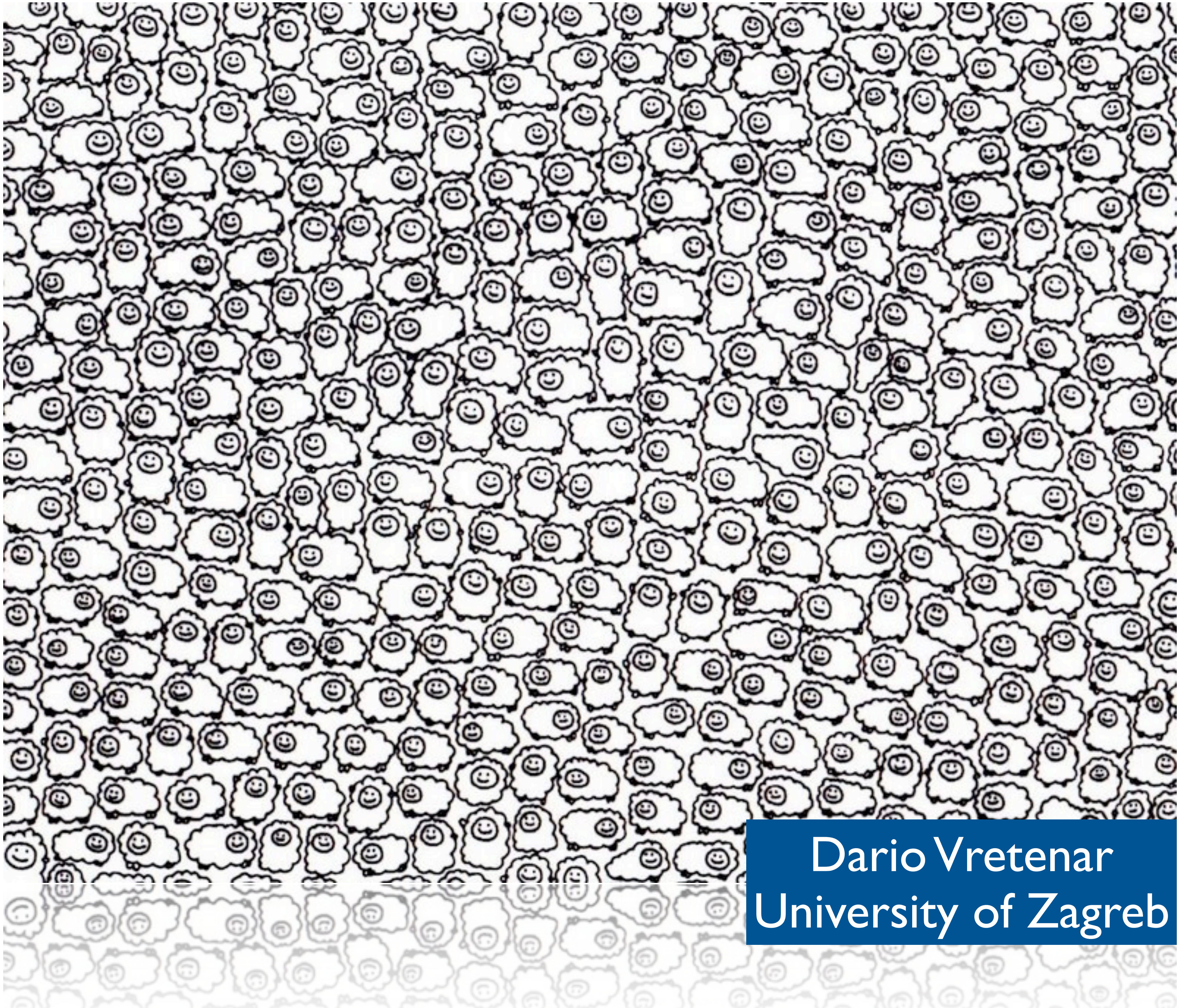
Relativistic EDFs: 5D Collective Hamiltonian



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Relativistic energy density functionals:

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

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

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

$$j_\mu = \langle\phi_0|\overline{\psi}\gamma_\mu\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\gamma_\mu\psi_k \ ,$$

$$\vec{j}_\mu = \langle\phi_0|\overline{\psi}\gamma_\mu\vec{\tau}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\gamma_\mu\vec{\tau}\psi_k \ ,$$

$$\rho_S = \langle\phi_0|\overline{\psi}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\psi_k \ ,$$

$$\vec{\rho}_S = \langle\phi_0|\overline{\psi}\vec{\tau}\psi|\phi_0\rangle = \sum_k \overline{\psi}_k\vec{\tau}\psi_k$$

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:

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

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

a_i ↙ Hartree

$(b_i + c_i x)e^{-d_i x}$ ↘ correlations

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

Semi-phenomenological functionals

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

... start from a favorite microscopic nuclear matter EOS

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

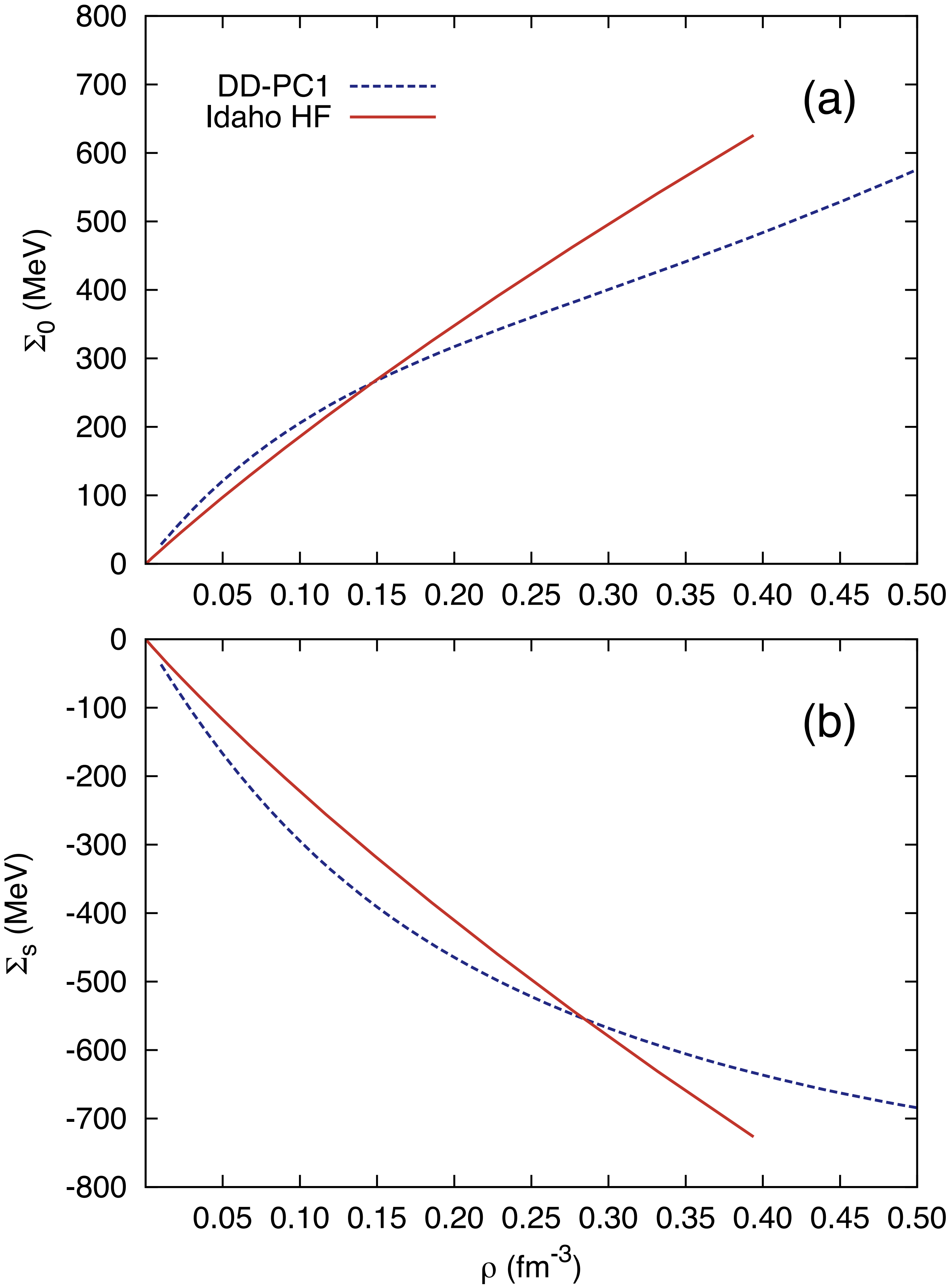
DD-PC1

... 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 ~ 150-180 and A ~ 230-250.

Density dependence of the DD-PC1 isoscalar vector and scalar nucleon self-energies in symmetric nuclear matter.

Starting approximation: Hartree-Fock self-energies calculated from the Idaho N^3LO NN-potential.



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

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

... 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:

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

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

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

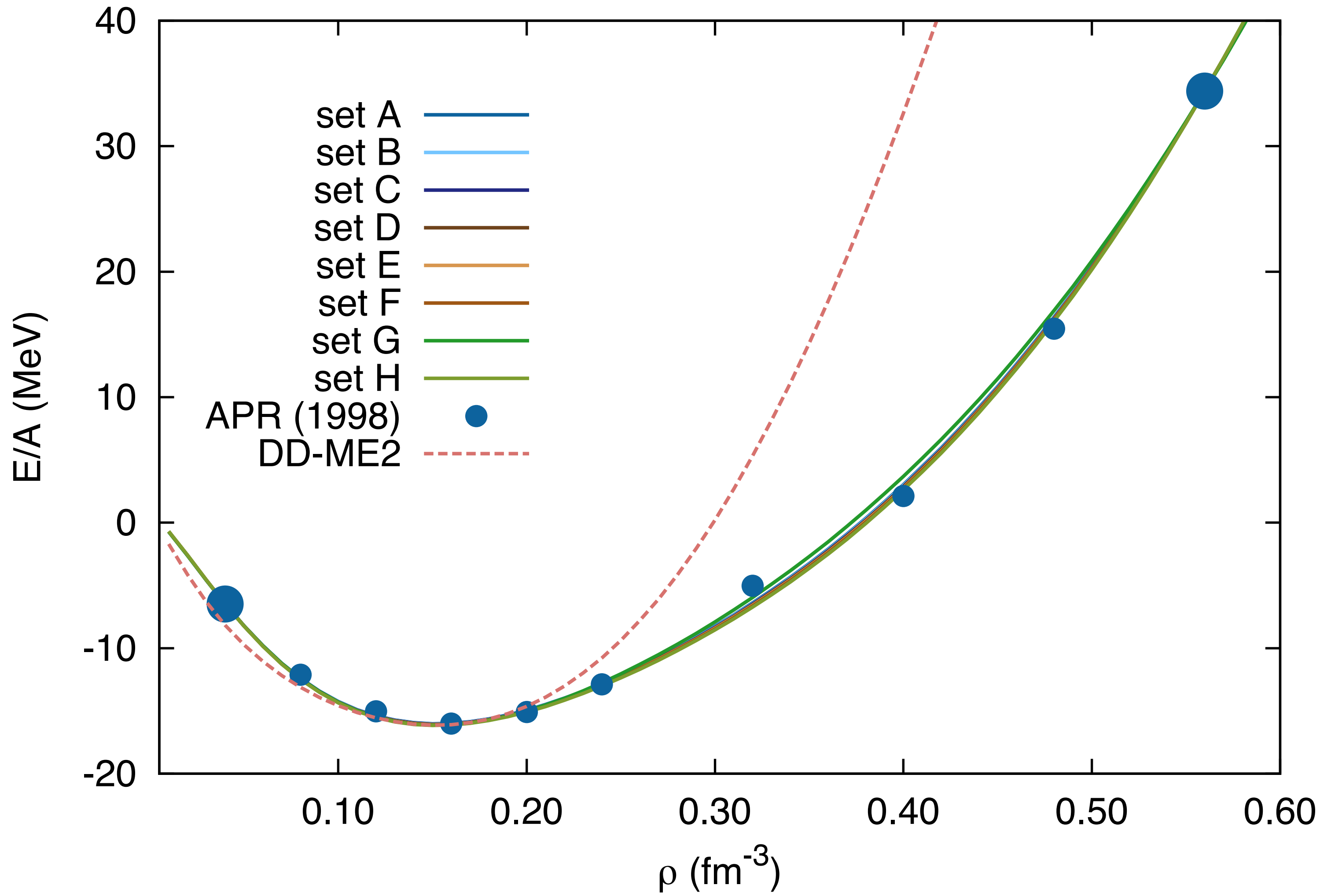
DD-ME1, DD-ME2

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:

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

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

Deformed nuclei

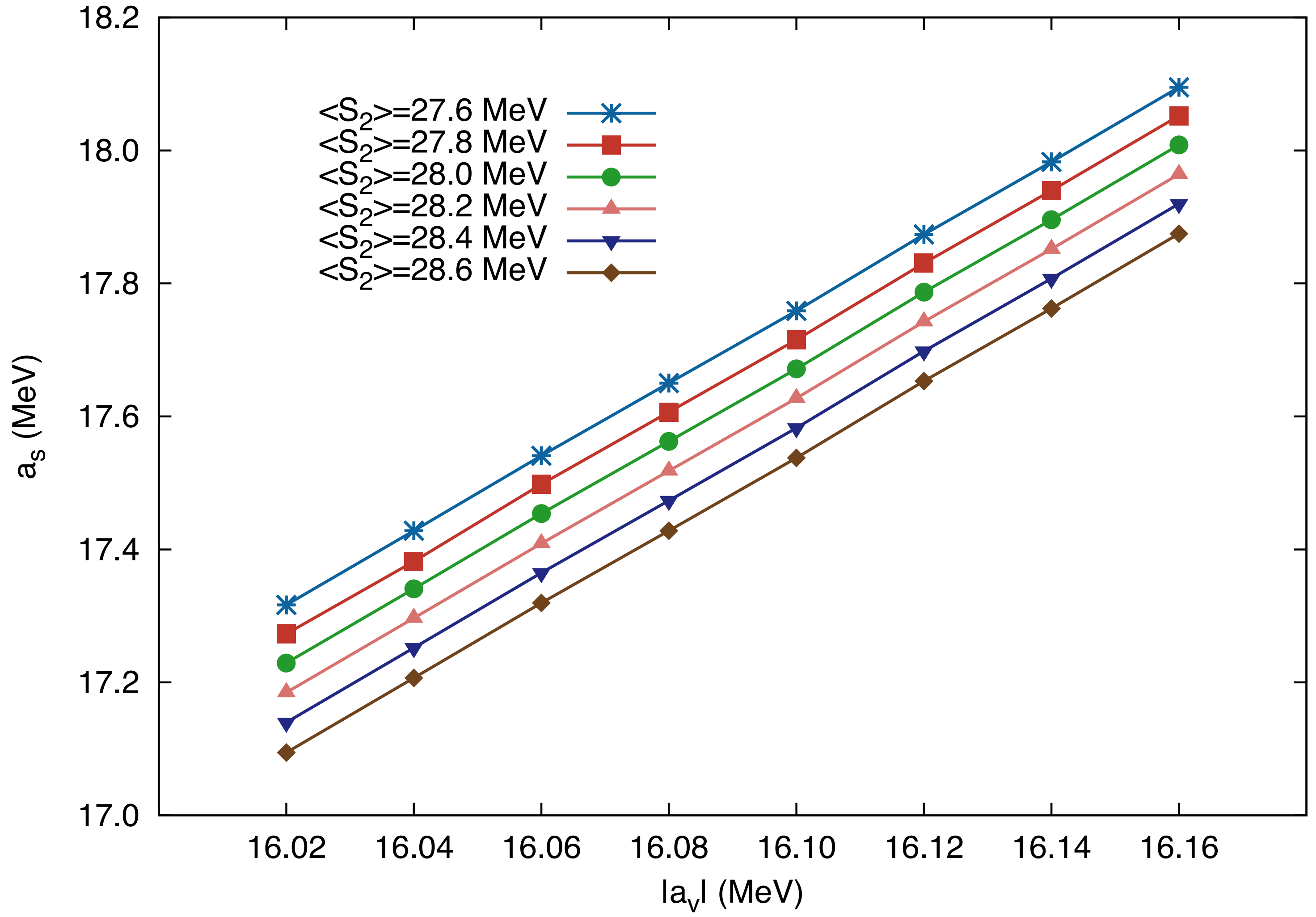
Binding energies used to adjust the parameters of the functional:

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.

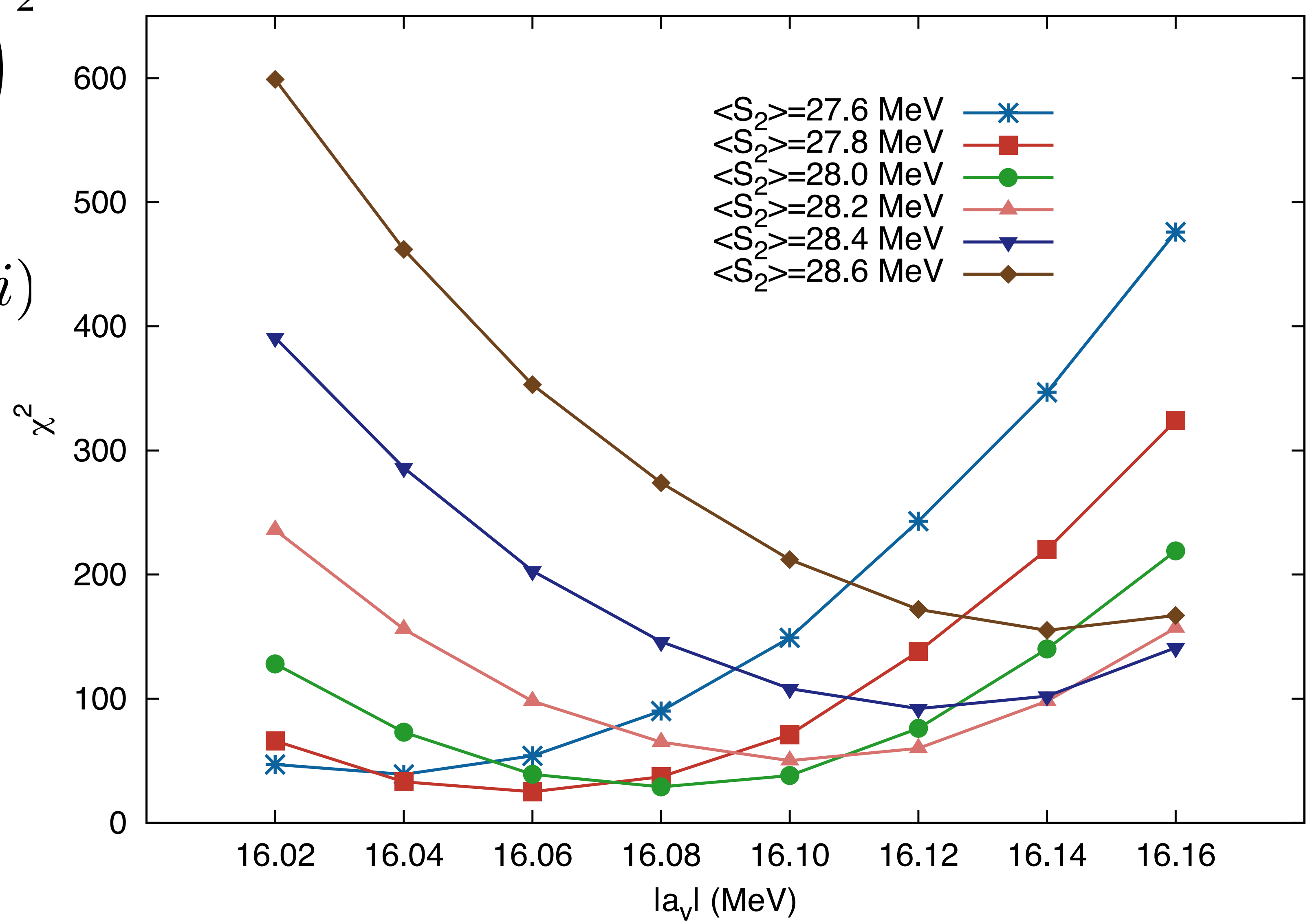
Required accuracy 0.05% ⇒ absolute error of ±1 MeV for the total binding energy



... 48 parameterizations of the energy density functional:

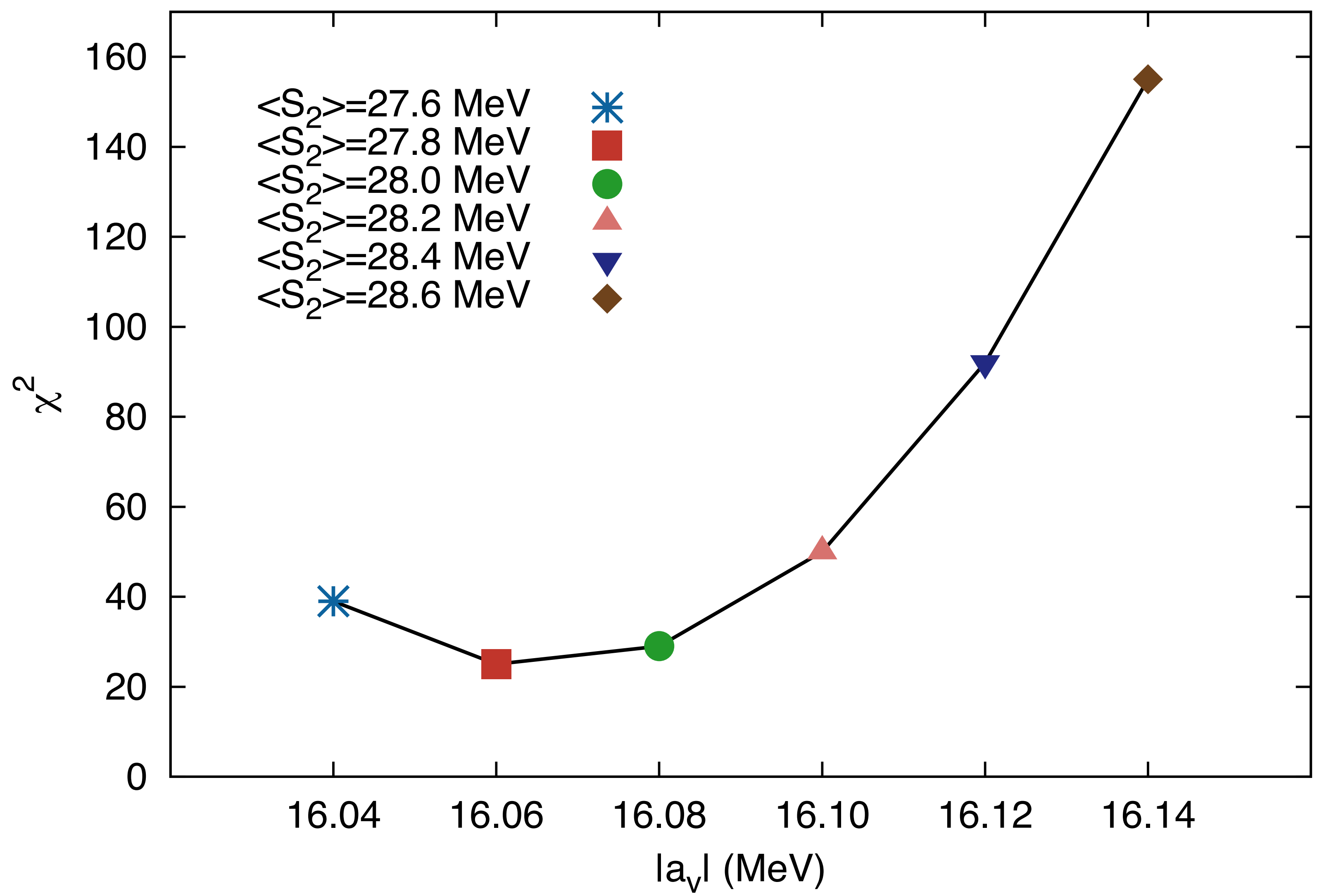
$$\chi^2 = \sum_i \left(\frac{E_B^{th}(i) - E_B^{exp}(i)}{\Delta E_B^{exp}(i)} \right)^2$$

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



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.

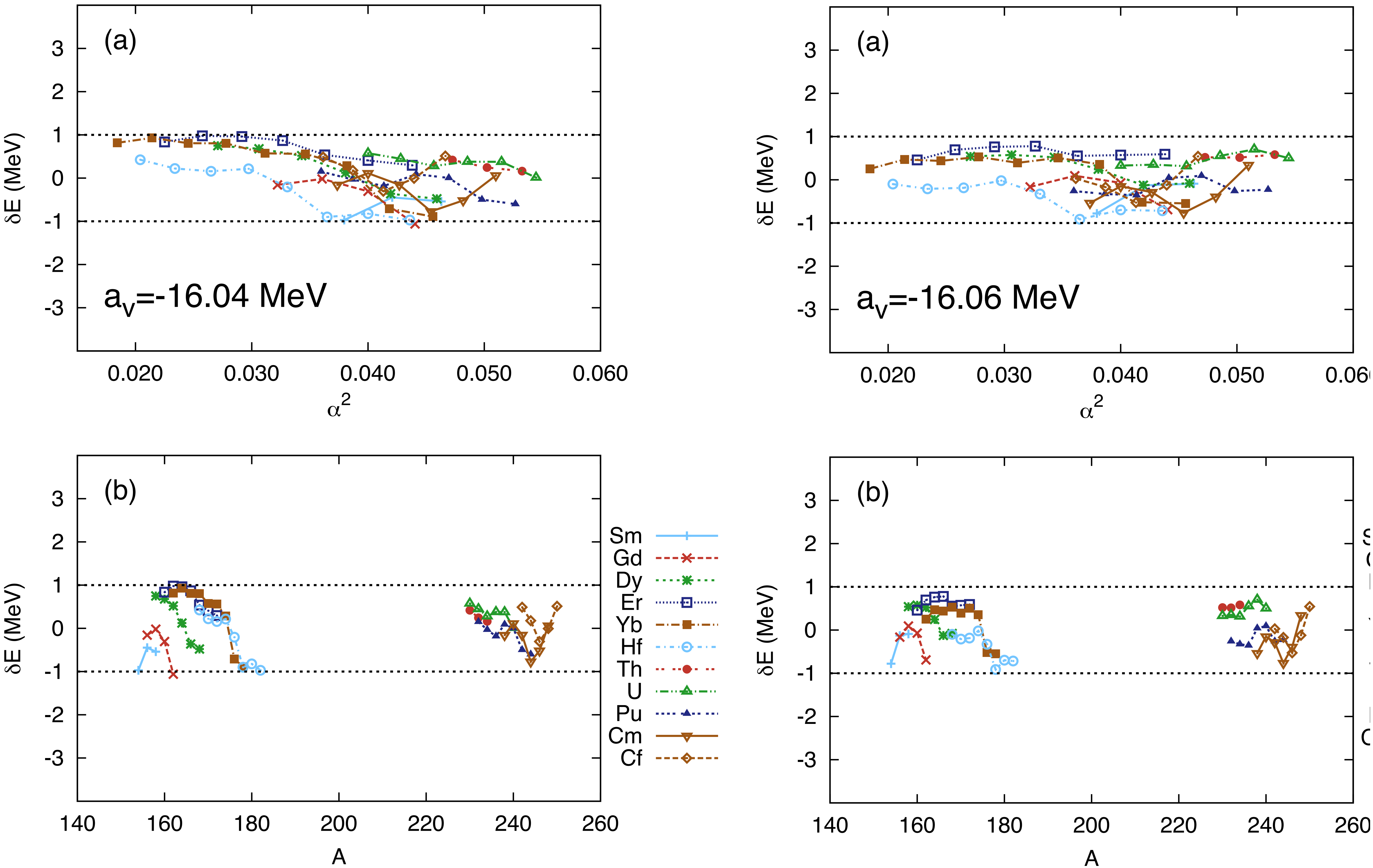
The minimum χ^2-deviation of the theoretical binding energies from data, as a function of the volume energy coefficient:



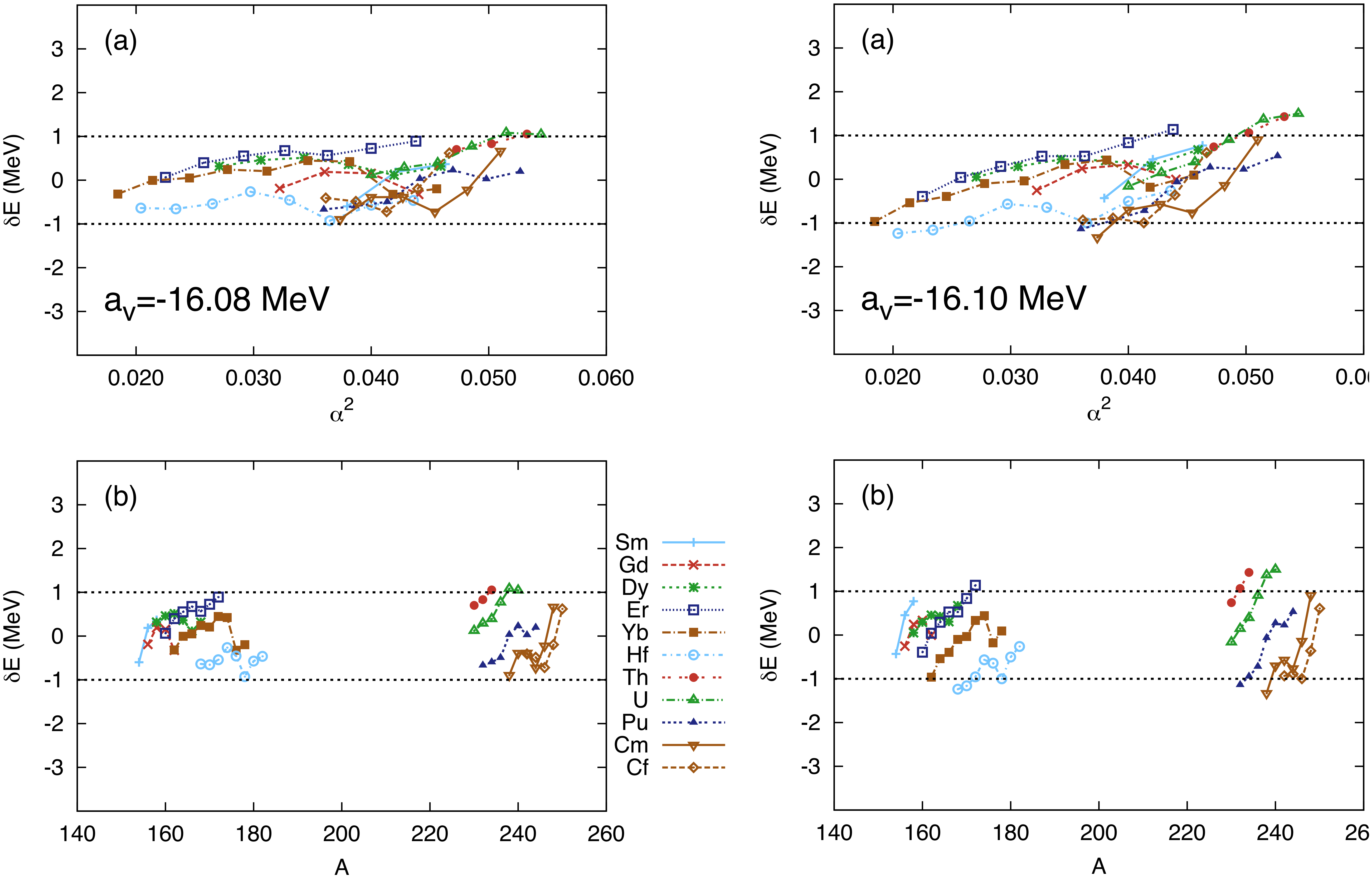
Absolute minimum:

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

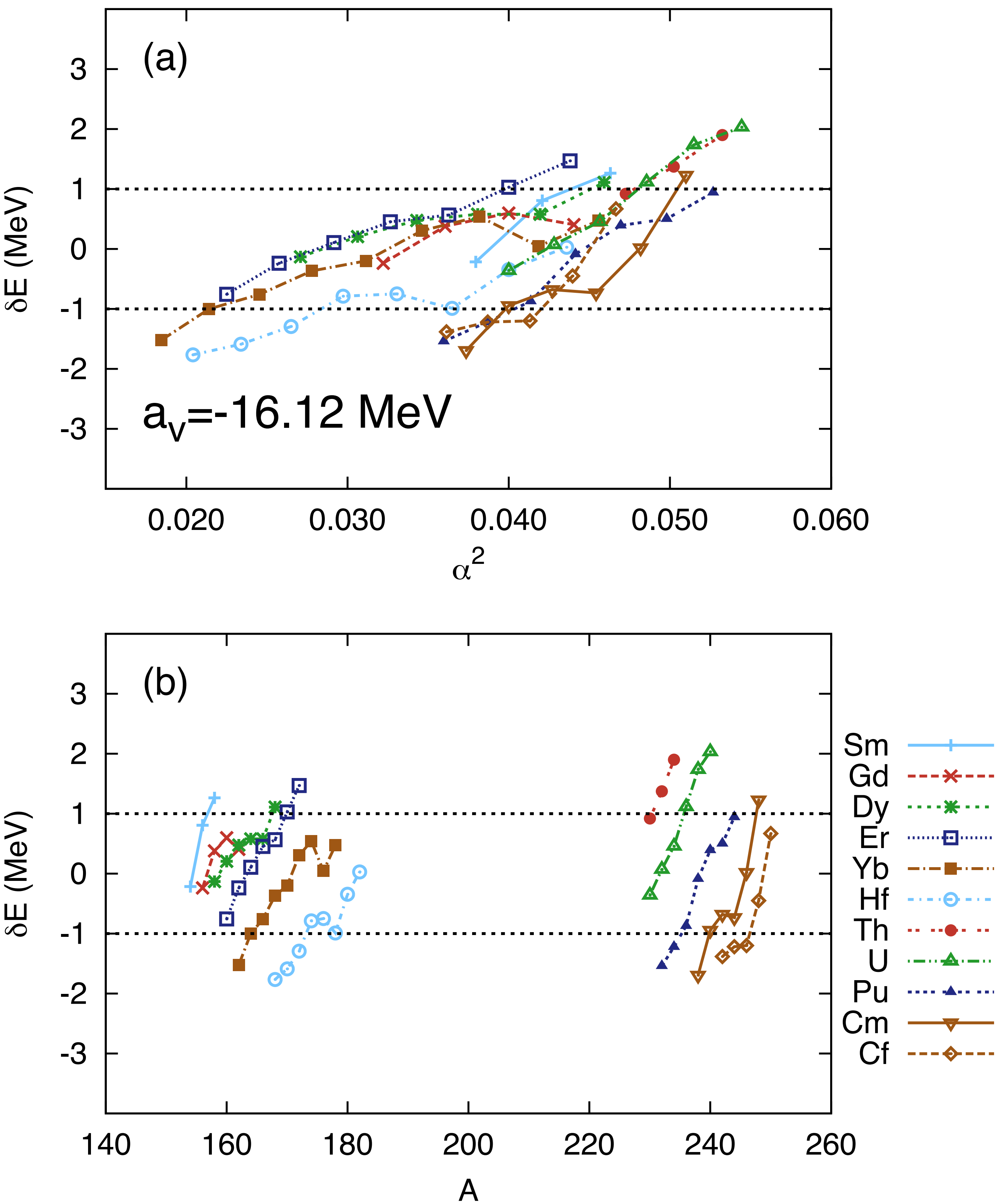
Absolute deviations of the calculated binding energies from data for 64 axially deformed nuclei:

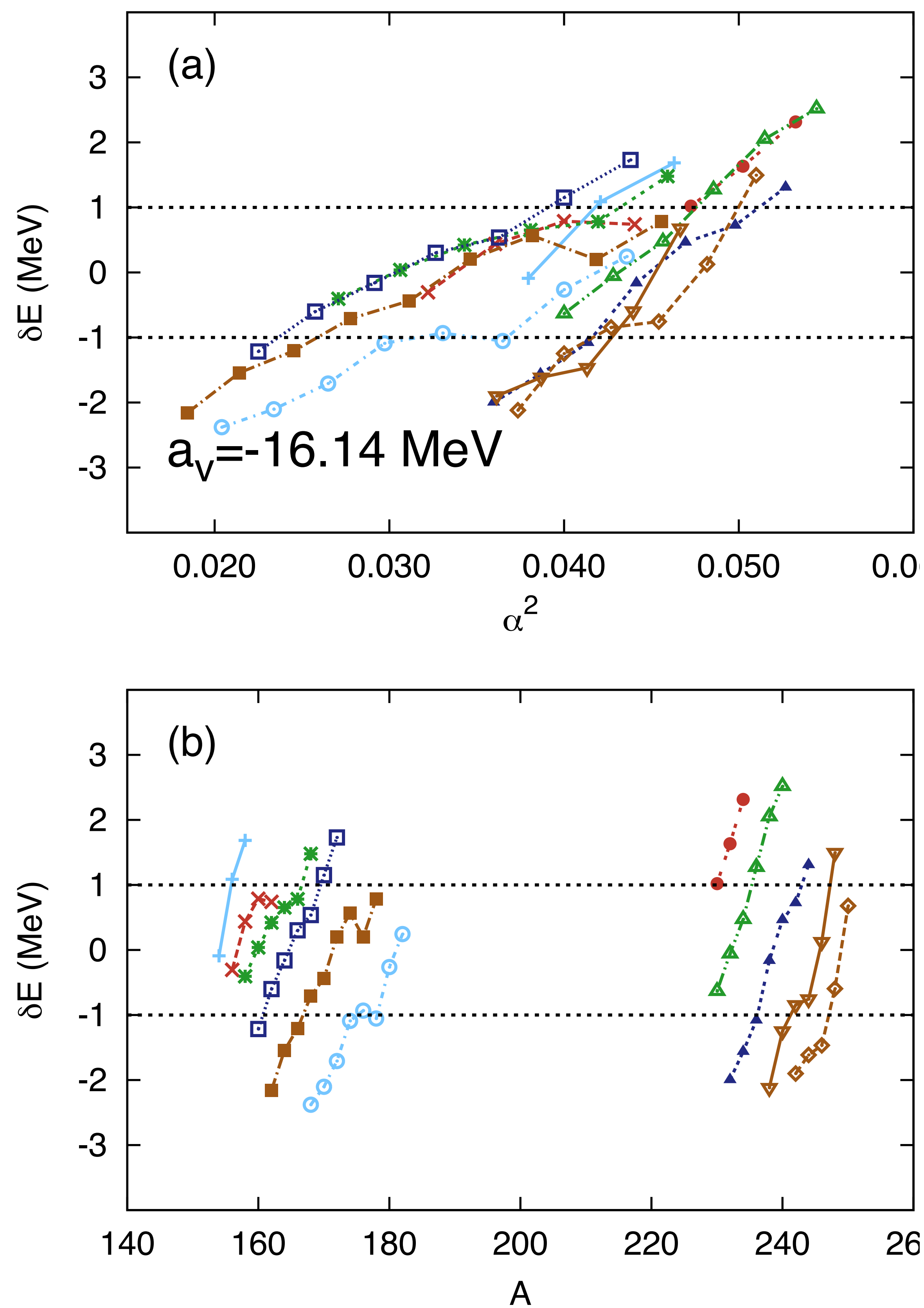


$$\alpha^2 = \frac{(N-Z)^2}{A^2}$$



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





The calculated masses are very sensitive (isospin and mass dependence) to the choice of nuclear matter binding energy at saturation.

... not possible to determine the parameters of a density functional already at nuclear matter level, without additional adjustment to low-energy data on finite medium-heavy and heavy nuclei.

DD-PC1

volume energy: $a_v = -16.06 \text{ MeV}$

surface energy: $a_s = 17.498 \text{ MeV}$

symmetry energy: $\langle S_2 \rangle = 27.8 \text{ MeV} \quad (a_4 = 33\text{MeV})$

Nuclear Many-Body Correlations

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

long-range
nuclear resonance modes

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

...vary smoothly with nucleon number!
Implicitly included in the universal EDF.

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

Five-dimensional collective Hamiltonian

Nikšić, Li, Vretenar, Prochniak, Meng, Ring, 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.

The quantized collective Hamiltonian: $\hat{H} = \hat{T}_{\text{vib}} + \hat{T}_{\text{rot}} + V_{\text{coll}}$

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

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

$$V_{\text{coll}}(q_0, q_2) = E_{\text{tot}}(q_0, q_2) - \Delta V_{\text{vib}}(q_0, q_2) - \Delta V_{\text{rot}}(q_0, q_2)$$

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

$$\Phi_{MK}^I(\Omega) = \sqrt{\frac{2I+1}{16\pi^2(1+\delta_{K0})}}\left[D_{MK}^{I*}(\Omega) + (-1)^I D_{M-K}^{I*}(\Omega)\right]$$

Microscopic parameters of the collective Hamiltonian:

In the simplest approximation the moments of inertia are calculated from the Inglis-Belyaev formula:

$$\mathcal{I}_k = \sum_{i,j} \frac{|\langle ij|\hat{J}_k|\Phi\rangle|^2}{E_i + E_j} \quad k = 1,2,3 \qquad |ij\rangle = \beta_i^\dagger \beta_j^\dagger |\Phi\rangle$$

quasiparticle vacuum

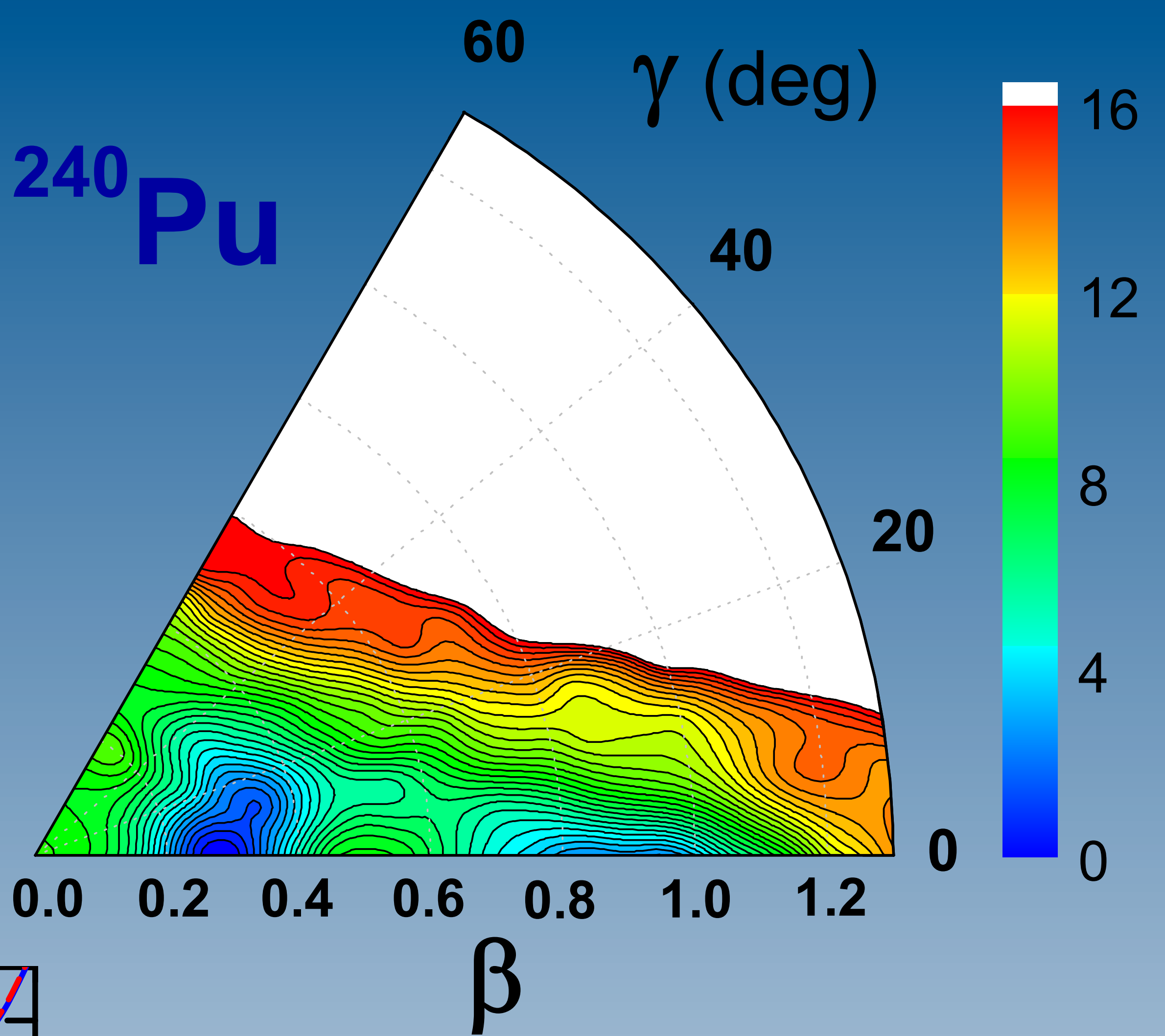
The mass parameters are calculated in the cranking approximation:

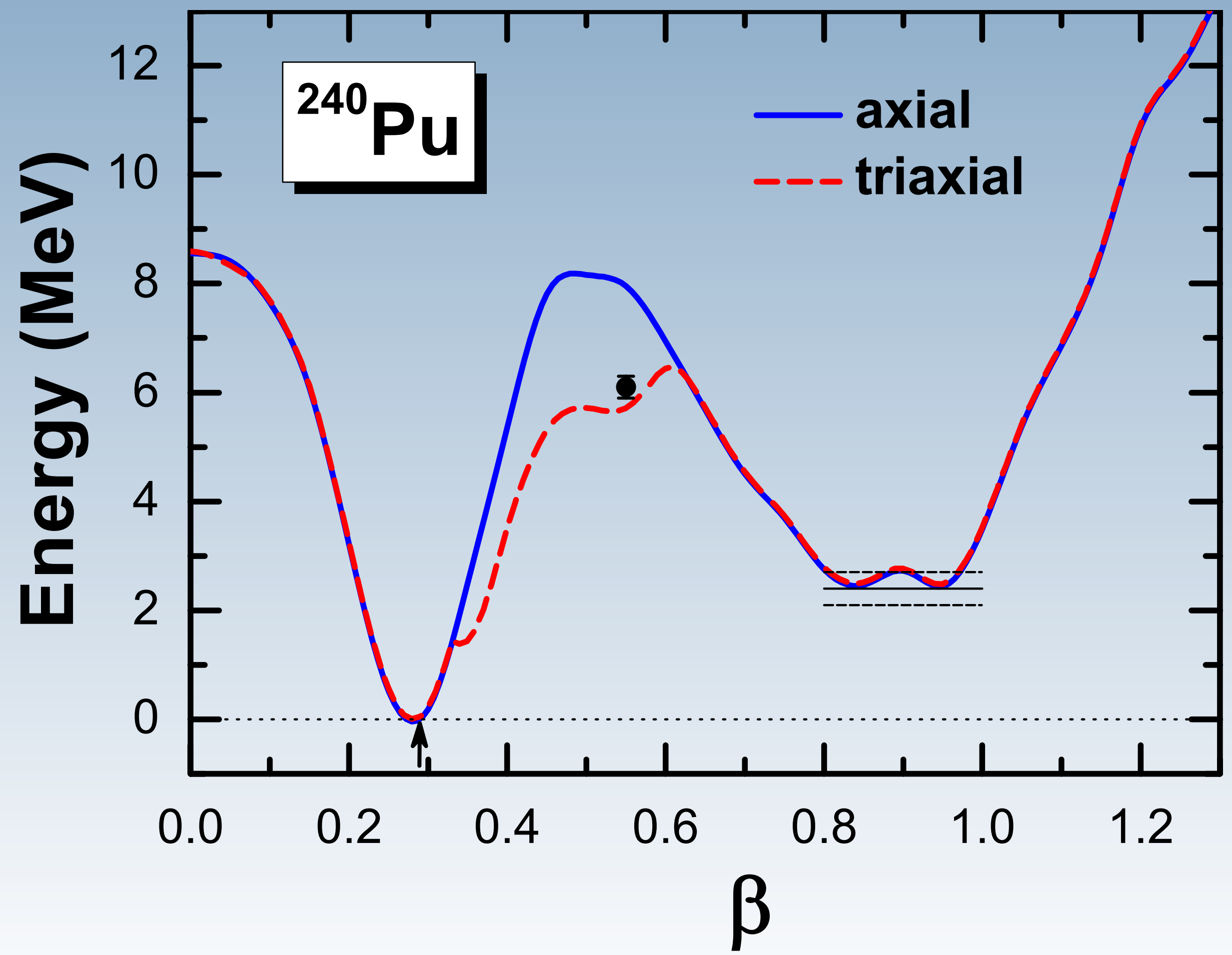
$$B_{\mu\nu}(q_0, q_2) = \frac{\hbar^2}{2}\left[\mathcal{M}_{(1)}^{-1}\mathcal{M}_{(3)}\mathcal{M}_{(1)}^{-1}\right]_{\mu\nu}$$

$$\mathcal{M}_{(n),\mu\nu}(q_0, q_2) = \sum_{i,j} \frac{\left|\langle\Phi|\hat{Q}_{2\mu}|ij\rangle\langle ij|\hat{Q}_{2\nu}|\Phi\rangle\right|}{(E_i + E_j)^n}$$

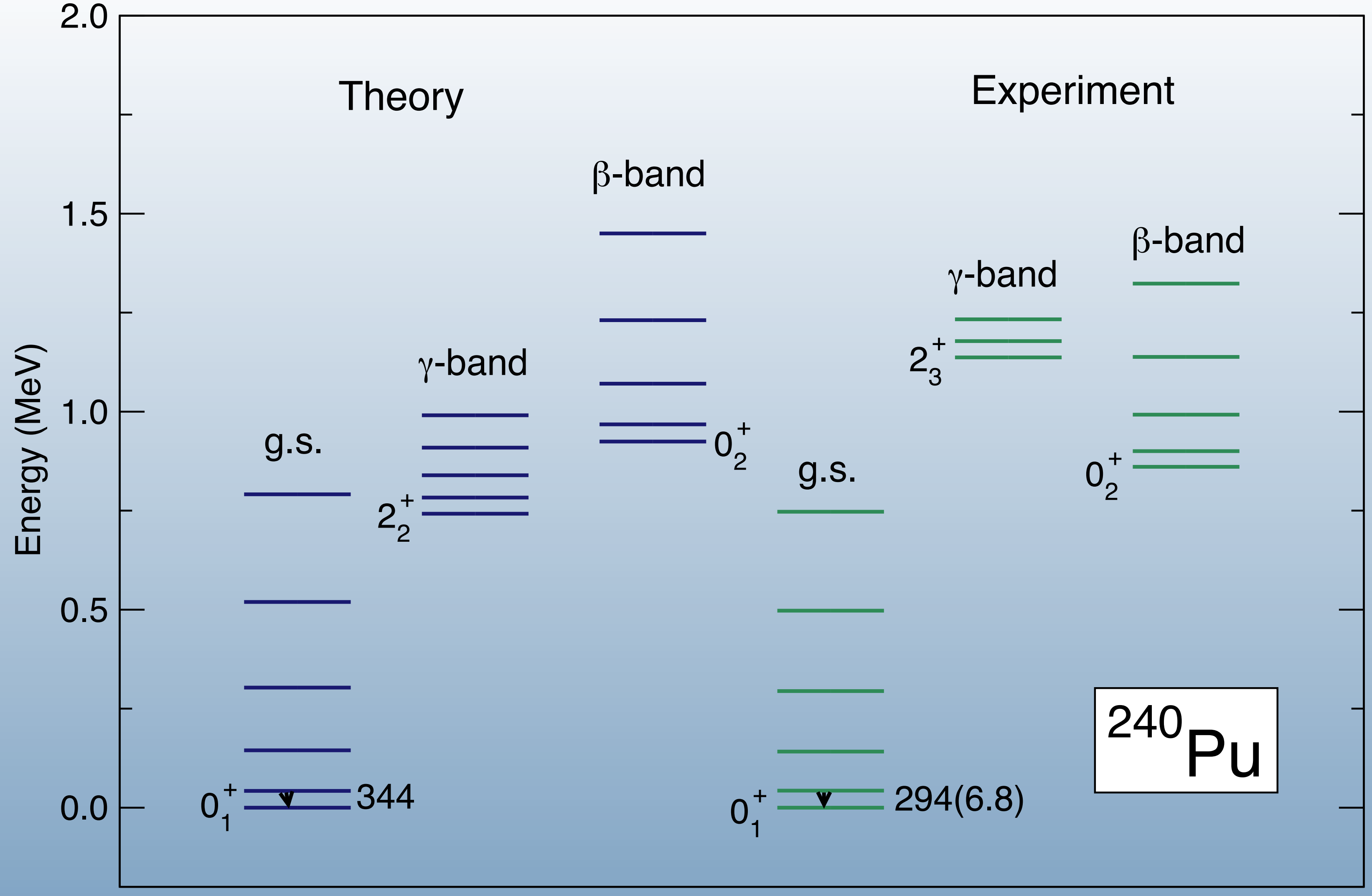
Test of DD-PC1:

Fission path and barriers:





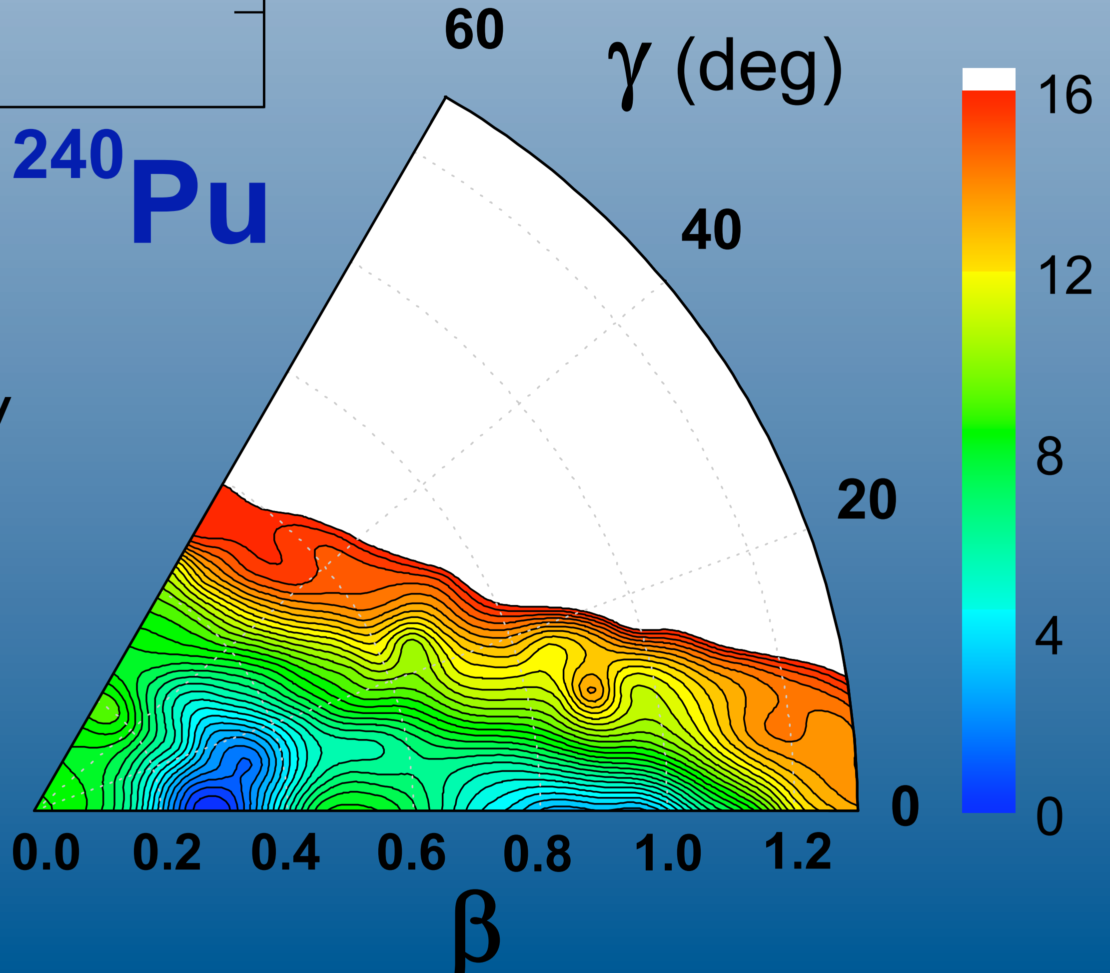
Li, Nikšić, Vretenar, Ring, Meng, Phys. Rev. C (2010)

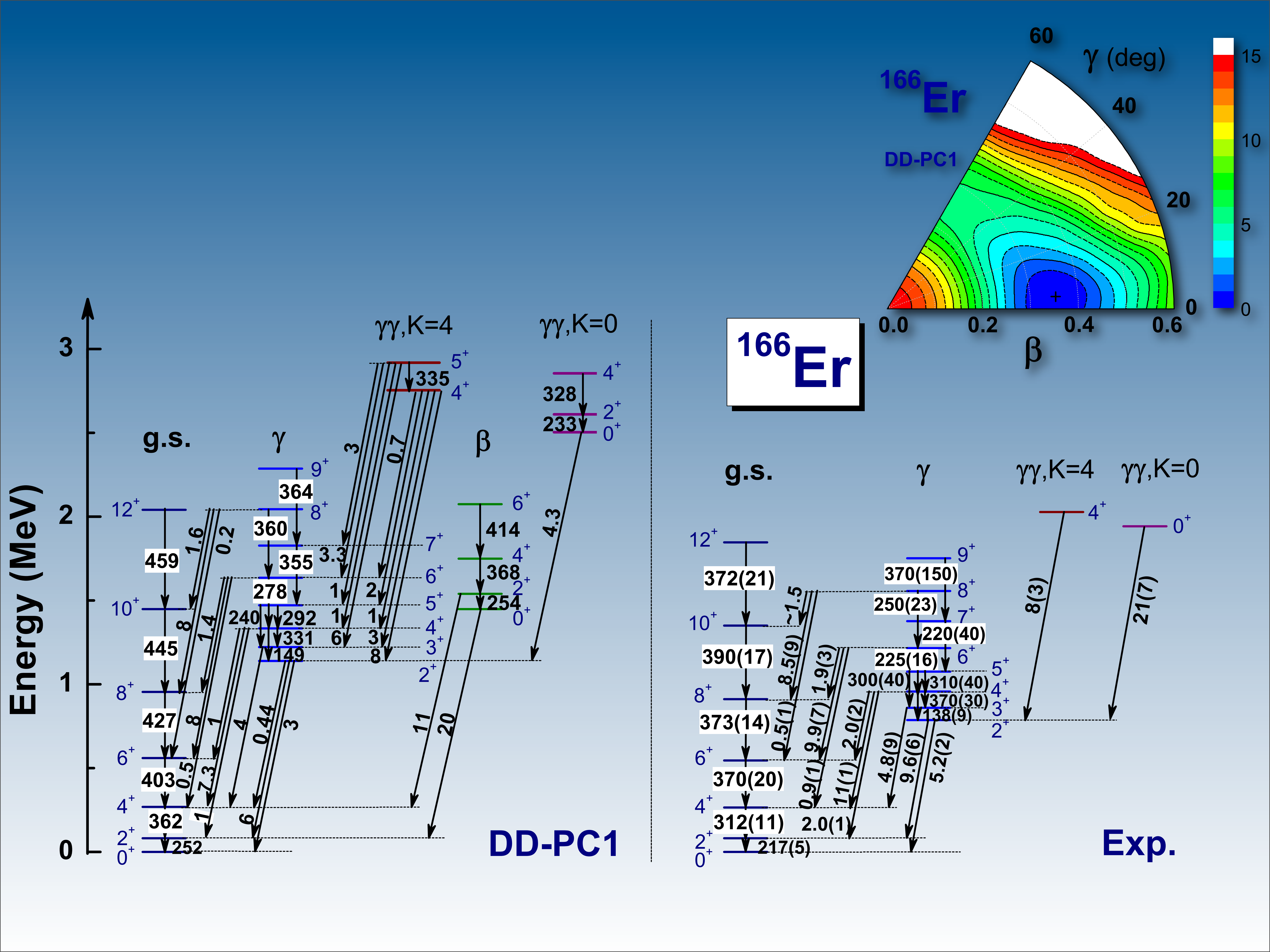


$$E^{th}_{4_1^+}/E^{th}_{2_1^+} = 3.33$$

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

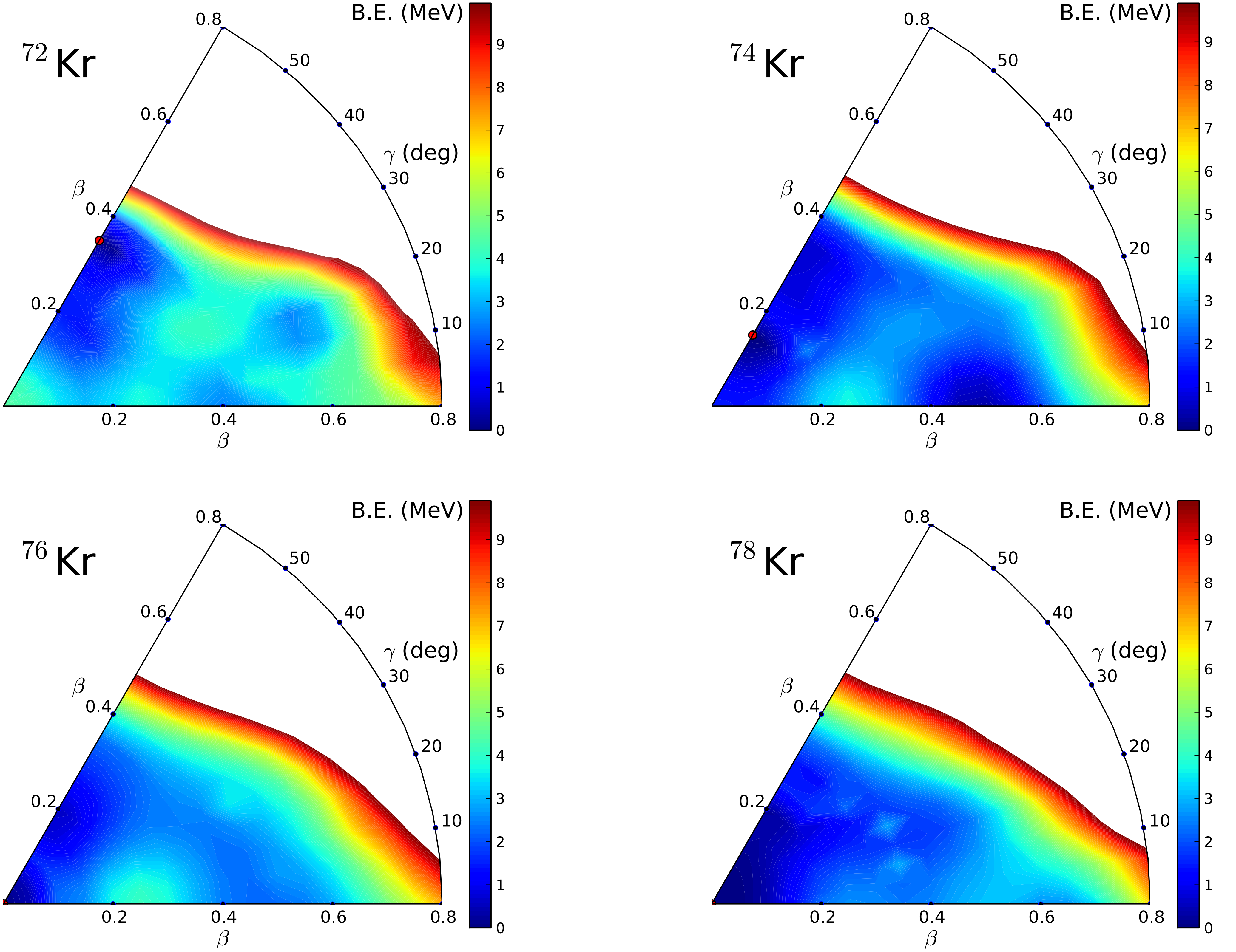
The moments of inertia are renormalized by a factor ≈ 1.3 (difference between the IB and TV moments of inertia).

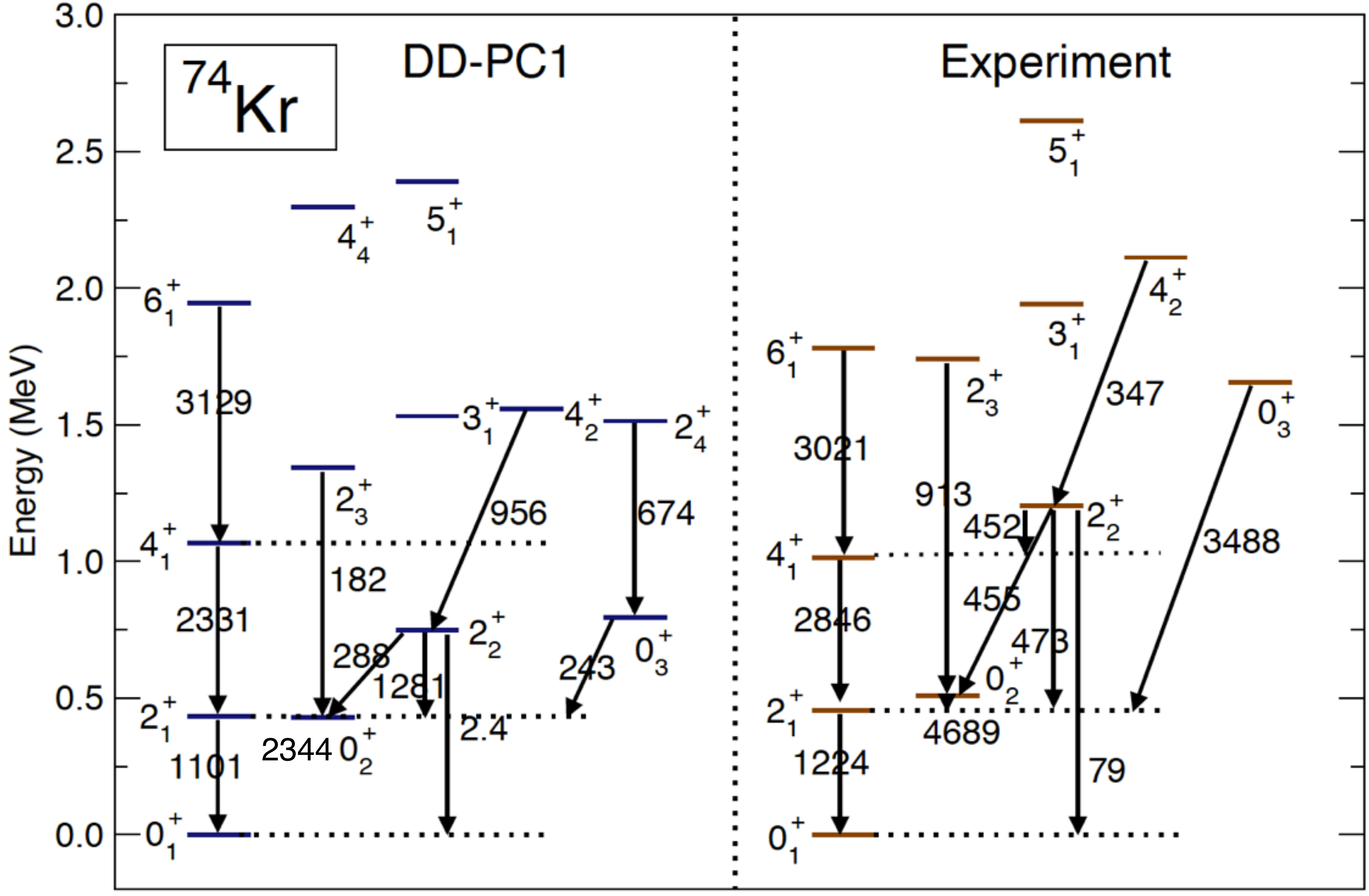




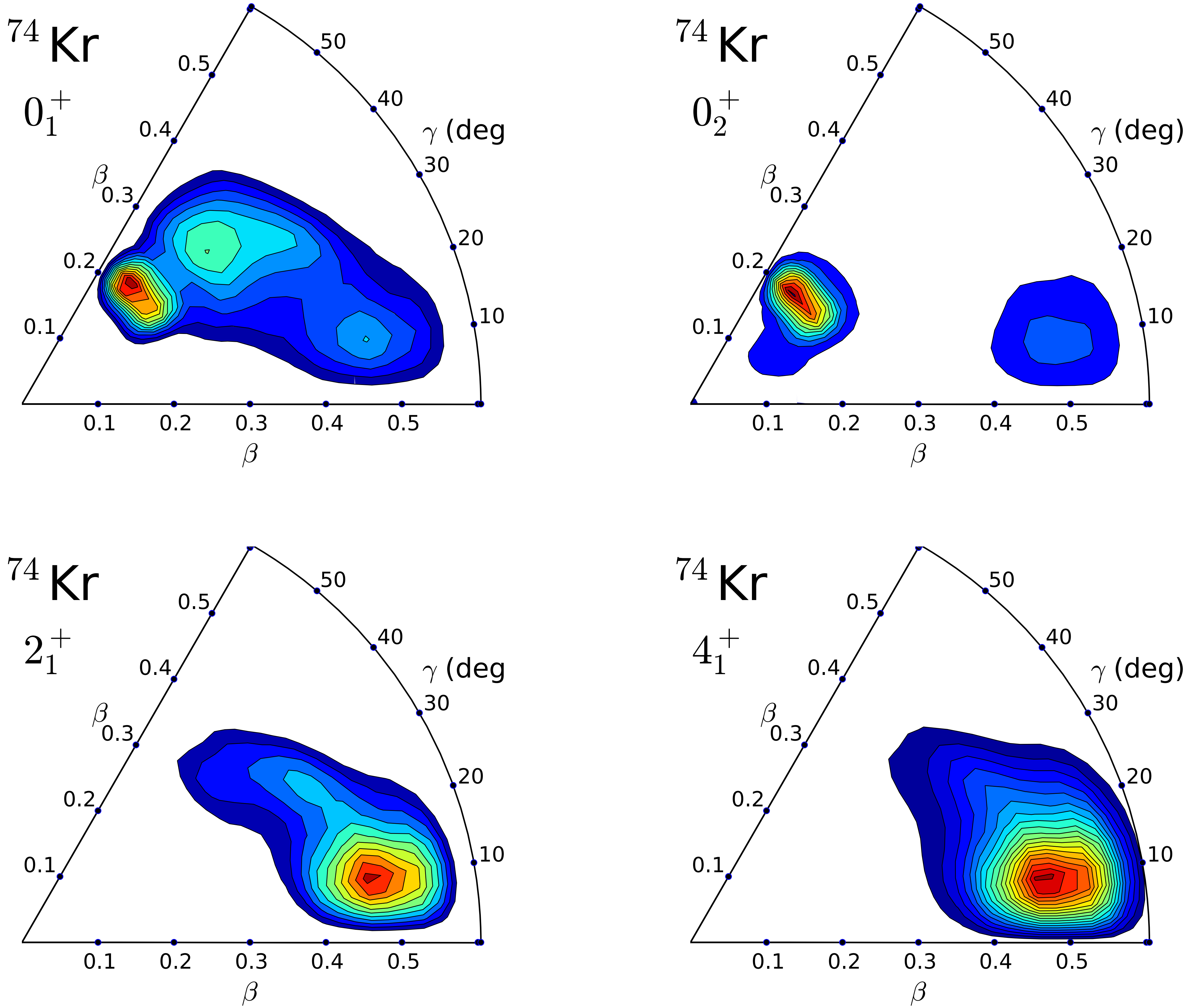
166Er
DD-PC1
γ (deg)
60
40
20
0
15
10
5
0
0.0
0.2
0.4
0.6
β
166Er
Energy (MeV)
0
1
2
3
g.s.
γ
γγ,K=4
γγ,K=0
β
459
445
427
403
362
252
364
360
355
278
240
292
331
149
335
414
368
254
328
233
DD-PC1
g.s.
γ
γγ,K=4
γγ,K=0
372(21)
390(17)
373(14)
370(20)
312(11)
217(5)
370(150)
250(23)
220(40)
225(16)
300(40)
310(40)
370(30)
138(9)
2.0(1)
8(3)
21(7)
Exp.

Shape-coexistence in neutron-deficient Kr isotopes



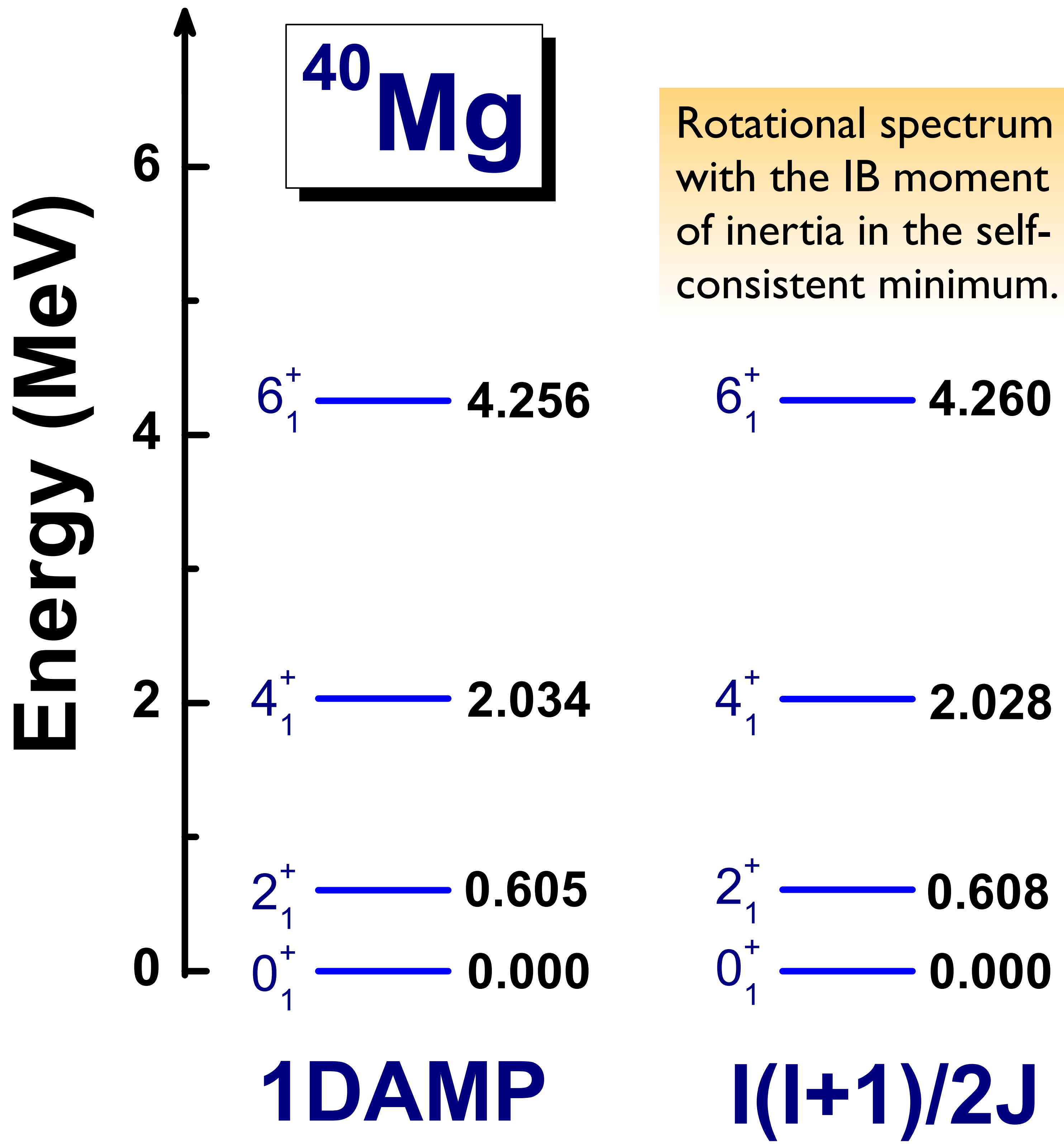


74Kr
DD-PC1
Experiment
Energy (MeV)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
3129
2331
1101
182
288
1281
2.4
956
674
243
2344
3021
2846
1224
913
452
455
473
347
3488
4689
79

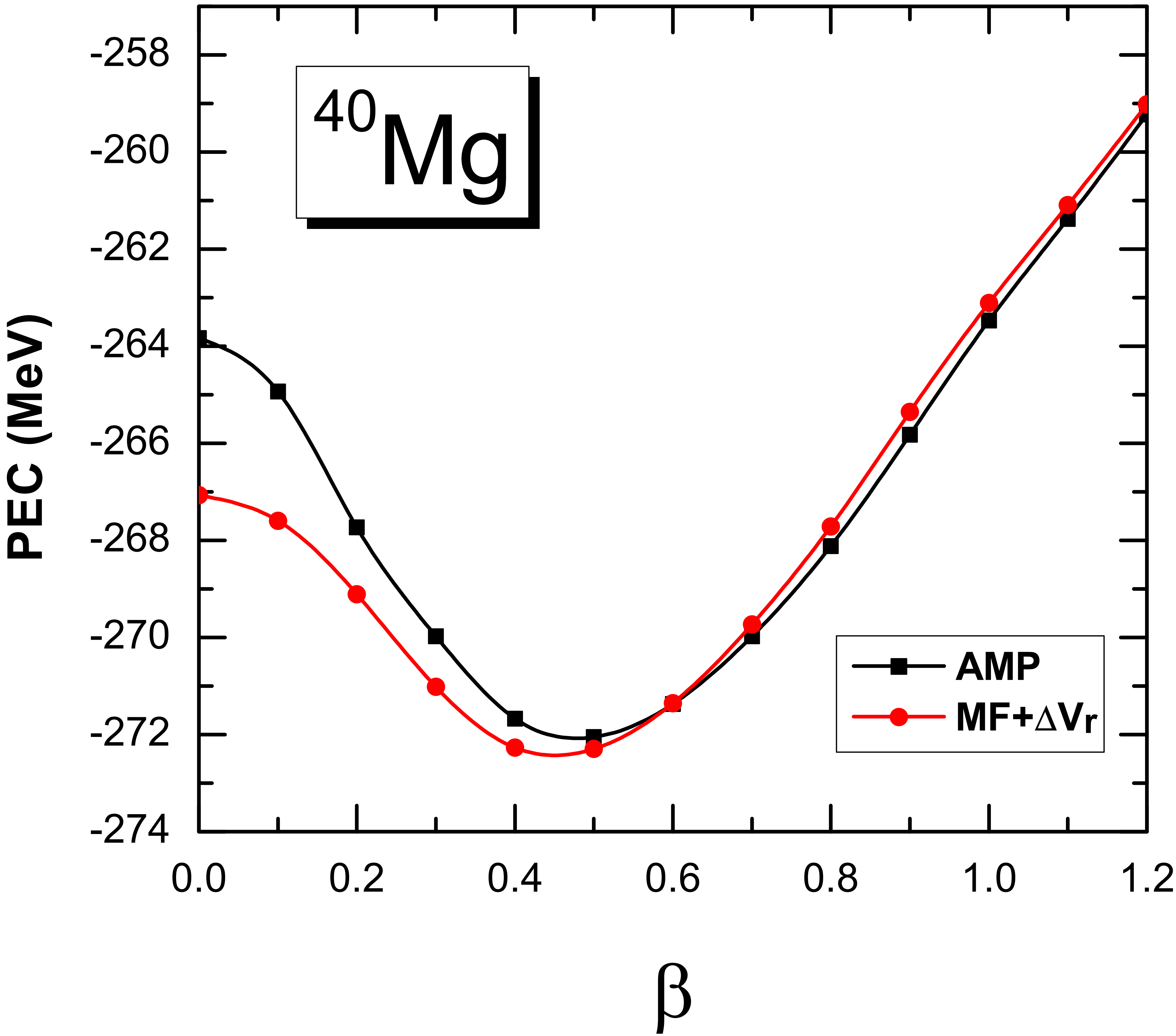


^{74}Kr
0_1^+
^{74}Kr
0_2^+
^{74}Kr
2_1^+
^{74}Kr
4_1^+
γ (deg
γ (deg)
50
40
30
20
10
β
0.1
0.2
0.3
0.4
0.5

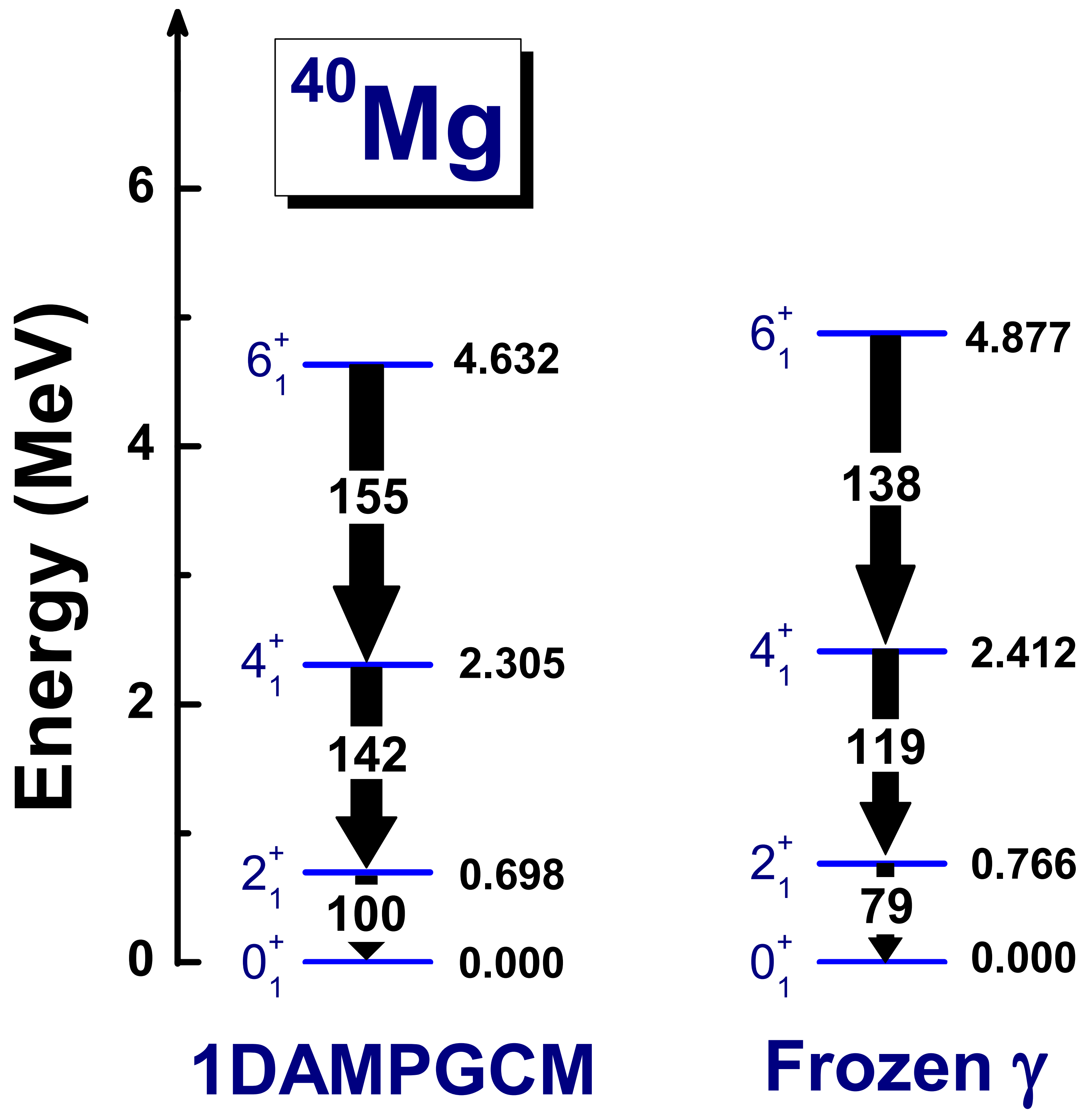
Collective Hamiltonian vs AMP+GCM: 1D case



Rotational spectrum with the IB moment of inertia in the self-consistent minimum.

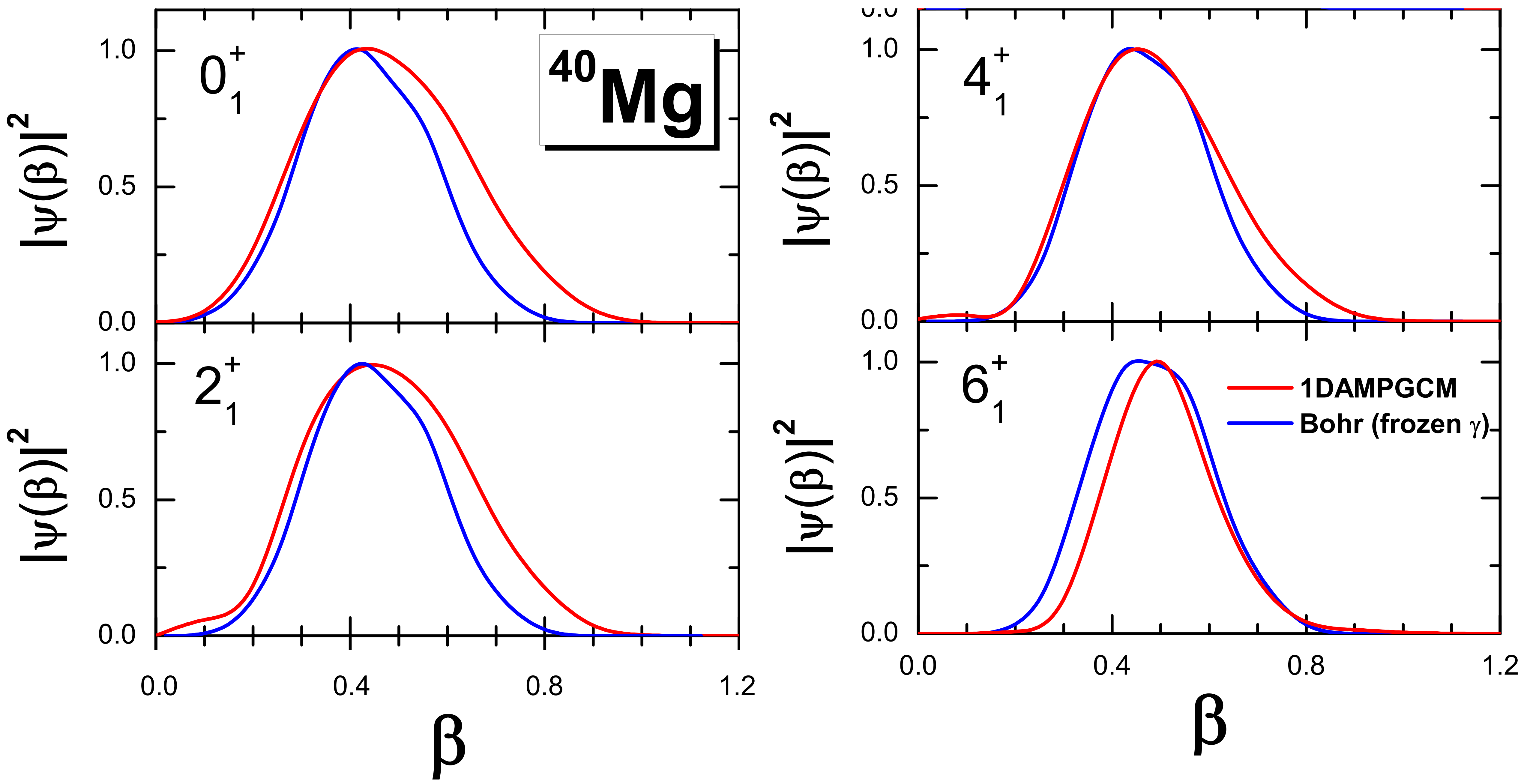


^{40}Mg
PEC (MeV)
-258
-260
-262
-264
-266
-268
-270
-272
-274
0.0
0.2
0.4
0.6
0.8
1.0
1.2
β
AMP
MF+ΔV$_r$



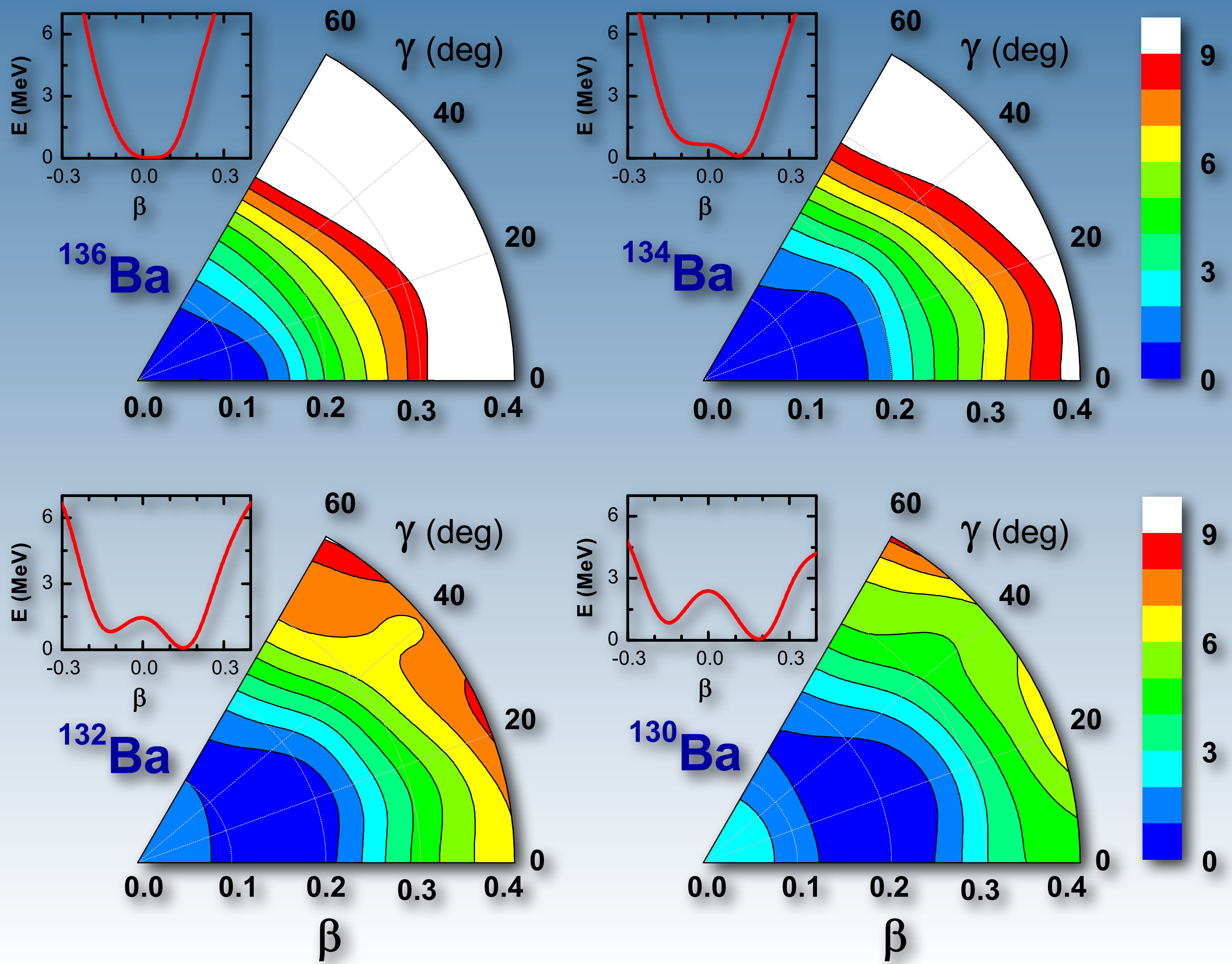
40Mg
Energy (MeV)
6
4
2
0
6+1
4.632
155
4+1
2.305
142
2+1
0.698
100
0+1
0.000
6+1
4.877
138
4+1
2.412
119
2+1
0.766
79
0+1
0.000
1DAMPGCM
Frozen γ

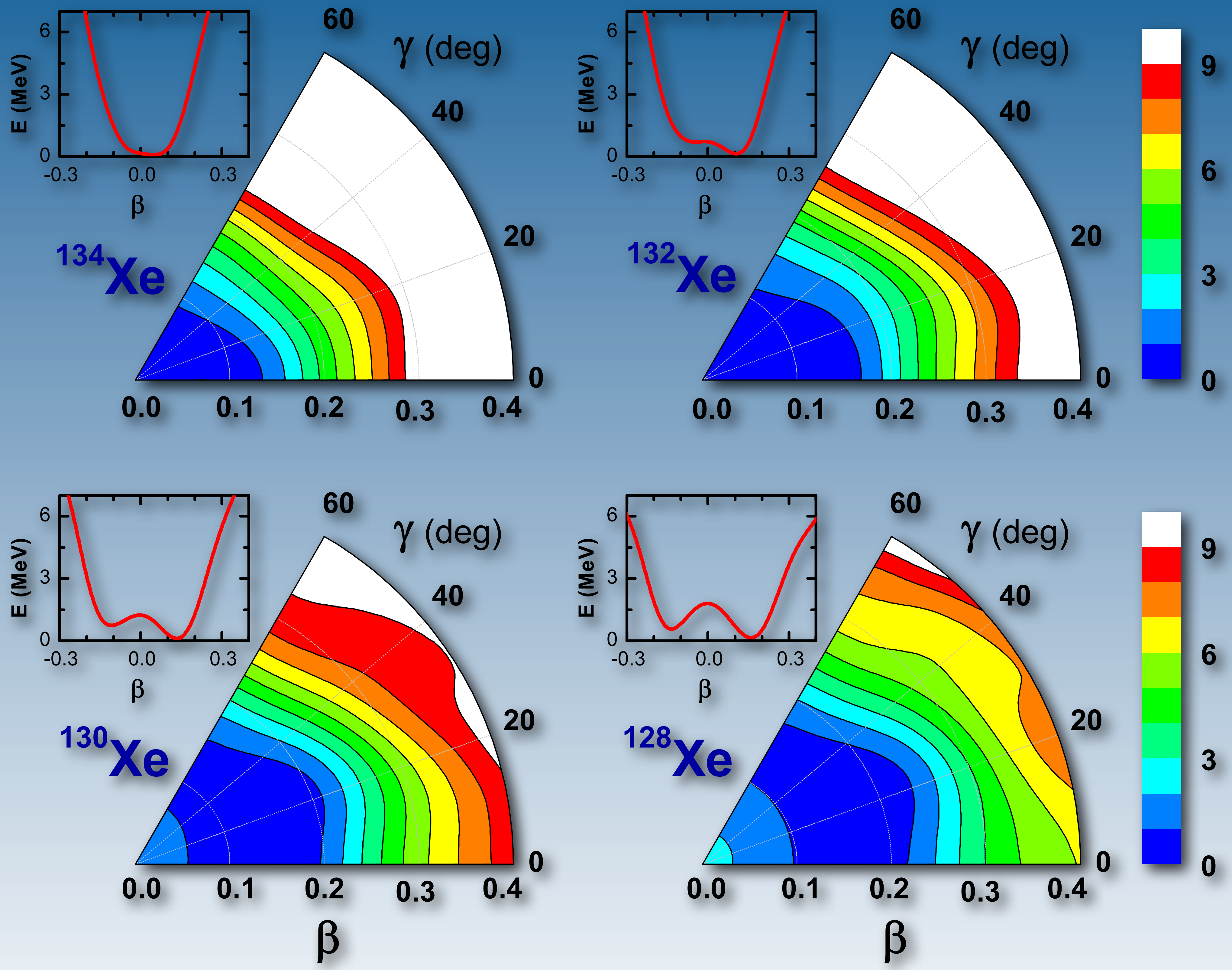
Collective wave functions:



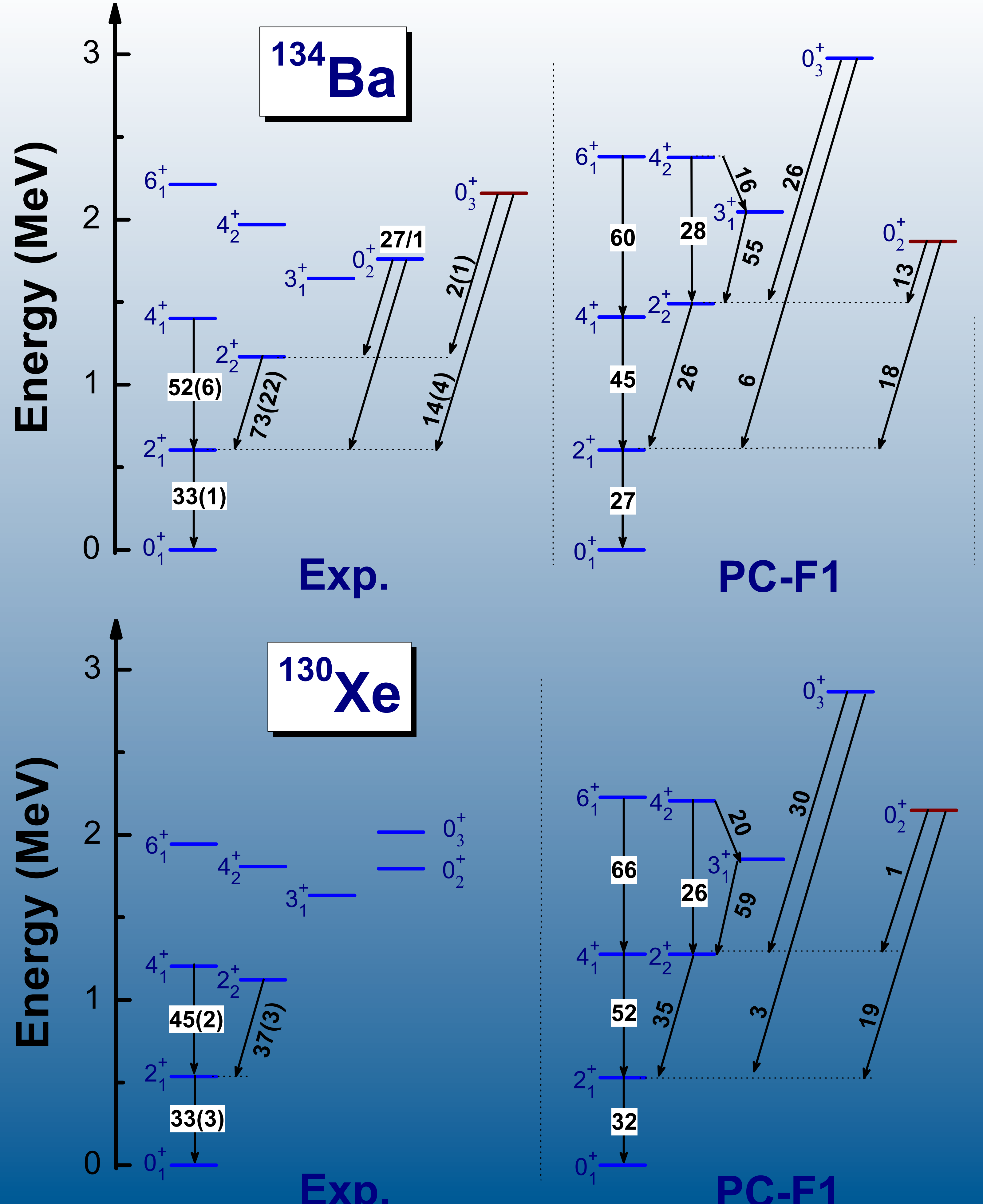
γ-soft nuclei in the mass A ≈ 130 region

Li, Nikšić, Vretenar, Meng, Phys. Rev. C **81**, 034316 (2010)



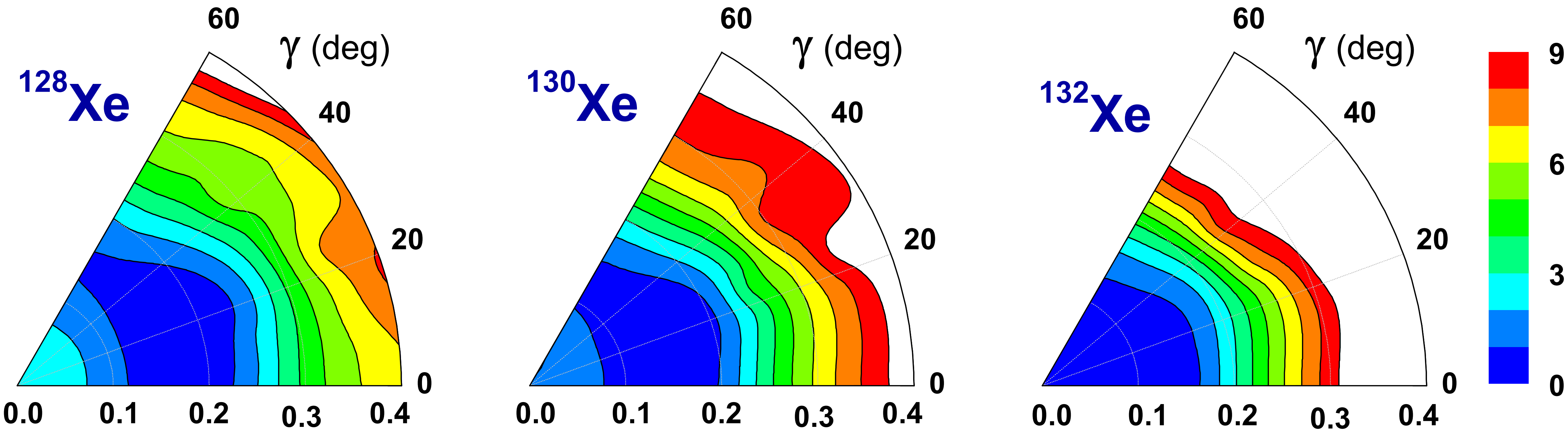


134Xe
132Xe
130Xe
128Xe
γ (deg)
60
40
20
0
0.0
0.1
0.2
0.3
0.4
β
E (MeV)
-0.3
0.3
9
6
3

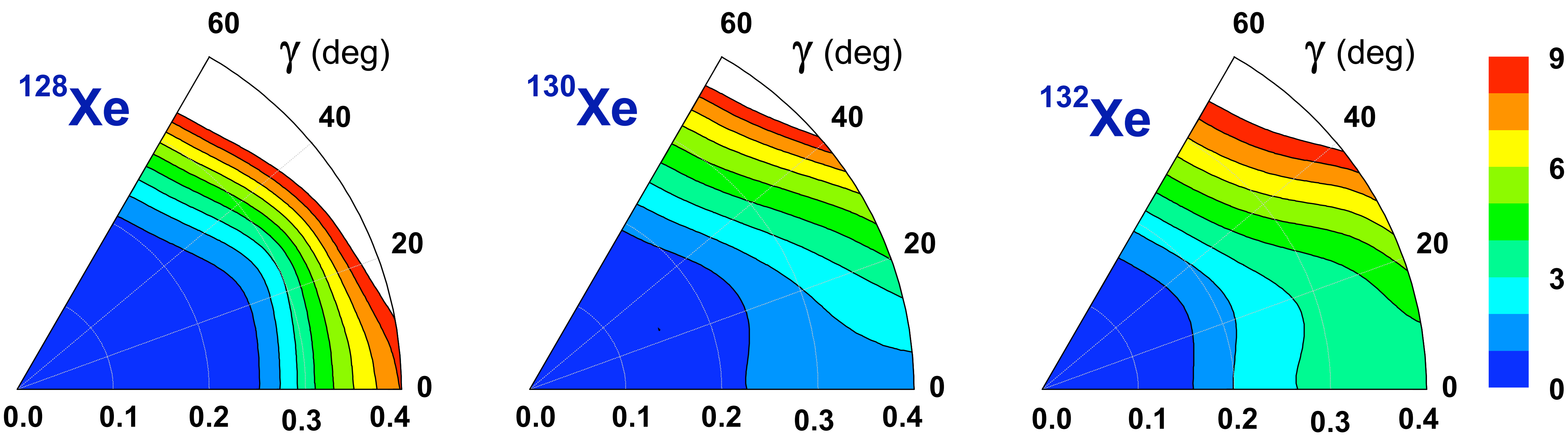


134Ba
Energy (MeV)
Exp.
PC-F1
52(6)
33(1)
73(22)
27/1
2(1)
14(4)
60
45
27
28
16
26
55
13
6
18
130Xe
45(2)
33(3)
37(3)
66
52
32
20
30
59
35
3
1
19

Effect of time-odd components:

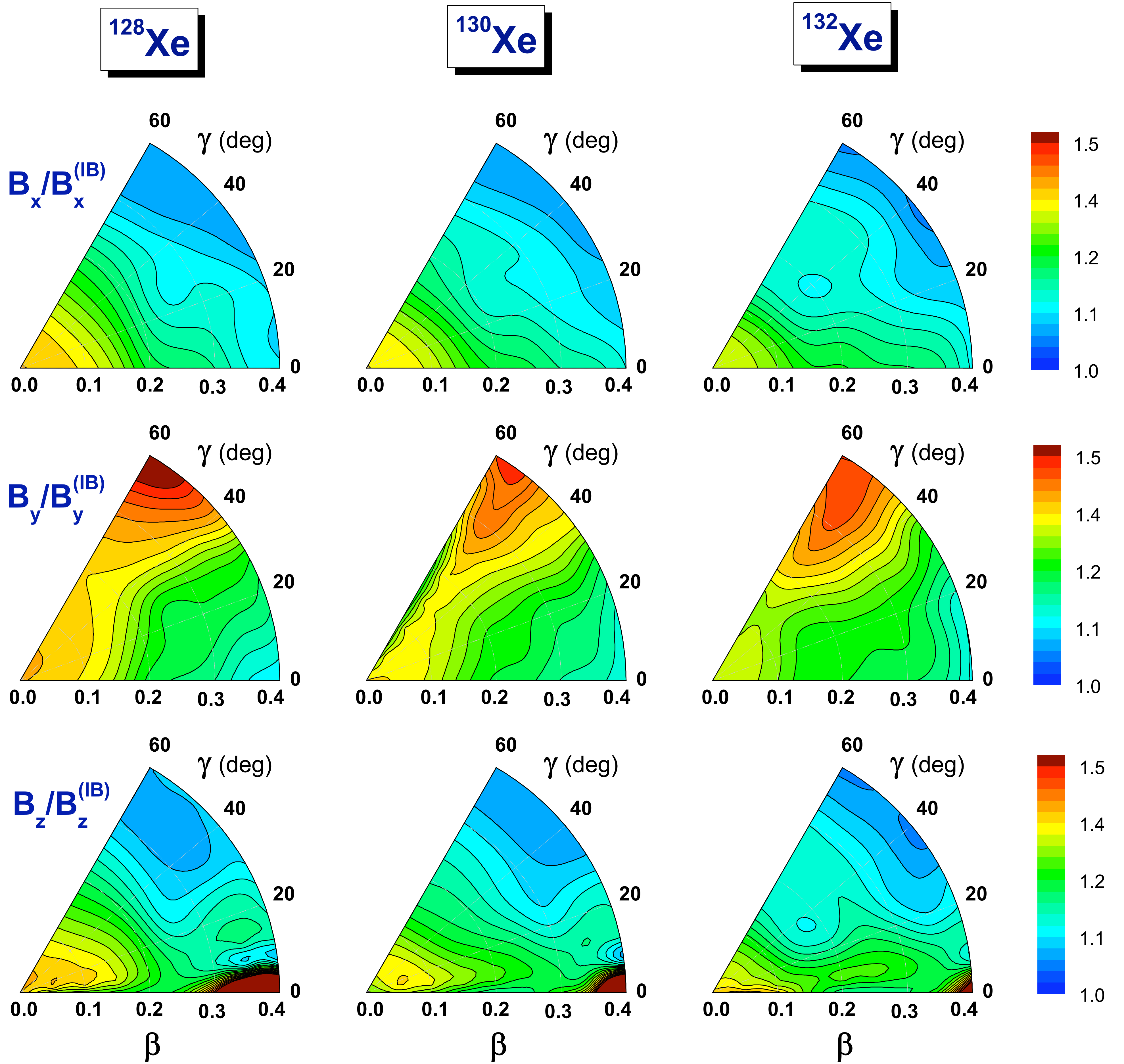


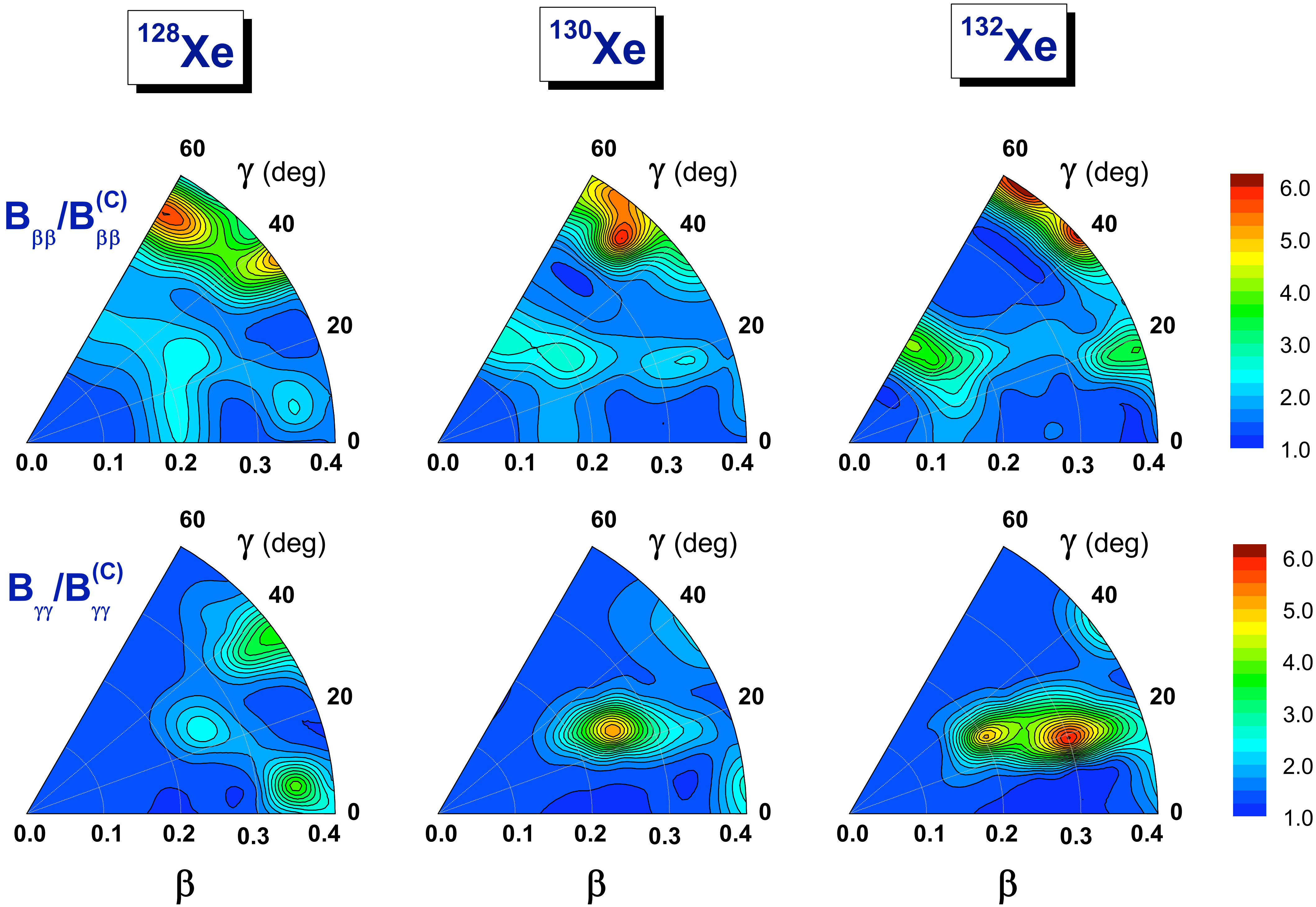
Self-consistent RHB triaxial quadrupole binding energy maps.



Quadrupole binding energy maps obtained from the P+Q Hamiltonian.

The ratios between the moments of inertia calculated from the LQRPA and the Inglis-Belyaev formula.

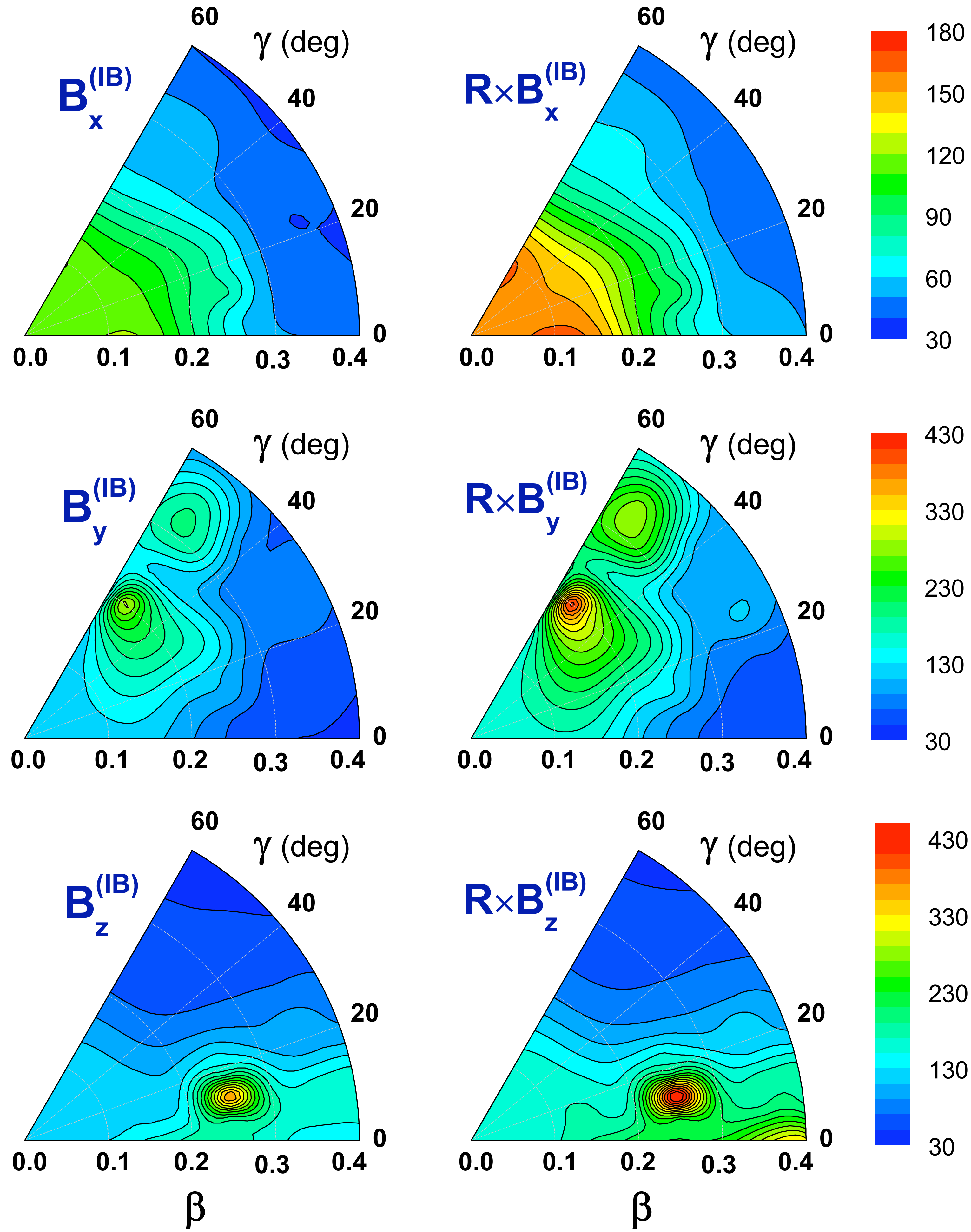


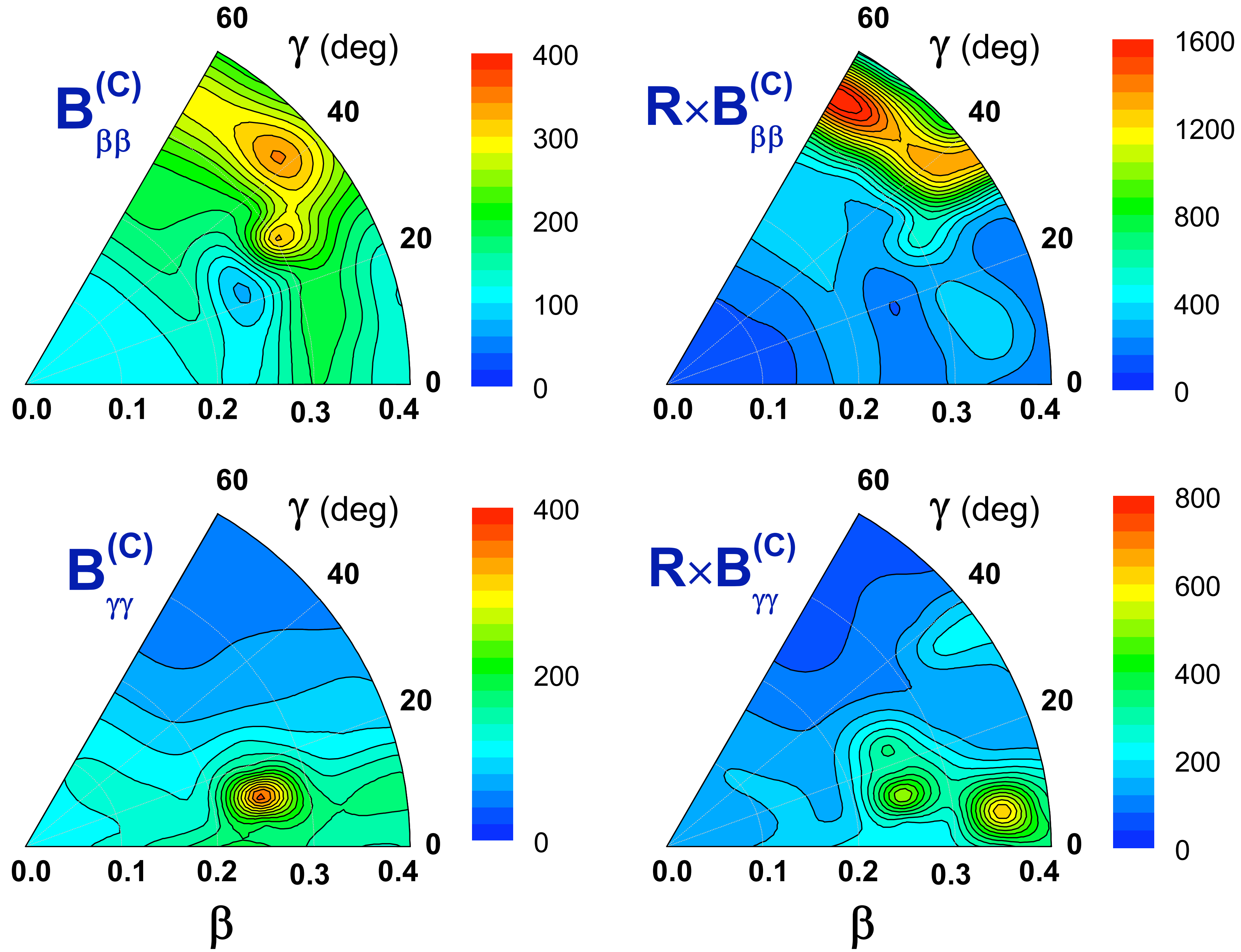


The ratios between the mass parameters calculated from LQRPA and the cranking approximation.

Moments of inertia calculated by the Inglis-Belyaev formula using the RHB input for 128Xe.

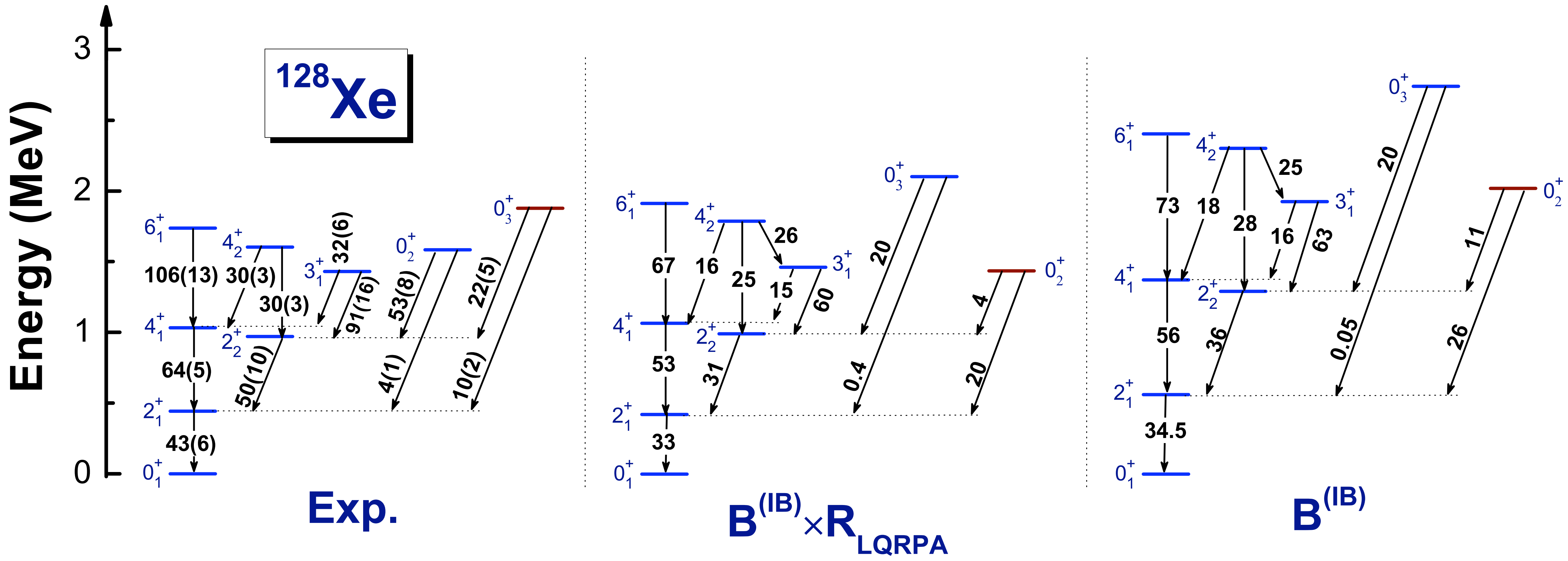
Moments of inertia multiplied by the corresponding ratios obtained from LQRPA.

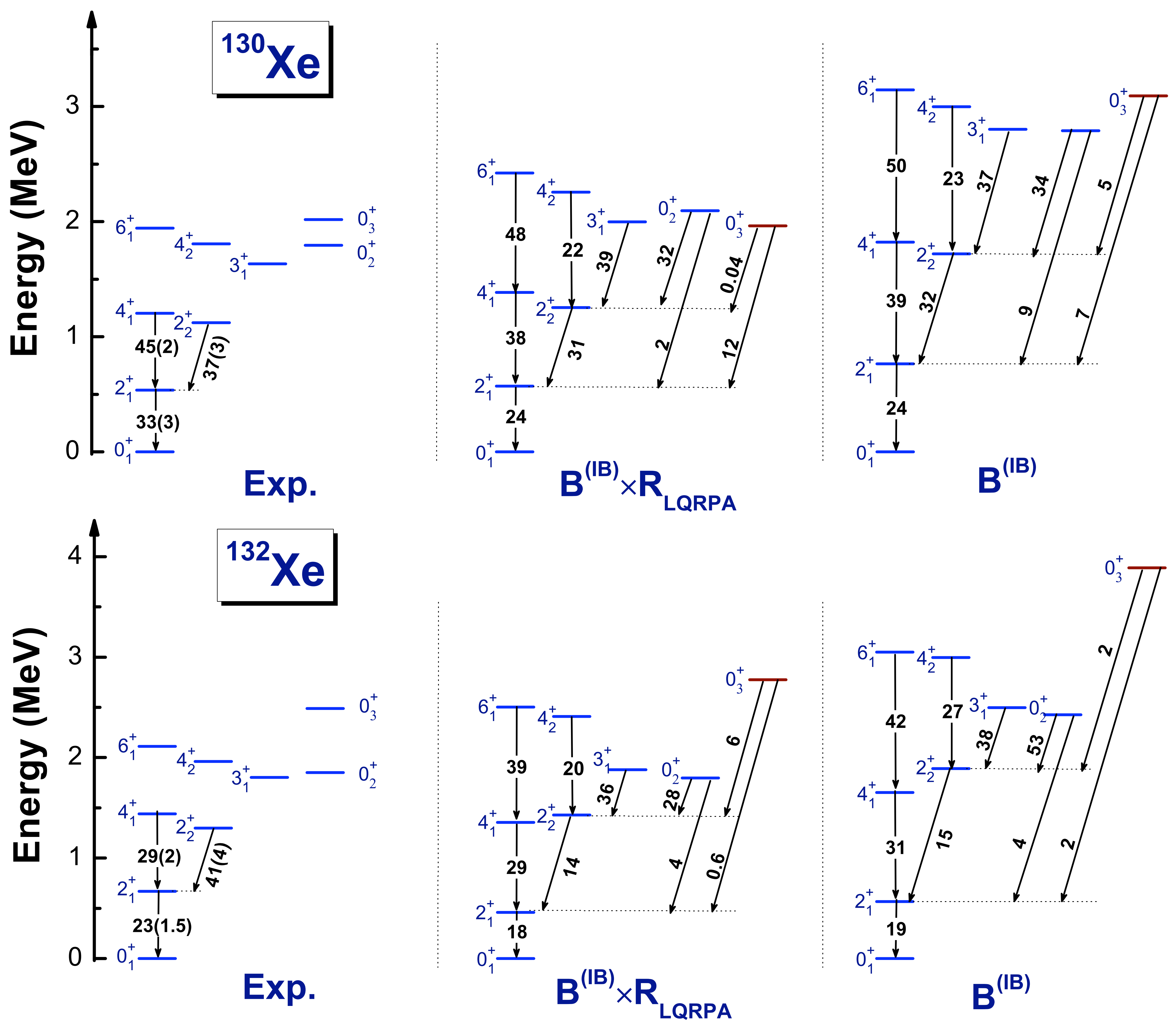




Mass parameters calculated in the cranking approximation using the RHB input for 128Xe, and mass parameters multiplied by the corresponding ratios obtained from LQRPA.

Effects of time-odd components on low-lying spectra:





130Xe
132Xe
Energy (MeV)
Exp.
B(IB)×R_LQRPA
B(IB)
45(2)
33(3)
37(3)
48
38
24
22
39
32
31
2
0.04
12
50
23
37
34
5
39
32
9
7
29(2)
23(1.5)
41(4)
39
20
36
28
6
29
14
4
0.6
18
42
27
38
53
2
31
15
19