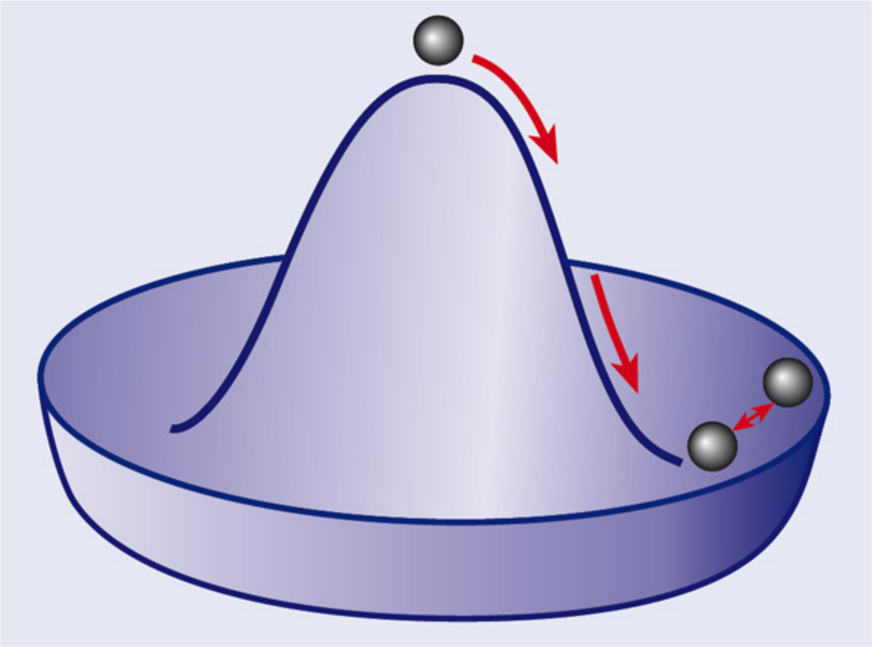
Symmetry Breaking and Correlations in Nuclei

II - Configuration Mixing

Configuration mixing



The most important correlation effects in nuclear structure originate from large amplitude collective motion. Low-lying excited states are admixed into the mean-field ground state. These admixtures can be removed by configuration mixing: superposition of mean-field states.
Correlations include nuclear surface vibrations (low-lying excitations) and zero-energy modes (translation, rotation, ...) related to restoration of symmetries which are broken by the mean-field ground state.

The Generator Coordinate Method

→ starting from a set of mean-field states $|\Phi(q)>$ that depend on the collective coordinate q, approximate eigenstates of the Hamiltonian H are obtained by GCM configuration mixing:

$$|\Psi_k\rangle = \int dq \; |\Phi(q)\rangle \; f_k(q)$$

Weight functions

Generator coordinate (collective variable)

Intrinsic (e.g. HFB) wave functions

The weight functions $f_k(q)$ are found by requiring that the expectation value:

$$E_k = \frac{\langle \Psi_k | \hat{H} | \Psi_k \rangle}{\langle \Psi_k | \Psi_k \rangle}$$

is stationary with respect to an arbitrary variation δf_k.

Hill-Wheeler equation:

$$\int dq' \; [\mathcal{H}(q,q') - E_k \mathcal{I}(q,q')] f_k(q') = 0$$

$$\mathcal{H}(q,q') = \langle \Phi(q)|\hat{H}|\Phi(q')\rangle \qquad \mathcal{I}(q,q') = \langle \Phi(q)|\Phi(q')\rangle$$

Hamiltonian kernel   overlap kernel

→ for any operator O:

$$\mathcal{O}(q,q') = \langle \Phi(q)|\hat{O}|\Phi(q')\rangle$$

The weight functions are not orthonormal and they cannot be interpreted as collective wave functions for the variable q. This role is assigned to the functions:

$$g_k(q) = \int dq' \, \mathcal{I}^{1/2}(q,q') \, f_k(q')$$

The matrix element of any operator between two GCM states can be expressed in terms of the g_k's as:

$$\langle \Psi_k|\hat{O}|\Psi_l\rangle = \iint dq \, dq' \, g_k^*(q) \, \tilde{\mathcal{O}}(q,q') \, g_l(q')$$

with: $$\tilde{\mathcal{O}}(q,q') = \iint dq''\, dq'''\, \mathcal{I}^{1/2}(q,q'')\, \mathcal{O}(q'',q''')\, \mathcal{I}^{1/2}(q''',q')$$

The GCM energies E_k and functions g_k are the eigenvalues and eigenvectors of the hermitian integral operator

$$\int dq'\, \tilde{\mathcal{H}}(q,q')\, g_k(q') = E_k g_k(q)$$

Gaussian Overlap Approximation: the overlap kernel is replaced by a Gaussian function of the form:

$$\mathcal{I}(q,q') \simeq \mathcal{I}_G(q,q') = \exp\left\{ -\frac{1}{2}\left[\frac{(q-q')}{a(\bar{q})}\right]^2 \right\}$$

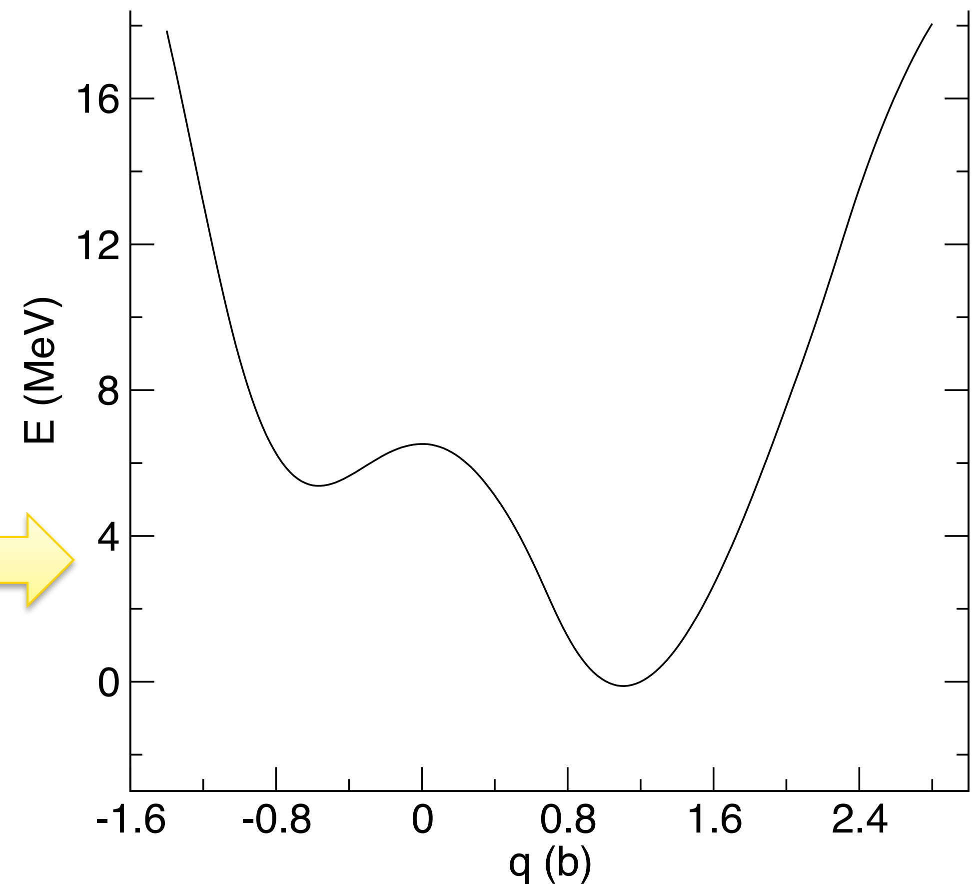
based on the rapid decrease of the matrix elements between wave functions corresponding to different values of the collective variable.

Choice of the collective coordinate

1. **RESTORATION OF BROKEN SYMMETRIES:** the family of wave functions $|\Phi(q)>$ is generated by the symmetry operations: rotation in coordinate space for angular momentum, rotation in gauge space for particle number. The functions $f_k(q)$ are a priori determined by the properties of the symmetry operator (this is strictly valid only for Abelian symmetry groups – U(1) particle number. For non-Abelian groups the weight functions are not completely determined by the symmetry).

2. SHAPE DEGREES OF FREEDOM: the collective space is generated by constrained mean-field calculations. The generating function is unknown and has to be determined by the diagonalization of the Hill-Wheeler equation.

The starting point is usually a constrained HFB calculation of the potential energy surface with the mass quadrupole components as constrained quantities.



Configuration mixing of mean-field wave functions projected on angular momentum and particle number:

$$|\Psi_\alpha^{JM}> = \sum_{j,K} f_\alpha^{JK}(q_j) \hat{P}^J_{MK} \hat{P}^Z \hat{P}^N |\phi(q_j)>$$

The weight functions are determined by requiring that the expectation value of the energy is stationary with respect to an arbitrary variation:

$$\delta E^J = \delta \frac{<\Psi_\alpha^{JM}|\hat{H}|\Psi_\alpha^{JM}>}{<\Psi_\alpha^{JM}|\Psi_\alpha^{JM}>} = 0$$

The Hill-Wheeler equation:

$$\sum_{j,K} f_\alpha^{JK}(q_j) \left(\langle\phi(q_i)| \hat{H} \hat{P}^J_{MK} \hat{P}^N \hat{P}^Z |\phi(q_j)\rangle - E_\alpha^J \langle\phi(q_i)| \hat{P}^J_{MK} \hat{P}^N \hat{P}^Z |\phi(q_j)\rangle \right) = 0$$

presents a generalized eigenvalue problem. The weight functions are not orthogonal and cannot be interpreted as collective wave functions for the variable *q*.

$$\sum_j \mathcal{H}^J(q_i, q_j) f_\alpha^J(q_j) = E_\alpha^J \sum_j \mathcal{N}^J(q_i, q_j) f_\alpha^J(q_j)$$

... define a new set of functions: $$g_\alpha^J(q_i) = \sum_j (\mathcal{N}^J)^{1/2}(q_i, q_j) f_\alpha^J(q_j)$$

With this transformation the Hill-Wheeler equation defines an ordinary eigenvalue problem:

$$\sum_j \tilde{\mathcal{H}}^J(q_i, q_j) g_\alpha^J(q_j) = E_\alpha g_\alpha^J(q_i)$$

with: $$\tilde{\mathcal{H}}^J(q_i, q_j) = \sum_{k,l} (\mathcal{N}^J)^{-1/2}(q_i, q_k) \mathcal{H}^J(q_k, q_l) (\mathcal{N}^J)^{-1/2}(q_l, q_j)$$

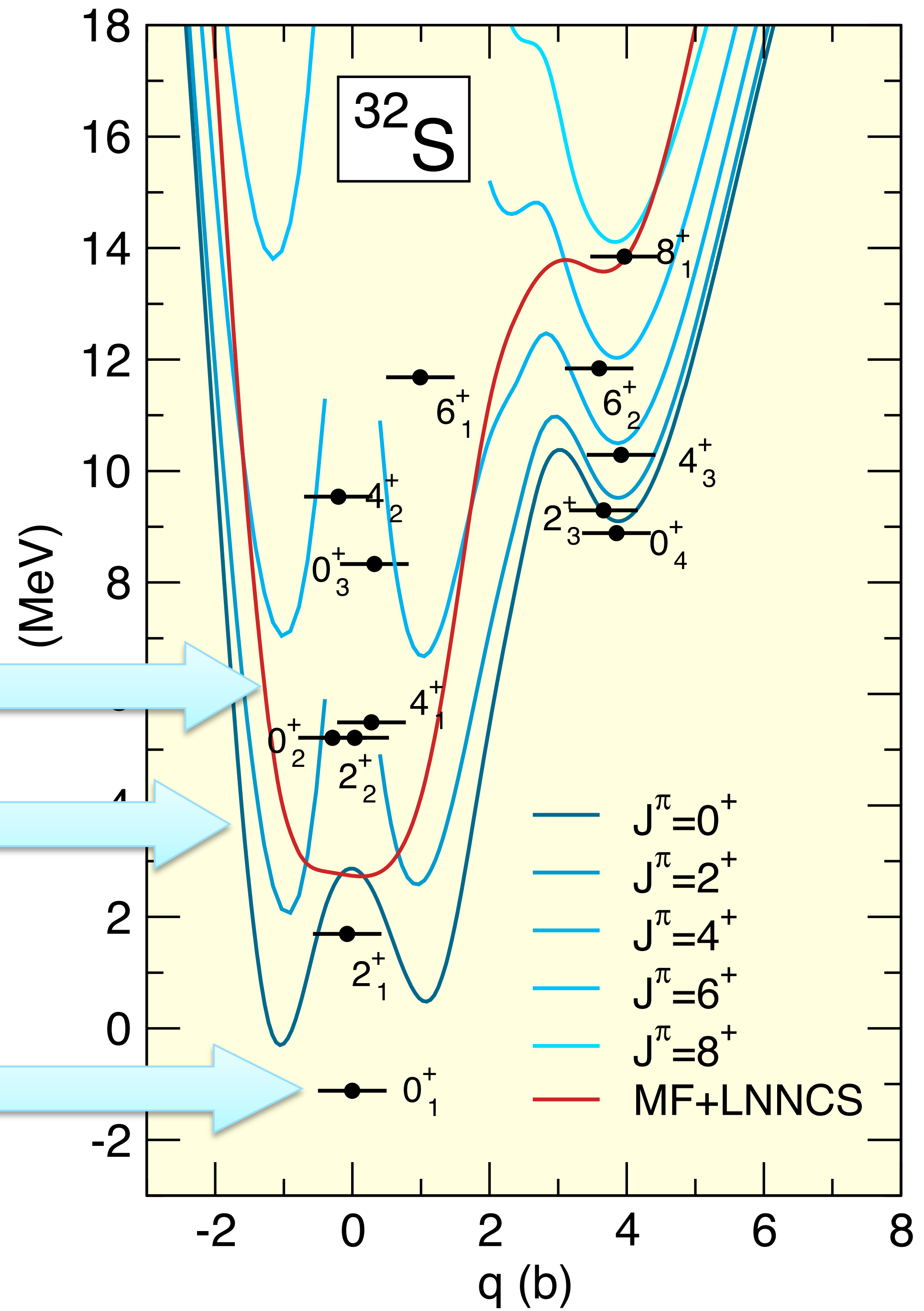
The functions $g^J_\alpha(q_i)$ are orthonormal and play the role of collective wave functions.

Example: Self-consistent mean-field calculation which includes correlations related to restoration of broken symmetries (rotational, particle number) and to fluctuations of collective variables (quadrupole deformation).

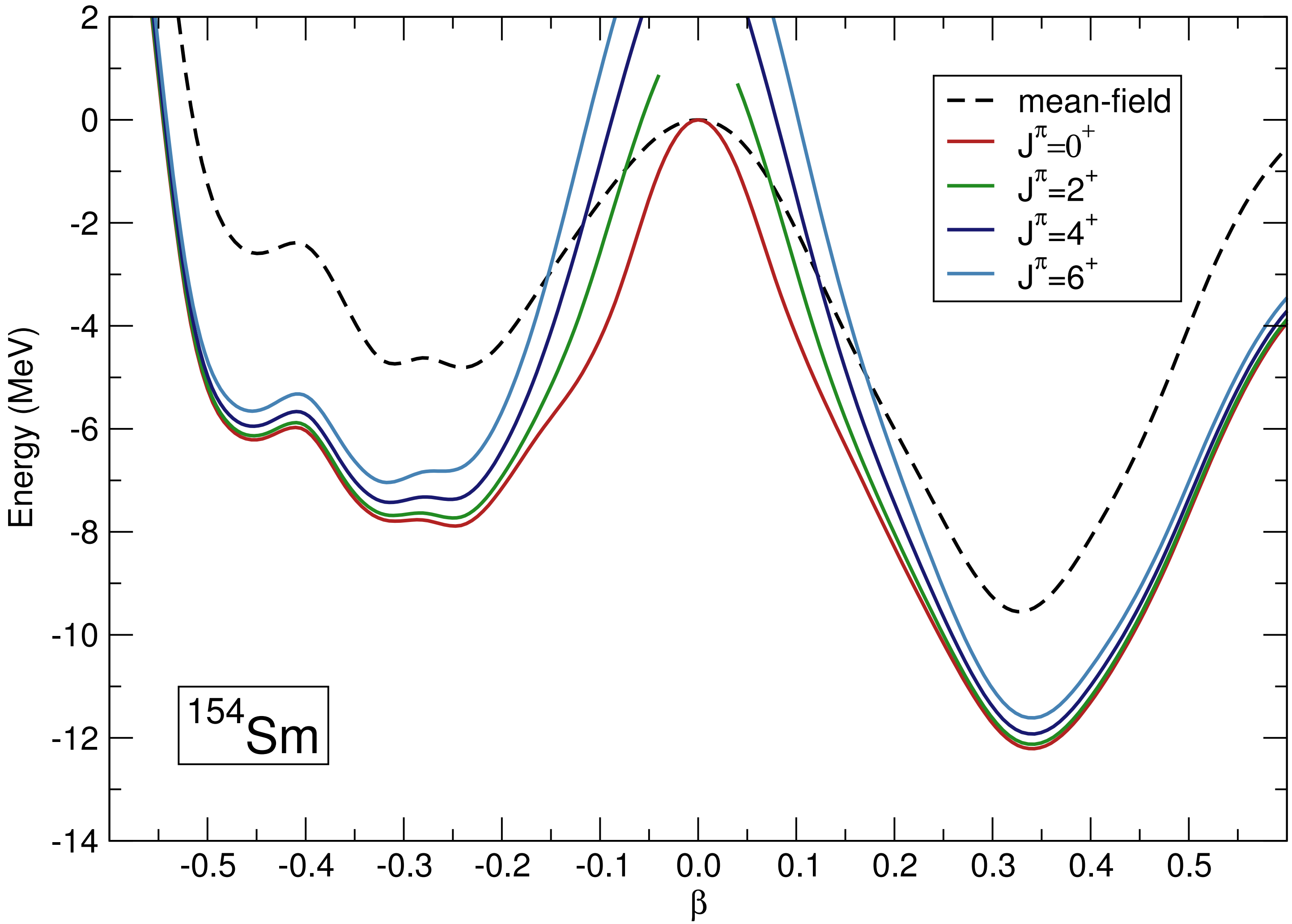
1. Mean-field potential energy curve calculated with a constraint on the quadrupole moment.

2. Angular-momentum and particle-number projected energy curves.

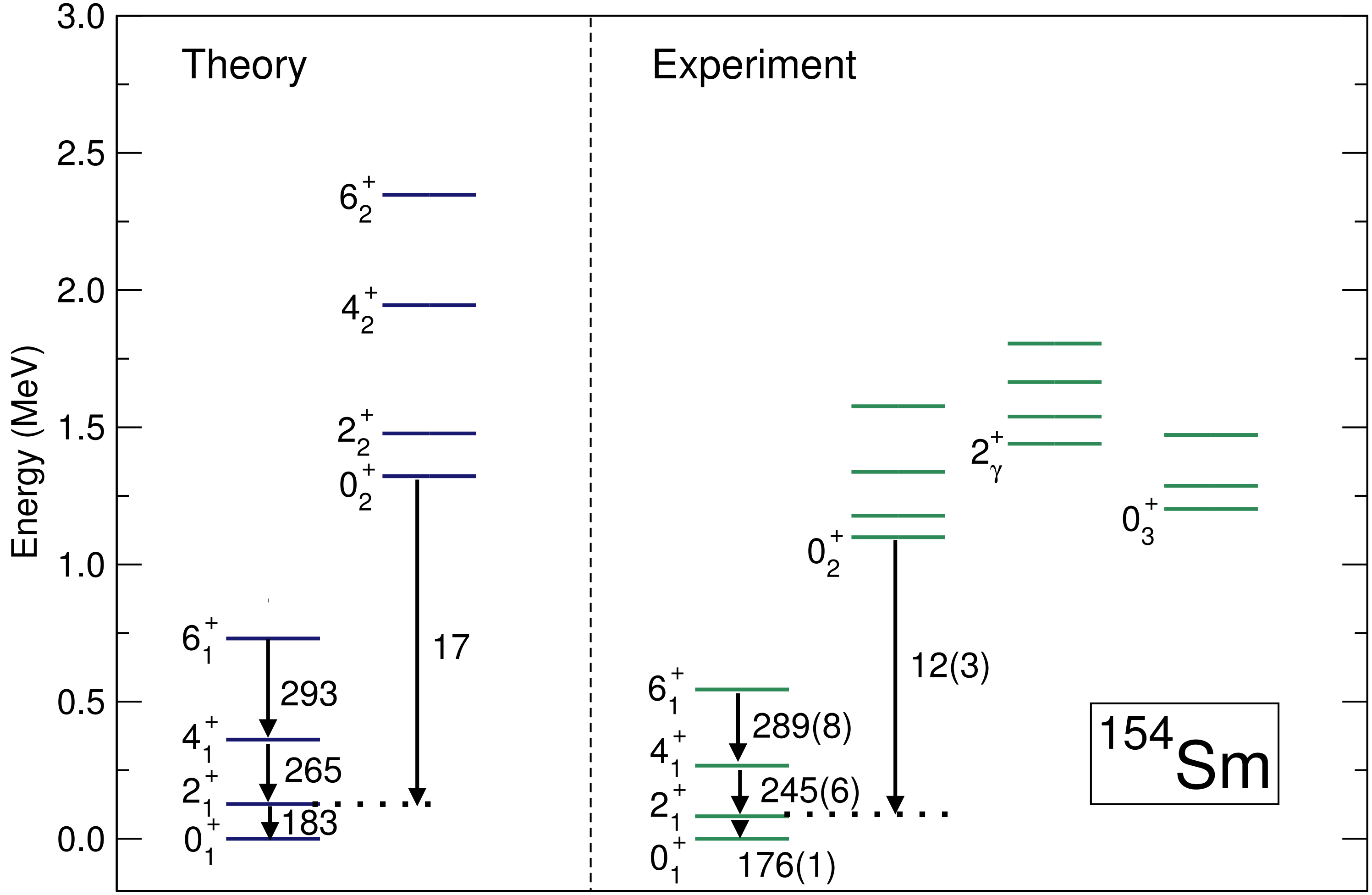
3. The Hamiltonian is diagonalized within each of the collective sub-spaces of the nonorthogonal bases |J, q> by using the Generator Coordinate Method.



Angular momentum projection and configuration mixing: ^{154}Sm



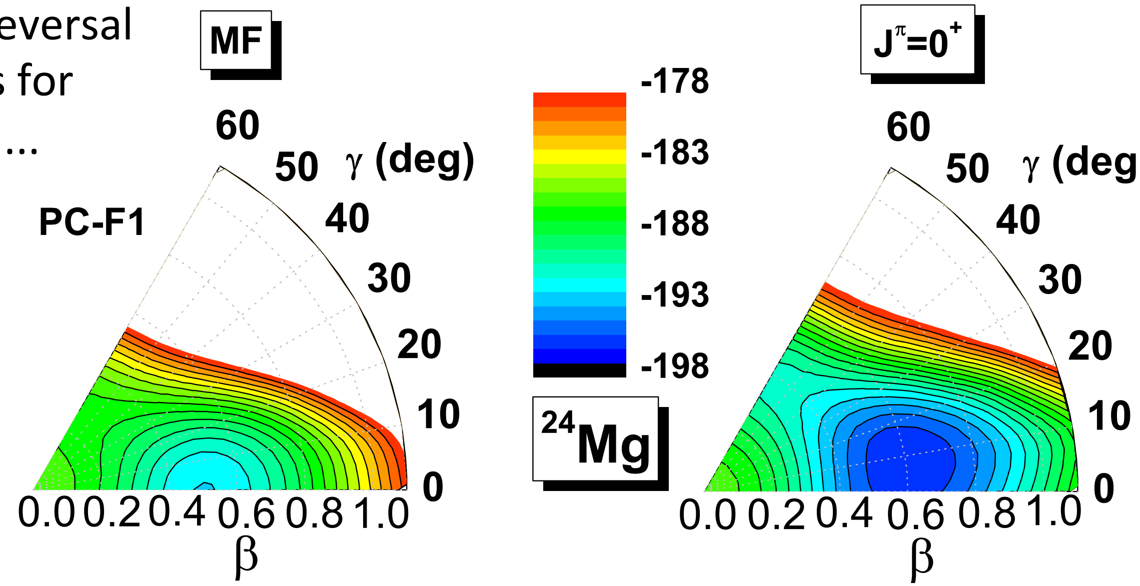
Men-field energy curve of ^{154}Sm (dashed), and the corresponding angular-momentum projected (J = 0+; 2+; 4+ , and 6+) energy curves, as functions of the axial deformation β.



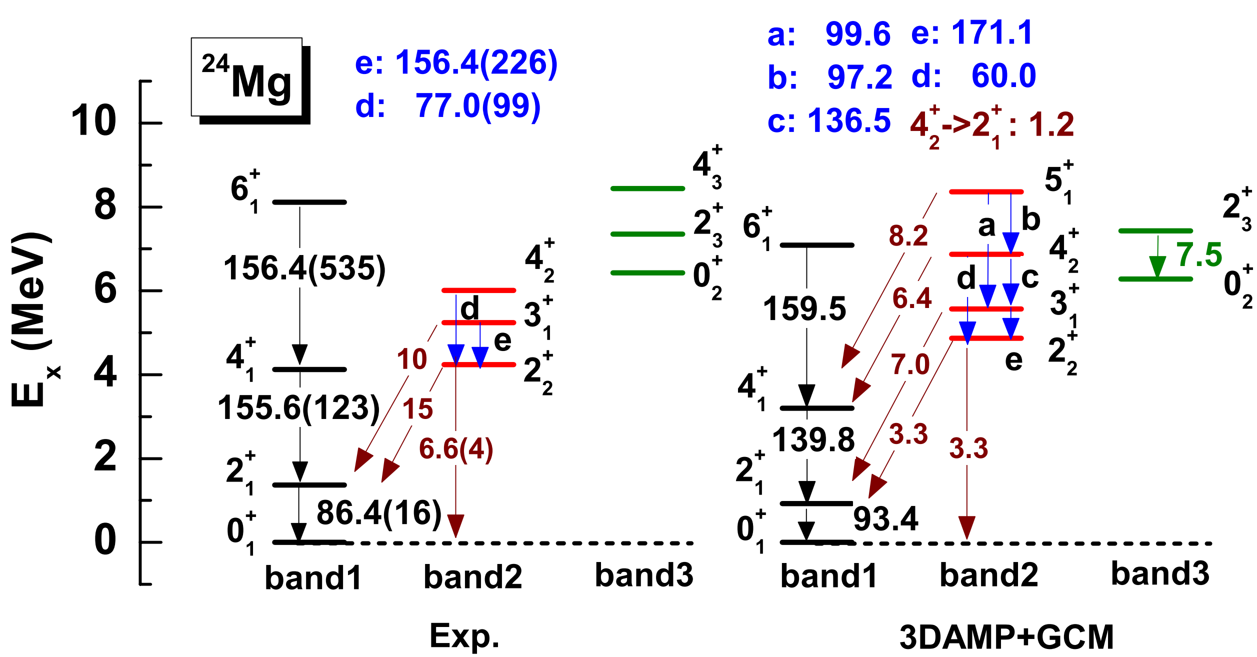
Angular-momentum projected GCM results for the excitation energies and B(E2) values (in Weisskopf units) of the lowest two bands in ^{154}Sm, in comparison to data.

→ larger variational space for projected GCM calculations!

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



3D AMP+GCM model



Collective Hamiltonian in five dimensions

S.G. Rohozinski, Phys. Scr. (2013)

→ quadrupole tensor: $\boldsymbol{\alpha} = \boldsymbol{\alpha}(d, \omega)$

Deformations: $d = (d_0, d_2)$ Euler angles: $\omega = (\omega_1, \omega_2, \omega_3)$

The volume element in the space of quadrupole coordinates:

$$\mathrm{d}\Omega(\boldsymbol{\alpha}) = \Pi_k \, \mathrm{d}a_k = \mathrm{d}\Omega(d)\, \mathrm{d}\Omega(\omega)$$

The GCM trial state:

$$|\Psi[\varphi]\rangle = \int \varphi(\boldsymbol{\alpha}) |\Phi(\boldsymbol{\alpha})\rangle \, \mathrm{d}\Omega(\boldsymbol{\alpha})$$

$$\Rightarrow \quad \int [\mathcal{H}(\boldsymbol{\alpha}, \boldsymbol{\alpha}') - E\mathcal{I}(\boldsymbol{\alpha}, \boldsymbol{\alpha}')]\varphi(\boldsymbol{\alpha}')\, \mathrm{d}\Omega(\boldsymbol{\alpha}') = 0.$$

The Gaussian overlap approximation

$$\boldsymbol{\beta} = \frac{1}{2}(\boldsymbol{\alpha} + \boldsymbol{\alpha}') \qquad \gamma_\mu = \alpha_\mu - \alpha'_\mu$$

→ approximate the overlap kernel by a Gaussian function:

$$\mathcal{I}(\boldsymbol{\beta} + \tfrac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \tfrac{1}{2}\boldsymbol{\gamma}) \approx \exp\left(-\tfrac{1}{2} g^{\mu\nu}(\boldsymbol{\beta})\gamma_\mu\gamma_\nu\right),$$

→ notation: $\alpha^\mu = \alpha^*_\mu = (-1)^\mu \alpha_{-\mu}$ $\qquad$ $\boldsymbol{\alpha} \cdot \boldsymbol{\beta} = \sum_\mu (-1)^\mu \alpha_\mu \beta_{-\mu}$

⇒ real, symmetric and positive definite matrix: $g^{\mu\nu}(\boldsymbol{\beta}) = -\dfrac{\partial^2 \mathcal{I}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial\gamma_\mu \partial\gamma_\nu}$

→ approximation for the energy kernel:

$$\begin{aligned}&\mathcal{H}(\boldsymbol{\beta} + \tfrac{1}{2}\boldsymbol{\gamma}, \boldsymbol{\beta} - \tfrac{1}{2}\boldsymbol{\gamma}) \\ &\qquad = \exp\left(-\tfrac{1}{2} g^{\mu\nu}(\boldsymbol{\beta})\, \gamma_\mu\gamma_\nu\right) \left[v(\boldsymbol{\beta}) - \tfrac{1}{2} h^{\mu\nu}(\boldsymbol{\beta})\gamma_\mu\gamma_\nu\right]\end{aligned}$$

$$v(\boldsymbol{\beta}) = \mathcal{H}(\boldsymbol{\beta}, \boldsymbol{\beta}),$$

$$h^{\mu\nu}(\boldsymbol{\beta}) = -\frac{\partial^2 \mathcal{H}(\boldsymbol{\beta}, \boldsymbol{\beta})}{\partial \gamma_\mu \partial \gamma_\nu} - g^{\mu\nu}(\boldsymbol{\beta}) v(\boldsymbol{\beta})$$

The square root kernel is defined:

$$\mathcal{R}(\boldsymbol{\alpha}, \boldsymbol{\xi}) = \left(\frac{2}{\pi}\right)^{5/4} \exp\left(-g^{\mu\nu}\left(\tfrac{1}{2}(\boldsymbol{\xi} + \boldsymbol{\alpha})\right)(\xi_\mu - \alpha_\mu)(\xi_\nu - \alpha_\nu)\right)$$

⇒ the integral Hill-Wheeler equation in the GOA reduces to an orthogonal eigenvalue equation for the collective wave function:

$$\psi(\boldsymbol{\alpha}) = \int \mathcal{R}(\boldsymbol{\alpha}, \boldsymbol{\alpha}')\varphi(\boldsymbol{\alpha}')\, \mathrm{d}\Omega(\boldsymbol{\alpha}')$$

⇒ the Bohr differential eigenvalue equation:

$$H(\boldsymbol{\xi})\psi(\boldsymbol{\xi}) = E\psi(\boldsymbol{\xi})$$

$$H = -\frac{1}{2\sqrt{g(\boldsymbol{\xi})}} \frac{\partial}{\partial \xi_\mu} \sqrt{g(\boldsymbol{\xi})} A_{\mu\nu}(\boldsymbol{\xi}) \frac{\partial}{\partial \xi_\nu} + V(\boldsymbol{\xi})$$

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

$$\hat{H} = \hat{T}_{\rm vib} + \hat{T}_{\rm rot} + V_{\rm coll}$$

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

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

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

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.

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

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

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

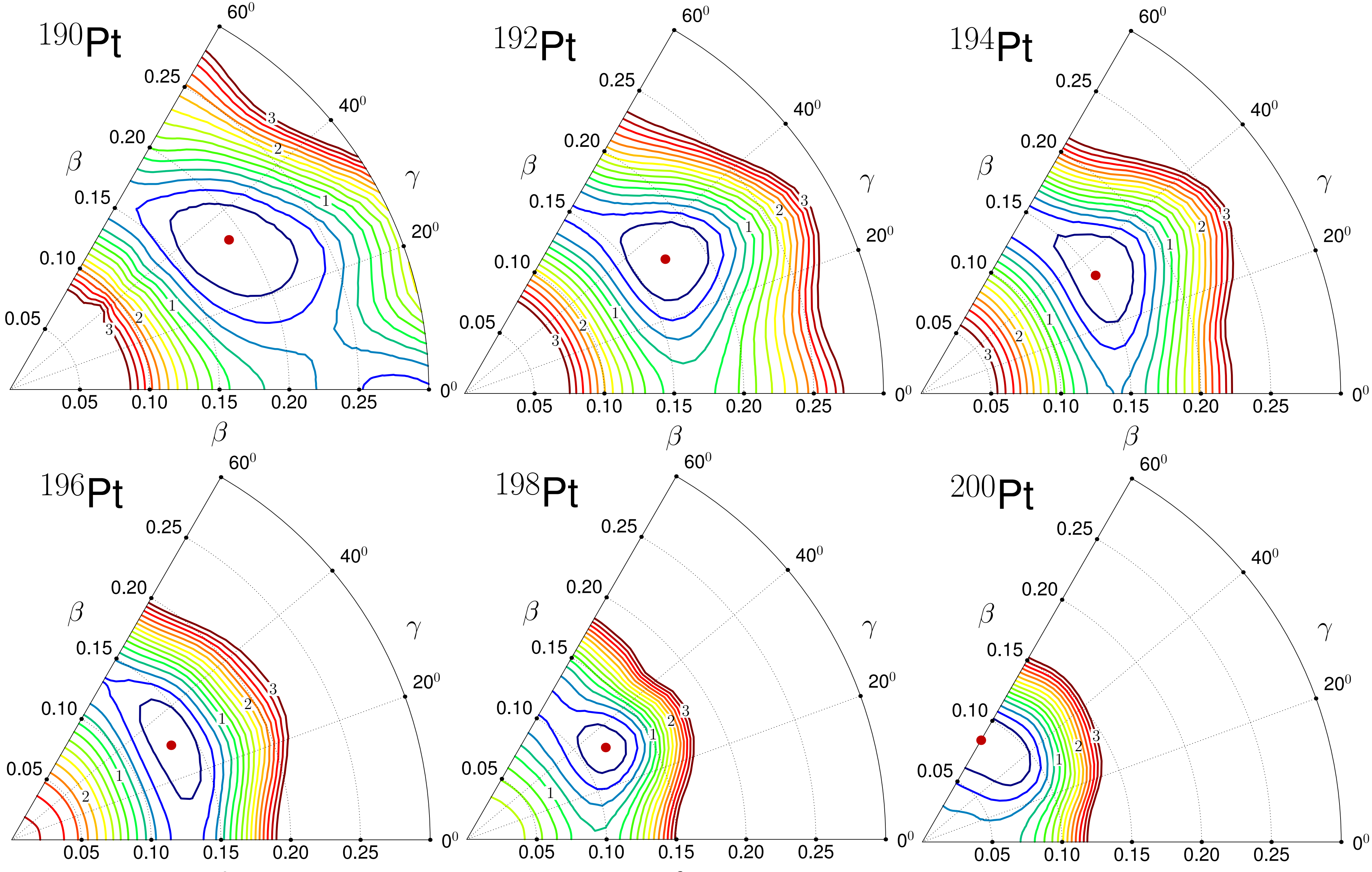
$$\mathcal{I}_k = \sum_{i,j} \frac{(u_i v_j - v_i u_j)^2}{E_i + E_j} |\langle i|\hat{J}_k|j\rangle|^2 \quad k = 1,2,3,$$

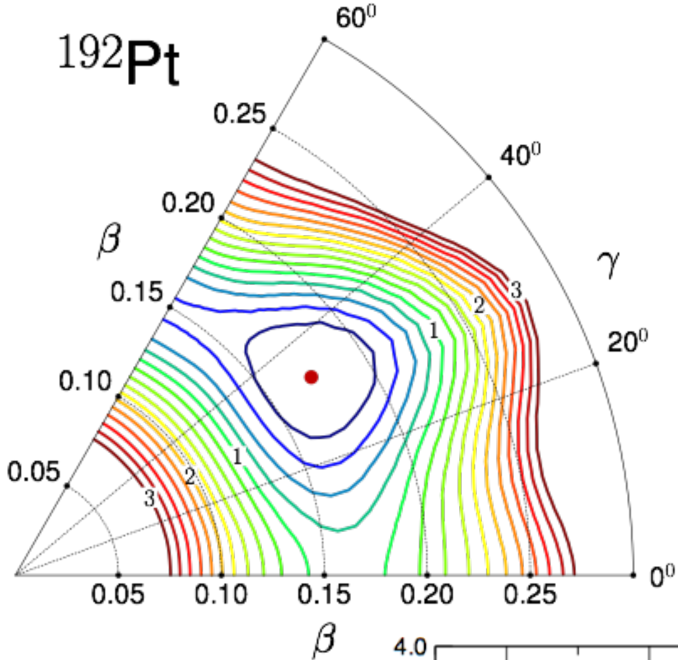
The mass parameters are calculated in the cranking approximation:

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

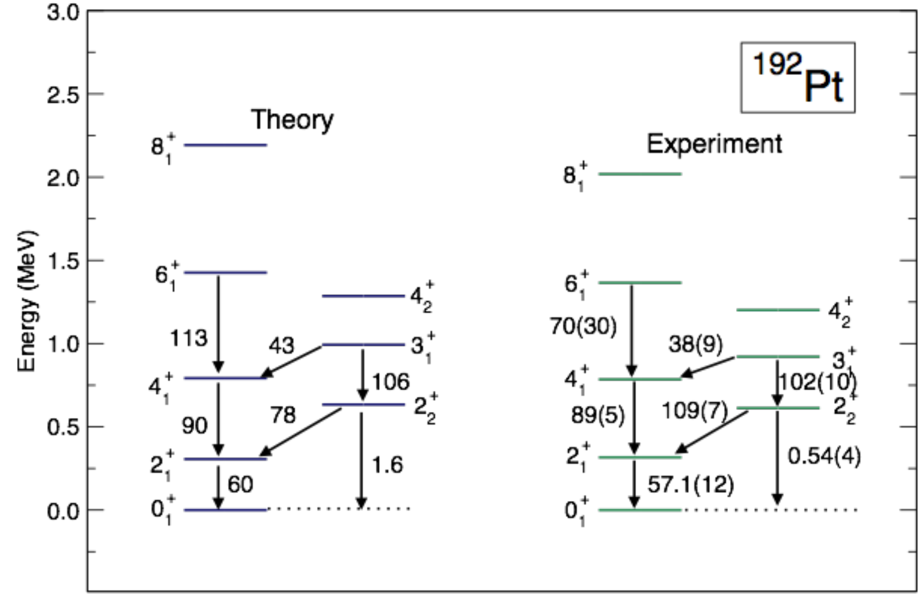
$$\mathcal{M}_{(n),\mu\nu}(q_0,q_2) = \sum_{i,j} \frac{\langle i|\,\hat{Q}_{2\mu}\,|j\rangle\,\langle j|\,\hat{Q}_{2\nu}\,|i\rangle}{(E_i+E_j)^n}(u_i v_j + v_i u_j)^2$$

Evolution of triaxial shapes in Pt nuclei:

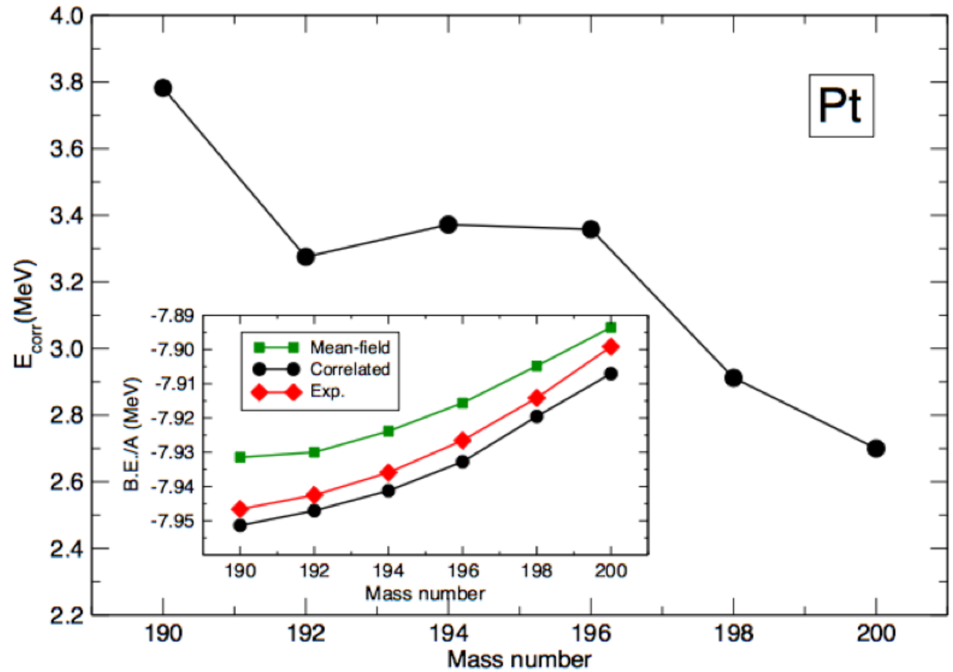




192Pt
β
γ
60⁰
40⁰
20⁰
0⁰
0.25
0.20
0.15
0.10
0.05
1
2
3
0.05 0.10 0.15 0.20 0.25
β

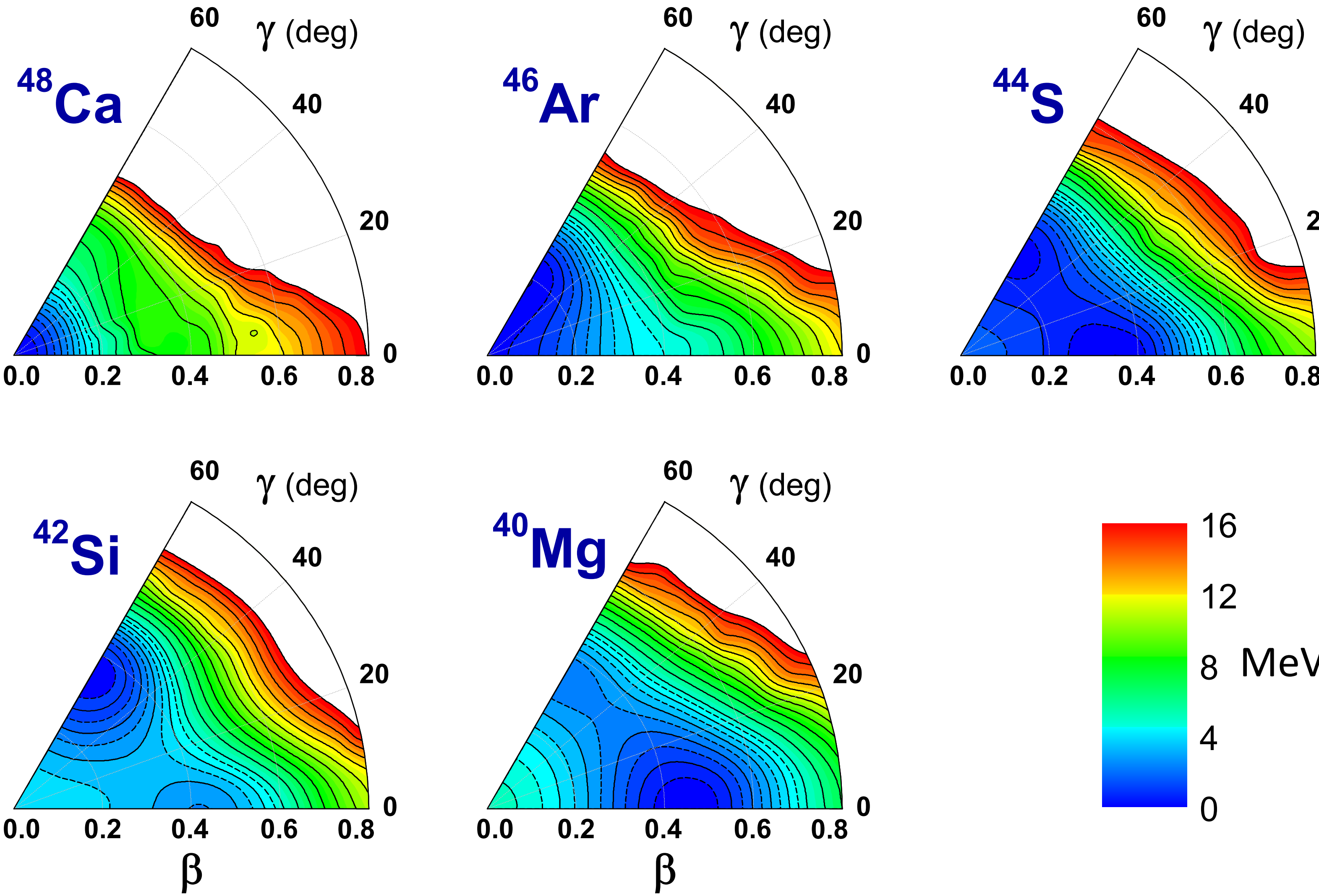


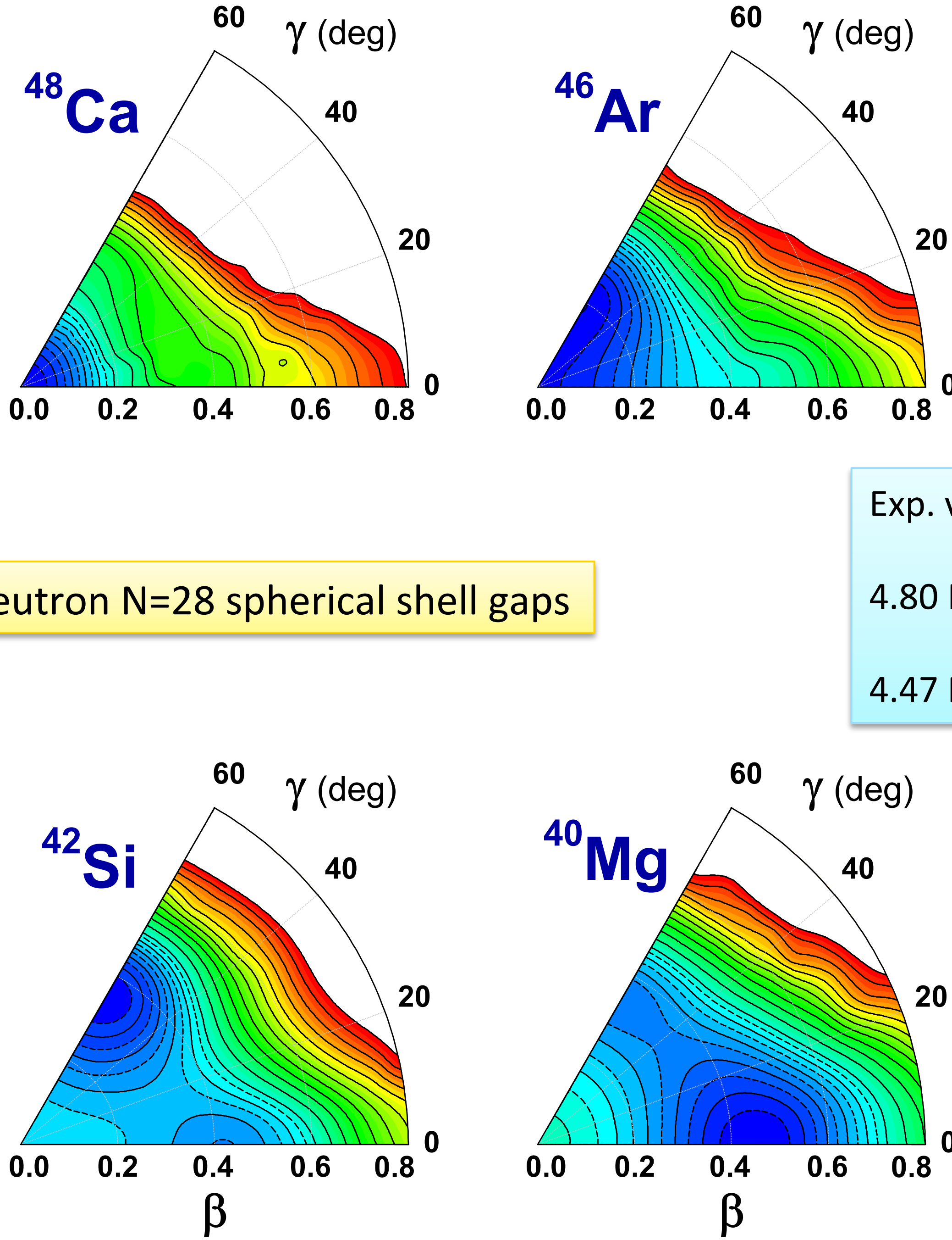
192Pt
Theory
Experiment
Energy (MeV)
3.0
2.5
2.0
1.5
1.0
0.5
0.0
8_1^+
6_1^+
4_1^+
2_1^+
0_1^+
4_2^+
3_1^+
2_2^+
113
43
106
90
78
60
1.6
70(30)
38(9)
102(10)
89(5)
109(7)
57.1(12)
0.54(4)



Pt
E_{corr}(MeV)
Mass number
4.0
3.8
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
190 192 194 196 198 200
Mean-field
Correlated
Exp.
B.E./A (MeV)
-7.89
-7.90
-7.91
-7.92
-7.93
-7.94
-7.95
190 192 194 196 198 200
Mass number

Coexisting shapes in the N=28 isotones

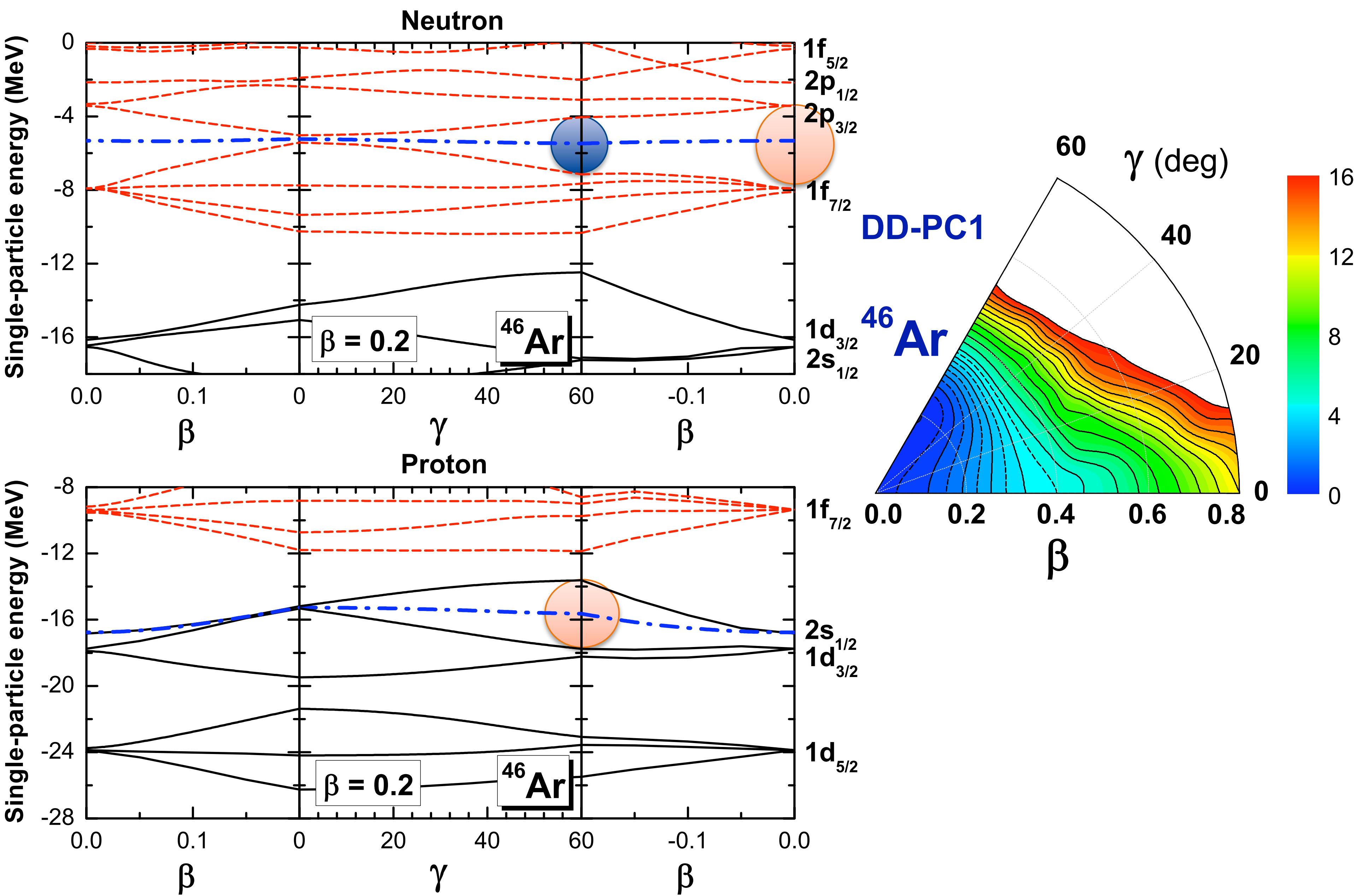




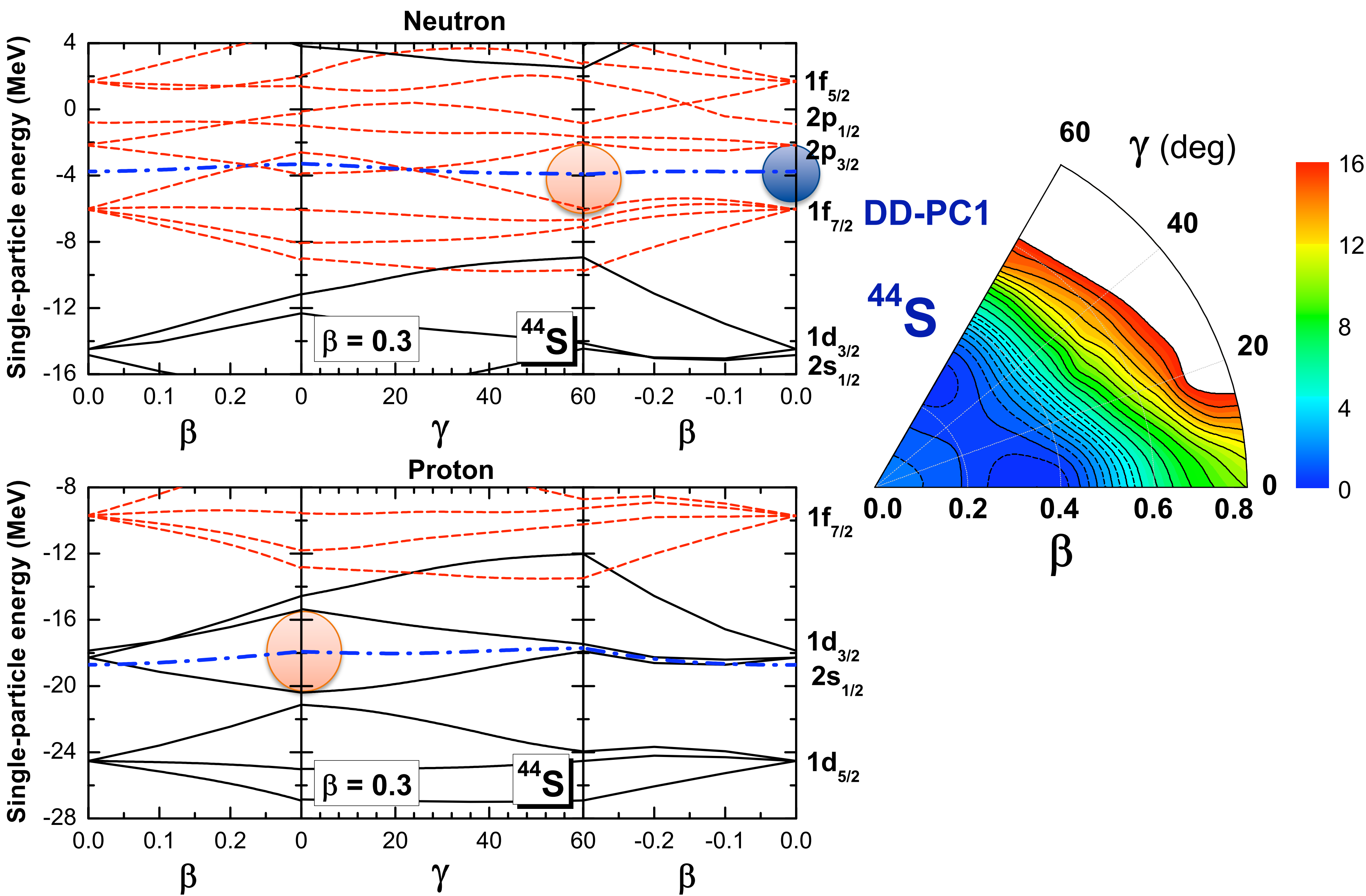
Neutron N=28 spherical shell gaps

	Exp. values	$\Delta^{sph.}_{N=28}$	β_{min}
^{48}Ca	4.80 MeV	4.73	0.00
^{46}Ar	4.47 MeV	4.48	-0.19
^{44}S		3.86	0.34
^{42}Si		3.13	-0.35
^{40}Mg		2.03	0.45

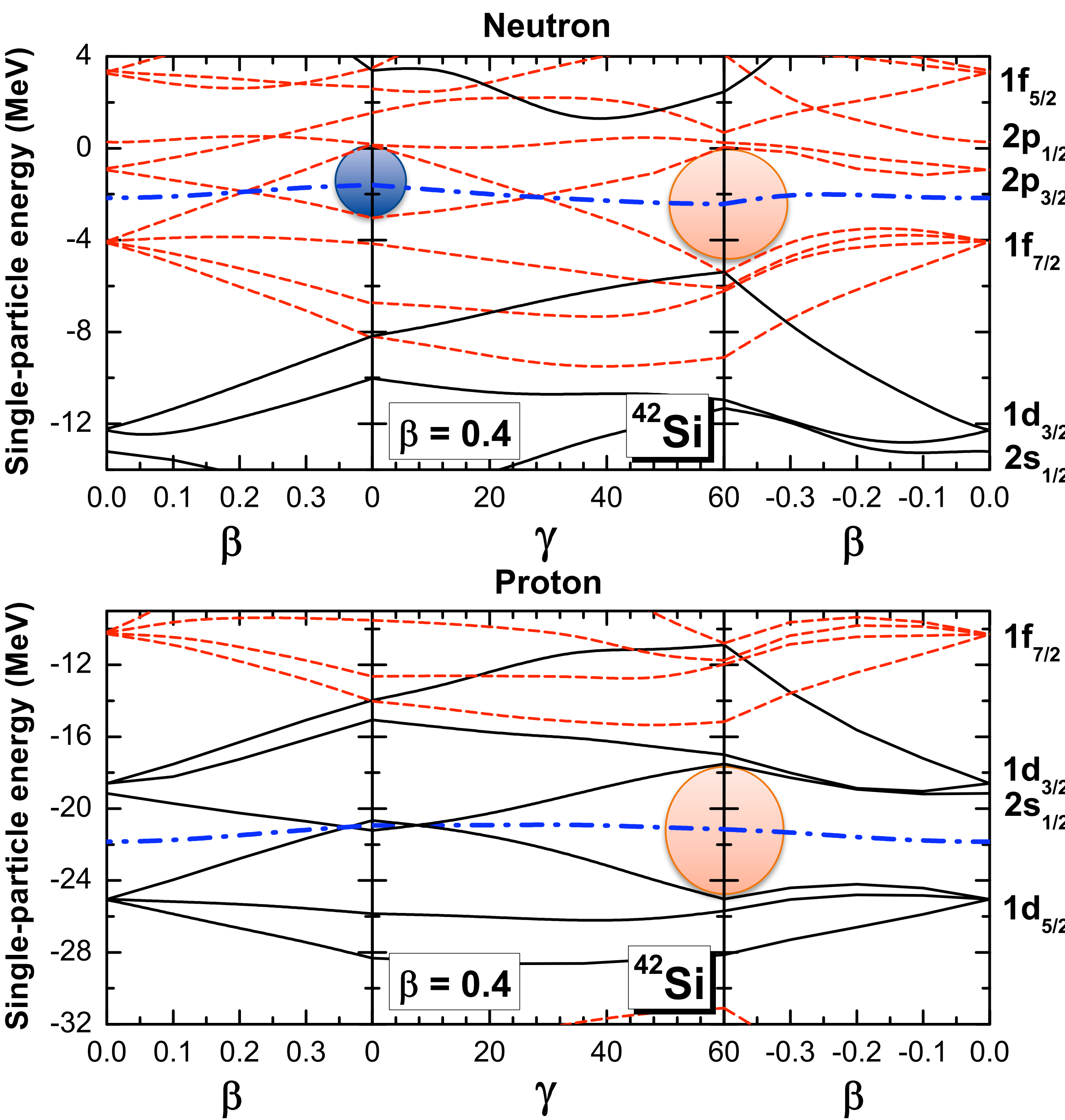
^{46}Ar: single-particle levels

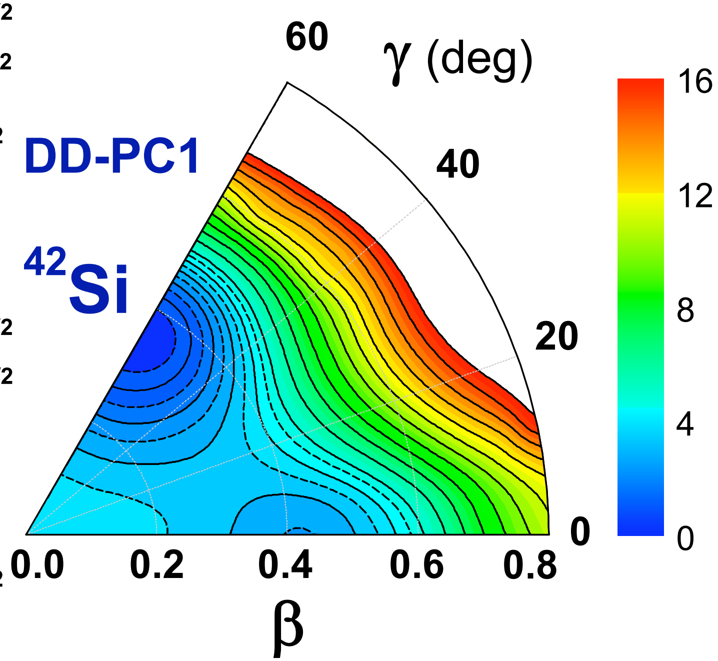


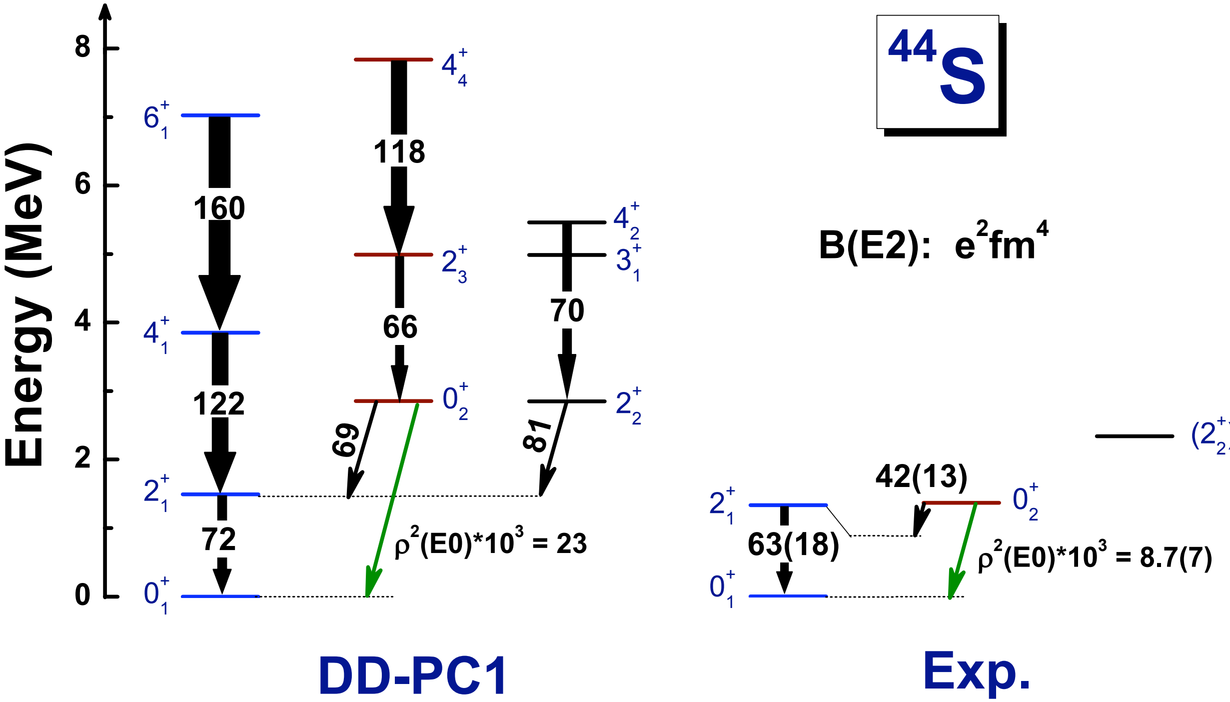
^{44}S: single-particle levels

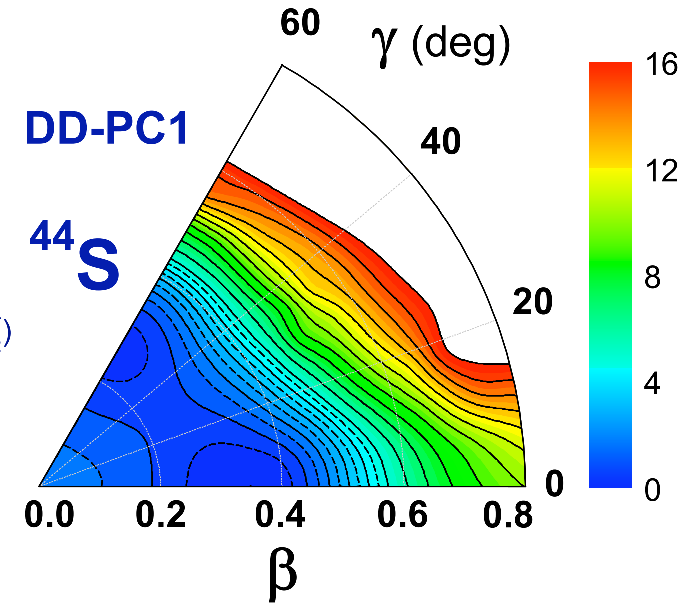


^{42}Si: single-particle levels

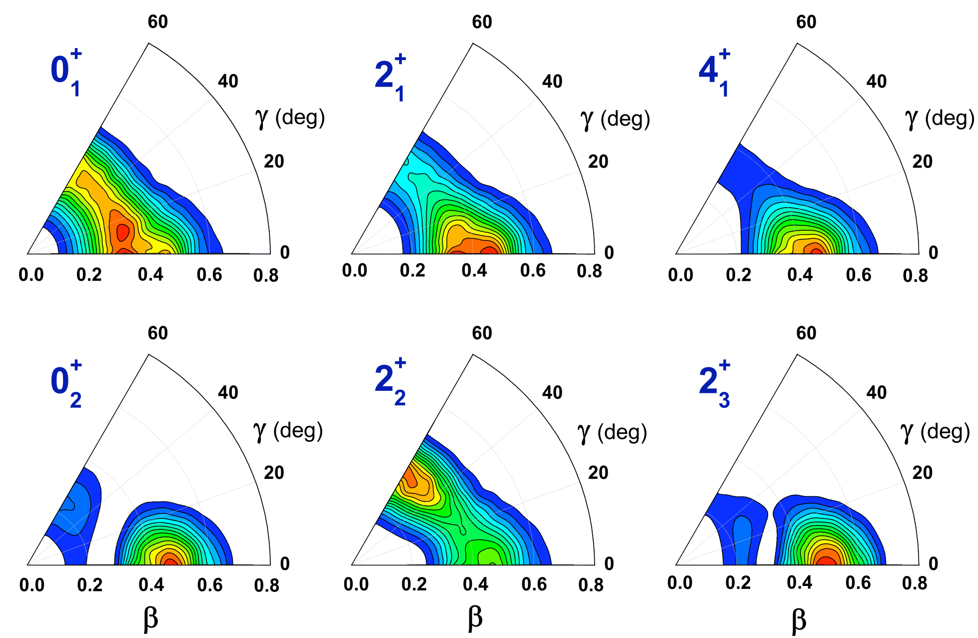








Probability density distributions:



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

Global study of quadrupole correlation effects

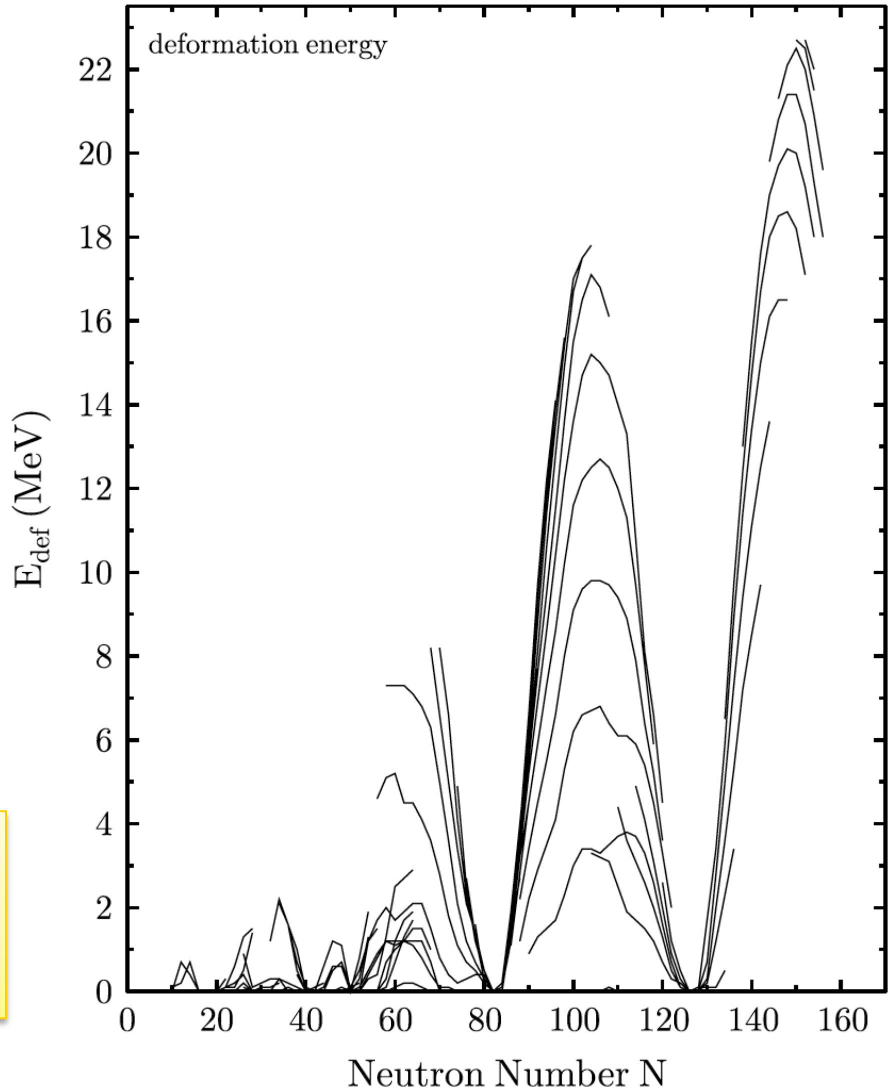
M. Bender, G. F. Bertsch, and P.-H. Heenen

Phys. Rev. C 73, 034322

Definition of correlation energies

1) The ***static deformation energy*** is the energy difference between a mean-field configuration q and the corresponding spherical state:

$$E_{\mathrm{def}}(q) = E(Q_2 = 0) - E(q)$$



Static deformation energy as a function of neutron number N. Isotopic chains are connected by lines.

2) The energy gained by the projection of a deformed mean-field state |q > (on angular momentum I=0) is its ***rotational energy***:

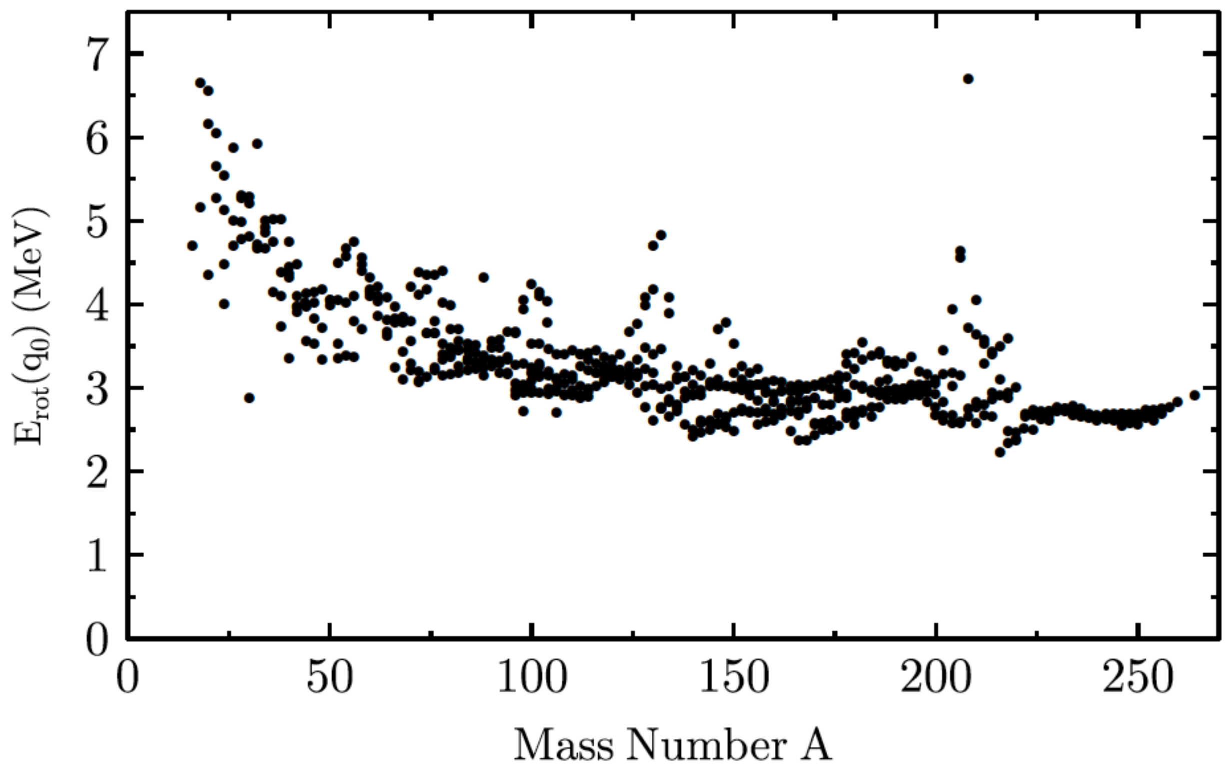
$$E_{\mathrm{rot}}(q) = E(q) - E_0(q)$$

3) The ***rotational energy correction***:

$$E_{I=0} = E(q_{\mathrm{mf}}) - E_0(q_0)$$

mean-field minimun

minimum after projection



Rotational energy $E_{rot}(q_0)$ at the minimum of the J = 0 projected energy curve.

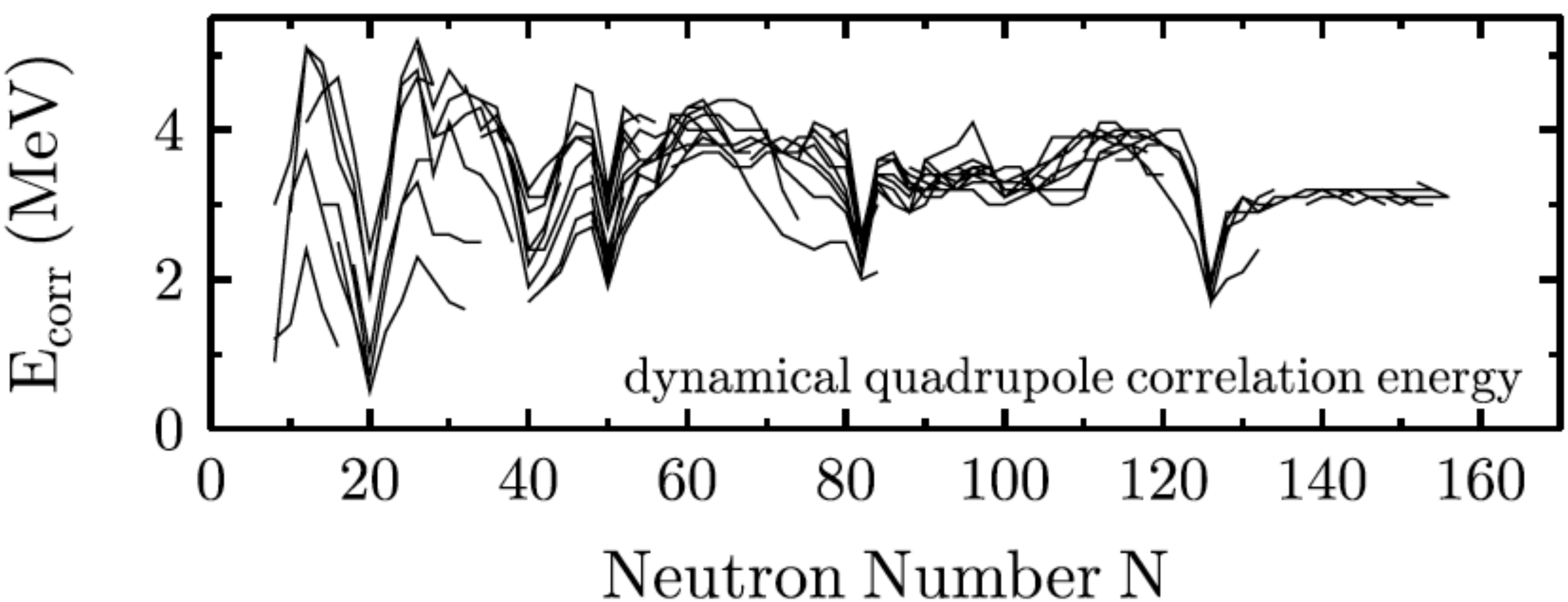
4) The correlation energy gained by configuration mixing:

$$E_{\mathrm{GCM}} = E_0(q_0) - E_{k=0}$$

GCM ground state

The total ***dynamical correlation energy*** is the energy difference between the mean-field ground state and the projected GCM ground state:

$$\begin{aligned} E_{\mathrm{corr}} &= E(q_{\mathrm{mf}}) - E_{k=0} \\ &= E_{I=0} + E_{\mathrm{GCM}} \end{aligned}$$



(i) The quadrupole correlation energy varies between a few 100 keV and about 5.5 MeV.

(ii) Projection on angular momentum J = 0 provides the major part of the energy gain of up to about 4 MeV; all nuclei gain energy by deformation.

(iii) the mixing of projected states with different intrinsic axial deformation adds a few 100 keV up to 1.5 MeV to the correlation energy.

(iv) Typically nuclei below mass A ≤ 60 have a larger correlation energy than static deformation energy, whereas the heavier deformed nuclei have larger static deformation energy than correlation energy.