# Symmetry breaking and symmetry restoration in mean-field based approaches

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Cliquez pour modifier le style des sous-titres du masque

With the kind help of
T. Duguet, D. Lacroix and M. Bender

## What is the problematic about ?

- Mean field approaches widely used to study nuclear structure properties. (the advantage of describing the system in terms of simple wave functions)

- However, it is not possible to take into account important correlations between nucleons by such wave functions, if we require simultaneously the proper symmetries.

-Thus, in practice correlations are treated by symmetry-violating mean field approaches.

- In a second stage, symmetries should be restored. Symmetry properties are currently treated with beyond mean field approaches by using projection techniques.

# OUTLINE

-1) The mean field approximation

-2) Some features about symmetry

-3) Symmetry-violating mean field

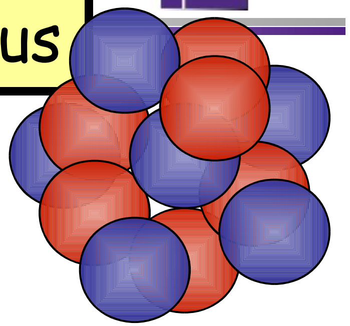
-4)  Symmetry restoration

-5) State of the art calculations

-6) Improvements

# 1) The mean field approximation

# Microscopic description of the atomic nucleus



**Nucleus = N nucleons in strong interaction**

**The many-body problem**
(the behavior of each nucleon influences the others)

Can be solved exactly for N < 12

For N >> 10 : approximations

**Shell model**
- valence space

**Approaches based on the mean field**
- no inert core
- hierarchy of the correlations

**Nucleon-Nucleon force unknown**

Bare Force

Effective Force

Phenomenological Effective Forces

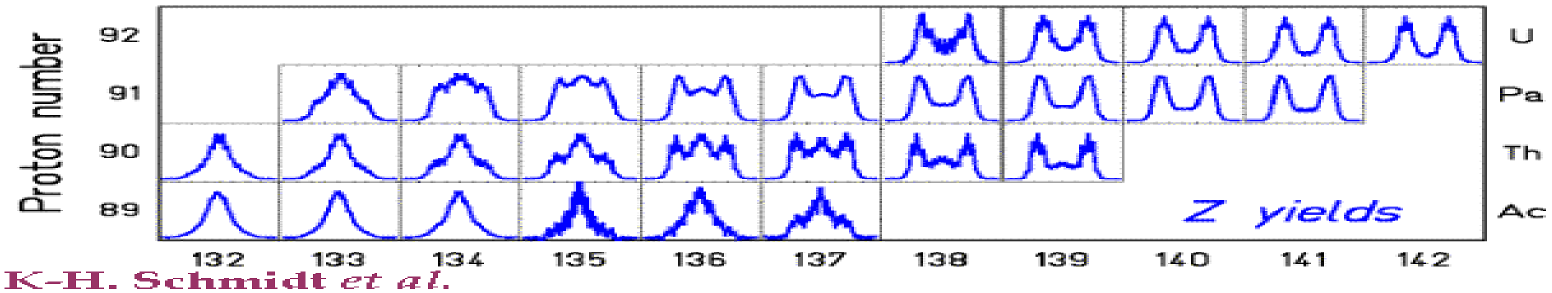
Zero range

Finite range

# Example of microscopic effects: Fission fragment yields

A heavy and a light fragment:

= asymmetric fission




Neutron number

Two identical fragments
= symmetric fission

*K-H Schmidt et al., Nucl. Phys. A665 (2000) 221*

# Mean field approach

The mean field approach is a theoretical tool for describing complex, open-shell nuclei for which the dimension of the configuration space becomes intractable for other methods of theoretical nuclear structure such as ab-initio or shell model approaches.


Main assumption: each particle is interacting with an average field generated by all the other particles : the mean field

The mean field is built from the individual excitations between the nucleons

No inert core is considered.

# The self consistent mean field approach
# The Hartree-Fock method

The basis ingredient is the effective Hamiltonian which governs the dynamics of the individual nucleons

$$H = \sum_{i=1}^{A} \frac{\vec{p}_i^{\,2}}{2M} + \frac{1}{2} \sum_{i \neq j = 1}^{A} v_{ij}^{eff}$$

Effective force

Wave function $\Phi(x_1, x_2, ..., x_A)$ = antisymmetrized product of A orbitals of the nucleons $\varphi_i(x_i)$ with $x_i = (\vec{r}_i, \sigma_i, \tau_i)$

Orbitals are obtained by minimizing the total energy of the nucleus

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

# The phenomenological effective finite-range Gogny force

$P_\tau$ : isospin exchange operator
$P_\sigma$ : spin exchange operator

$$v_{12} = \sum_{j=1}^{2} \exp\left[ - \frac{\left| \mathbf{r}_1 - \mathbf{r}_2 \right|^2}{p_j} \right] \left( \mathbf{W}_j + \mathbf{B}_j \mathbf{P}_\sigma - \mathbf{H}_j \mathbf{P}_\tau - \mathbf{M}_j \mathbf{P}_\sigma \mathbf{P}_\tau \right)$$

Finite range central term

$$+ t_3 \left(1 + x_0 P_s\right) \delta\left(\vec{r}_1 - \vec{r}_2\right) \rho^\alpha \left(\vec{r}_1 + \vec{r}_2\right)$$

Density dependent term

$$+ iW_{ls} \overleftarrow{\nabla}_{12.} \delta\left(\vec{r}_1 - \vec{r}_2\right) \Lambda \vec{\nabla}_{12} . \left(\vec{\sigma}_1 + \vec{\sigma}_2\right)$$

Spin orbit term

$$+ \left(1 + 2t_{1z}\right)\left(1 + 2t_{2z}\right) \frac{e^2}{\left|\vec{r}_1 - \vec{r}_2\right|}$$

Coulomb term

back

# The Hartree Fock equations

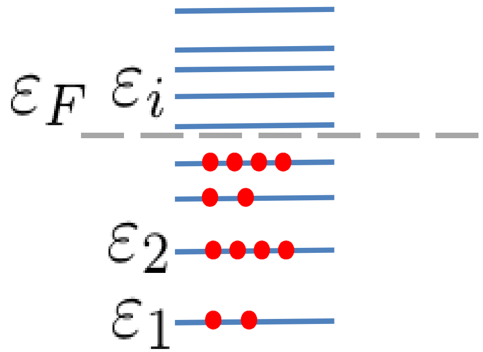
Hartree-Fock equations

(A set of coupled Schrodinger equations)

$$\left[\frac{-\hbar^2}{2M}\nabla^2 + U_{HF}(\varphi_\alpha)\right]\varphi_i(x_i) = \varepsilon_i \varphi_i(x_i)$$

Hartree-Fock potential

Single particle wave functions

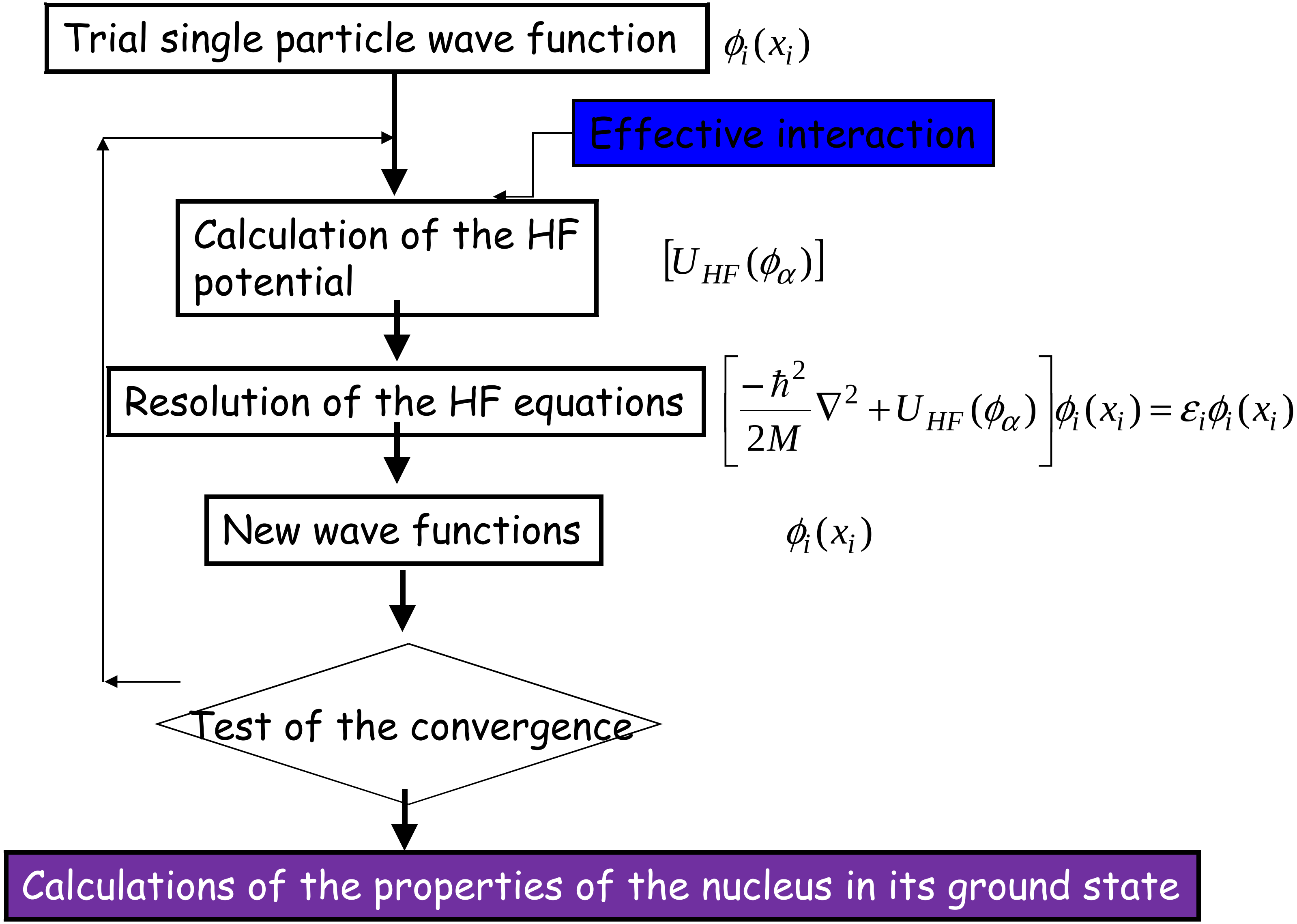



Self consistent mean field :

the Hartree Fock potential depends on the solutions (the single particle wave functions)

-> Resolution by iteration

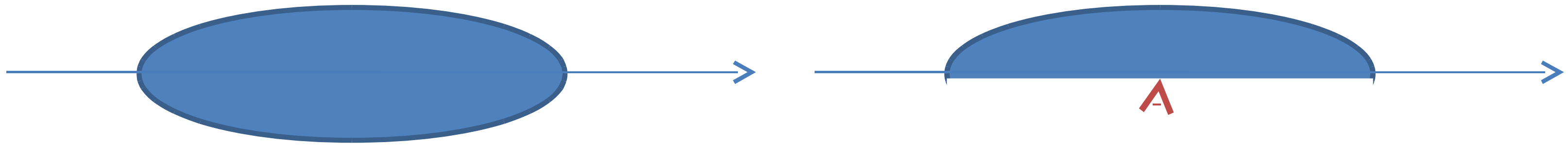
# Resolution of the Hartree Fock equations



·Symmetry imposed : for a sake of simplicity symmetries can be enforced

-spherical nuclei : calculation of 1/8 of the nucleus
axial symmetry + parity enforced : calculation of ¼
triaxial shapes but parity enforced : ½

- spherical nuclei : 1 state should be treated instead of (2J+1)



* Intrinsic symmetries: [H,S]=0

Warning : if the first trial wave function does not break the symmetry S, the solution will not break the symmetry, even if it should !!

-> Solution : to start with a w.f as general as possible

# Symmetry breaking Hartree-Fock solutions

## Symmetries of the exact Hamiltonian and symmetries of the Hartree-Fock Hamiltonian"

Mean-field approximation: to describe the system in terms of simple wave functions (Slater determinant).

<u>Problems with symmetries:</u>

<u>Example of the translational invariance strongly broken in ALL nuclei :</u>

transitional invariant wave functions are products of plane waves

-> not adequate for the description of a (self-bound) finite nuclei

But many correlations between nucleons are missing by so simple wave functions if we require simultaneously the proper symmetry behavior

$$[H_{exact}, S] = 0 \quad \text{but} \quad [\mathrm{H}_{\mathrm{HF}}, S] \neq 0$$

# Philosophy

Some correlations can be treated by a symmetry-violating mean-field approach:

Such as for instance:
- The long range particle-hole (ph) correlations responsible for stable deformations
- particle-particle (pp) correlations for superfluidity

-> can be treated by the Hartree-Fock-Bogoliubov theory that violates J and N.

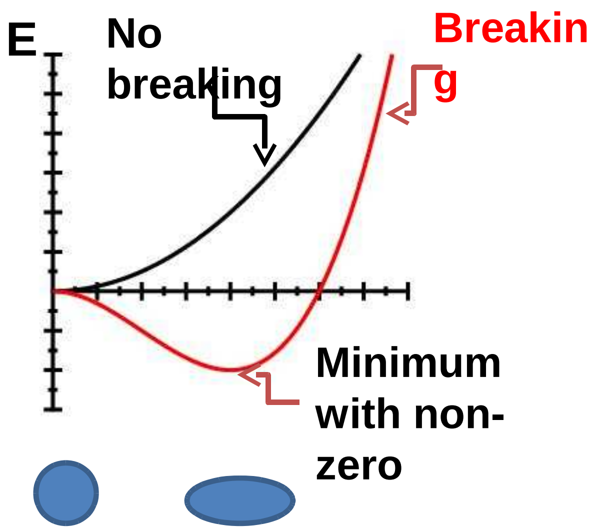
The stronger the correlations, the better such an approximation.

# Symmetry violation and phase transition (1/2)

With strong correlations a symmetry-violating minimum develops

In analogy to solid state physics, the system undergoes a phase transition to a symmetry-violating state such as to a deformed state or to superfluid phase

**Illustration of symmetry**




Caution : The concept of phase transition is only valid for infinite systems.
In finite nuclei such effects are smoothed.

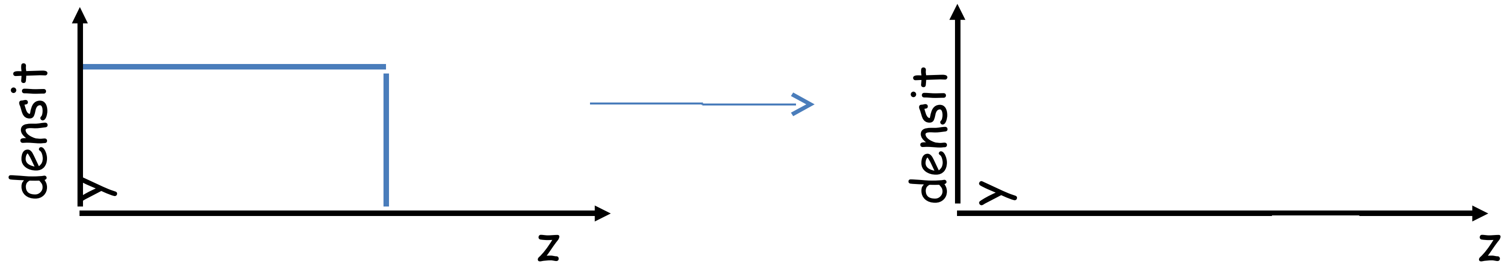
# Symmetry violation and phase transition 2/2
## Why a phase transition ?

Phase transition are due to a collective mode that becomes softer and softer:

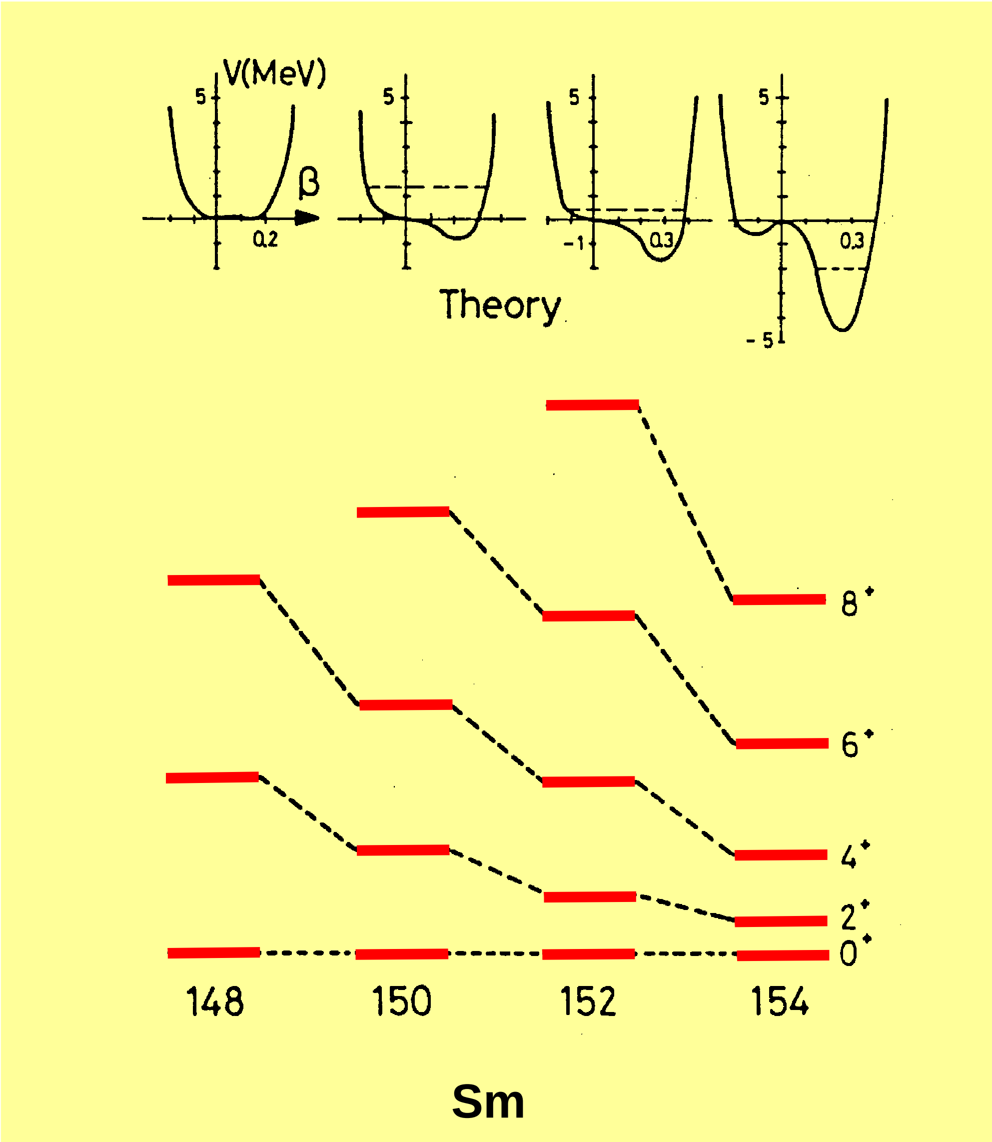
* Breaking of the rotational invariance related to the spherical-deformed transition due to quadrupole vibration

* Breaking of the particle number related to a transition from normal to superfluid due to the pair vibration mode.

* Breaking of the translational invariance related to the liquid-gas transition and to fragmentation due to fluctuations of the density.



# HFB deformation and experimental spectra




Slide from D. Goutte

# Angular velocity of a rotating nucleus

For a rotating nucleus, the energy of a level is given by* :

$$E_{rot}(I) = \frac{I(I+1)}{2J}\hbar^2$$

With J the moment of inertia

We also have $E_{cin} = \frac{1}{2}J\omega^2$ so $\omega = \sqrt{\frac{2E}{J}}$

With $\hbar = 6.582 \times 10^{22}$ Mev · s

$$\omega_{^{160}Gd}(2^+) = \sqrt{\frac{2 \times 75.26 \times 10^{-3}}{39.86(6.582 \times 10^{-22})^2}} = 9.336 \times 10^{20}\ \mathrm{rad \cdot s^{-1}} = 1.486 \times 10^{19}\ \mathrm{tr \cdot s^{-1}}$$

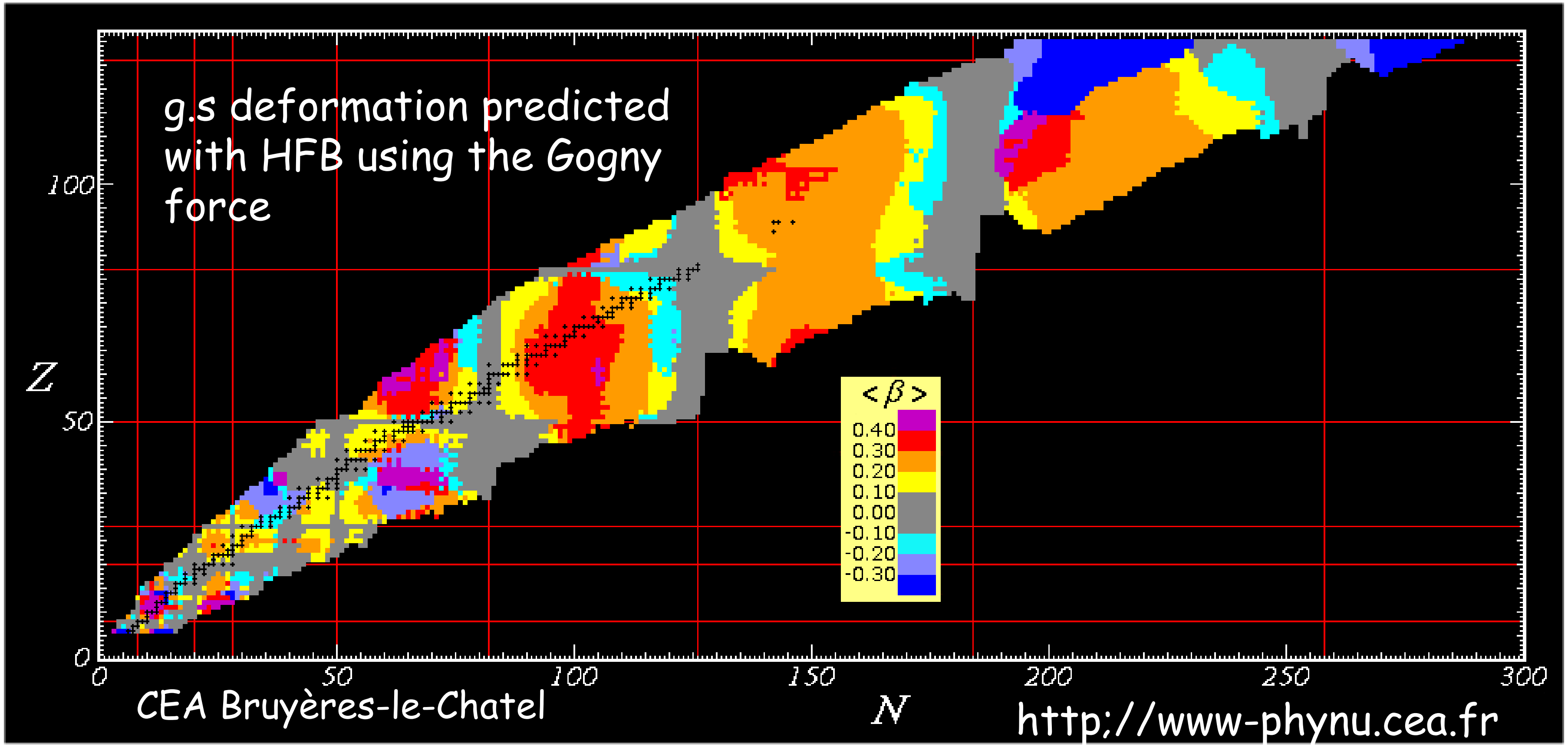
To compare with a wash machine: 1300 tpm

* Mécanique quantique by C. Cohen-Tannoudji, B. Diu, F. Laloe)

Illustration of the symmetry breaking in HFB:

Breaking
of the rotational invariance

# Static ground state deformation from HFB



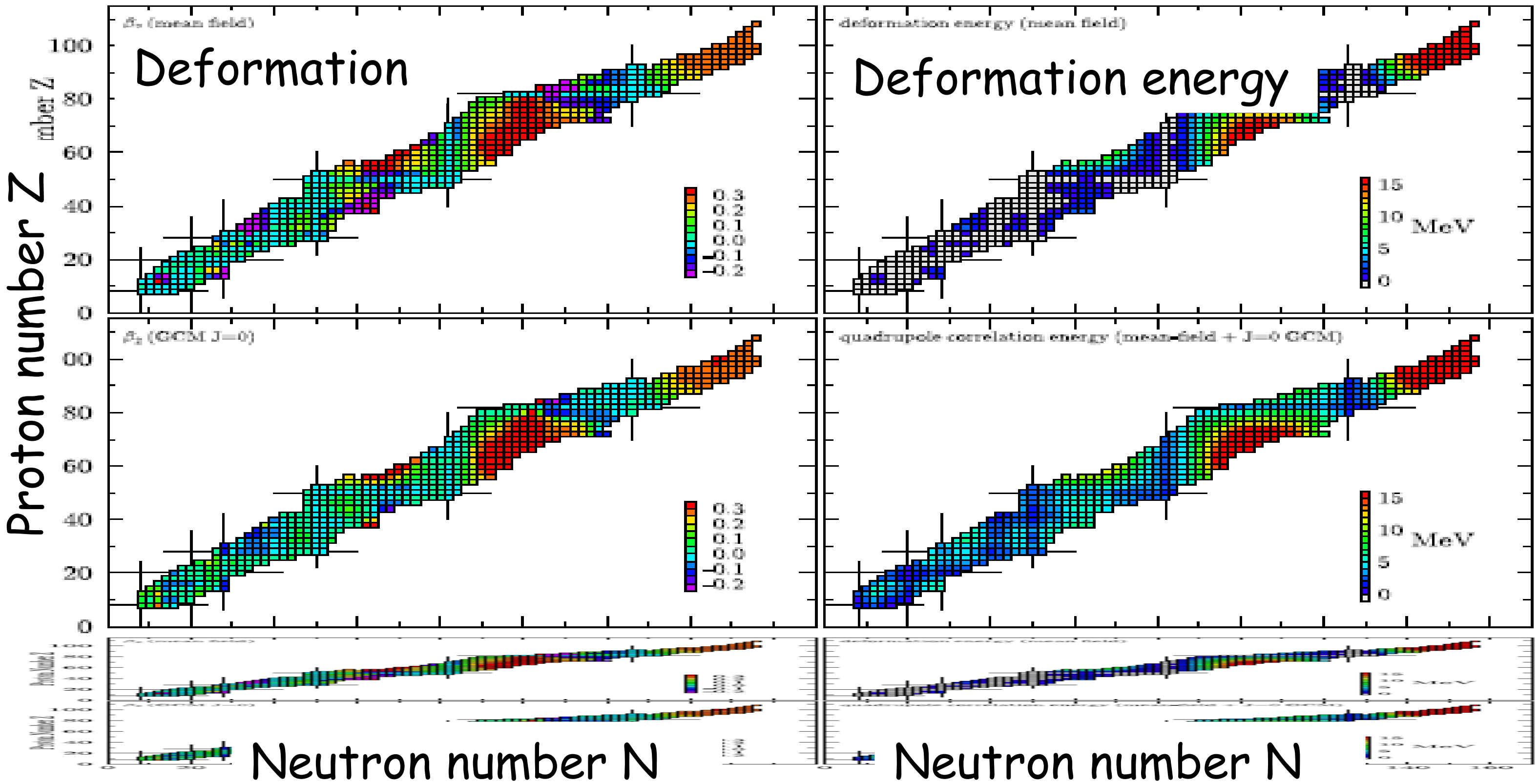

with β characterizing the axial quadrupole deformation

β =0 spherical β> 0 prolate β <0 oblate

# Static deformation energy from HFB (1/2)

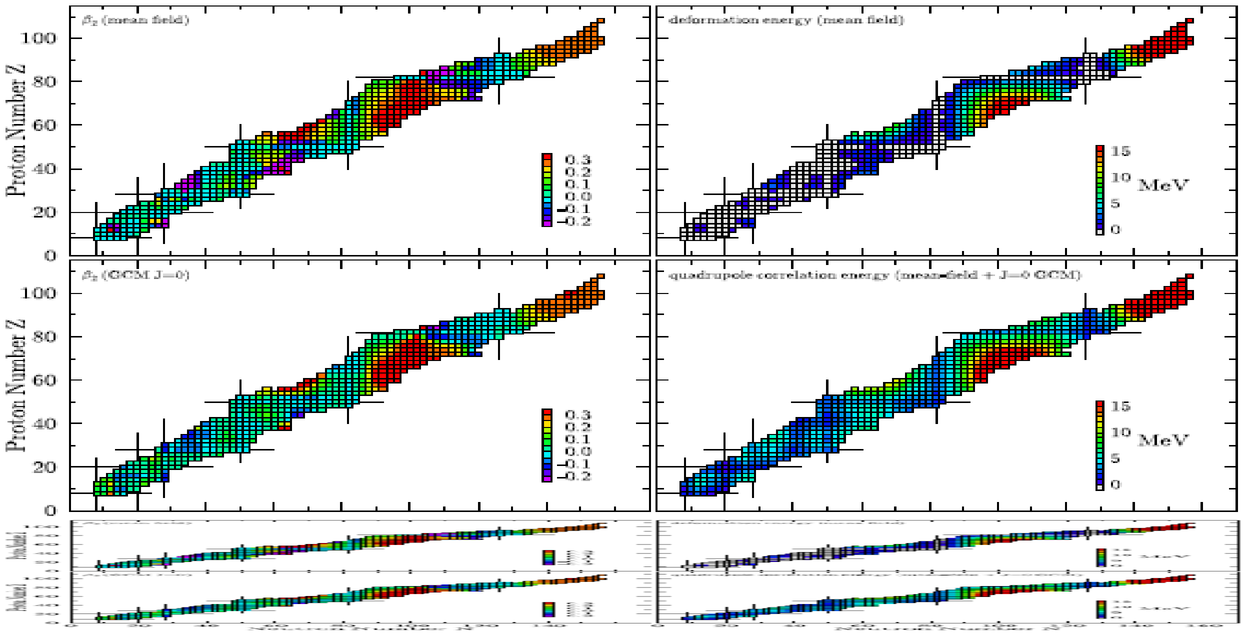
The energy gained by static deformation is :

$$E_{stat\ def} = E(\beta=0) - E_{min}$$




"Global Study of quadrupole correlation effects", M. Bender, G.F. Bertsch and P.-H. Heenen, Phys. Rev. C73, 034322 (2006)

# Static deformation energy from HFB(2/2)




<u>Main features:</u>

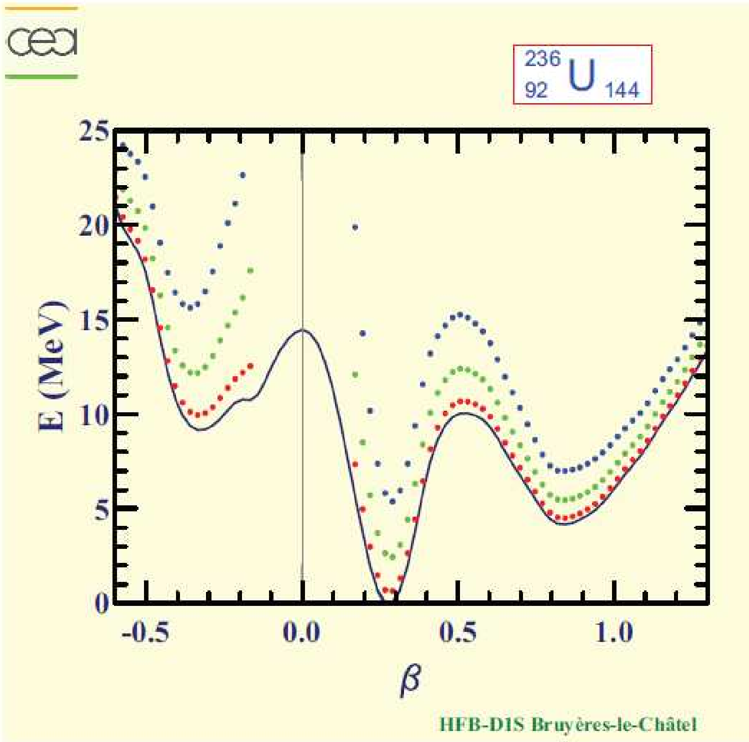
* above Z=50 three regions of well-deformed prolate nuclei :
  mid shell nuclei

* up to a 15 MeV energy gain

In many nuclei, the minimum of the energy is found for  ≠ 0.

The deformed ground state solution violates the rotational invariance

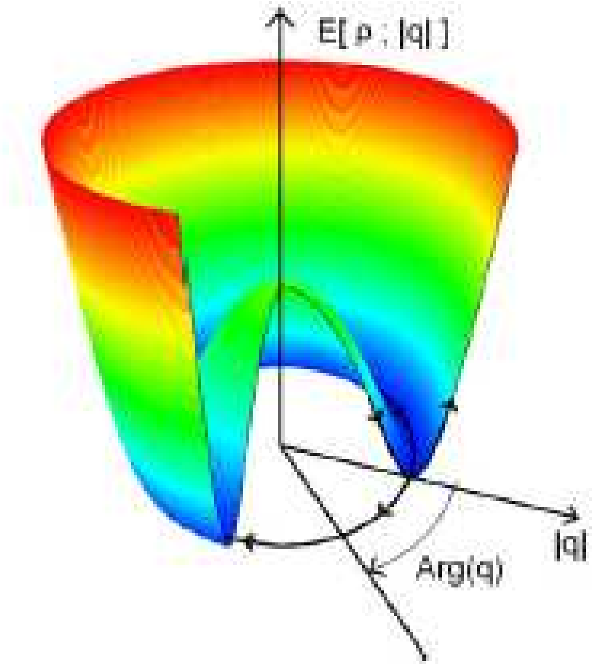
$$\left[\mathrm{H}_{\mathrm{HF}}, \hat{J}\right] \neq 0$$



# Order parameter

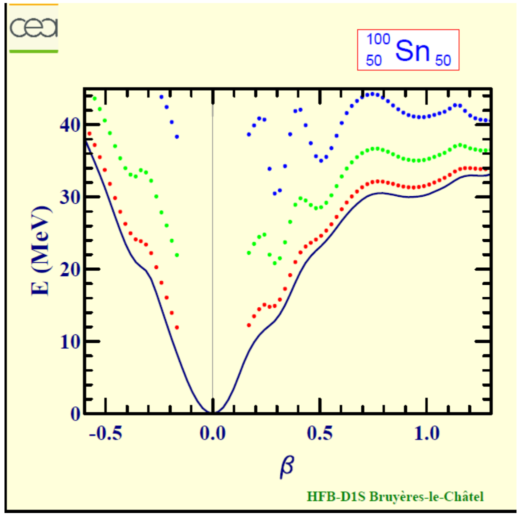
-> the breaking of the symmetry is monitored by the magnitude (and the phase) of an order parameter q.

-> In such a continuous symmetry breaking, the energy is independent of the phase (Mexican hat)

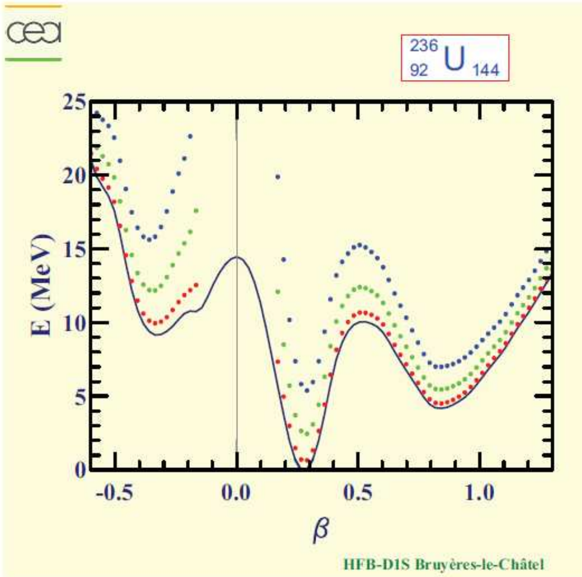



For the spherical-deformed phase transition the order parameter q is the deformation

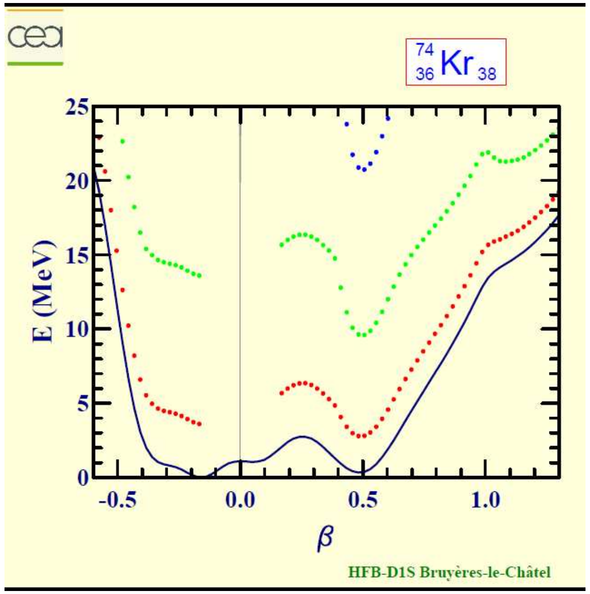
# Typical cases of symmetry violations




Rigid spherical:
So symmetry violation



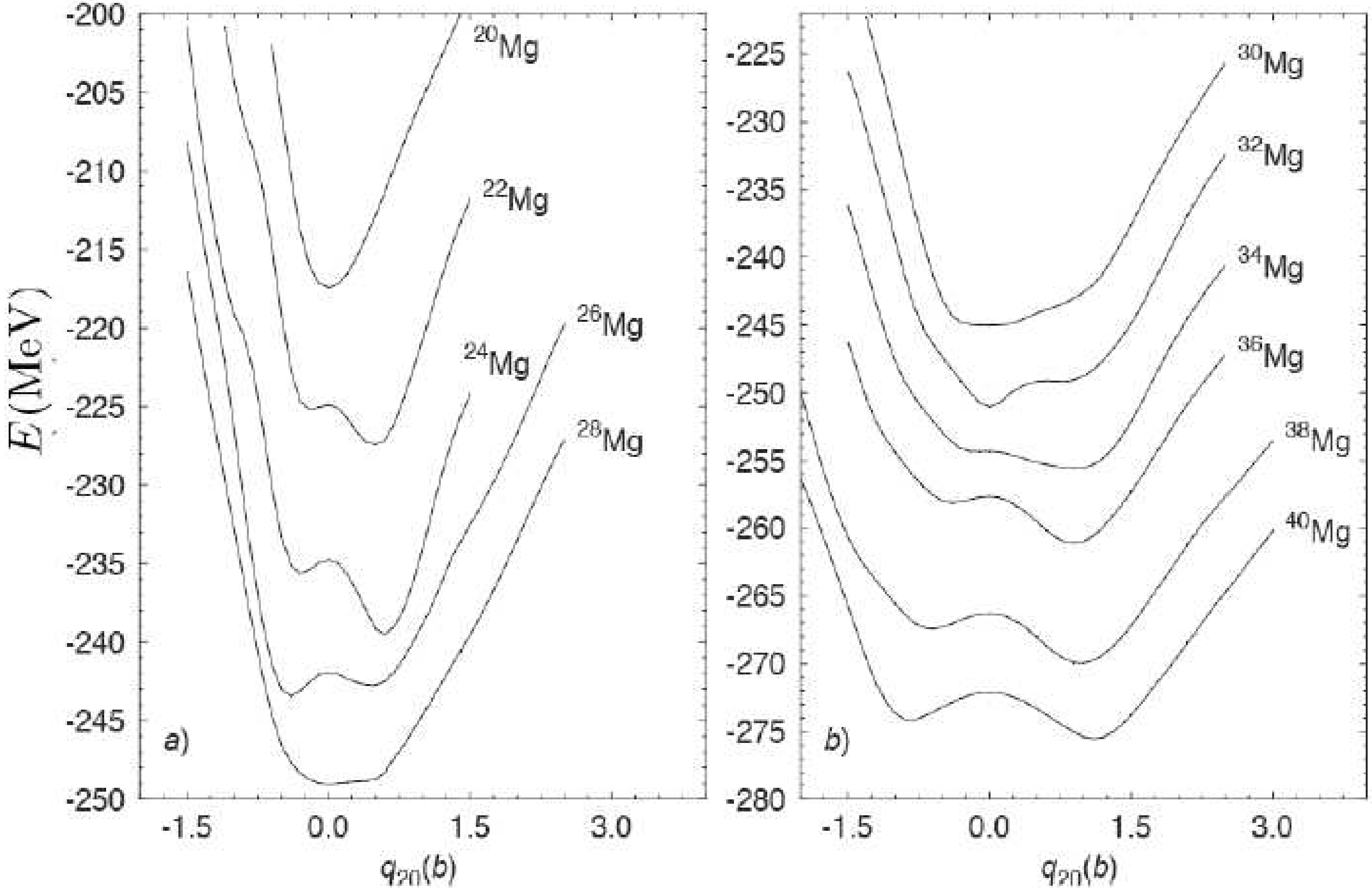

Well-deformed




Soft

HFB results using the Gogny force from CEA Bruyères-le-Châtel
http://www-phynu.cea.fr

# Evolution of the g.s. deformation along an isotopic chain




Slide from L. Egido, workshop on shell effects 3-5 May 2010 ESNT Saclay

# Symmetry restoration

# Need for symmetry restoration

* The HFB state is a wave packet and quantum fluctuations make such a wave packet to relax into the symmetry conserving g.s.

* Symmetry breaking wave-functions do not carry good quantum numbers

-> restoring symmetries amounts to using an enriched trial wave function that carries good quantum numbers (mandatory to calculate for instance transition probabilities …)

-> the concept of symmetry breaking is only an intermediate description of the system and symmetries must be restored.

# Restoration of the translational symmetry breaking (1/2)

Exact Hamiltonian $H = -\frac{\hbar^2}{2m}\sum_i (\frac{\partial}{\partial r_i})^2 + V$

Coordinate transformation
(R collective coordinate,
x coordinate in the C.M. frame)

$$\begin{cases} x_i = r_i - R \\ R = \frac{1}{A}\sum_i r_i \end{cases}$$

$$H = \frac{1}{2Am}P^2 + \sum_i \frac{p_i^2}{2m} + V - \frac{1}{2Am}(\sum_i p_i)^2$$

with

$$\begin{cases} p_i = \frac{\hbar}{i}\frac{\partial}{\partial x_i} \\ P = \frac{\hbar}{i}\frac{\partial}{\partial R} \end{cases}$$

-> Definition of an Intrinsic Hamiltonian

$$H_{\text{int}} = \sum_i \frac{p_i^2}{2m} + V - \frac{1}{2Am}(\sum_i p_i)^2$$

# Restoration of the translational symmetry breaking (2/2)

-> Intrinsic Hamiltonian

$$H_{\mathrm{int}} = \sum_i \frac{p_i^2}{2m} + V - \frac{1}{2Am}\left(\sum_i p_i\right)^2$$

* If we are in the intrinsic system we don't have to worry about translational invariance

* Using Hartree-Fock we get a localized potential and a localized wave function.

* We have to subtract from the usual HF Hamiltonian the term $\frac{1}{2Am}\left(\sum_i p_i\right)^2$

-> Warning : this "correction" contains a 2-body interaction which is often omitted !!!!!!

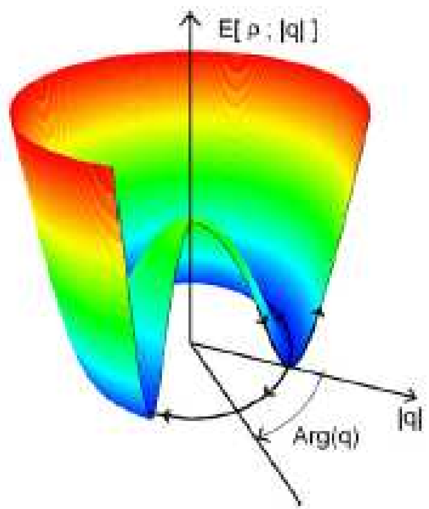
Except for translation, the transformation to the intrinsic system and the construction of a collective Hamiltonian are difficult.

Because

A complete separation between collective and intrinsic degrees of freedom can not be achieved

A more general way to treat symmetry violations is to use projection technique

# The Goldstone boson and the Godstone mode




For dynamically broken symmetry, there must exist a massless boson : the Goldstone boson.

If we put a particle in the Mexican hat potential and treat it within the small –vibration approximation one obtains a zero-frequency mode that corresponds to uniform motion around the hat :the Goldstone boson.

-> In the deformed nuclei we have an excitation spectrum: ie . a rotational band

The collective motion associated to the Goldstone mode in the breaking of the rotational invariance due to deformation is given by the rotations.

The Goldstone mode in an even-even nucleus is the T=0 rotational band 0+, 2+, 4+ …

# A few features associated to symmetry breaking

| Name | Operator | In which nuclei ? | Due to | Order parameter | Goldstone mode |
|---|---|---|---|---|---|
| Translational symmetry | $[H_{HF}, \hat{P}] \neq 0$ | All | Density fluctuation | d | I=1- T=0 |
| Rotational symmetry | $[H_{HF}, \hat{J}^2] \neq 0$ | deformed | Quadrupole vibration I=2+ T=0 | Quadrupole deformation | I=0+,2+,4+ … T=0 |
| Particle number | $[H_{HFBCS}, \hat{N}] \neq 0$ | All but doubly magic | Pair vibrations I=0+ T=1 | gap | I=0+ T=T0,T0±2 , … |

$$d = \left\langle \sum_{k,k'} a_{k'}^{+} a_k - \sum_k a_k^{+} a_k \right\rangle$$

with k related to plane waves

# Projection methods (1/2)

Let's take a symmetry-violating wave function $|\phi\rangle$ for instance HFB wave function

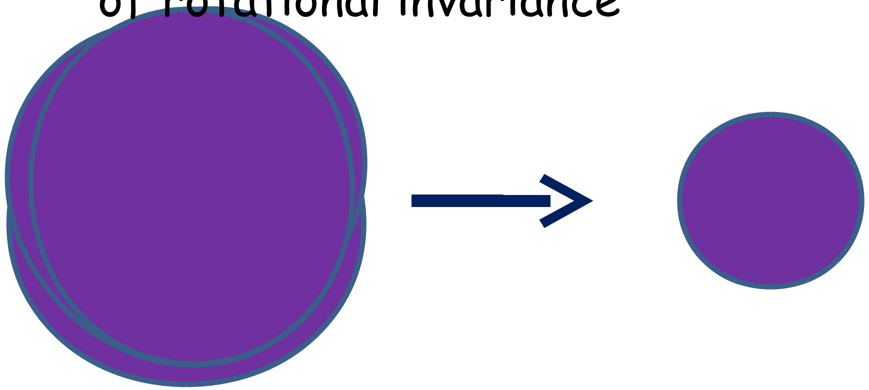
And apply the elements R(Ω) of the group onto $|\phi\rangle$

$$|\phi(\Omega)\rangle = R(\Omega)|\phi\rangle$$

$$|\Psi\rangle = \int d\Omega \; f(\Omega)|\phi(\Omega)\rangle$$

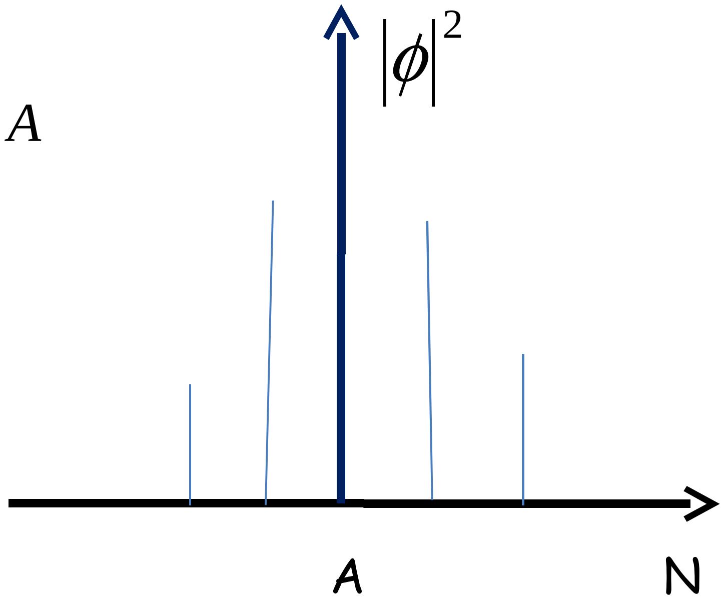
It exists f(□) which causes $|\psi\rangle$ to have the proper symmetry.

Schematic illustration of the restoration of rotational invariance



# Projection methods (2/2)
## Example of particle number projection

Let's take a HFB wave function $|\phi\rangle$ with $\langle N\rangle = A$




$$|\Psi\rangle = \sum_n f_n \hat{P}^{2n} |\phi\rangle$$

$$P^A = \frac{1}{2\pi} \int_0^{2\pi} e^{i\varphi(\hat{N}-A)} d\varphi$$

Of course if we are only interested in $|\Psi\rangle$ with the proper A,
we have fn=0, 2n≠A

"Global Study of quadrupole correlation effects"
M. Bender, G.F. Bertsch and P.-H. Heenen
Phys. Rev. C73, 034322 (2006)

Main goal of the study ?

How large are the correlation energies associated with broken symmetries ?

A 4-steps approach :

1) Constrained HFB calculations
2) Projection onto good particle numbers
3) Projection onto good angular momentum
4) Axial quadrupole configuration mixing

## Eigenstates of J2, Jz N and Z

$$\left| JMKN_0Z_0q \right\rangle = P^J_{MK} P_{N_0} P_{Z_0} \left| \Phi_q \right\rangle$$

HFB state,
(deformation q)

Angular-momentum projection

Huge simplifications in the axial case:
only one Euler angle, and no K mixing

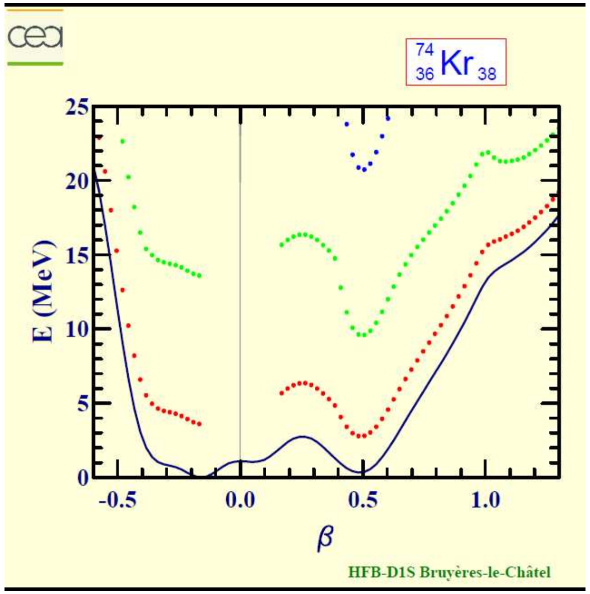
Particle number projection

+

The next step in treating quadrupole correlations is to mix configurations of different deformations. (Generator Coordinate Method)

$$\left| JMKN_0Z_0k \right\rangle = \sum_q f_{Jk}(q) \left| JMKN_0Z_0q \right\rangle$$

# Configuration mixing : why ?

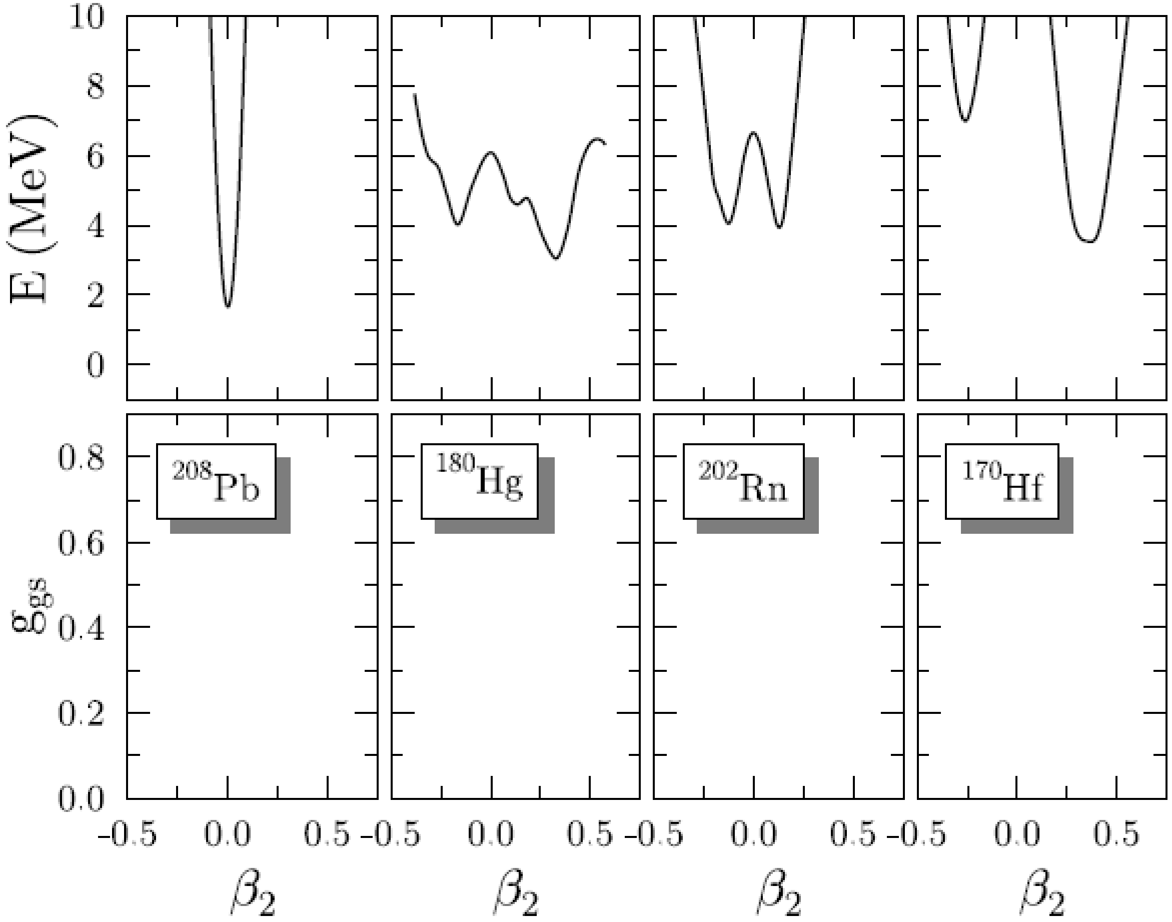



Why ?

-Take into account more correlations

- give access to ground state and excited states

## Typical situations



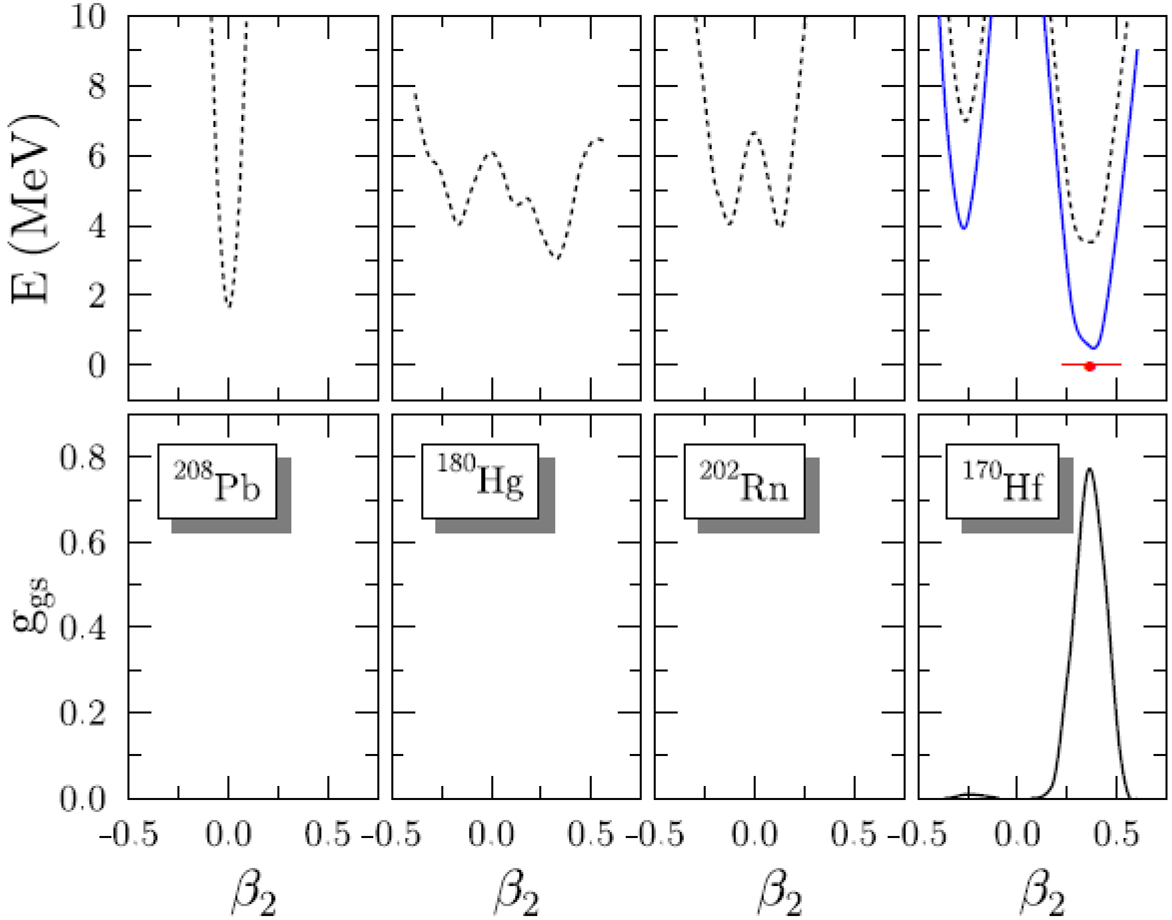

HFB results projected on N and Z

+ projection on J

+ configuration mixing

M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

## Typical situations

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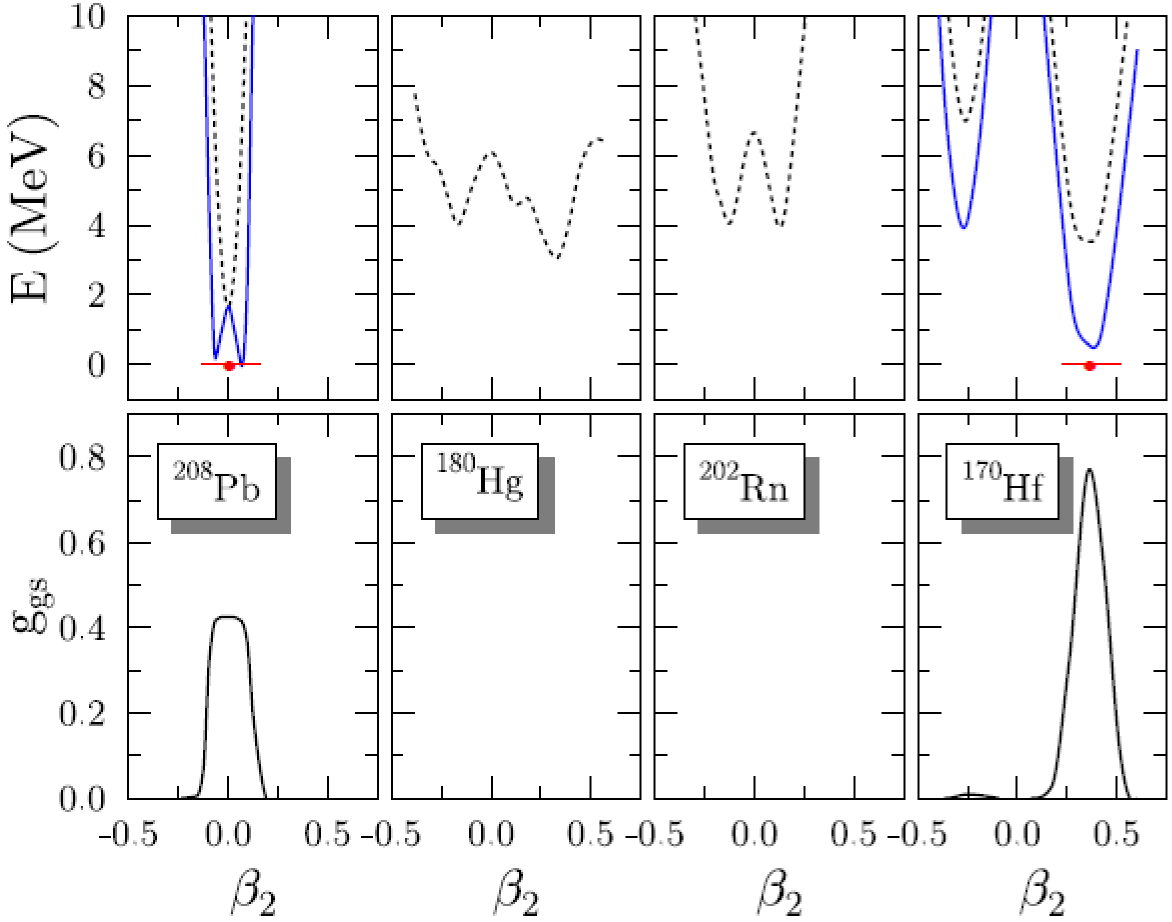


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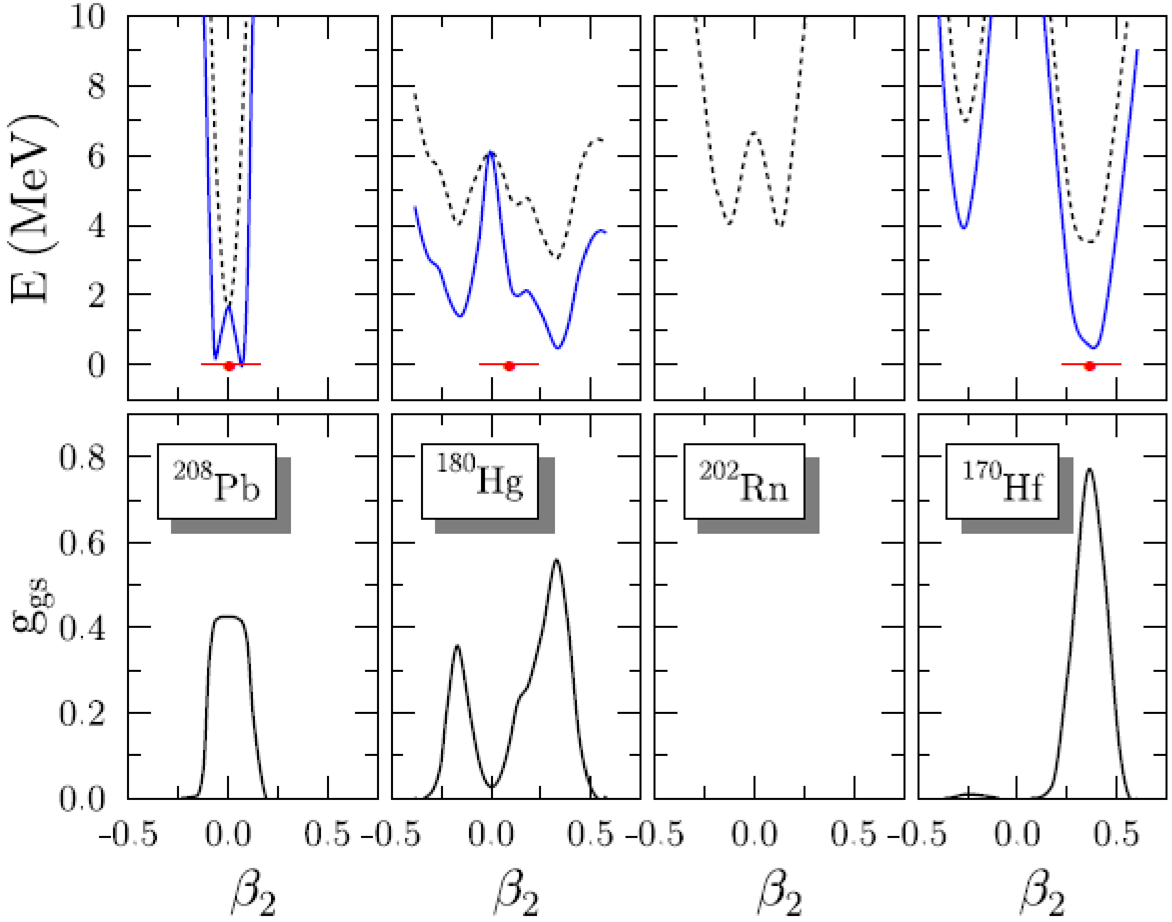


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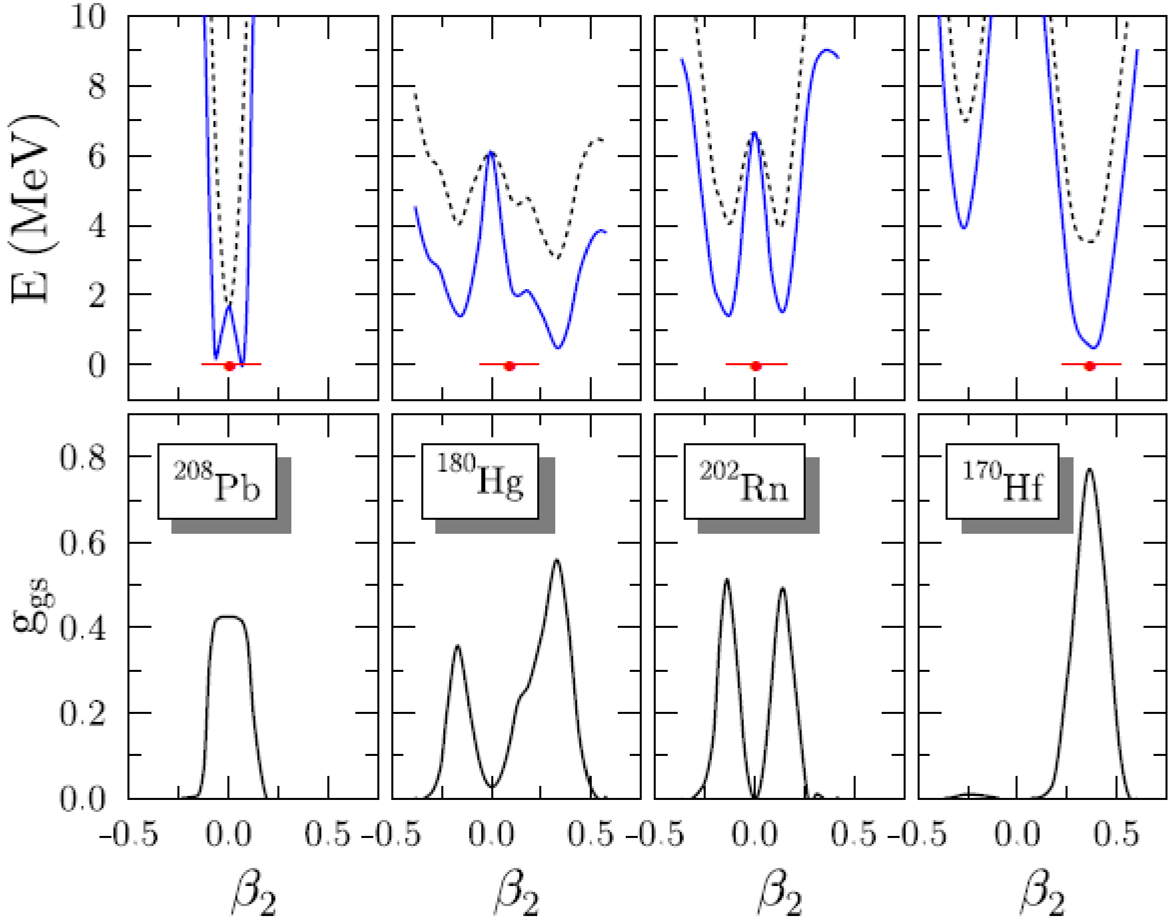


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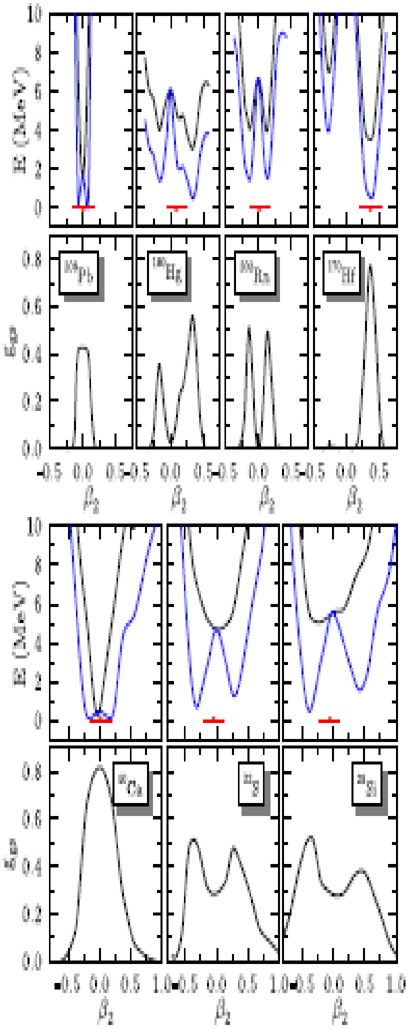
# Orders of magnitude

## Typical Situations



| nucleus | $E_{def}$ | $E_{J=0}$ | $E_{GCM}$ | $E_{corr}$ |
|---|---|---|---|---|
| $^{208}$Pb | 0.0 | 1.7 | 0.0 | 1.7 |
| $^{180}$Hg | 3.0 | 2.6 | 0.5 | 3.1 |
| $^{170}$Hf | 12.2 | 2.9 | 0.5 | 3.4 |
| $^{202}$Rn | 2.6 | 2.7 | 1.4 | 4.0 |
| $^{48}$Ca | 0.0 | 1.4 | 0.7 | 2.0 |
| $^{32}$S | 0.0 | 3.8 | 0.9 | 4.7 |
| $^{28}$Si | 0.7 | 4.2 | 0.6 | 4.9 |

- $E_{def}$: static deformation energy
- $E_{J=0}$: energy gain from projection
- $E_{GCM}$: energy gain from mixing projected states
- $E_{corr} = E_{J=0} + E_{GCM}$: total dynamical correlation energy

M. B., G. F. Berts From M. Bender

## State of the art calculations example 2
## J.-P. Delaroche et al., PRC 81 014303 (2010)

A **systematic study** of low-energy nuclear structure has been carried out using the 5DCH (5 dimensional collective Hamiltonian ) formalism based on HFB basis states and the D1S interaction

**Results for nuclei with Z=10 -110 and N < 200**

* Ground state : rc, S2n, S2p
  -> Ecor, Q20

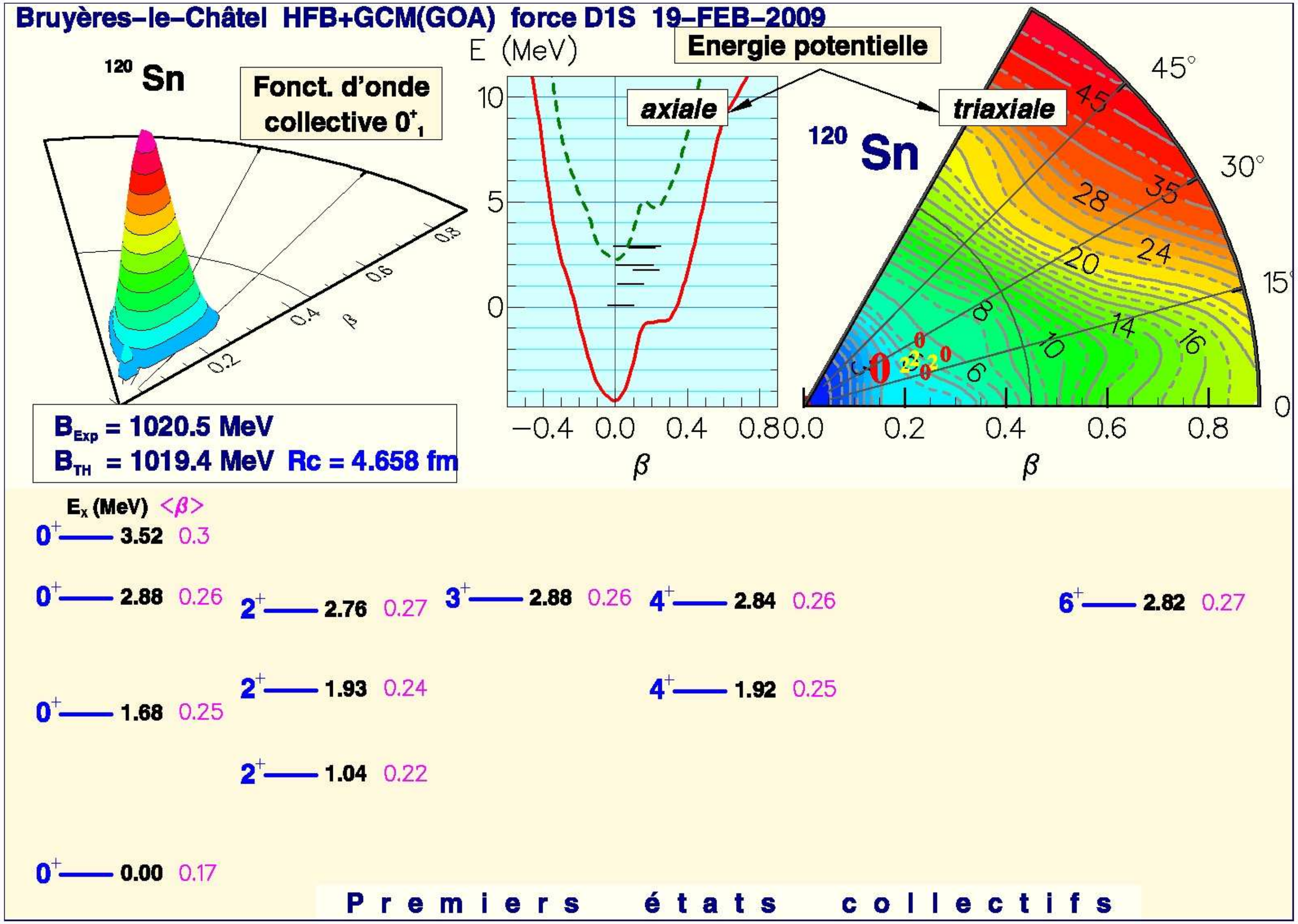
* Y-rast band 0+1, 2+1, 4+1, 6+1 energy, transition probabilities, quadrupole deformation

* Y-rare states 0+2, 2+2, 2+3

-> **Data available** CEA website
EPAPS repository

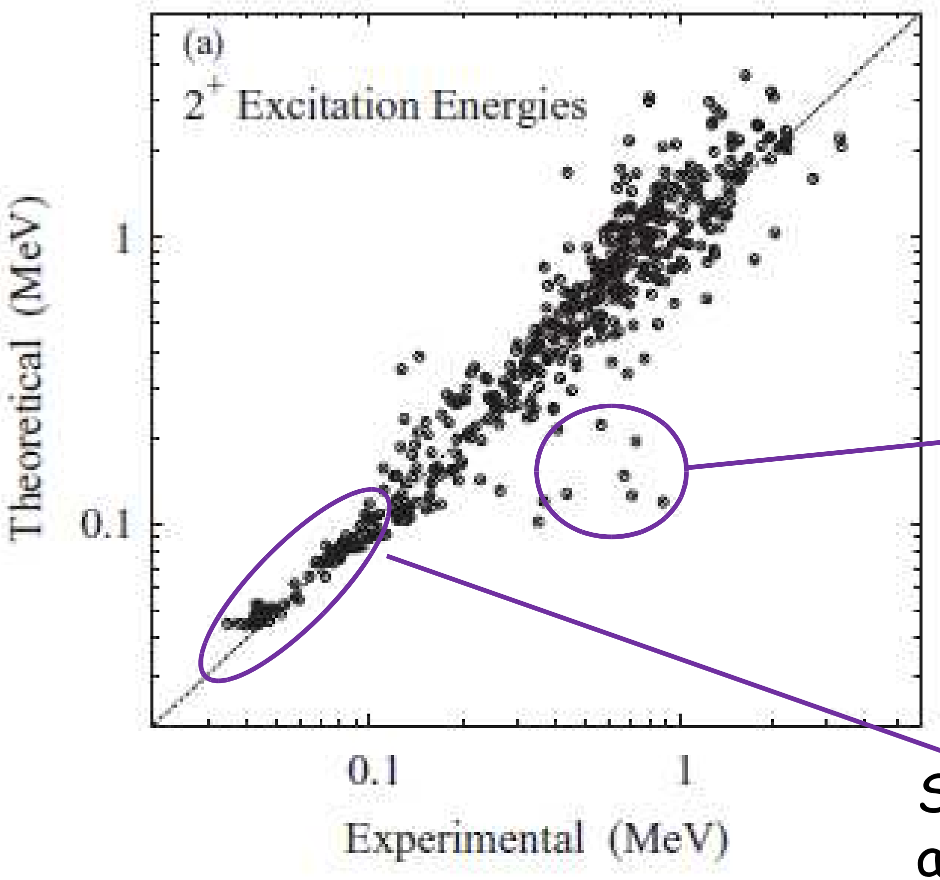
http://www-phynu.cea.fr/HFB-5DCH-table.htm

http://link.aps.org/supplemental/10.1103/PhysRevC.81.014303



Bruyères-le-Châtel HFB+GCM(GOA) force D1S 19-FEB-2009
120 Sn
Fonct. d'onde collective 0+1
E (MeV)
Energie potentielle
axiale
triaxiale
120 Sn
β
45°
30°
15°
B_Exp = 1020.5 MeV
B_TH = 1019.4 MeV Rc = 4.658 fm
Ex (MeV) <β>
0+ 3.52 0.3
0+ 2.88 0.26
2+ 2.76 0.27
3+ 2.88 0.26
4+ 2.84 0.26
6+ 2.82 0.27
2+ 1.93 0.24
4+ 1.92 0.25
0+ 1.68 0.25
2+ 1.04 0.22
0+ 0.00 0.17
Premiers états collectifs

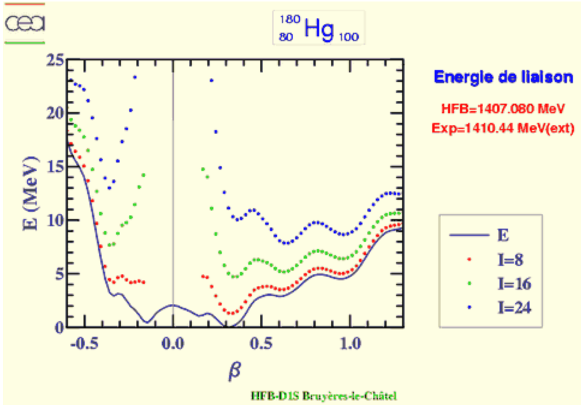
# First 2+ state: Excitation energy

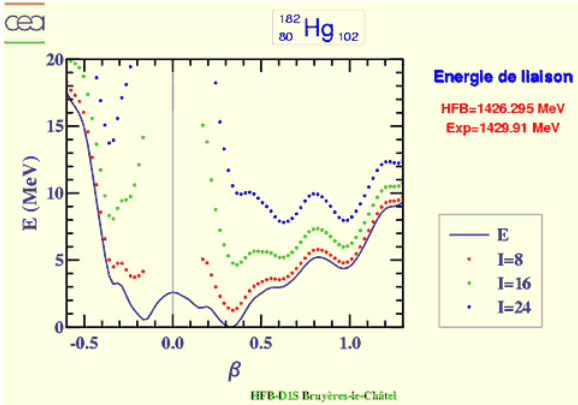


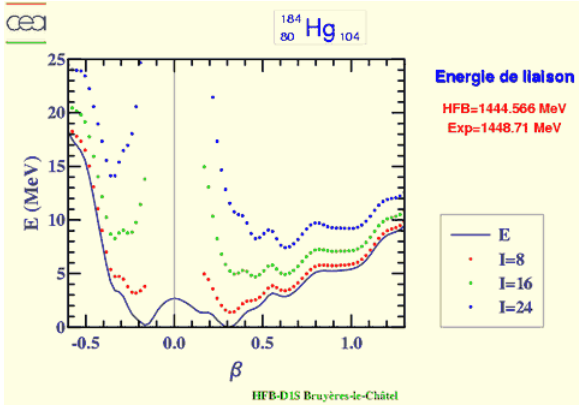

Z = 80 – 82 , N = 104

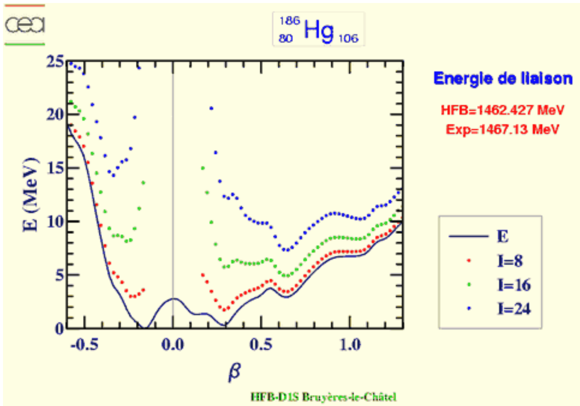
Strongly deformed actinides

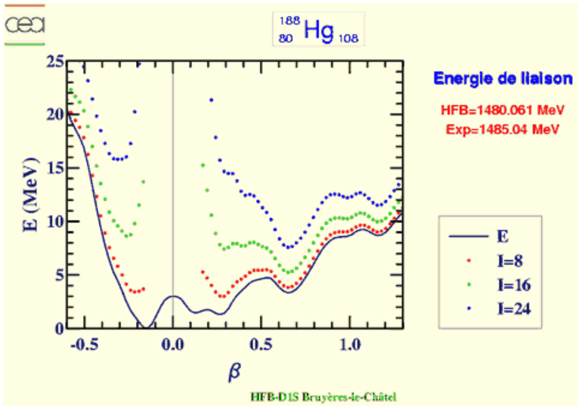
# Shape coexistence in N ~ 104 Hg and Pb isotopes

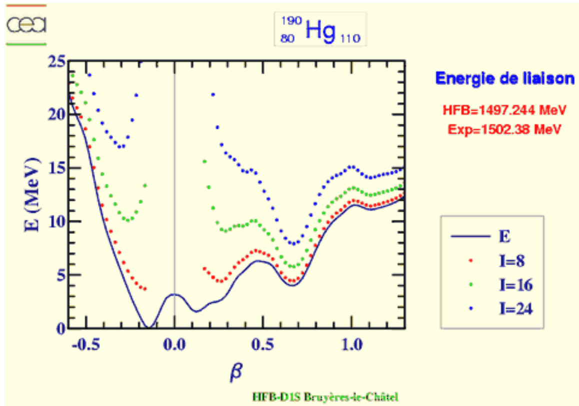



See also J.P. Delaroche *et al.*, PRC (1994)

## Search for β-vibrations

If the spectrum truly exhibits a β-vibrational band, the quadrupole transitions between it and the g.s. should be governed by a single parameter, the quadrupole operator between the two intrinsic states.

$$\left\langle \beta J_\beta \left\| M(E2) \right\| g J_g \right\rangle = (2J_g+1)^{1/2} (J_g 020 | J_\beta 0) \left\langle \beta \left| M(E2) \right| g \right\rangle$$

$$|M_{02}| = |M_{20}| = \sqrt{\frac{7}{10}} |M_{22}|$$

The ratio of these three quantities to their total has been plotted. The fraction are given by the distance to a side of the triangle.

# Search for □-vibrations

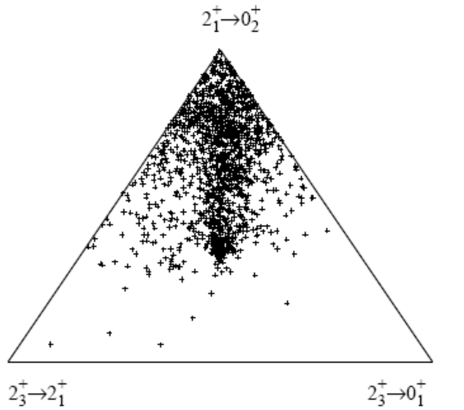



FIG. 23: Crossover matrix elements. Relative magnitudes of the three quantities $|M_{02}|, |M_{20}|, \sqrt{\frac{7}{10}}|M_{22}|$ are shown by distances to the sides of the triangle. The vertexes of the triangle correspond to the case where only the labeled transition is nonzero.

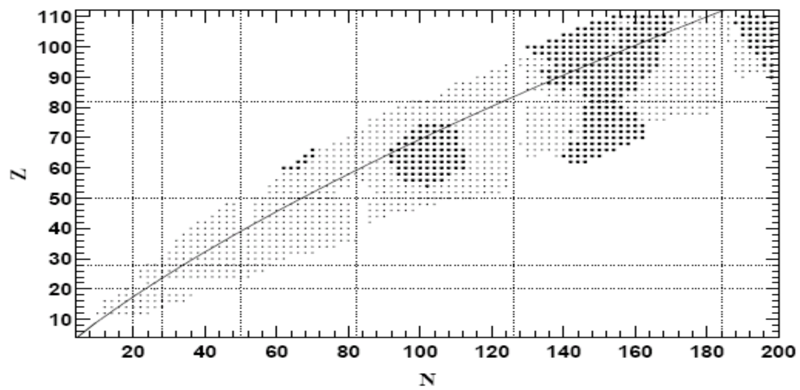



FIG. 24: Chart of nuclei (full circles) in the vicinity of the center point of the triangle shown in Fig. 23. The continuous curve is for the $\beta$-stability line, and dots are for nuclei between driplines as shown in the left-hand panel of Fig. 3.

Relative magnitude are shown by distances to the sides of the triangle

Four regions where the condition is well satisfied, including the strongly deformed rare earths and actinides.

5DCH predicts that the conditions for the existence of the □-vibrational bands should be quite common.

# New developments

1) Full triaxial angular momentum projection (see Bender et al, and Egido et al.)

2) Full variation after projection calculations ★

3) Derivation of a formal framework for GCM-type calculations to avoid surprises from spurious contributions to the energy density functional when using clever tricks originally invented for operators
(D. Lacroix, T. Duguet, M. B., PRC 79 (2009) 044318)

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4) Particle number and angular momentum projection in odd nuclei

5) Projection during reaction mechanisms. What about projection on particle number during fission ?? ★

## Projection after variation

1) Variation

$$\partial\langle\phi|H|\phi\rangle = 0$$

2) Projection

$$P|\phi\rangle$$

Advantages:

simple …

Drawbacks:

violates the variational principle

## Variation after projection

1) Projection

$$P|\phi\rangle$$

2) Variation

$$\partial\langle\phi|PHP|\phi\rangle = 0$$

Advantages:

* proper variational principle

Drawbacks:

* more complicated

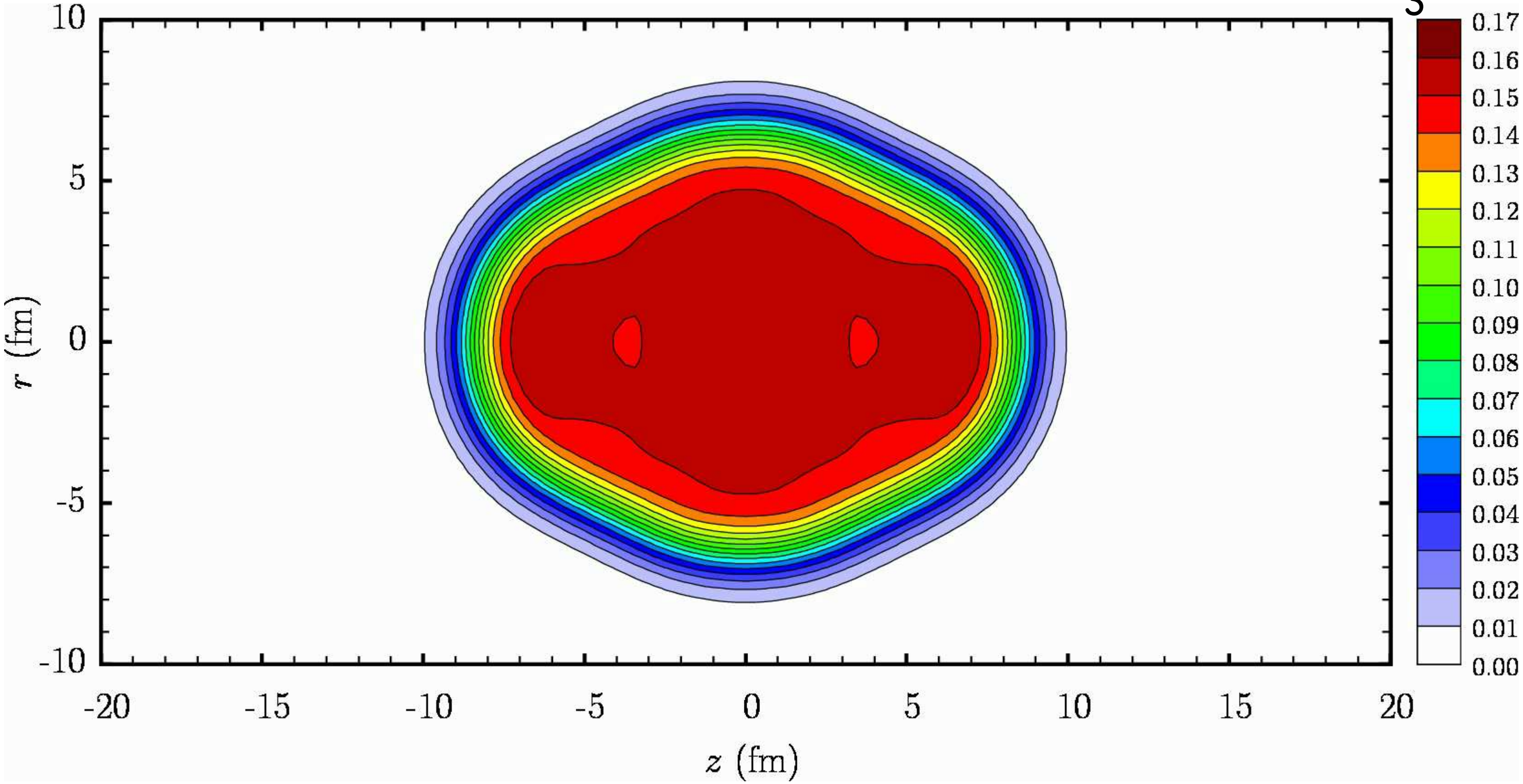
(repeat the variation for all I or N)

* PHP is a multi-body operator …

Nucleon density

240Pu  134Sn + 106Ru

N fm-3




HFB code from J-F. Berger, CEA Bruyères-le-Chatel

## Bibliography

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M. Bender, G.F. Bertsch and P.-H. Heenen
Phys. Rev. C73, 034322 (2006).

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