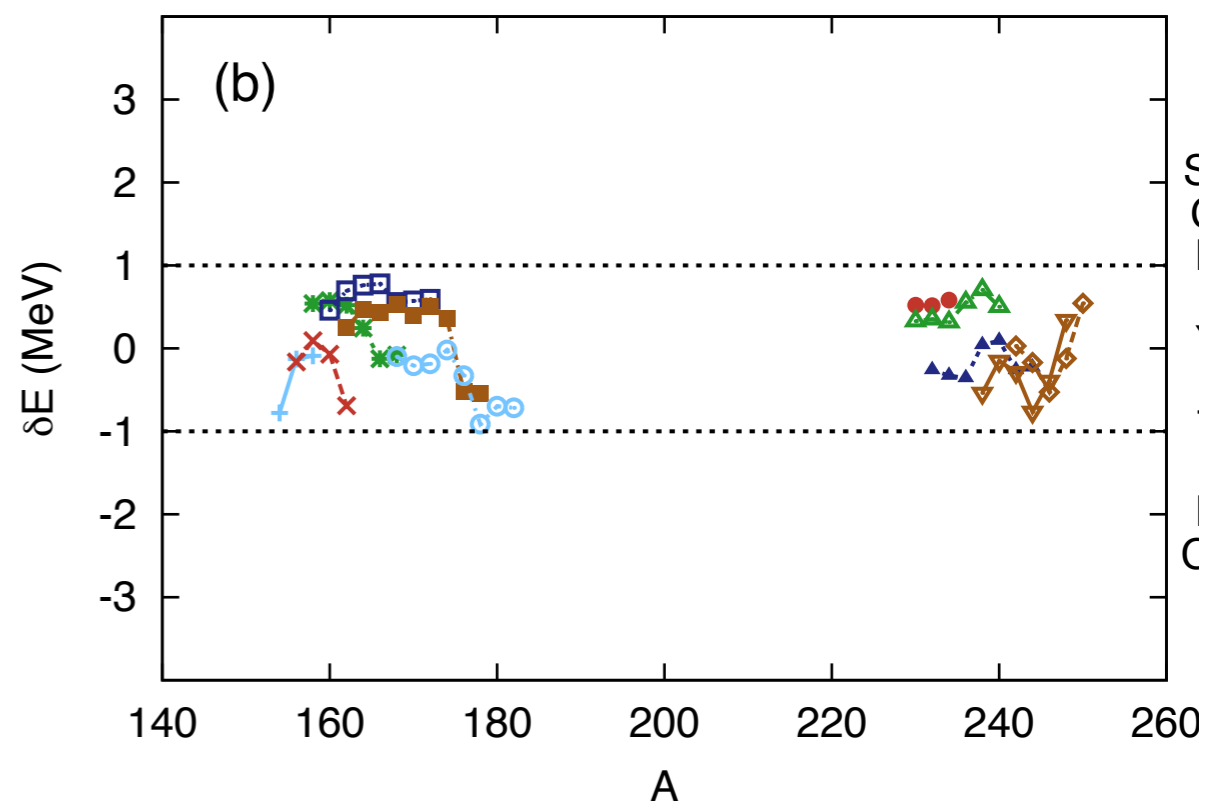
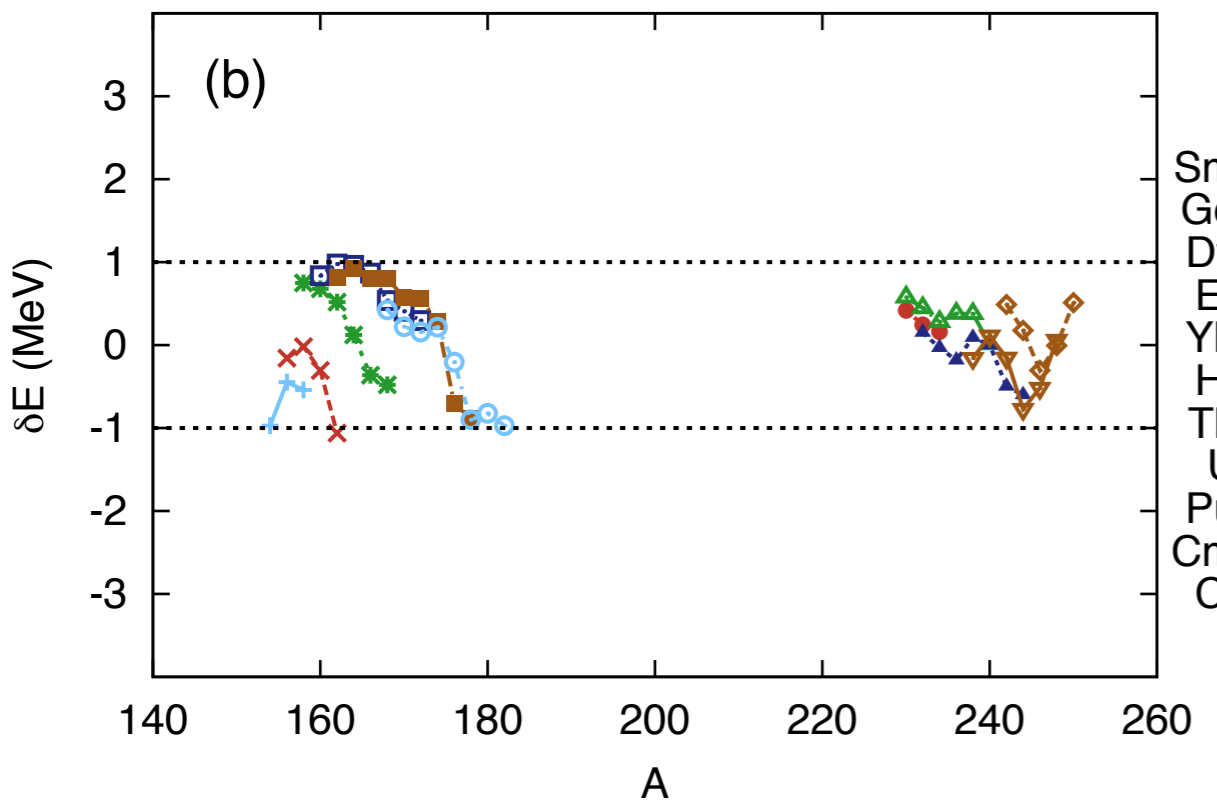
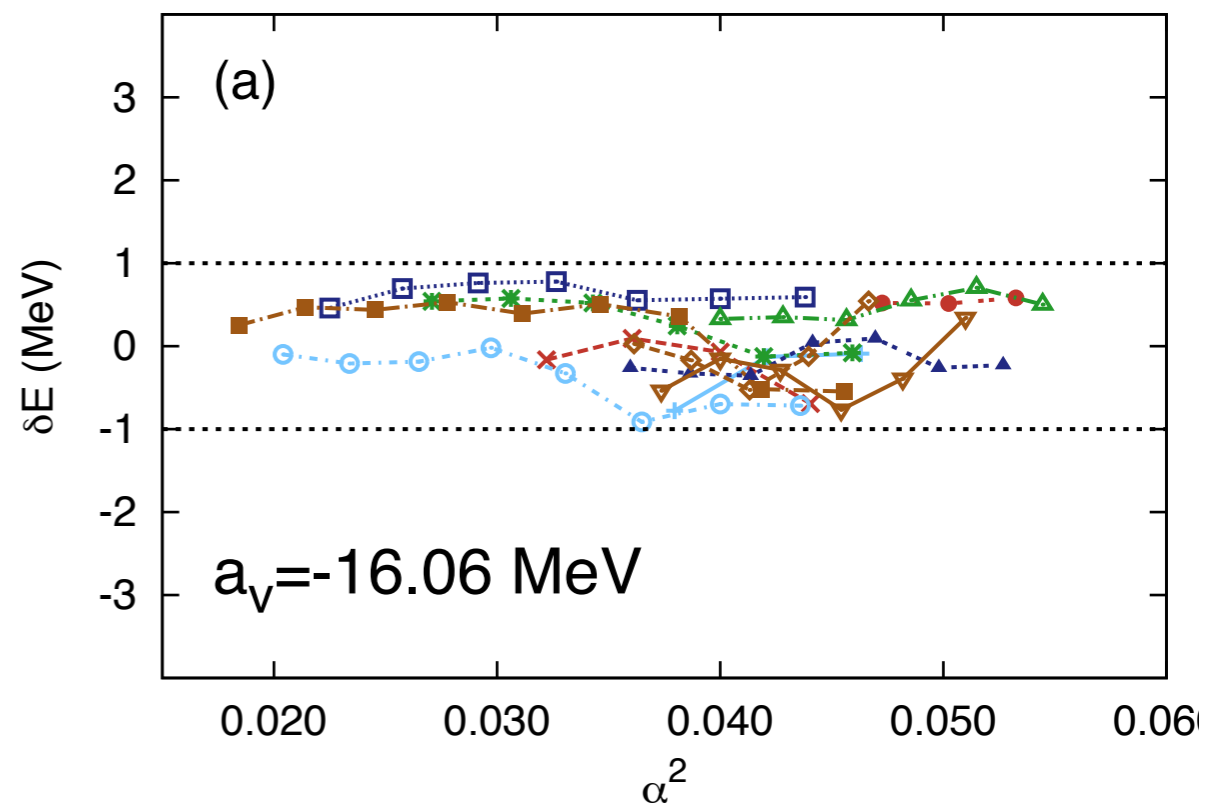
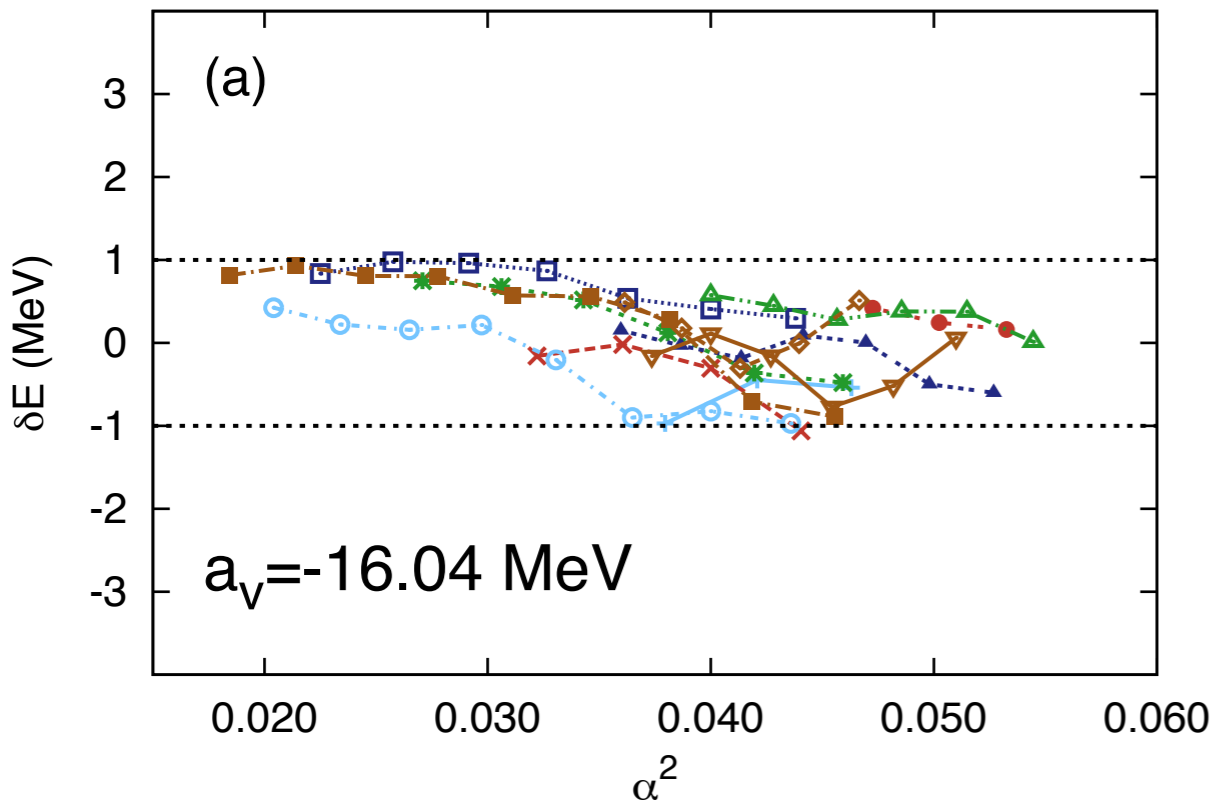
The minimum χ^2 -deviation of the theoretical binding energies from data, as a function of the volume energy coefficient:



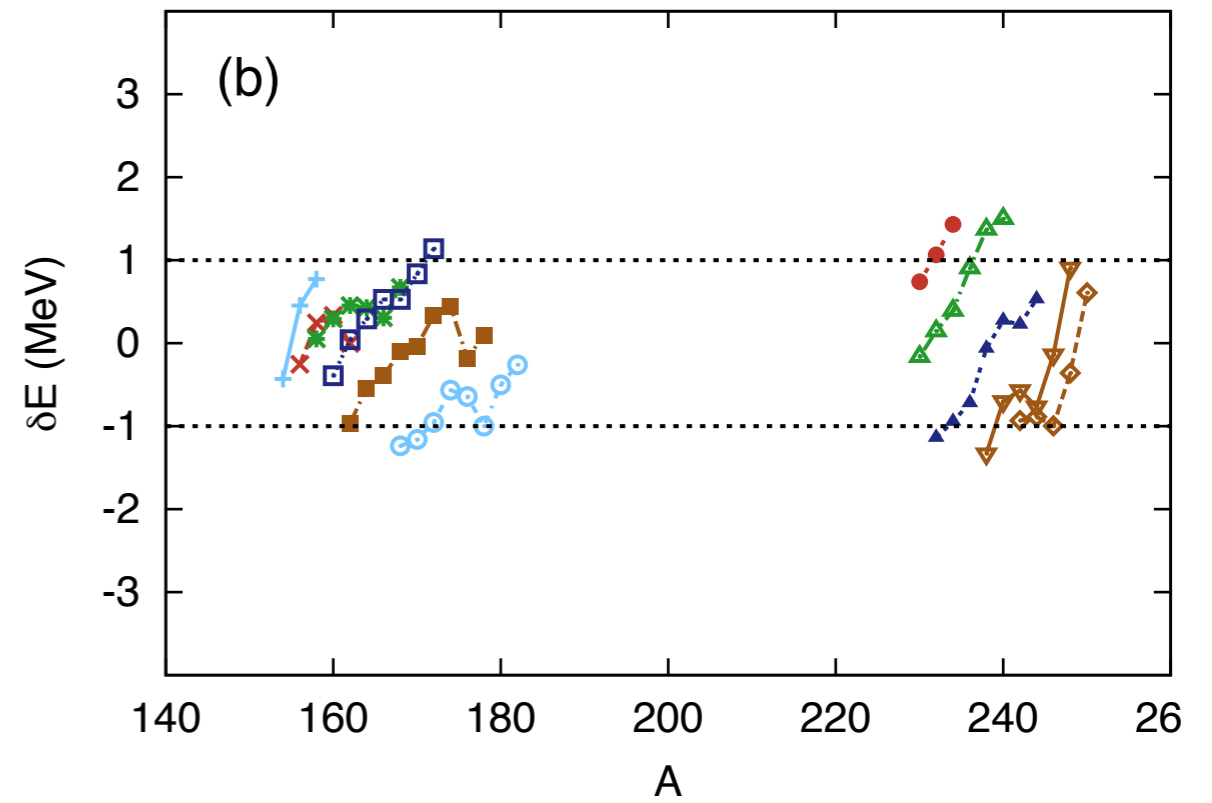
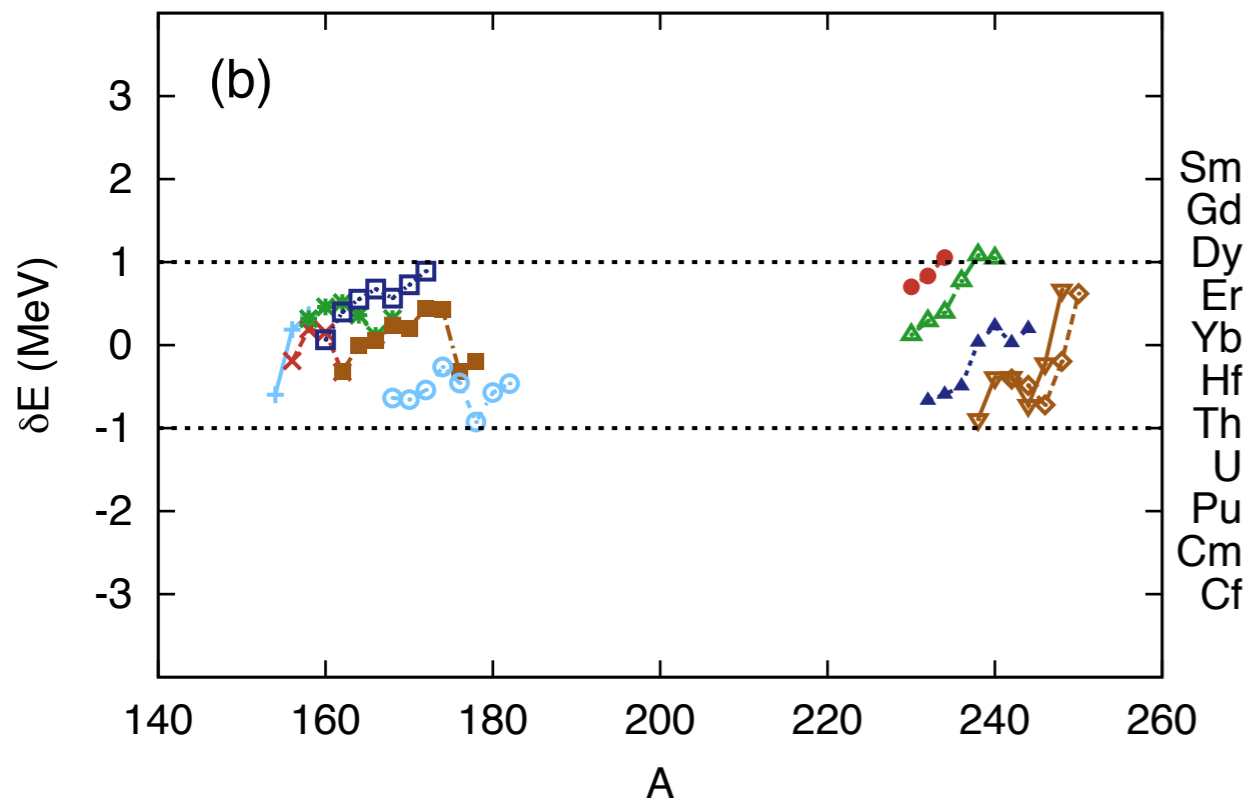
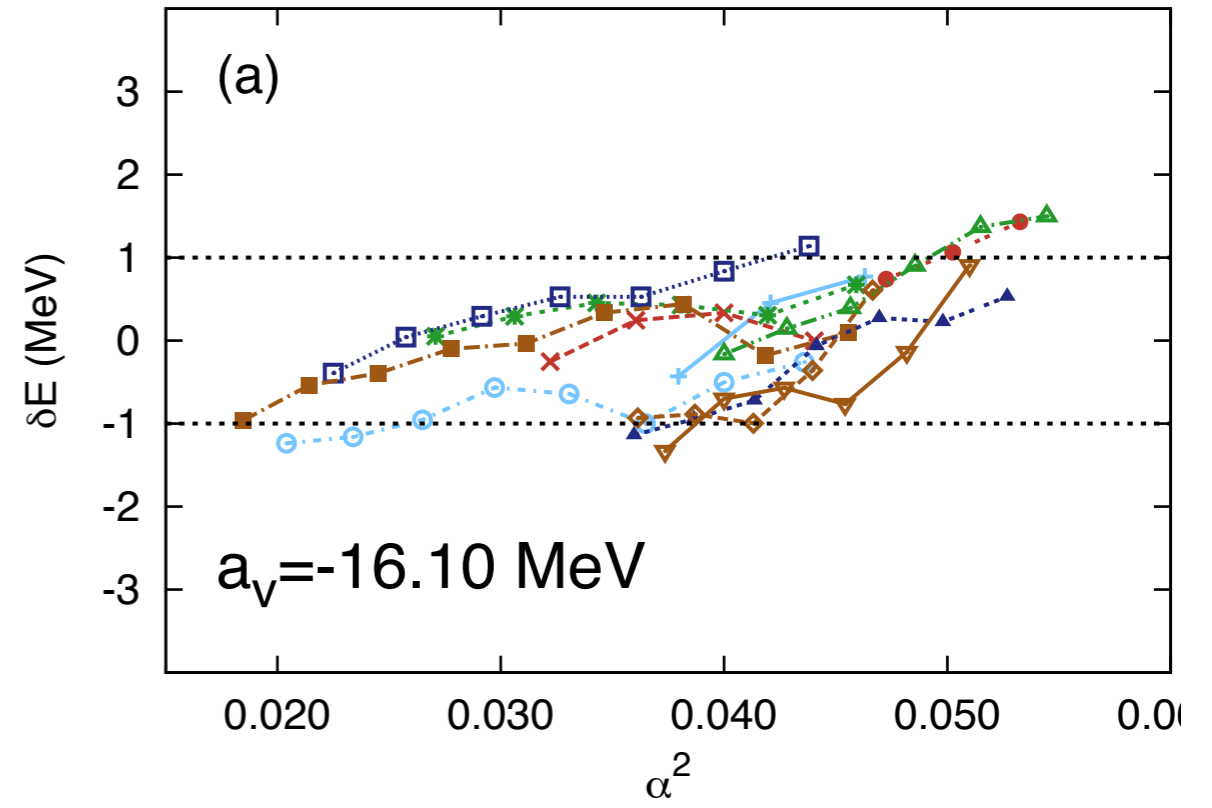
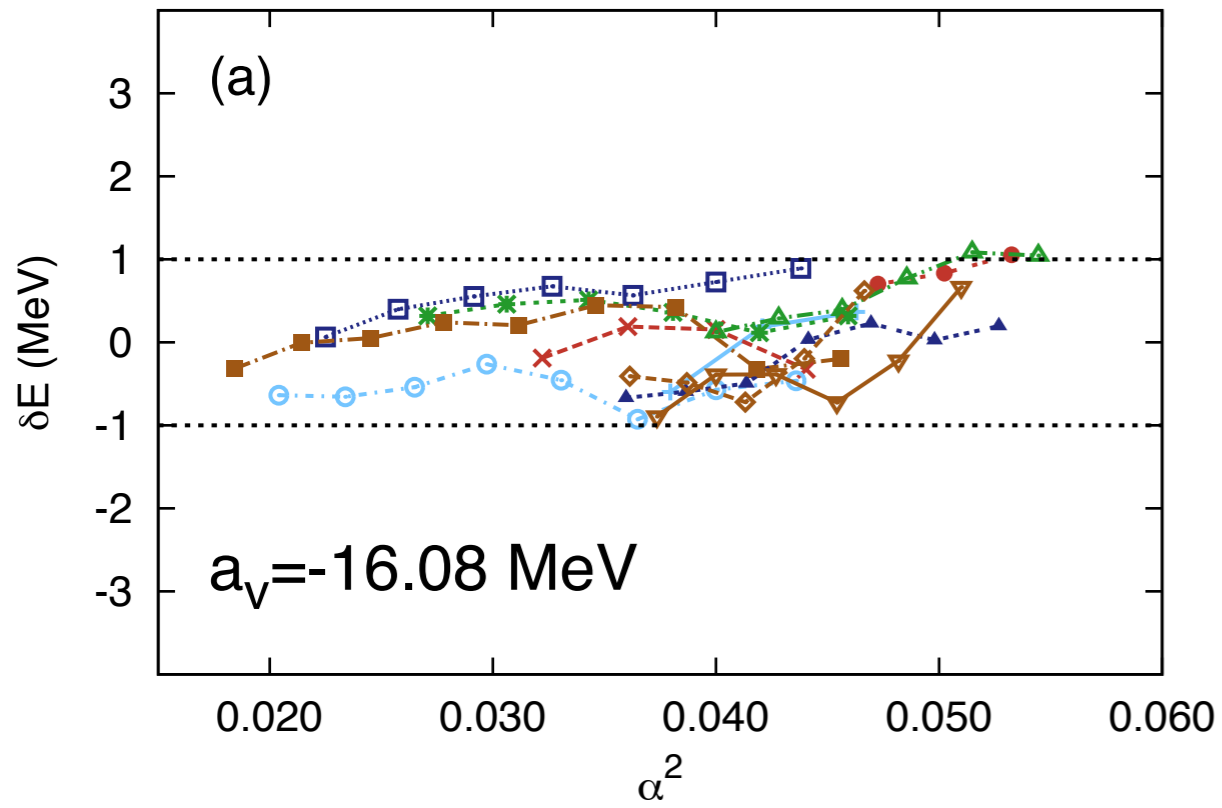
Absolute minimum:

$$a_v = -16.06 \text{ MeV} \quad \langle S_2 \rangle = 27.8 \text{ MeV} \quad a_s = 17.498 \text{ MeV}$$

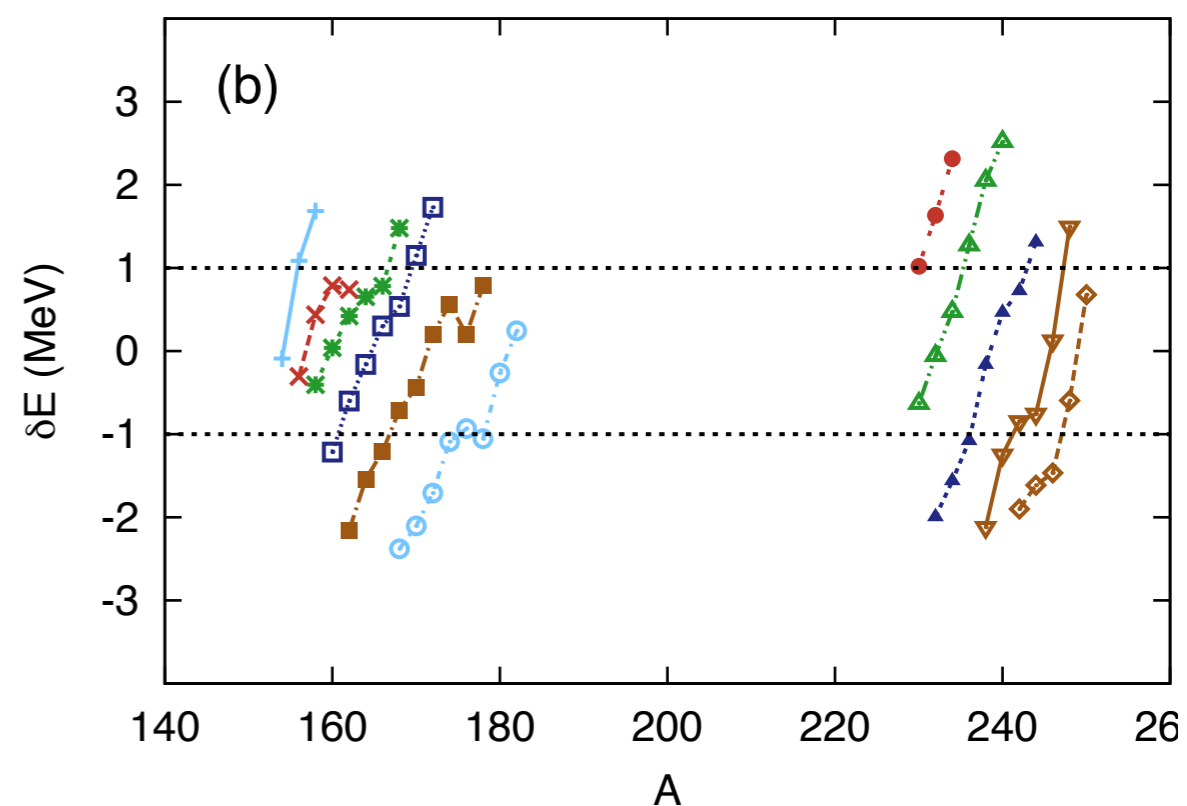
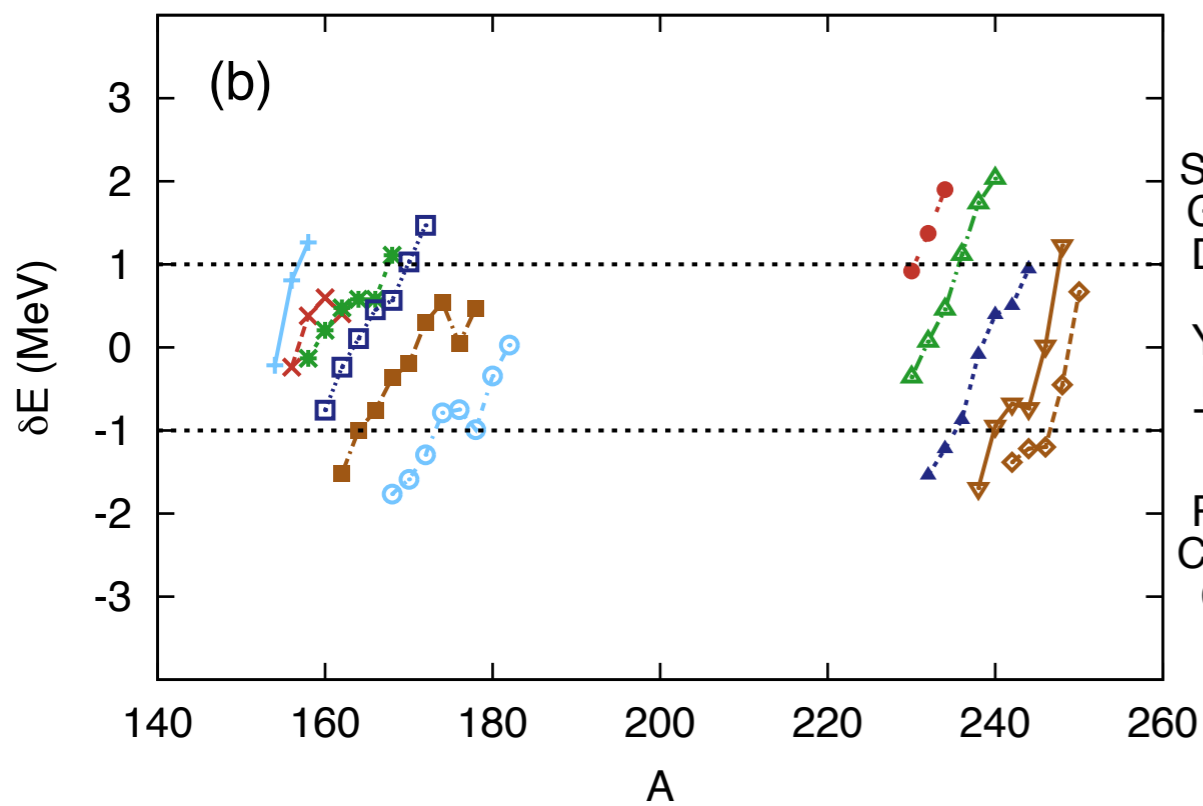
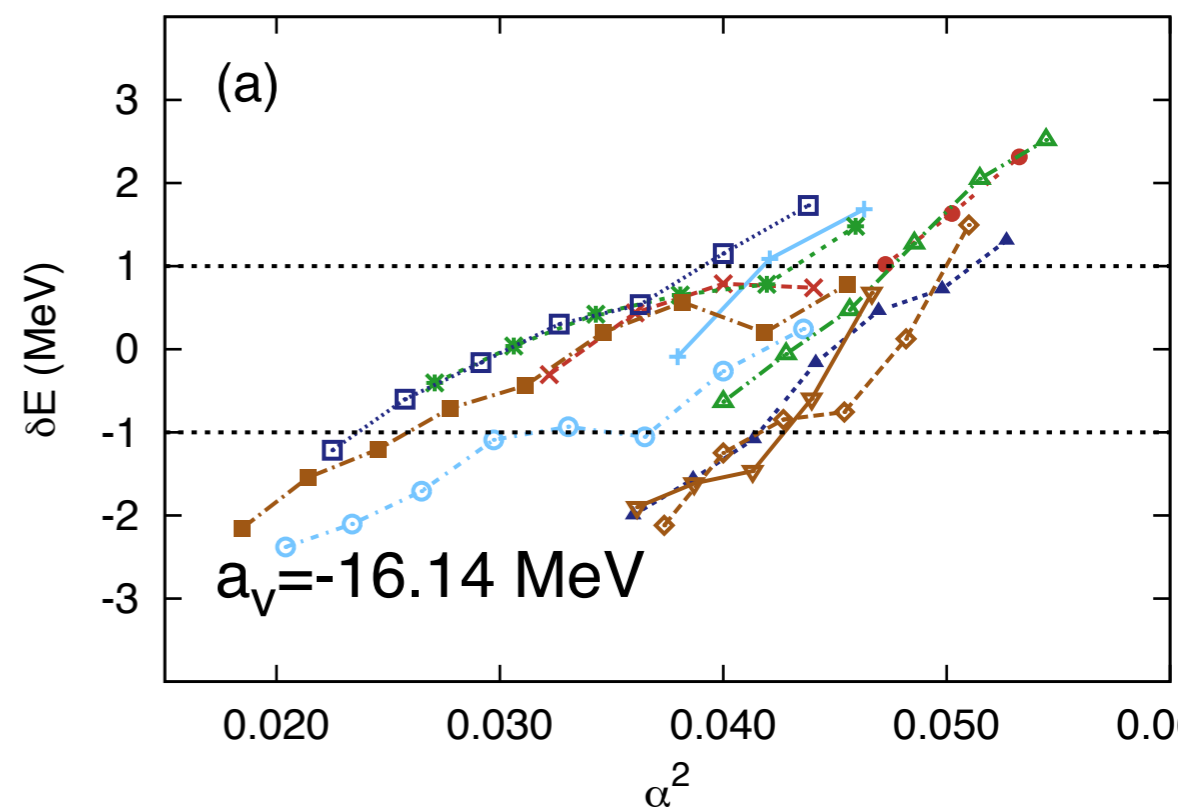
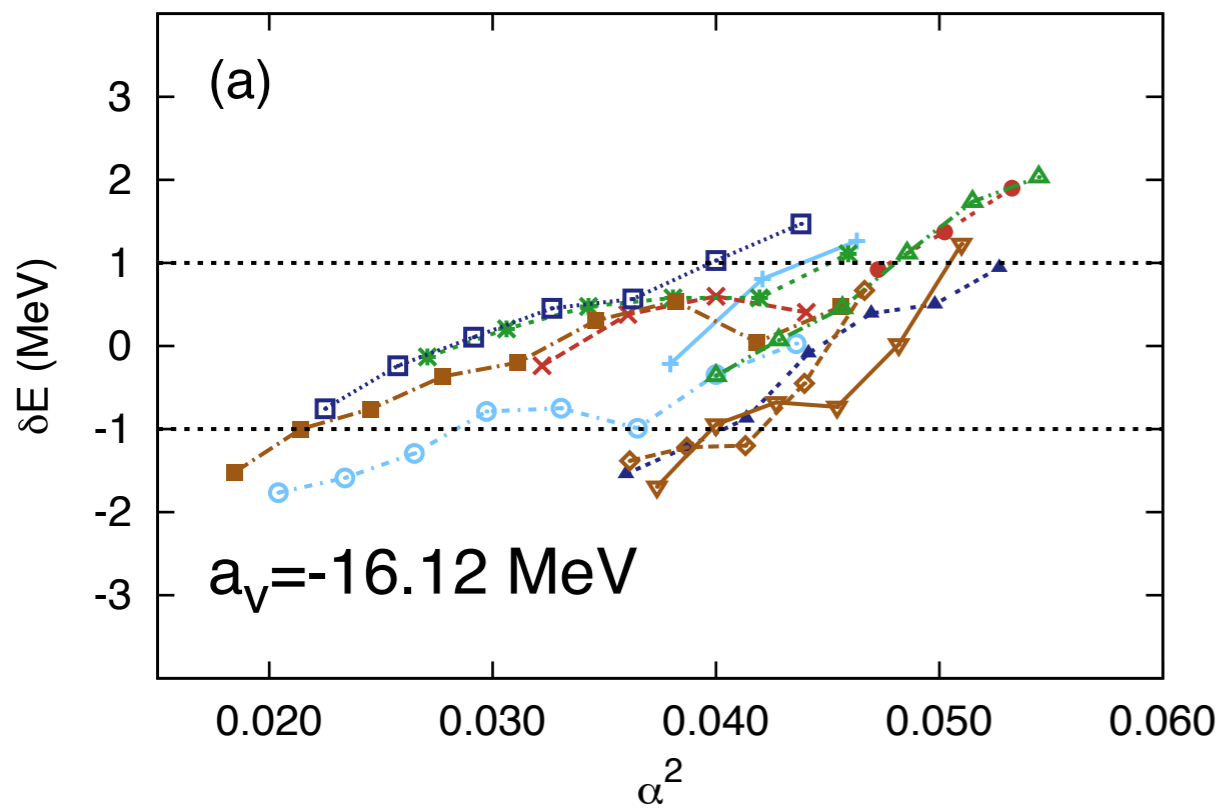
Absolute deviations of the calculated binding energies from data for 64 axially deformed nuclei:



$$\alpha^2 = \frac{(N - Z)^2}{A^2}$$



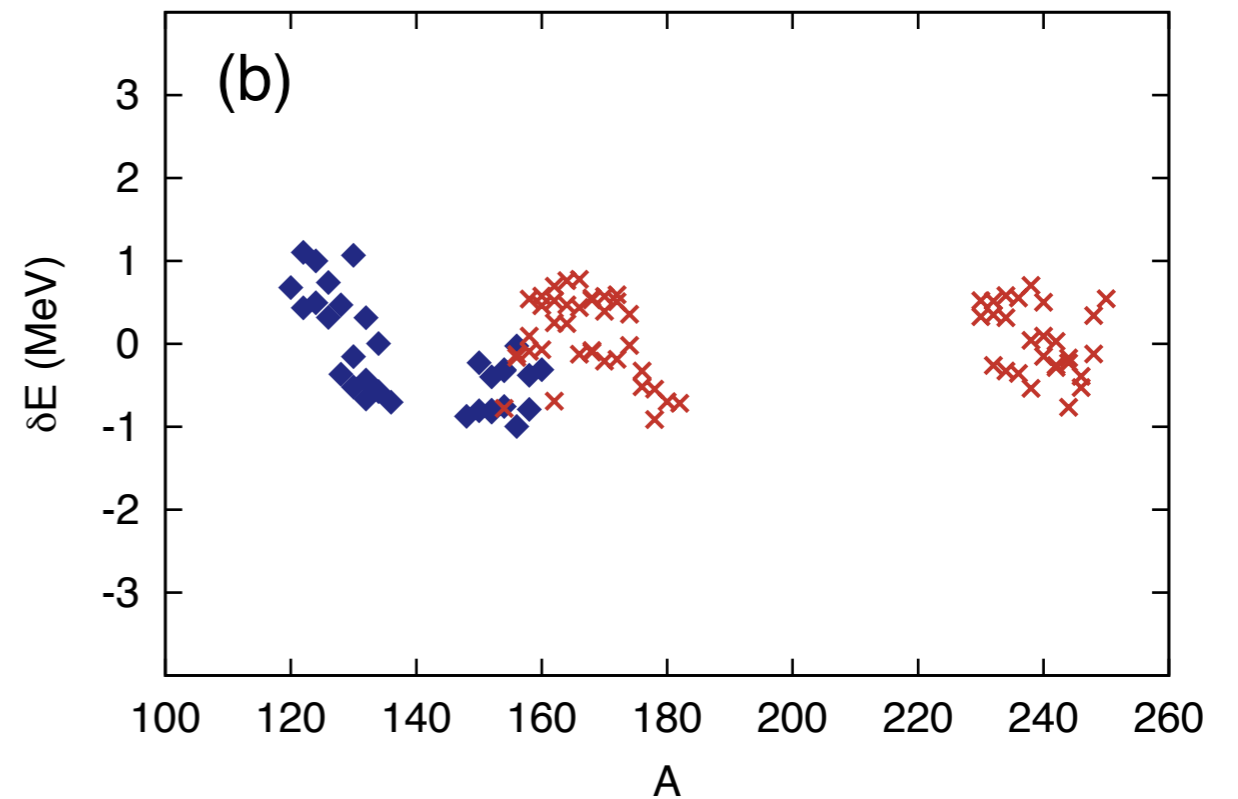
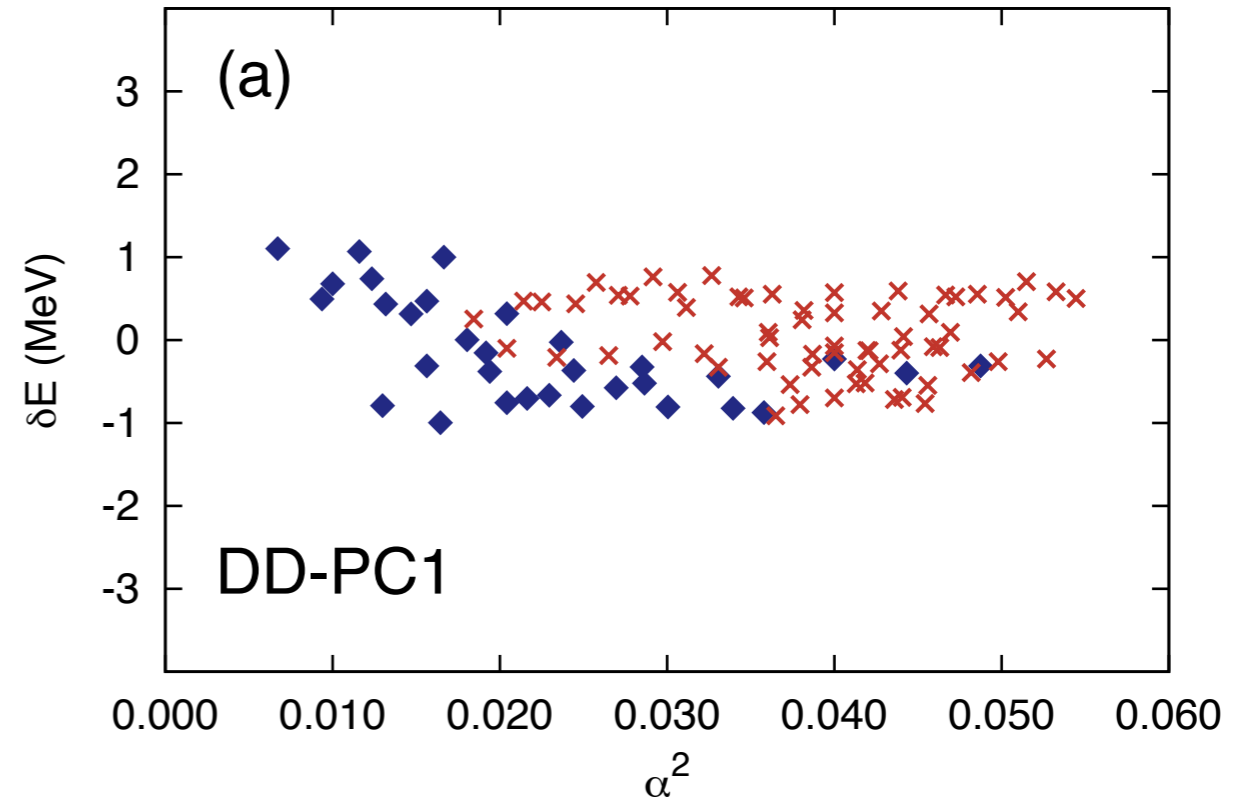
$$\alpha^2 = \frac{(N - Z)^2}{A^2}$$



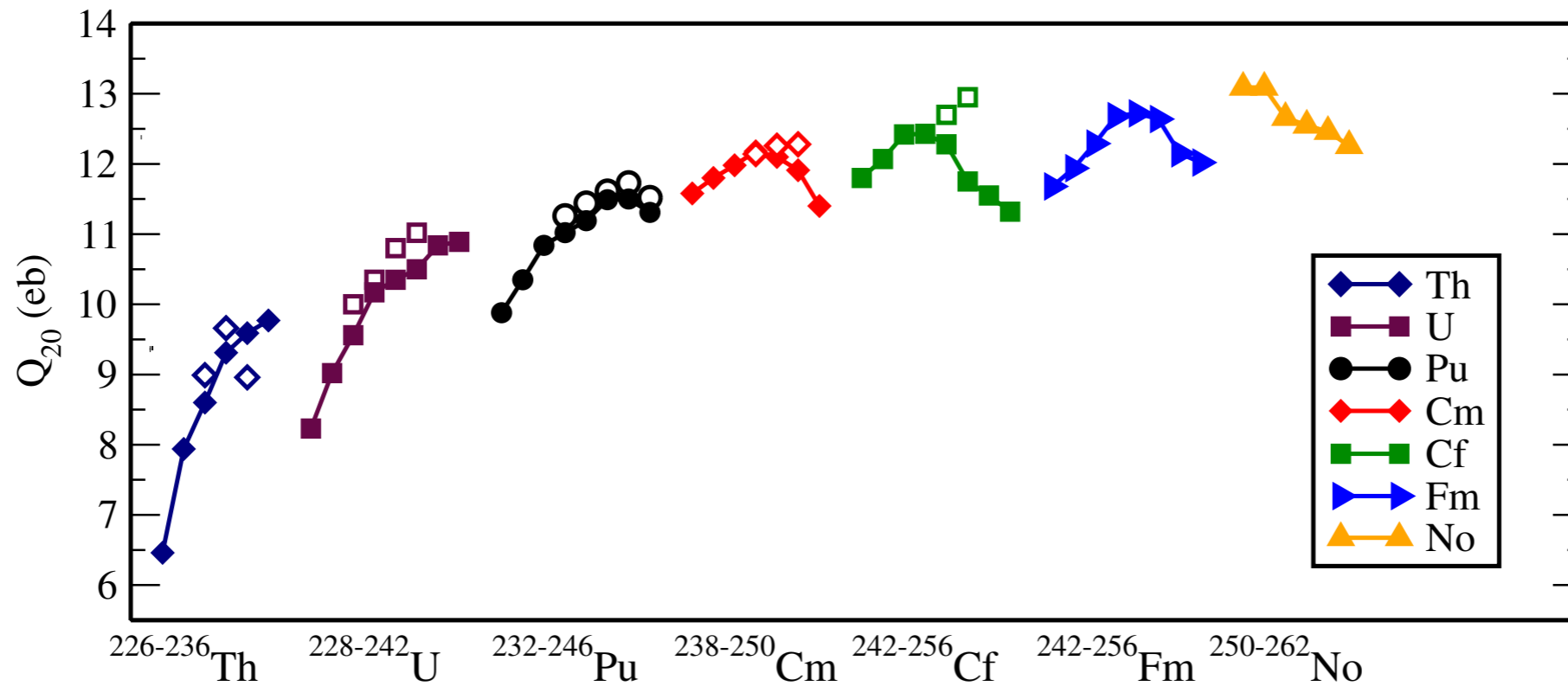
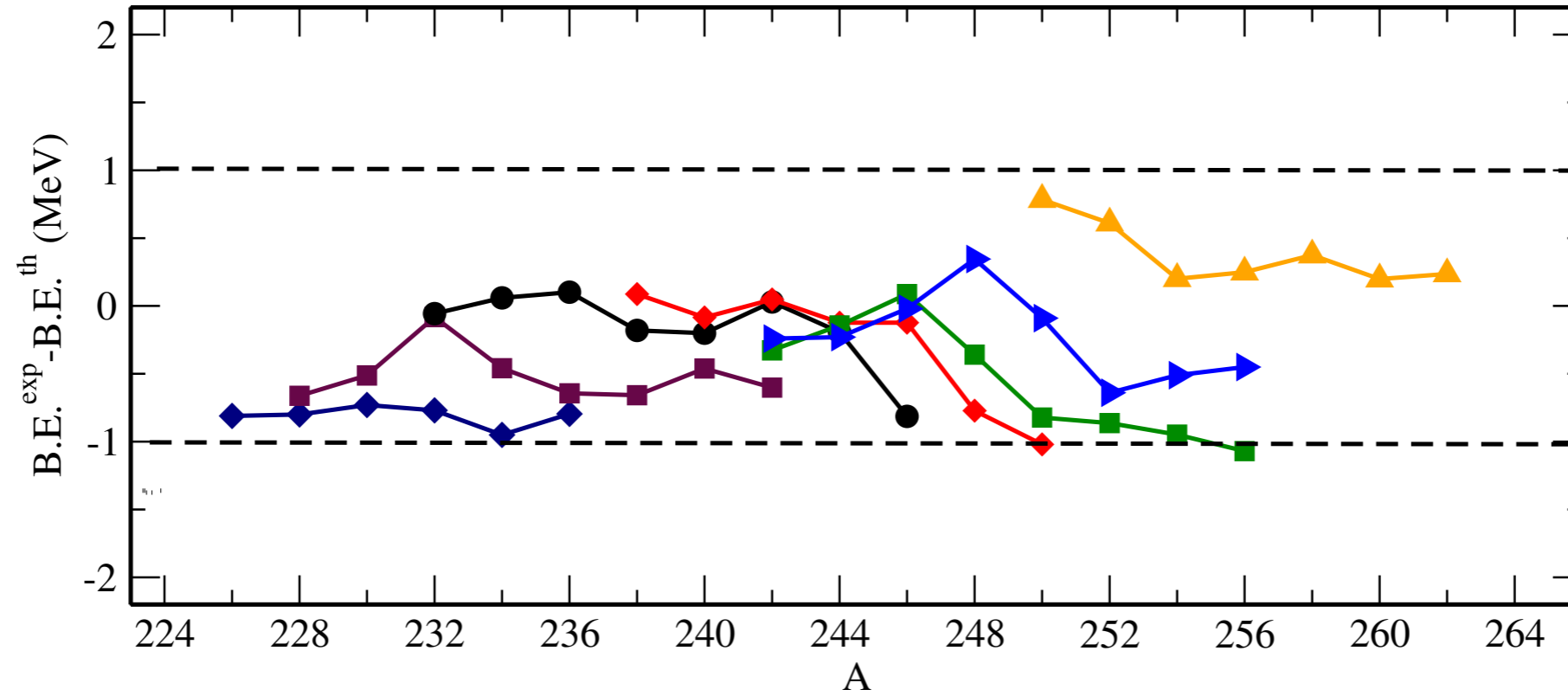
... calculated masses are extrapolated to a lower mass region not included in the fit and to lower values of the asymmetry parameter.

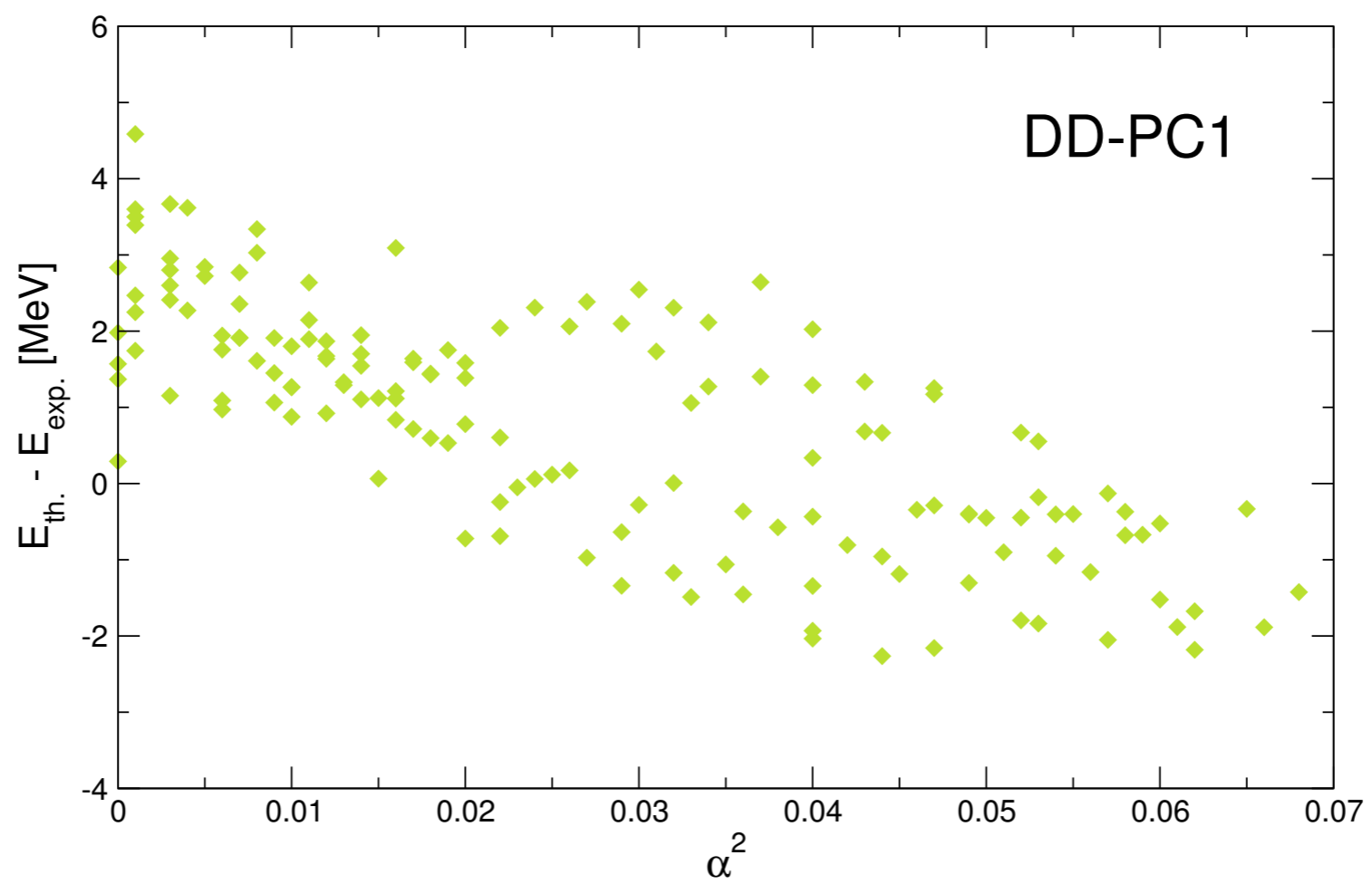
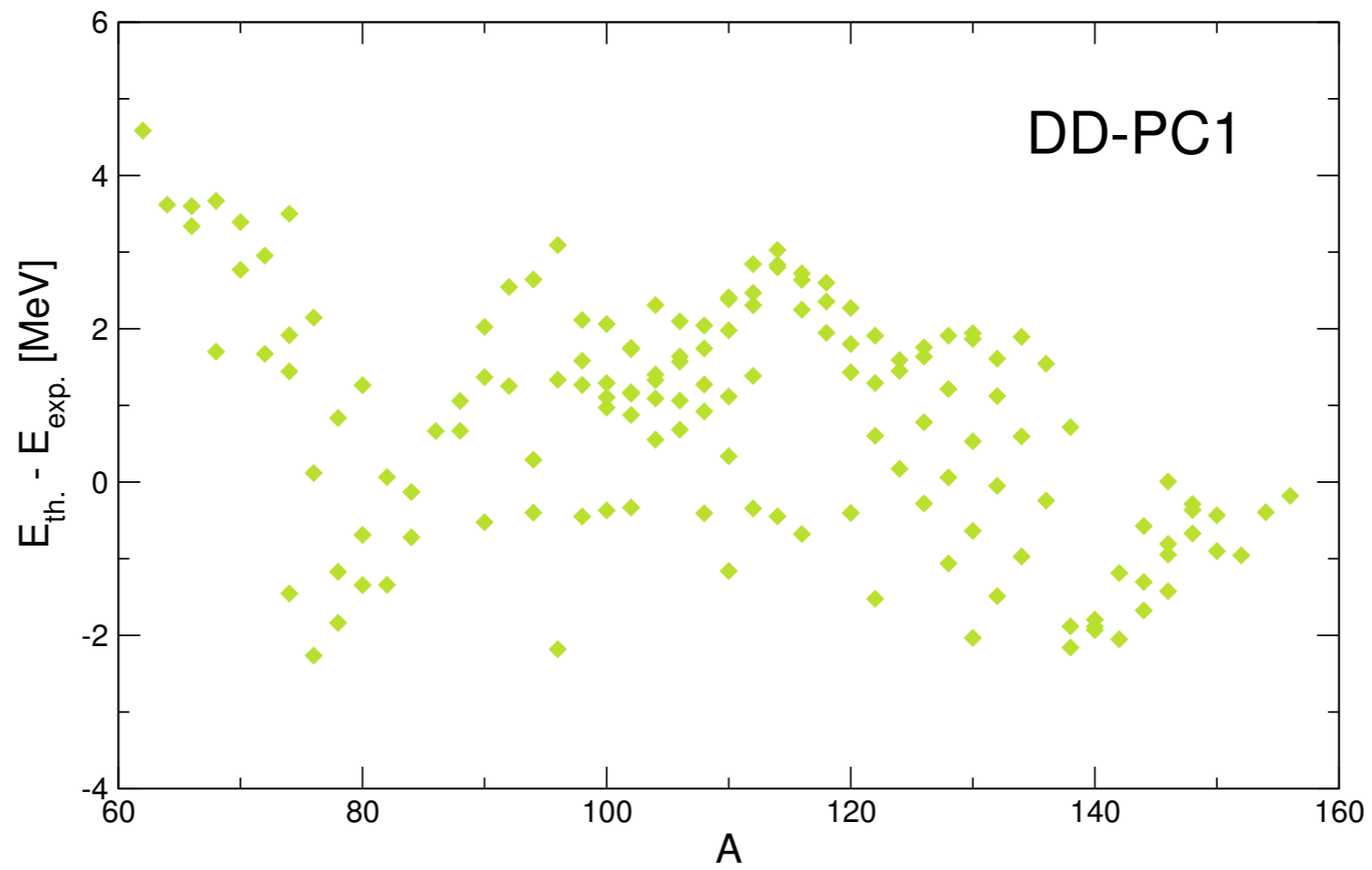
- ✗ fitted values
- ◆ extrapolated values

Nikšić, Vretenar, and Ring, Phys. Rev. C **78**, 034318 (2008)

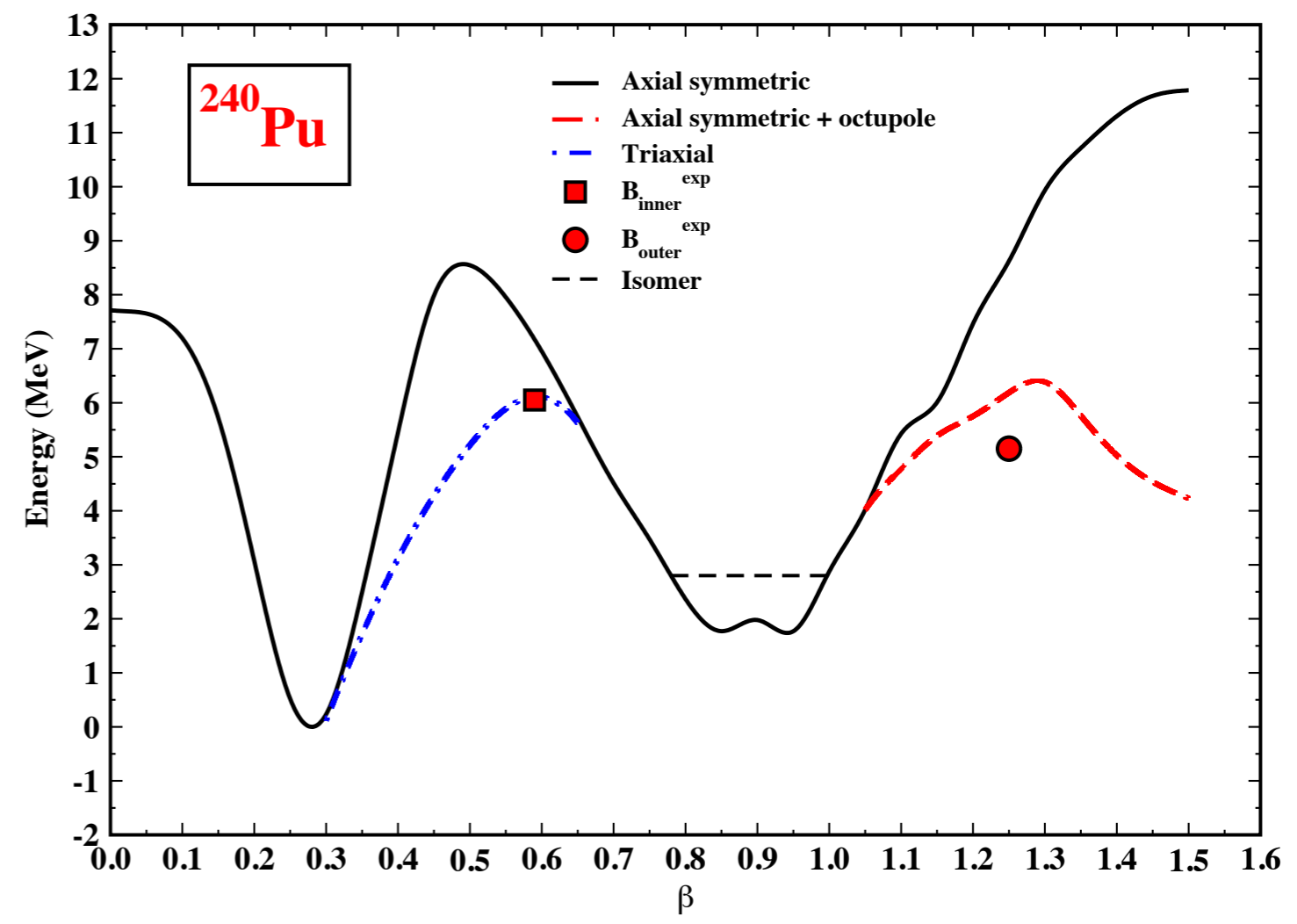
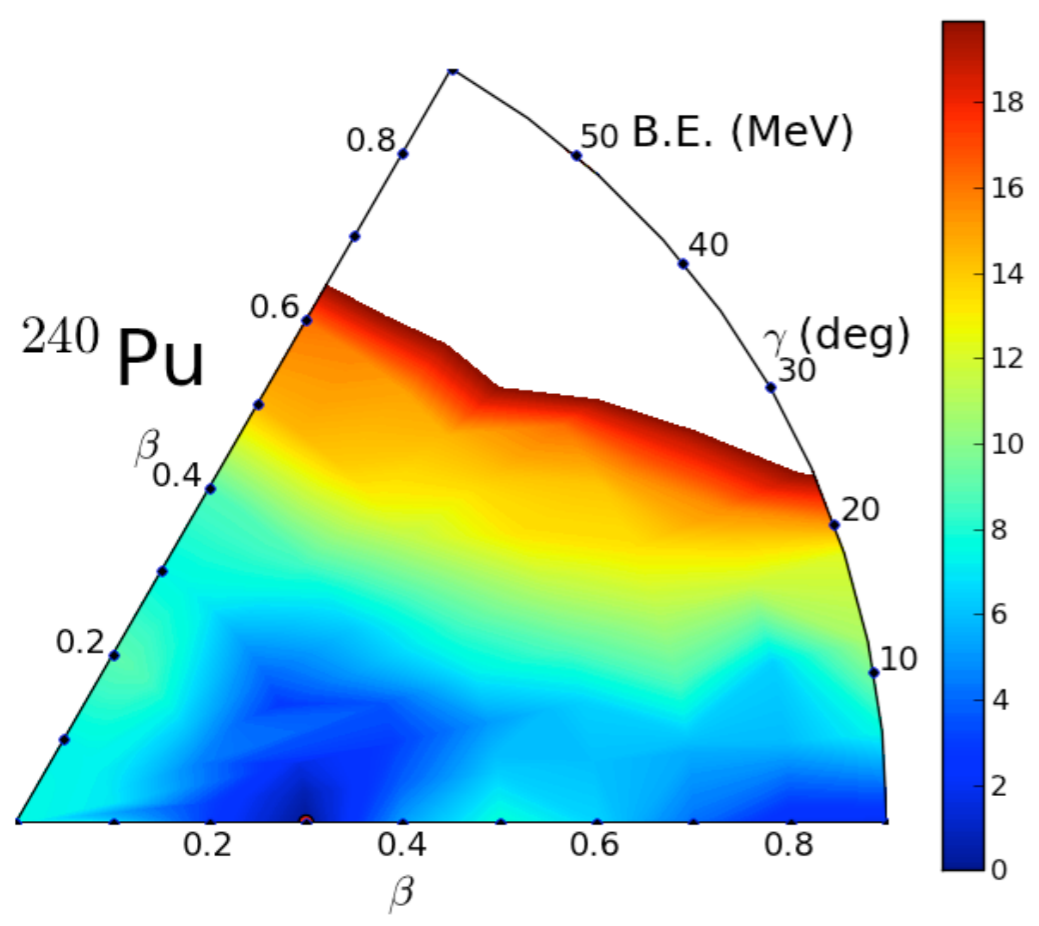


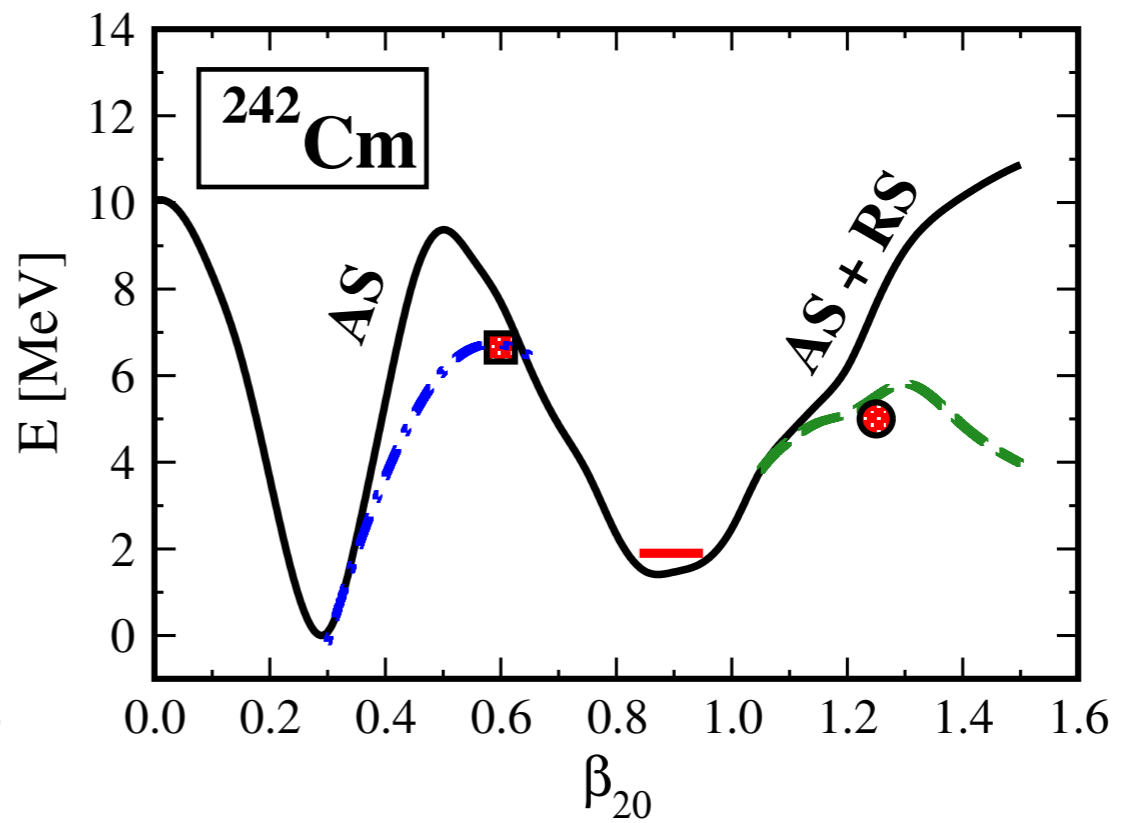
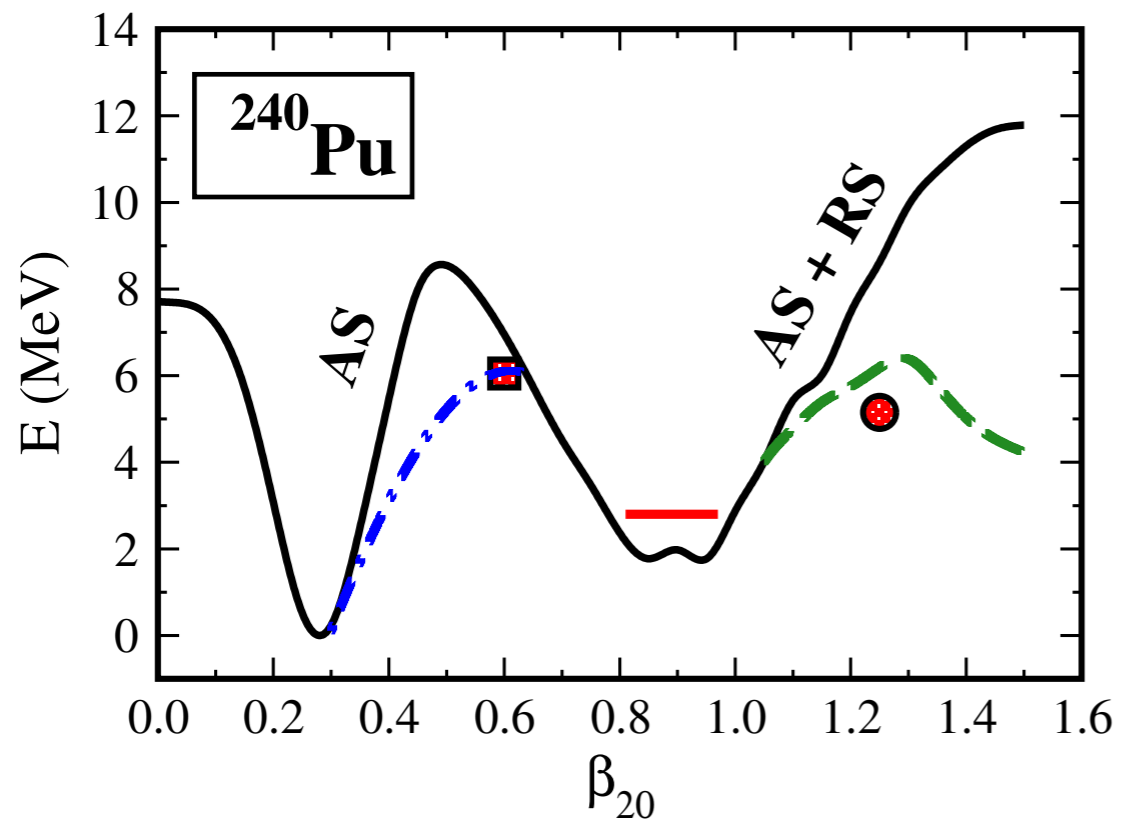
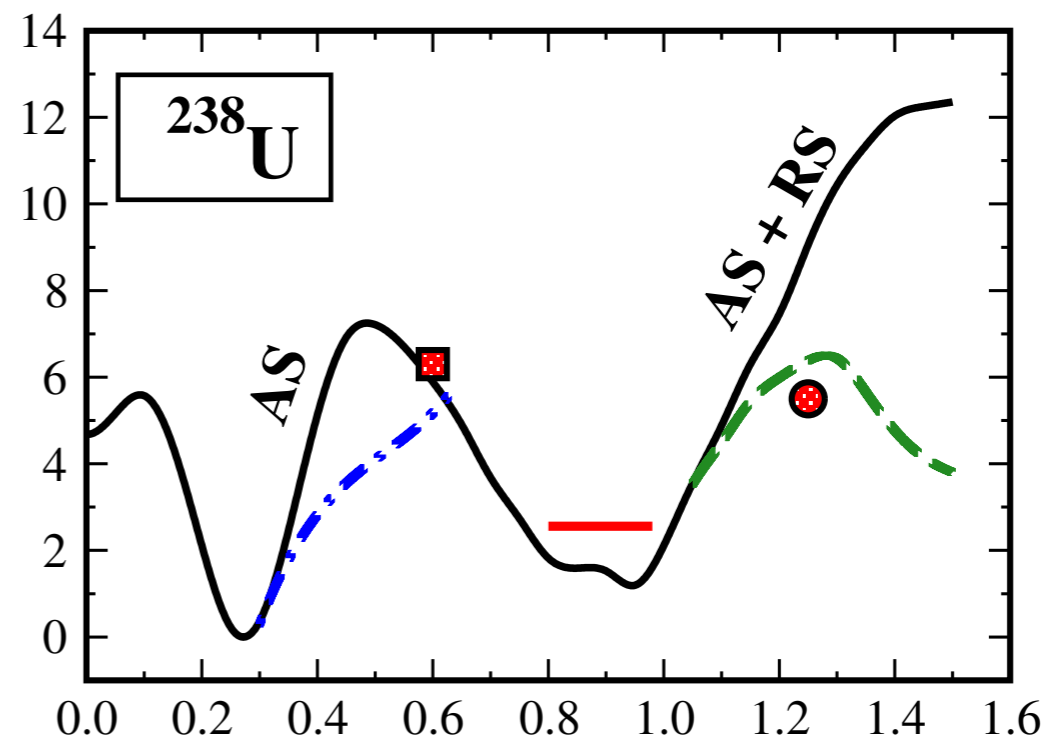
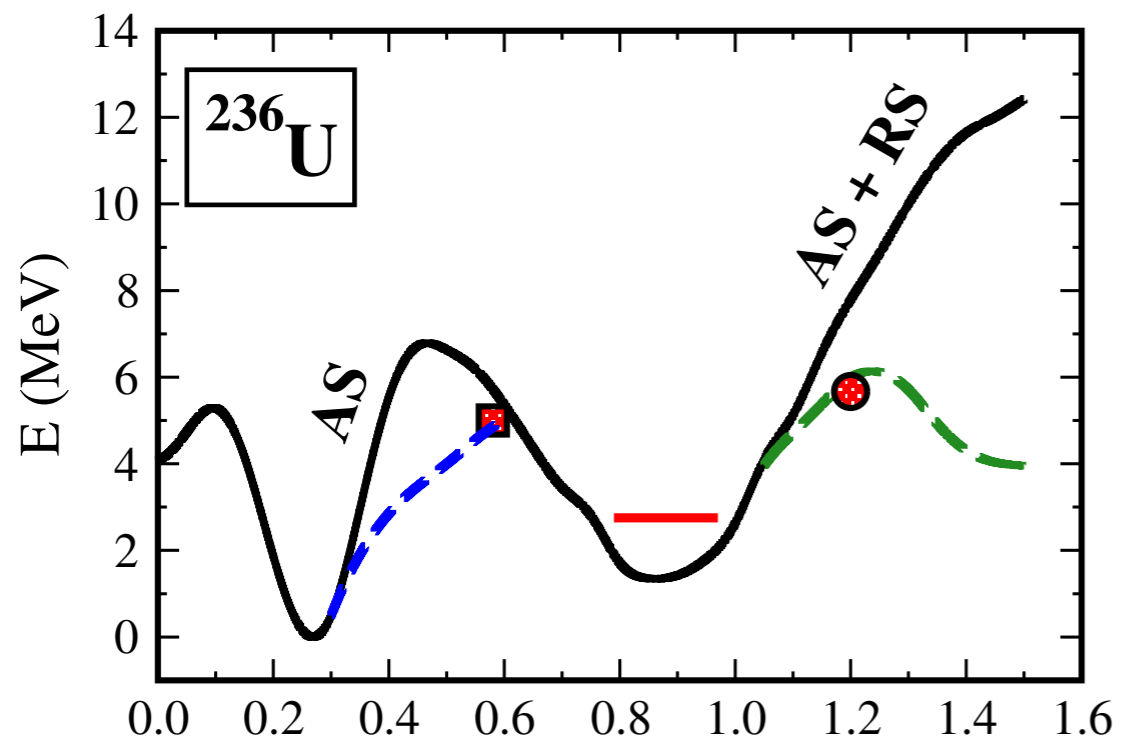
Test: ground-state properties of actinides



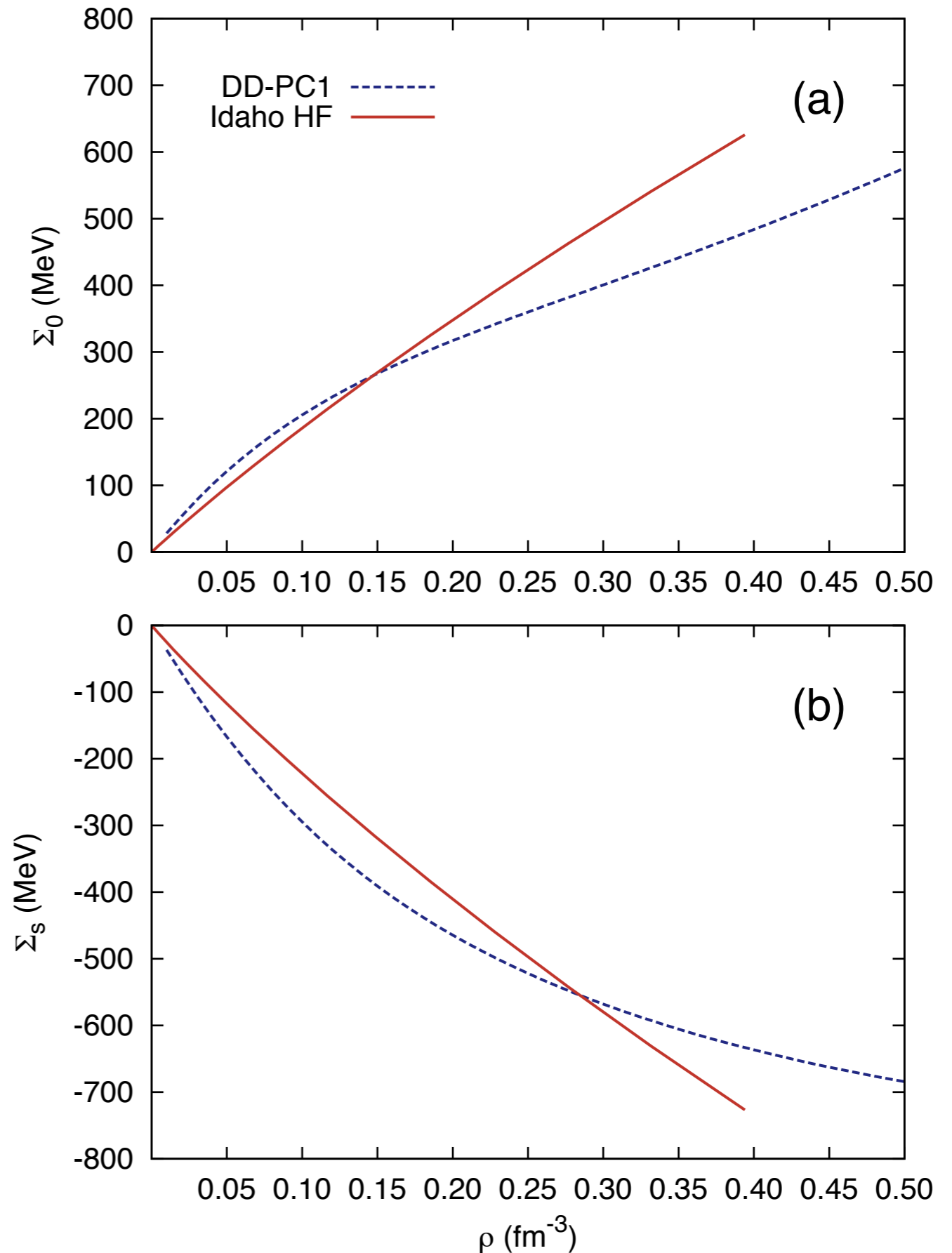


Test: "double-humped" fission barriers of actinides





Density dependence of the DD-PC1 isoscalar vector and scalar nucleon self-energies in symmetric nuclear matter, compared with the starting approximation: the Hartree-Fock self-energies calculated from the Idaho $N^3\text{LO}$ NN-potential.



Nuclear Many-Body Correlations



short-range
(hard repulsive core of
the NN-interaction)

long-range
nuclear resonance
modes
(giant resonances)

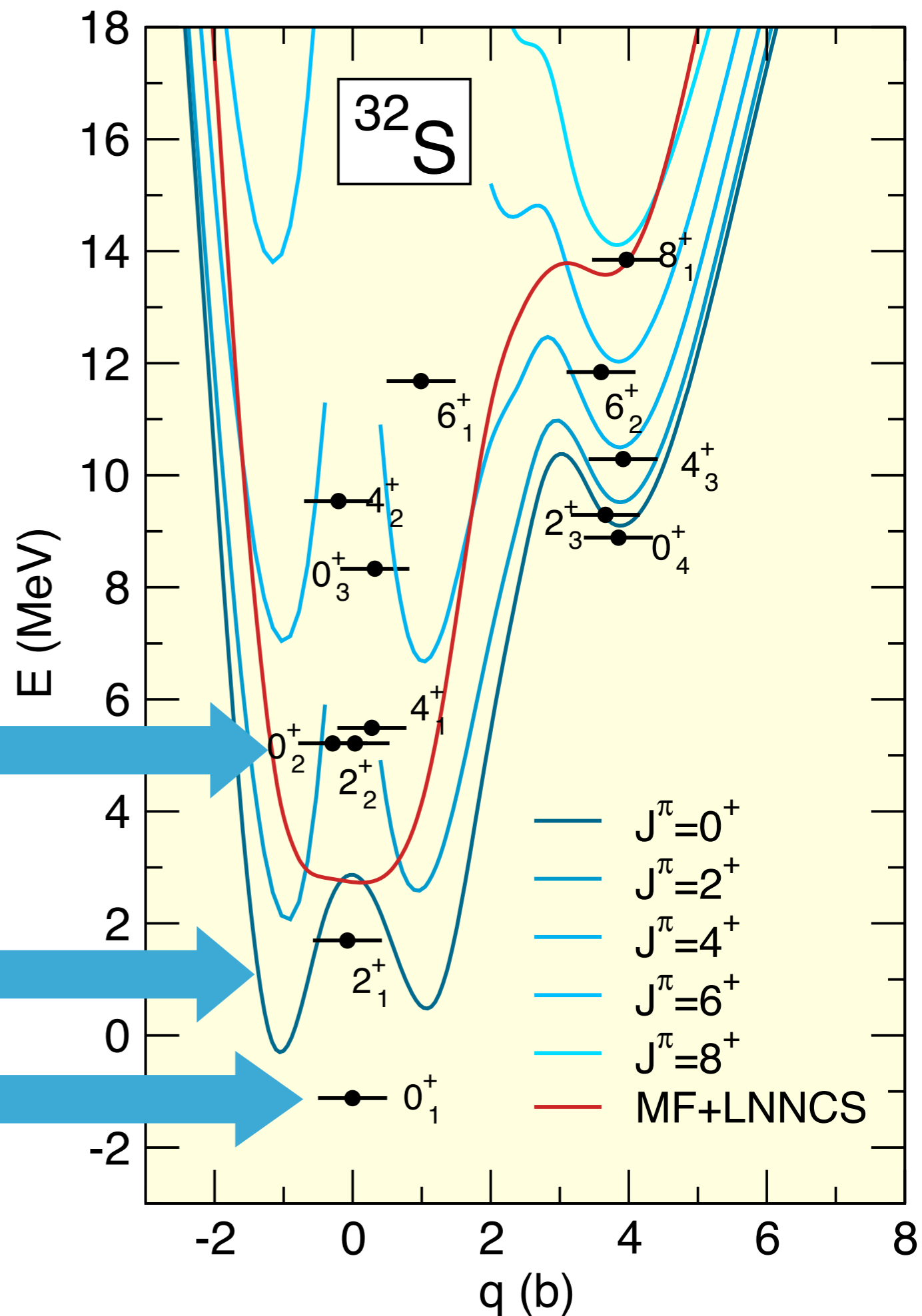
collective correlations
large-amplitude soft modes:
(center of mass motion, rotation,
low-energy quadrupole vibrations)

...vary smoothly with nucleon number!
Implicitly included in an effective EDF.

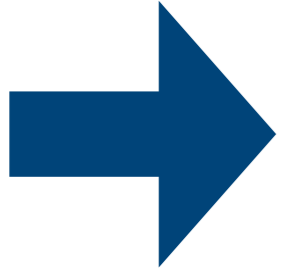
...sensitive to shell-effects and strong variations
with nucleon number!
Cannot be included in a simple Kohn-Sham EDF
framework.

Restoration of broken symmetries and fluctuations of collective variables

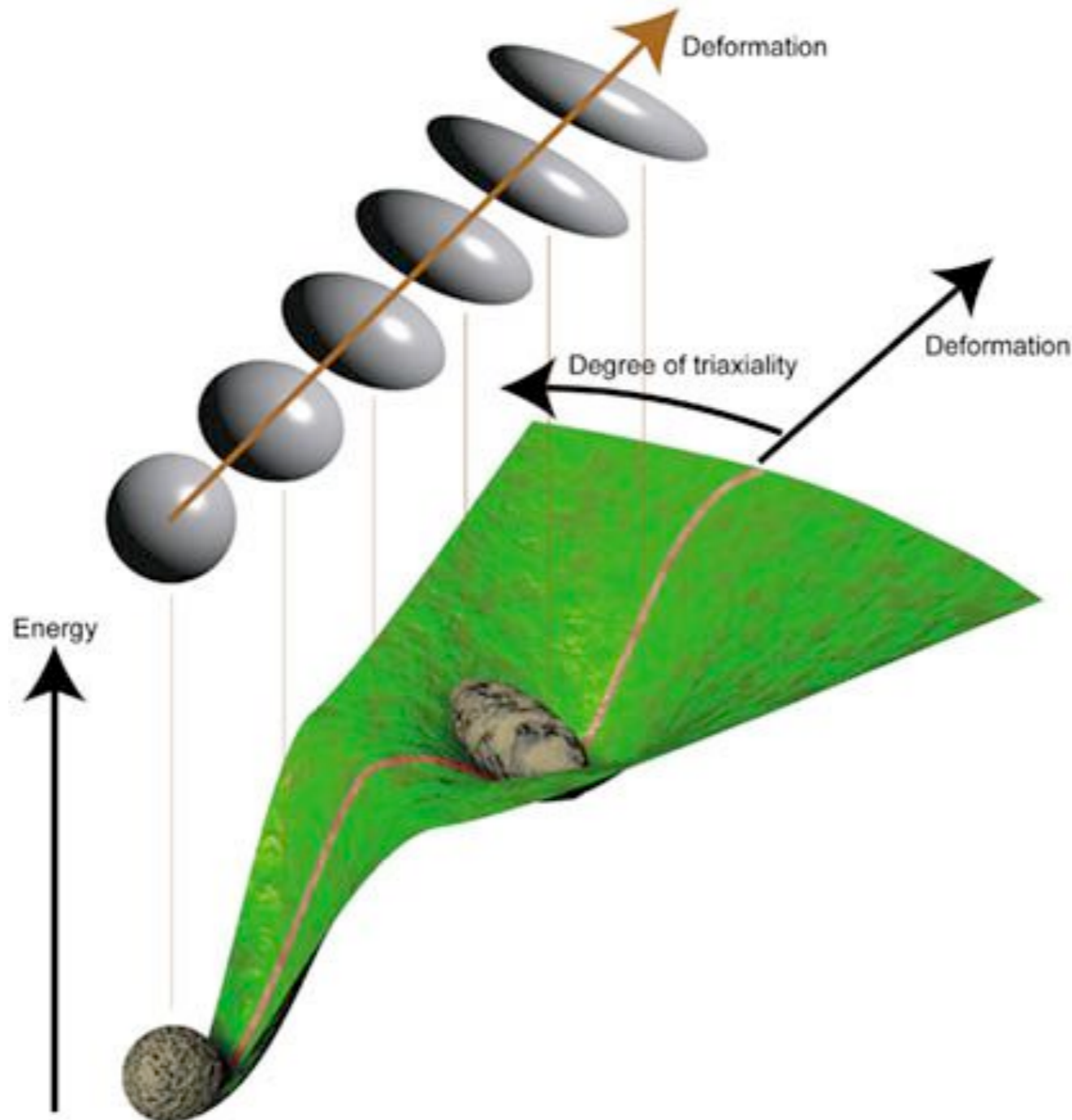
1. Mean-field calculations, with a constraint on the quadrupole moment.
2. Angular-momentum and particle-number projection.
3. Generator Coordinate Method \Rightarrow configuration mixing



... larger variational space for projected GCM calculations!



triaxial shapes, breaking time-reversal invariance, different deformations for proton and neutron distributions, ...



Five-dimensional collective Hamiltonian

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

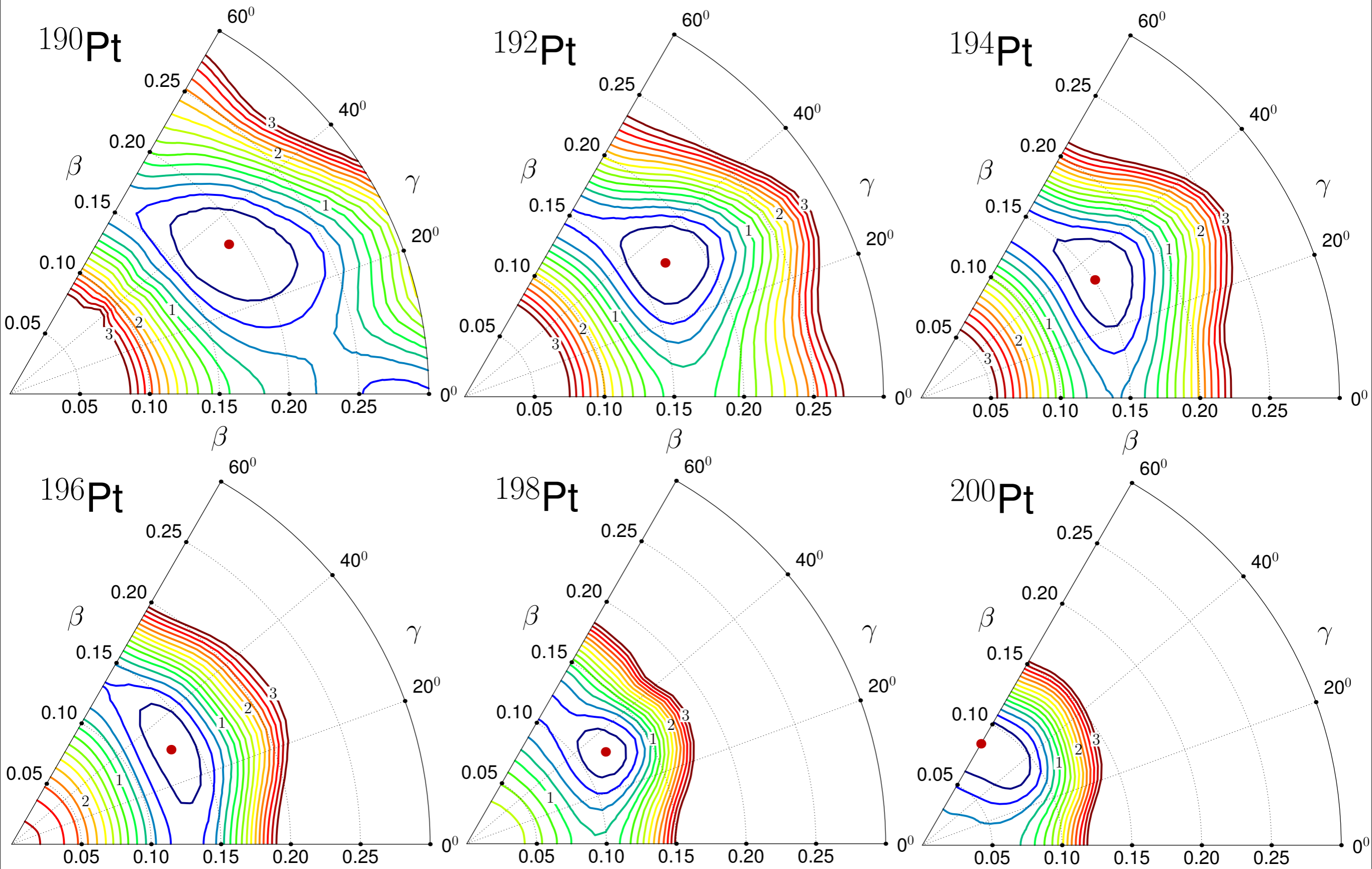
$$H_{\text{coll}} = \mathcal{T}_{\text{vib}}(\beta, \gamma) + \mathcal{T}_{\text{rot}}(\beta, \gamma, \Omega) + \mathcal{V}_{\text{coll}}(\beta, \gamma)$$

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

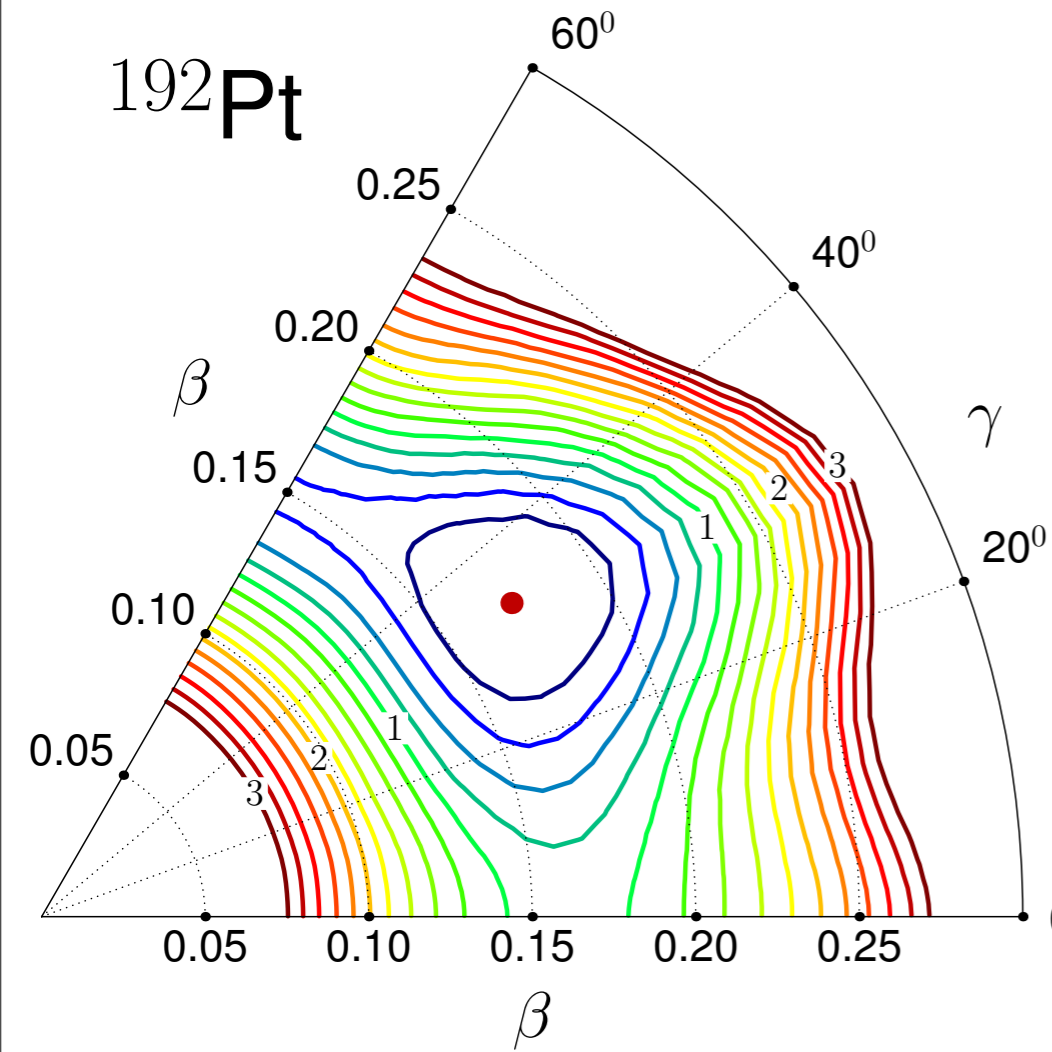
$$\mathcal{T}_{\text{rot}} = \frac{1}{2} \sum_{k=1}^3 \mathcal{I}_k \omega_k^2$$

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 \mathcal{I}_k .

Evolution of triaxial shapes in Pt nuclei:

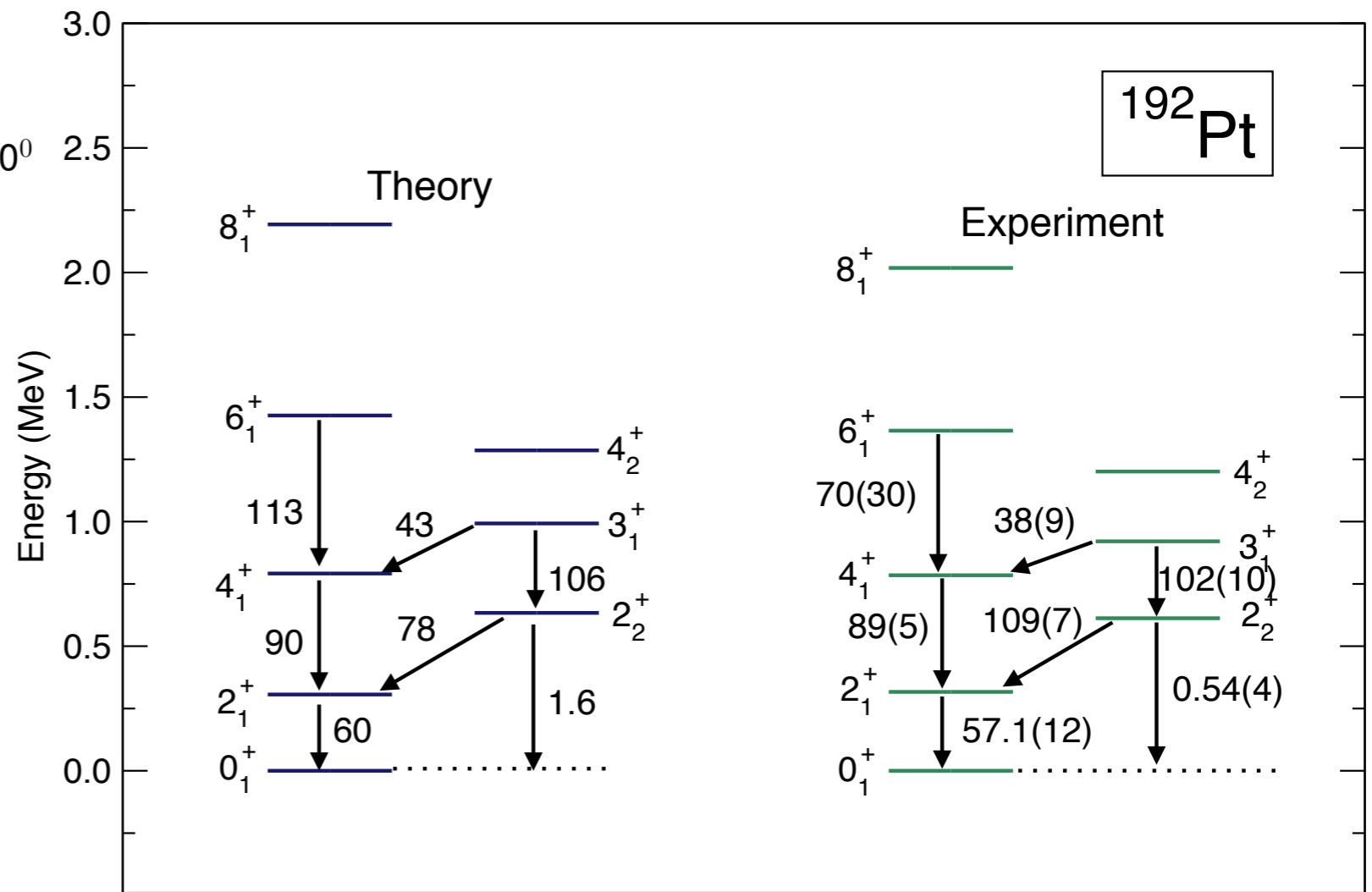


^{192}Pt

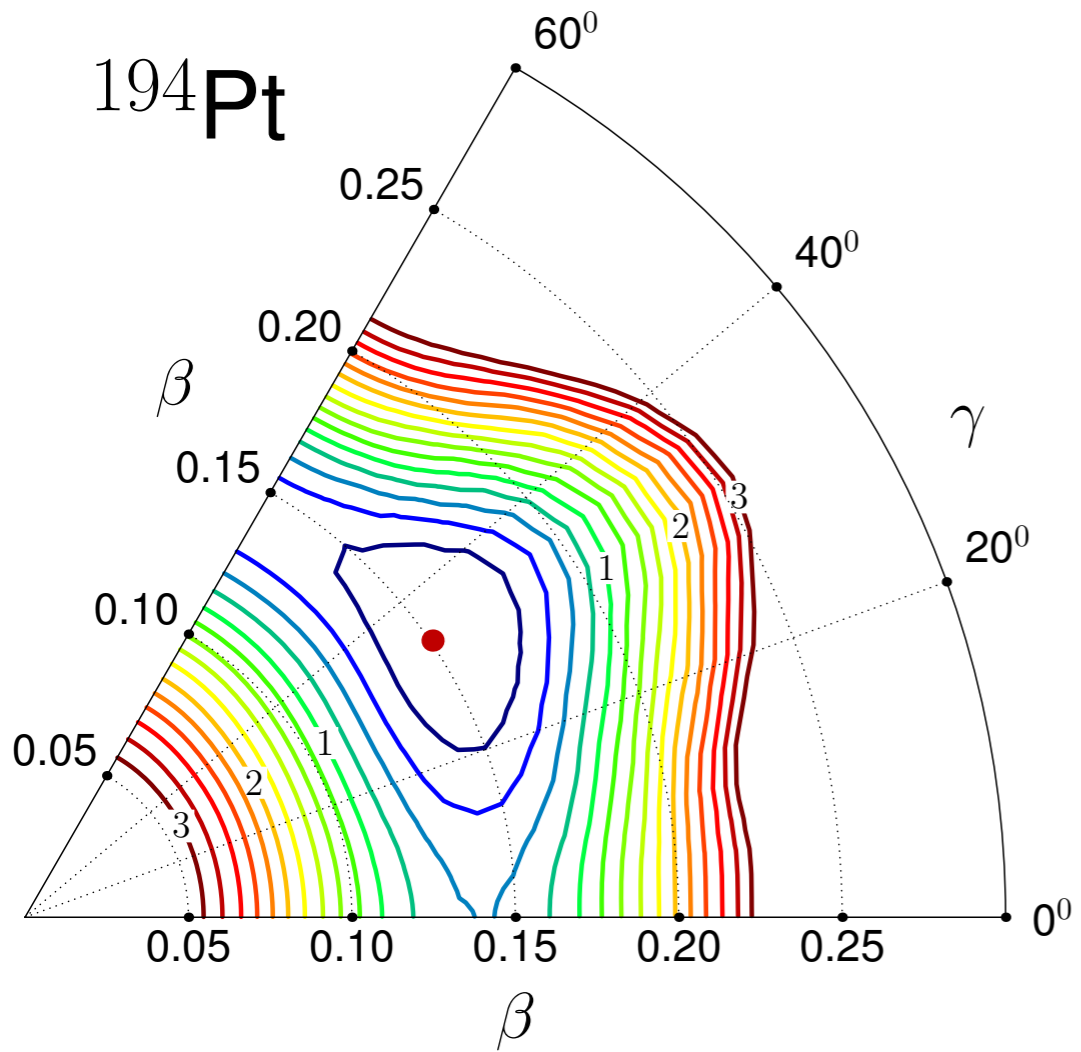


$$E_{4_1^+}^{th} / E_{2_1^+}^{th} = 2.58$$

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

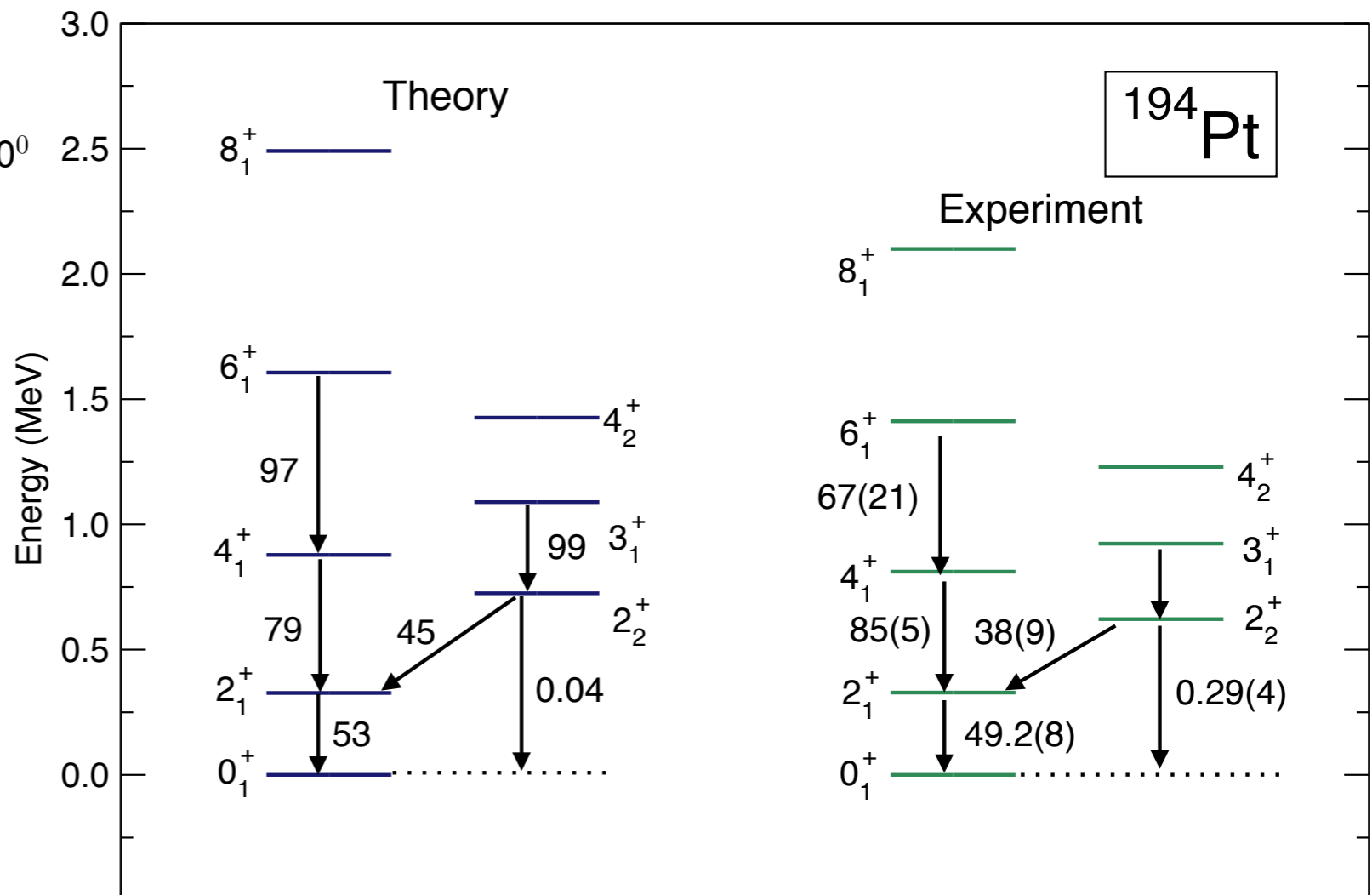


^{194}Pt

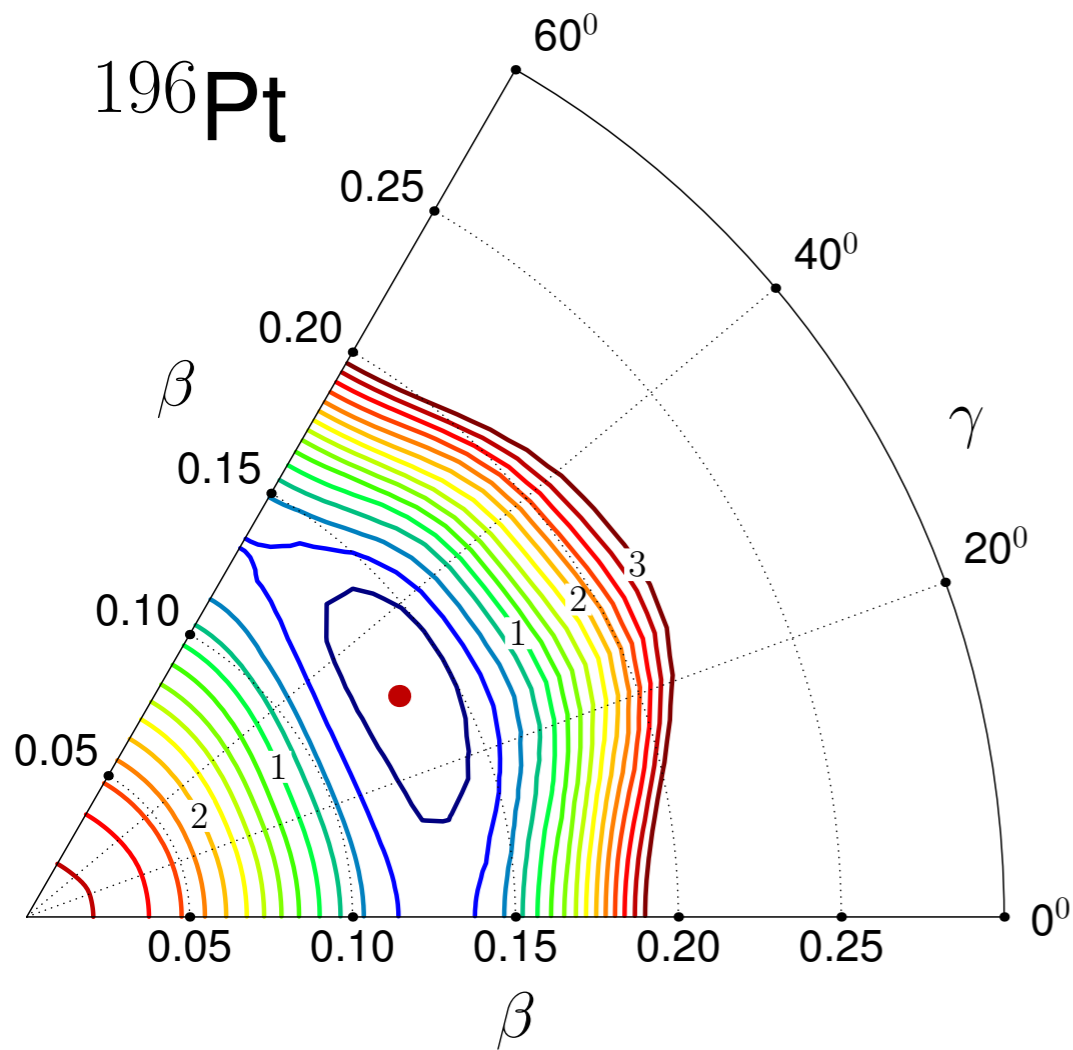


$$E_{4_1^+}^{th} / E_{2_1^+}^{th} = 2.68$$

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

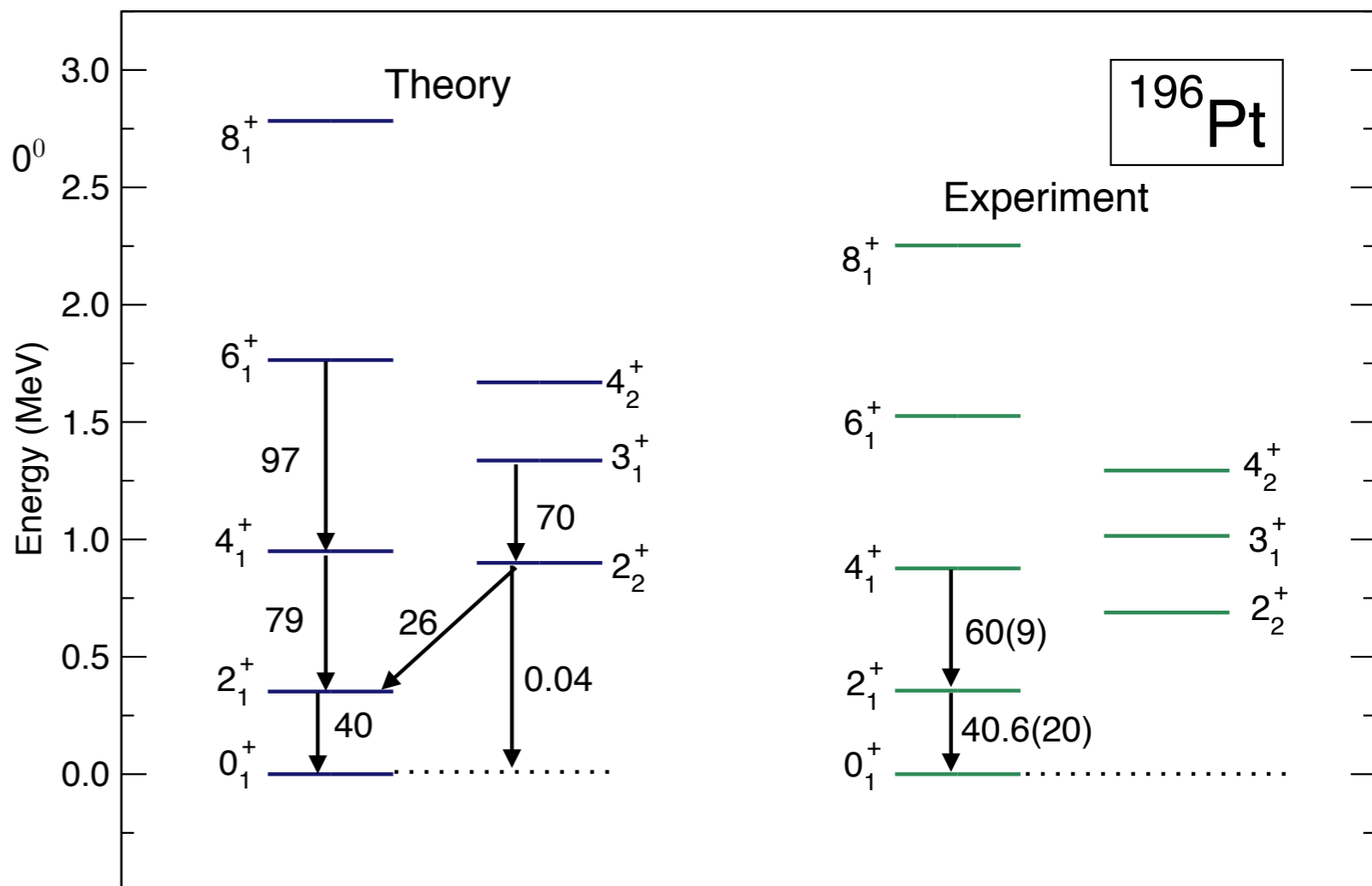


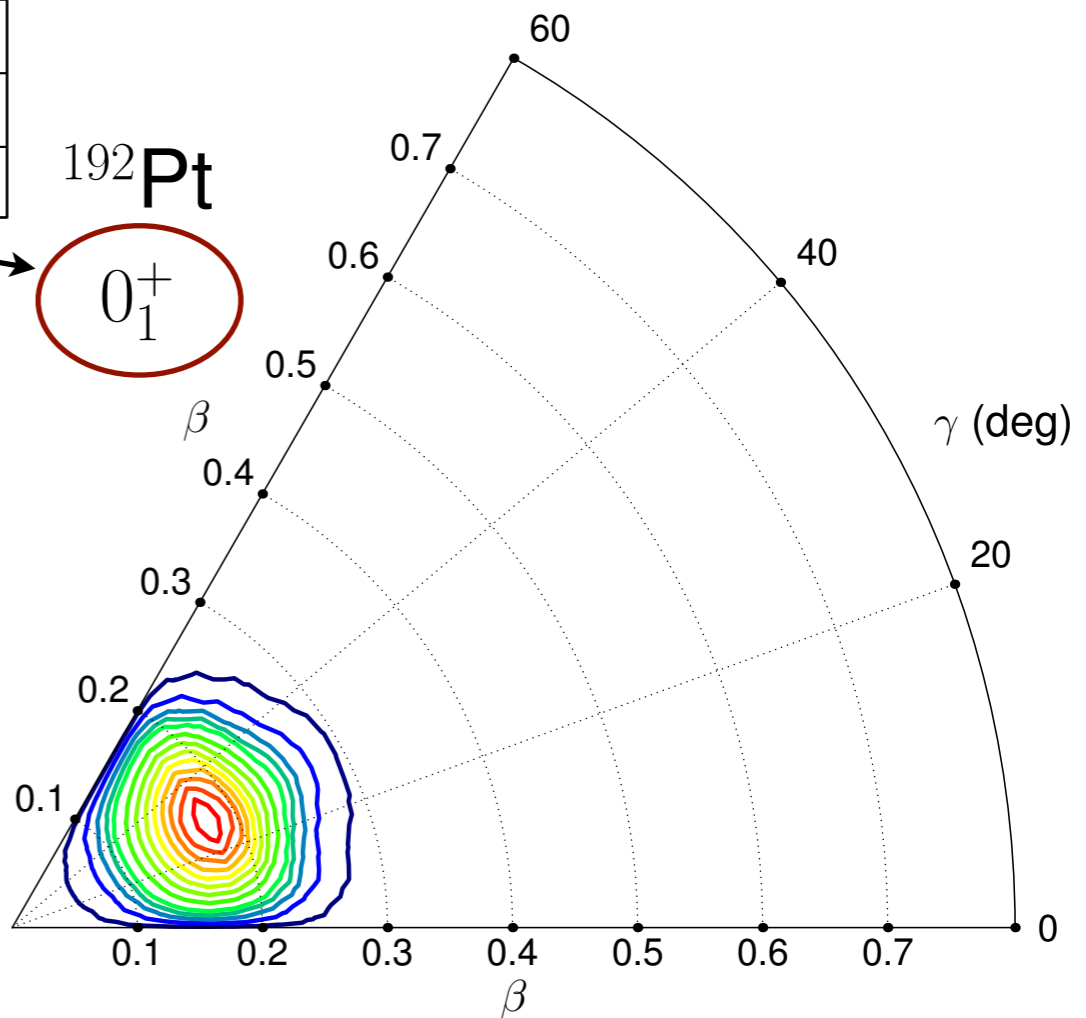
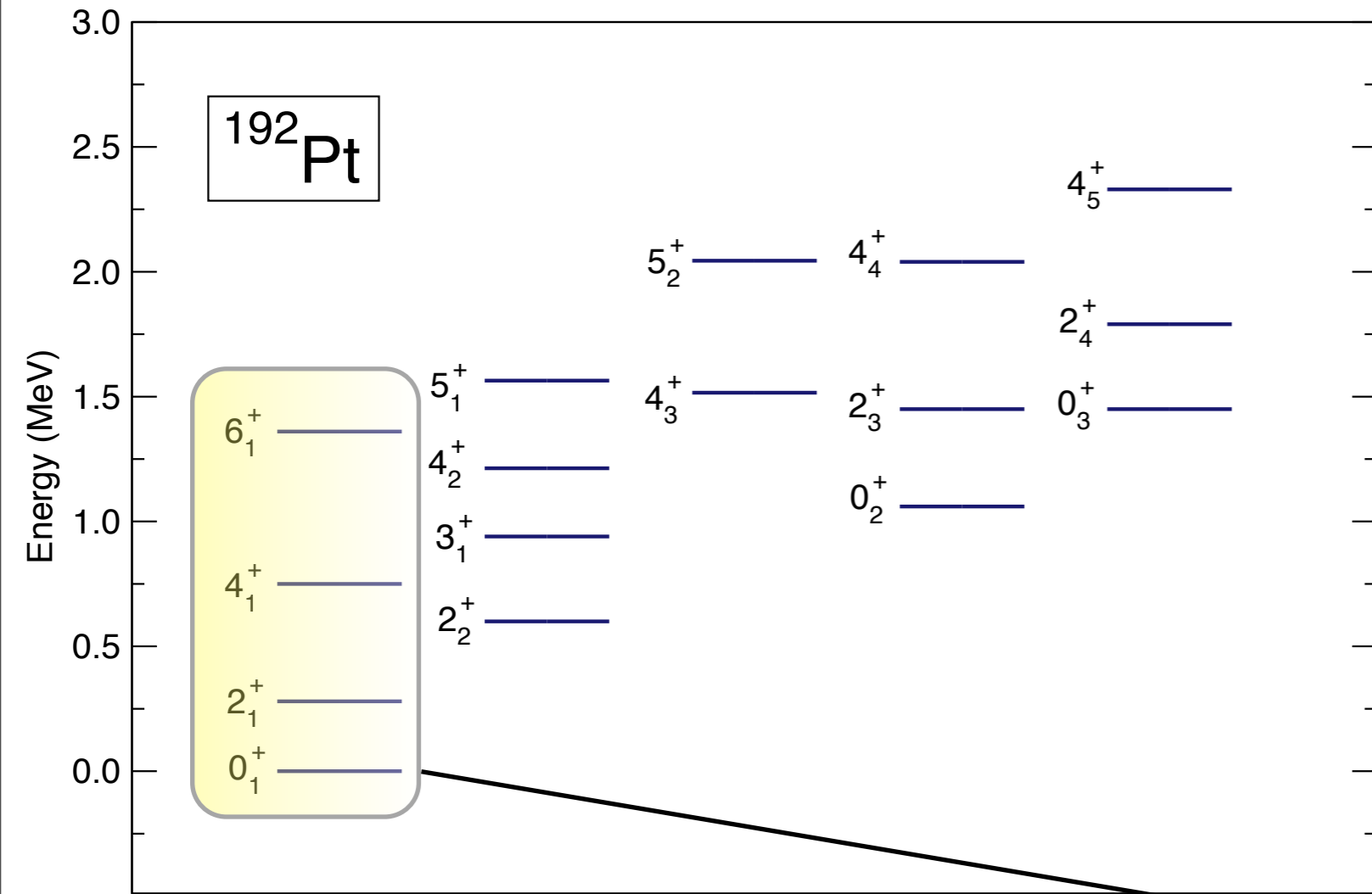
^{196}Pt



$$E_{4_1^+}^{th} / E_{2_1^+}^{th} = 2.69$$

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



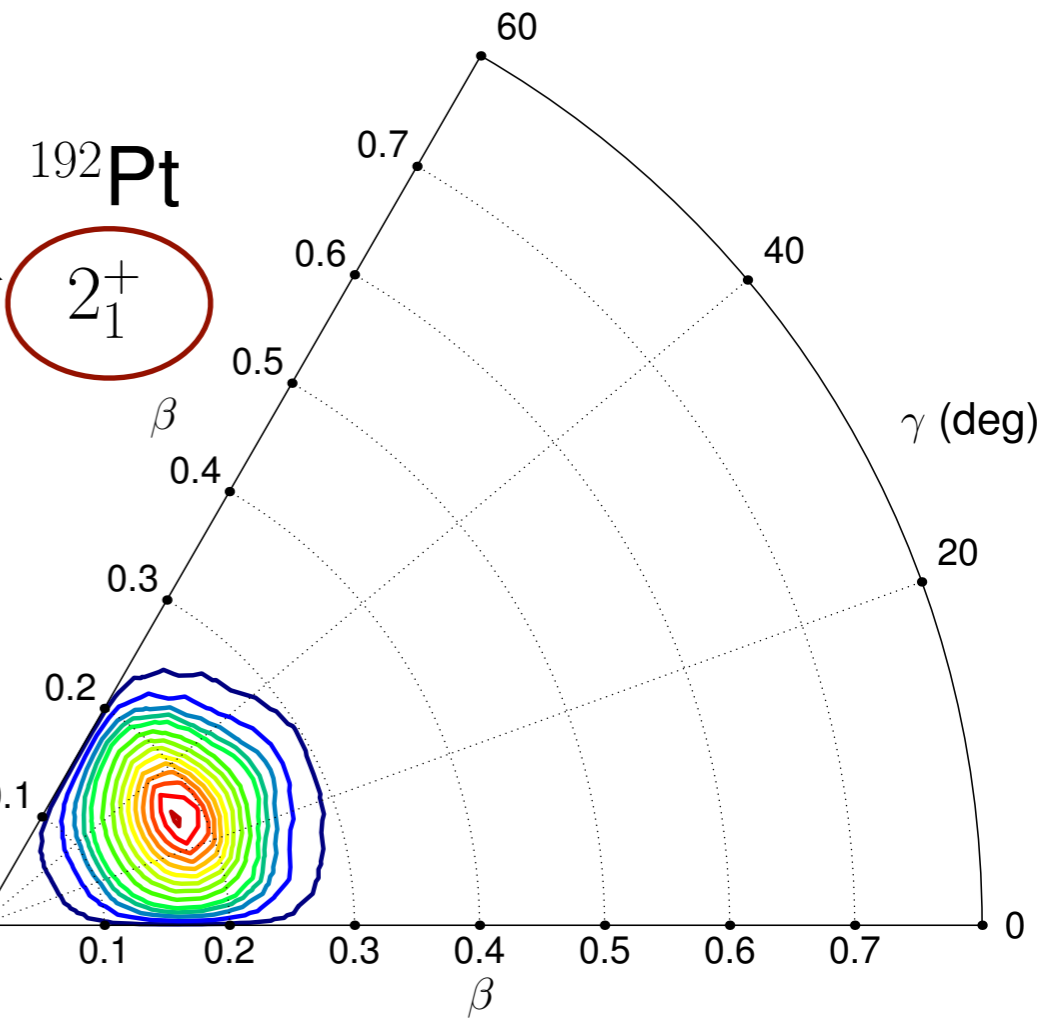
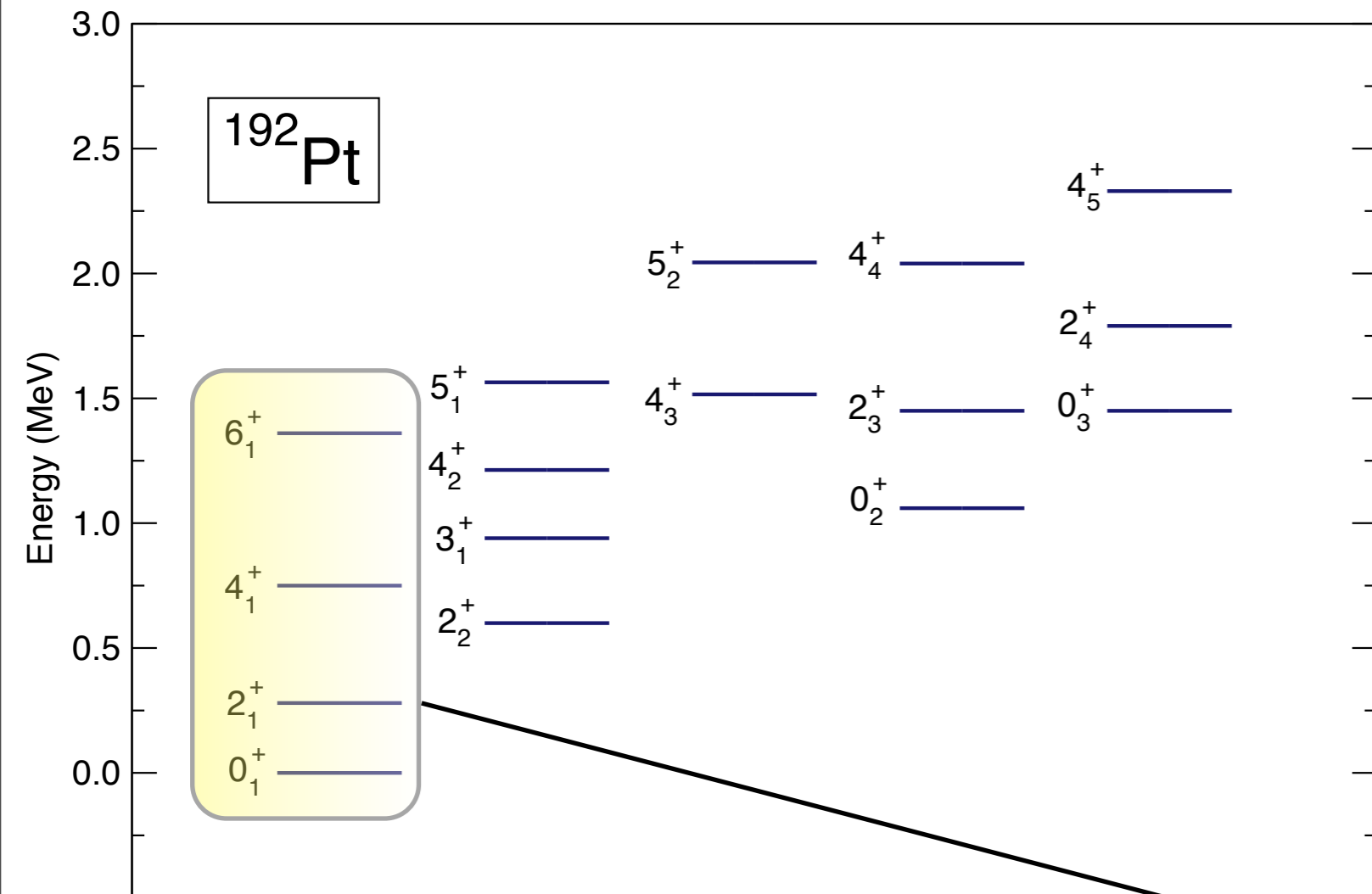


Collective wave function:

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

Probability density distribution in the (β, γ) plane:

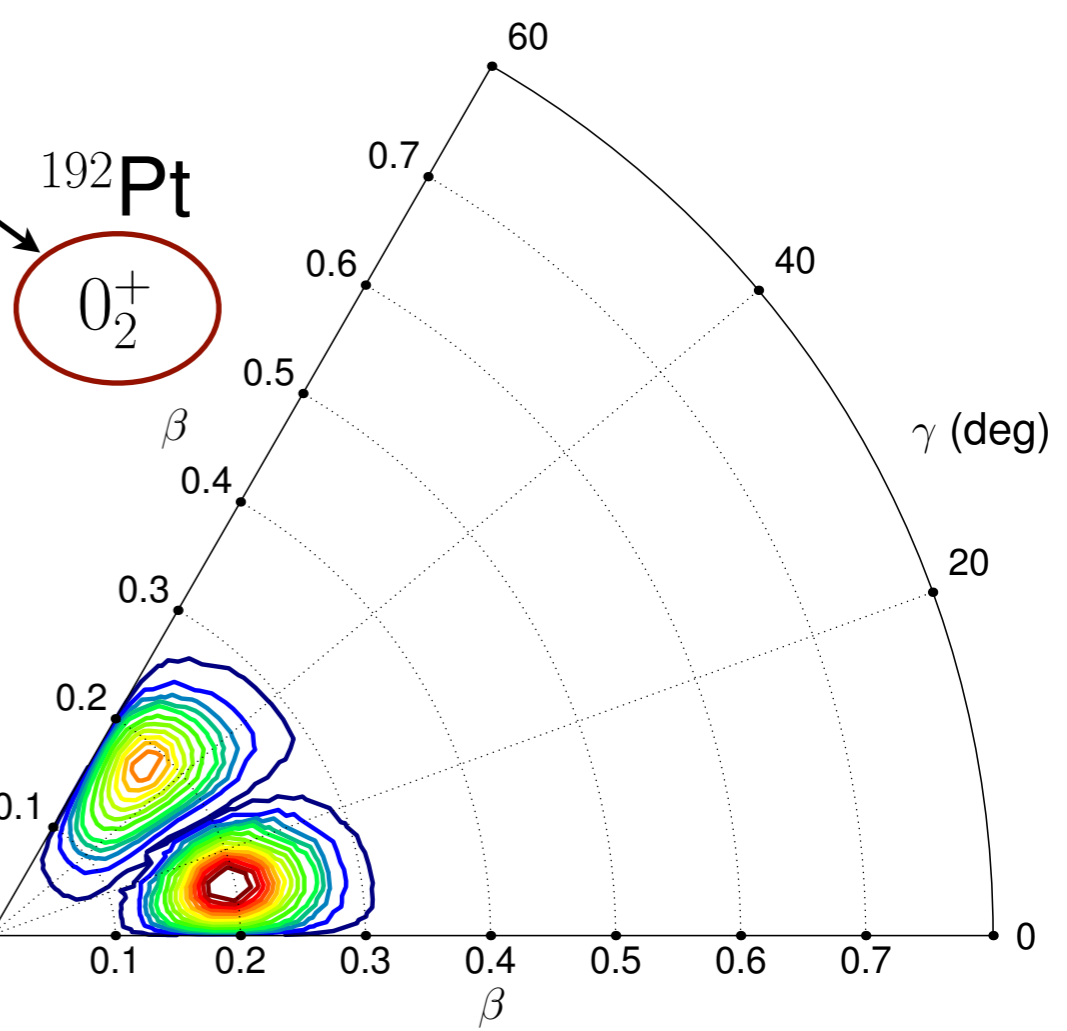
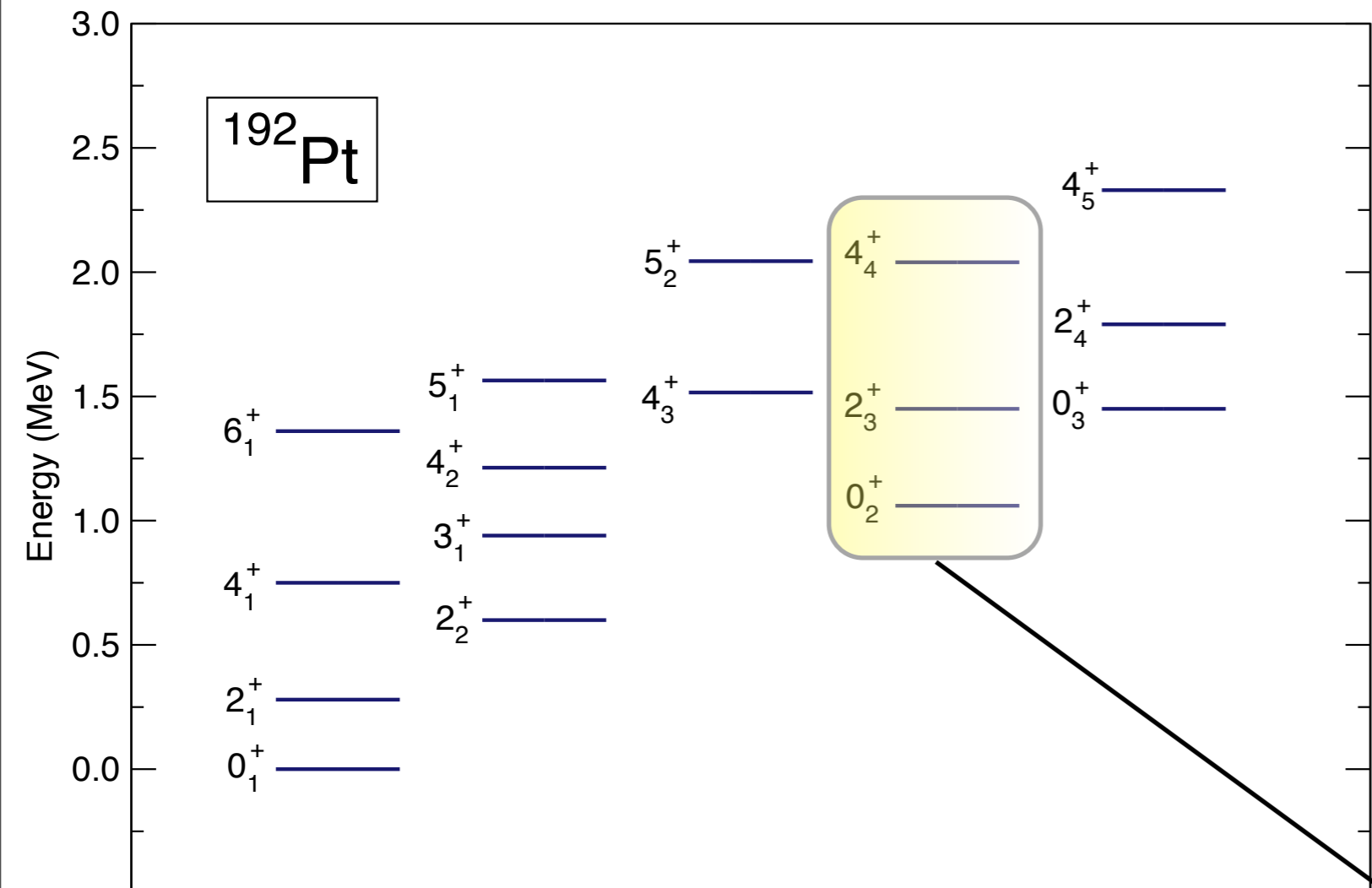
$$\rho_{I\alpha}(\beta, \gamma) = \sum_{K \in \Delta I} |\psi_{\alpha K}^I(\beta, \gamma)|^2 \beta^3 |\sin 3\gamma|$$



Probability density distribution in the (β, γ) plane:

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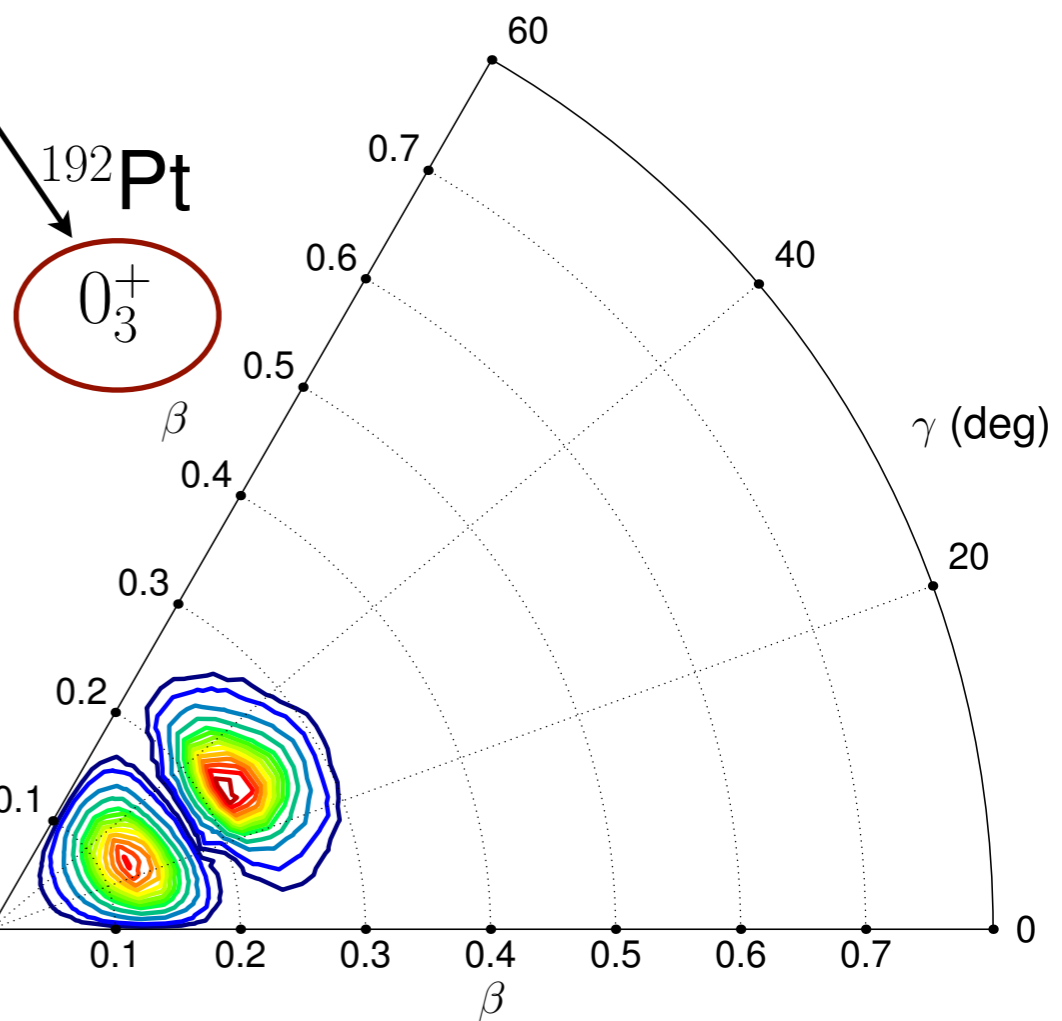
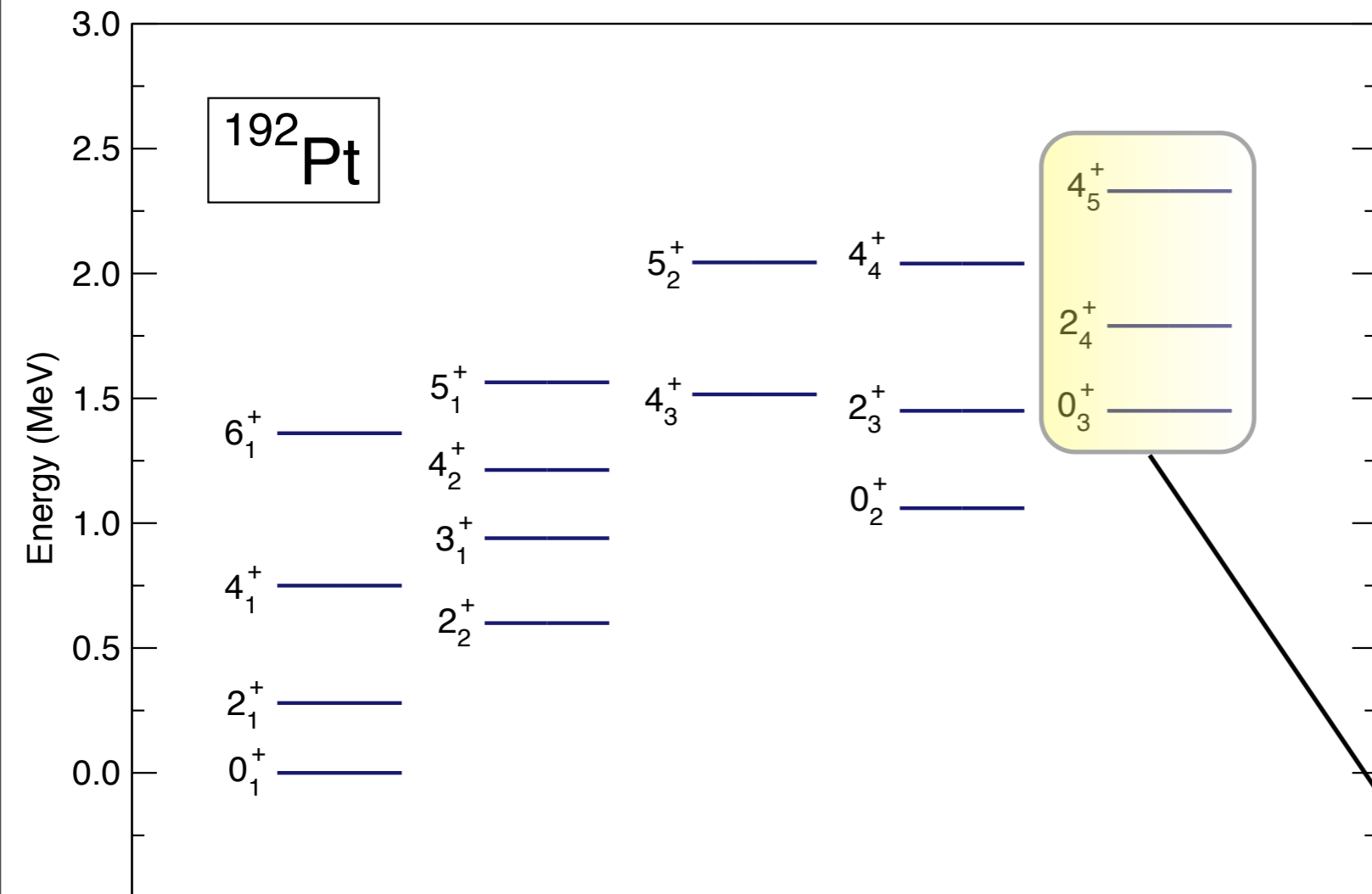
$$\int_0^\infty \beta d\beta \int_0^{2\pi} d\gamma \rho_{I\alpha}(\beta, \gamma) = 1$$



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

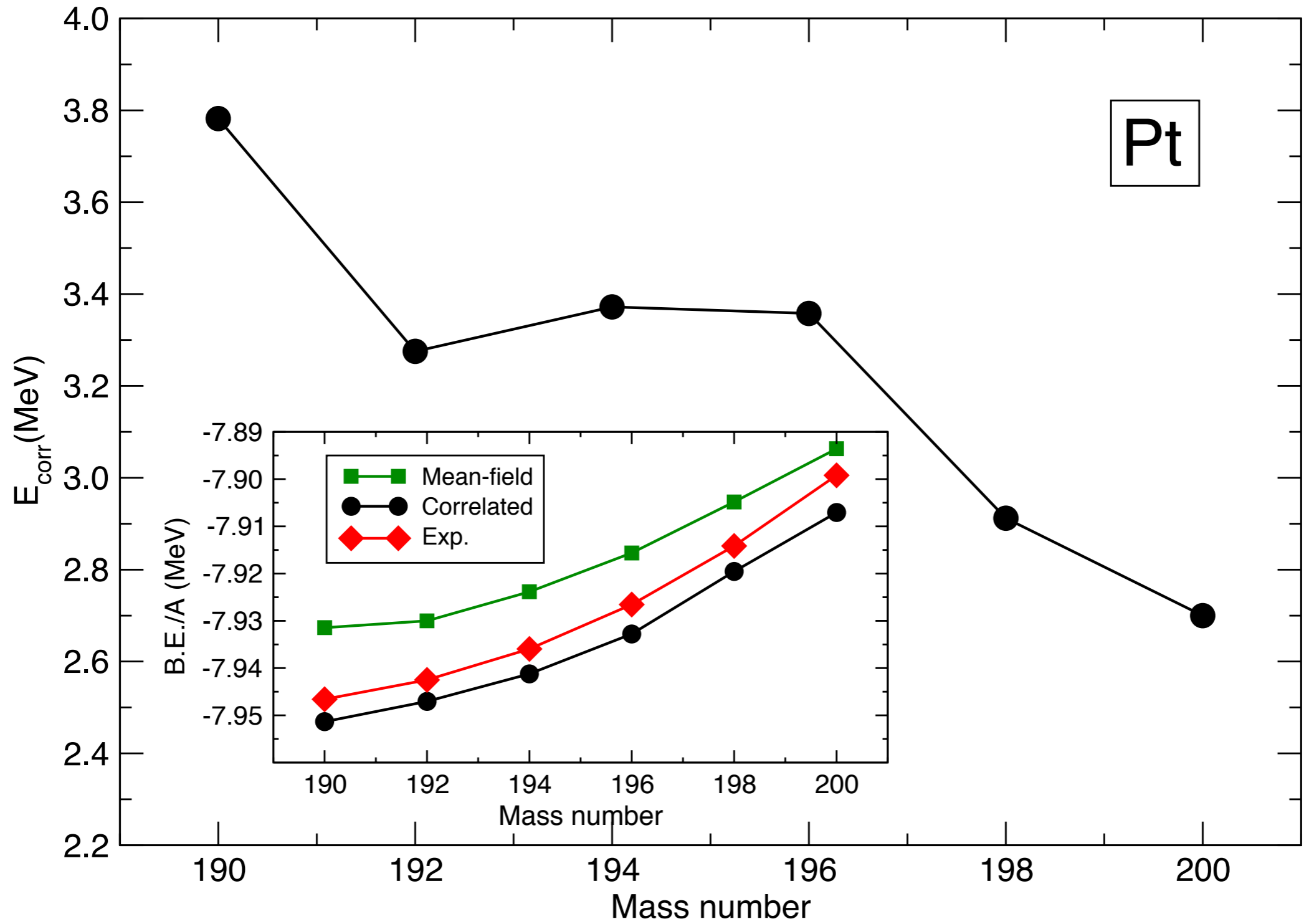
$$\int_0^\infty \beta d\beta \int_0^{2\pi} d\gamma \rho_{I\alpha}(\beta, \gamma) = 1$$



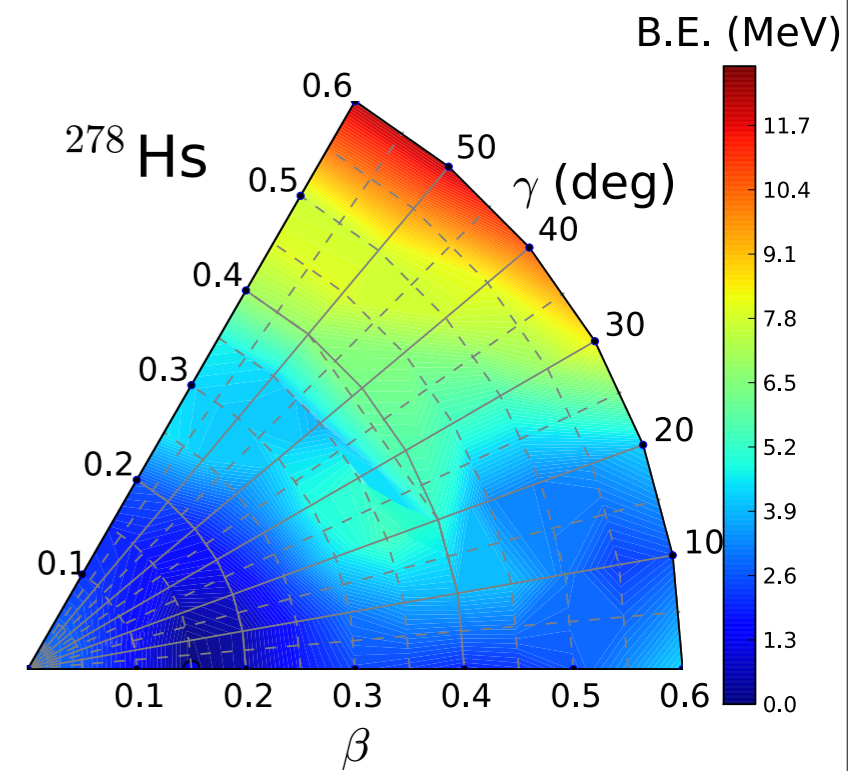
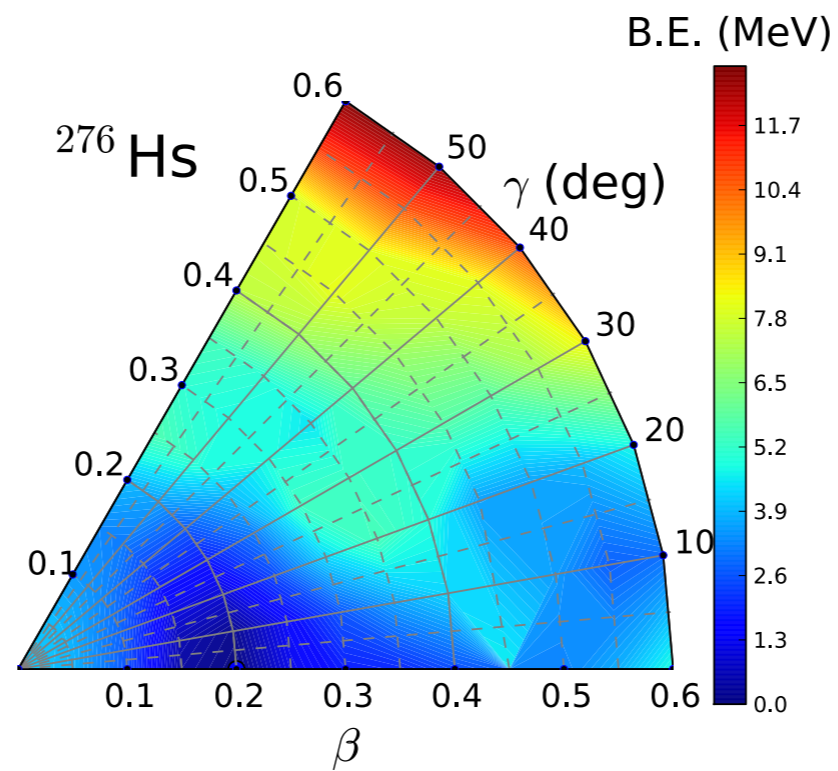
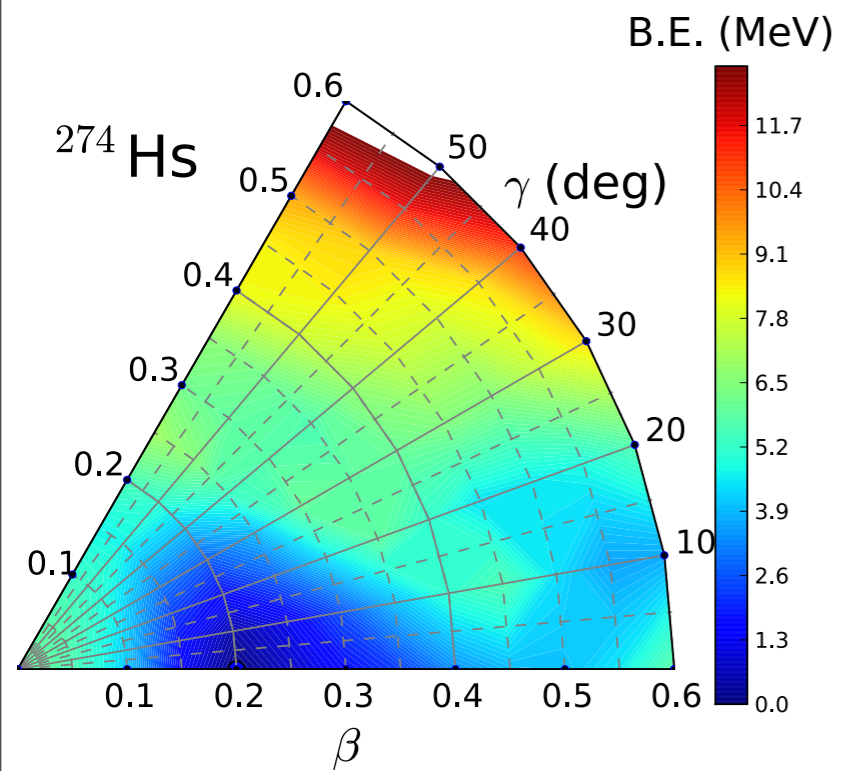
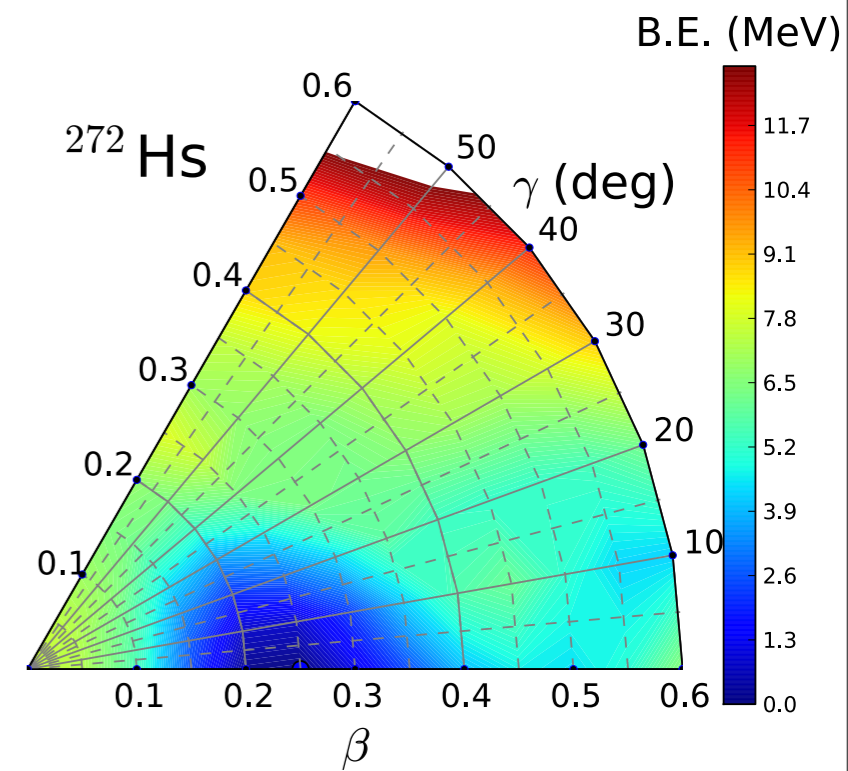
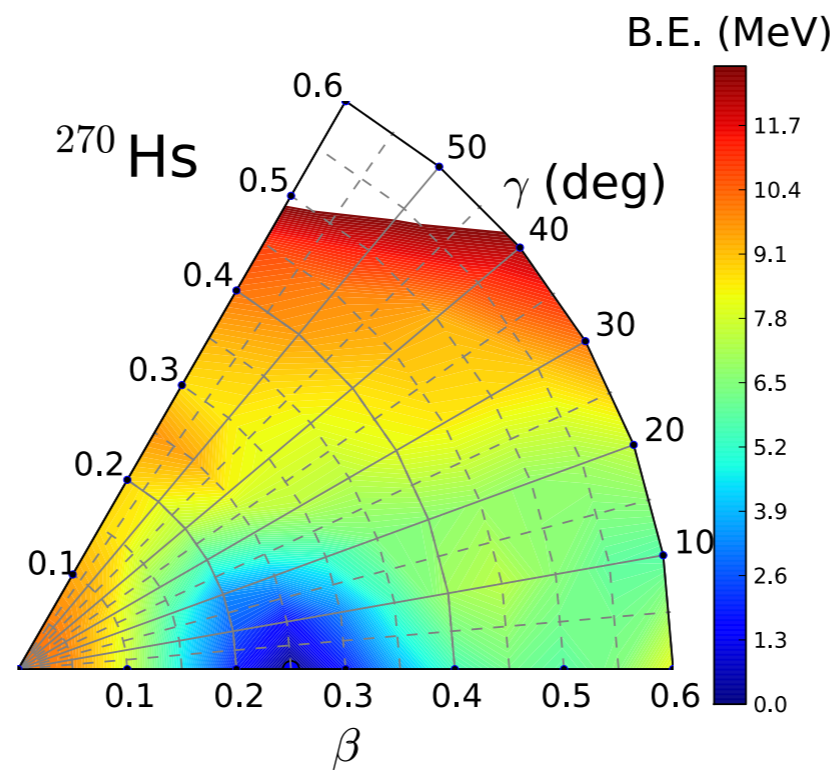
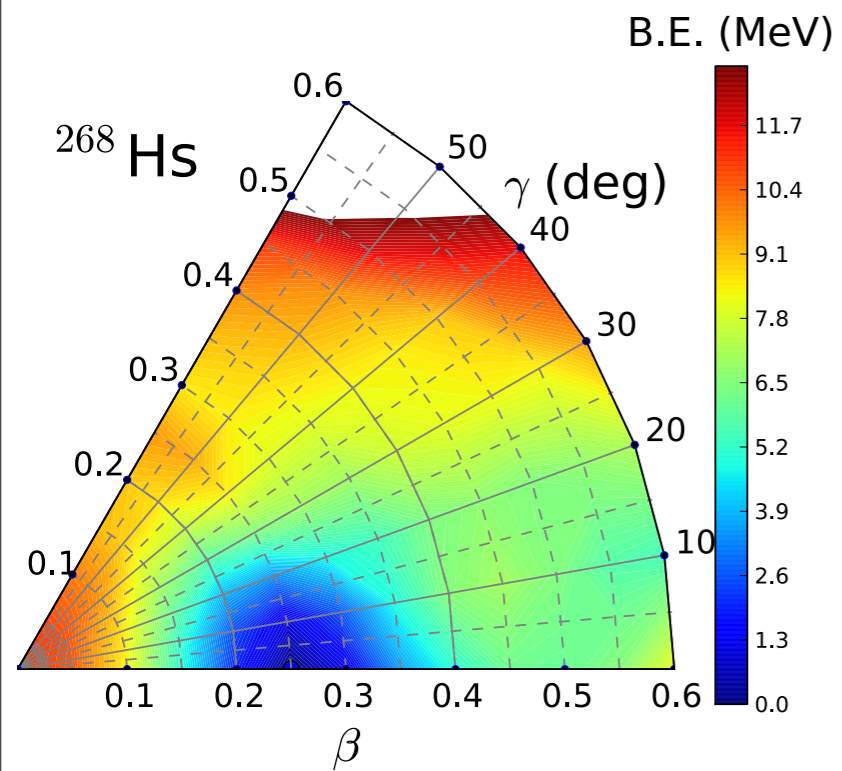
Probability density distribution in the (β, γ) plane:

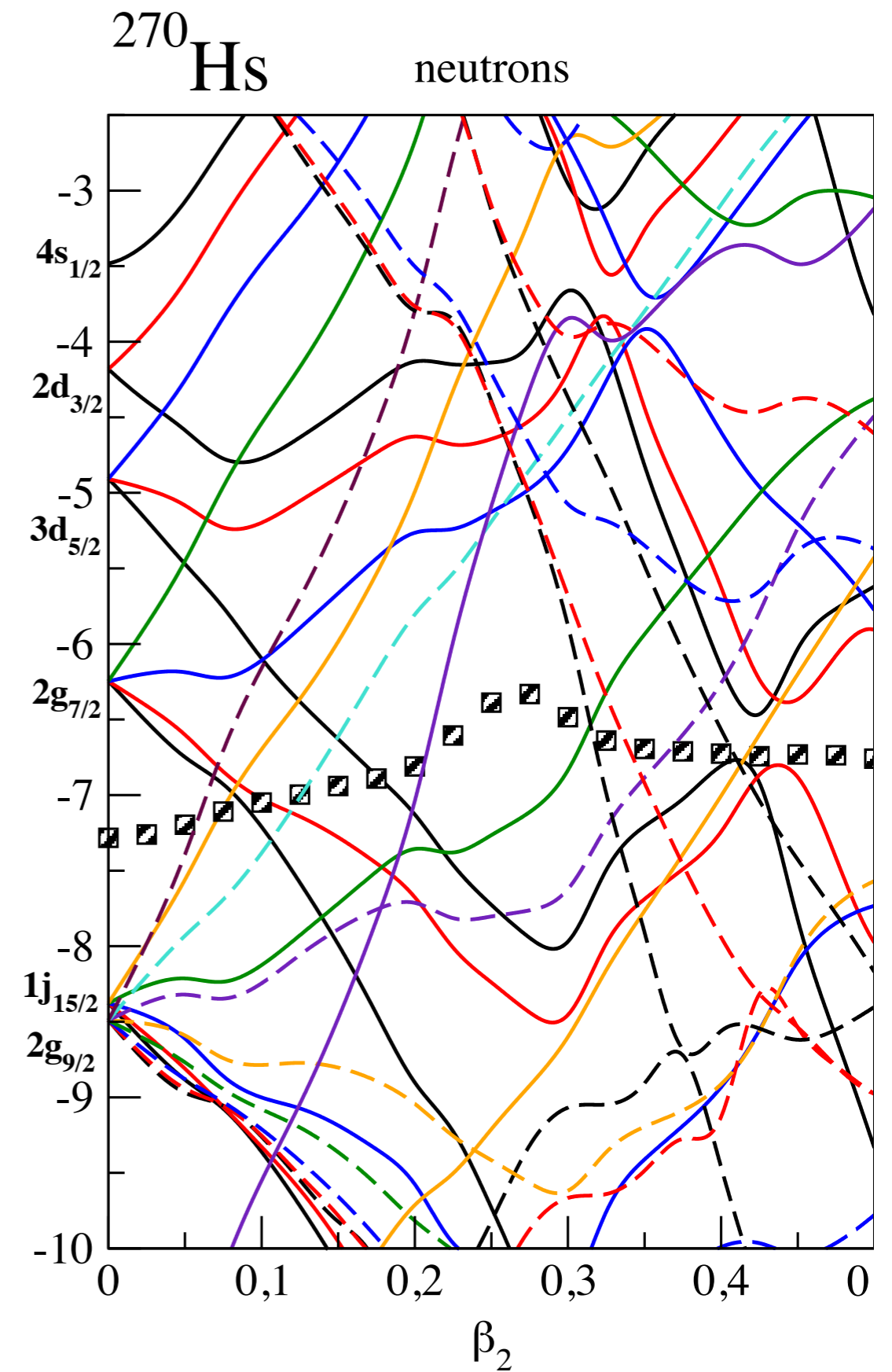
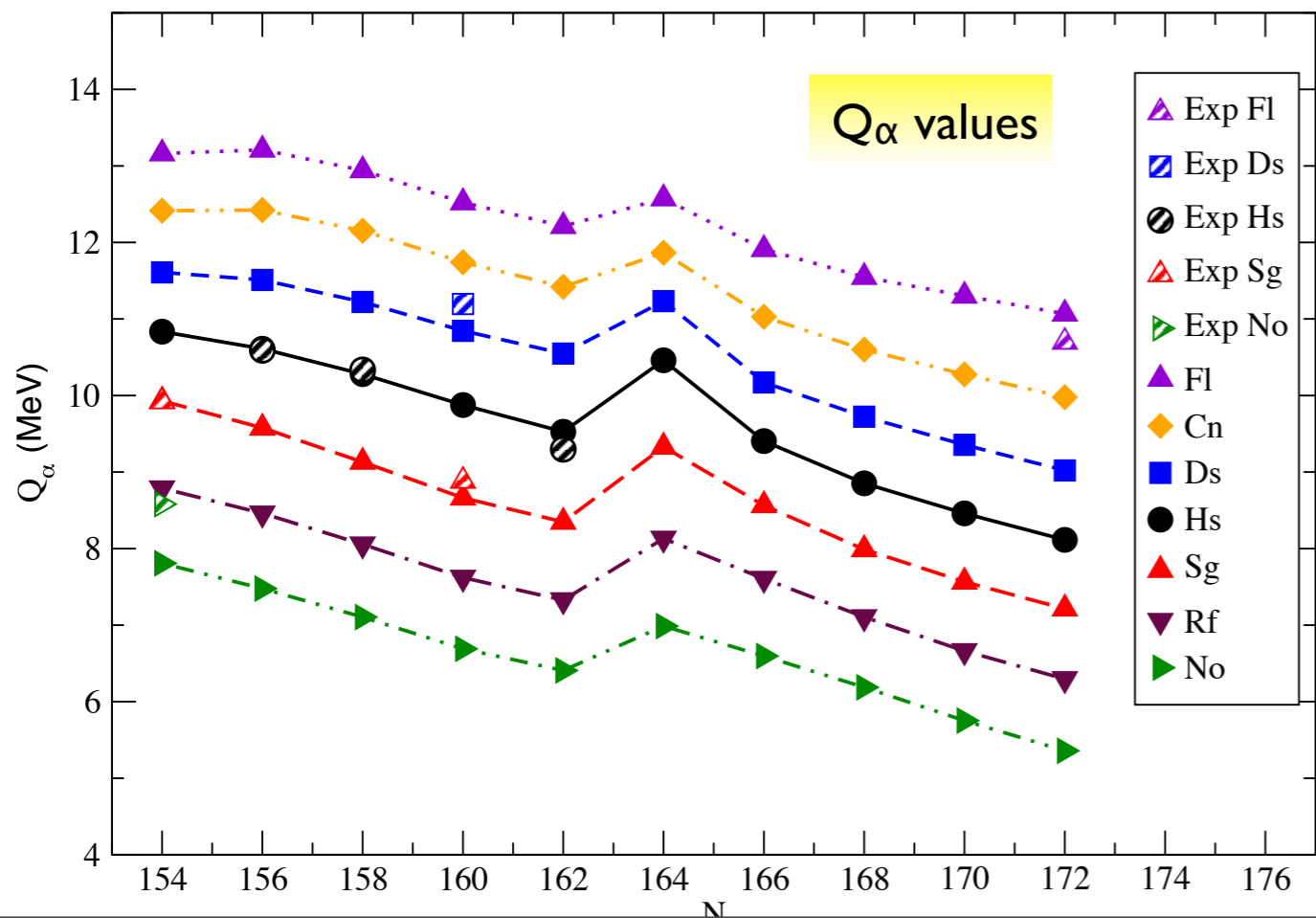
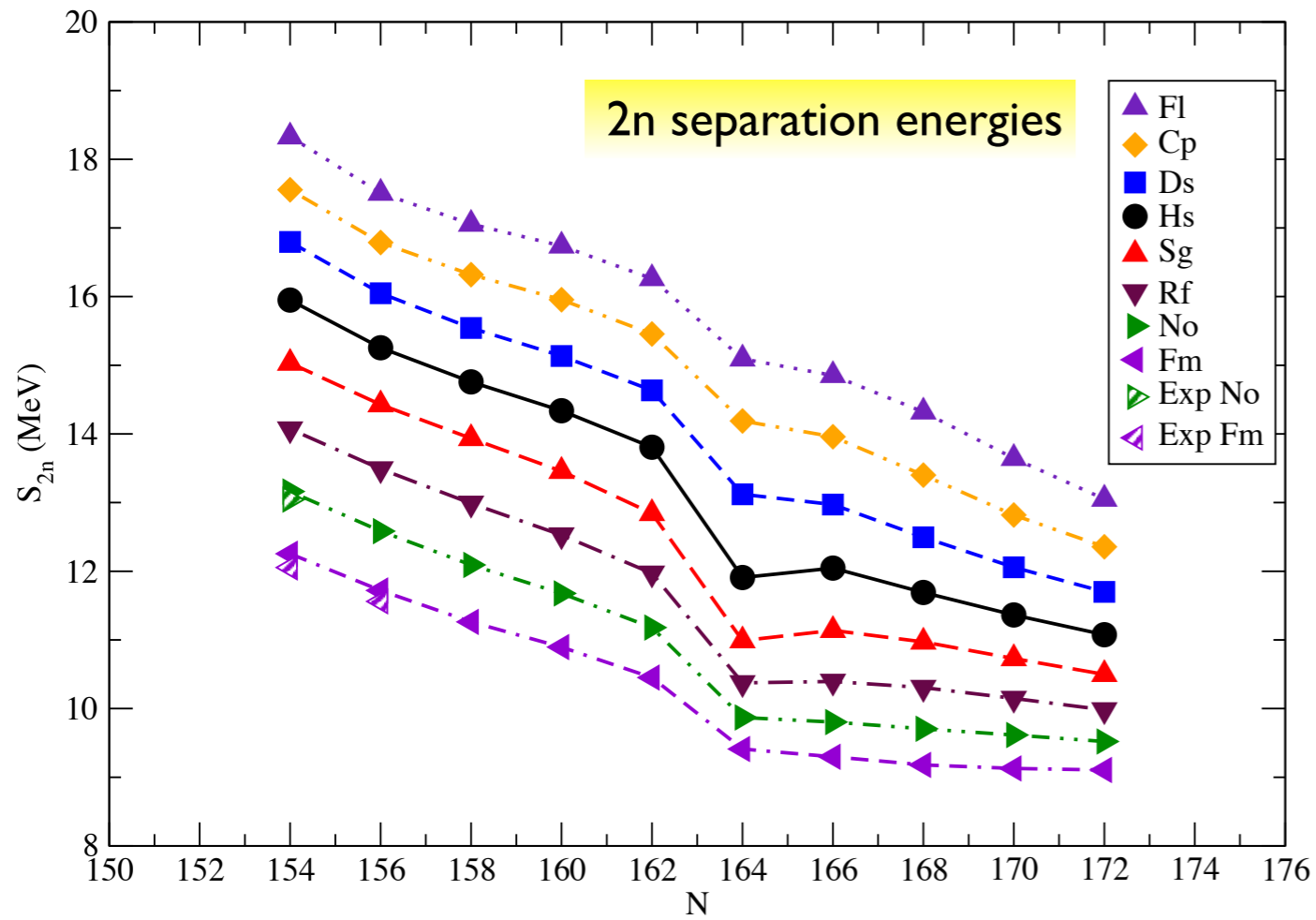
$$\rho_{I\alpha}(\beta, \gamma) = \sum_{K \in \Delta I} |\psi_{\alpha K}^I(\beta, \gamma)|^2 \beta^3 |\sin 3\gamma|$$

$$\int_0^\infty \beta d\beta \int_0^{2\pi} d\gamma \rho_{I\alpha}(\beta, \gamma) = 1$$

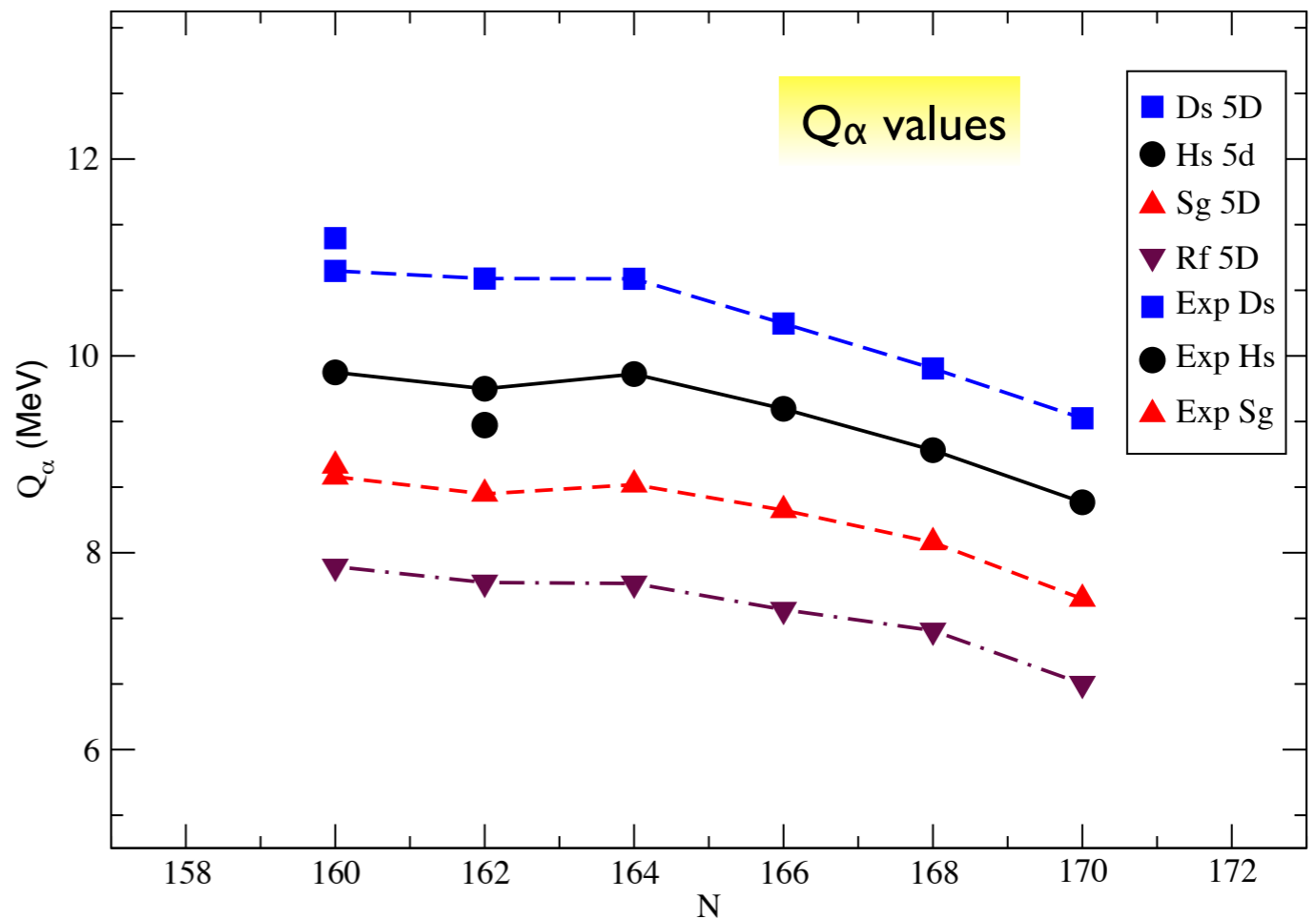
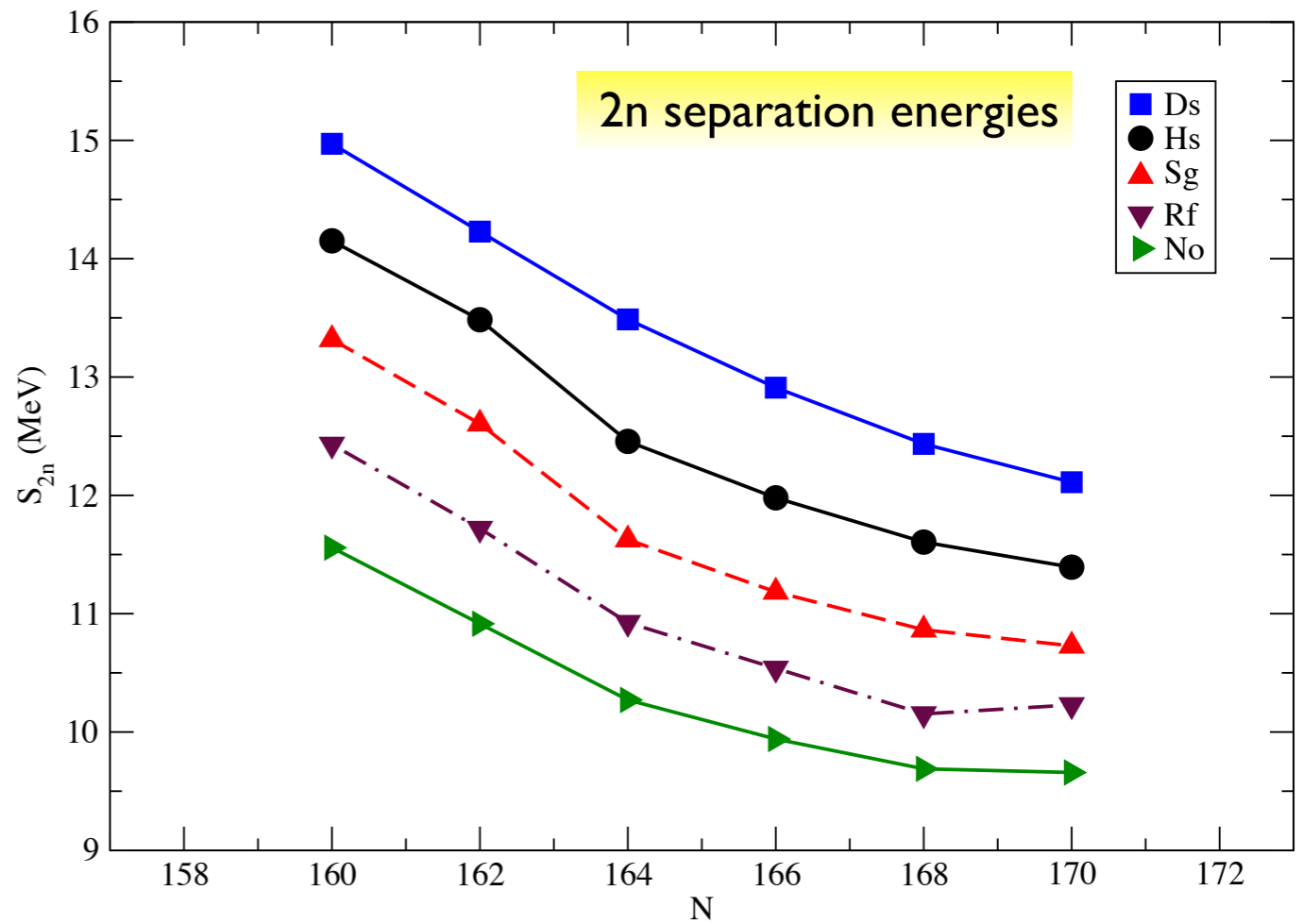


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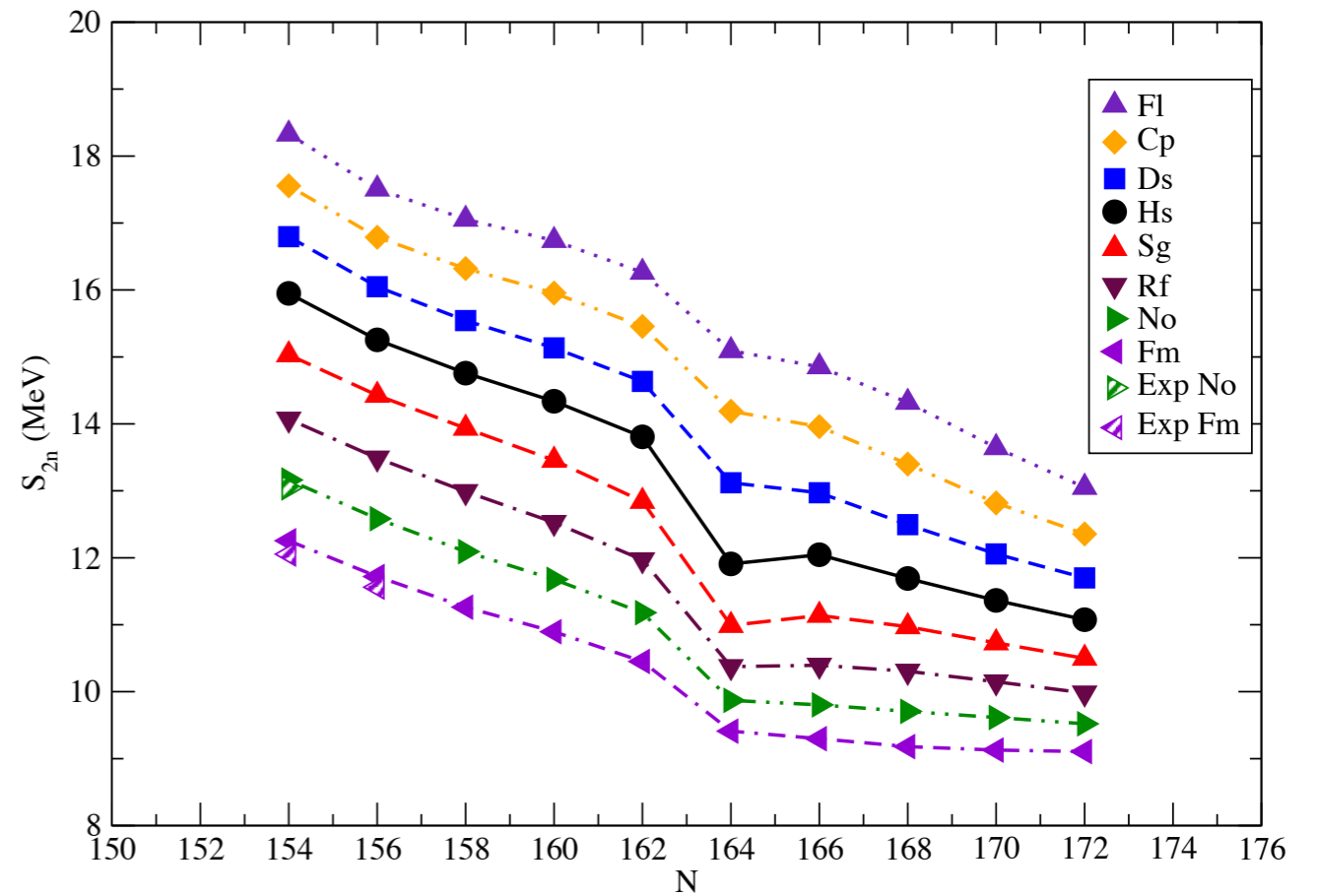


Inclusion of collective correlations \Rightarrow
 5D collective Hamiltonian

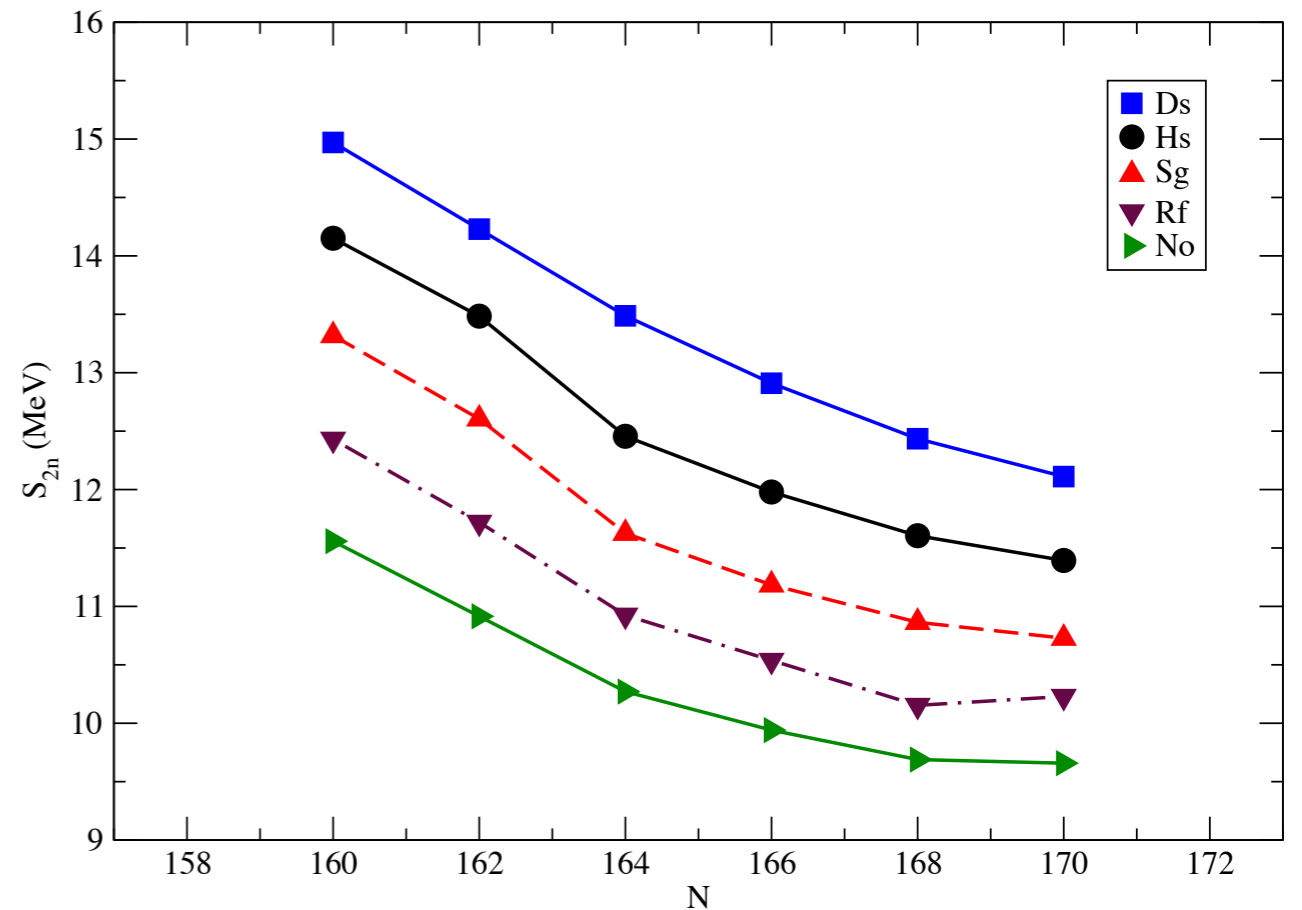


2n separation energies

Axially-deformed RHB calculation



5D collective Hamiltonian



Nuclear Energy Density Functional Framework

- ✓ unified microscopic description of the structure of stable and nuclei far from stability, and reliable extrapolations toward the drip lines.
- ✓ fully self-consistent (Q)RPA analysis of giant resonances, low-energy multipole response in weakly-bound nuclei, weak-interaction processes.
- ✓ extended to take into account collective correlations → quantitative description of ground-state properties, excitation spectra and electromagnetic transition rates.