

# Beyond the Static Mean-Field Approach

**Symmetry Restoration and  
Configuration Mixing**

# 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!  
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.**

# Restoration of Broken Symmetries

A self-consistent mean-field (SCMF) wave function breaks necessarily several symmetries of the nuclear Hamiltonian (translational, rotational).

**EXAMPLE:** the only translational invariant product wave functions are products of plane waves, but they cannot be used to describe strong correlations between nucleons and their clustering into a finite nucleus.

## A. Symmetry of a Hamiltonian and Broken Symmetry

→ symmetry of the hamiltonian of the system:

$$UHU^+ = H \quad [H, U] = 0$$

-unitary transformation: preserves the norm of state vectors and the matrix elements of observables.

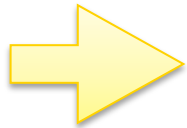
-symmetry group of H: the eigenvectors of H are classified according to the irreducible representation of the symmetry group.

State of broken symmetry (deformed state): cannot be classified according to an irreducible representation of the symmetry group of the Hamiltonian  $H$ .

$$U(\alpha)$$

→ set of unitary operators (representing the symmetry group of the Hamiltonian).  
The parameter  $\alpha$  can be discrete or continuous.

$$|\Phi\alpha\rangle = U(\alpha)|\Phi\rangle$$



$$\begin{aligned}\langle\Phi\alpha|H|\Phi\alpha\rangle &= \langle\Phi|U^\dagger(\alpha)HU(\alpha)|\Phi\rangle \\ &= \langle\Phi|H|\Phi\rangle \quad \forall\alpha\end{aligned}$$

⇒ all deformed states  $|\Phi\alpha\rangle$  are DEGENERATE.

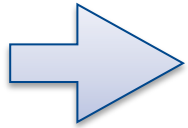
## B. Symmetries of the Hartree-Fock field

$|\Phi\rangle \rightarrow$  independent-particle state with the associated single-particle density  $\rho$

$$\rho_{ij} = \langle \Phi | a_j^\dagger a_i | \Phi \rangle \equiv \langle \Phi | \rho | \Phi \rangle$$

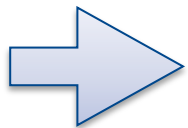
$\rightarrow$  consider a unitary transformation:

$$|\bar{\Phi}\rangle = U|\Phi\rangle$$



$$\bar{\rho}_{ij} \equiv \langle \bar{\Phi} | a_j^\dagger a_i | \bar{\Phi} \rangle$$

$\rightarrow$  with:  $U^\dagger a_j^\dagger U = \sum_k U_{jk}^* a_k^\dagger$   $U^\dagger a_i U = \sum_k U_{ik} a_k$



$$\bar{\rho} = U \rho U^\dagger$$

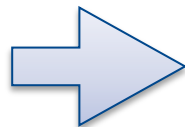
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$\rightarrow$  in the HF approximation:

$$E[\rho] = \langle \Phi | H | \Phi \rangle$$

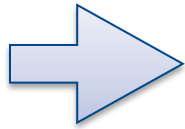
$\rightarrow$  if

$$U H U^\dagger = H$$



$$E[\bar{\rho}] = E[\rho]$$

$$E[\bar{\rho}] = E[\rho]$$



$$h[\bar{\rho}] = U h[\rho] U^+$$

transformation of the Hartree-Fock hamiltonian

1) the density matrix  $\rho$  is invariant under the transformation  $U$ :

$$\bar{\rho} = \rho \quad \Longrightarrow \quad h[\bar{\rho}] = h[\rho]$$

$U$  represents a ***self-consistent symmetry*** of the HF hamiltonian.

$$2) \quad \bar{\rho} \neq \rho \quad [h[\rho], U] \neq 0$$

$U$  represents a ***broken symmetry*** of the HF hamiltonian.

***Example:*** translational symmetry is always broken by the HF potential of a bound finite system.

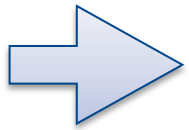
## C. Symmetries in the presence of pairing fields

In the Hartree-Fock-Bogoliubov (HFB) approximation the quasiparticle vacuum is characterized by the generalized density matrix:

$$\mathcal{R} = \begin{pmatrix} \rho & \kappa \\ -\kappa^* & \mathbb{1} - \rho^* \end{pmatrix}$$

→ unitary transformation:

$$|\bar{\Phi}\rangle = U|\Phi\rangle$$

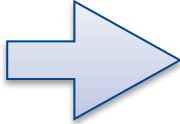


$$\bar{\rho}_{ij} = \langle \bar{\Phi} | a_j^\dagger a_i | \bar{\Phi} \rangle = (U \rho U^\dagger)_{ij}$$

$$\bar{\kappa}_{ij} = \langle \bar{\Phi} | a_j a_i | \bar{\Phi} \rangle = (U \kappa \tilde{U})_{ij}$$

$$\bar{\mathcal{R}} = \mathcal{U} \mathcal{R} \mathcal{U}^\dagger \quad \mathcal{U} = \begin{pmatrix} U & 0 \\ 0 & U^\dagger \end{pmatrix}$$

If  $U$  represents a symmetry of the Hamiltonian  $H \Rightarrow E[\bar{\mathcal{R}}] = E[\mathcal{R}]$

  $\mathcal{H}[\bar{\mathcal{R}}] = U\mathcal{H}[\mathcal{R}]U^+$  transformation of the HFB Hamiltonian

1) self-consistent symmetry of the HFB Hamiltonian

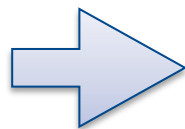
$$[\mathcal{R}, U] = 0 \quad \bar{\mathcal{R}} = \mathcal{R} \quad U\mathcal{H}U^+ = \mathcal{H}$$

2) broken symmetry

$$[\mathcal{R}, U] \neq 0 \quad \bar{\mathcal{R}} \neq \mathcal{R} \quad U\mathcal{H}U^+ \neq \mathcal{H}$$

The pairing field breaks the invariance with respect to the transformation induced by the operator:

$$U = e^{iN\phi} \quad N = \sum_i a_i^+ a_i$$



$$\bar{\mathcal{R}} = U\mathcal{R}U^+ = \begin{pmatrix} \rho & \kappa e^{2i\phi} \\ -\kappa^* e^{-2i\phi} & \mathbb{1} - \rho^* \end{pmatrix}$$

## D. Broken symmetries in finite systems

In *finite systems* broken symmetries arise only as a result of approximations (variational principle applied to a restricted set of trial wave functions).

A broken symmetry implies a degeneracy of the solutions of variational equations.

$$|\Phi\alpha\rangle \equiv U(\alpha)|\Phi\rangle$$

**SYMMETRY RESTORATION** → the new trial wave function is a linear superposition of the degenerate deformed states.

$$|\psi\rangle = \int d\alpha f(\alpha) |\Phi\alpha\rangle$$

The *minimization of the energy* with respect to the expansion coefficients  $f(\alpha)$  is equivalent to the *projection* of states of good symmetry from the deformed state  $|\Phi\rangle$ . The resulting states can be classified according to the *irreps* of the symmetry group.

**EXAMPLE:** *parity* - discrete broken symmetry

$|\Phi\rangle$  a normalized state that is not an eigenstate of the **parity operator**  $\Pi$ .  $[H, \Pi] = 0$  implies that the linearly independent states  $|\Phi\rangle$  and  $\Pi|\Phi\rangle$  are degenerate.

→ new trial function:  $|\psi(\lambda)\rangle = |\Phi\rangle + \lambda\Pi|\Phi\rangle$

→ parameter to be evaluated by minimizing the energy expectation value

$$E(\lambda) = \frac{\langle \Psi(\lambda) | H | \Psi(\lambda) \rangle}{\langle \Psi(\lambda) | \Psi(\lambda) \rangle} = \langle H \rangle \frac{1 + \lambda^2 + 2\lambda \langle H\Pi \rangle / \langle H \rangle}{1 + \lambda^2 + 2\lambda \langle \Pi \rangle}$$

$$\frac{dE(\lambda)}{d\lambda} = 0 \quad \Rightarrow \quad [\langle H\Pi \rangle - \langle H \rangle \langle \Pi \rangle](1 - \lambda^2) = 0$$

If  $|\Phi\rangle$  is not an eigenstate of the parity operator:

$$\langle H\Pi\rangle \neq \langle H\rangle\langle\Pi\rangle \implies \lambda = \pm 1$$

→ parity eigenstates:

$$|\Psi_{\pm}\rangle = \frac{1}{\sqrt{2}}(1 \pm \Pi)|\Phi\rangle \implies \Pi|\Psi_{\pm}\rangle = \pm|\Psi_{\pm}\rangle$$

The same states are obtained by simply acting with the projection operators:

$$P_{\pm} = \frac{1}{\sqrt{2}}(1 \pm \Pi)$$

on the deformed state  $|\Phi\rangle$ . The degeneracy of the deformed states  $|\Phi\rangle$  and  $\Pi|\Phi\rangle$  has been removed:

$$E_+ - E_- = 2 \frac{\langle H\Pi\rangle - \langle H\rangle\langle\Pi\rangle}{1 - \langle\Pi\rangle^2}$$

## E. Non-conservation of particle number

$|\Phi\rangle$  a normalized state, not an eigenstate of the **particle number operator**  $N$ .

$$[H, N] = 0 \quad \Longrightarrow \quad e^{-i\alpha N} |\Phi\rangle \quad \alpha \in [0, 2\pi]$$

**degenerate states!**

→ new trial  
function:

$$|\Psi\rangle = \int_0^{2\pi} \frac{d\alpha}{2\pi} f(\alpha) e^{-i\alpha \hat{N}} |\Phi\rangle \equiv \int_0^{2\pi} \frac{d\alpha}{2\pi} f(\alpha) |\Phi\alpha\rangle$$

def.  $\hat{N} = N - \bar{n}, \quad |\Phi\alpha\rangle \equiv e^{-i\alpha \hat{N}} |\Phi\rangle$

The projection on states with good particle number is equivalent to the requirement that the energy:

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

is stationary with  
respect to variations  
of  $f^*(\alpha)$  and  $f(\alpha)$ .

$$= \frac{\int_0^{2\pi} d\alpha \int_0^{2\pi} d\alpha' f^*(\alpha) \langle \Phi\alpha | H | \Phi\alpha' \rangle f(\alpha')}{\int_0^{2\pi} d\alpha \int_0^{2\pi} d\alpha' f^*(\alpha) \langle \Phi\alpha | \Phi\alpha' \rangle f(\alpha')}$$



$$\int_0^{2\pi} \frac{d\alpha'}{2\pi} \langle \Phi | e^{i\hat{N}(\alpha - \alpha')} (H - E) | \Phi \rangle f(\alpha') = 0$$

**Hill-Wheeler equation**

the solutions are eigenstates of the particle number operator!

Fourier transform:

$$f(\alpha) = \sum_{n=0}^{\infty} f_n e^{i(n-\bar{n})\alpha} \quad \Rightarrow \quad f_n = \int_0^{2\pi} \frac{d\alpha}{2\pi} e^{-i(n-\bar{n})\alpha} f(\alpha)$$



HW equation:

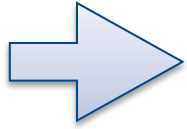
$$\sum_{n=0}^{\infty} f_n \langle \Phi | (H - E) P_n | \Phi \rangle e^{i(n-\bar{n})\alpha} = 0$$

where:

$$P_n \equiv \int_0^{2\pi} \frac{d\alpha}{2\pi} e^{-i(N-n)\alpha}$$

→ operator projecting onto states with particle number n.

The Hill-Wheeler equation is valid for all angles  $\alpha$ :



$$f_n \langle \Phi | (H - E) P_n | \Phi \rangle = 0$$

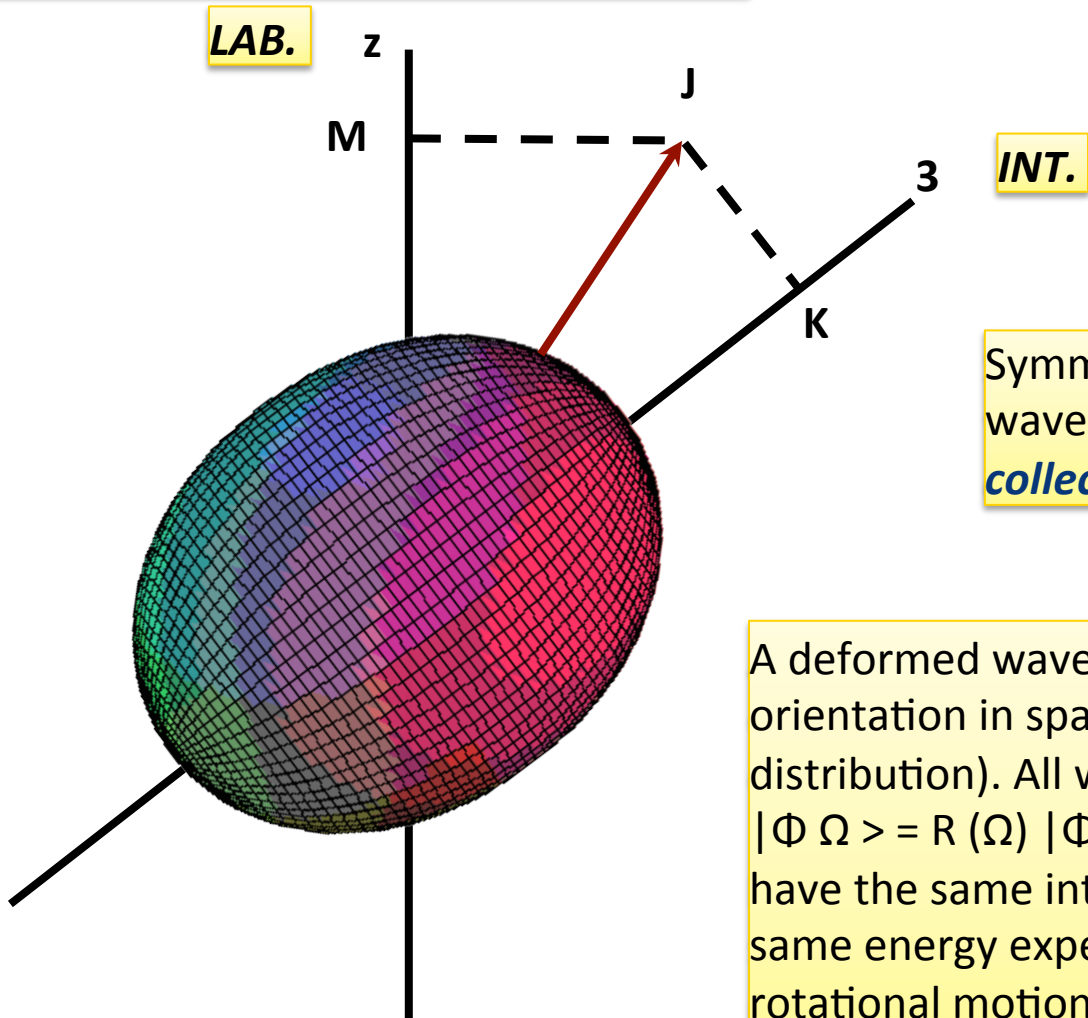
nonvanishing coefficients exist only if the energy  $E$  equals:

$$E_n = \frac{\langle \Phi | H P_n | \Phi \rangle}{\langle \Phi | P_n | \Psi \rangle}$$

The solution of the HW equation is the projected state:

$$|\Psi\rangle = f_n |\Psi_n\rangle, \quad |\Psi_n\rangle \equiv P_n |\Phi\rangle$$

## F. Angular momentum projection



Symmetry violation in many-particle wave functions can be related to **collective motion**.

A deformed wave function  $|\Phi\rangle$  defines a fixed orientation in space (principal axes of the mass distribution). All wave functions:  
 $|\Phi\Omega\rangle = R(\Omega)|\Phi\rangle$   
have the same internal structure and yield the same energy expectation value  $\Rightarrow$  collective rotational motion approximately preserves the intrinsic structure.

## Angular momentum operators in the laboratory and intrinsic frames

INT.  $\hat{e}_a \quad (a = 1, 2, 3) :$   $\hat{e}_a \cdot \hat{e}_b = \delta_{ab}, \quad \hat{e}_a \times \hat{e}_b = \epsilon_{abc} \hat{e}_c$

LAB.  $\hat{u}_i \quad (i = x, y, z) :$   $\hat{e}_a = \tilde{\mathcal{R}}_{ai}(\Omega) \hat{u}_i, \quad \Omega = \{\alpha, \beta, \gamma\}$

Euler angles

The Euler angles are dynamical variables which specify the orientation of the intrinsic frame.

Def. intrinsic angular momentum operators:

$$I_a = \hat{e}_a \cdot \vec{J}$$

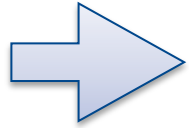
$$[I_a, J_i] = 0 \quad \forall a, i$$

$$[I_a, I_b] = -i\epsilon_{abc} I_c$$

$$\vec{I}^2 = \sum_a I_a^2 = \sum_i J_i^2 = \vec{J}^2$$

$$\vec{I}^2 = \vec{J}^2, I_3, J_z$$

set of commuting operators,  
can be diagonalized simultaneously

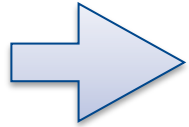


$$\begin{aligned}
\vec{I}^2 |IKM\rangle &= I(I+1) |IKM\rangle \\
I_3 |IKM\rangle &= K |IKM\rangle \quad -I \leq K \leq I \\
J_z |IKM\rangle &= M |IKM\rangle \quad -I \leq M \leq I
\end{aligned}$$

$$\sum_{IKM} |IKM\rangle \langle IKM| = 1, \quad \langle IKM | I'K'M' \rangle = \delta_{II'} \delta_{KK'} \delta_{MM'}$$

The states  $|IKM\rangle$  can be represented by the wave functions  $\langle \Omega | IKM \rangle$ , which depend on the Euler angles  $\Omega = \{\alpha, \beta, \gamma\}$ . With the definition of the state  $|\Omega\rangle$ :

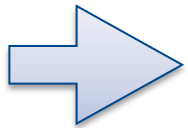
$$|\Omega\rangle = \mathcal{R}(\Omega) |\Omega = 0\rangle$$



$$\begin{aligned}
\langle \Omega | IKM \rangle &= \langle \Omega = 0 | \mathcal{R}^+(\Omega) | IKM \rangle \\
&= \sum_{I'K'M'} \langle \Omega = 0 | I'K'M' \rangle \langle I'K'M' | \mathcal{R}^+(\Omega) | IKM \rangle
\end{aligned}$$

The rotation does not change the intrinsic angular momenta  $\Rightarrow K=K'$  and  $I=I'$ . If the Euler angles are chosen in such a way that the INT and LAB frames coincide for  $\Omega=0$ :

$$\langle \Omega = 0 | I K M \rangle = c_I \delta_{K M} \quad c_I = \sqrt{(2I + 1)/8\pi^2}$$



$$\begin{aligned} \langle \Omega | I K M \rangle &= \sqrt{(2I + 1)/8\pi^2} D_{MK}^I(\Omega) \\ &= \sqrt{(2I + 1)/8\pi^2} e^{i\alpha M} d_{MK}^I(\beta) e^{i\gamma K} \end{aligned}$$

$$\begin{aligned} \langle I K M | I' K' M' \rangle &= \frac{2I + 1}{8\pi^2} \int d\Omega D_{M'K'}^{I'}(\Omega) D_{MK}^{I*}(\Omega) \\ &= \delta_{II'} \delta_{KK'} \delta_{MM'} \end{aligned}$$

## Variational principle and angular momentum projection

Deformed state  $|\Phi\rangle$ , not an eigenstate of  $\vec{J}^2, J_3$

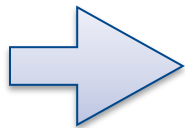
$$\mathcal{R}(\alpha, \beta, \gamma) = e^{-i\alpha J_z} e^{-i\beta J_y} e^{-i\gamma J_z}$$

$$[H, \mathcal{R}] = 0 \quad \Longrightarrow \quad |\Phi\Omega\rangle = \mathcal{R}(\Omega)|\Phi\rangle \text{ degenerate states}$$

$$\rightarrow \text{new trial function: } |\Psi\rangle = \int d\Omega f(\Omega) |\Phi\Omega\rangle \equiv \int d\Omega f(\Omega) \mathcal{R}(\Omega) |\Phi\rangle$$

The weight function  $f(\Omega)$  is determined by requiring that the energy expectation:

$$E = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \quad \text{is stationary with respect to variations of } f^* \text{ and } f.$$



Hill-Wheeler  
equation

$$\int d\Omega' \langle \Phi\Omega | H - E | \Phi\Omega' \rangle f(\Omega') = 0$$

The solutions of the HW equation are eigenstates of the operators  $\vec{J}^2, J_3$

$$f(\Omega) = \sum_{IMK} \frac{2I+1}{8\pi^2} f_{MK}^I D_{MK}^I(\Omega) \Rightarrow f_{MK}^I = \int d\Omega f(\Omega) D_{MK}^{I*}(\Omega)$$


$$|\Psi\rangle = \sum_{IMK} f_{MK}^I P_{MK}^I |\Phi\rangle$$

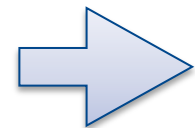
where:

$$P_{MK}^I = \frac{2I+1}{8\pi^2} \int d\Omega D_{MK}^I(\Omega) \mathcal{R}(\Omega)$$

$$(P_{MK}^I)^+ = P_{KM}^I \quad (P_{MK}^I)^+ P_{M'K'}^{I'} = \delta_{II'} \delta_{MM'} P_{KK'}^I$$

not quite a projector!

with:  $[H, P_{MK}^I] = 0$



HW equation:

$$\sum_{K'} \langle \Phi | (H - E) P_{KK'}^I | \Phi \rangle f_{MK'}^I = 0$$

⇒ eigenvalues determined by the equation:

$$\det [\langle \Phi | (H - E) P_{KK'}^I | \Phi \rangle] = 0$$

- a) the HW equation is equivalent to the diagonalization of the hamiltonian in the basis  $P_{MK}^I | \Phi \rangle$   
b) H does not connect states with  $I \neq I'$ , and the eigenvalues do not depend on M

⇒ eigenstates:

$$|\Psi_{IM}\rangle = \sum_K f_{MK}^I P_{MK}^I | \Phi \rangle$$

## G. Projection before and after variation

How do we determine the deformed (symmetry-violating) intrinsic function  $|\Phi\rangle$ ?

### i) Variation before the projection (VBP)

$|\Phi\rangle$  is determined by the variational principle:

$$\delta \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0$$

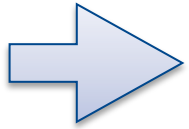
The deformed solution is a superposition of eigenstates of the corresponding symmetry operator (for example, angular momentum). The wave function:

$$|\Psi_I\rangle = P^I |\Phi\rangle$$

is no longer a product wave function, but a complicated superposition of Slater determinants. It contains many more correlations than the function  $|\Phi\rangle$ .

This method violates the variational principle, because we do not vary the projected wave function. It does not allow for changes in the self-consistent mean-field for different values of  $I$  (within a rotational band).

## ii) Variation after projection (VAP)



$$\delta \frac{\langle \Psi_I | H | \Psi_I \rangle}{\langle \Phi_I | \Psi_I \rangle} = \delta \frac{\langle \Phi | P^I H P^I | \Phi \rangle}{\langle \Phi | P^I P^I | \Phi \rangle} = 0$$

⇒ minimize the expectation value of the projected energy  $P^I H P^I$  within the set of product wave functions  $|\Phi\rangle$ .

This method corresponds to a double variation, using the ansatz:

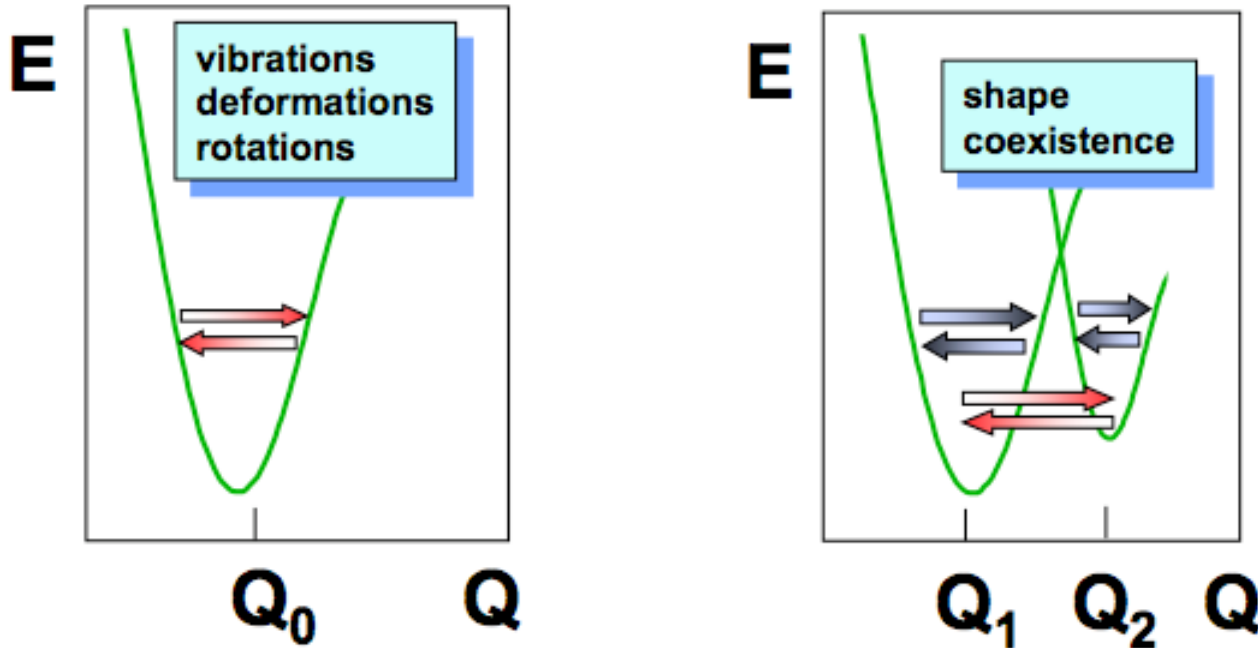
$$|\Psi\rangle = \int d\Omega f(\Omega) \mathcal{R}(\Omega) |\Phi\rangle$$

and varying the energy with respect to both the weight function  $f(\Omega)$  and the generating function  $|\Phi\rangle$ .

**Much more complicated than VBP!**

- (1) must repeat the variation for each value of  $I$
- (2)  $P^I H P^I$  is a multi-particle operator

# Configuration Mixing



The most important correlation effects in nuclear structure stem 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 several 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.

## A. The Generator Coordinate Method

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

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

Diagram illustrating the Generator Coordinate Method (GCM) configuration mixing equation:

- $|\Psi_k\rangle$ : Approximate eigenstate of the Hamiltonian  $H$ .
- $\int dq$ : Integration over the collective coordinate  $q$ .
- $|\Phi(q)\rangle$ : Mean-field states (intrinsic wave functions) that depend on the collective coordinate  $q$ .
- $f_k(q)$ : Weight functions.

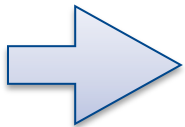
Labels in the diagram:

- Generator coordinate (collective variable) points to  $q$ .
- Intrinsic (e.g. HFB) wave functions points to  $|\Phi(q)\rangle$ .
- Weight functions points to  $f_k(q)$ .

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  $\delta f_k$ .



Hill-Wheeler equation

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

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

Hamiltonian kernel

overlap kernel

→ for any operator  $\hat{O}$ :

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

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.

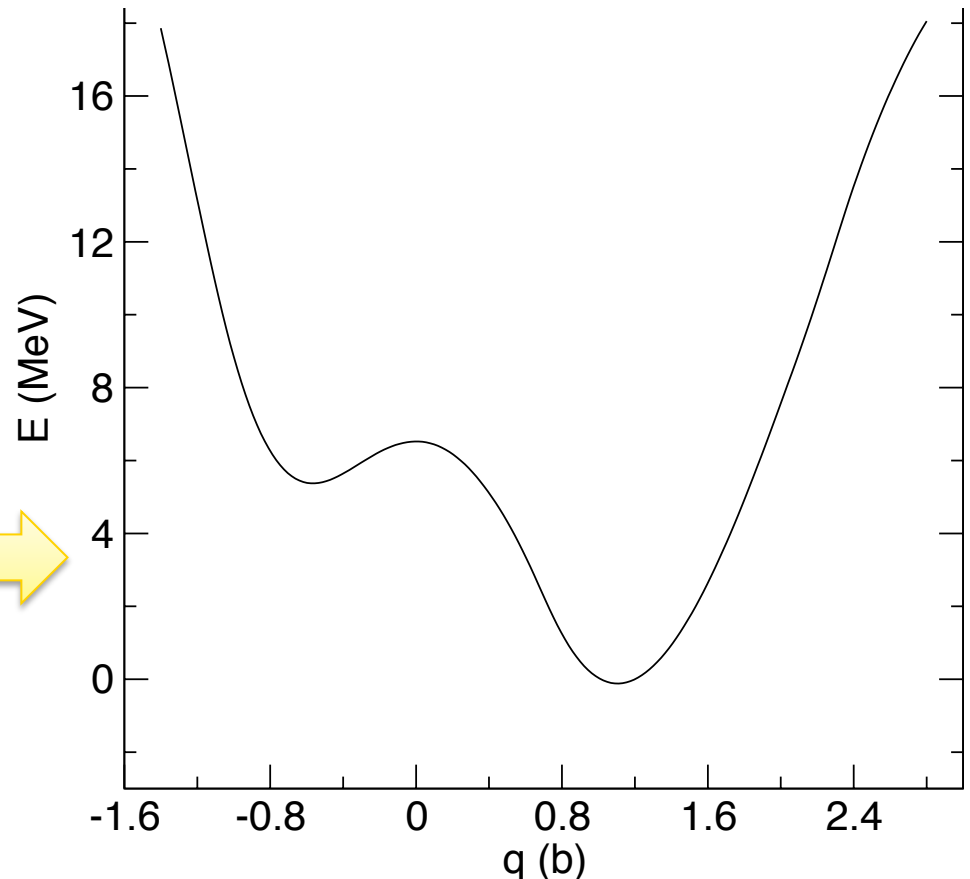
## B. Choice of the collective coordinate

**1. RESTORATION OF BROKEN SYMMETRIES:** the family of wave functions  $|\Phi(q)\rangle$  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.

### **2. SHAPE DEGREES OF FREEDOM:**

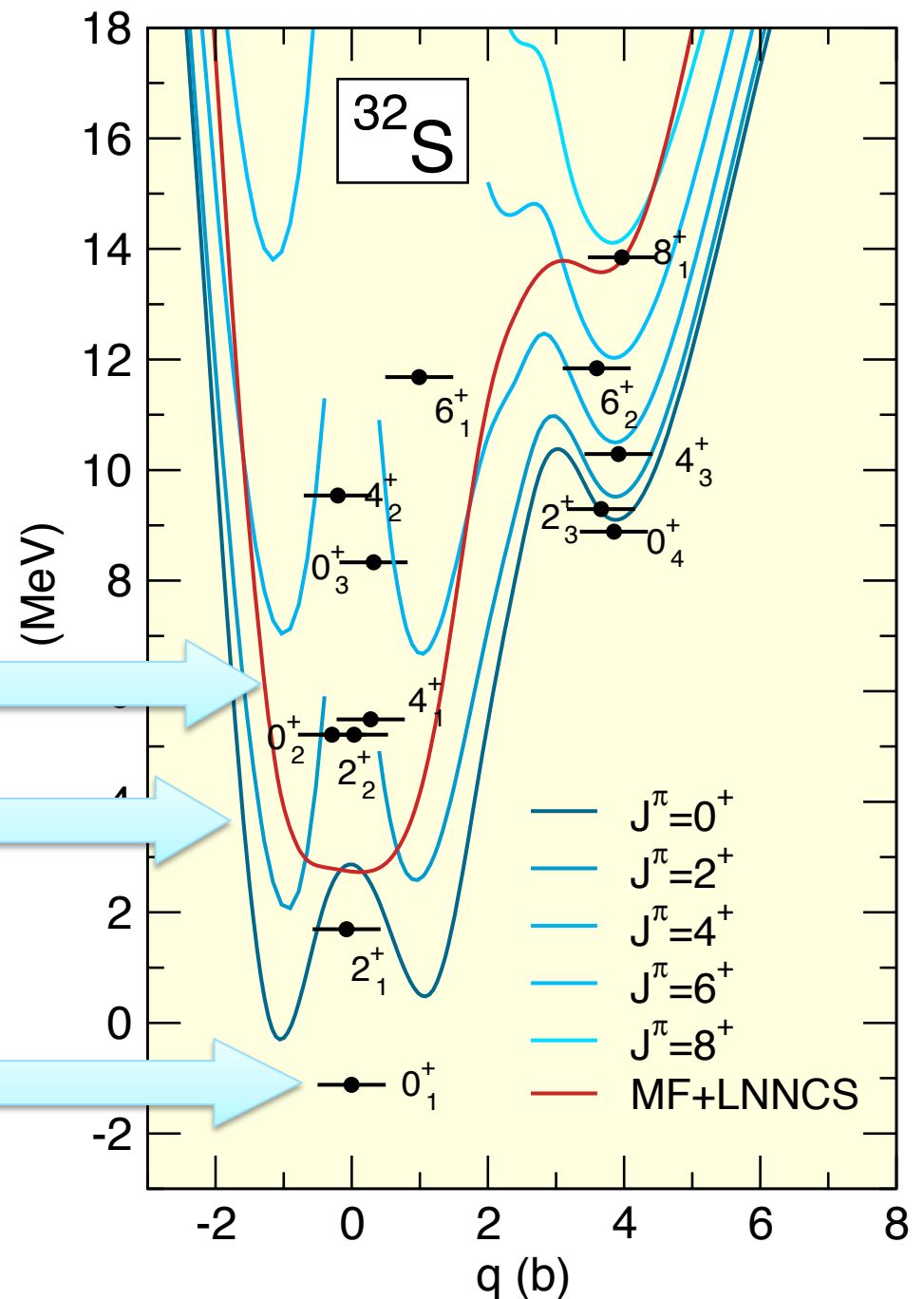
the collective space is generated by constrained mean-field calculations. The generating function is unknown and has to be determined by the diagonalization of the Hill-Wheeler equation.

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

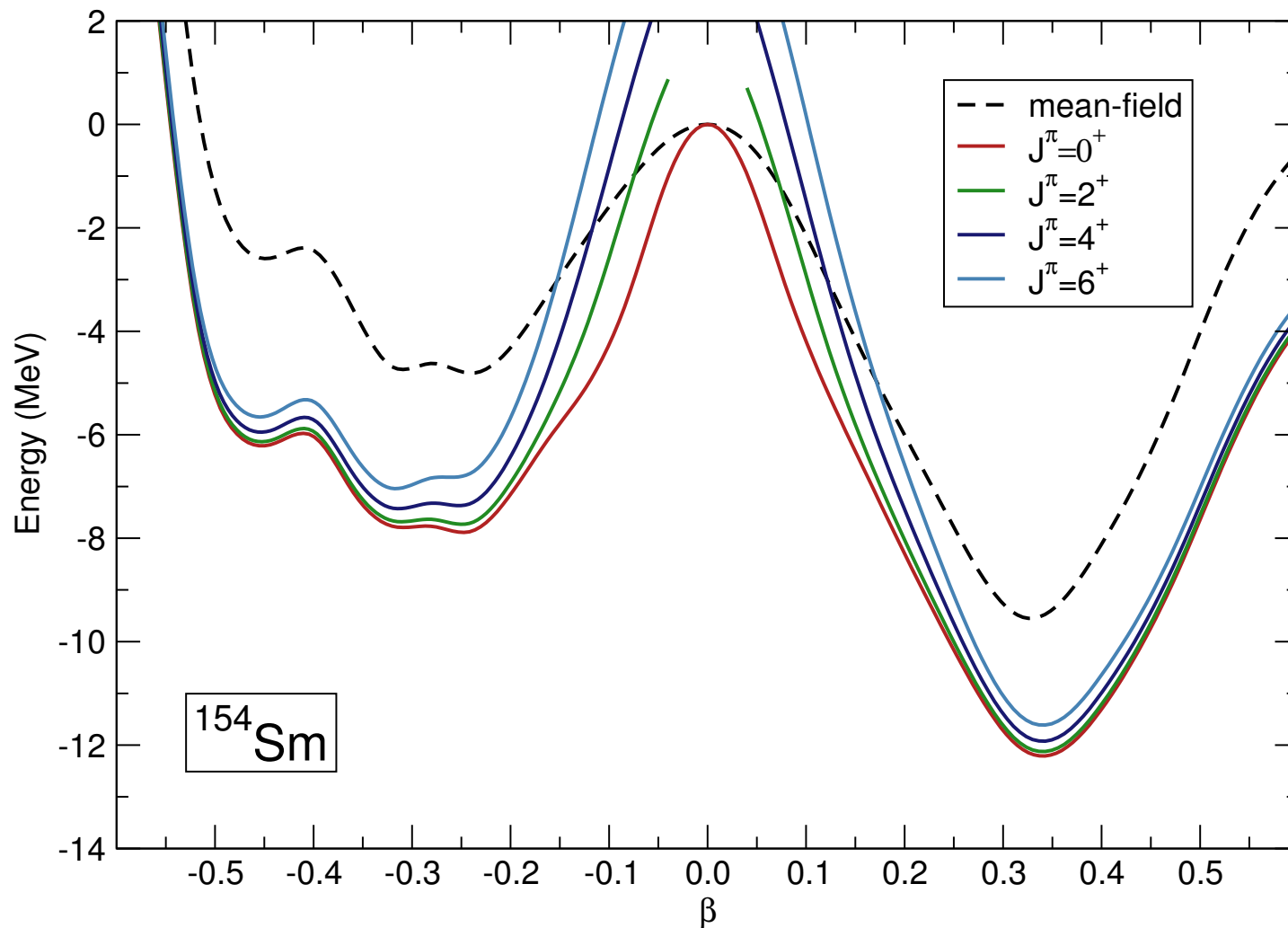


**Example:** Self-consistent mean-field calculation which includes correlations related to restoration of broken symmetries (**rotational, particle number**) and to fluctuations of collective variables (**quadrupole deformation**).

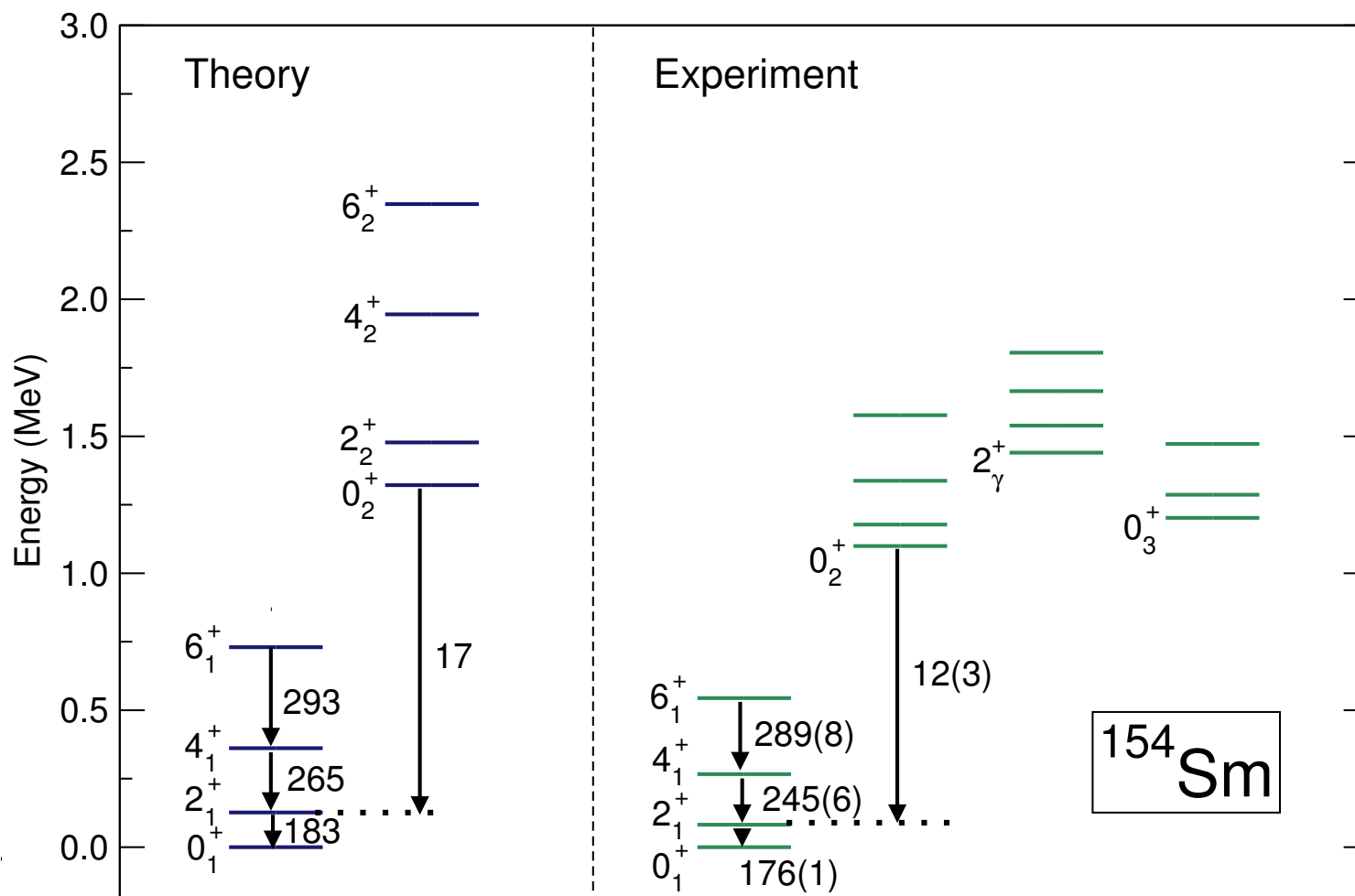
1. Mean-field potential energy curve calculated with a constraint on the quadrupole moment.
2. Angular-momentum and particle-number projected energy curves.
3. The Hamiltonian is diagonalized within each of the collective subspaces of the nonorthogonal bases  $|J, q\rangle$  by using the Generator Coordinate Method.



## C. Angular momentum projection and configuration mixing: $^{154}\text{Sm}$



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

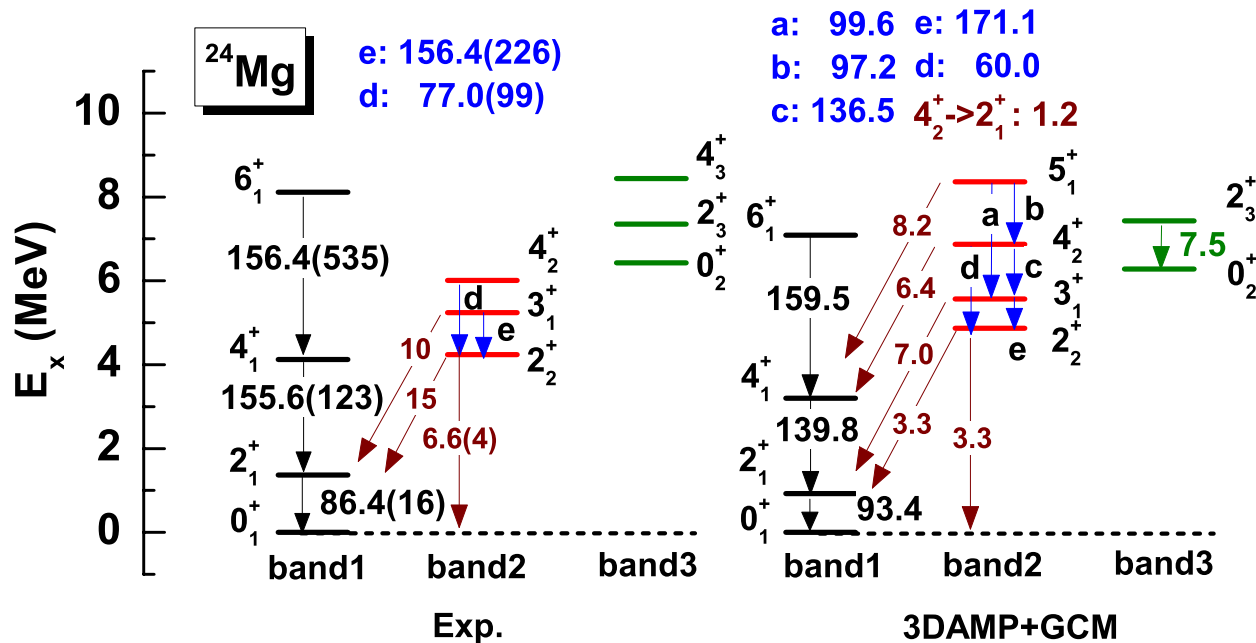
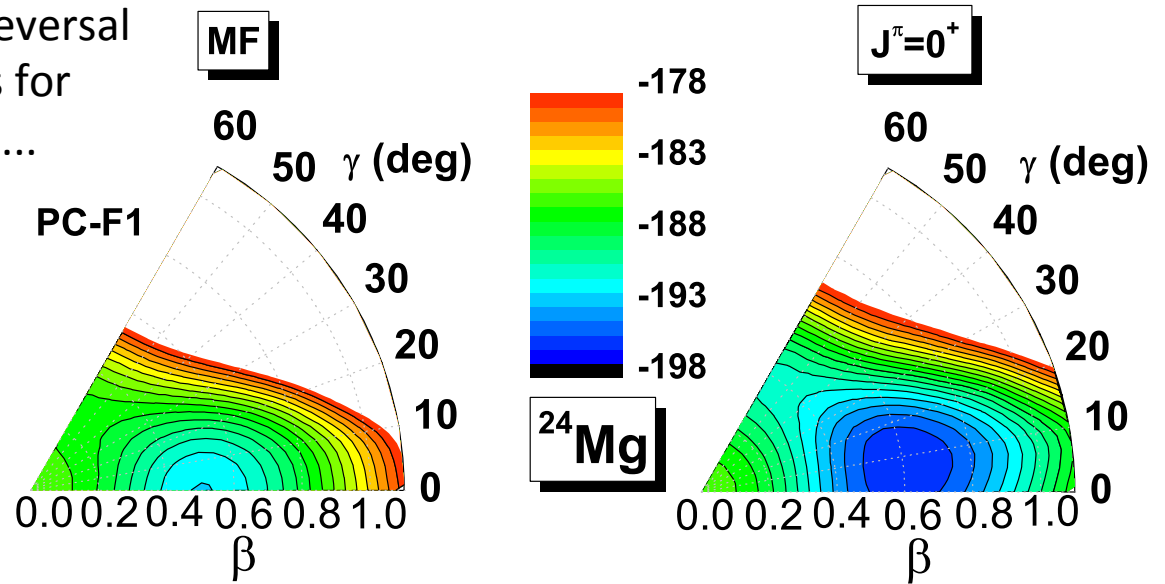


Angular-momentum projected GCM results for the excitation energies and B(E2) values (in Weisskopf units) of the lowest two bands in  $^{154}\text{Sm}$ , in comparison to data.

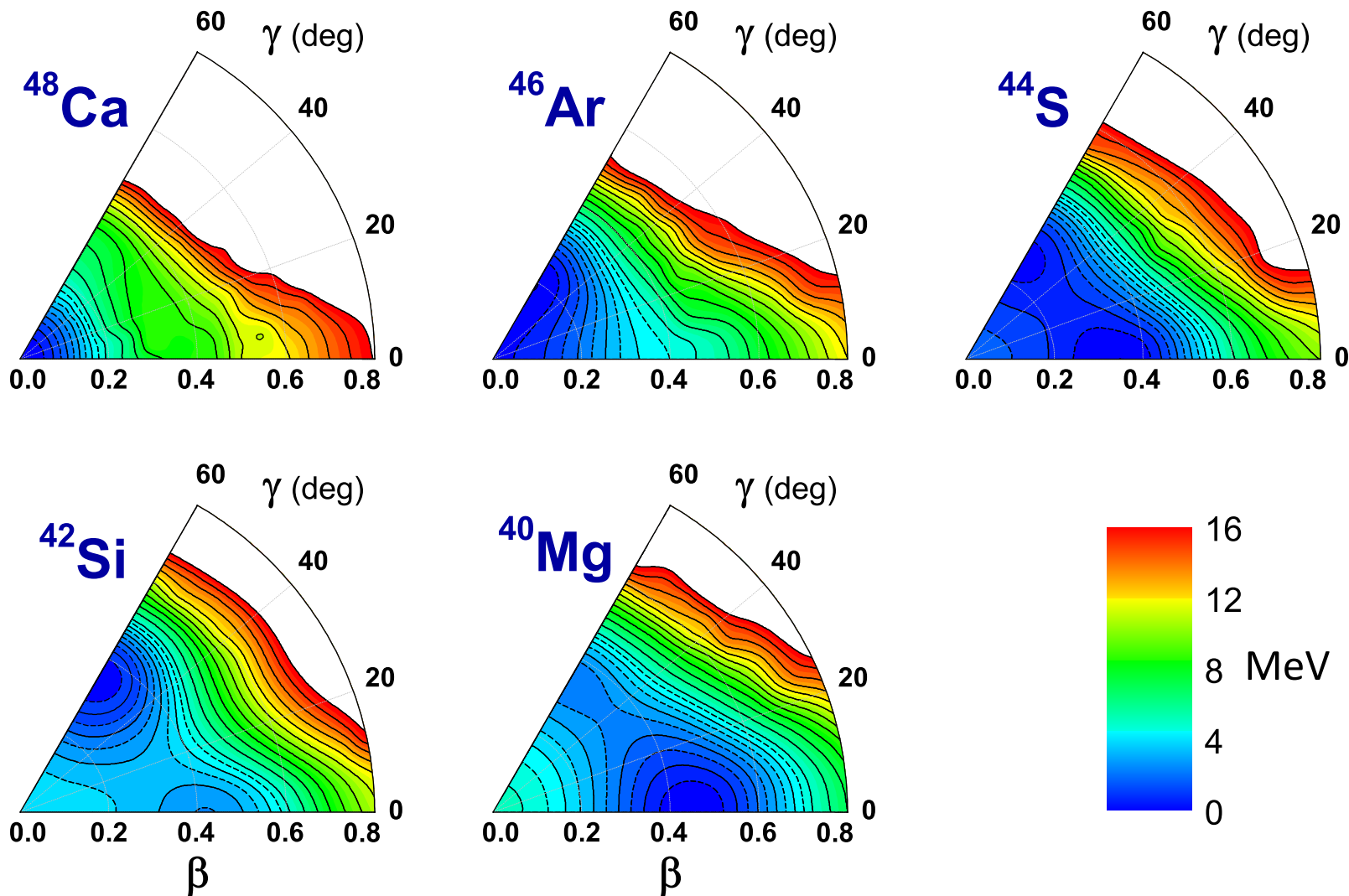
→ larger variational space for projected GCM calculations!

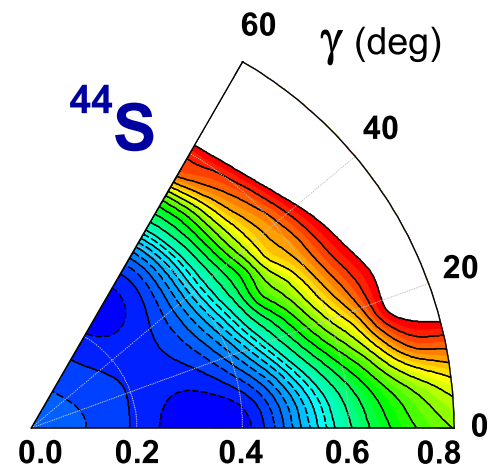
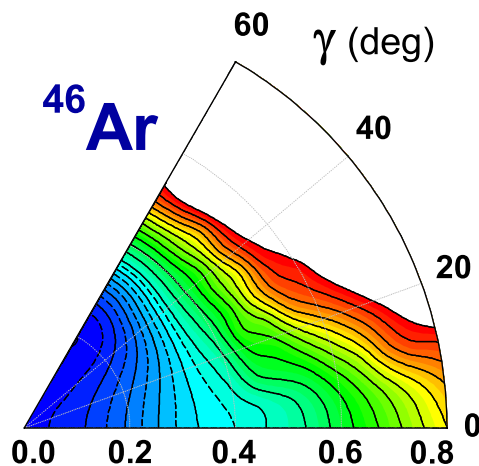
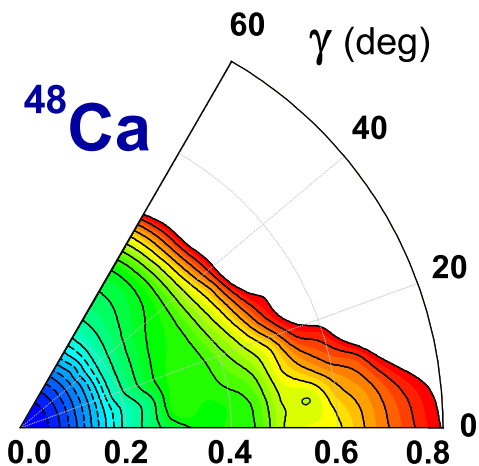
→ triaxial shapes, breaking time-reversal invariance, different deformations for proton and neutron distributions, ...

3D AMP+GCM model



## D. Coexisting shapes in the N=28 isotones





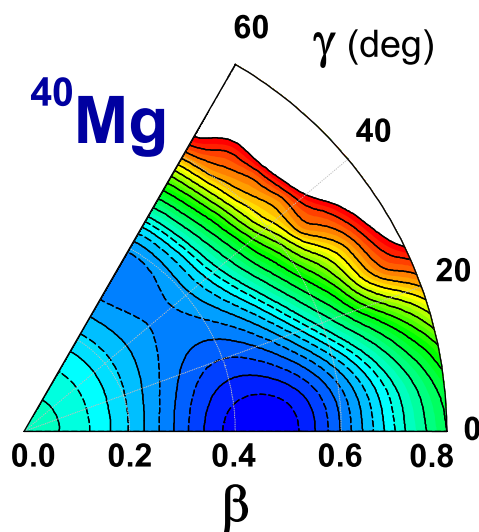
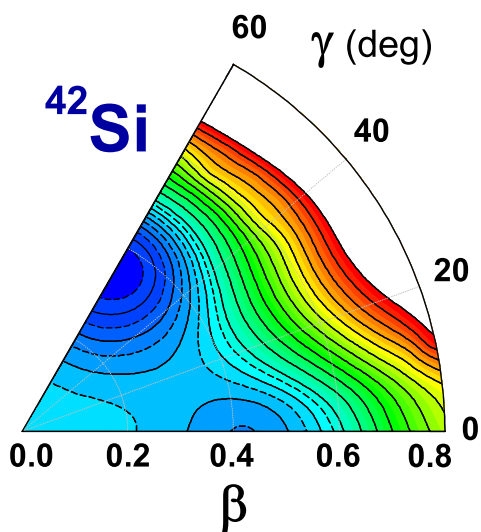
Neutron N=28 spherical shell gaps

Exp. values

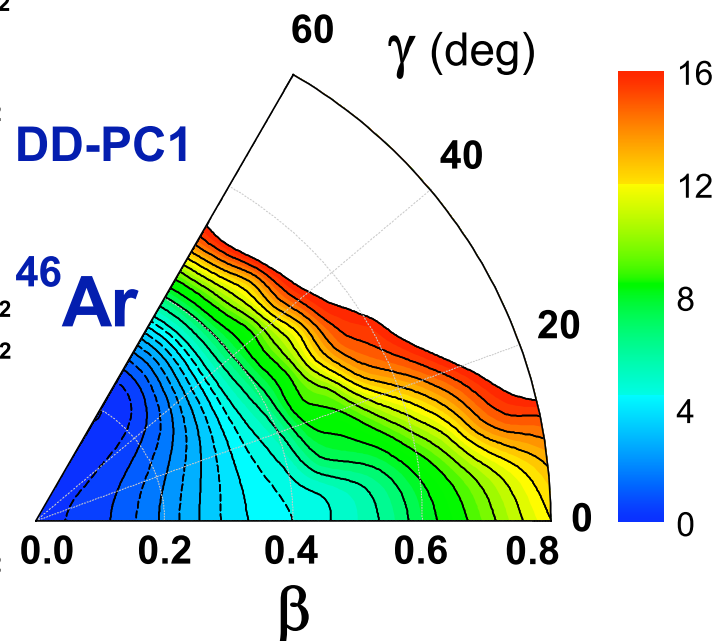
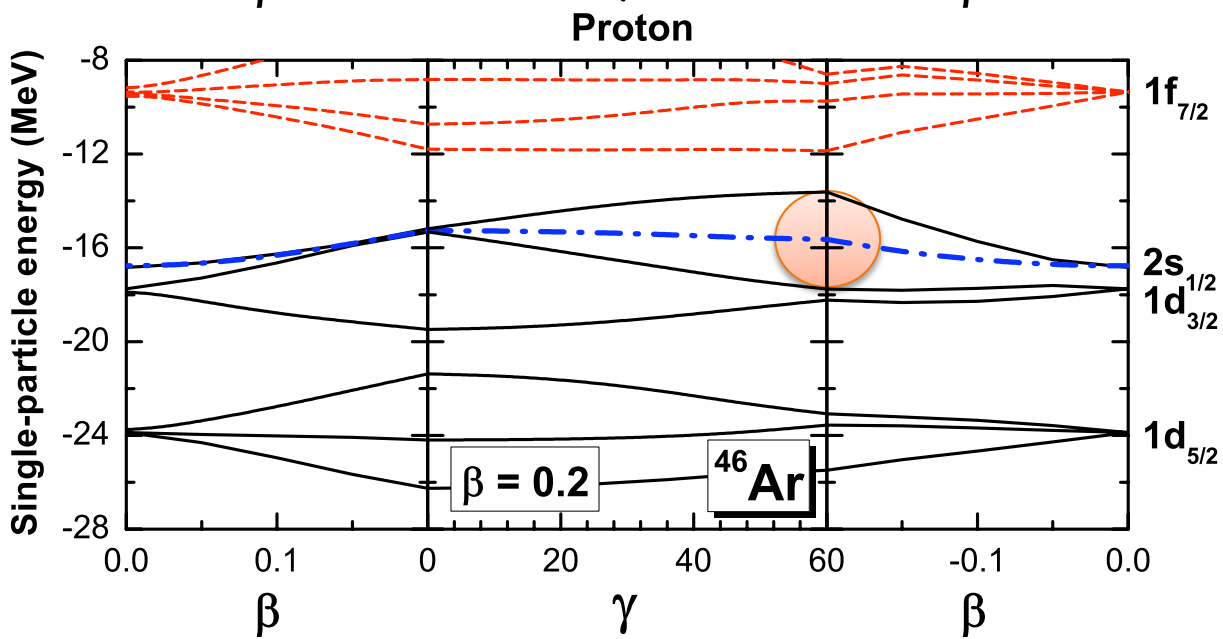
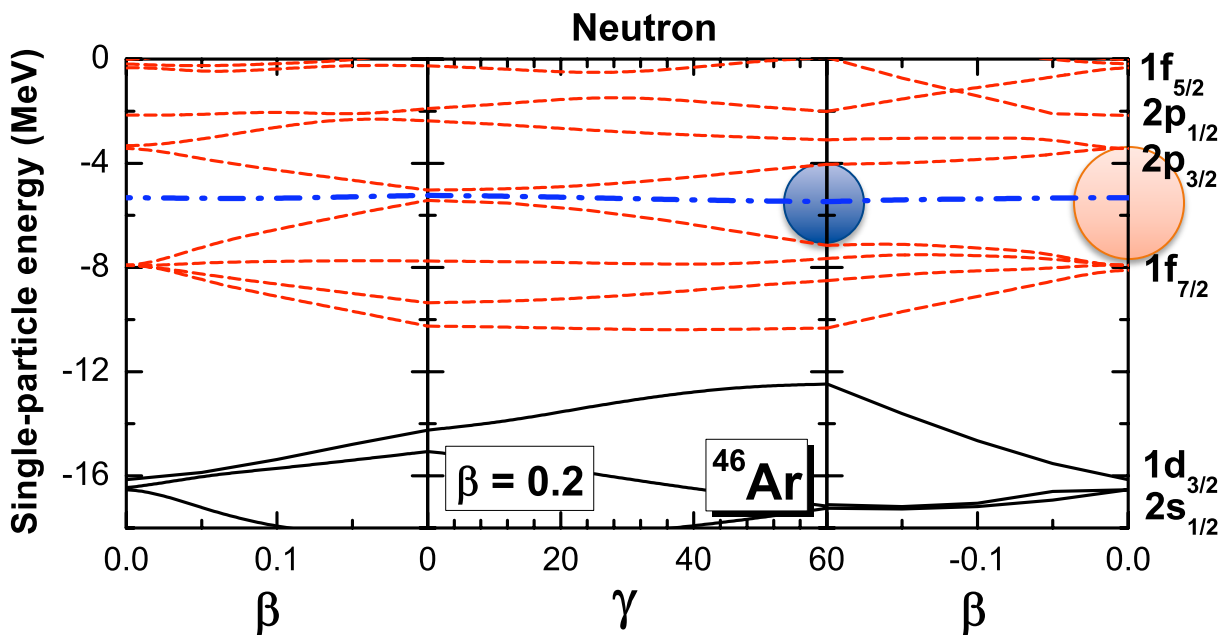
4.80 MeV

4.47 MeV

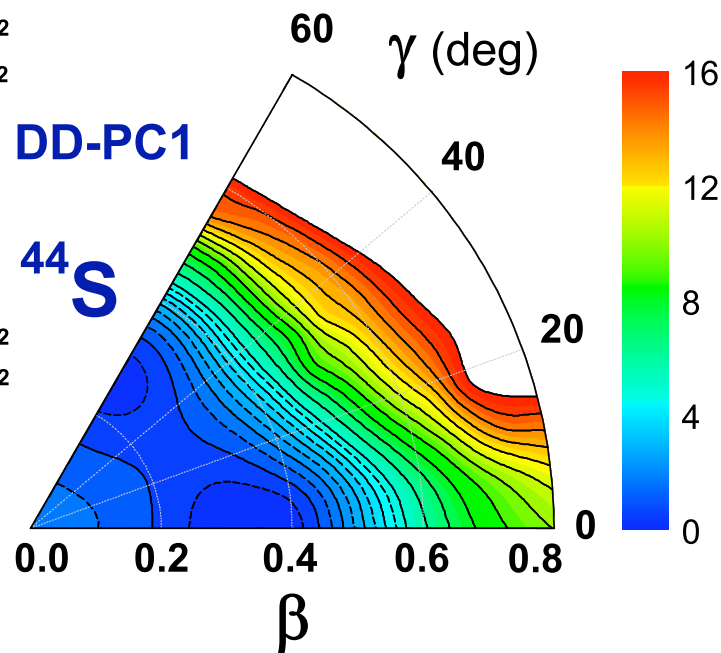
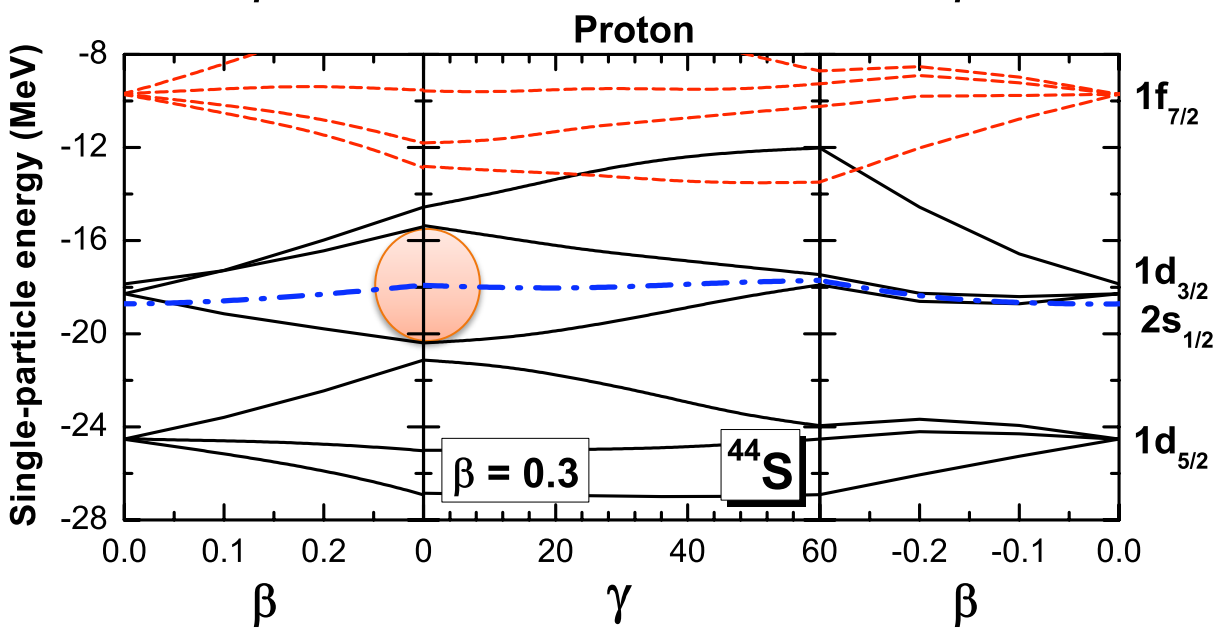
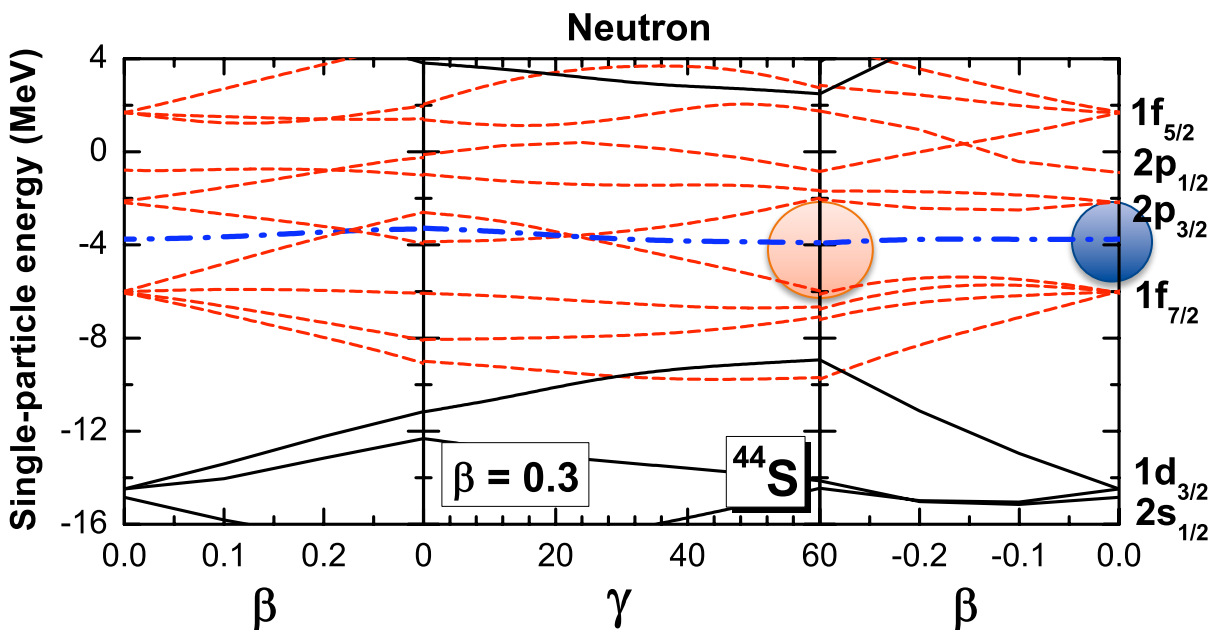
	$\Delta_{N=28}^{\text{sph.}}$	$\beta_{\text{min}}$
$^{48}\text{Ca}$	4.73	0.00
$^{46}\text{Ar}$	4.48	-0.19
$^{44}\text{S}$	3.86	0.34
$^{42}\text{Si}$	3.13	-0.35
$^{40}\text{Mg}$	2.03	0.45



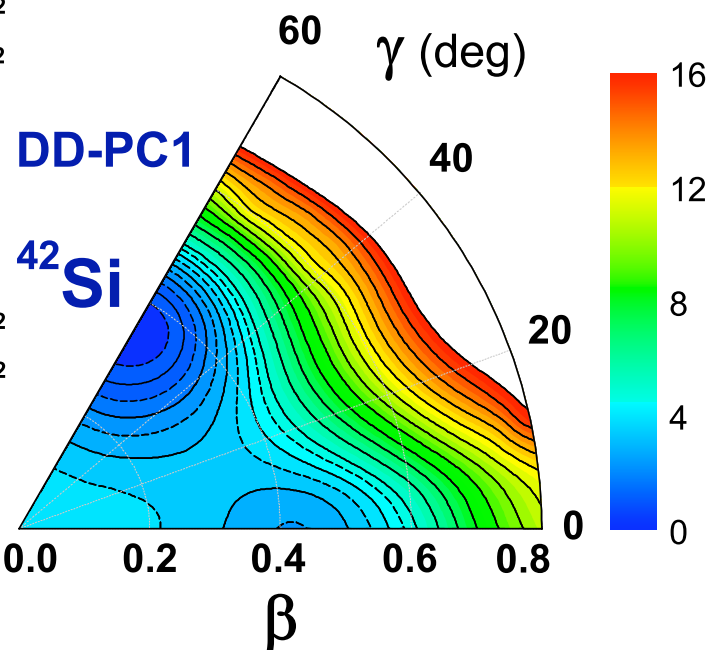
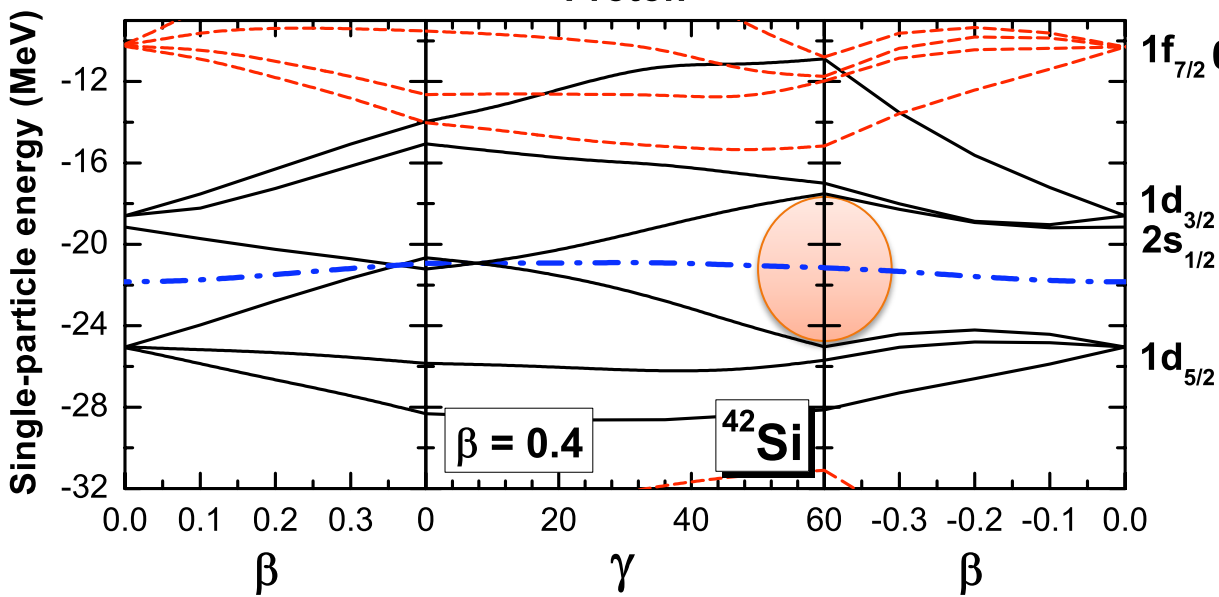
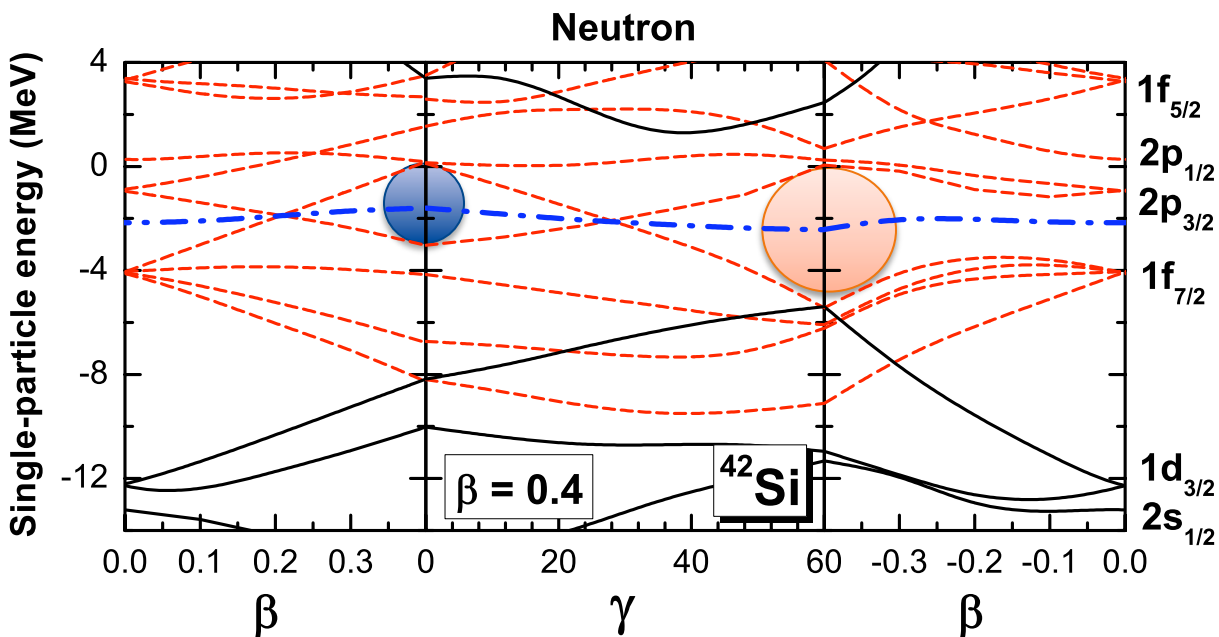
# $^{46}\text{Ar}$ : single-particle levels

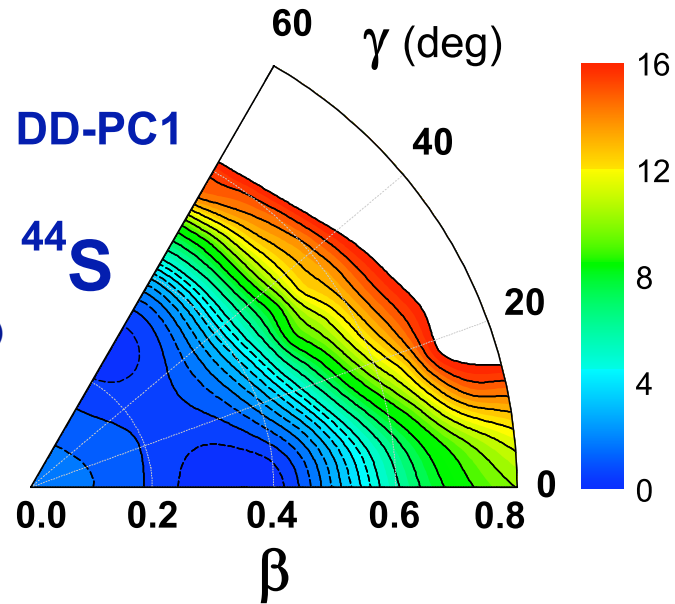
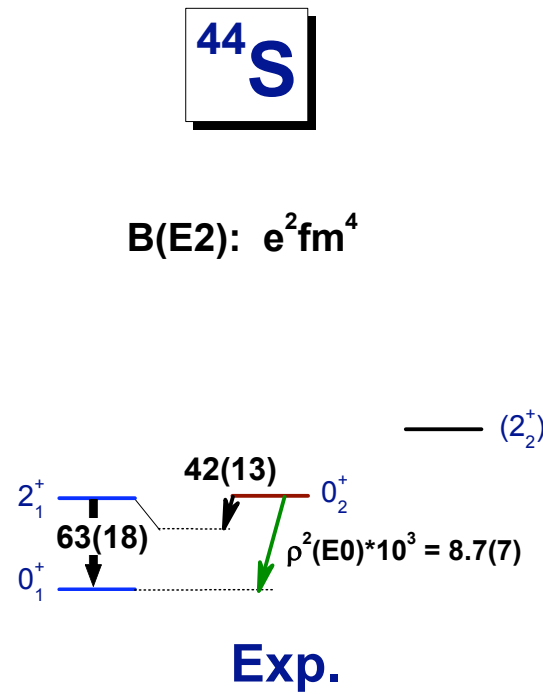
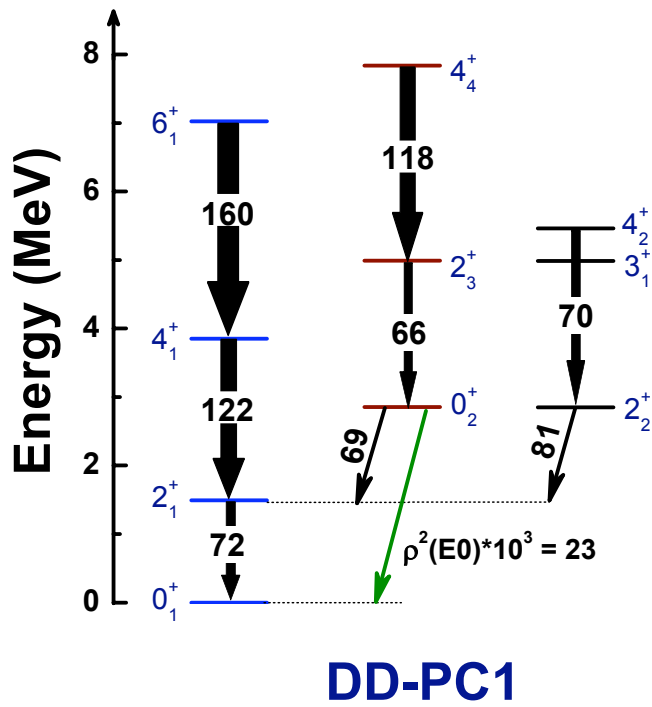


# $^{44}\text{S}$ : single-particle levels



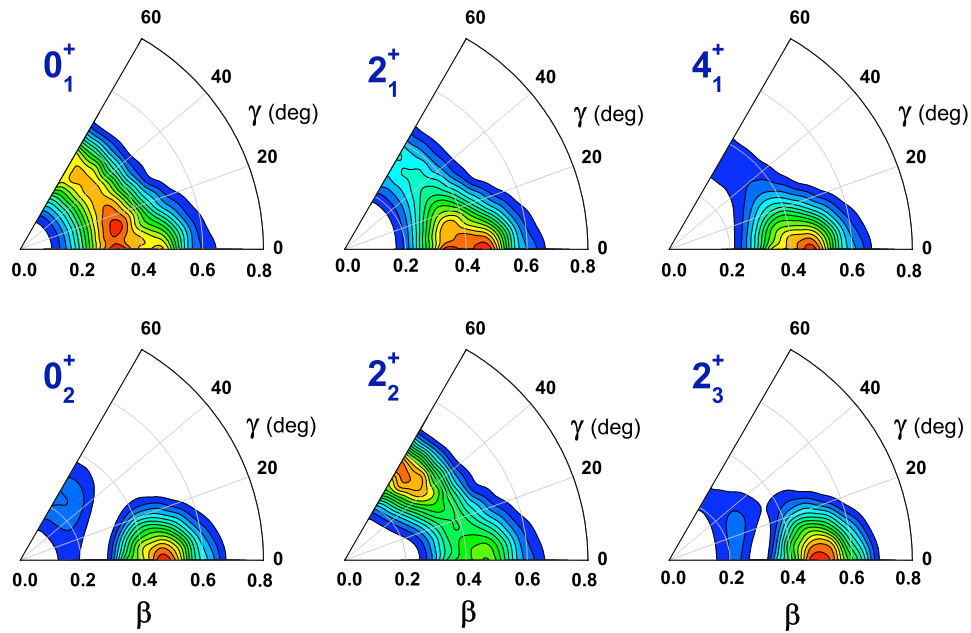
# $^{42}\text{Si}$ : single-particle levels





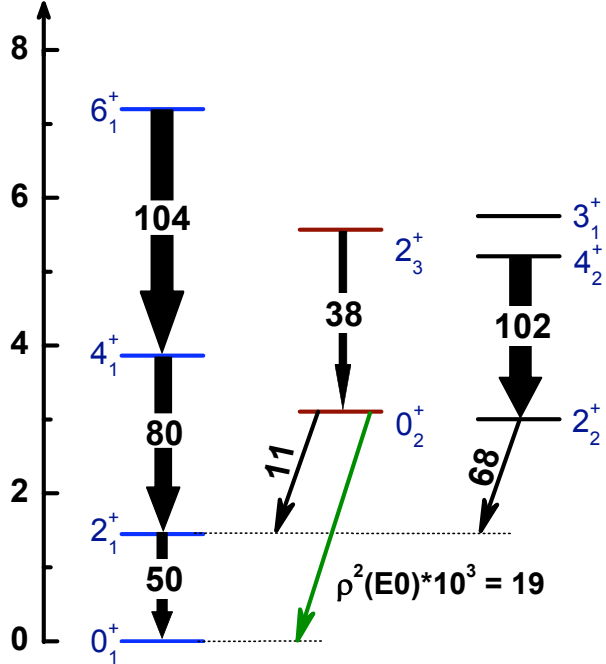
Probability density distributions:

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



**$^{42}\text{Si}$**

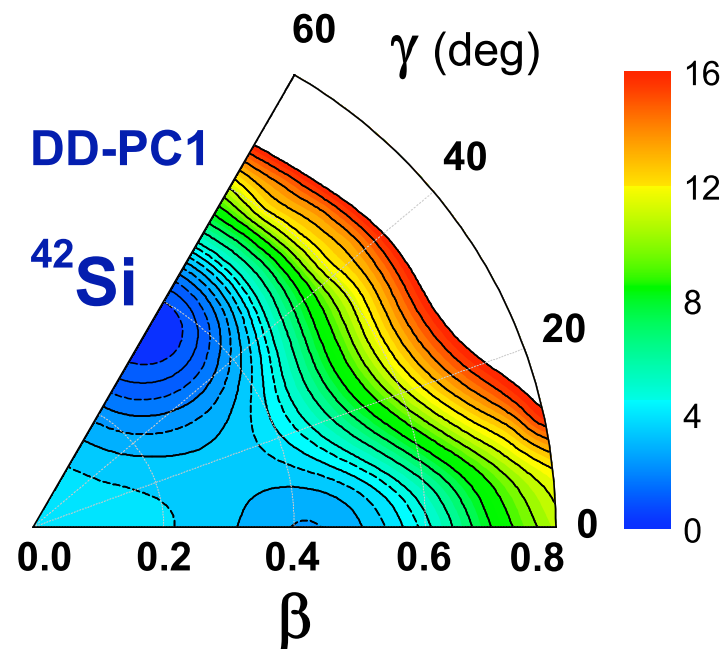
Energy (MeV)



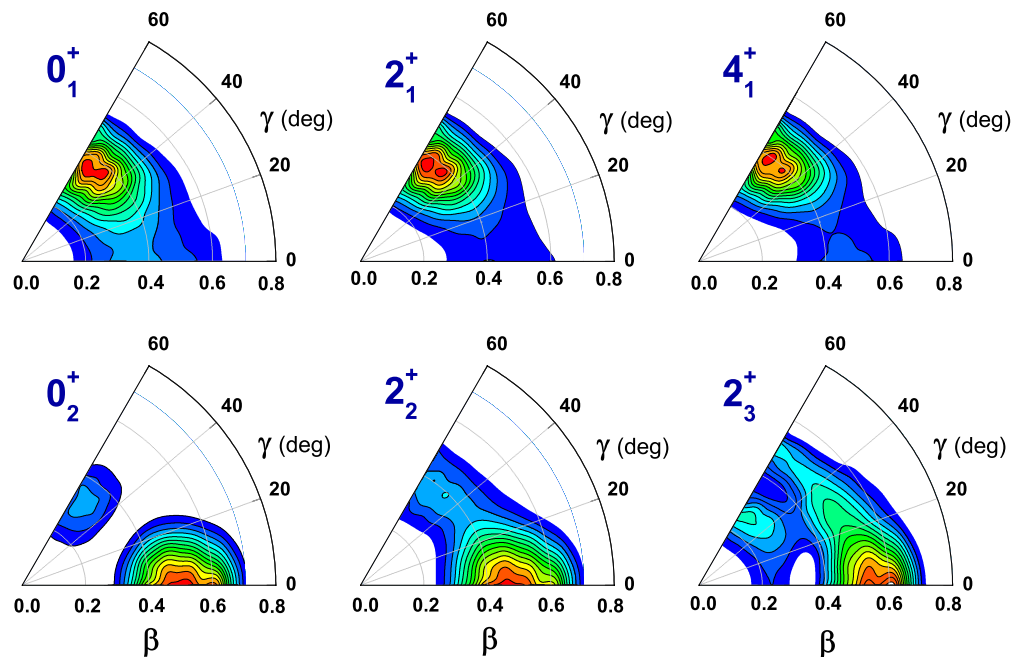
**DD-PC1**

$2_1^+$  —  
 $0_1^+$  —

**Exp.**



Probability density distributions:



## E. Global study of quadrupole correlation effects

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

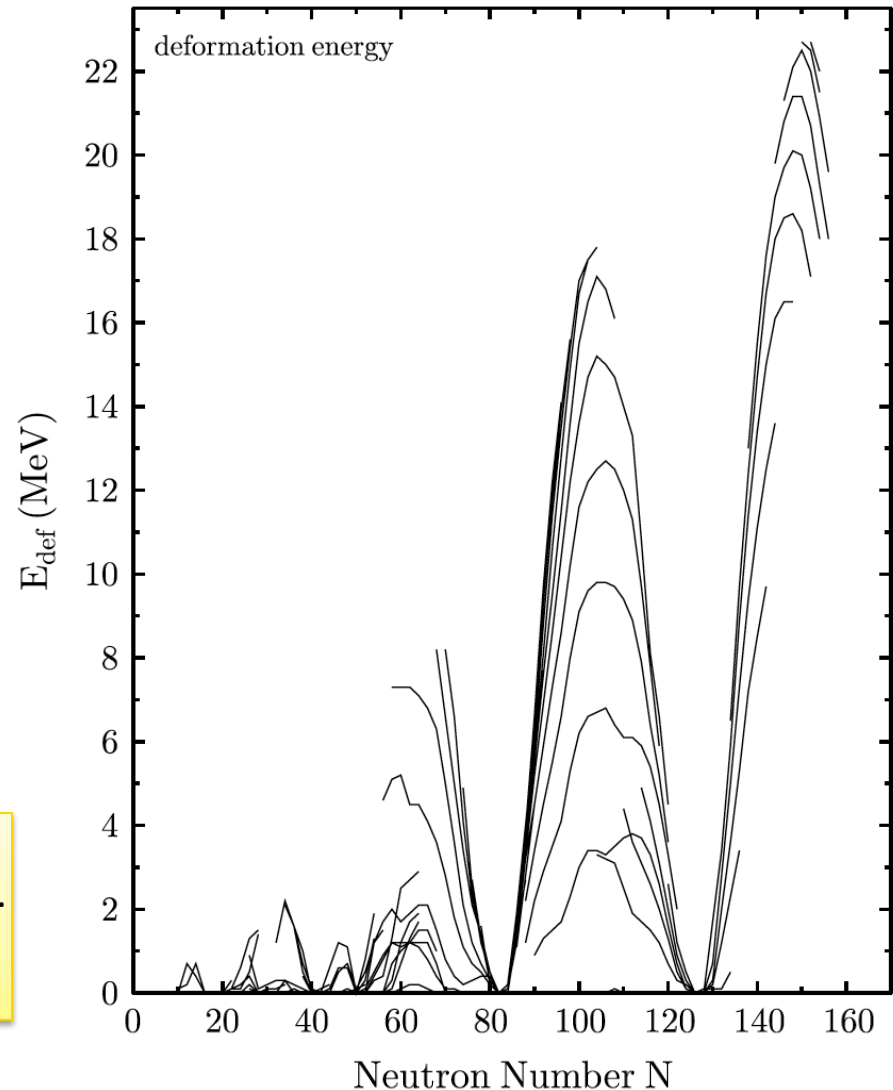
Phys. Rev. C 73, 034322

### Definition of correlation energies

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

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

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  $|q\rangle$  (on angular momentum  $I=0$ ) is its **rotational energy**:

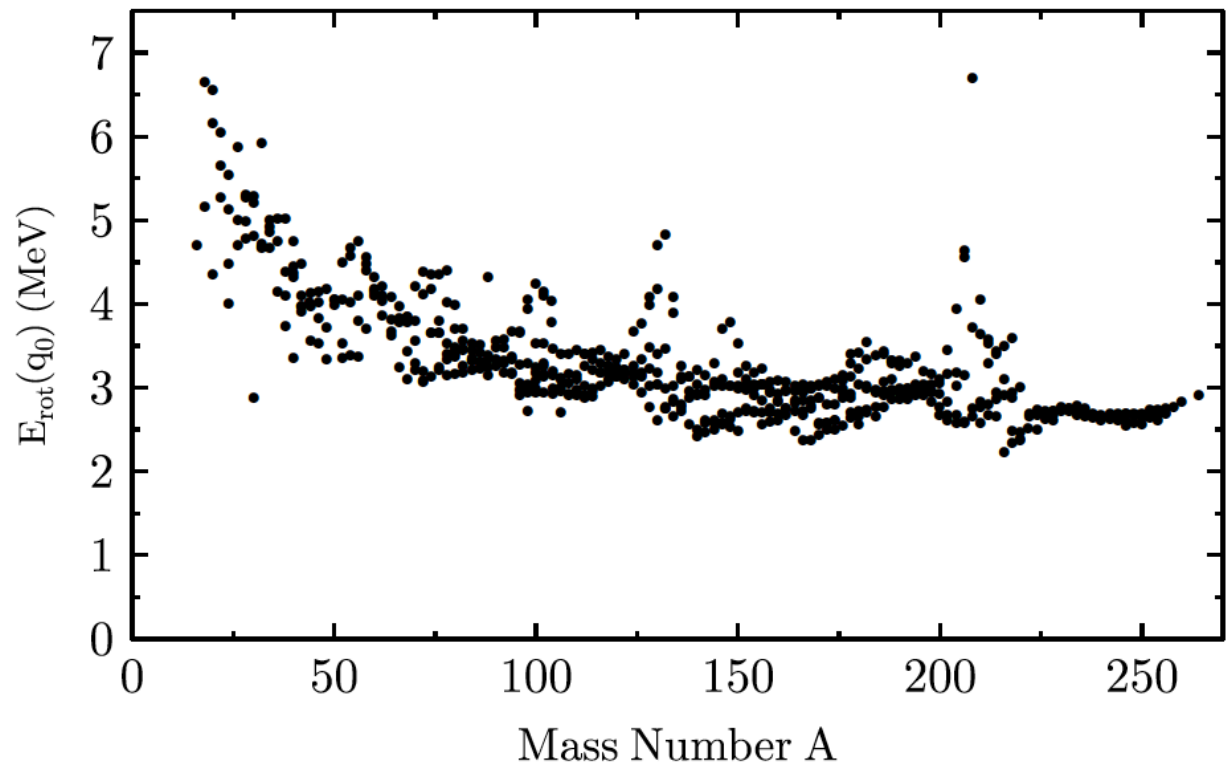
$$E_{\text{rot}}(q) = E(q) - E_0(q)$$

3) The **rotational energy correction**:

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

mean-field  
minimum

minimum  
after projection



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

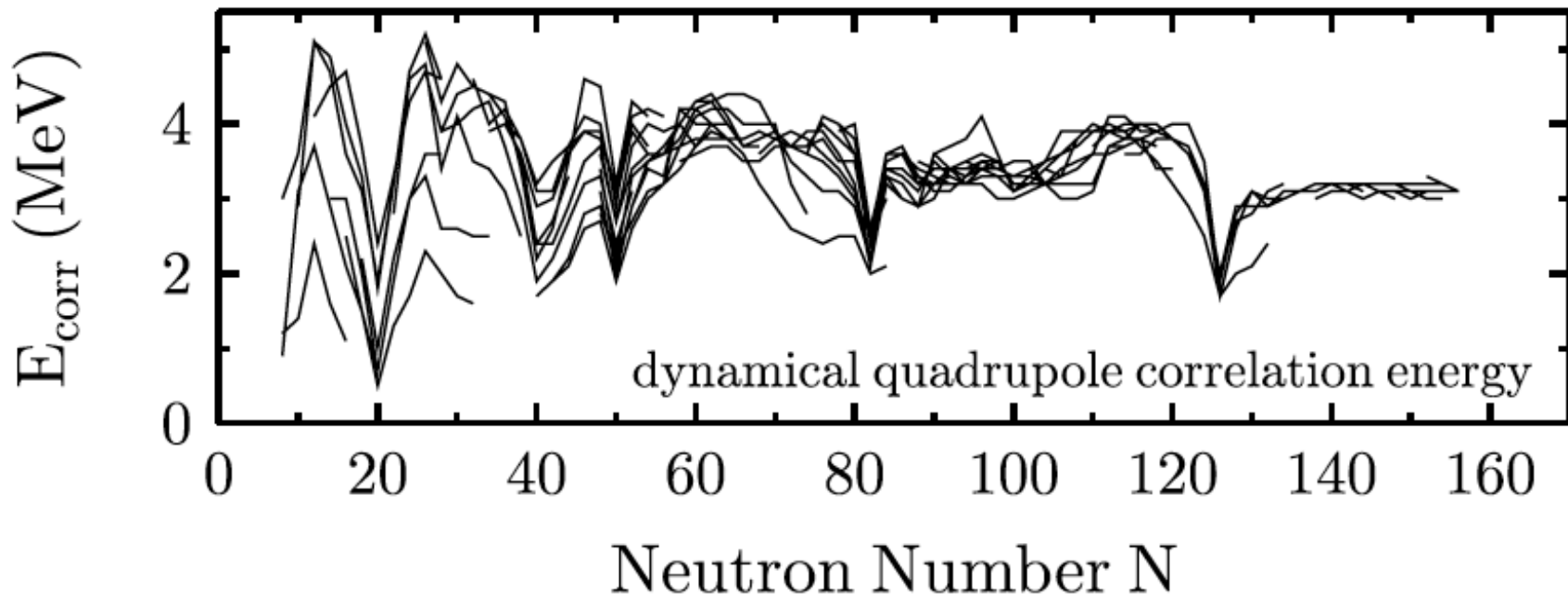
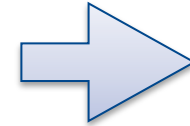
4) The correlation energy gained by configuration mixing:

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

GCM ground state

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

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



- (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  $A \leq 60$  have a larger correlation energy than static deformation energy, whereas the heavier deformed nuclei have larger static deformation energy than correlation energy.

