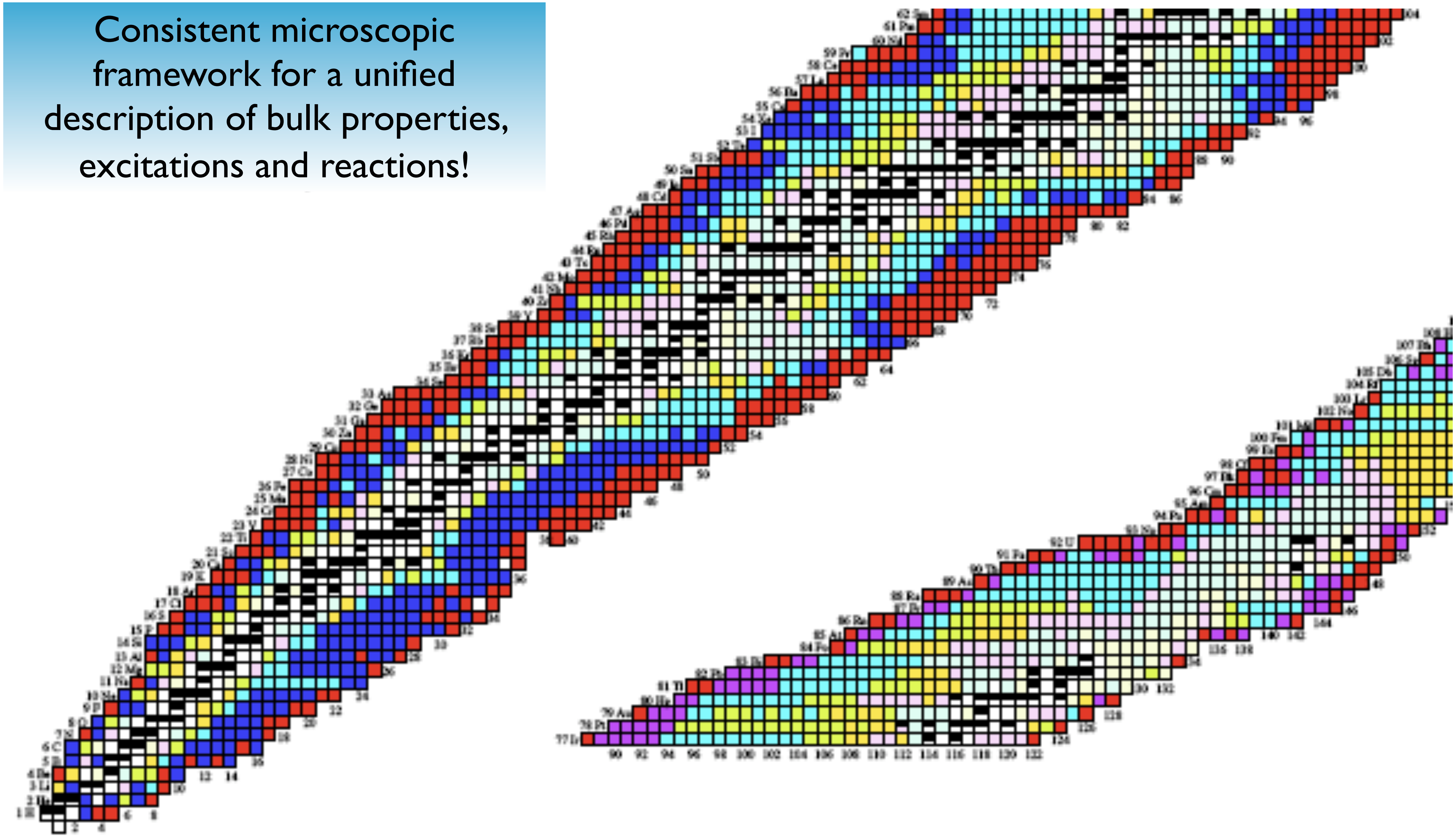
Nuclear Energy Density Functionals

Dario Vretenar
University of Zagreb

Energy Density Functionals

Consistent microscopic framework for a unified description of bulk properties, excitations and reactions!



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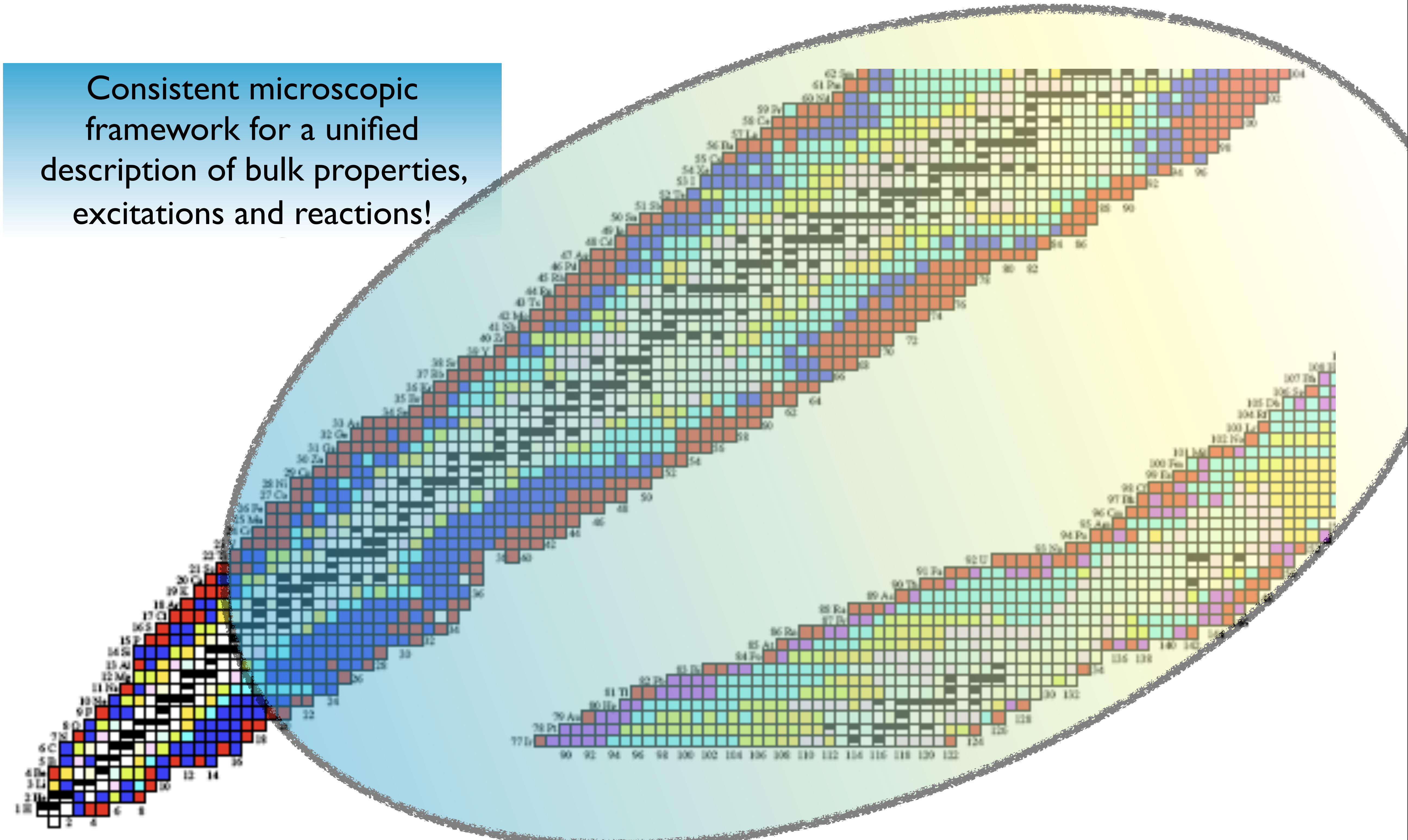

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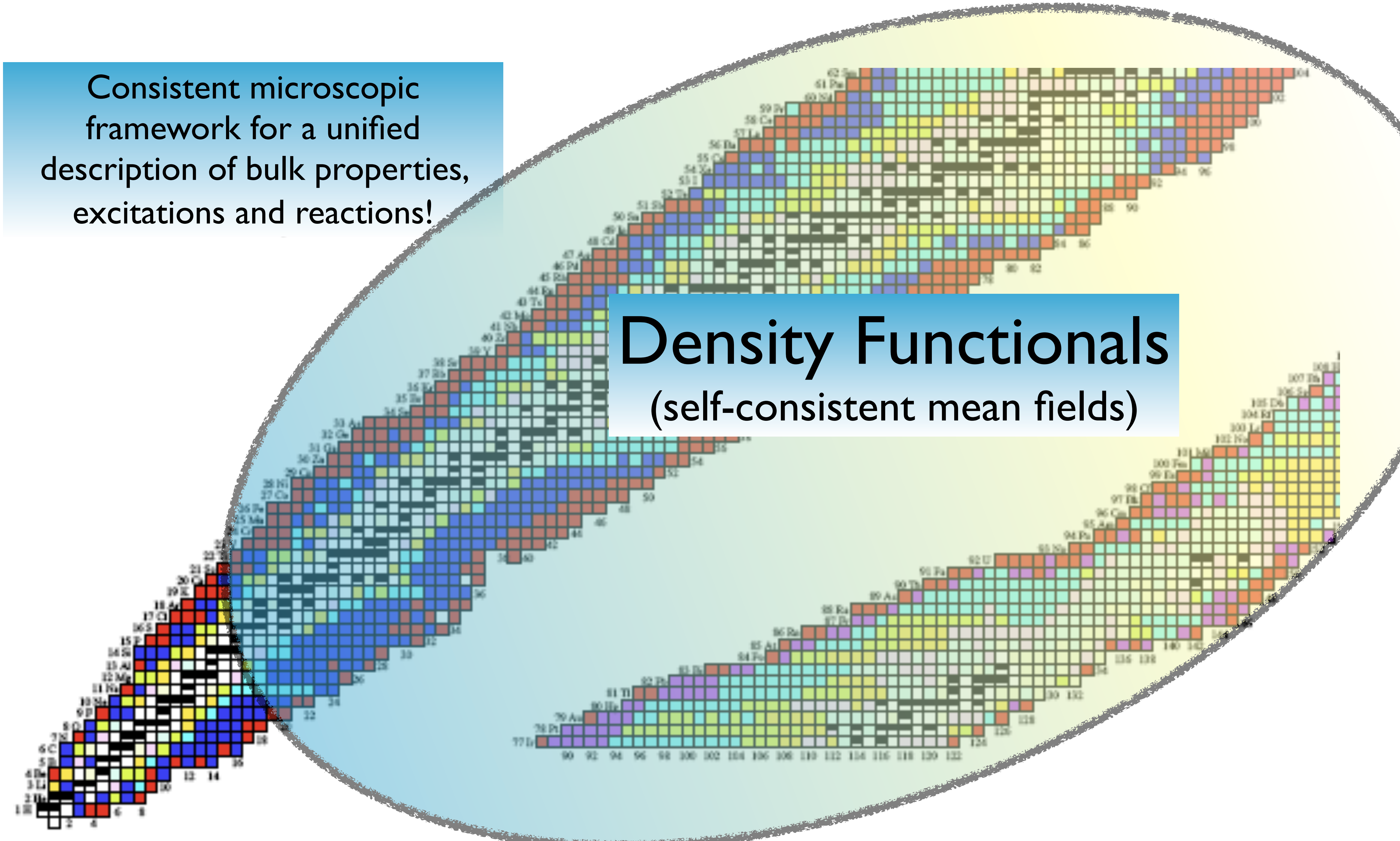

Density Functionals
(self-consistent mean fields)

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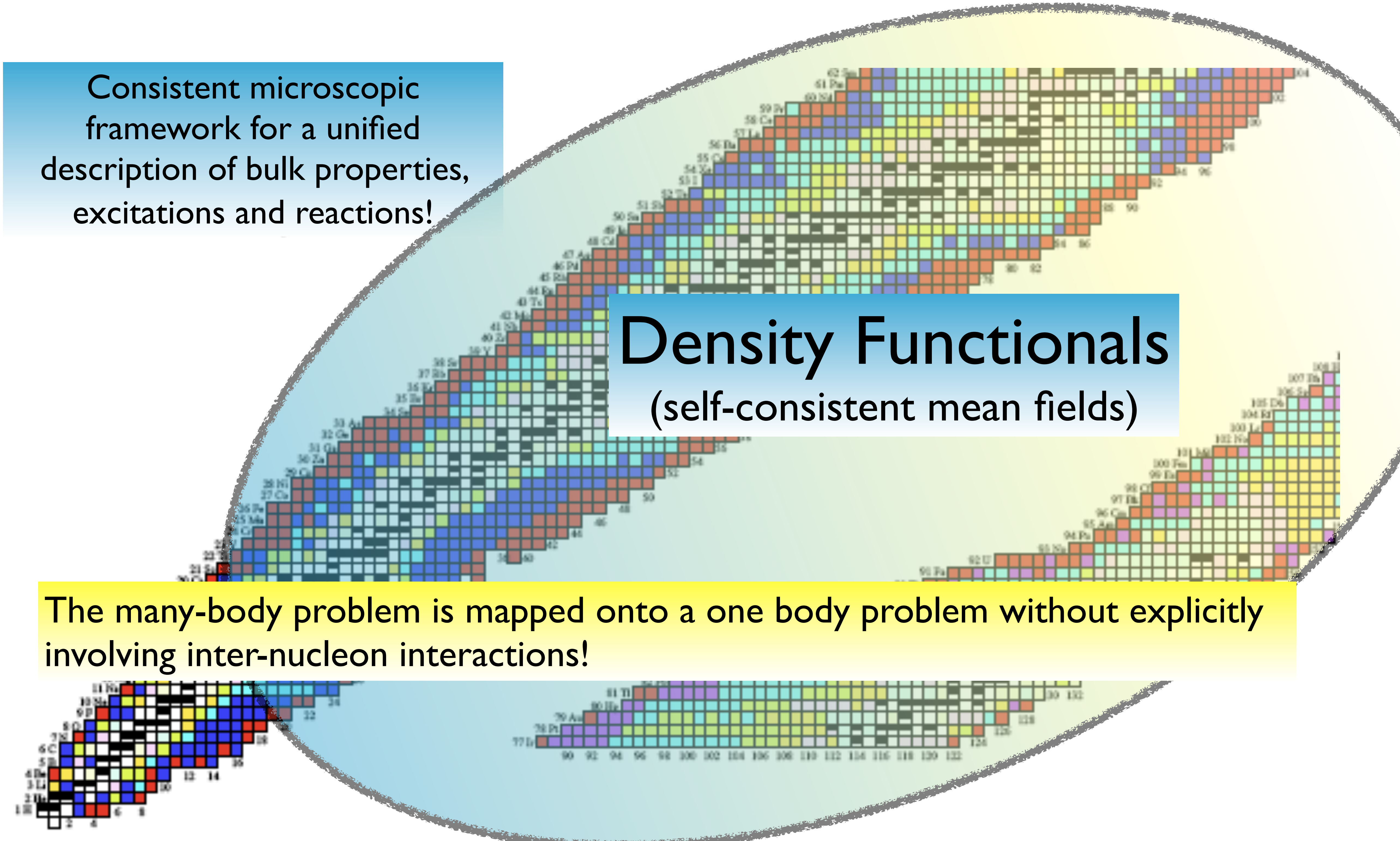

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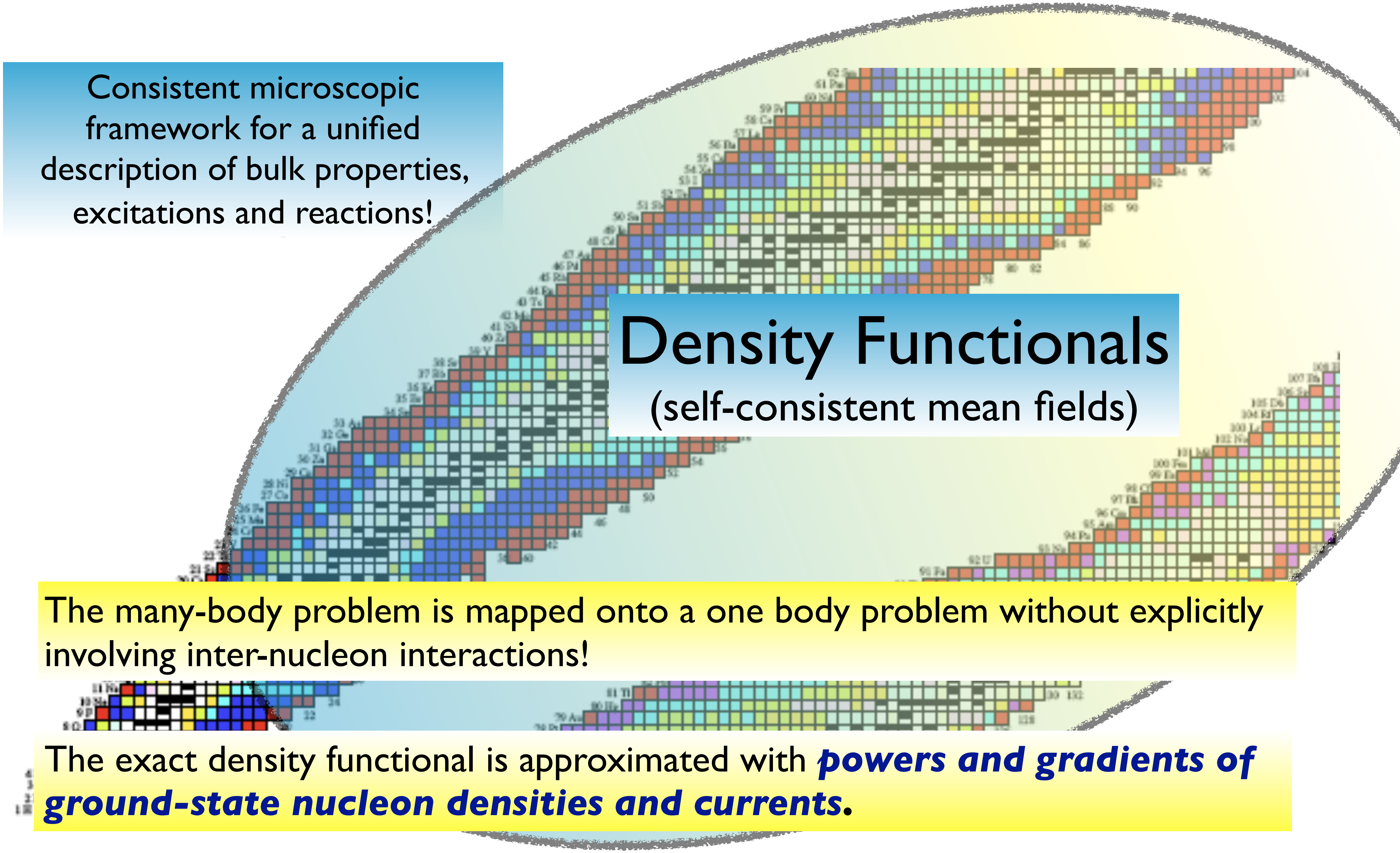

Density Functionals

(self-consistent mean fields)

The many-body problem is mapped onto a one body problem without explicitly involving inter-nucleon interactions!

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

Local densities and currents:

T=0 density: $$\rho_0(\mathbf{r}) = \rho_0(\mathbf{r},\mathbf{r}) = \sum_{\sigma\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma\tau)$$

T=1 density: $$\rho_1(\mathbf{r}) = \rho_1(\mathbf{r},\mathbf{r}) = \sum_{\sigma\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma\tau)\,\tau$$

T=0 spin density: $$\mathbf{s}_0(\mathbf{r}) = \mathbf{s}_0(\mathbf{r},\mathbf{r}) = \sum_{\sigma\sigma'\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma'\tau)\,\boldsymbol{\sigma}_{\sigma'\sigma}$$

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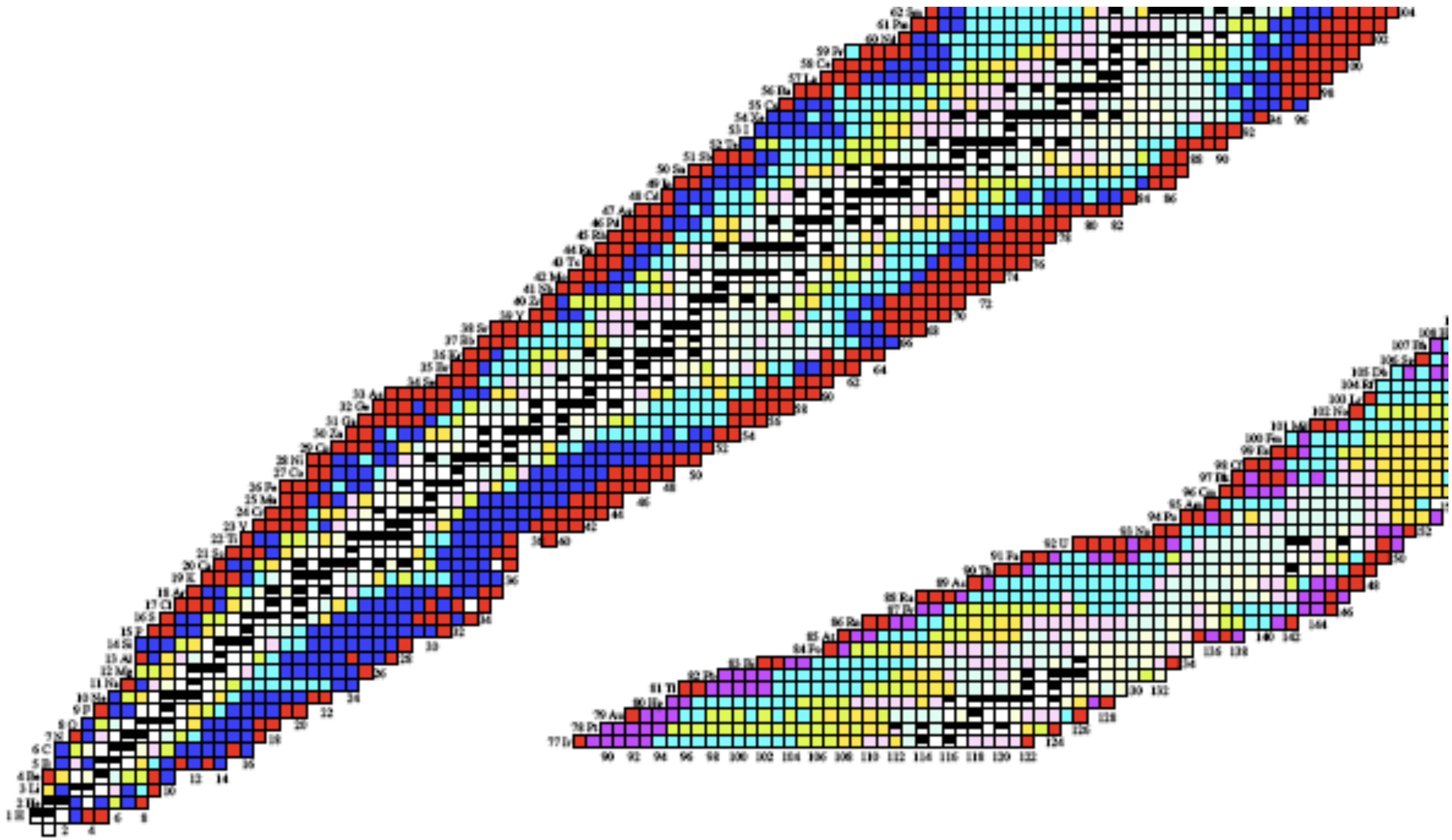
Current: $$\mathbf{j}_T(\mathbf{r}) = \frac{i}{2}(\nabla' - \nabla)\,\rho_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Spin-current tensor: $$\mathcal{J}_T(\mathbf{r}) = \frac{i}{2}(\nabla' - \nabla)\otimes\mathbf{s}_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Kinetic density: $$\tau_T(\mathbf{r}) = \nabla\cdot\nabla'\,\rho_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

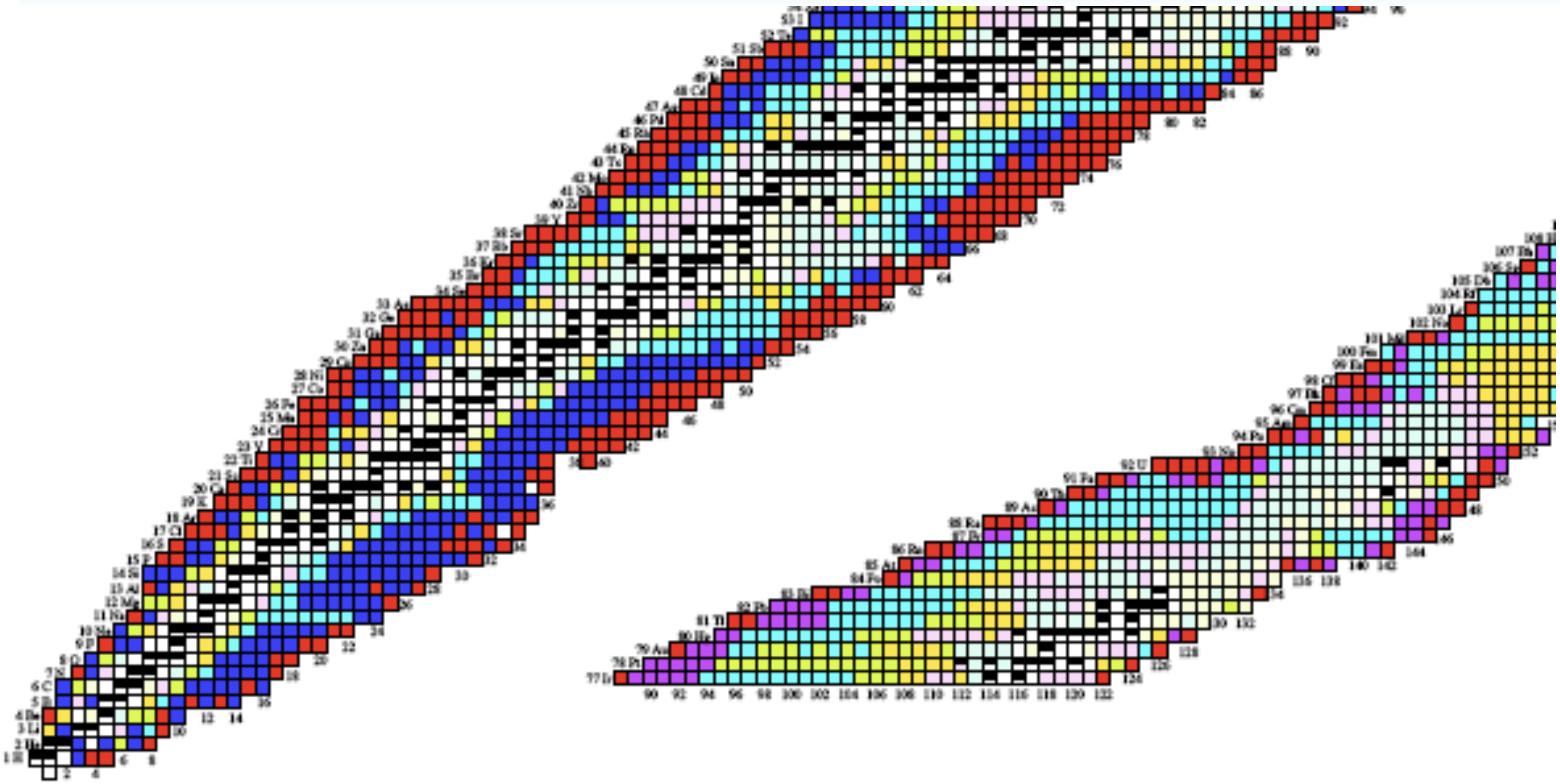
Kinetic spin-density: $$\mathbf{T}_T(\mathbf{r}) = \nabla\cdot\nabla'\,\mathbf{s}_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Relativistic Energy Density Functionals



Relativistic Energy Density Functionals

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



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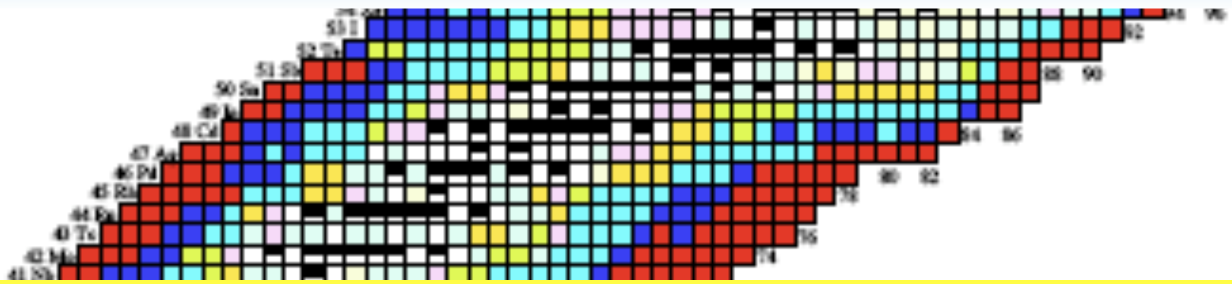
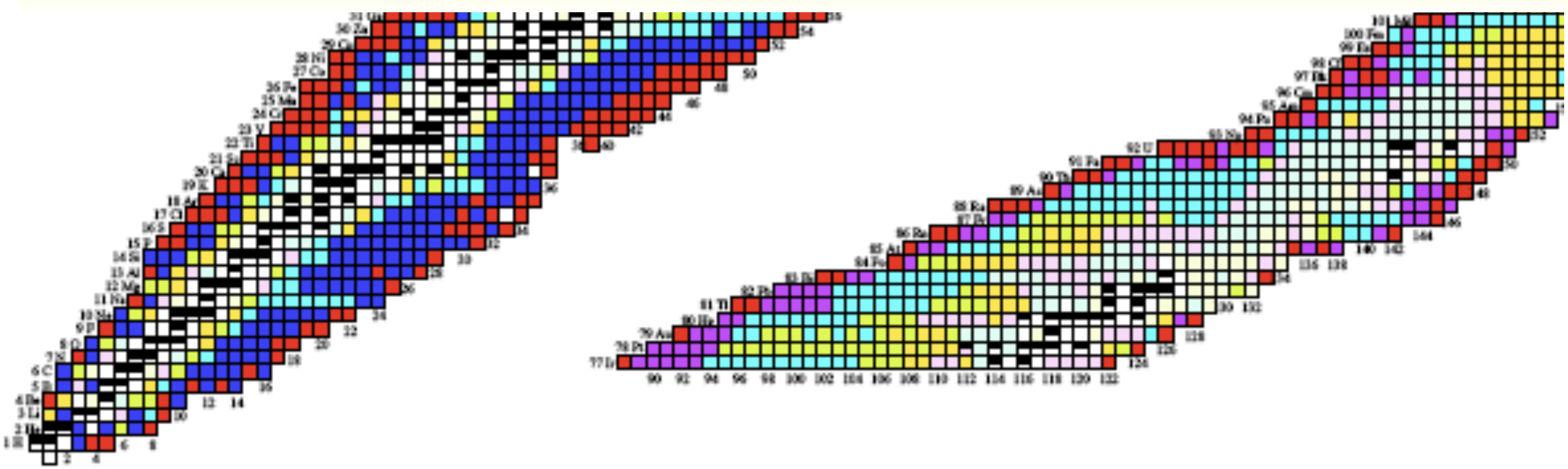


✔ unique parameterization of **time-odd components** (currents) of the nuclear mean-field



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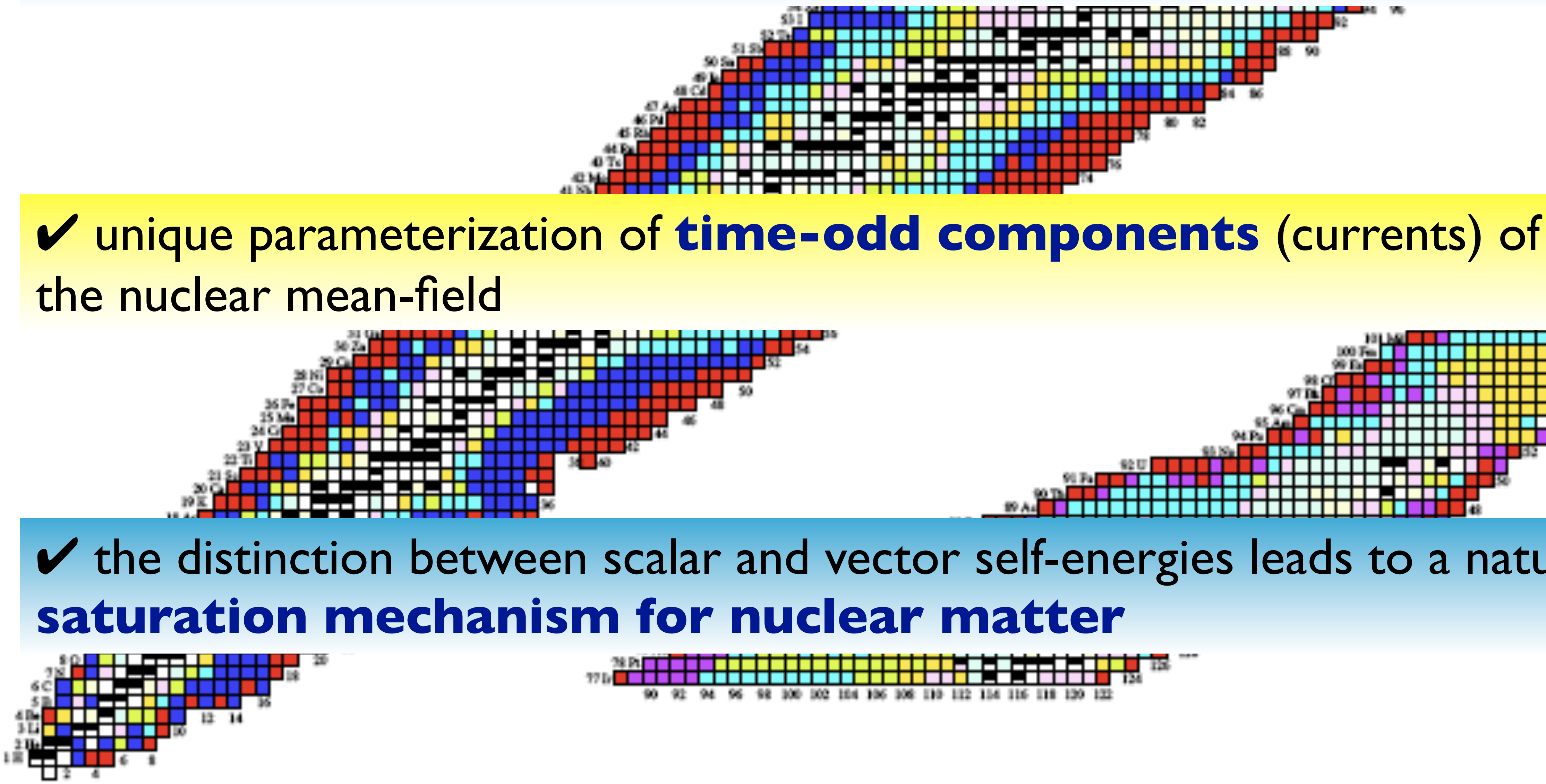
✔ the distinction between scalar and vector self-energies leads to a natural **saturation mechanism for nuclear matter**



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Important for extrapolations to regions far from stability!

... microscopic foundation for a universal EDF framework, related to and constrained by low-energy QCD

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... correlations related to restoration of broken symmetries and fluctuations of collective coordinates

Semi-empirical 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

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

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... 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.

... 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.

DD-PC1

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

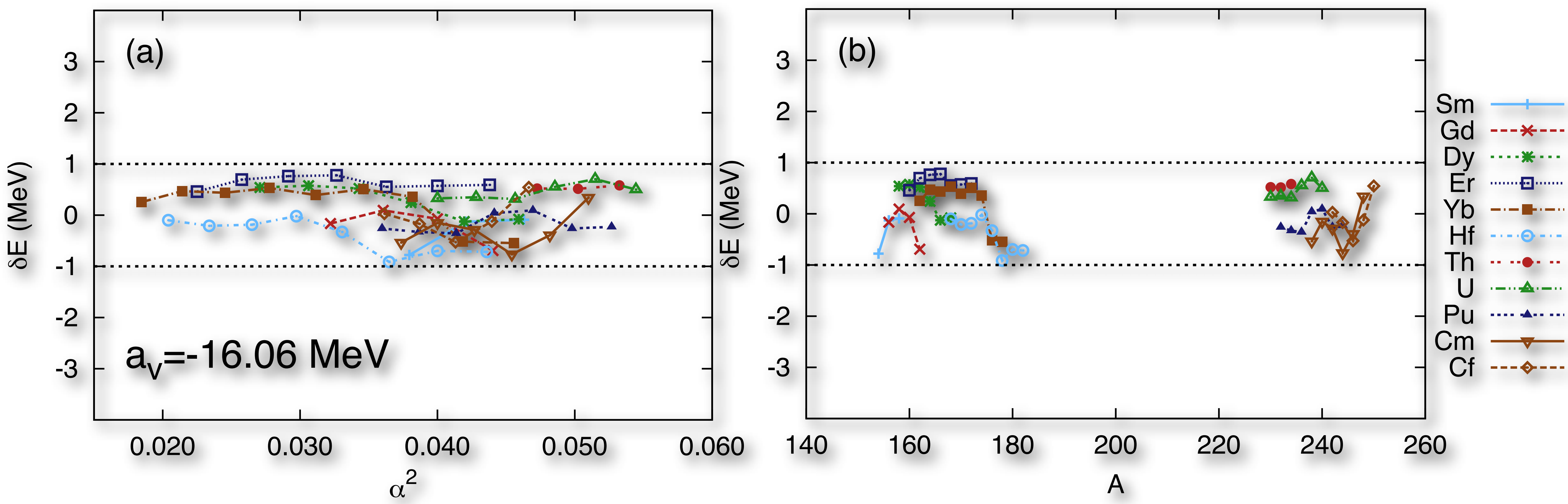
surface energy: $a_s = 17.498 \text{ MeV}$

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

Deformed nuclei

Binding energies used to adjust the parameters of the functional:

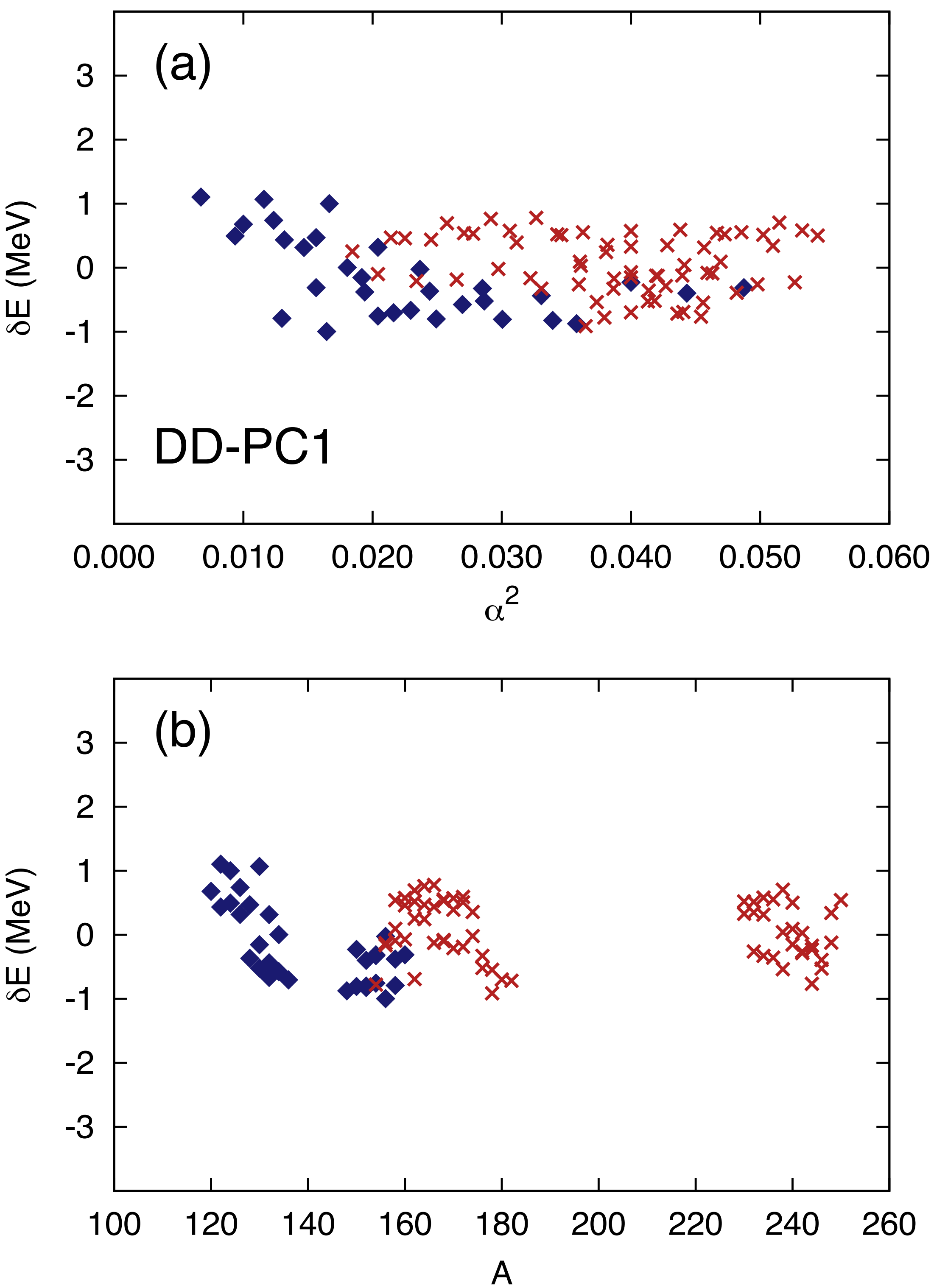
Z	62	64	66	68	70	72	90	92	94	96	98
N_{min}	92	92	92	92	92	72	140	138	138	142	144
N_{max}	96	98	102	104	108	110	144	148	150	152	152



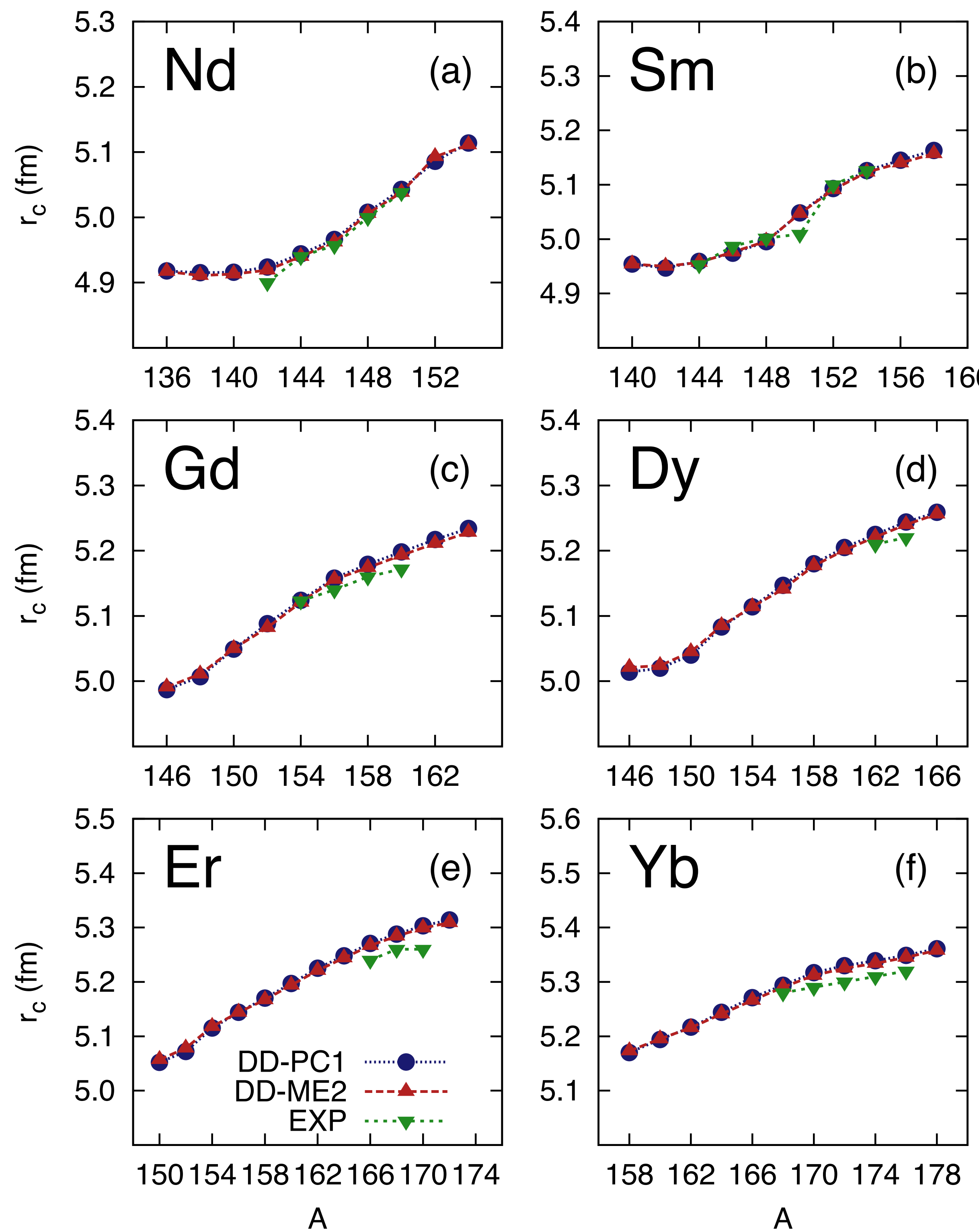
Nikšić, Vretenar, and Ring, Phys. Rev. C **78**, 034318 (2008)

Systematic calculation of ground-state properties:

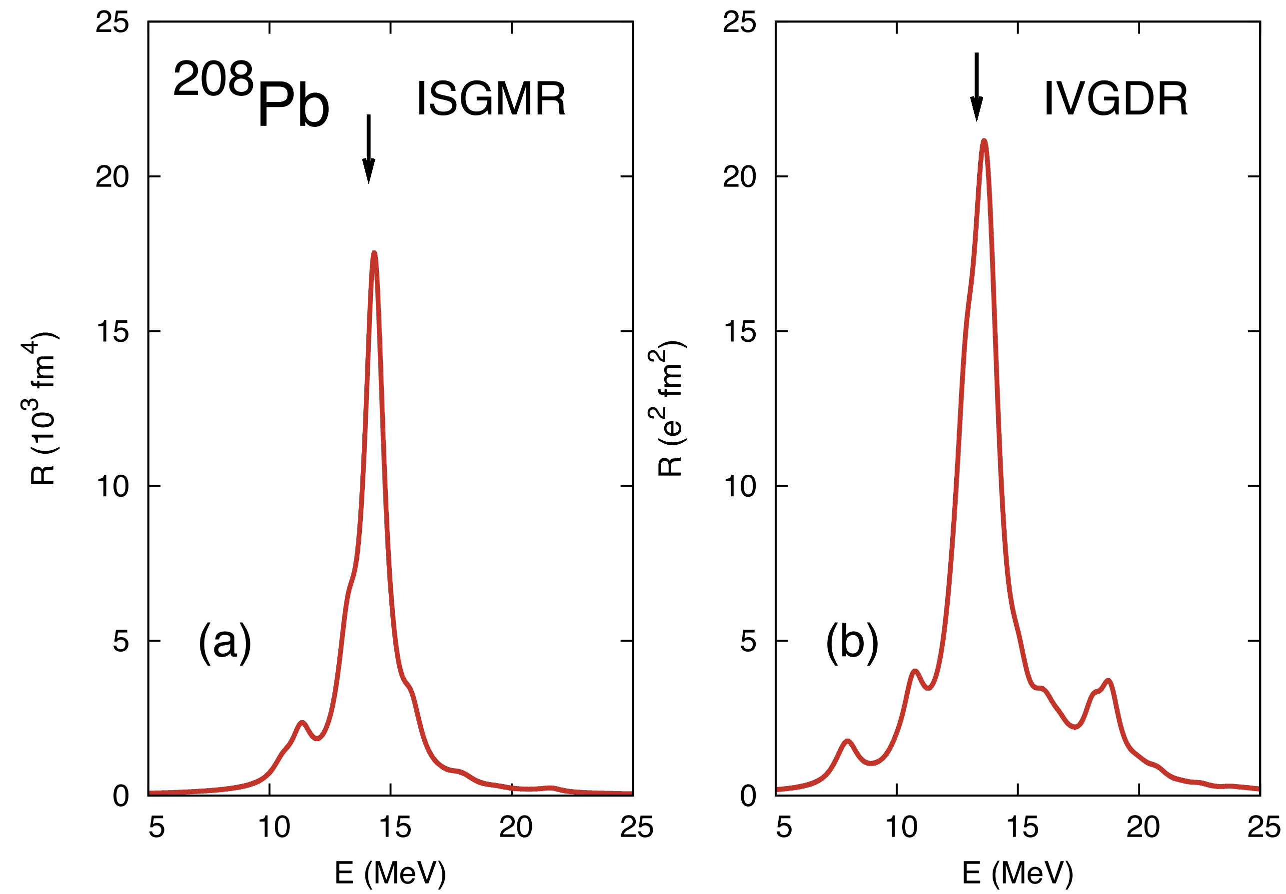
Absolute error of calculated masses:



Charge radii:

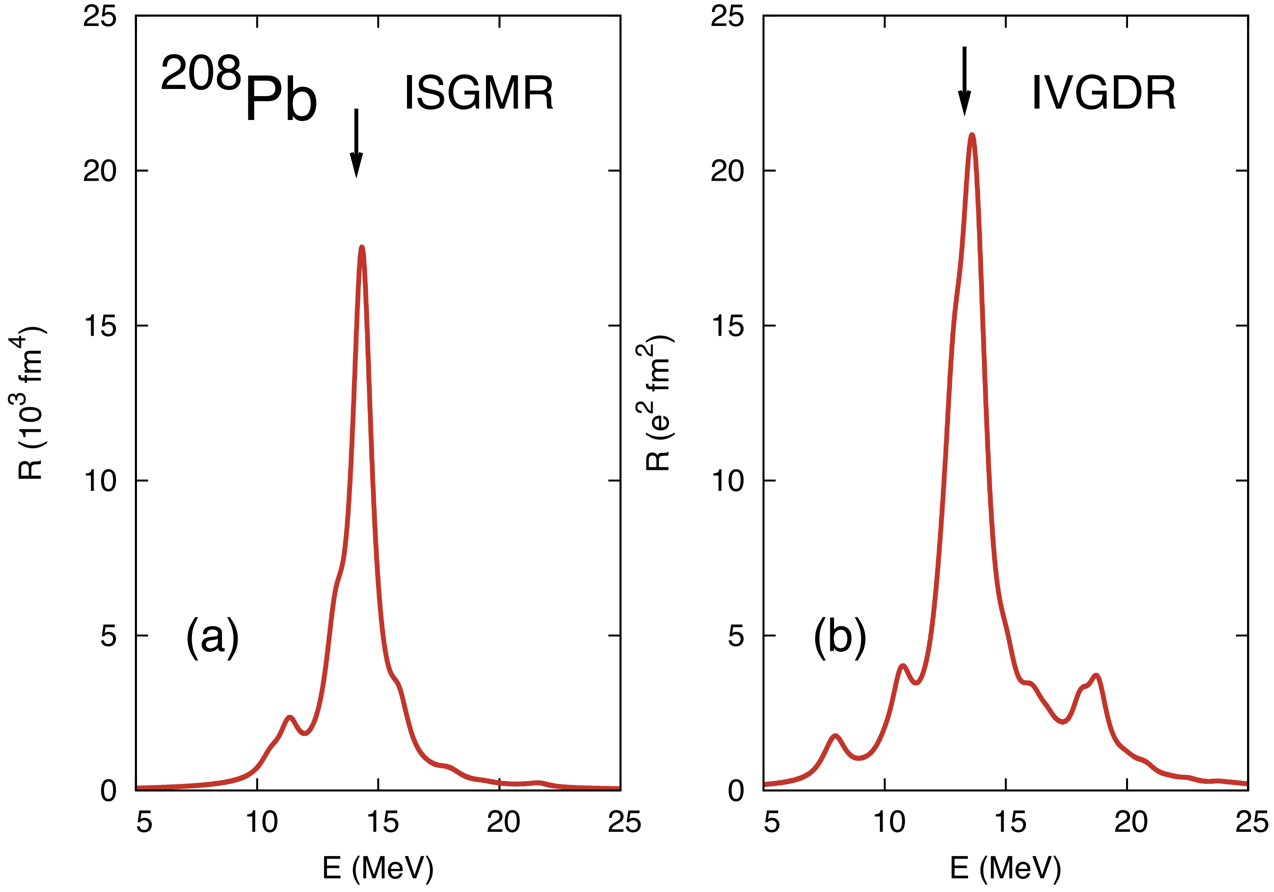


Excitation energies of collective modes:



Excitation energies of collective modes:

IVGDR



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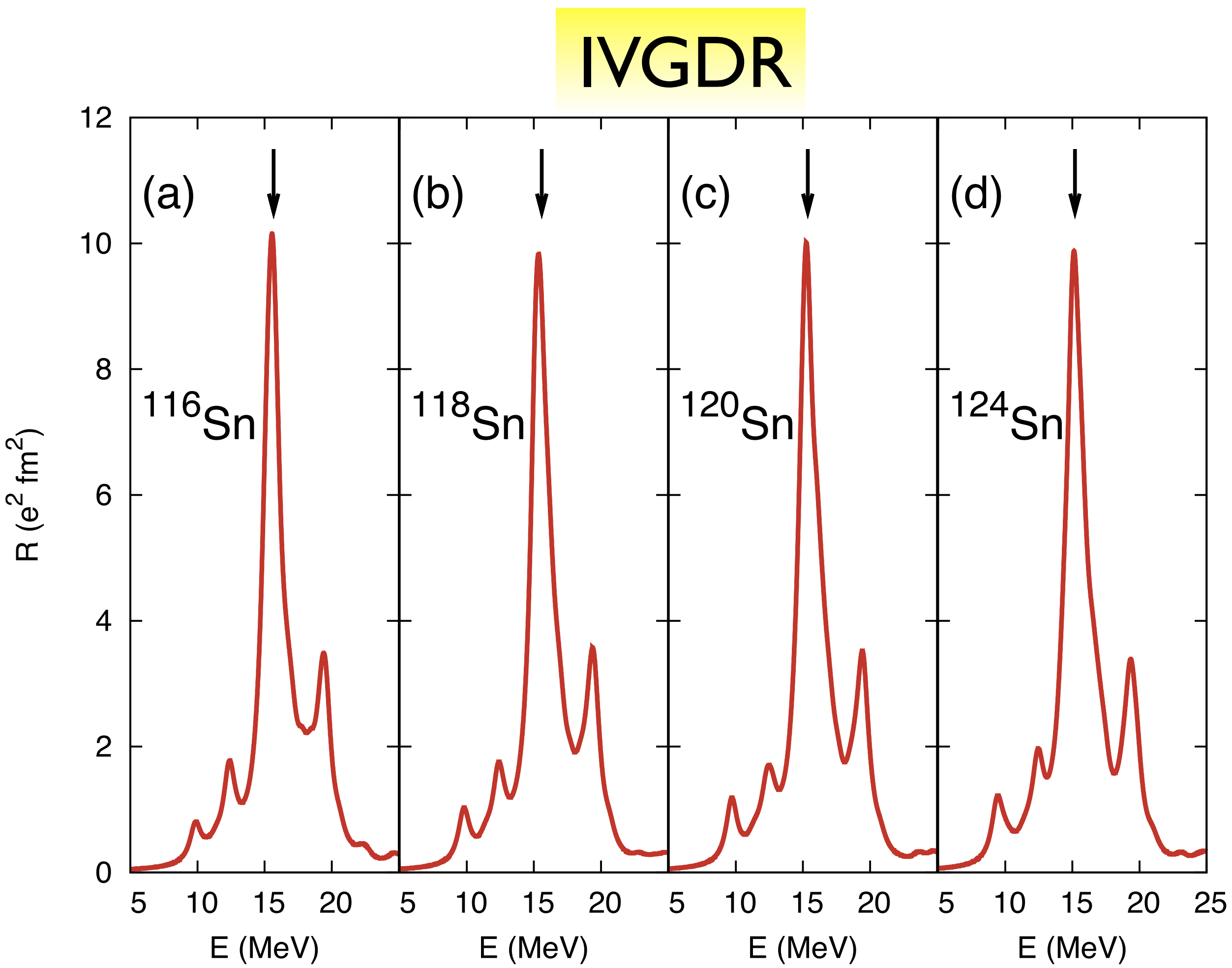

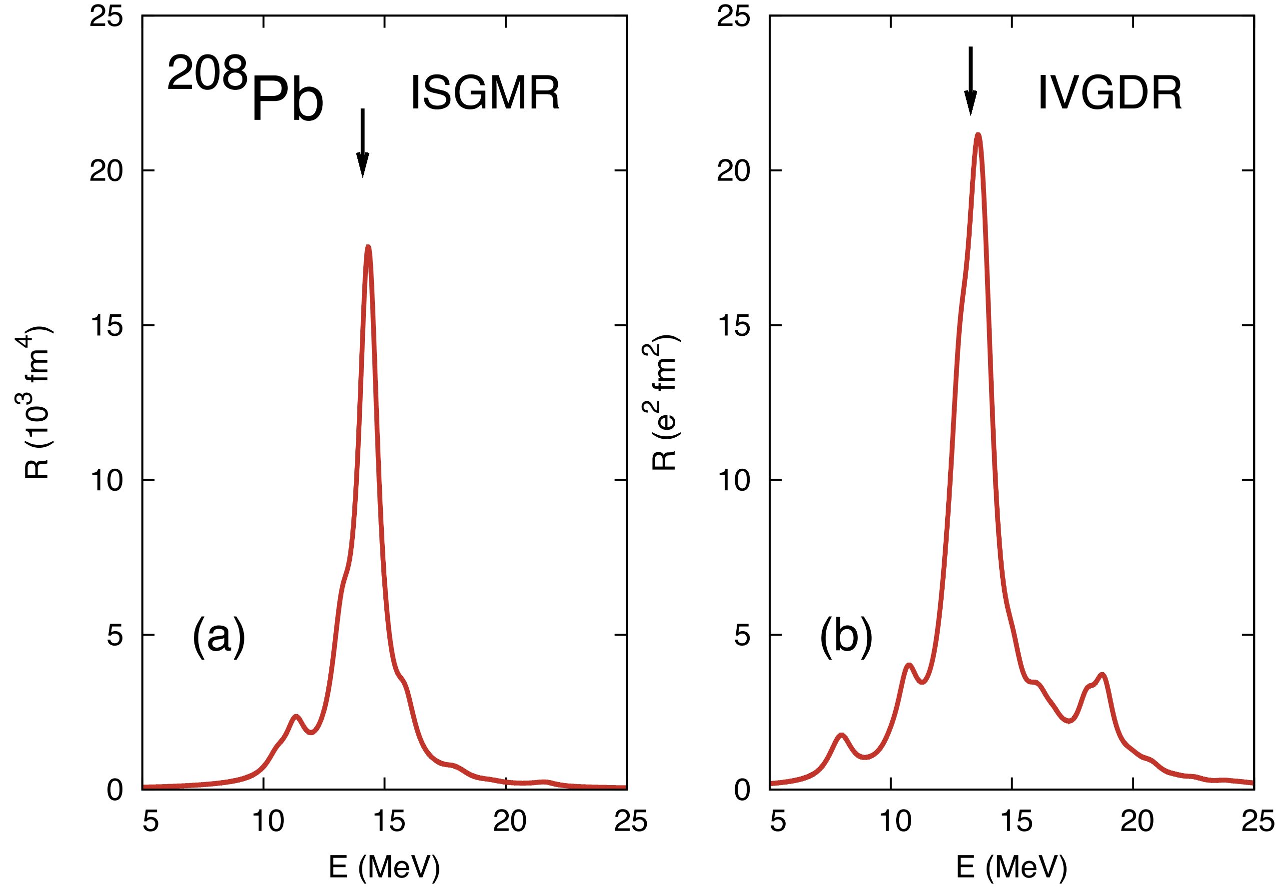

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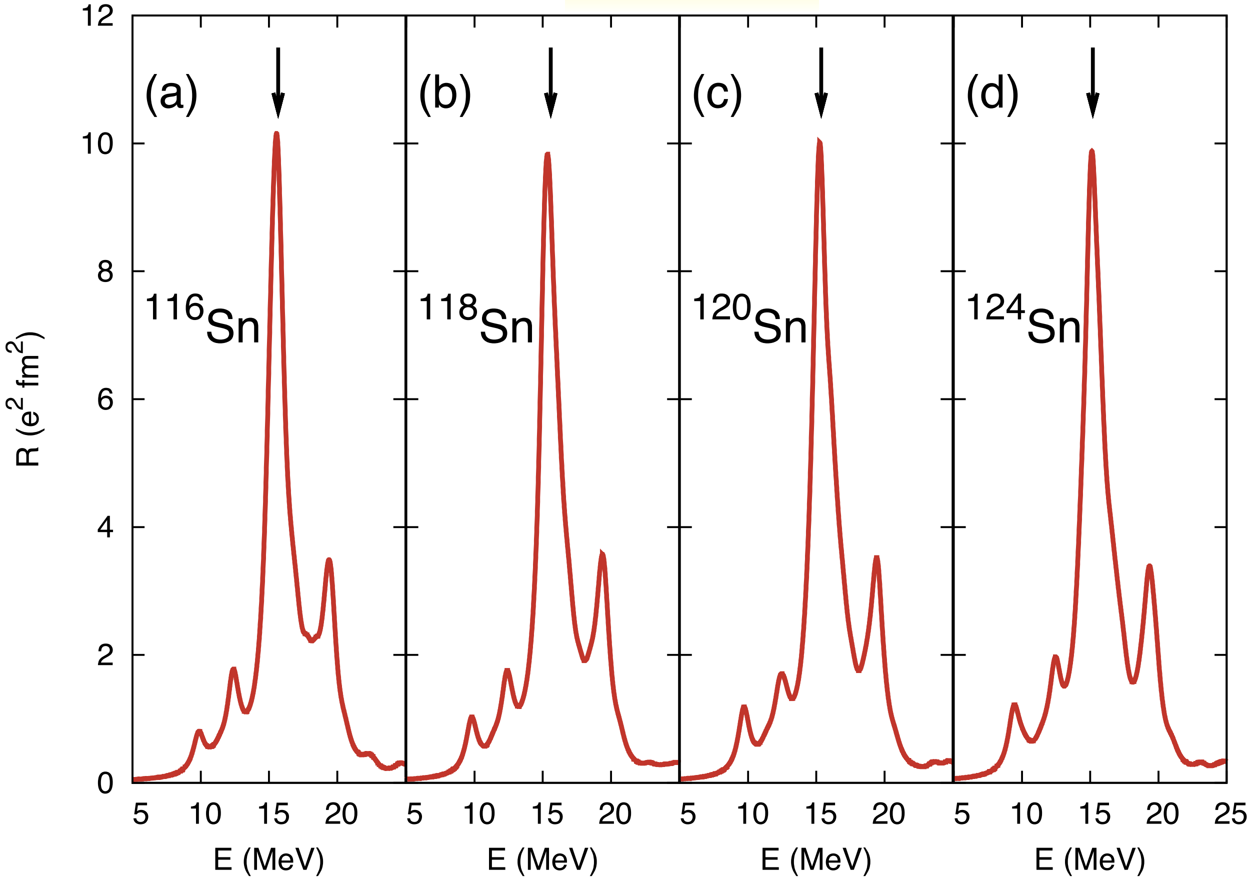

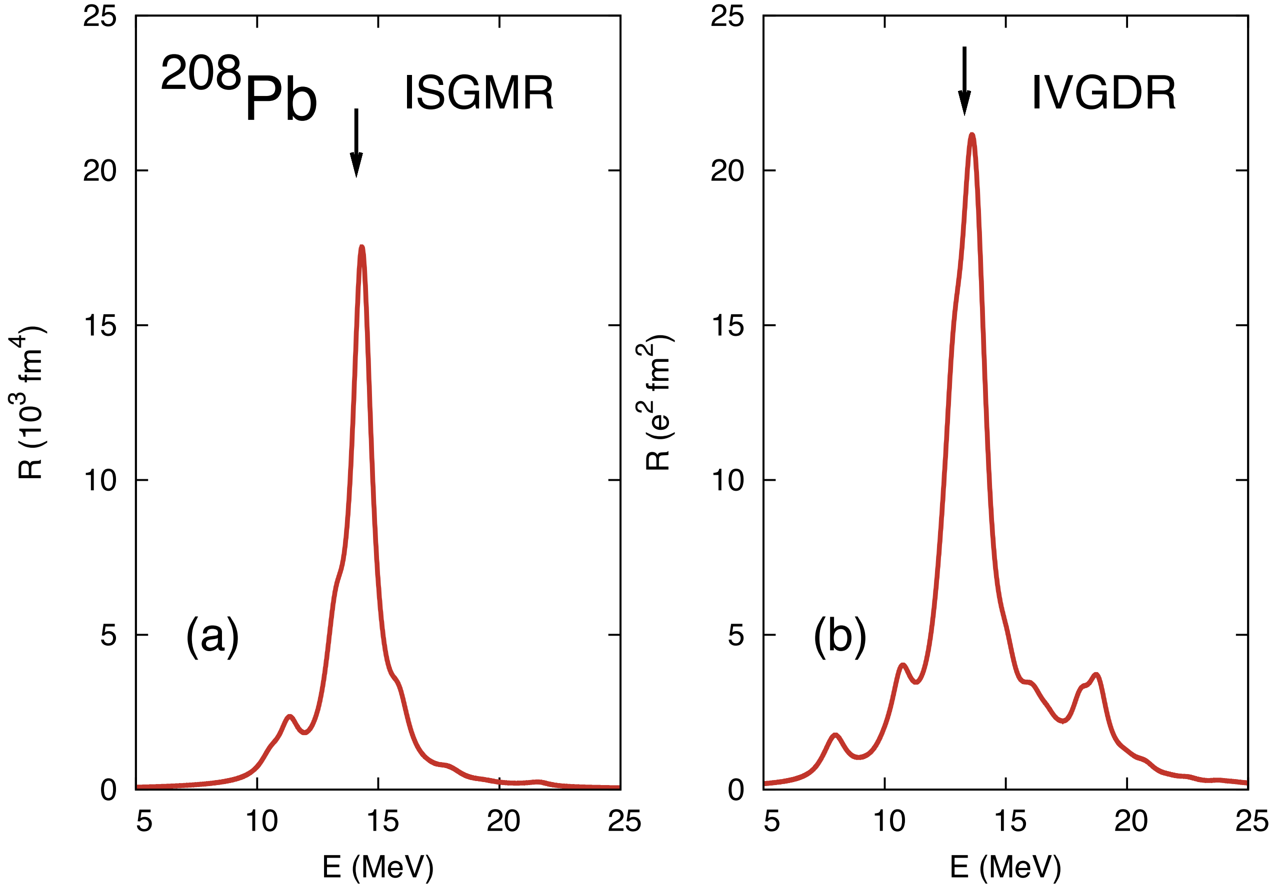

ISGMR

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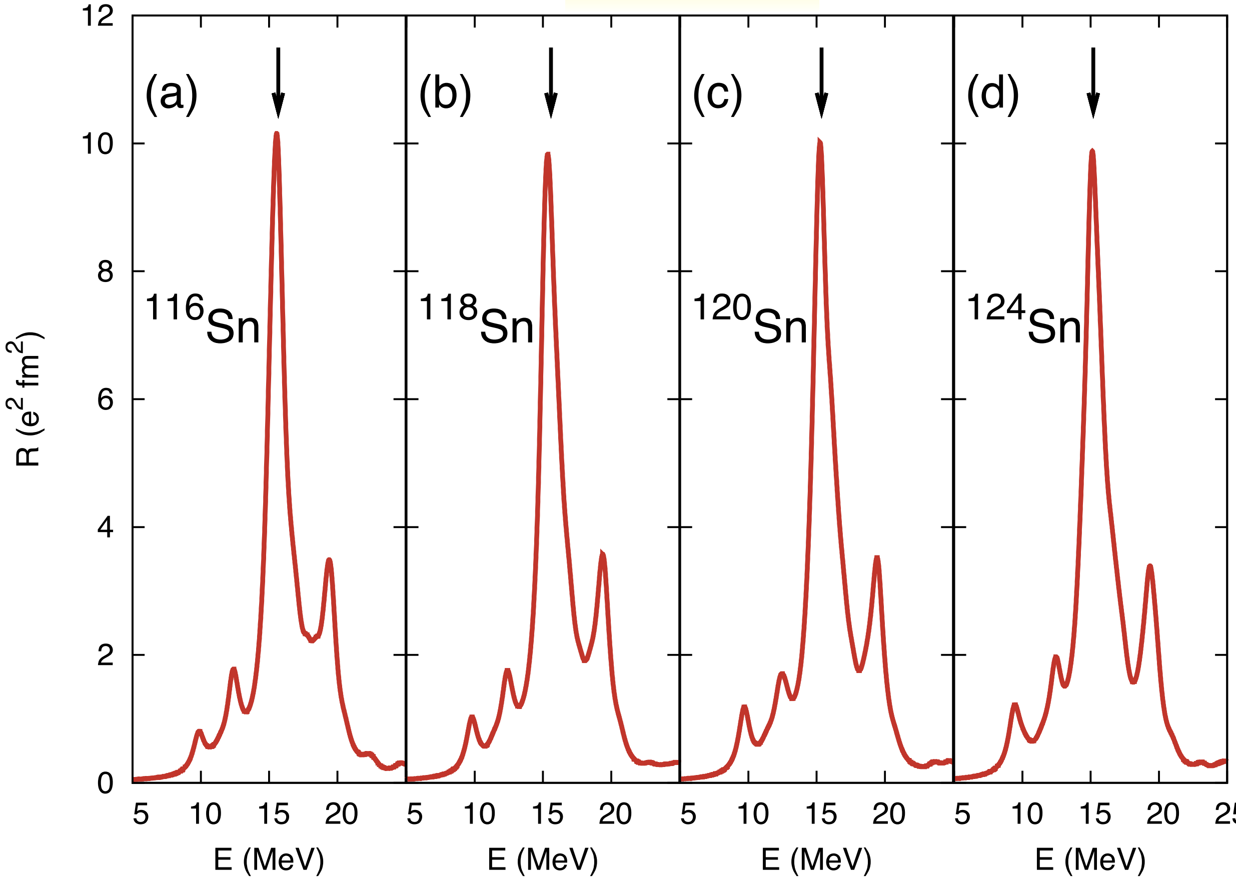

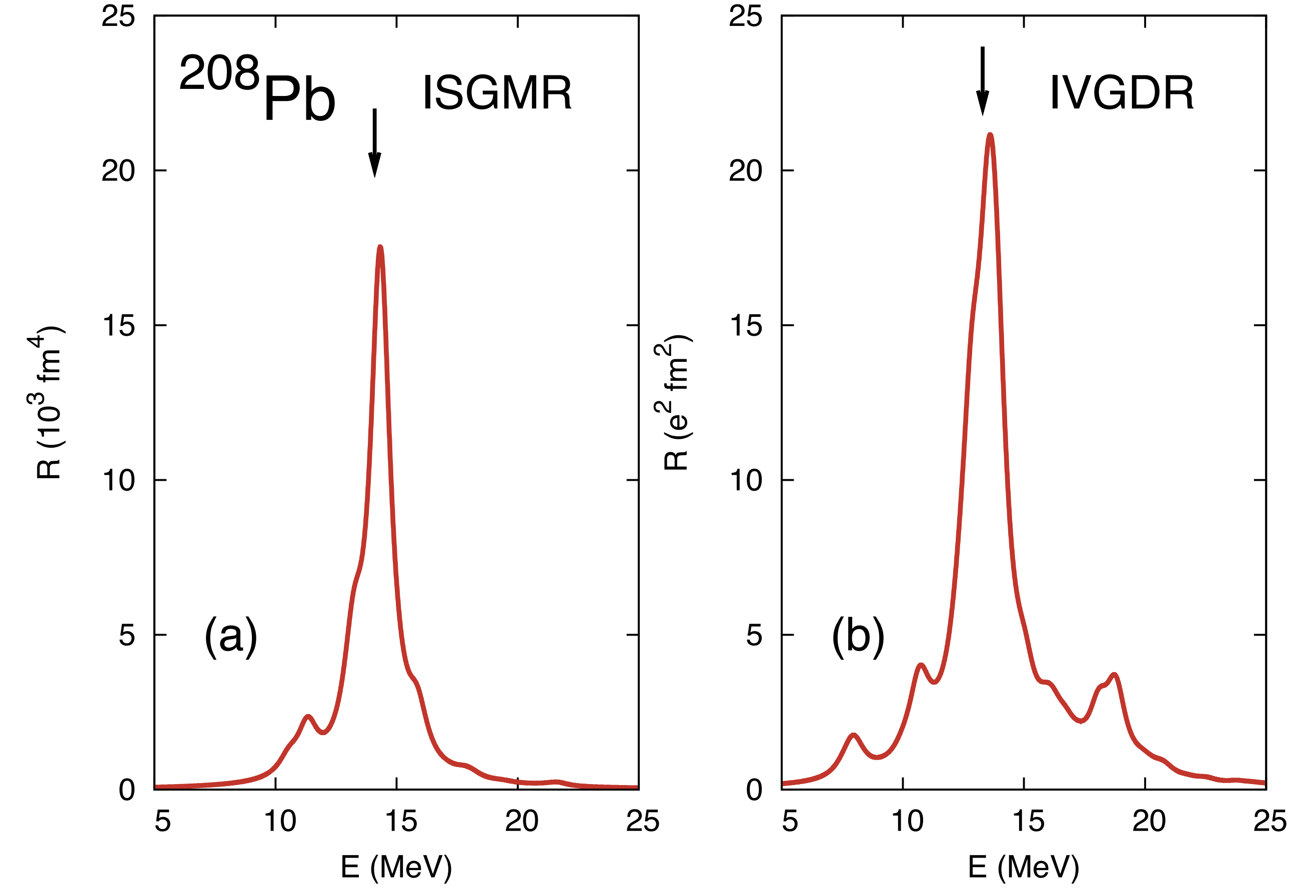

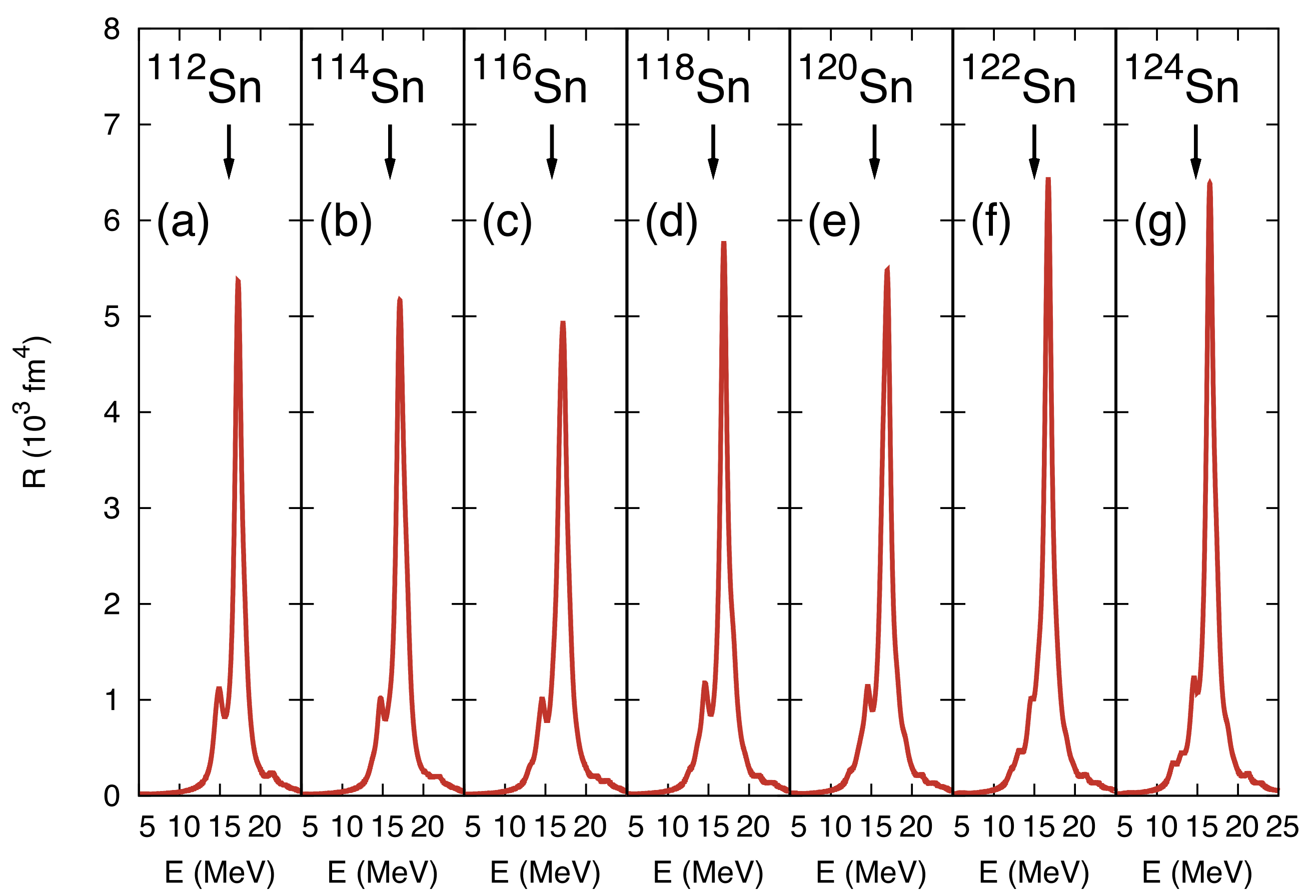

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Nuclear Many-Body Correlations

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)

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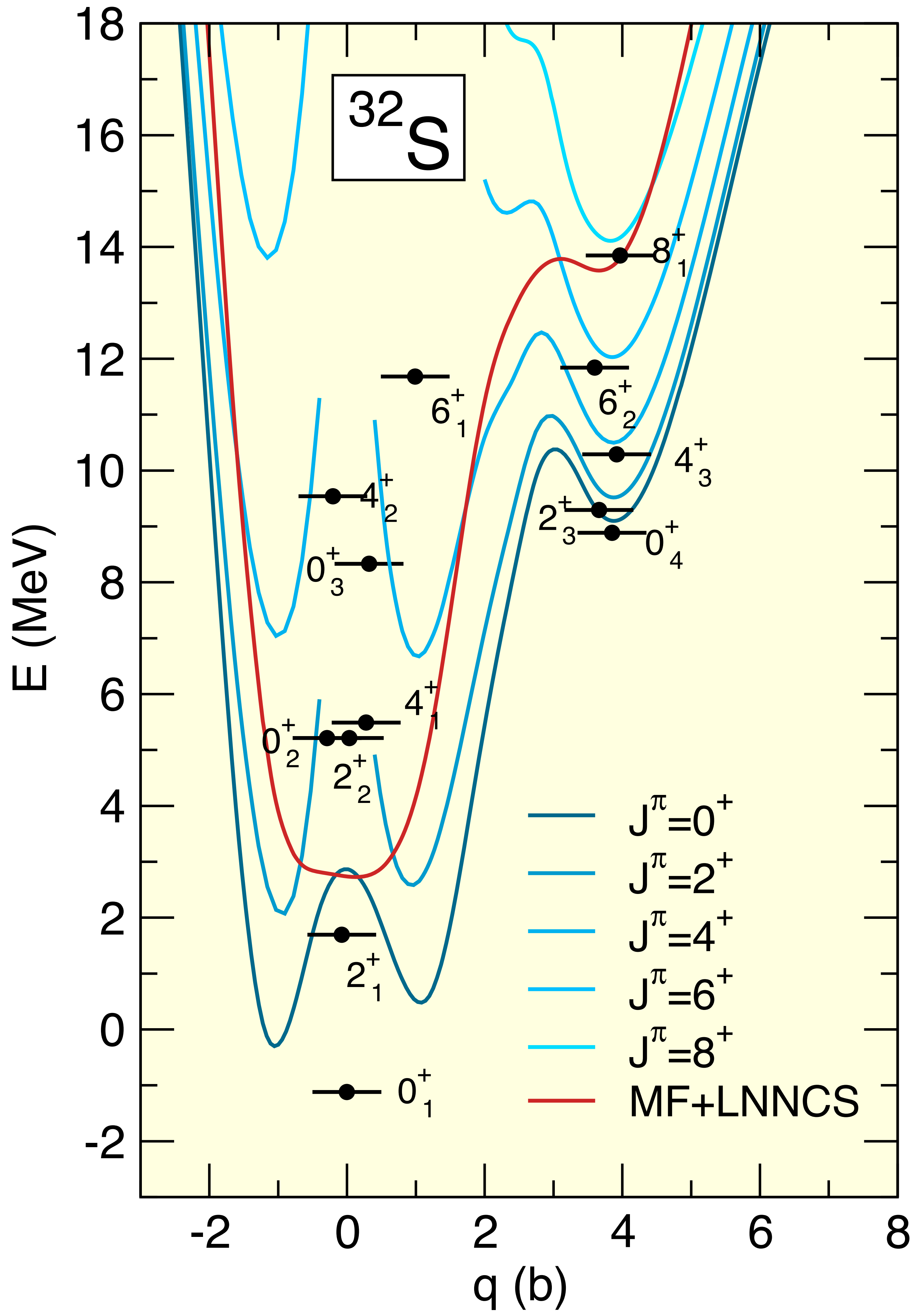
Can be included implicitly in an effective Energy Density Functional.

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

Collective correlations → restoration of broken symmetries and fluctuations of collective variables



Collective correlations → restoration of broken symmetries and fluctuations of collective variables

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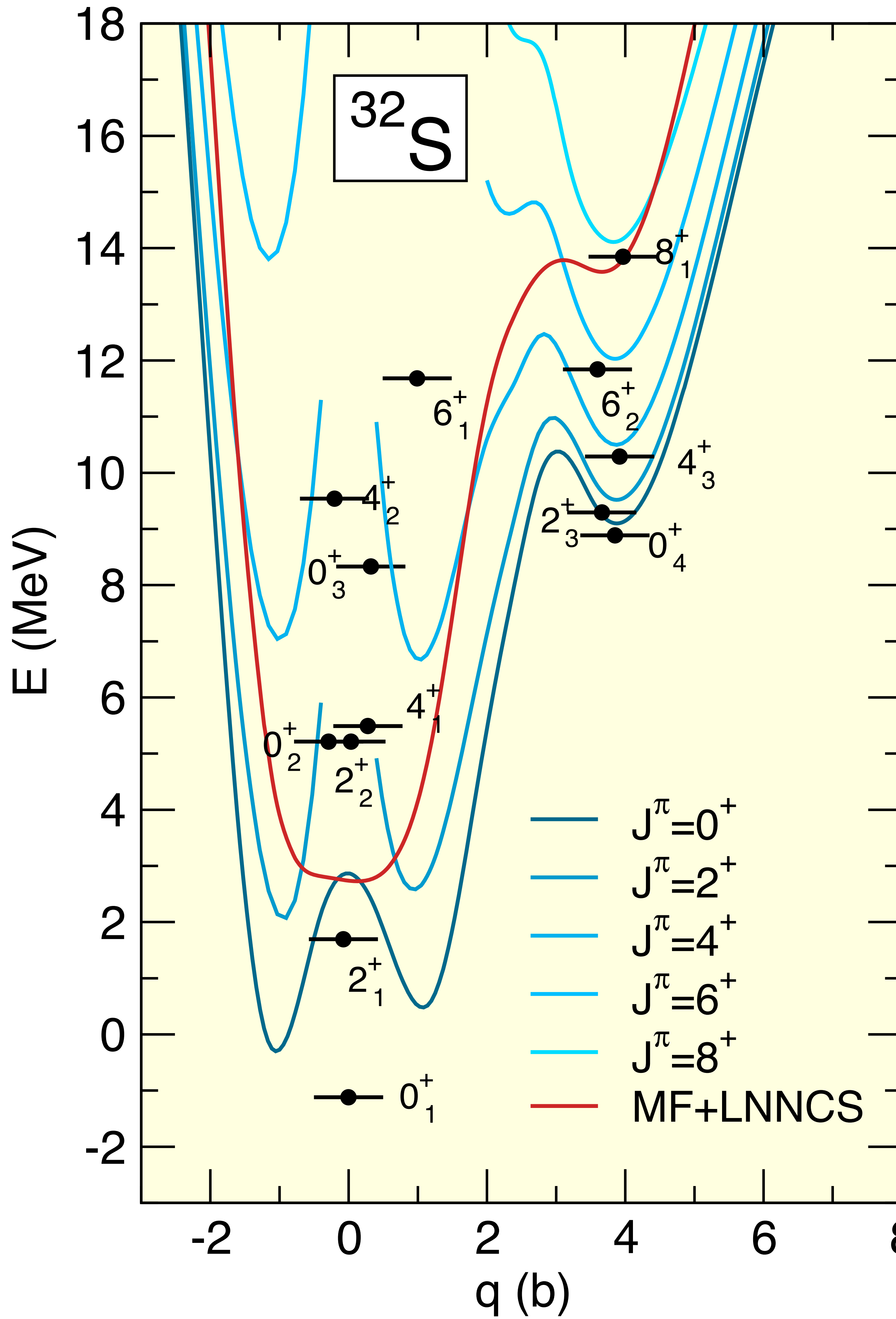
2. Angular-momentum and particle-number projection.

3. Generator Coordinate Method ⇒ configuration mixing



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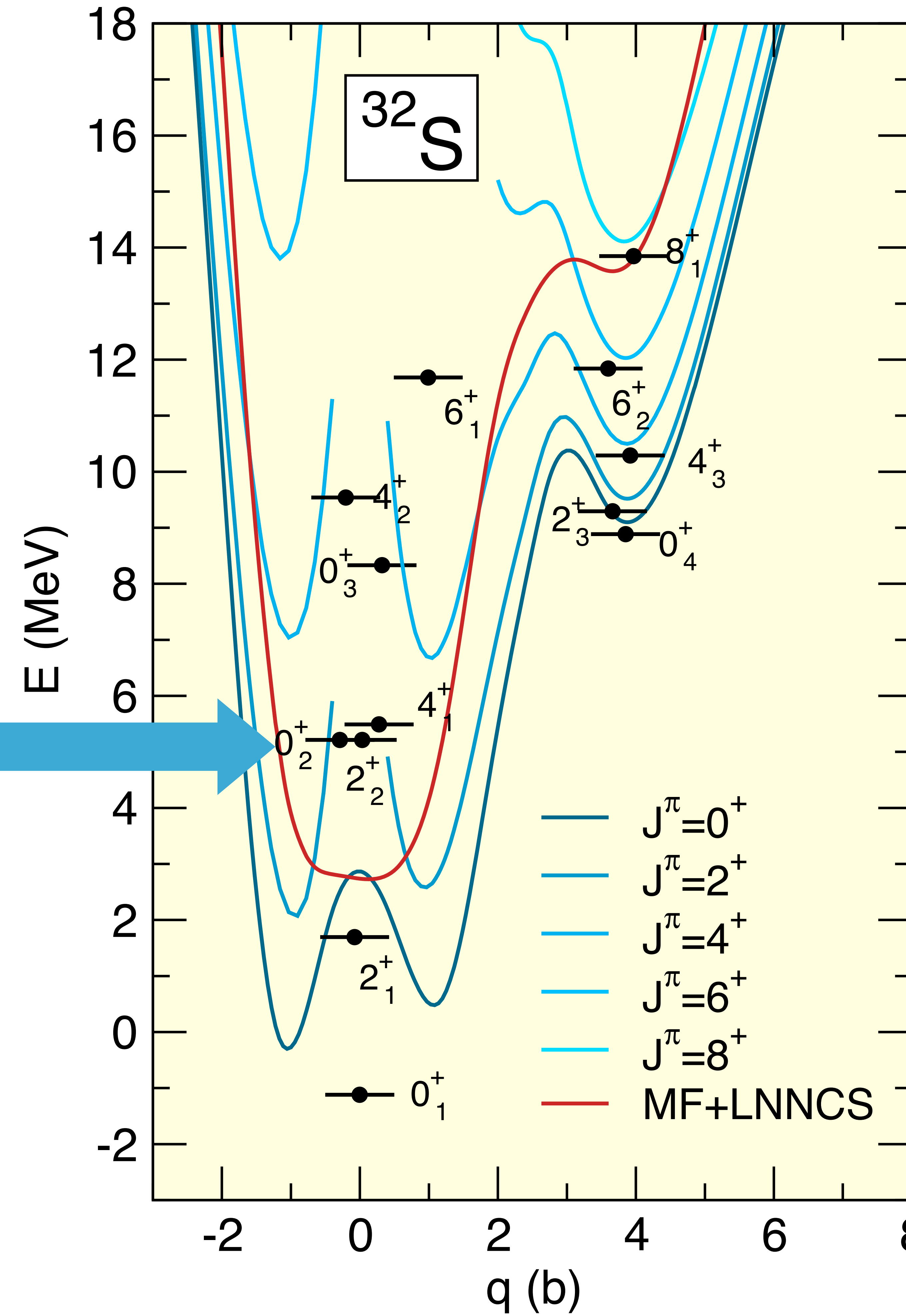

Monday, June 27, 2011

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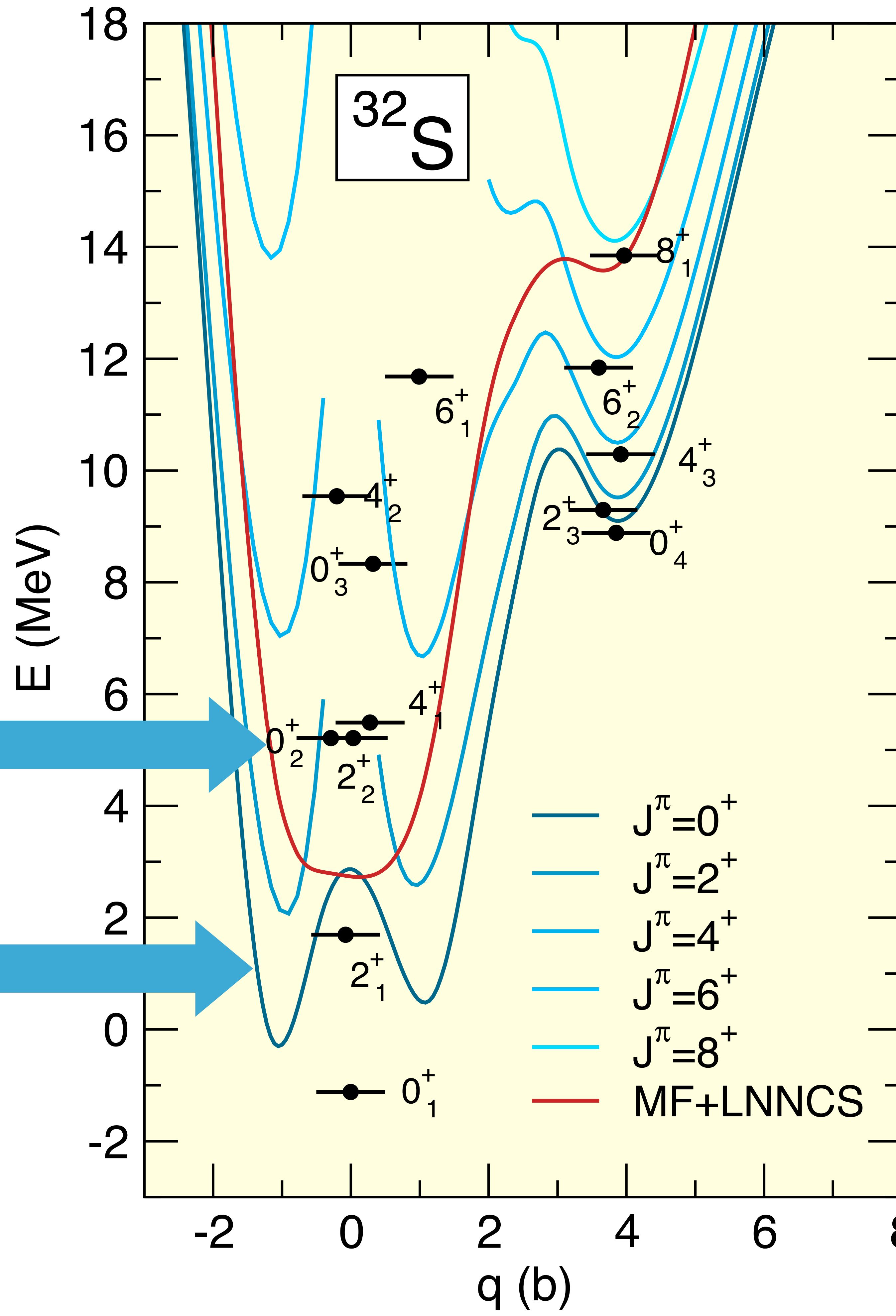

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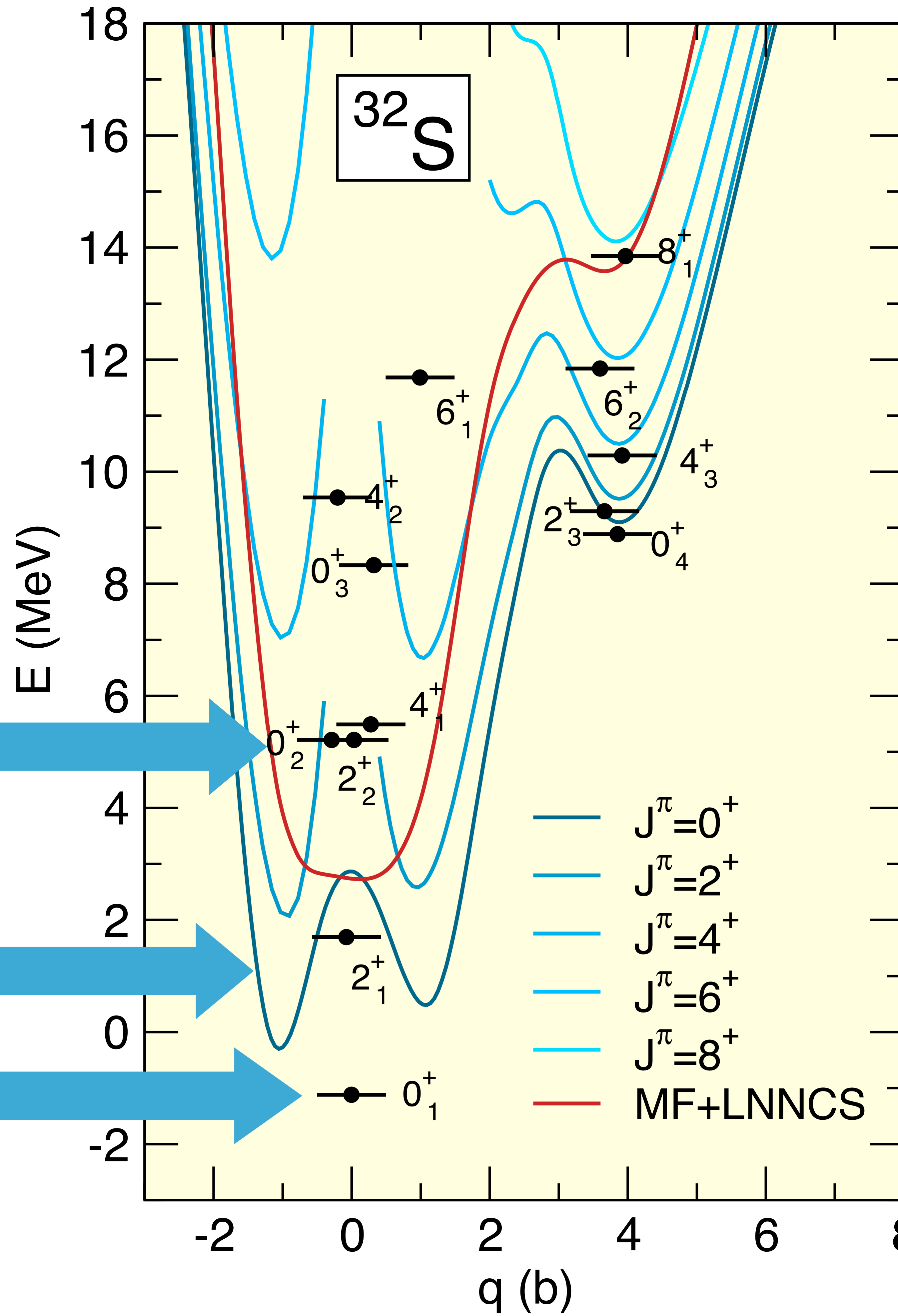
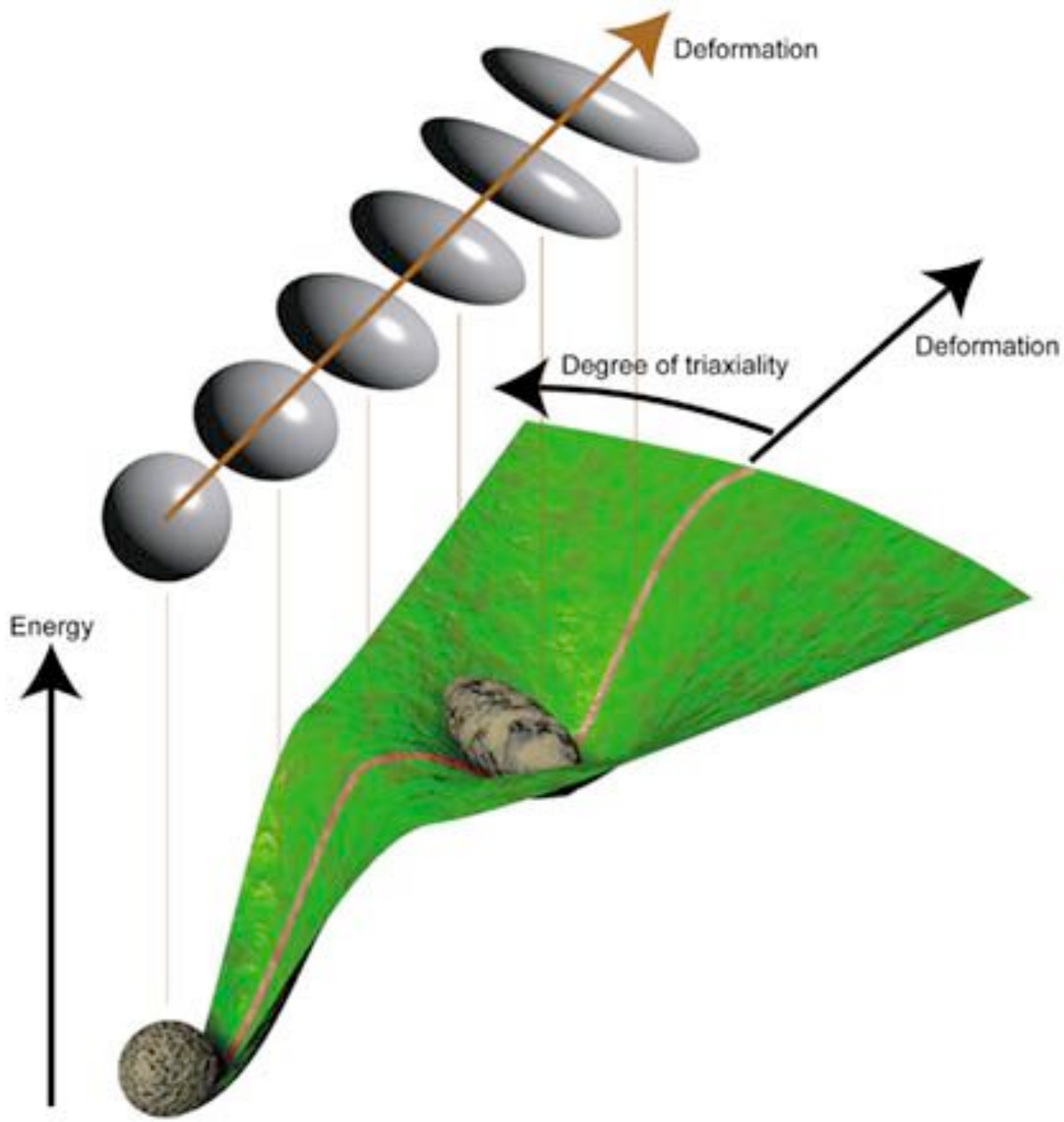


... larger variational space for projected GCM calculations!

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



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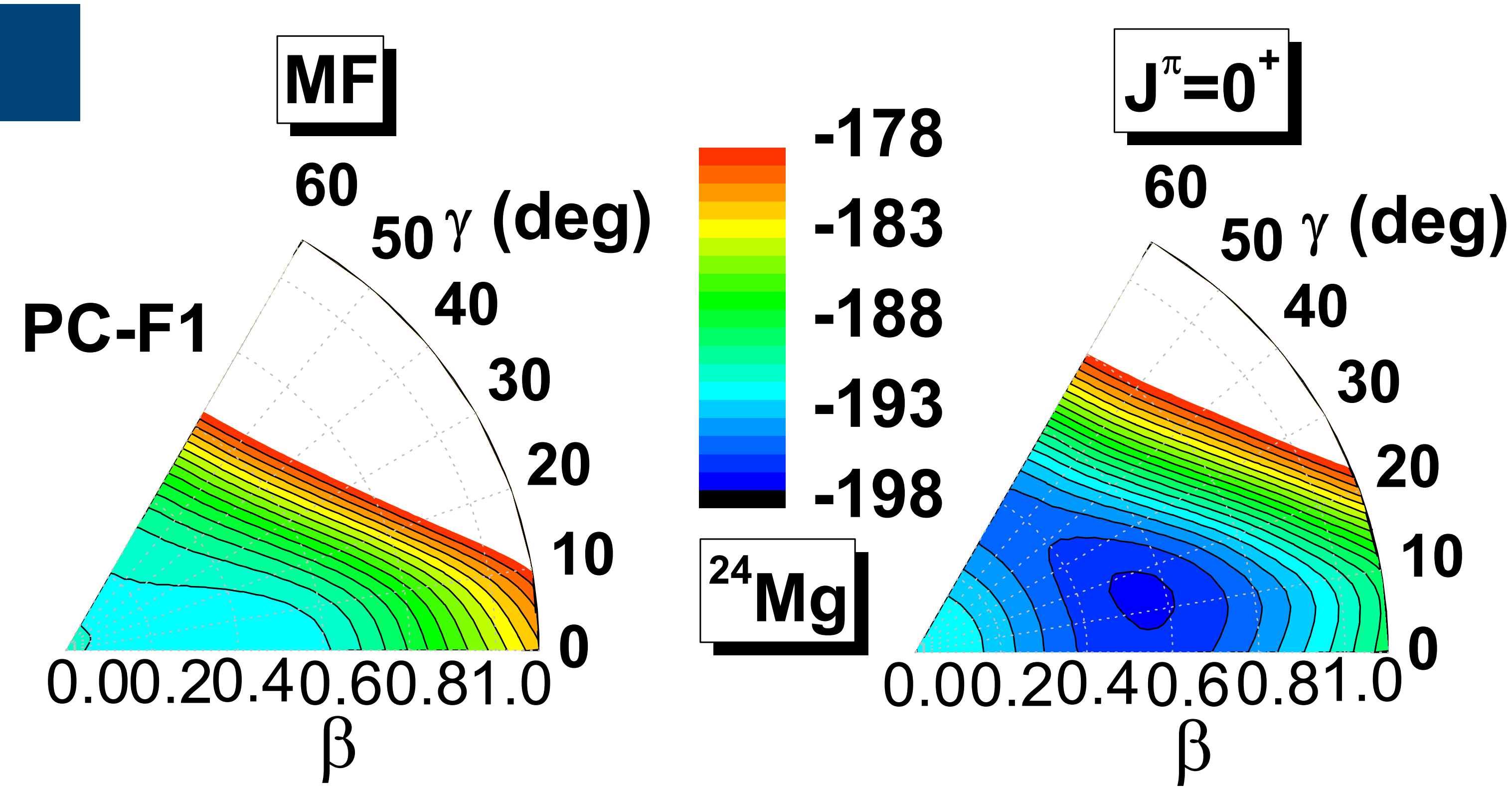

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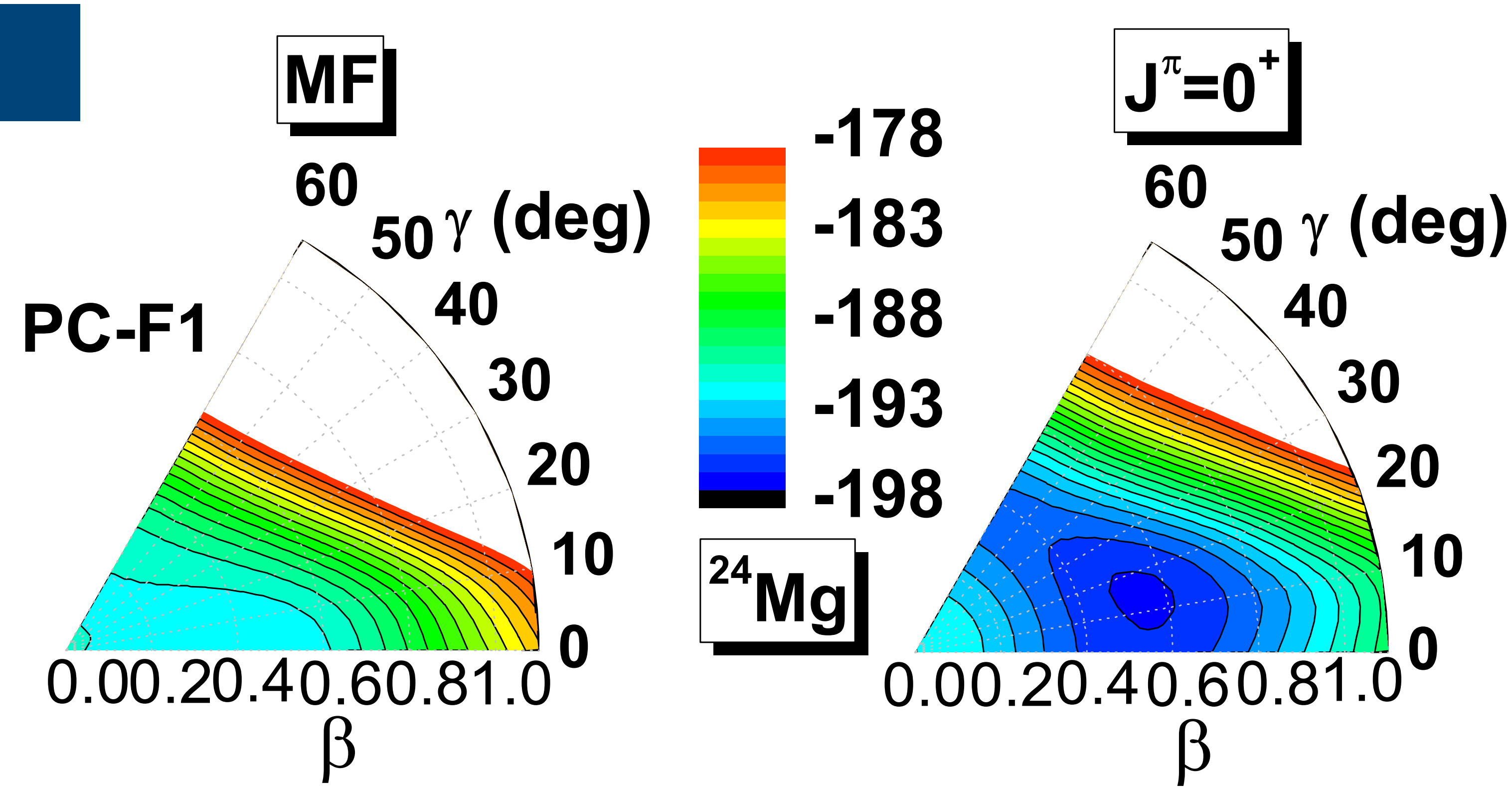

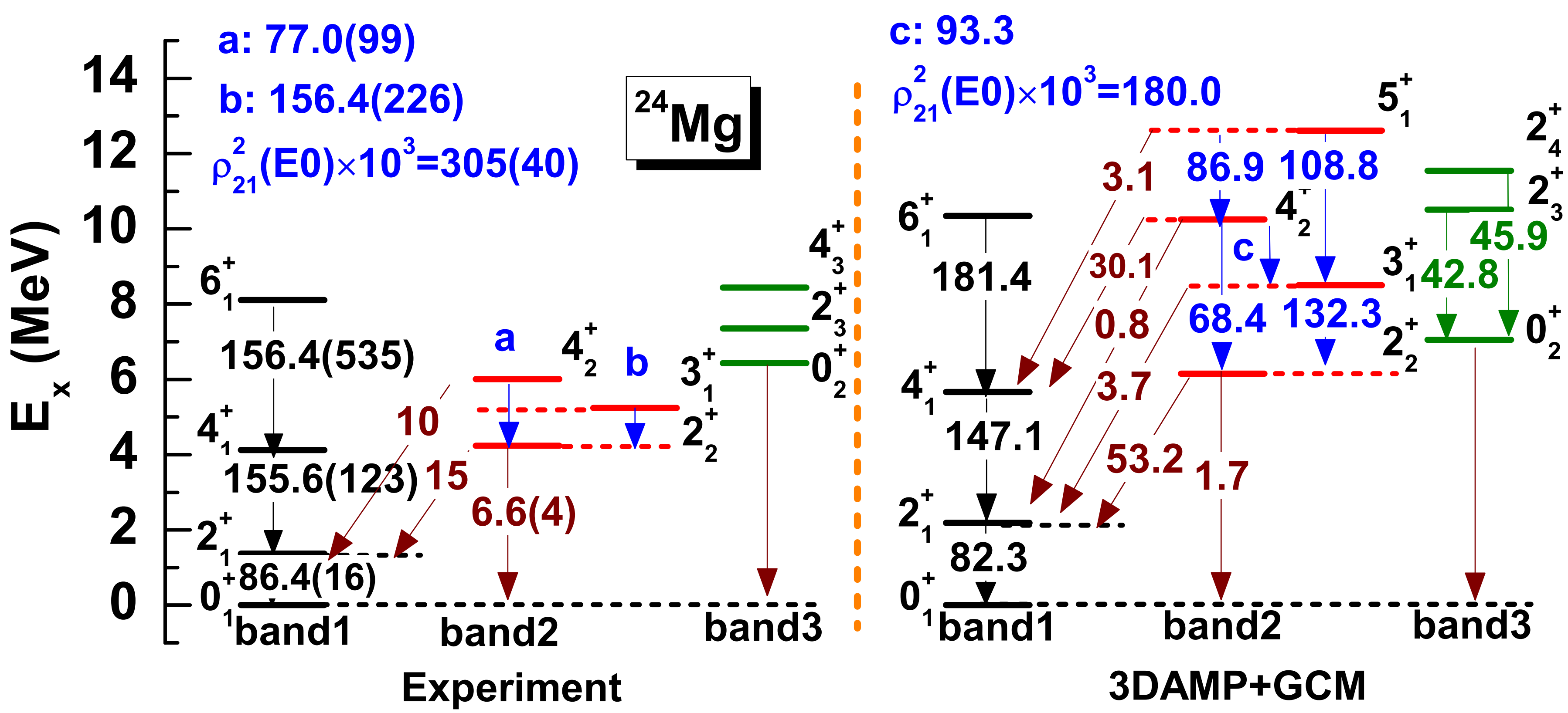

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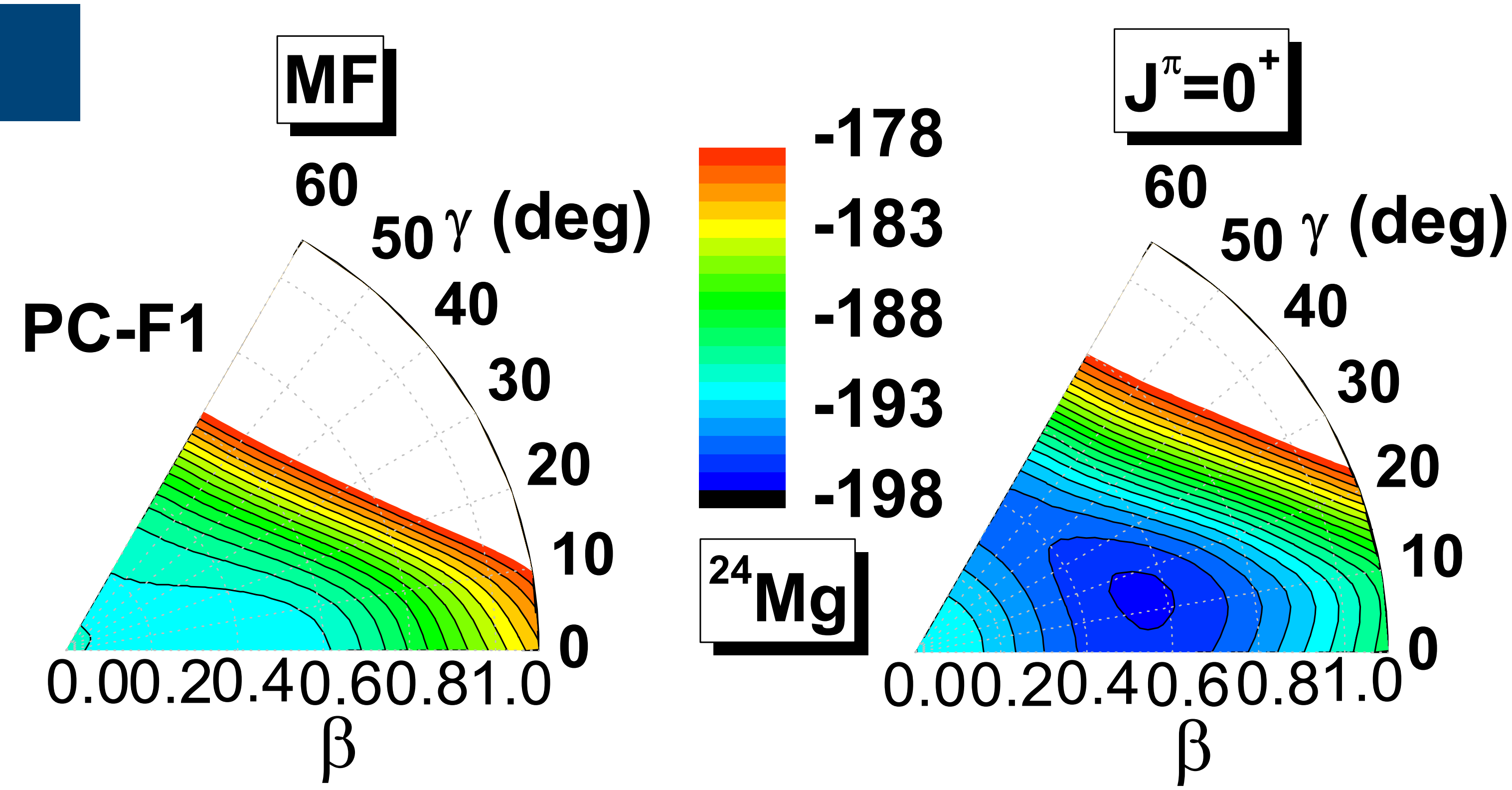

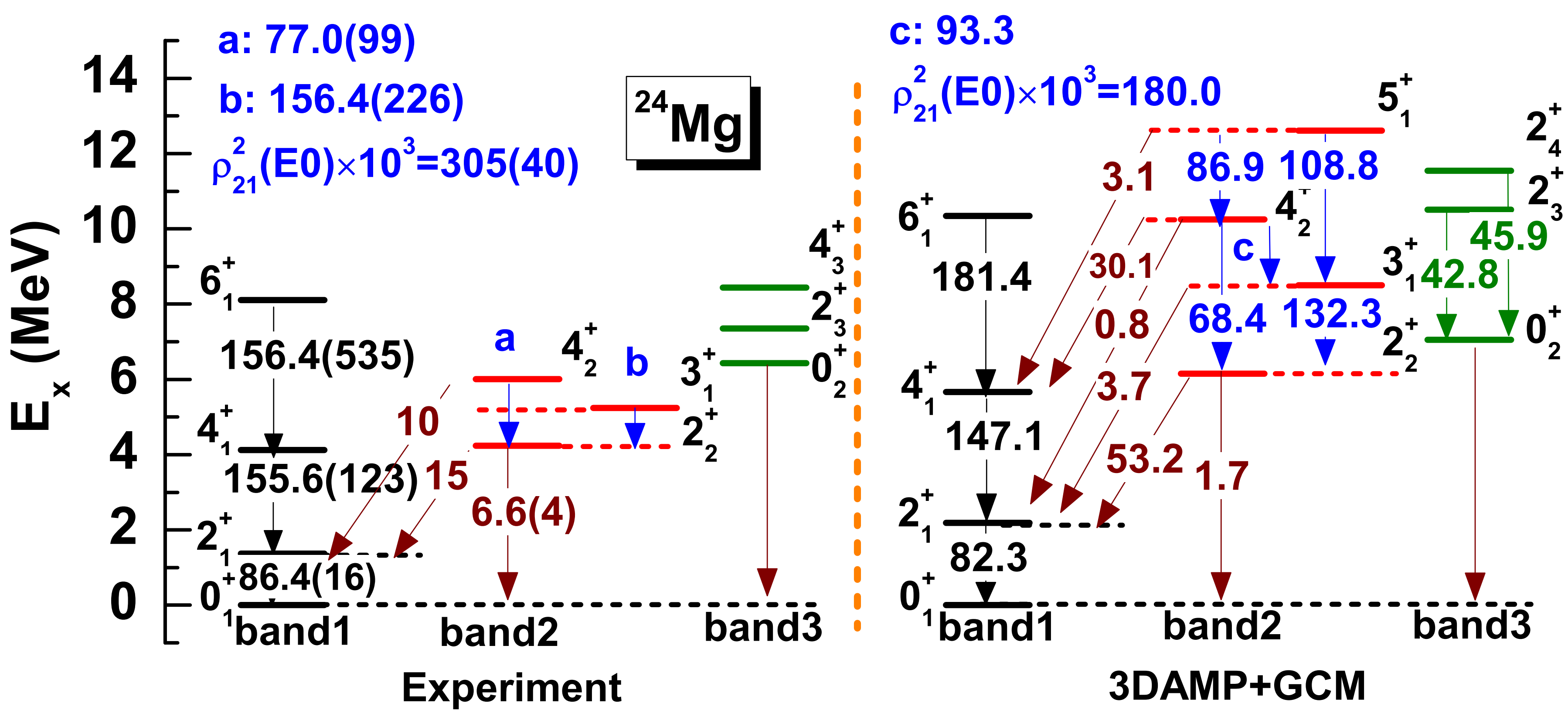

Yao, Meng, Ring, Vretenar,
Phys. Rev. C **81**, 044311 (2010)

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

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

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

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

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

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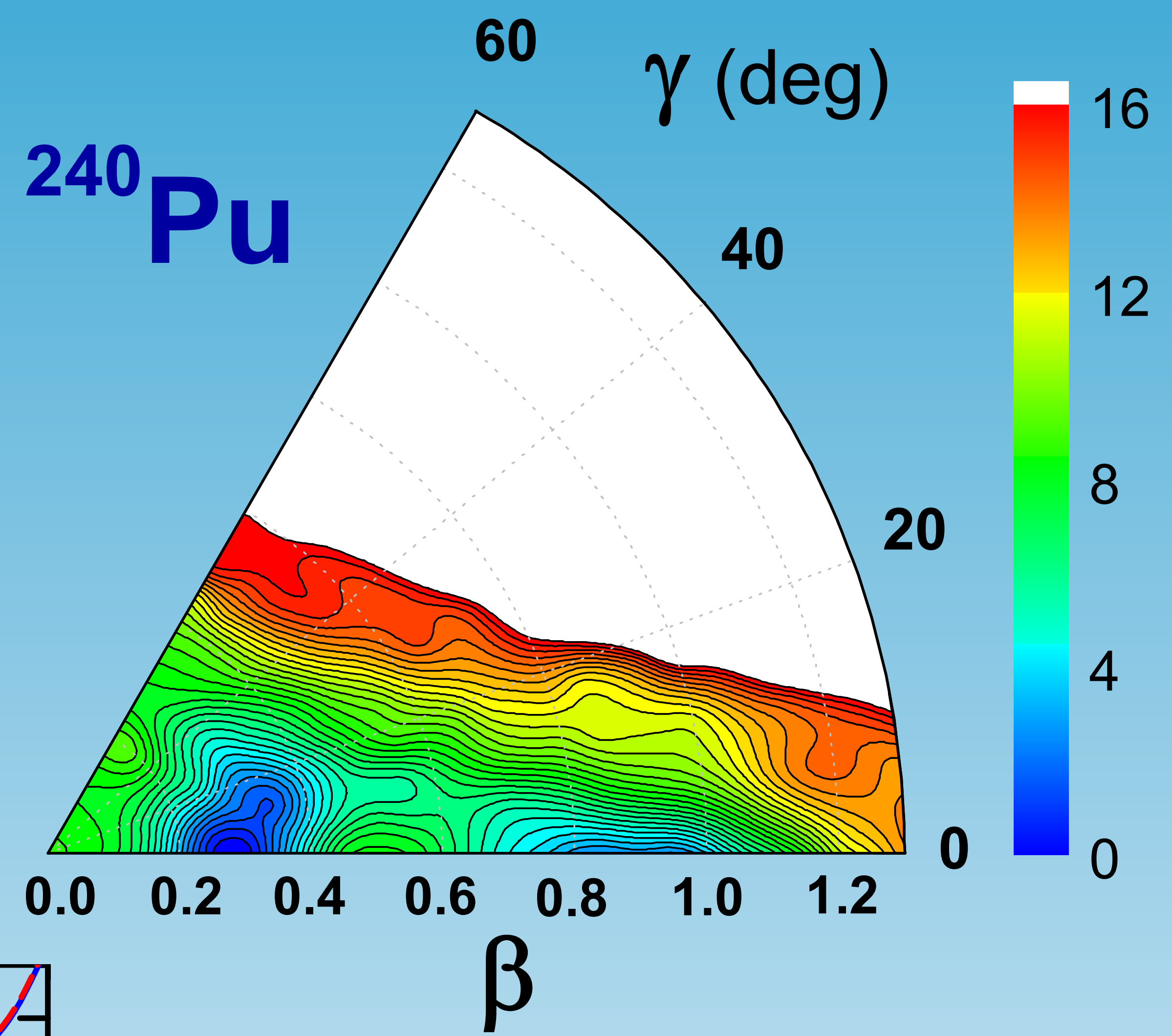
$$\mathcal{T}_{\rm rot} = \frac{1}{2}\sum_{k=1}^{3}\mathcal{I}_k\omega_k^2$$

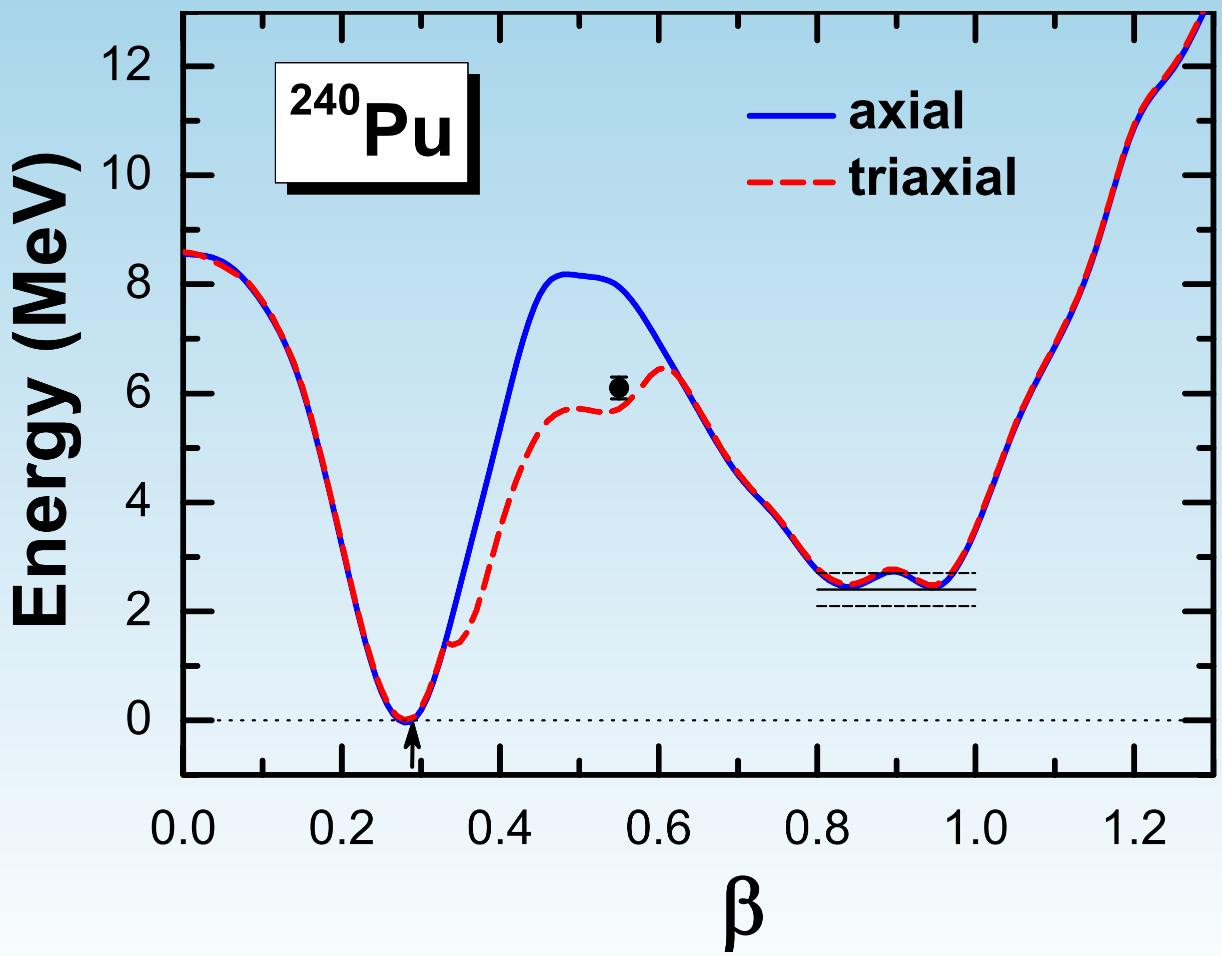
$$\mathcal{V}_{\rm coll}(\beta,\gamma) = E_{\rm tot}(\beta,\gamma) - \Delta V_{\rm vib}(\beta,\gamma) - \Delta V_{\rm rot}(\beta,\gamma)$$

The quasiparticle wave functions and energies generated from constrained self-consistent solutions of a mean-field model, provide the microscopic input for the parameters of the collective Hamiltonian.

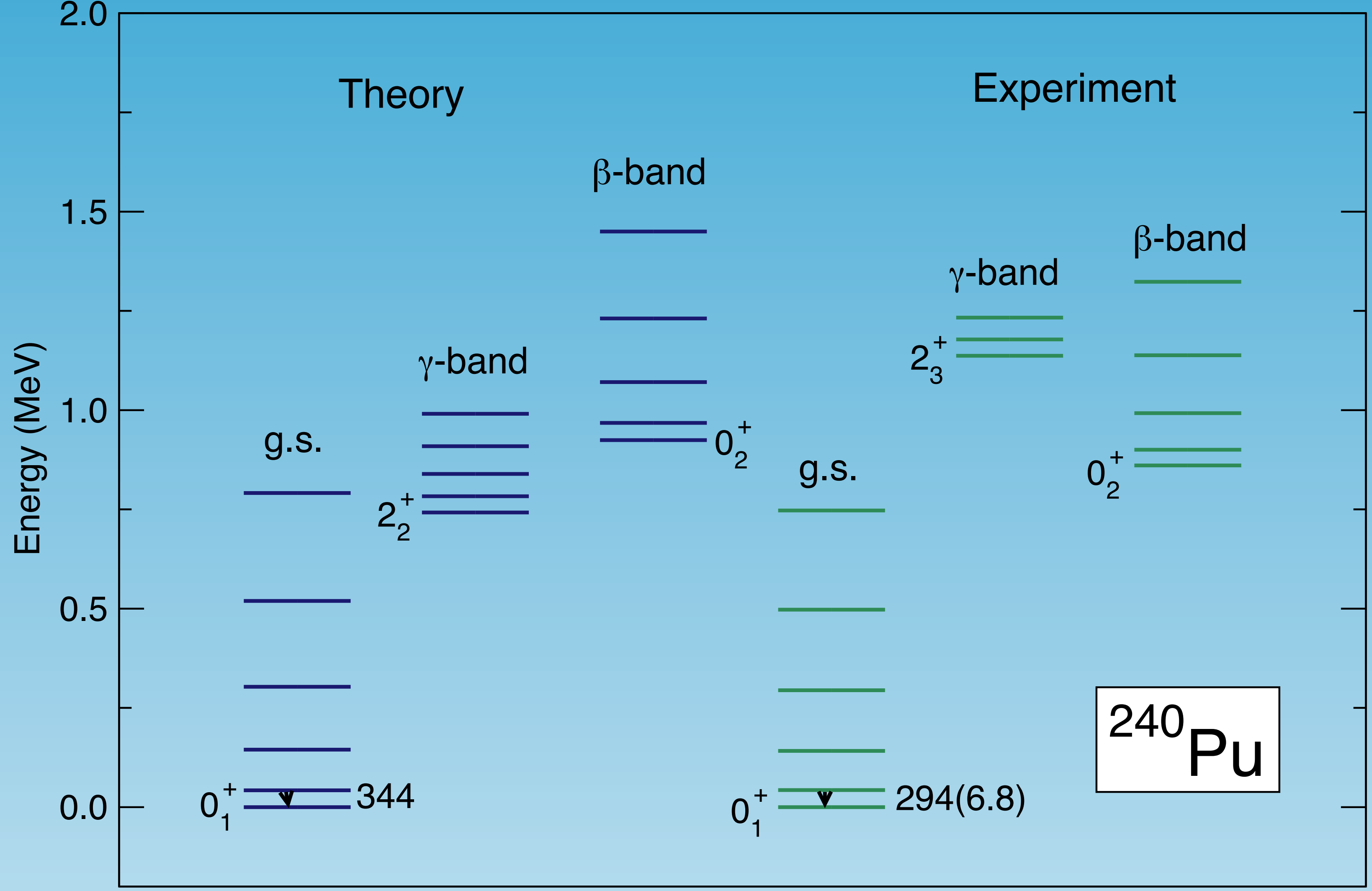
Test of DD-PC1:

Fission path and barriers:



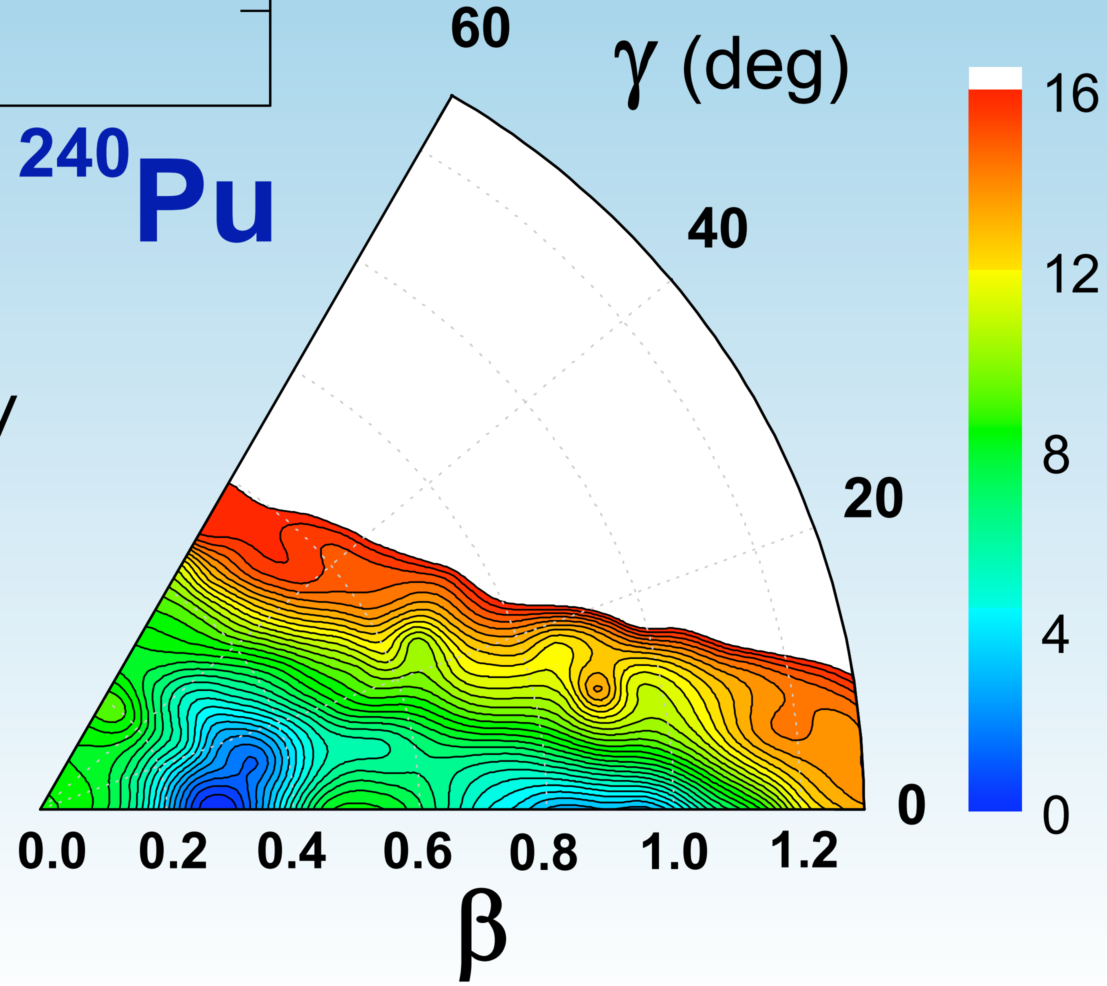


Li, Nikšić, Vretenar, Ring, Meng, Phys. Rev. C (2010)



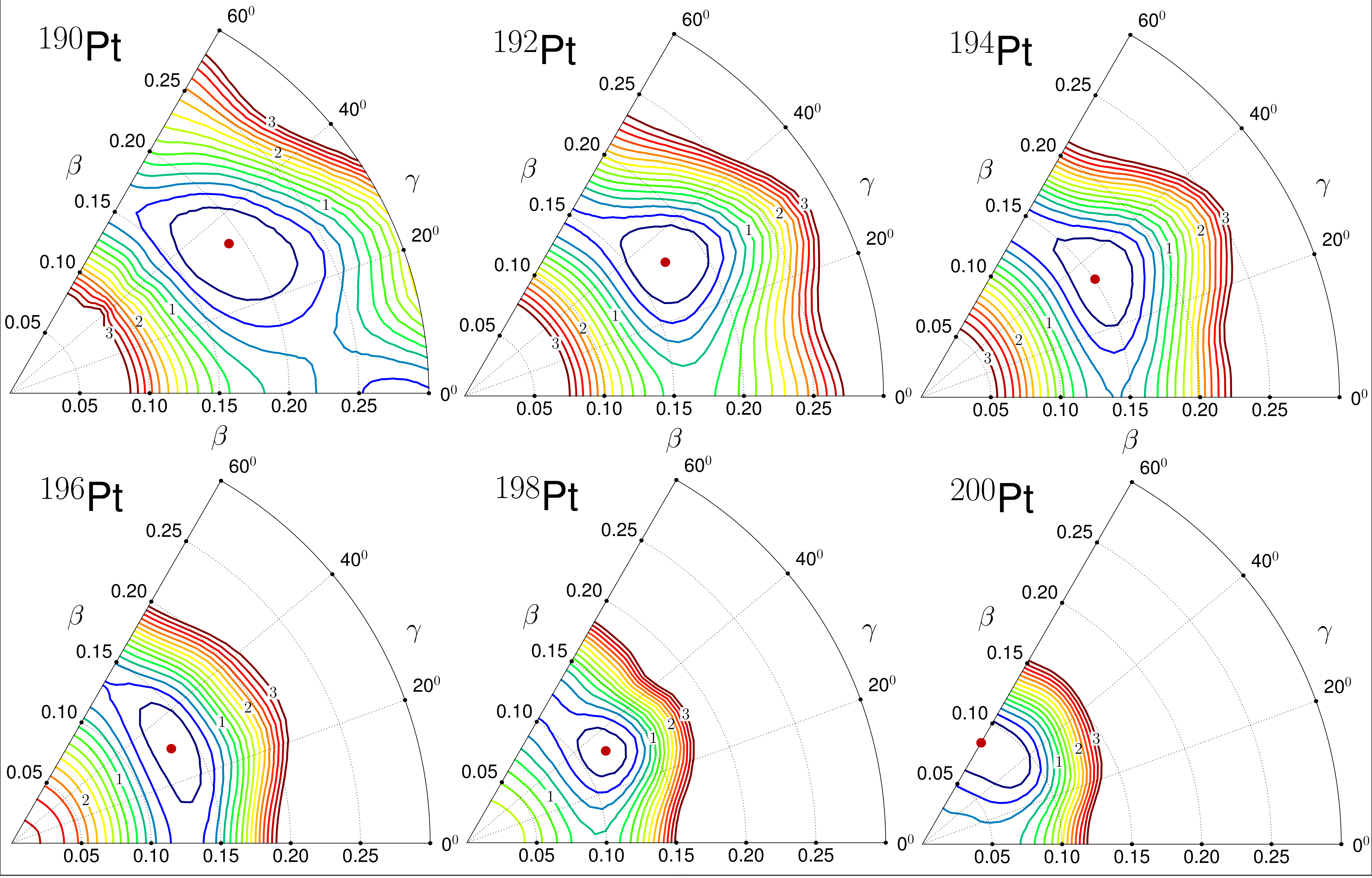
$$E^{th}_{4_1^+}/E^{th}_{2_1^+} = 3.33$$

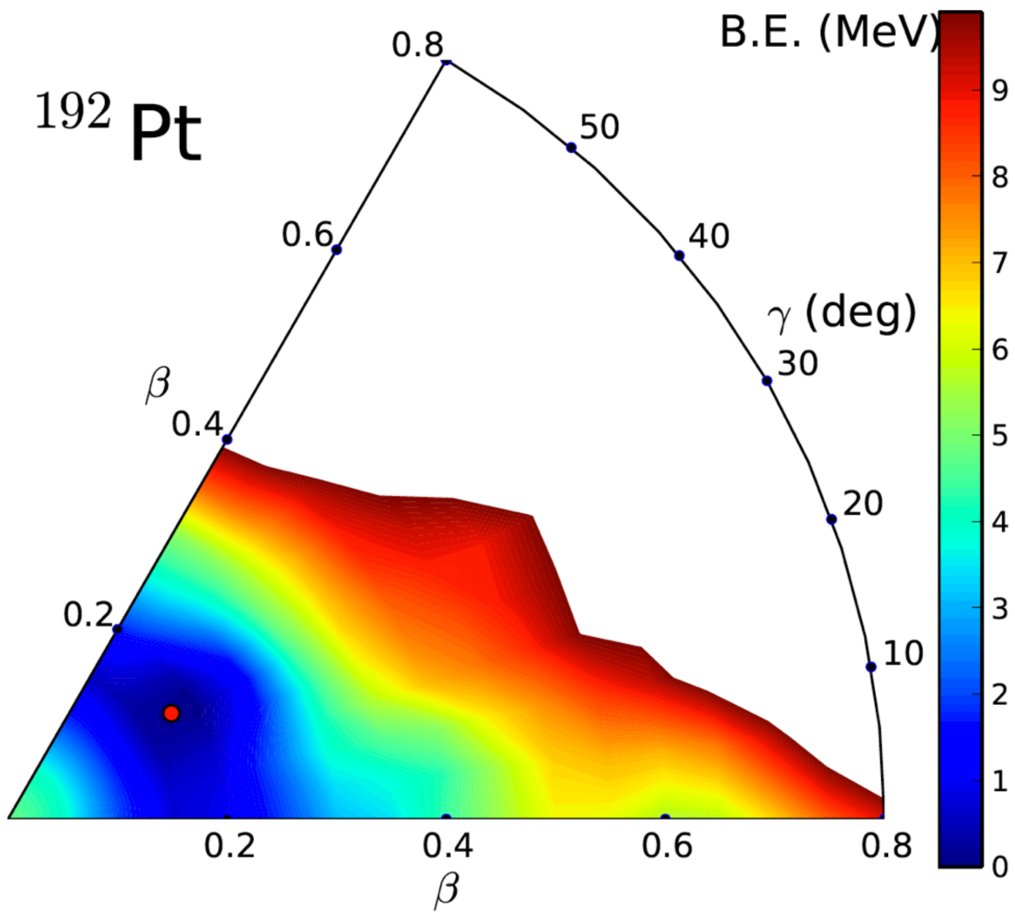
$$E^{exp}_{4_1^+}/E^{exp}_{2_1^+} = 3.31$$



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

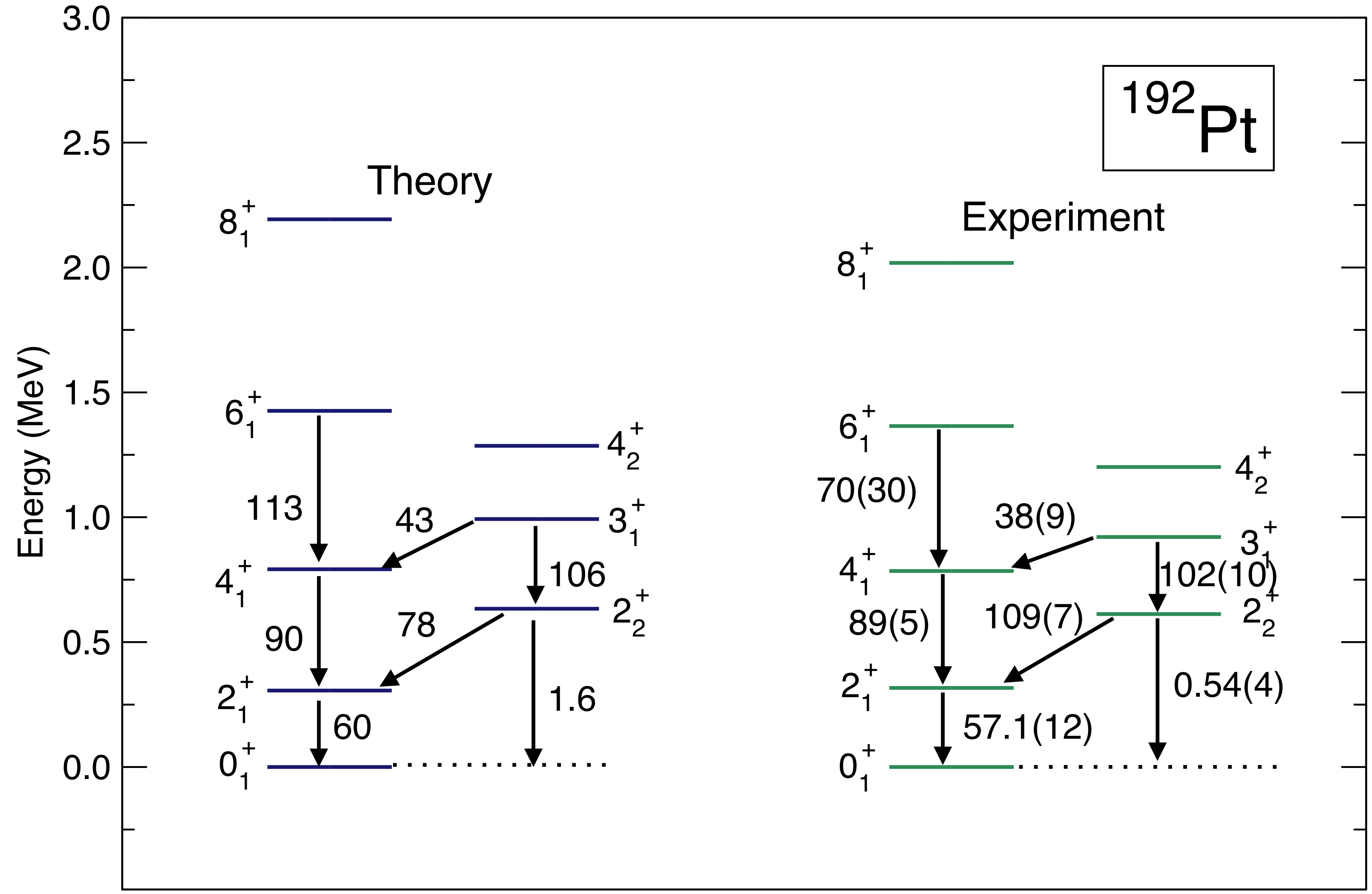
Evolution of triaxial shapes in Pt nuclei:

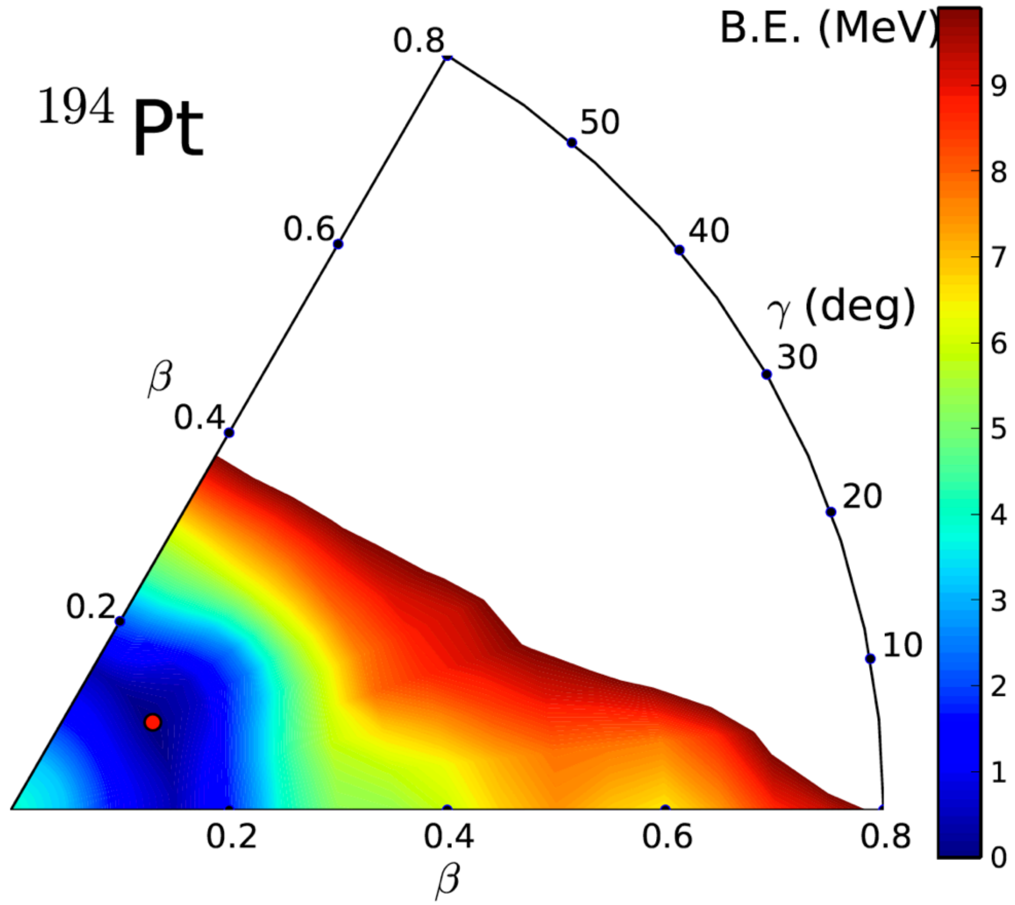




$$E^{th}_{4_1^+}/E^{th}_{2_1^+} = 2.58$$

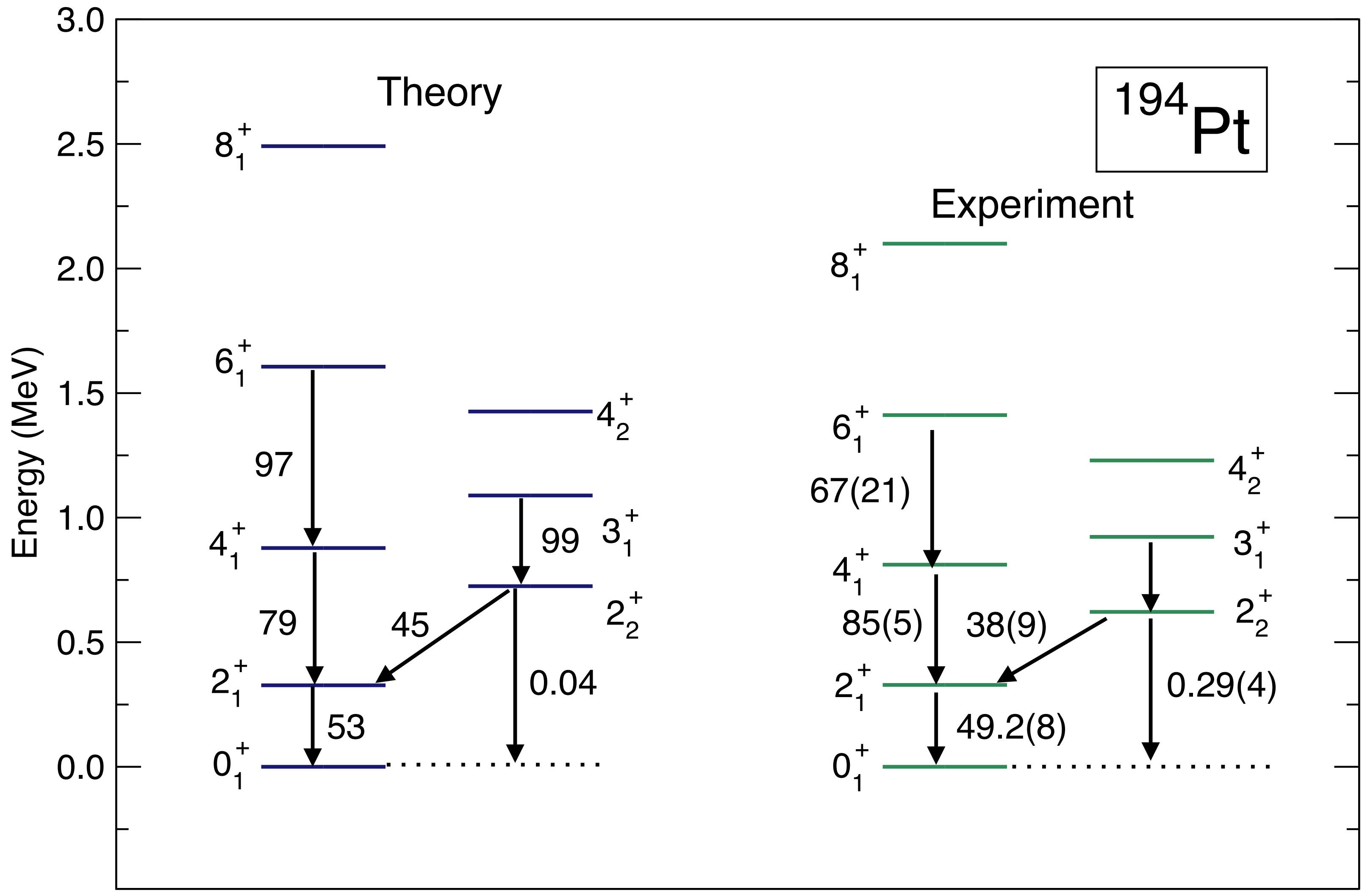
$$E^{exp}_{4_1^+}/E^{exp}_{2_1^+} = 2.48$$

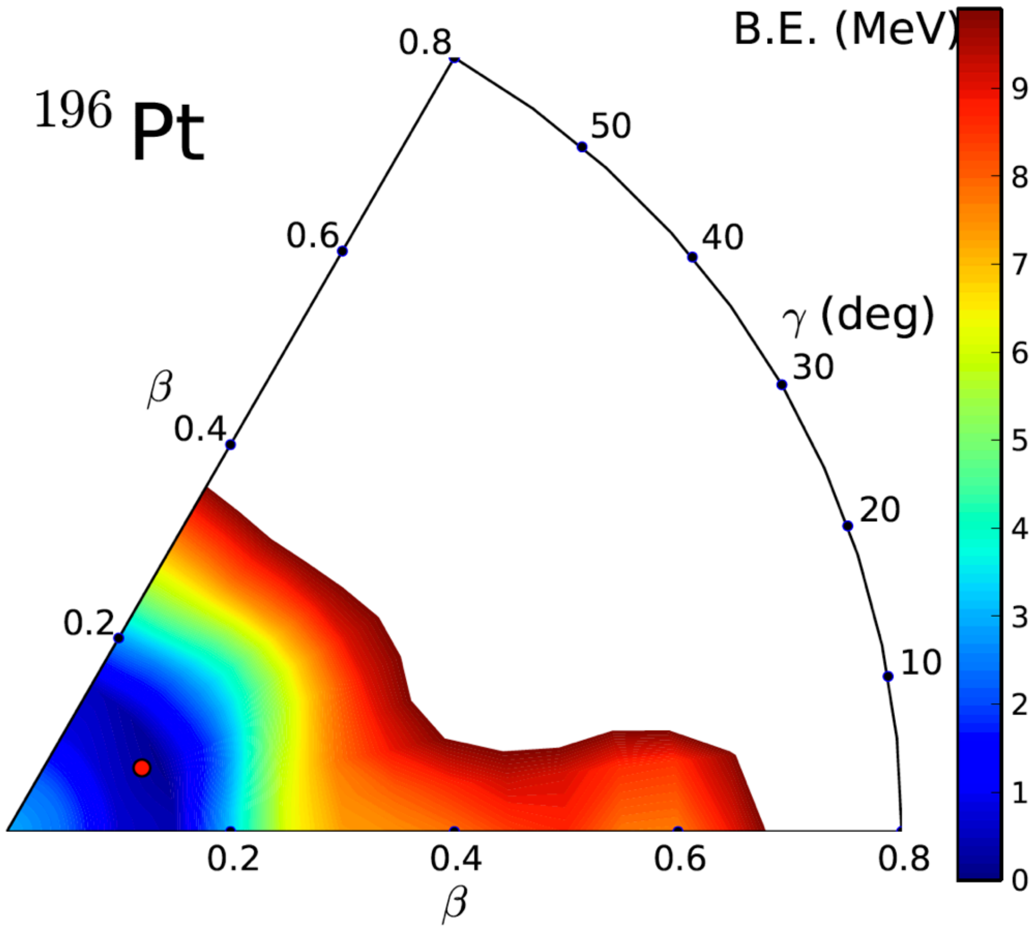




$$E^{th}_{4_1^+}/E^{th}_{2_1^+} = 2.68$$

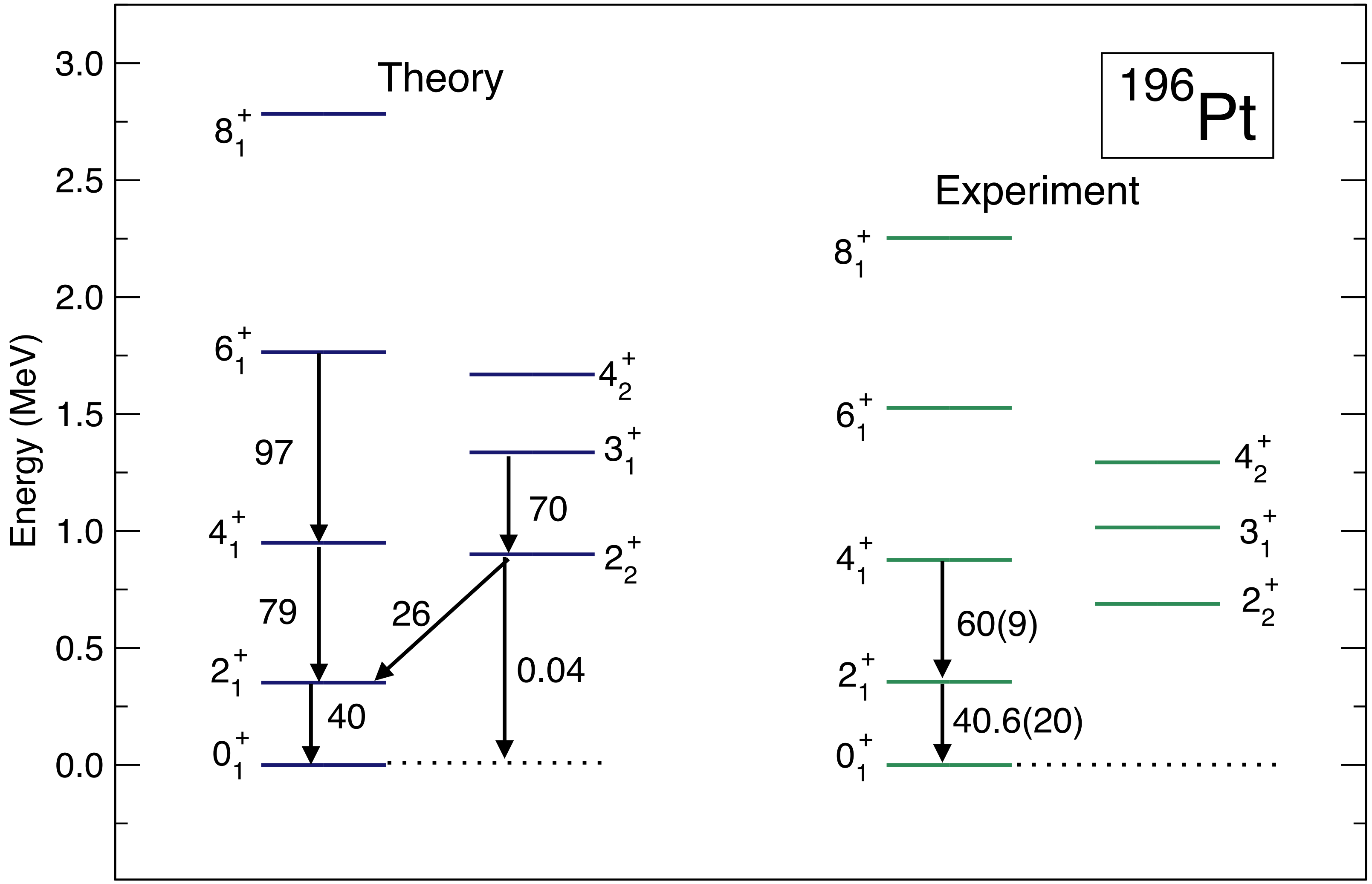
$$E^{exp}_{4_1^+}/E^{exp}_{2_1^+} = 2.47$$

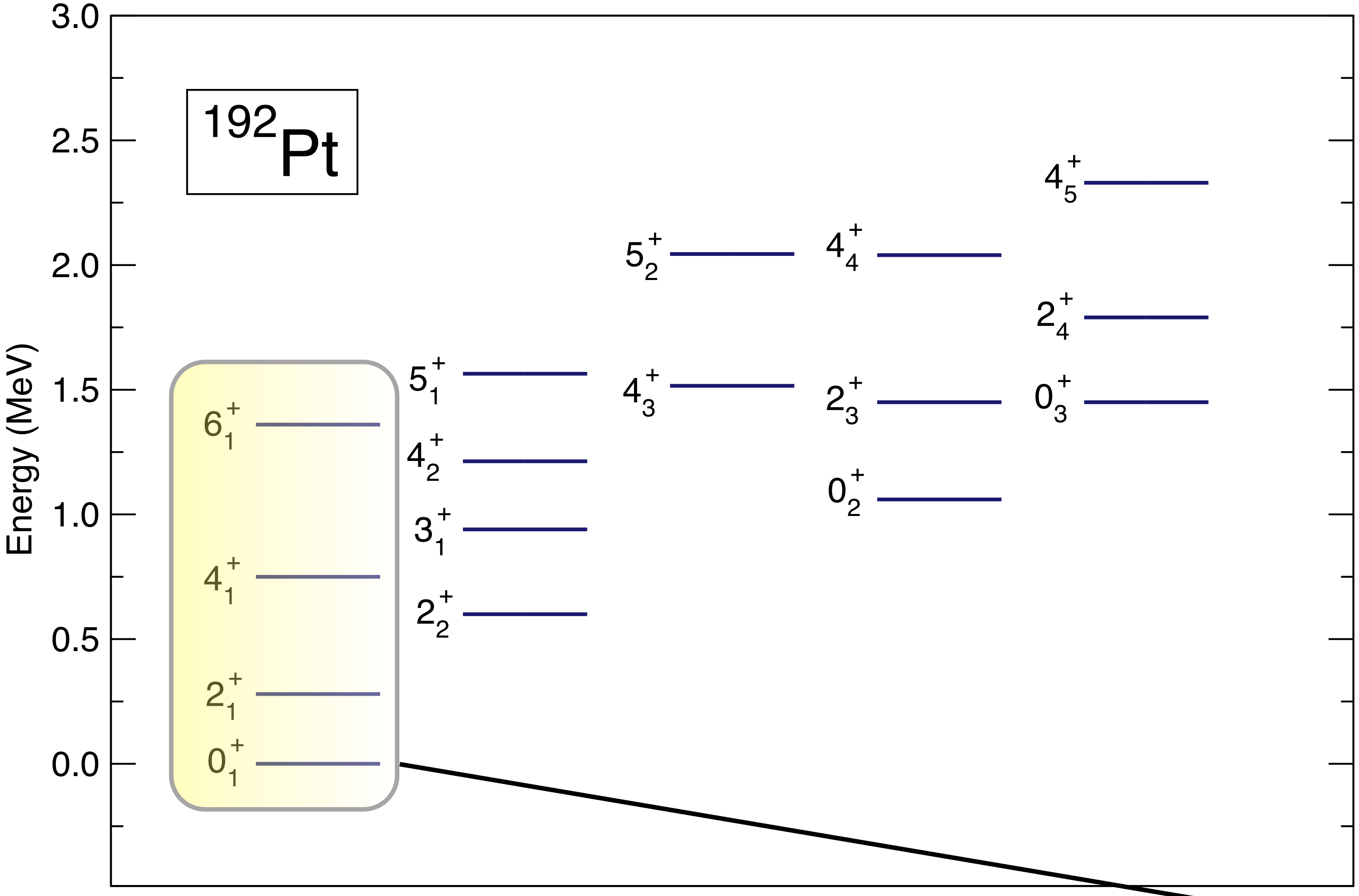


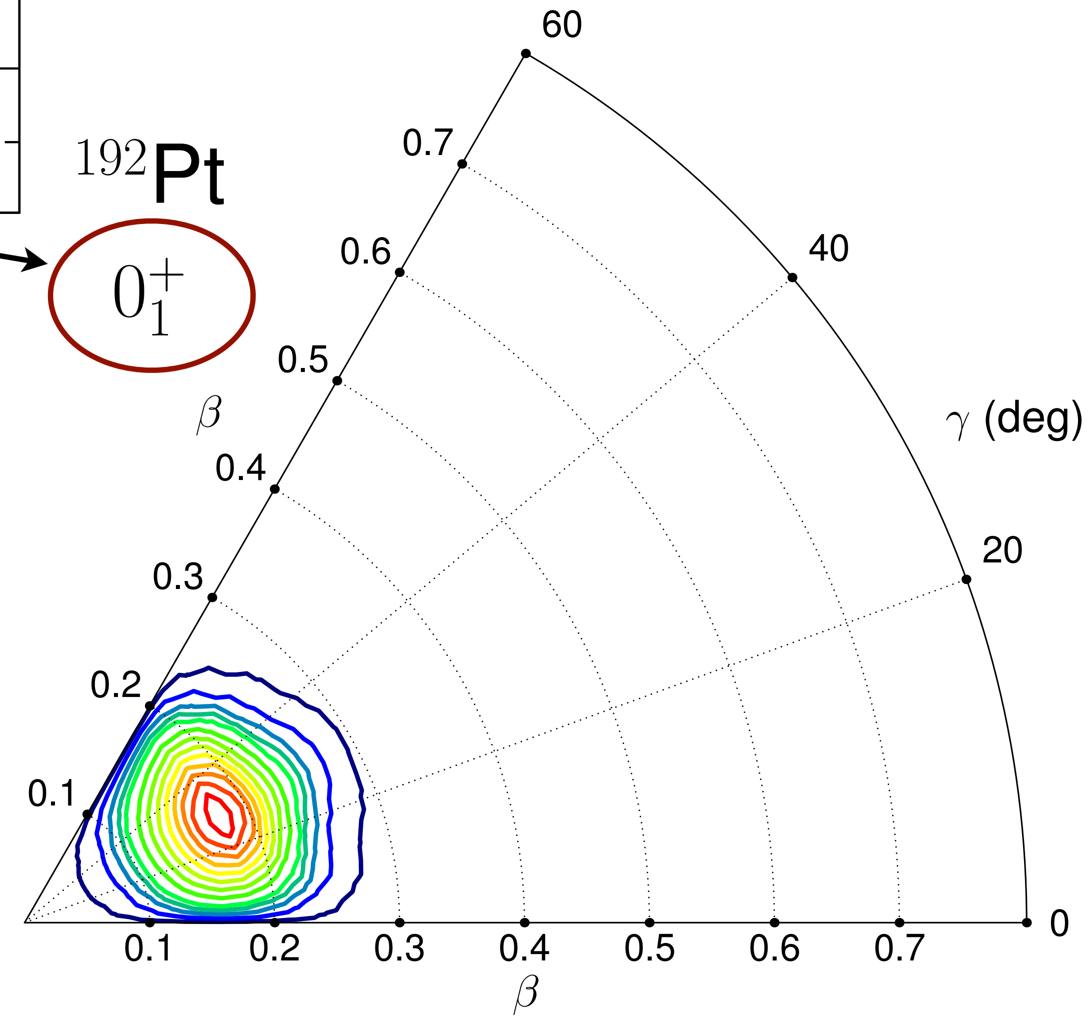


$$E^{th}_{4_1^+}/E^{th}_{2_1^+} = 2.69$$

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





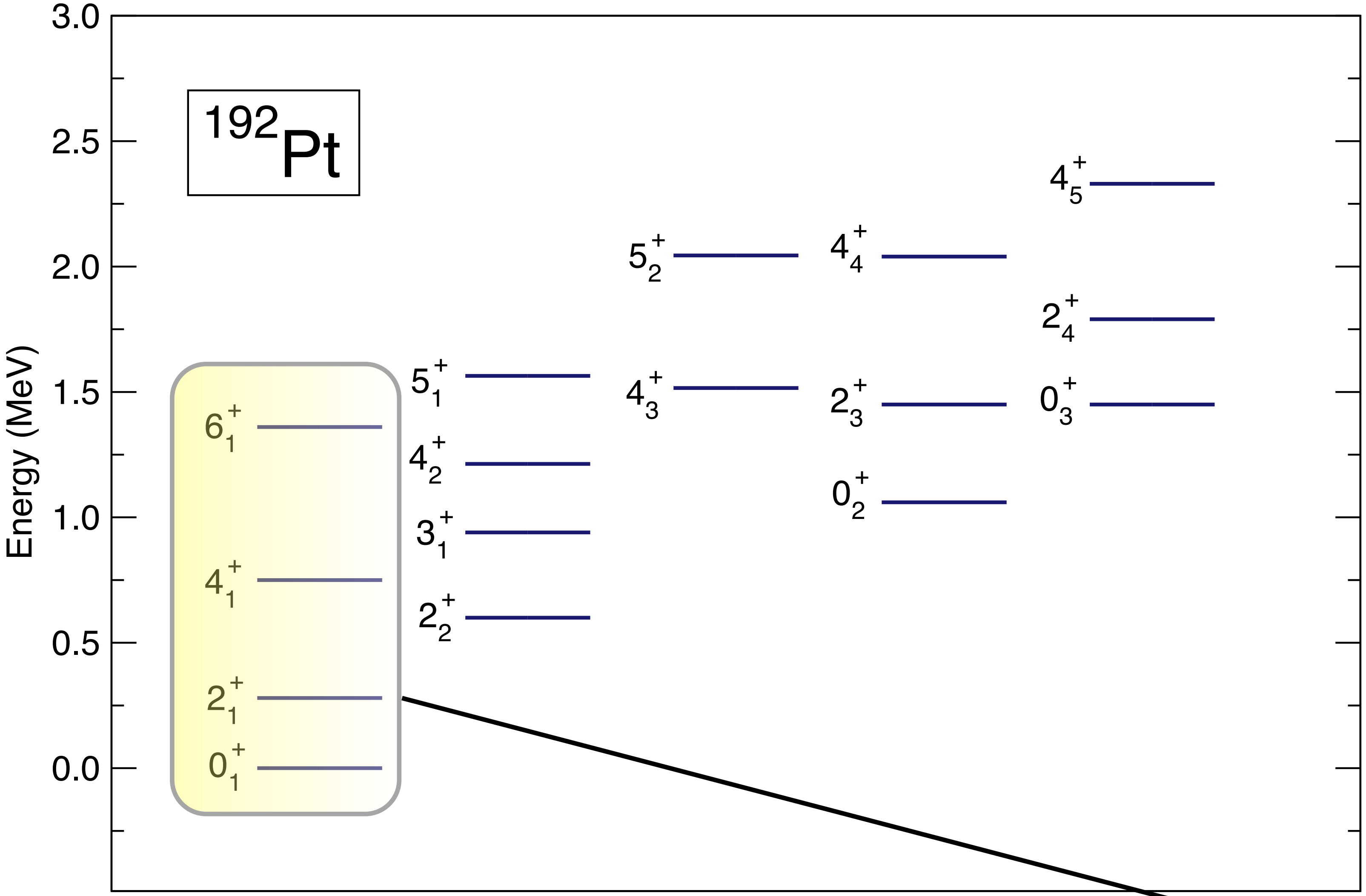


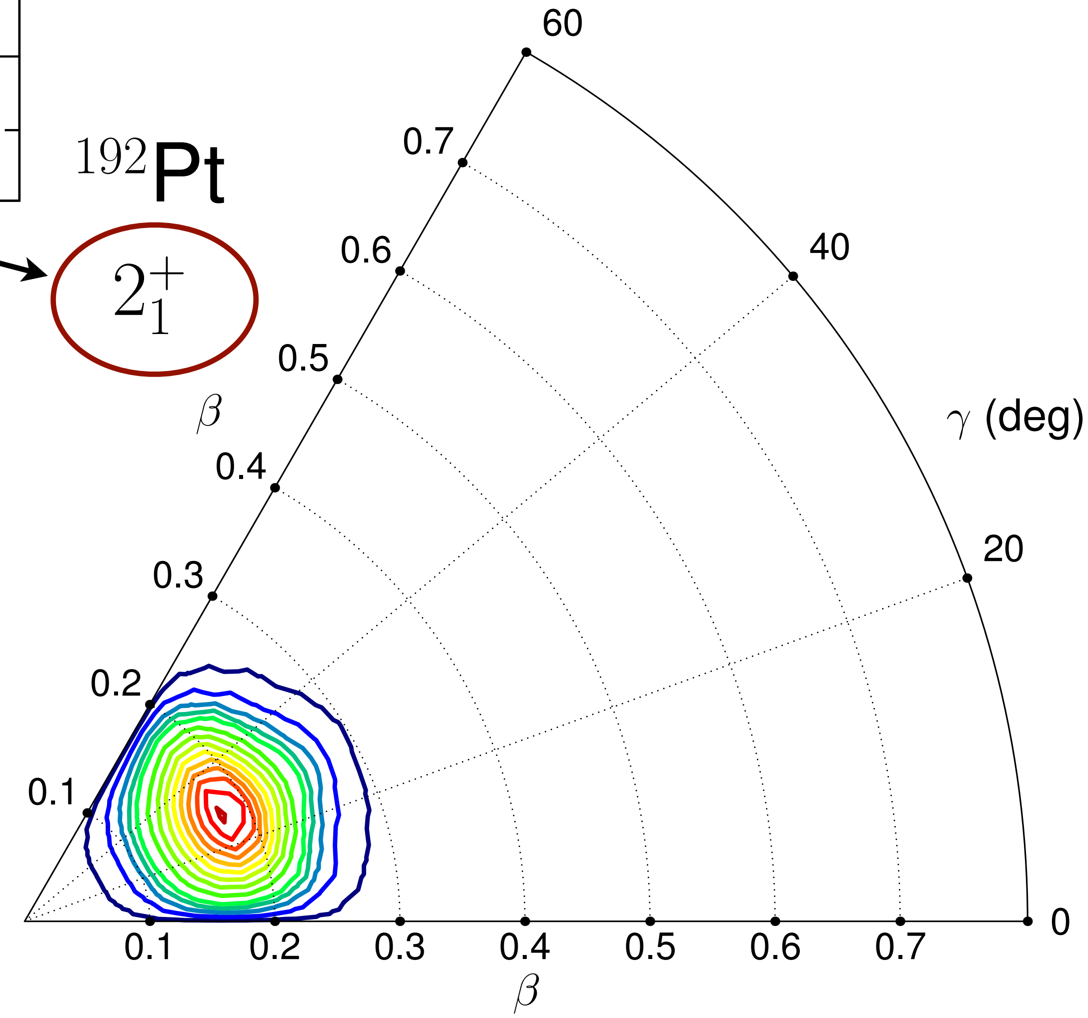
Collective wave function:

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

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

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

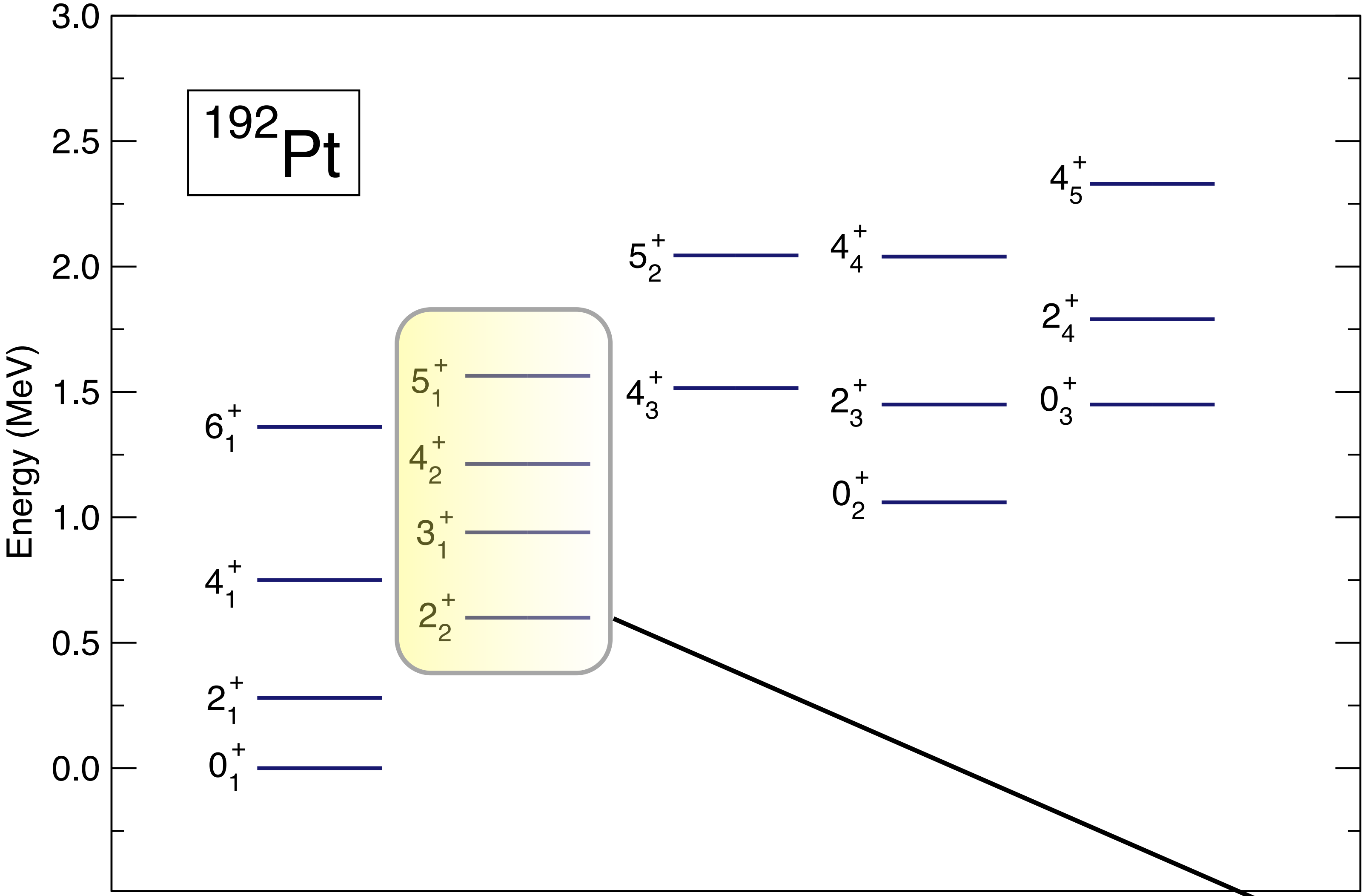


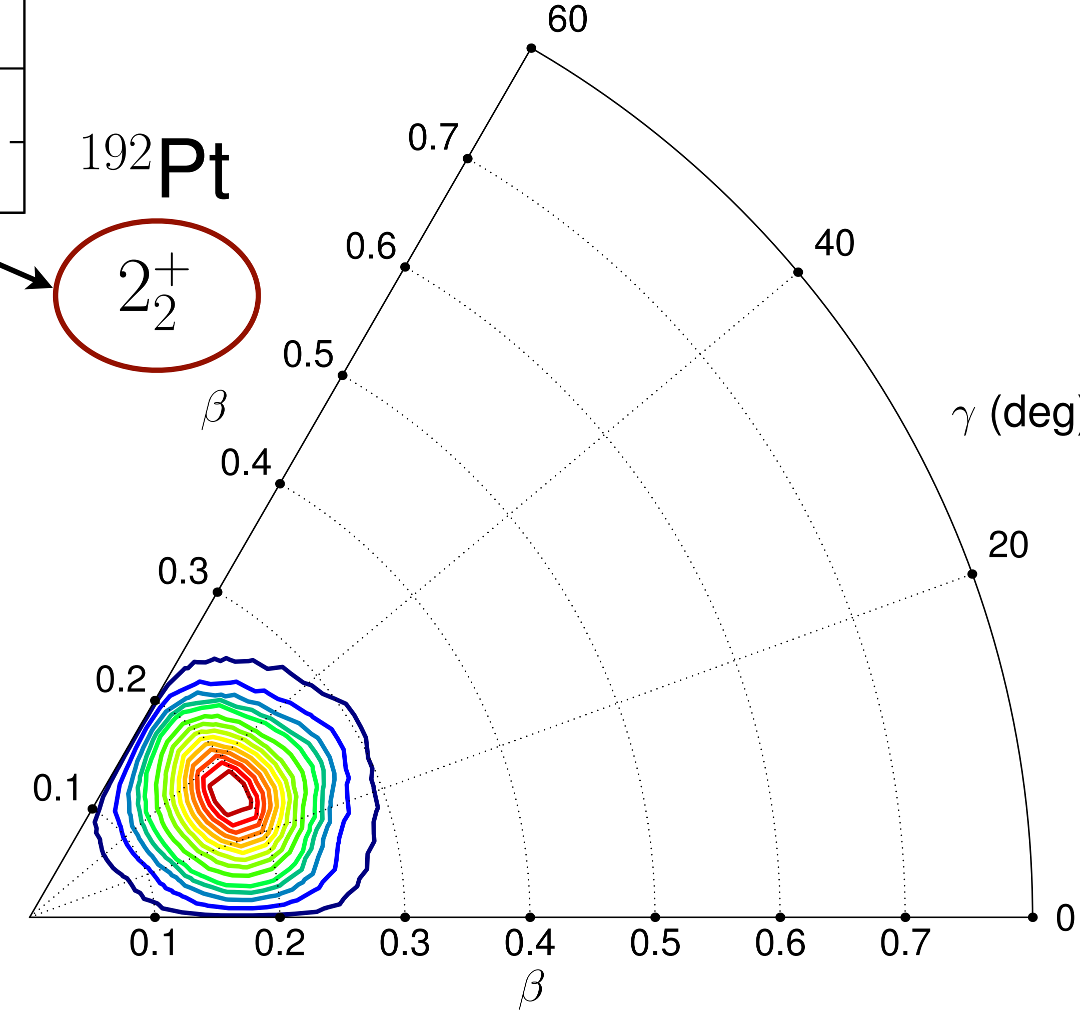


Probability density distribution in the (β,γ) plane:

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

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

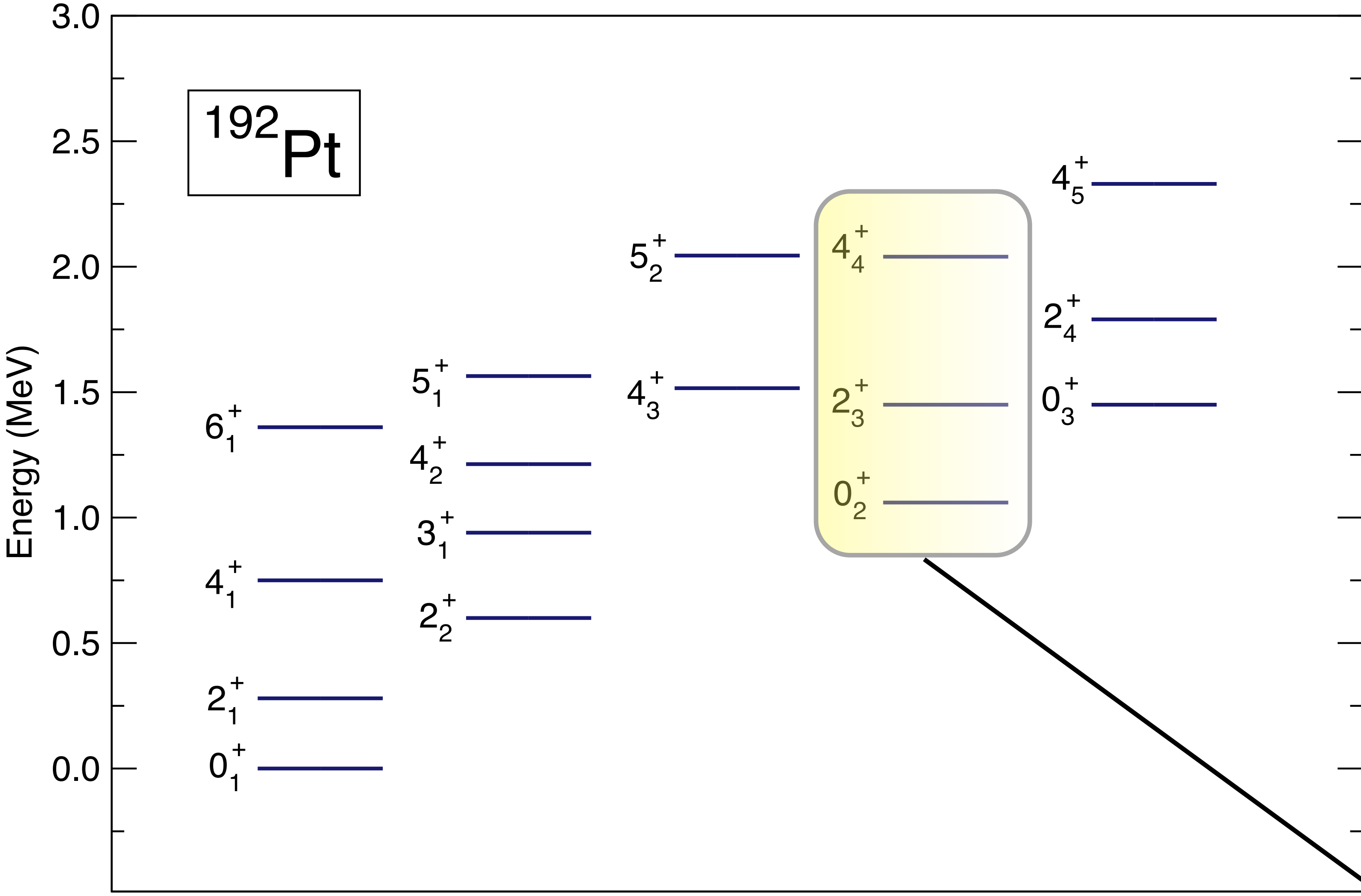


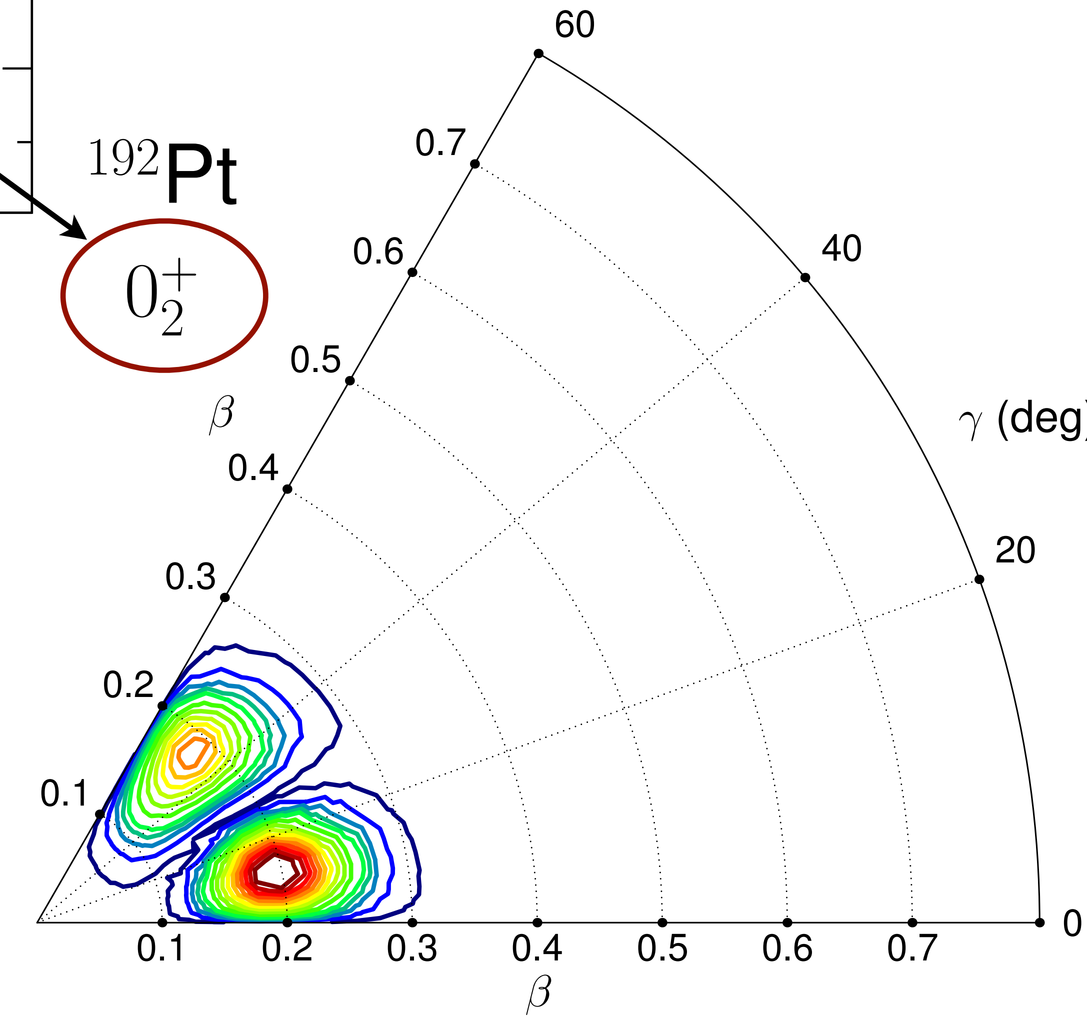


Probability density distribution in the (β,γ) plane:

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

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

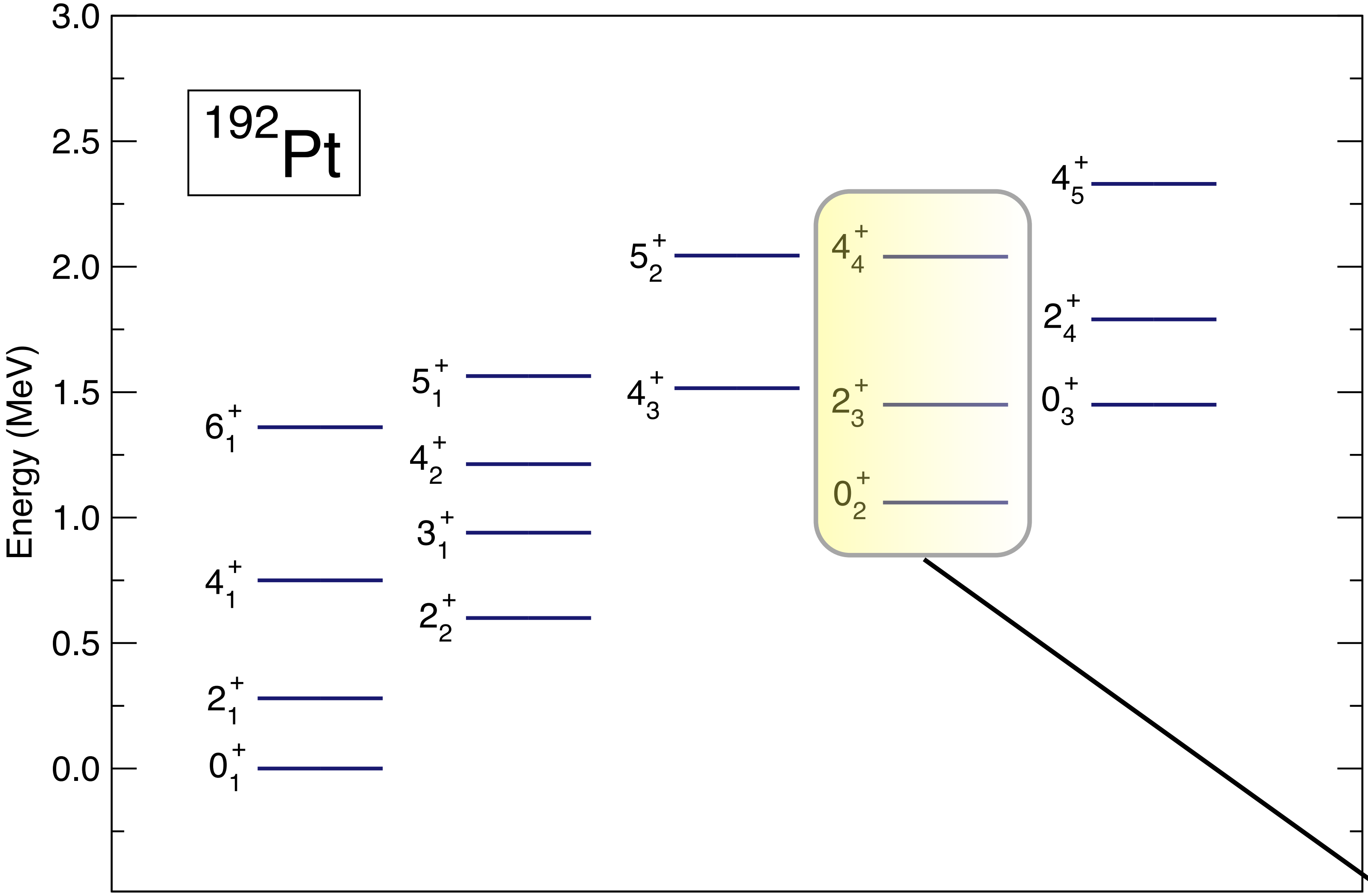


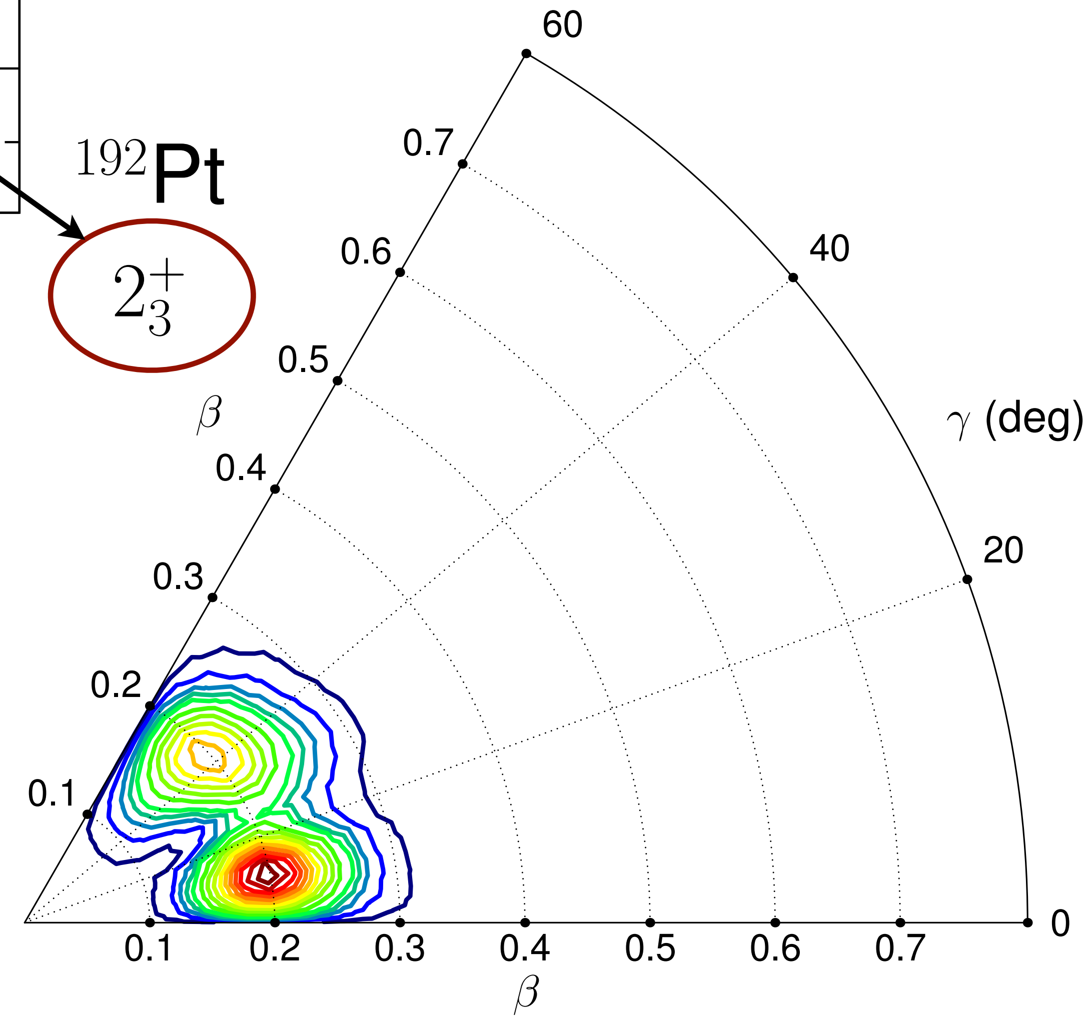


Probability density distribution in the (β,γ) plane:

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

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

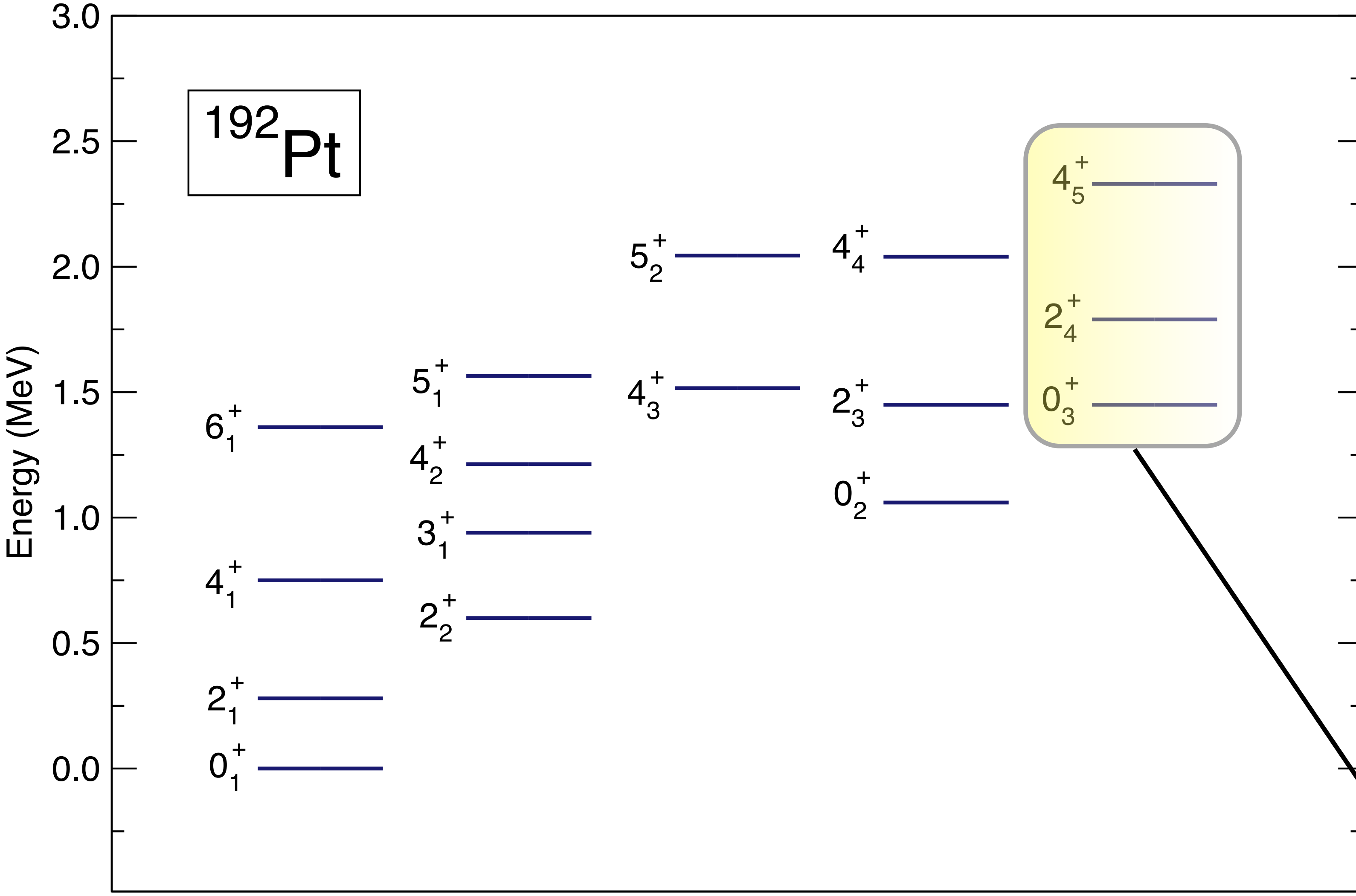


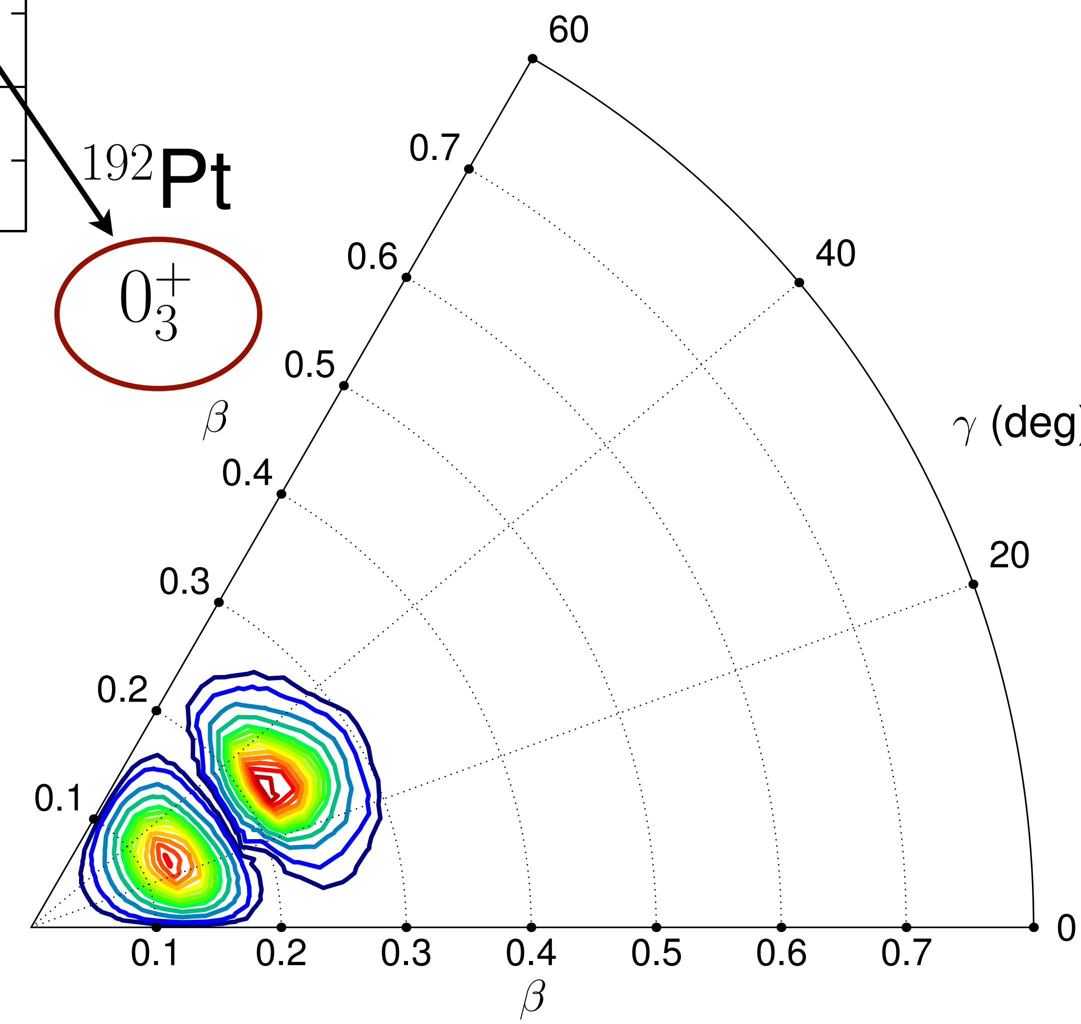


Probability density distribution in the (β,γ) plane:

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

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

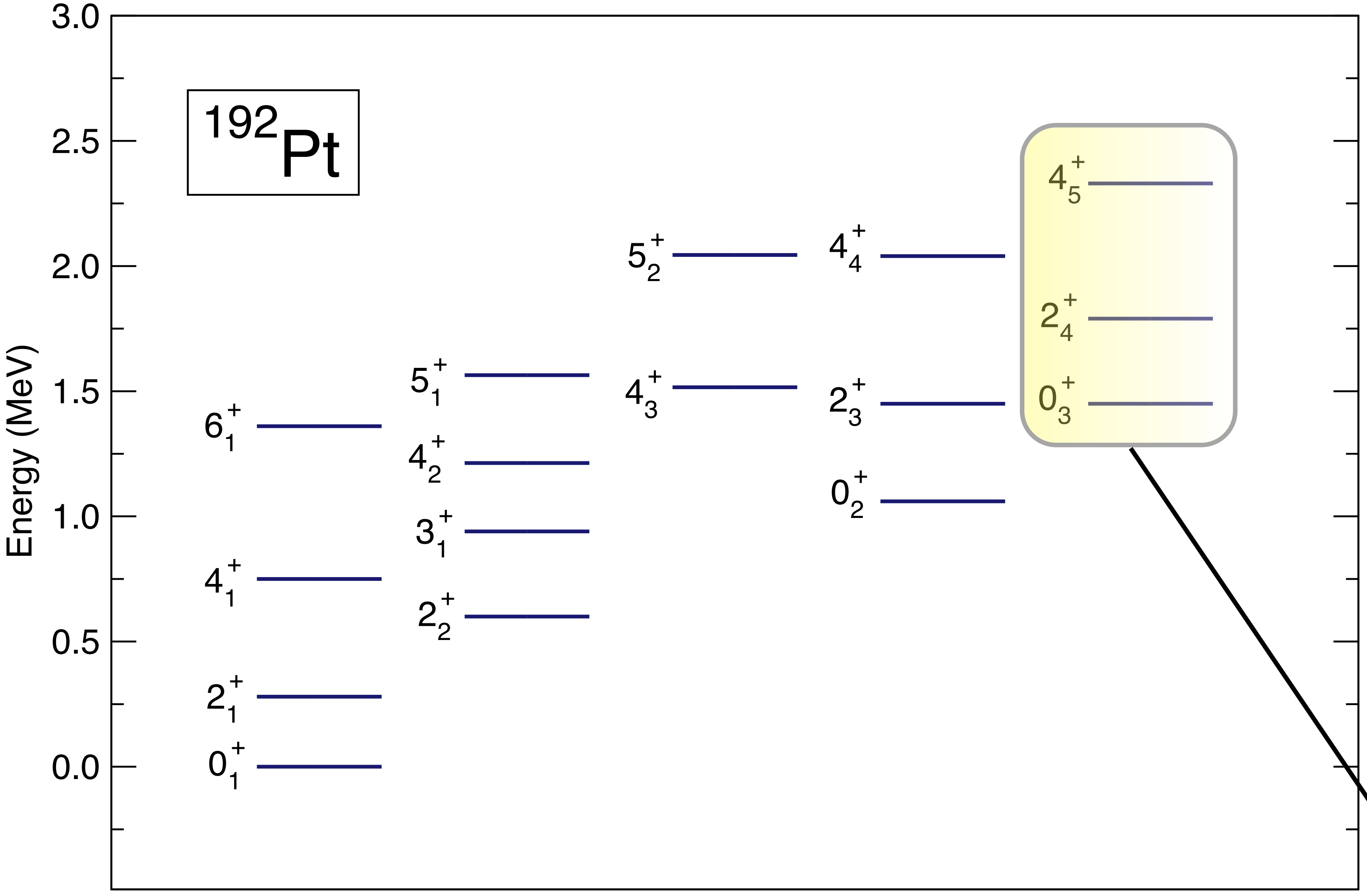


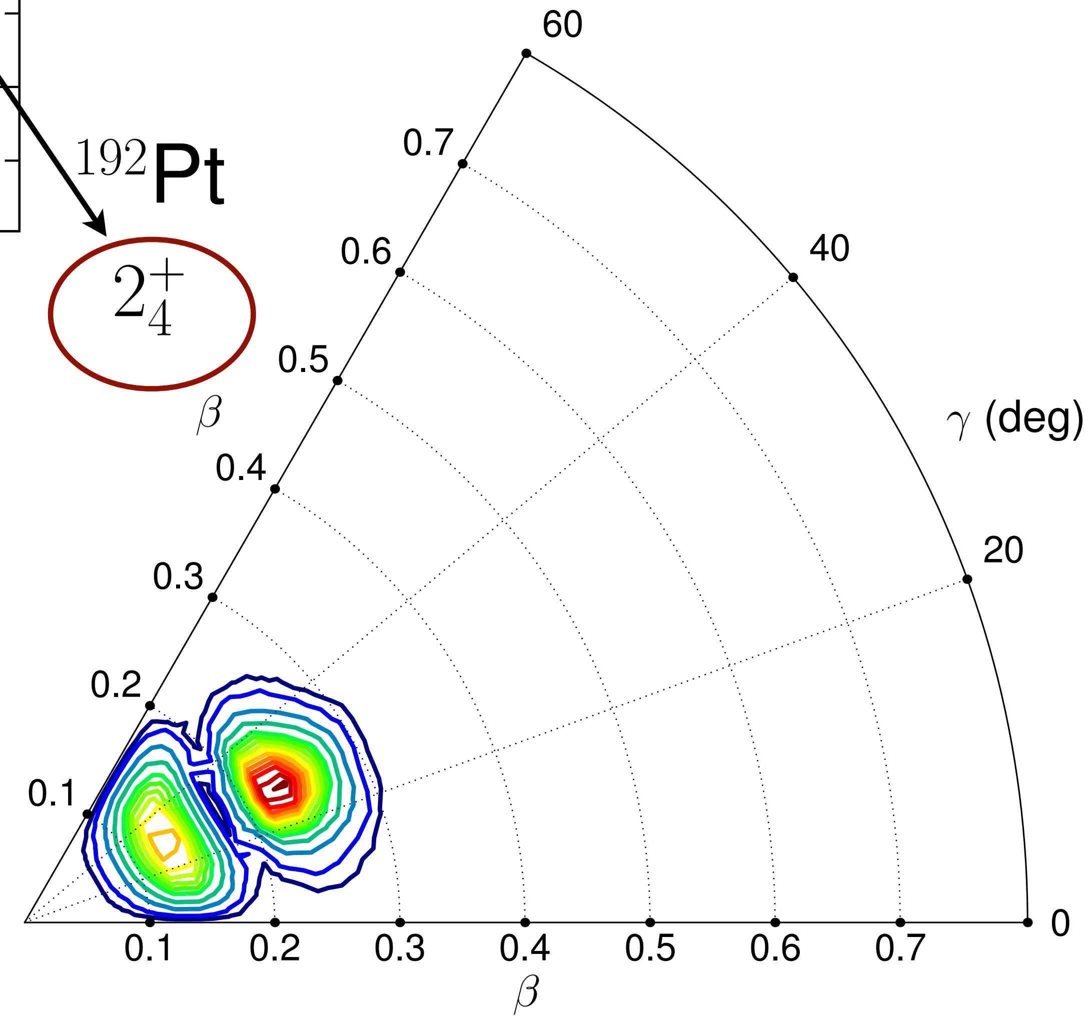


Probability density distribution in the (β,γ) plane:

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

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





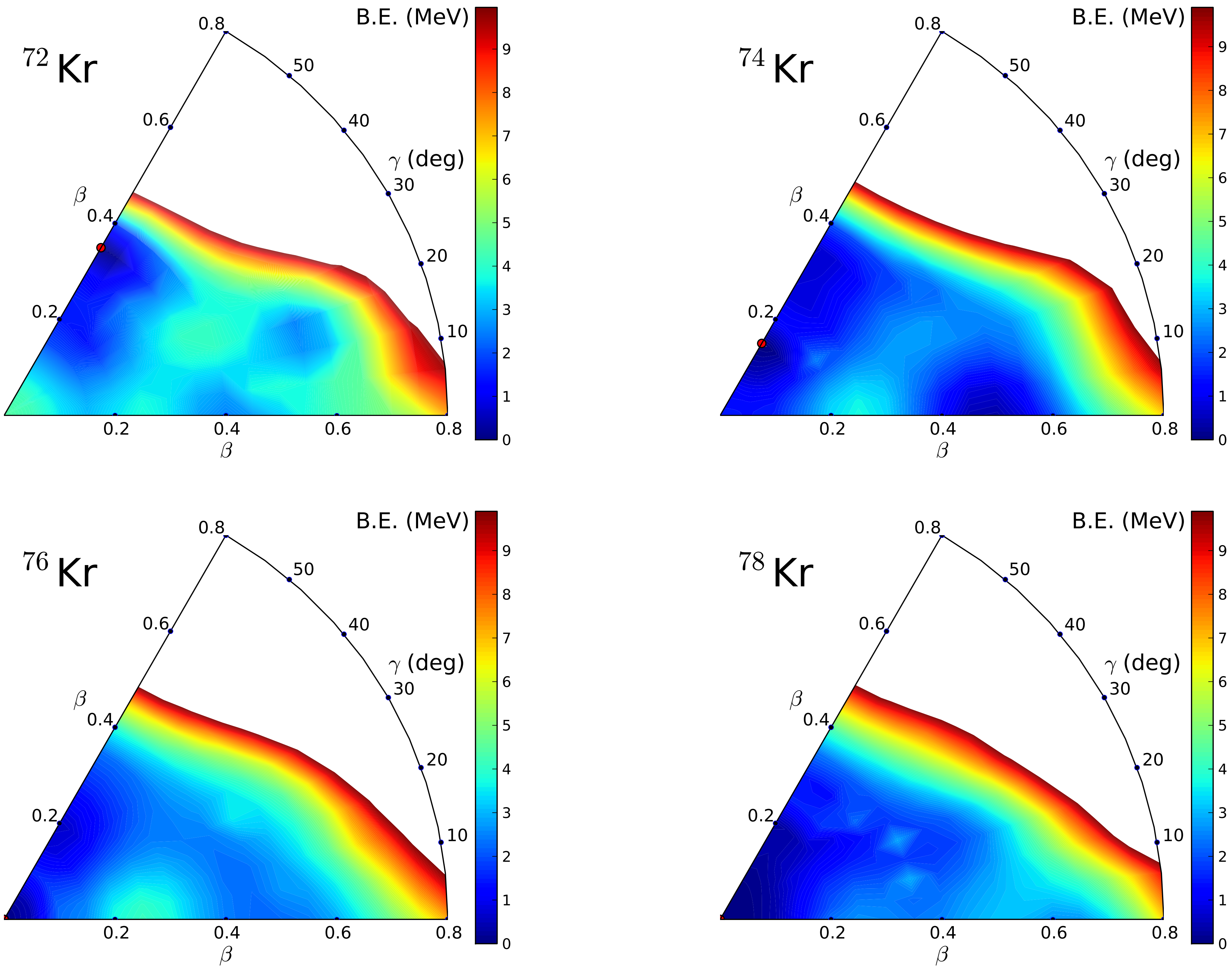
Probability density distribution in the (β,γ) plane:

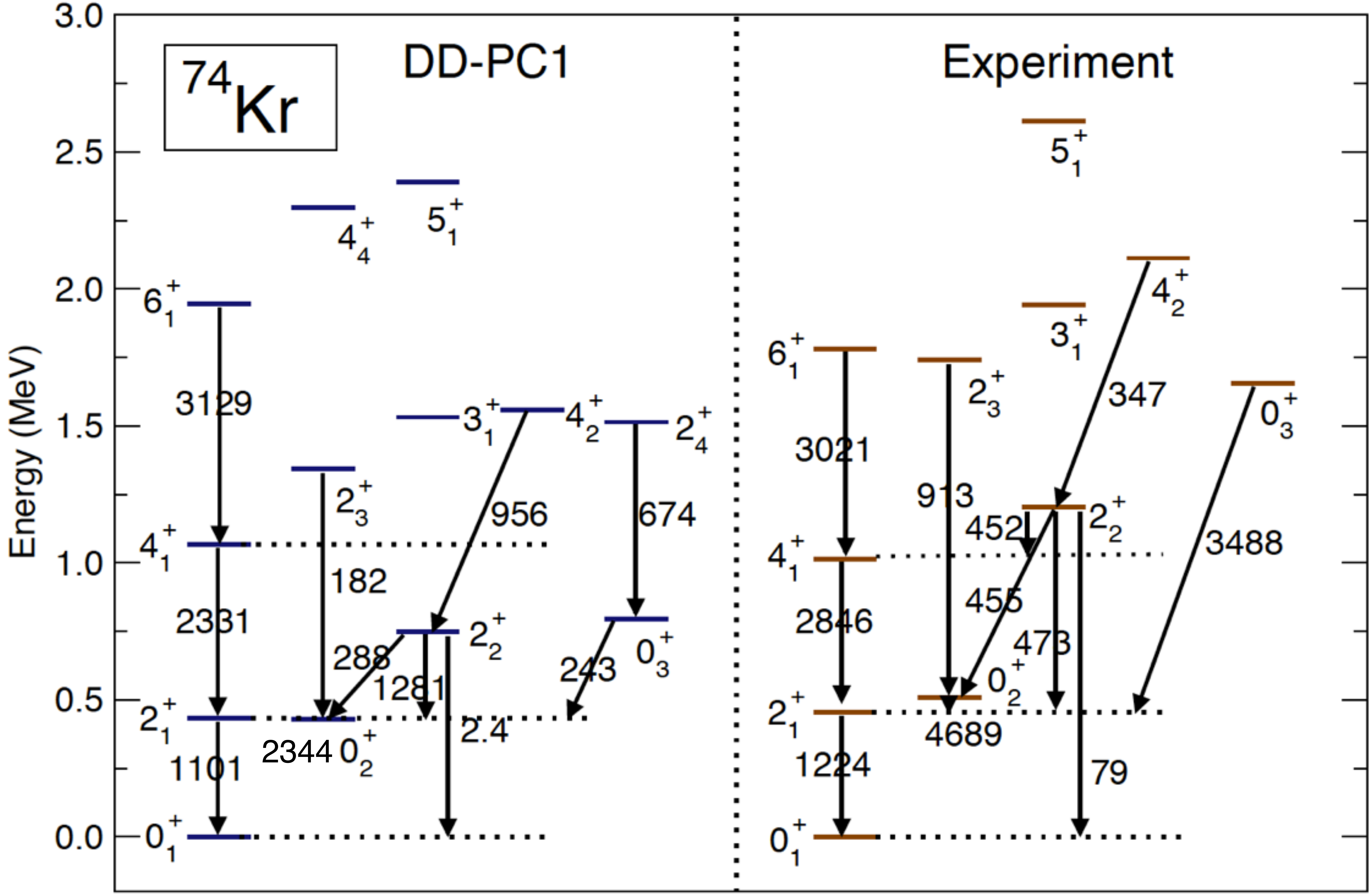
$$\rho_{I\alpha}(\beta,\gamma) = \sum_{K\in\Delta I} |\psi^I_{\alpha K}(\beta,\gamma)|^2\beta^3|\sin 3\gamma|$$

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

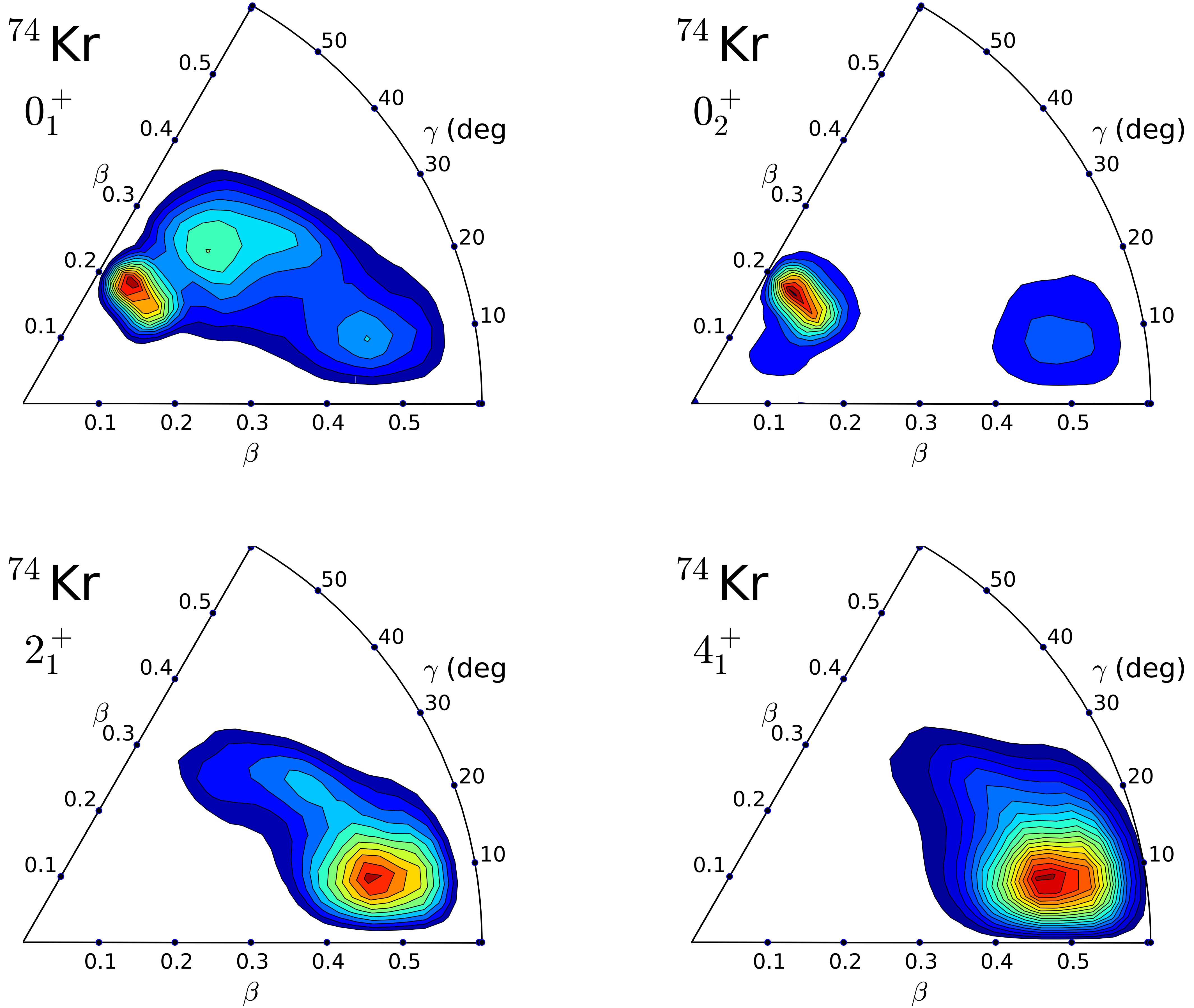
How does the functional DD-PC1 extrapolate to other mass regions?

Shape-coexistence in neutron-deficient Kr isotopes



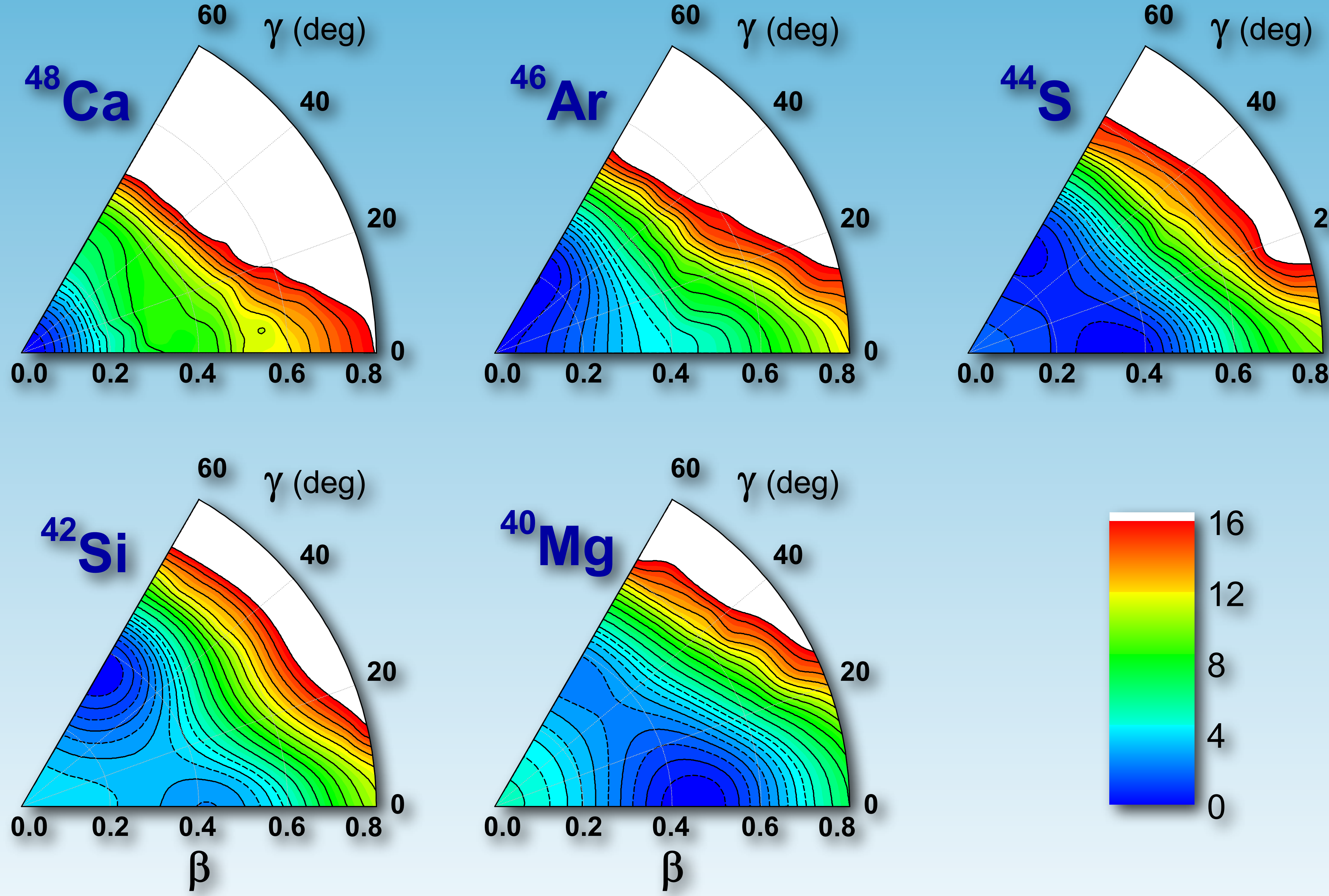


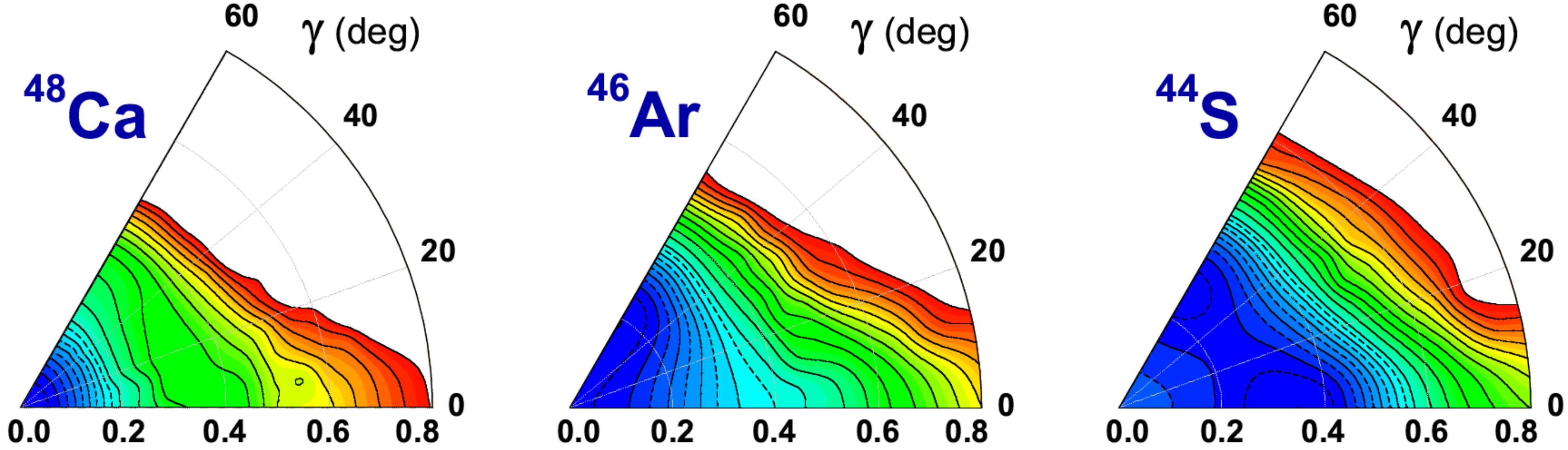
74Kr
DD-PC1
Experiment
Energy (MeV)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
3129
2331
1101
182
288
2344
1281
2.4
956
674
243
3021
2846
1224
913
4689
452
455
473
79
347
3488



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

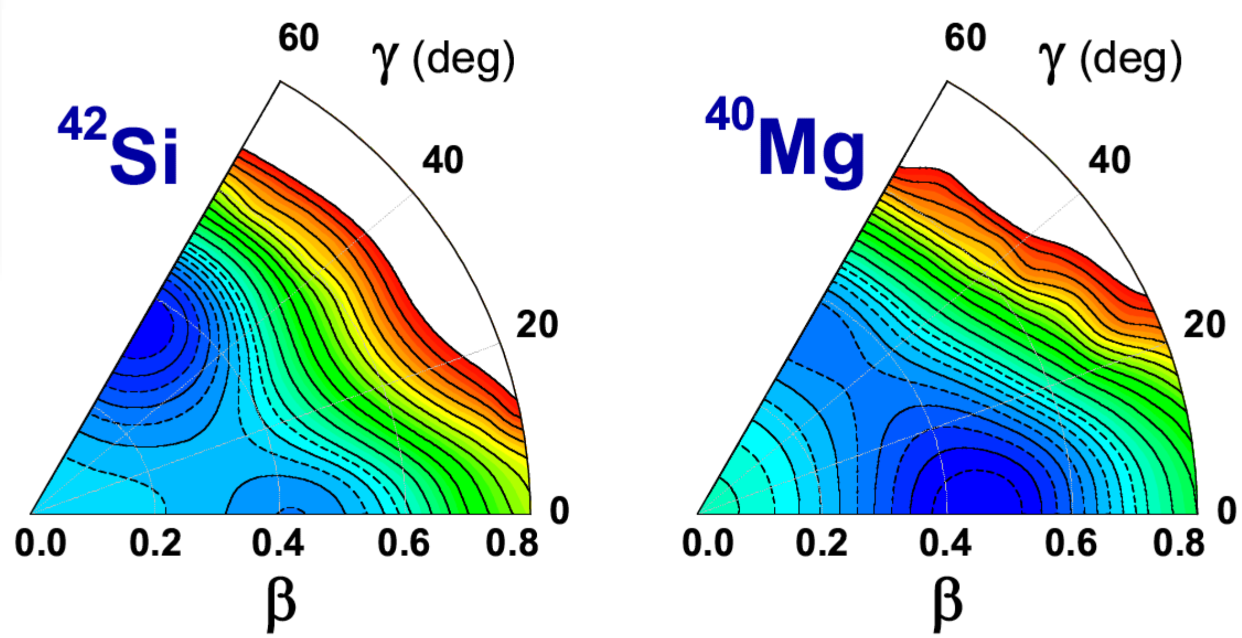
Coexisting shapes in the N=28 isotones

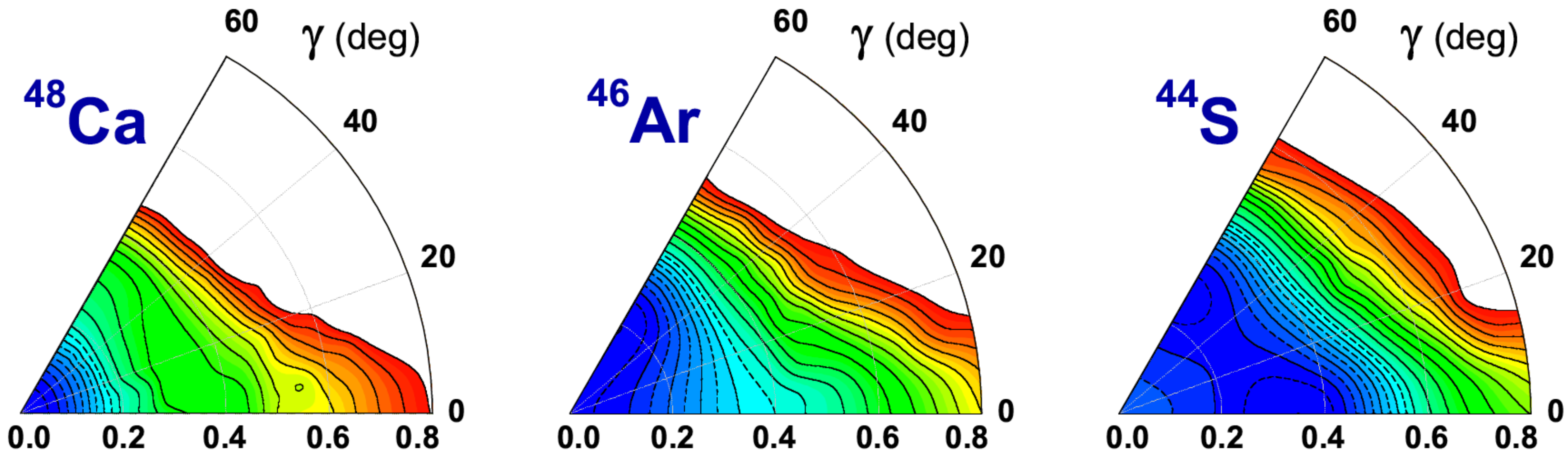




Neutron N=28 spherical energy gaps

	$\Delta^{\text{sph.}}_{N=28}$	β_{min}
^{48}Ca	4.73	0.00
^{46}Ar	4.48	-0.19
^{44}S	3.86	0.34
^{42}Si	3.13	-0.35
^{40}Mg	2.03	0.45





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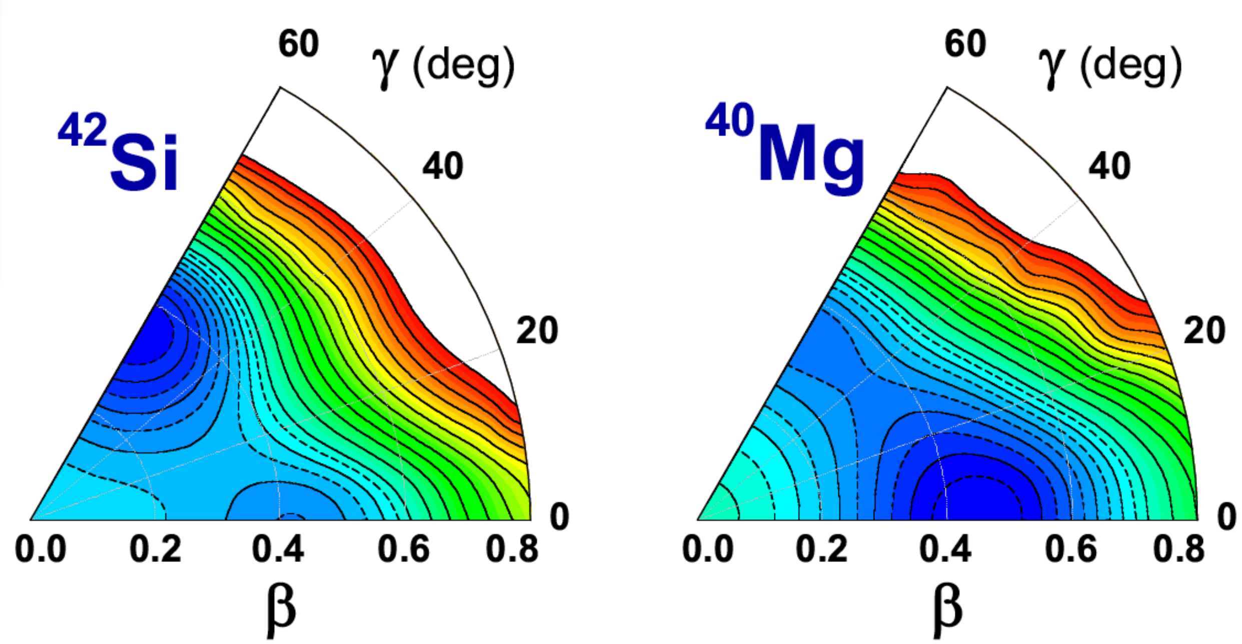
^{48}Ca	4.73	0.00
^{46}Ar	4.48	-0.19
^{44}S	3.86	0.34
^{42}Si	3.13	-0.35
^{40}Mg	2.03	0.45

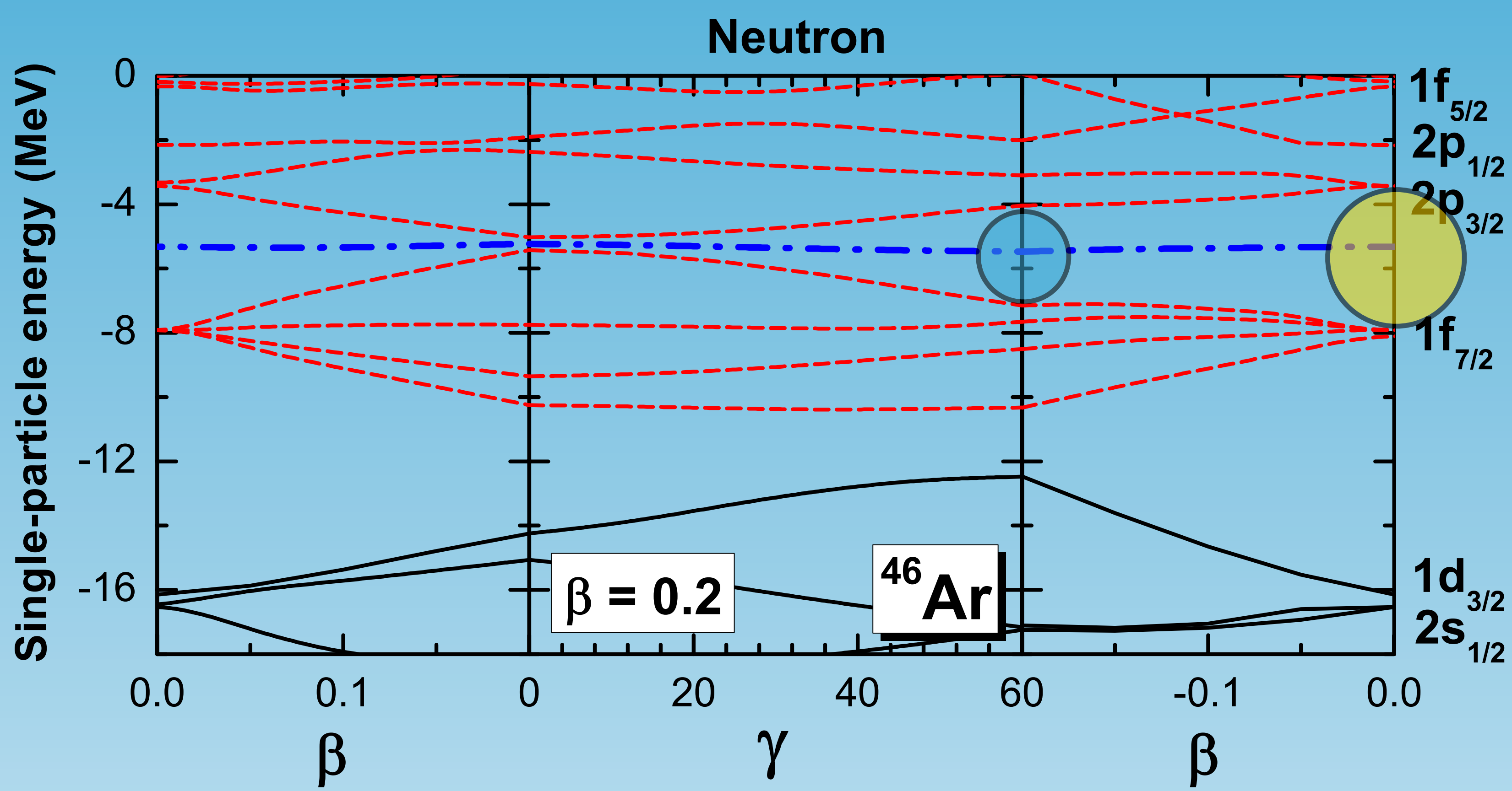
Experimental values:

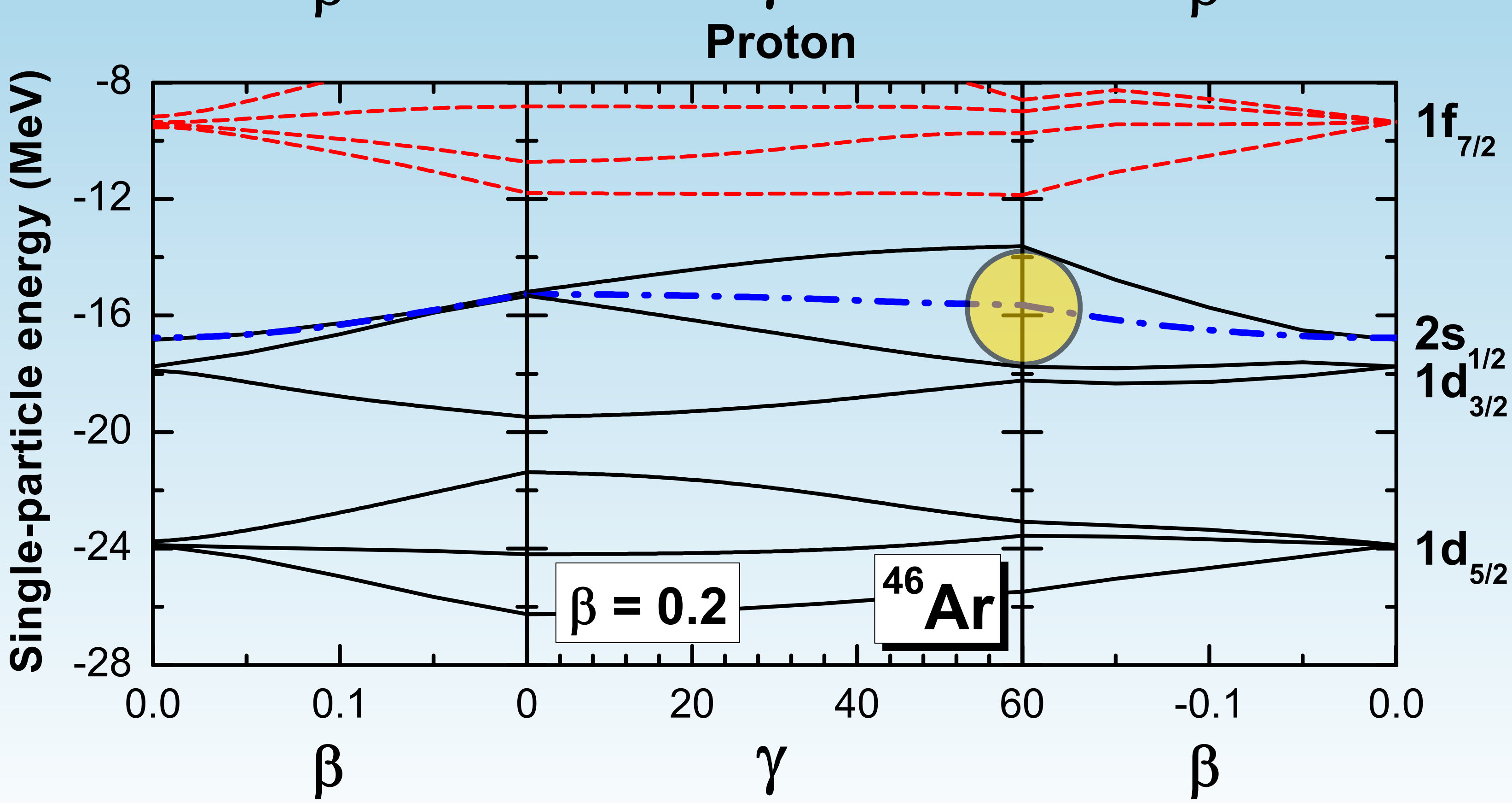
4.80 MeV

4.47 MeV

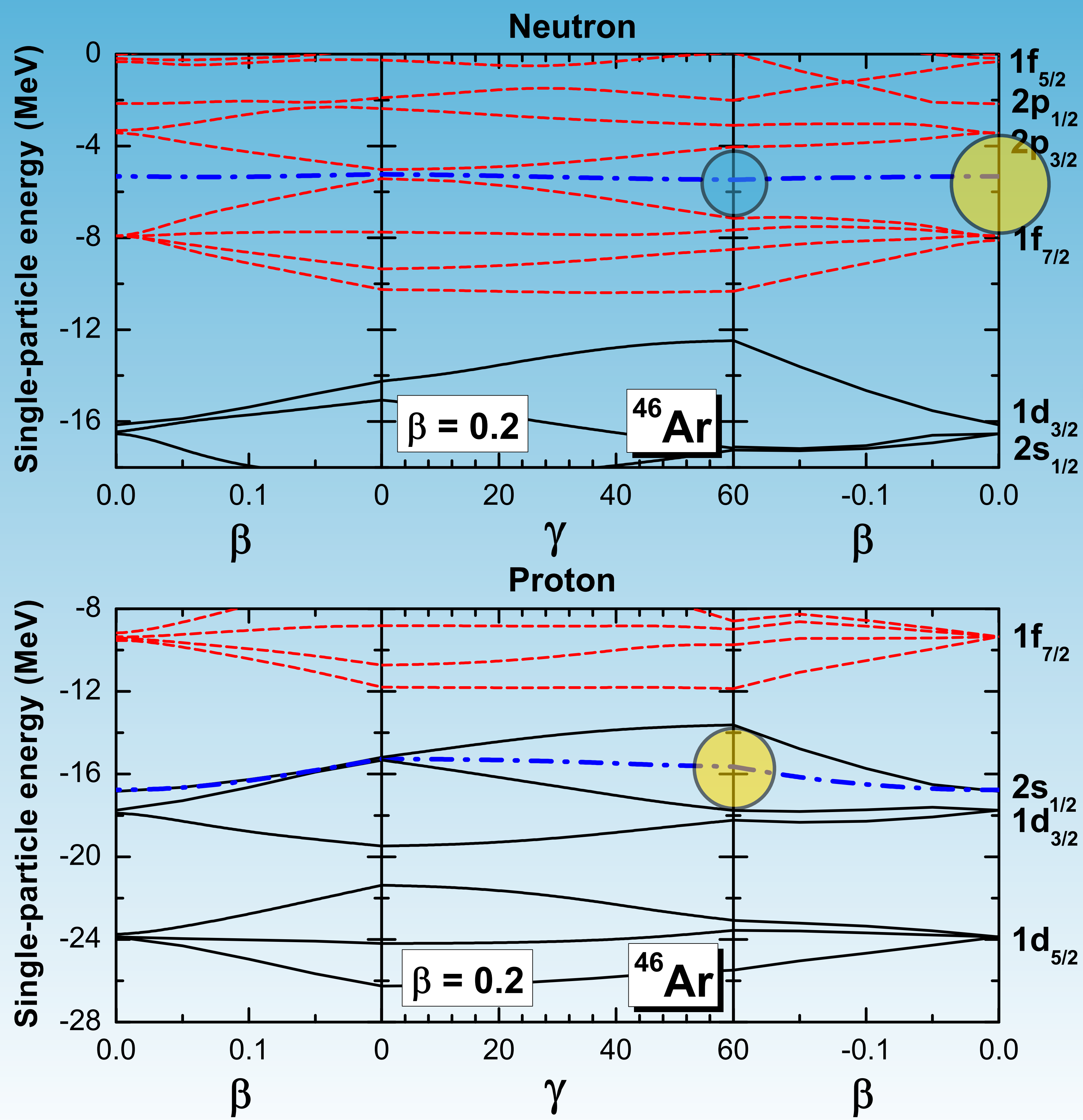


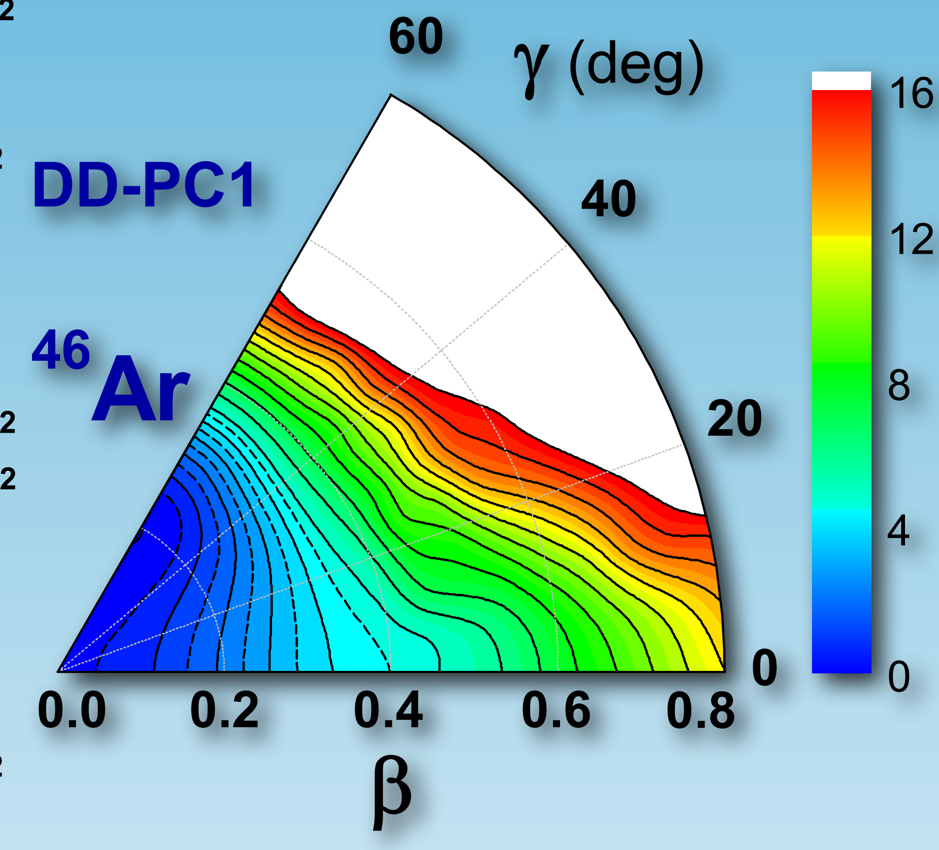
^{46}Ar: single-particle levels





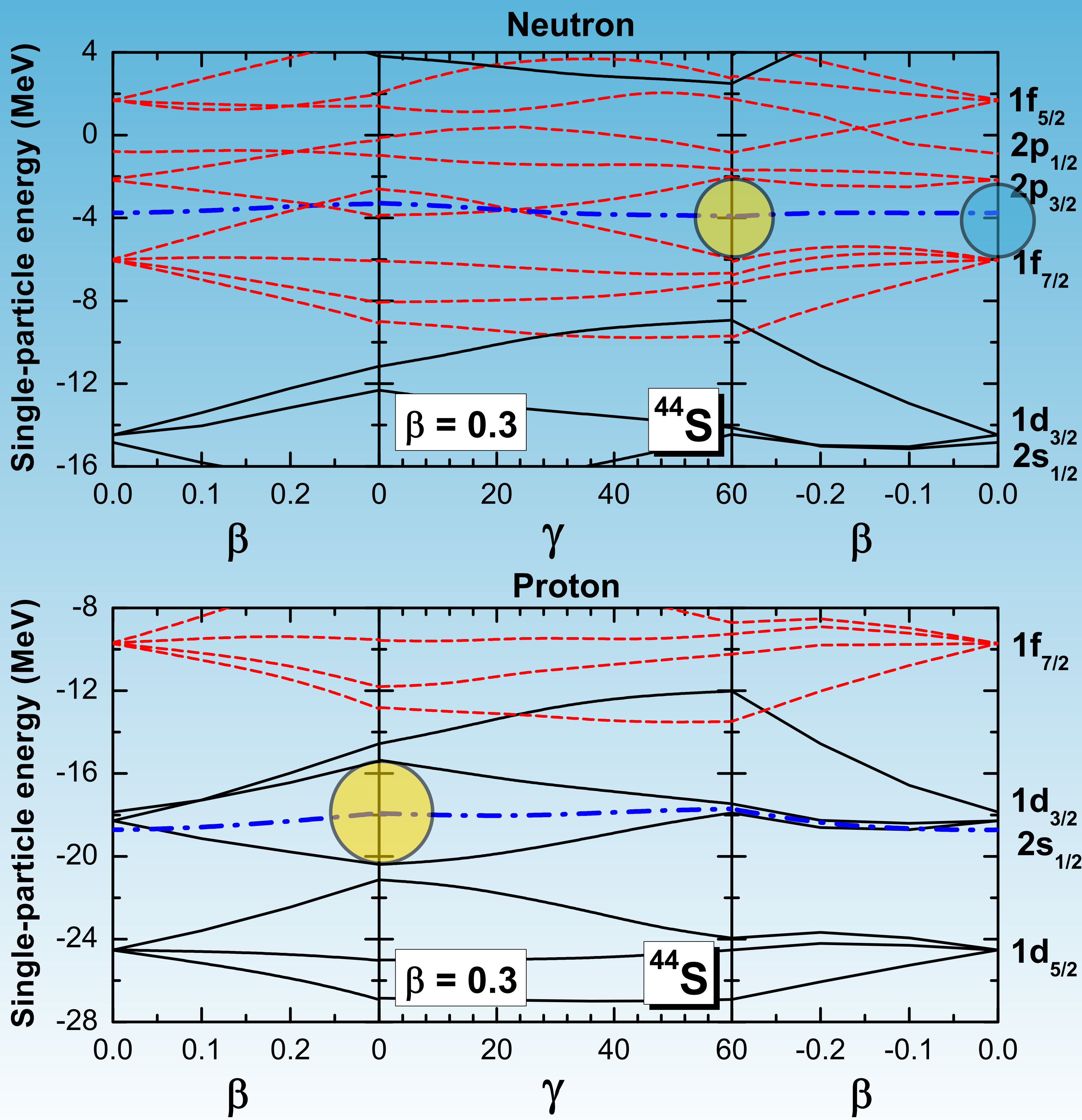
^{46}Ar: single-particle levels



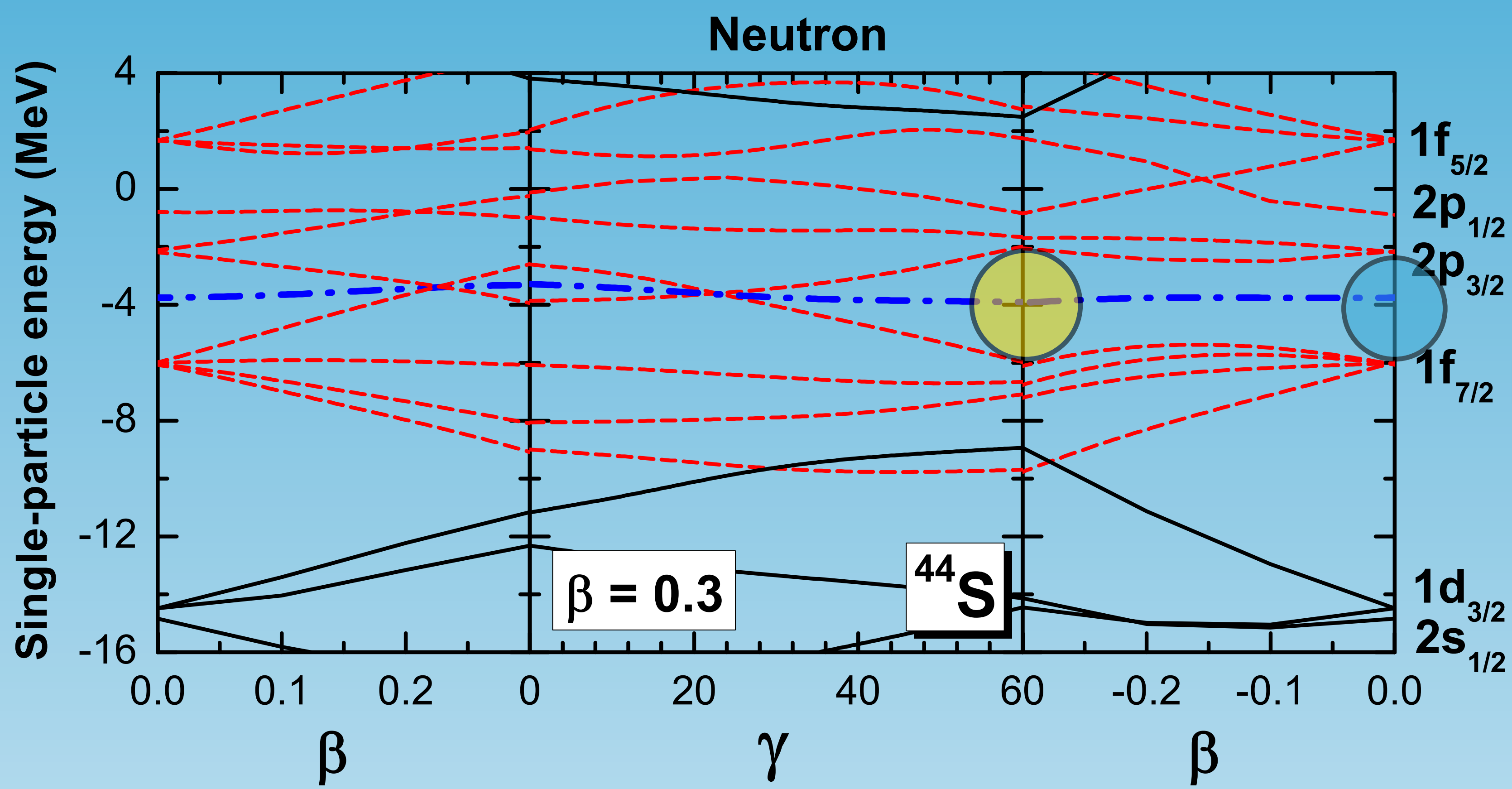


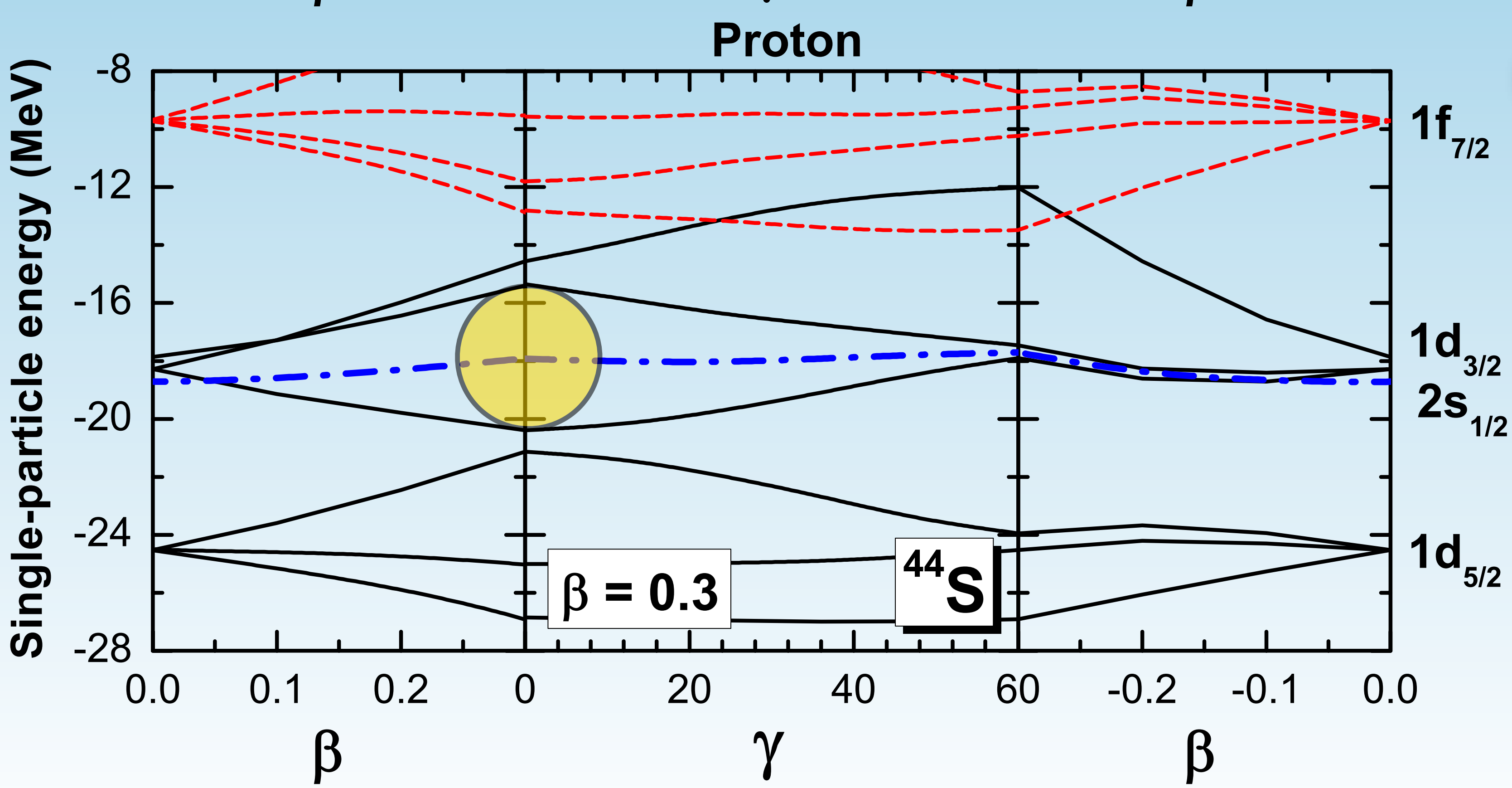
Monday, June 27, 2011

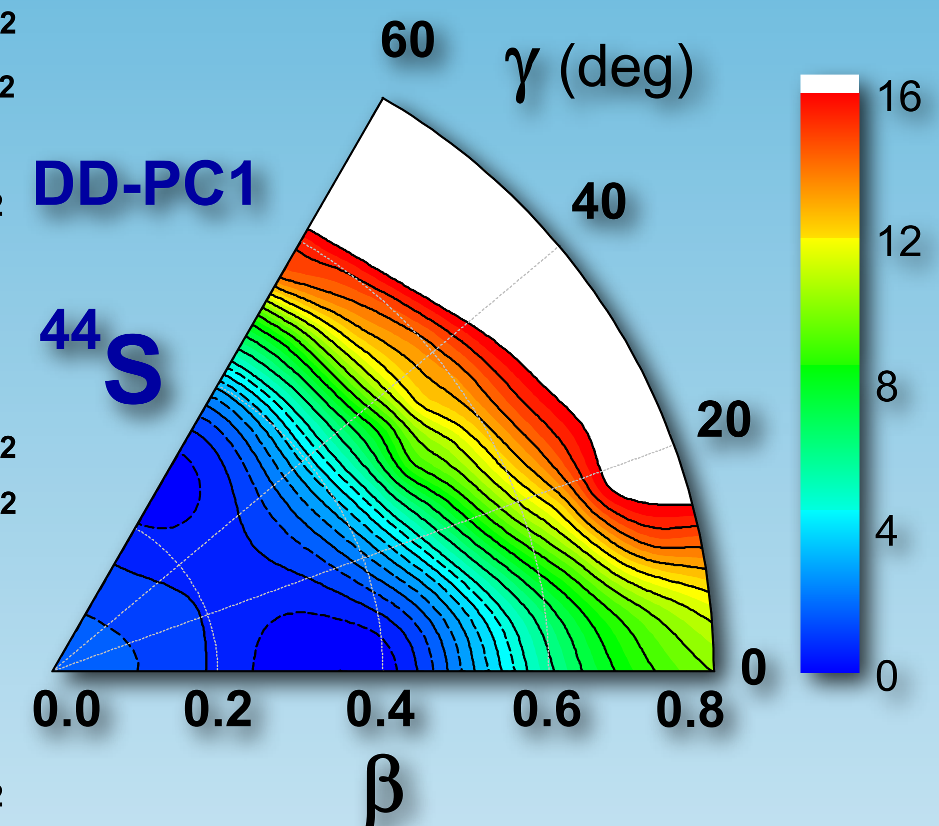
^{44}S: single-particle levels



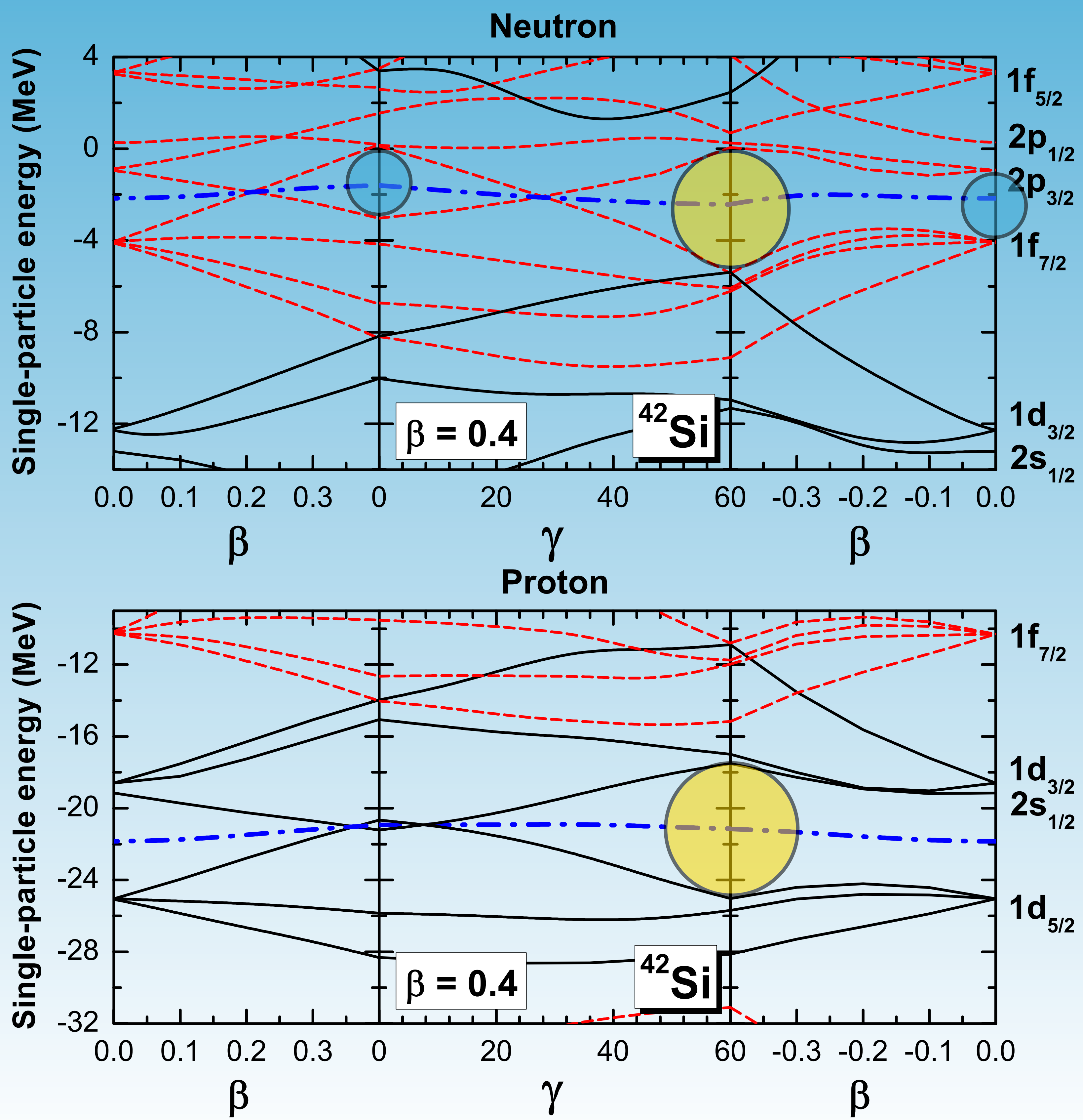
^{44}S: single-particle levels



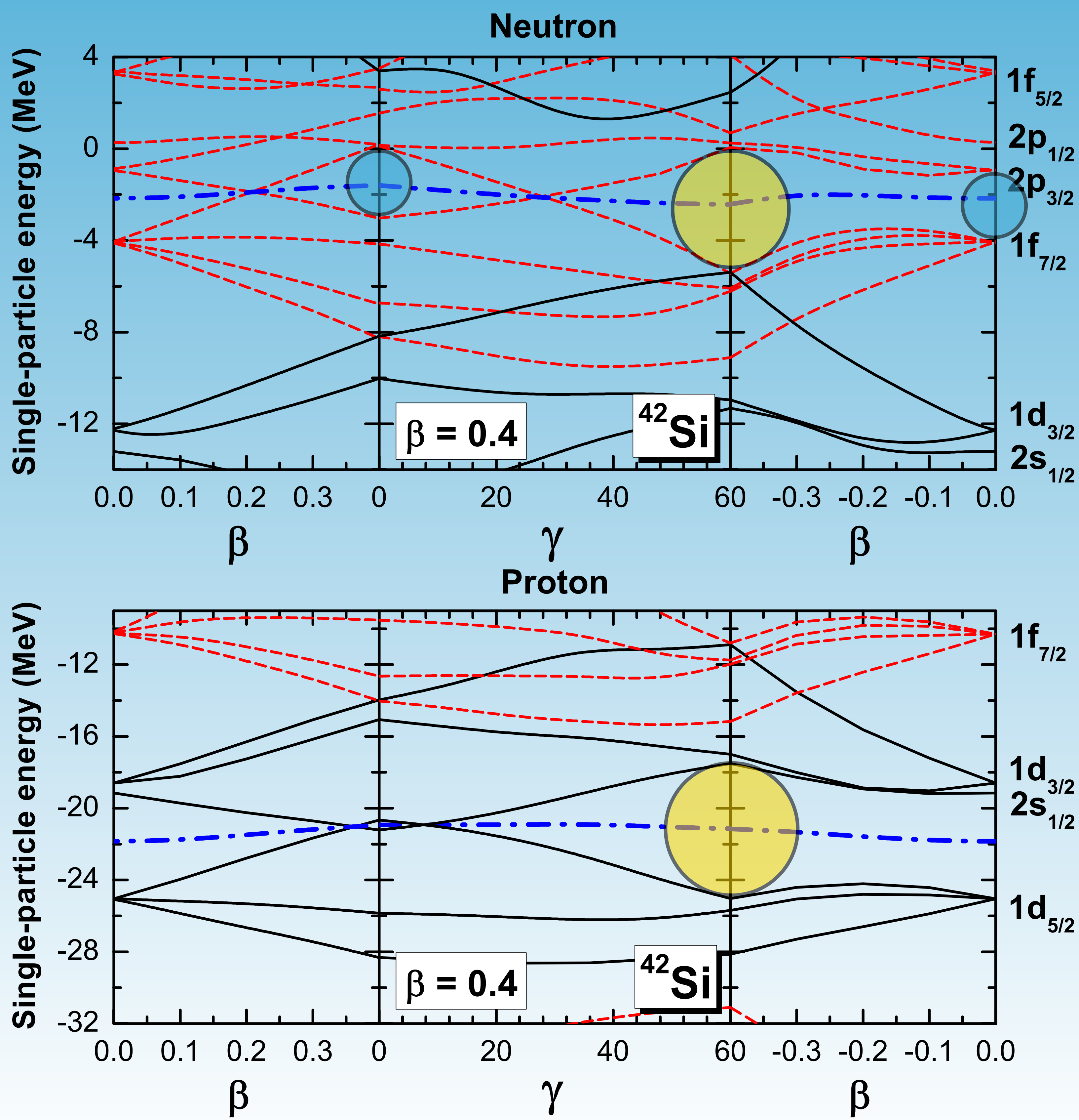


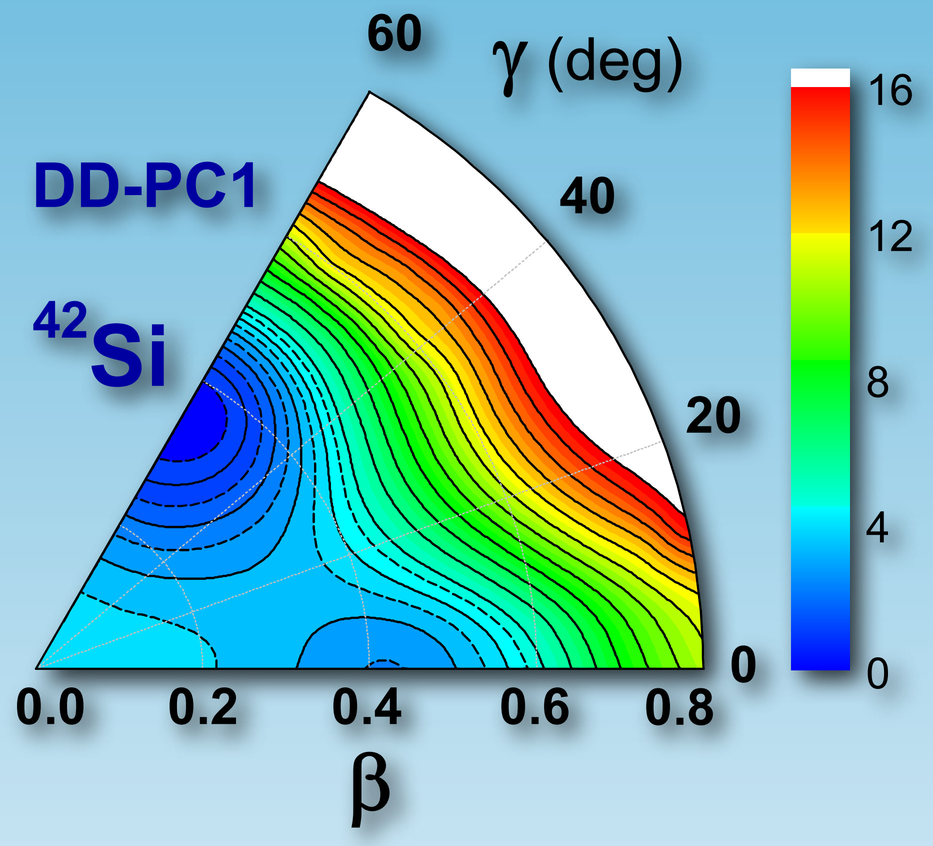


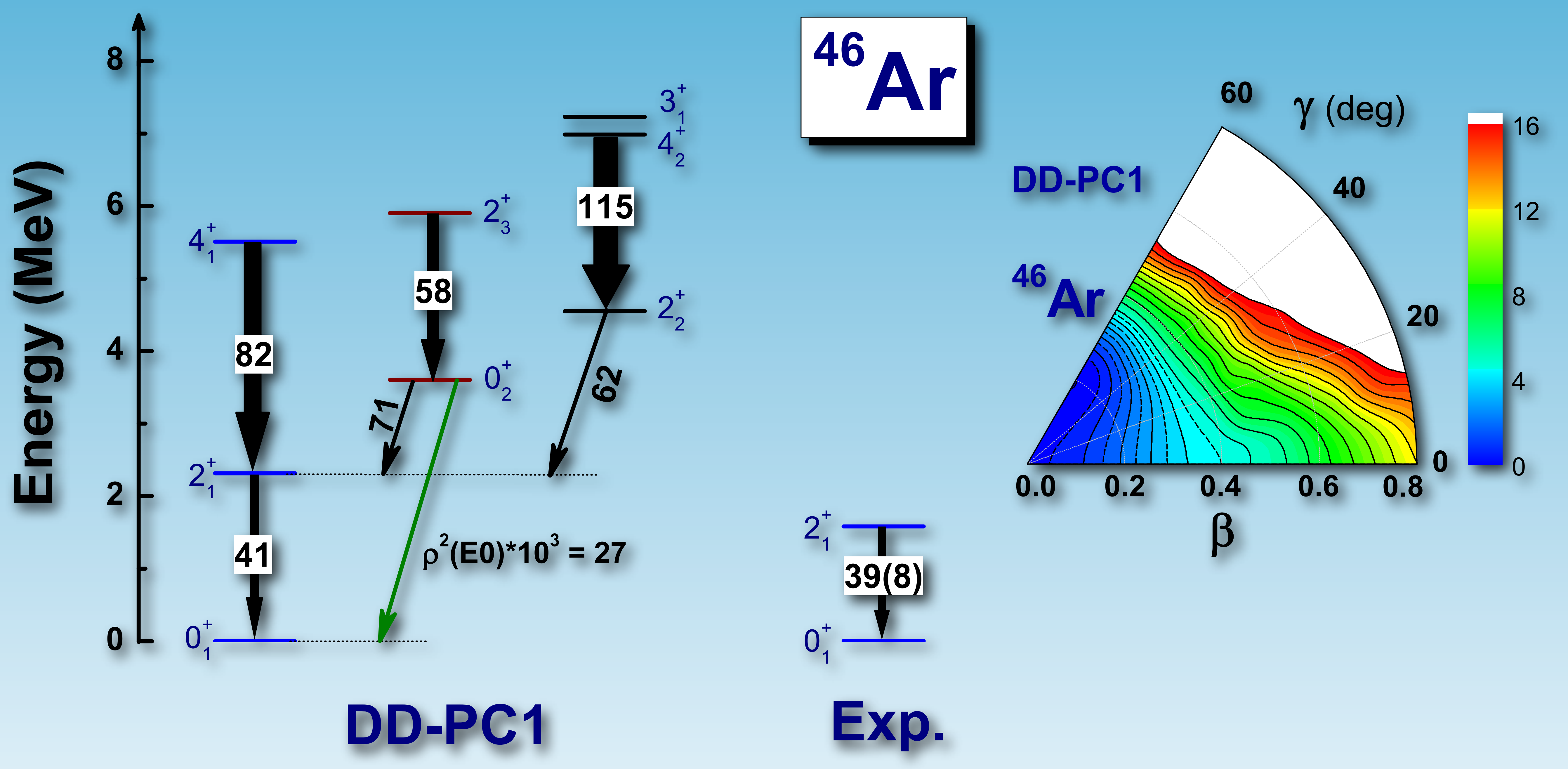
^{42}Si: single-particle levels



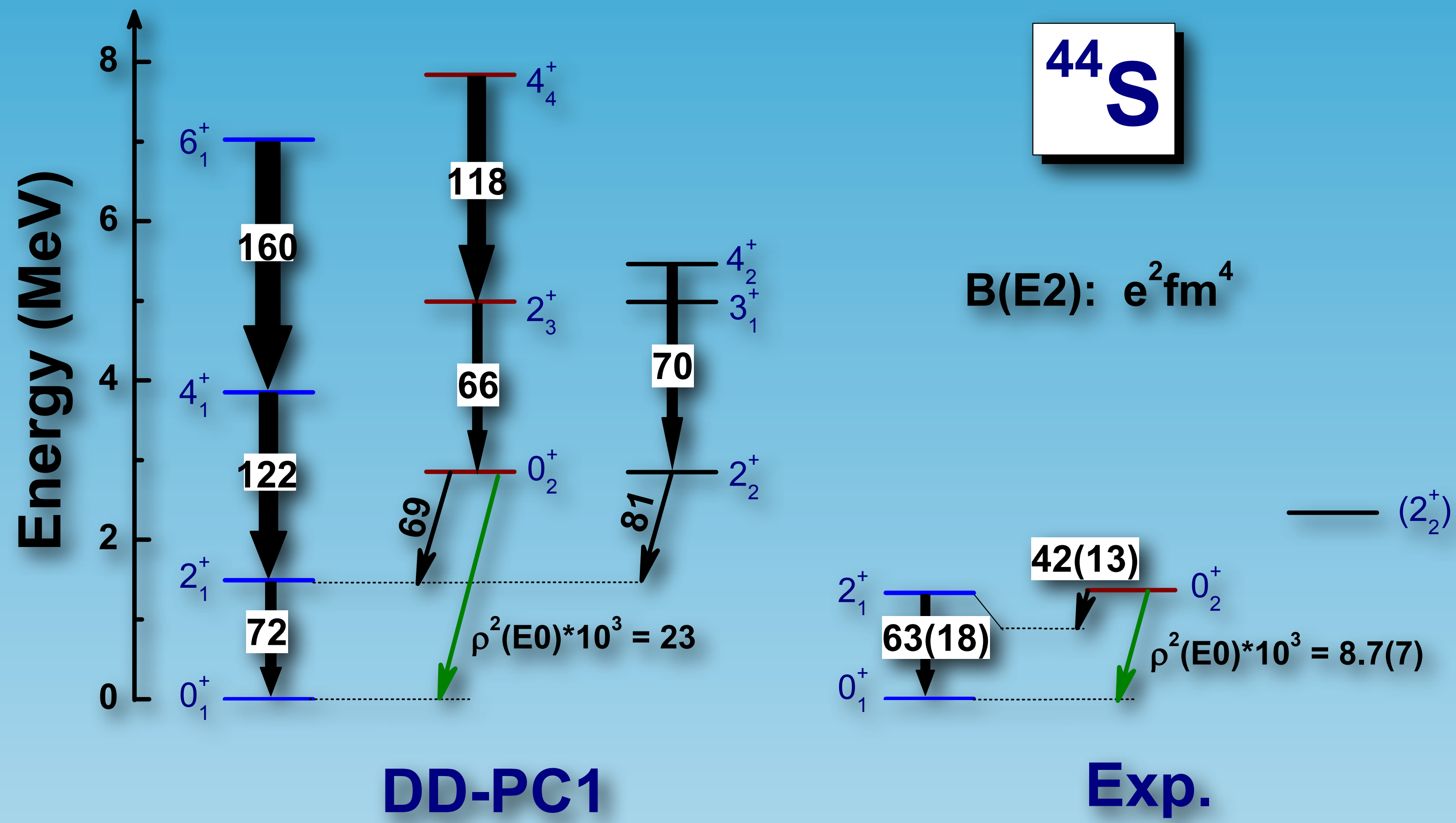
^{42}Si: single-particle levels

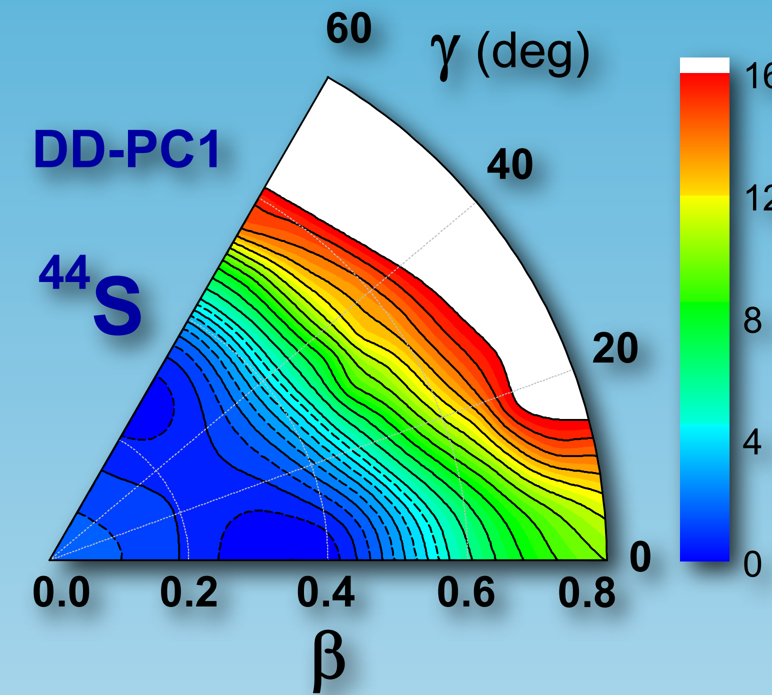





46Ar
Energy (MeV)
8
6
4
2
0
4^+_1
2^+_1
0^+_1
82
41
2^+_3
0^+_2
58
71
$\rho^2(E0)*10^3 = 27$
3^+_1
4^+_2
2^+_2
115
62
DD-PC1
2^+_1
39(8)
0^+_1
Exp.
DD-PC1
46Ar
60
40
20
0
γ (deg)
0.0
0.2
0.4
0.6
0.8
β
16
12
8
4
0

Monday, June 27, 2011

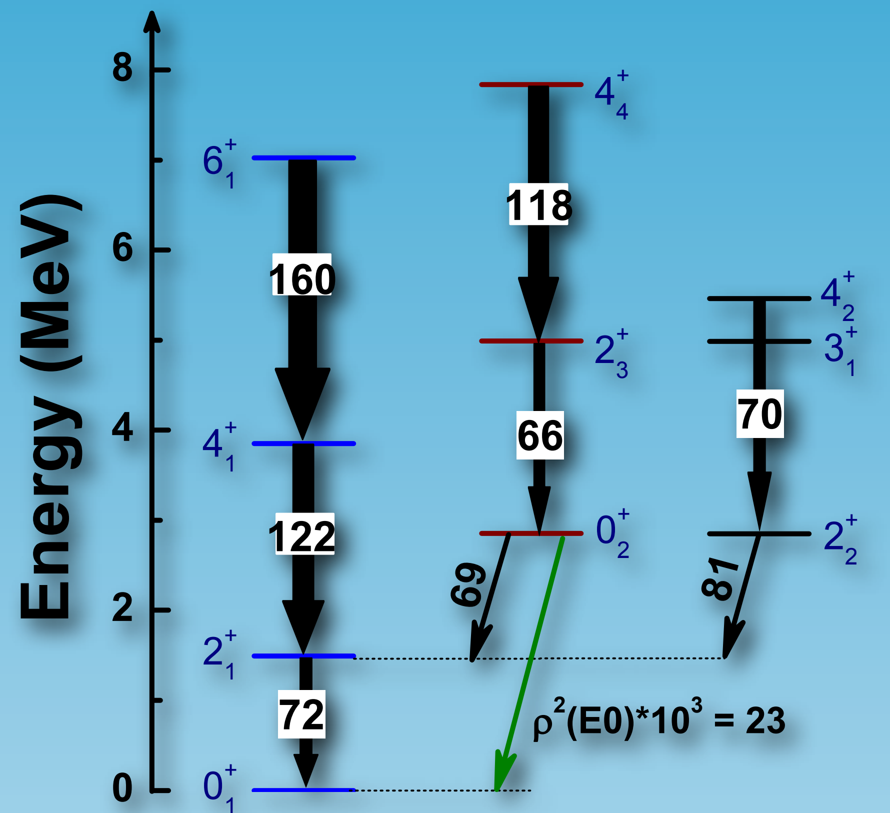




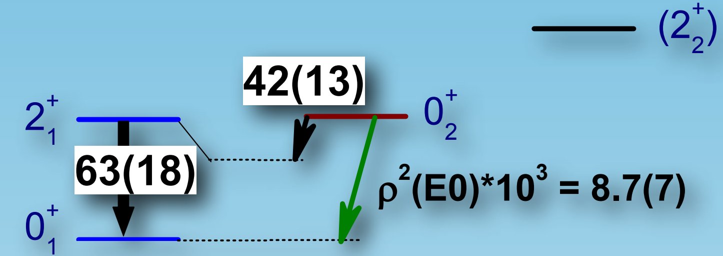
Probability density distributions:

^{44}S

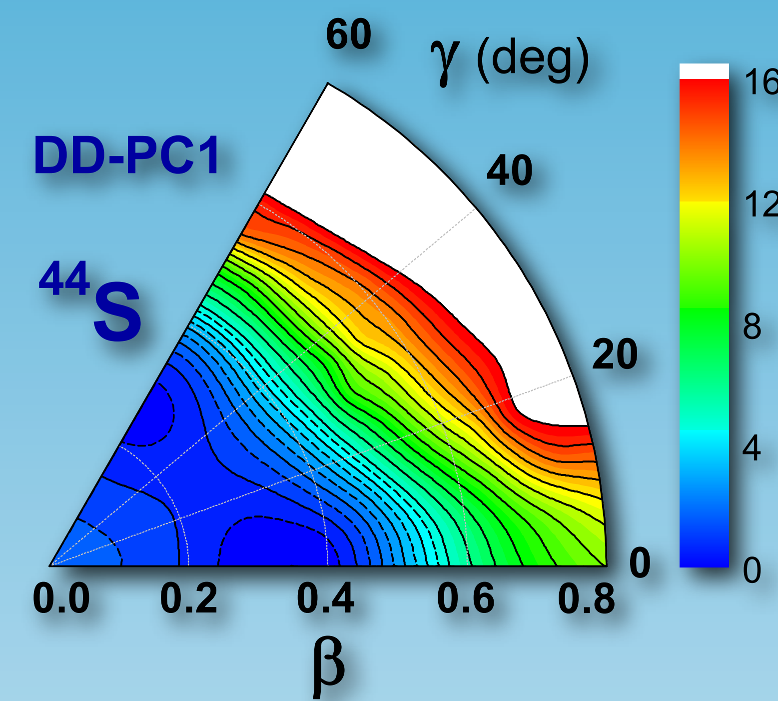
B(E2): e^2fm^4



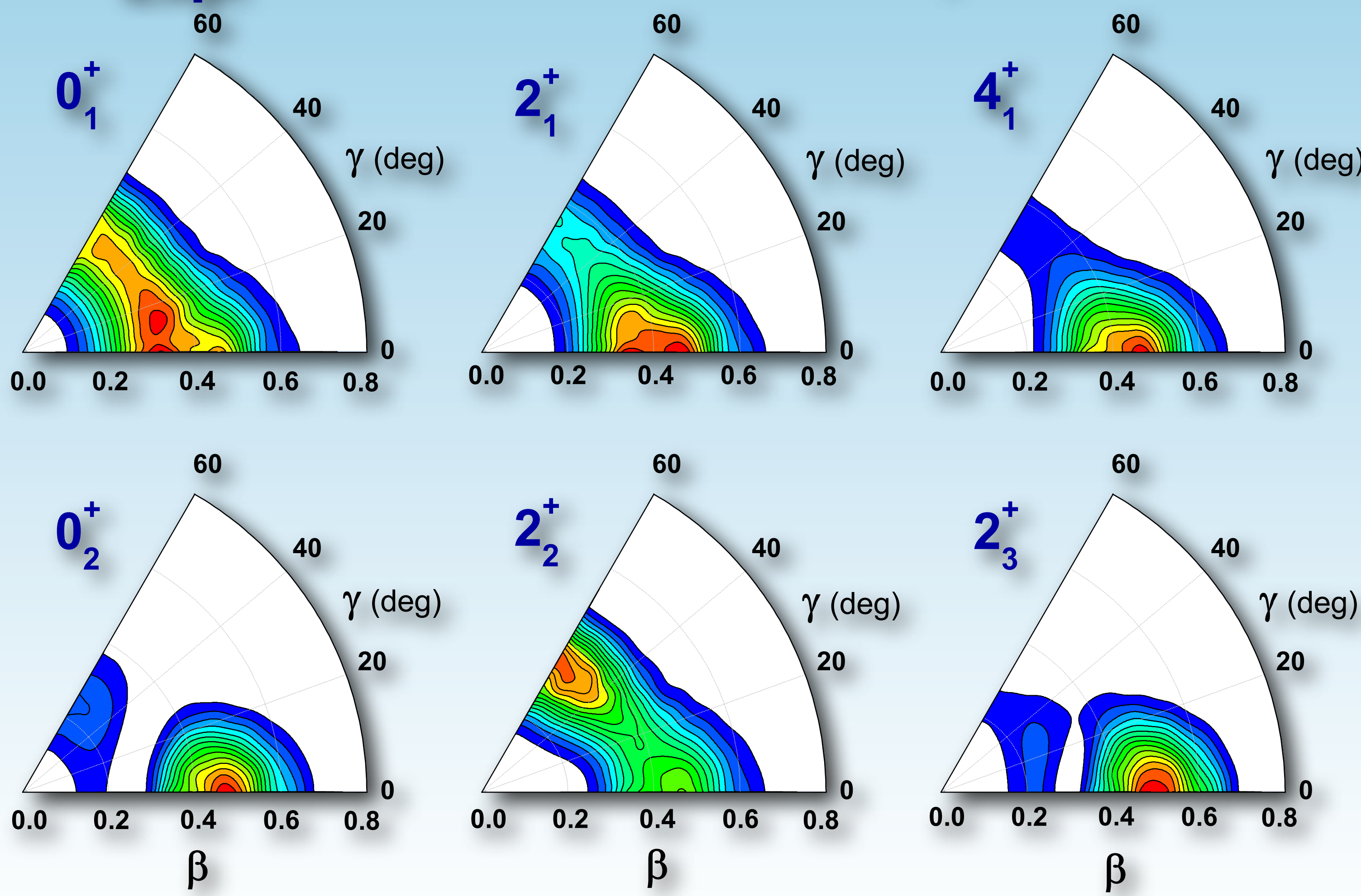
DD-PC1



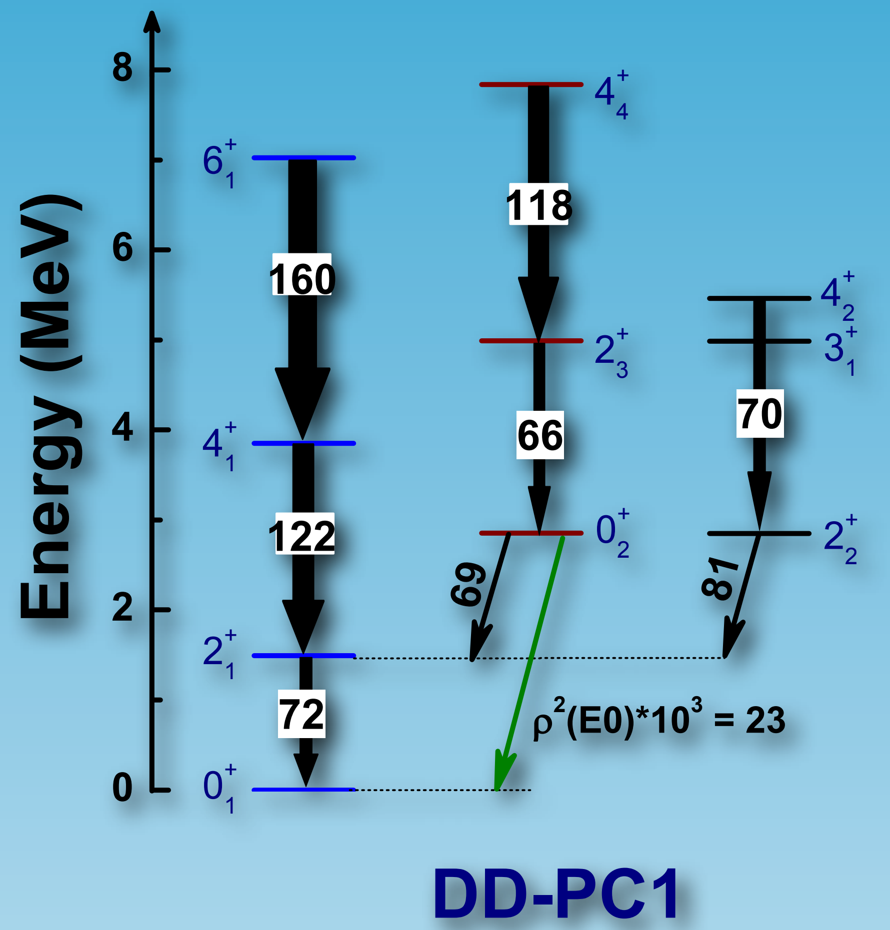
Exp.

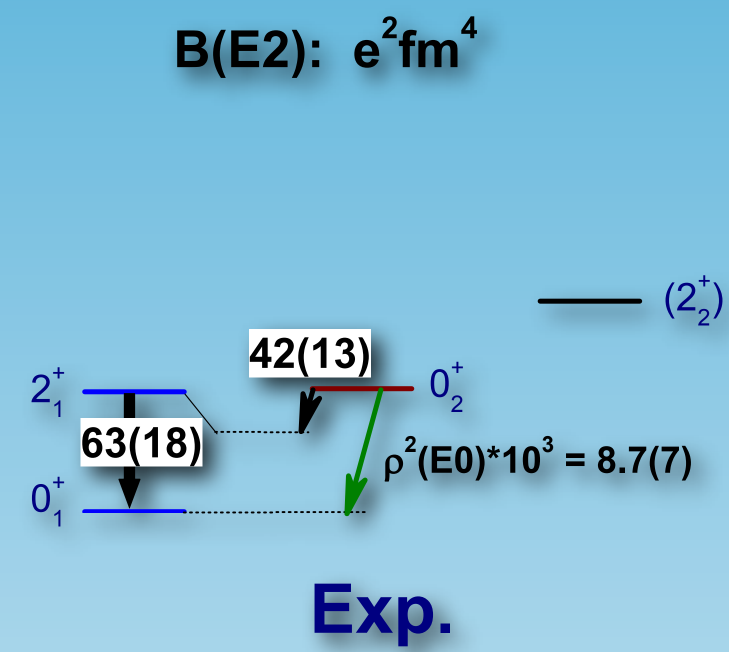


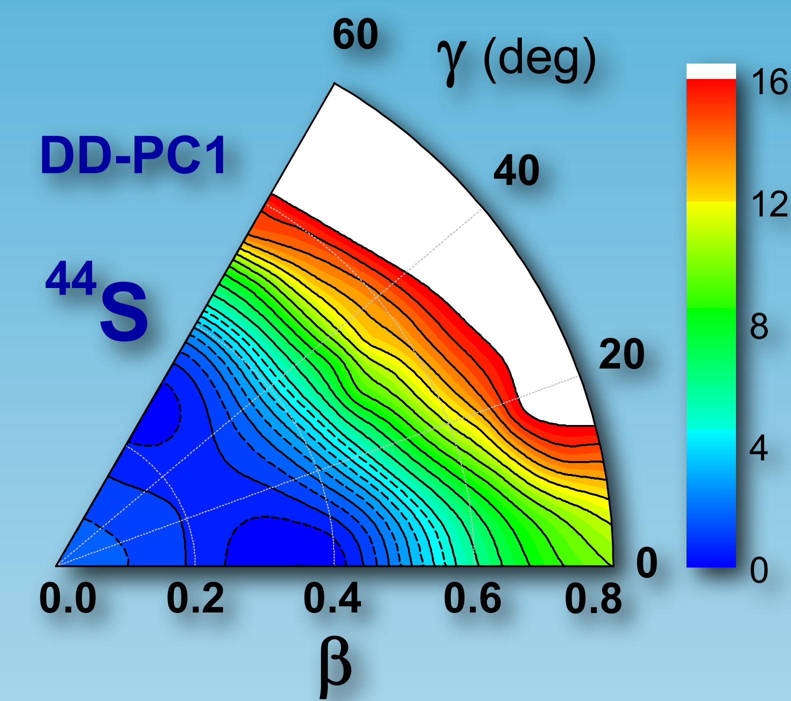
Probability density distributions:



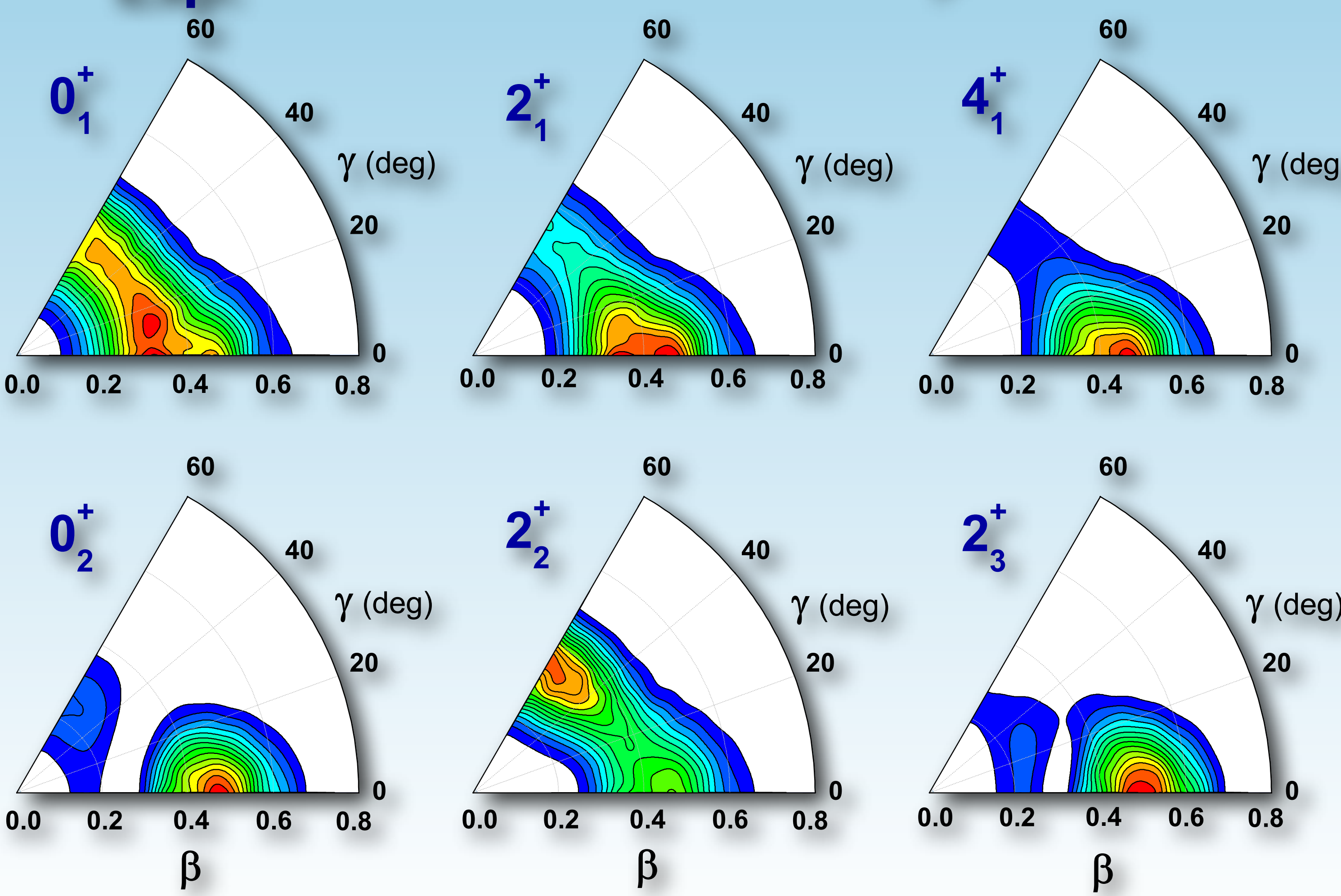
^{44}S





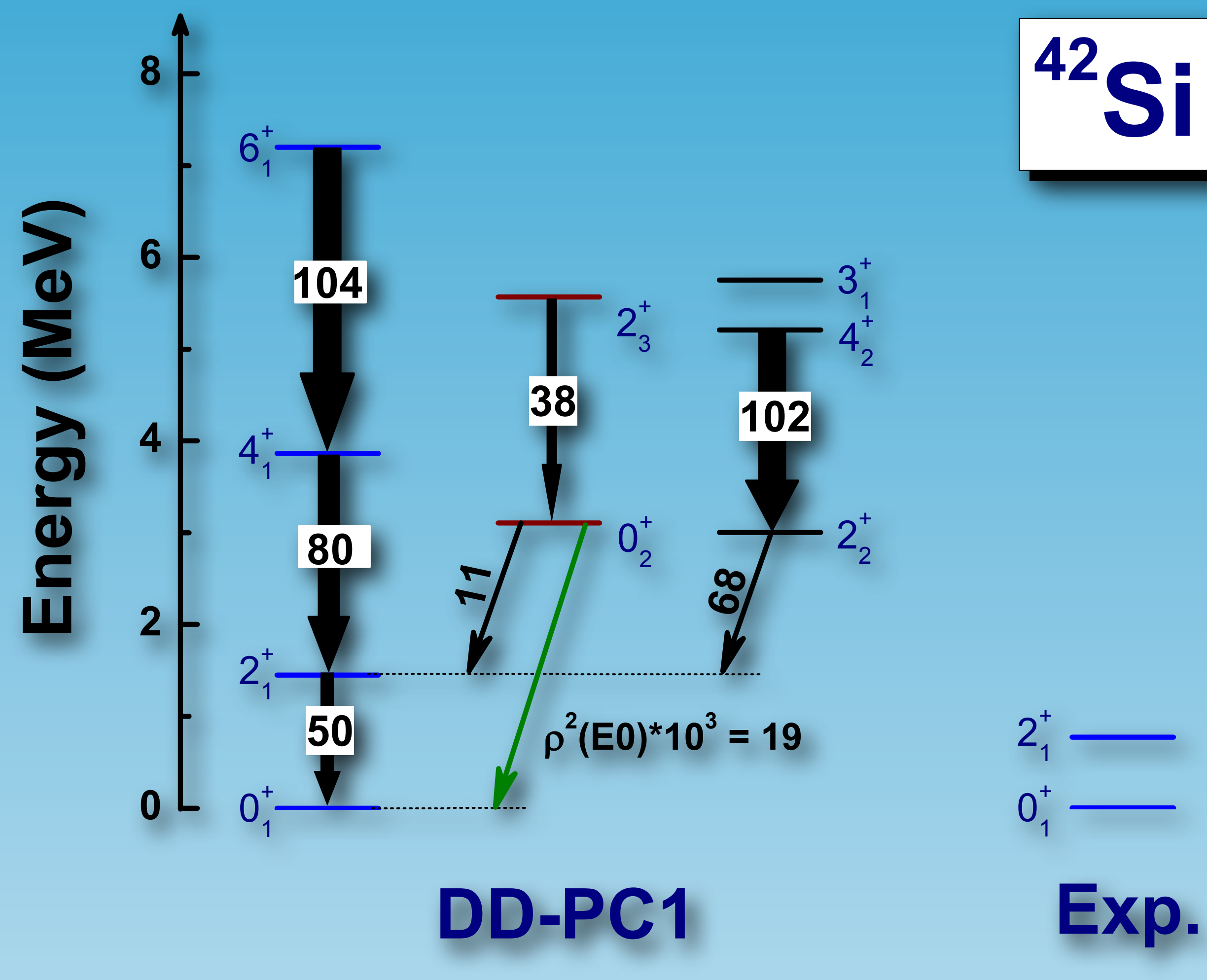


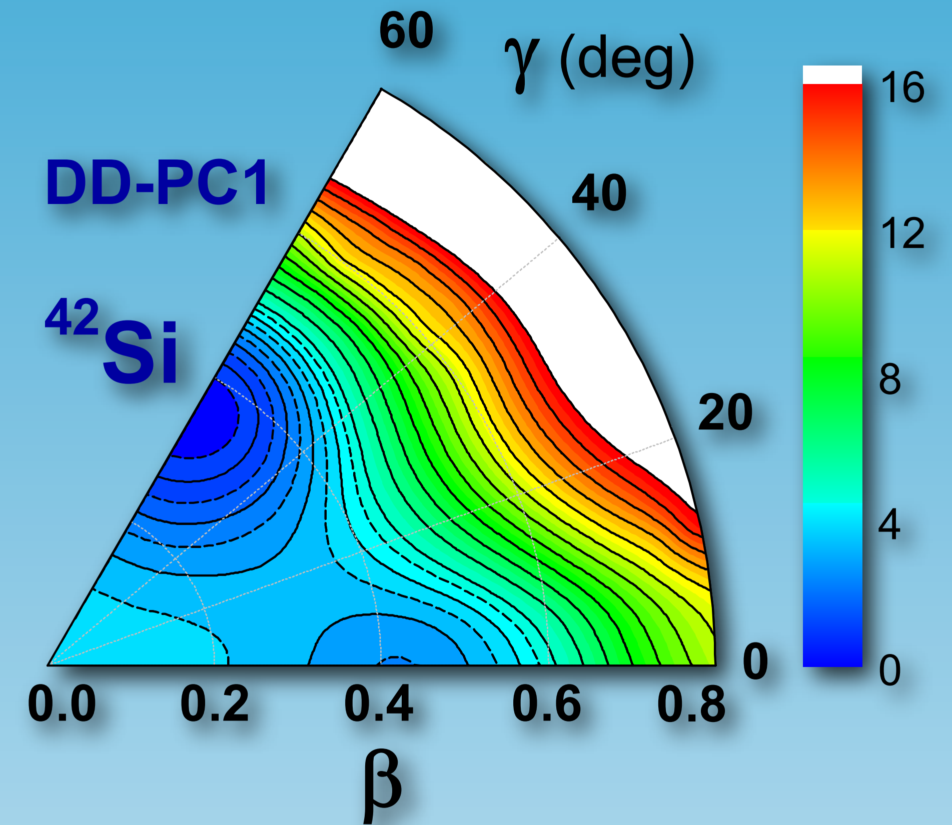
Probability density distributions:



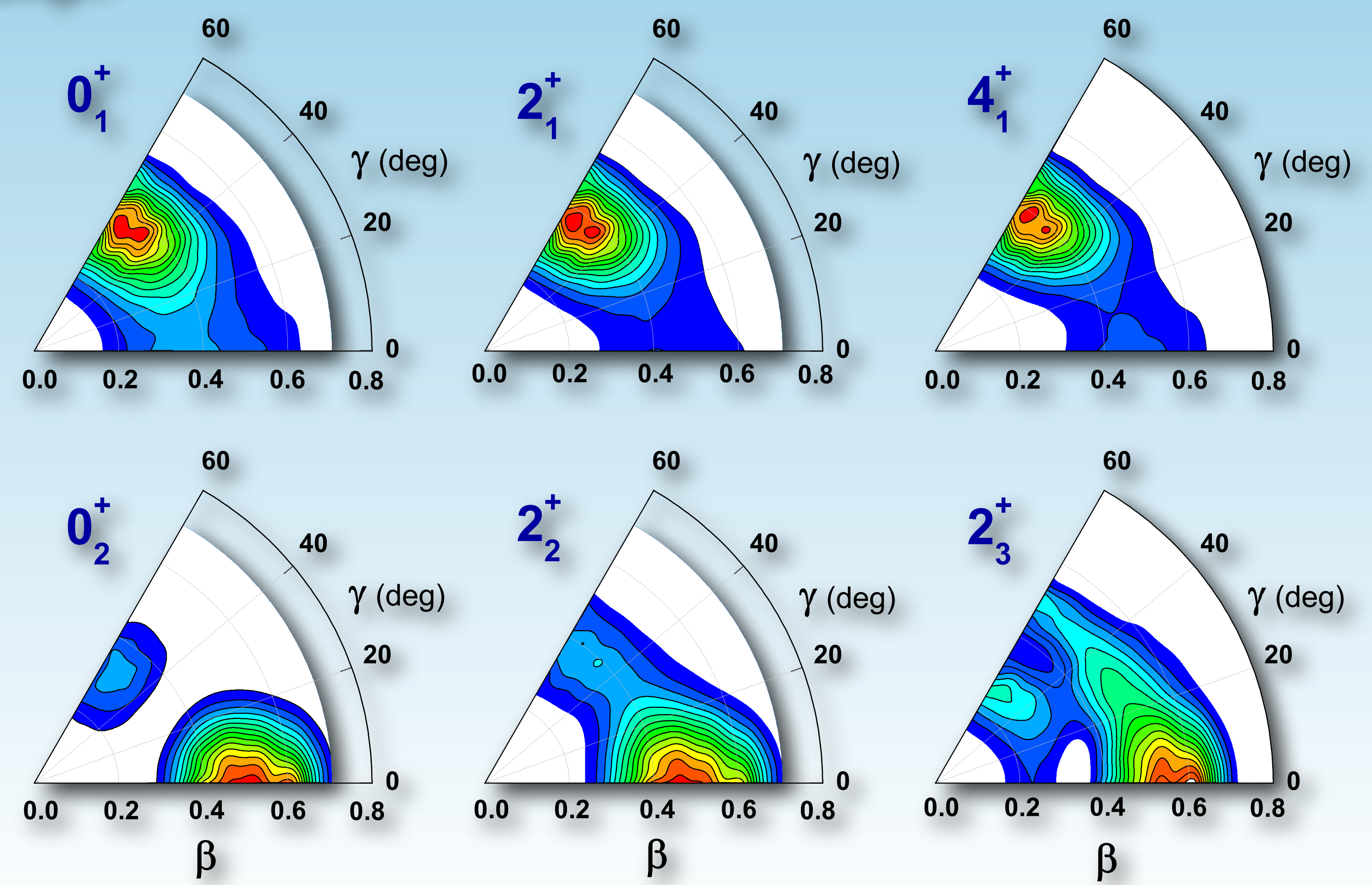
	$K=0$	$K=2$	$Q_{spec.}$
2^+_1	88.4	11.6	-10.9
2^+_2	21.5	78.5	7.8
2^+_3	80.0	20.0	-9.6

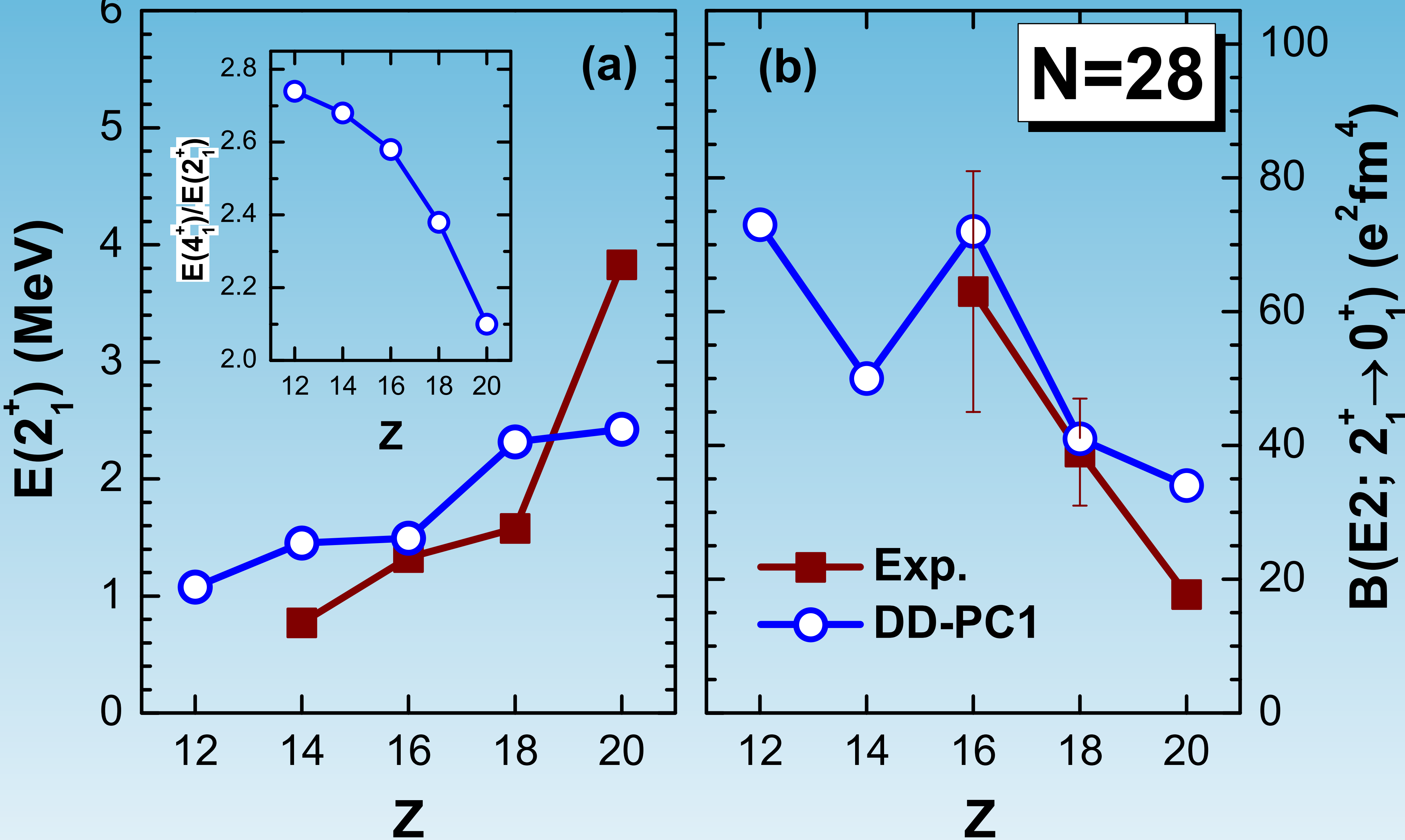
^{42}Si





Probability density distributions:





(a)
(b)
N=28
E(2_1^+) (MeV)
$E(4_1^+)/E(2_1^+)$
Z
B(E2; $2_1^+ \rightarrow 0_1^+$) (e^2fm^4)
Exp.
DD-PC1
0
1
2
3
4
5
6
2.0
2.2
2.4
2.6
2.8
12
14
16
18
20
20
40
60
80
100

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, dynamics of exotic modes of excitation.

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

NUCLEAR ENERGY DENSITY FUNCTIONALS for DUMMIES

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N. Paar
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