Symmetry breaking and symmetry restoration in mean-field based approaches

Héloise Goutte
GANIL
Caen, France
goutte@ganil.fr

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

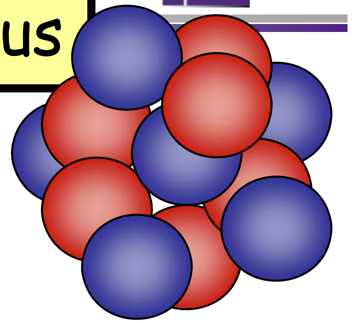
-4) Symmetry restoration

-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

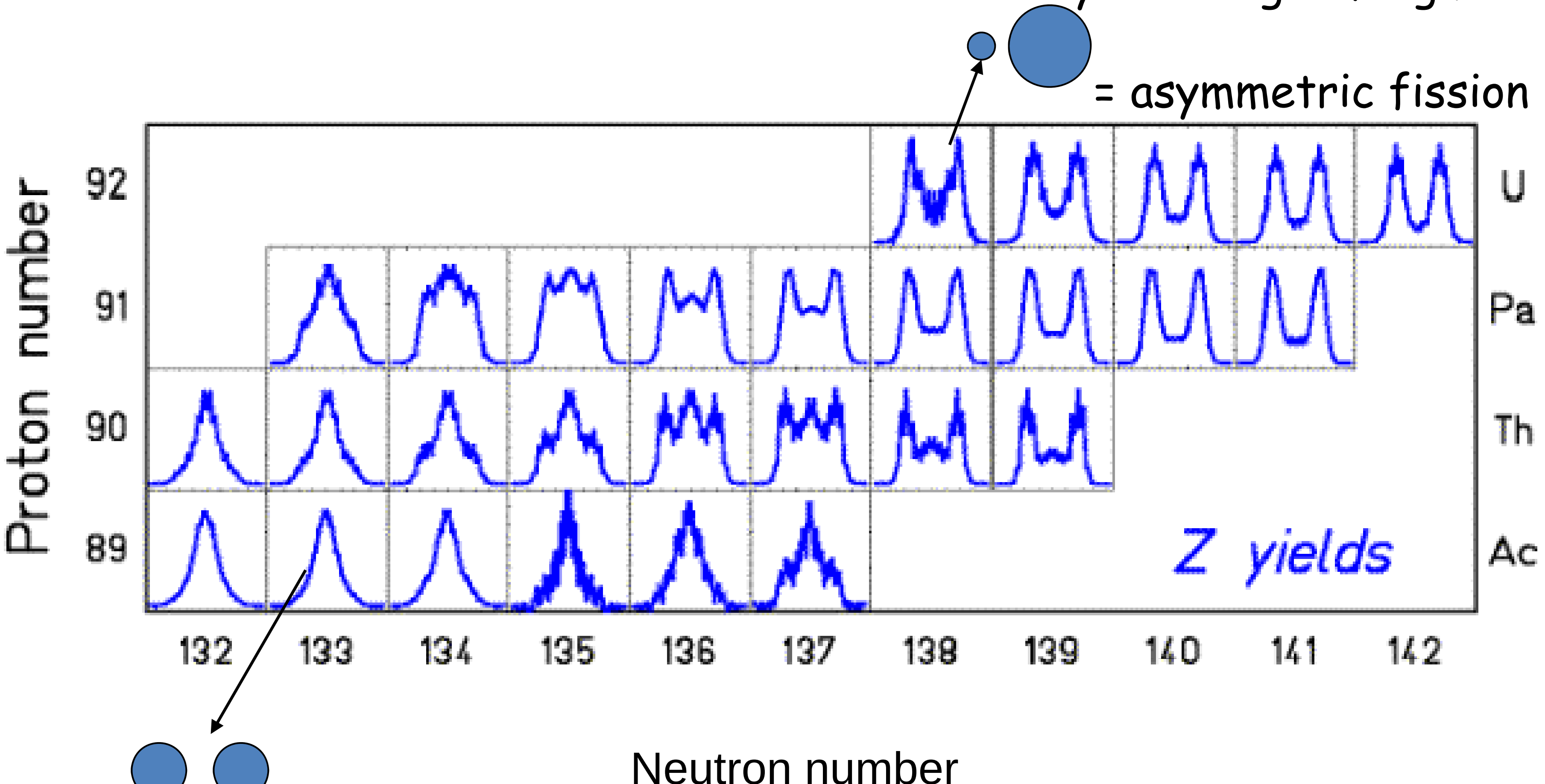
Zero range

Finite range

Example of microscopic effects: Fission fragment yields

A heavy and a light fragment:

= asymmetric fission



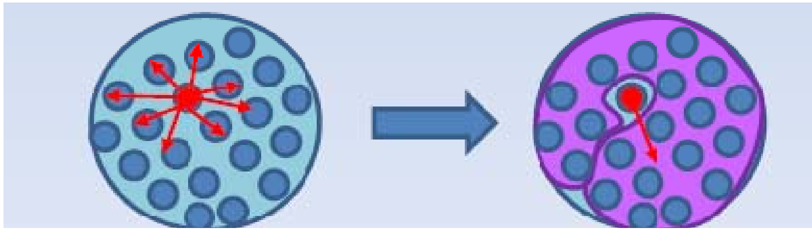
Neutron number

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 $\Phi(x_1, x_2, \ldots, x_A)$ = 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

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

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

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

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

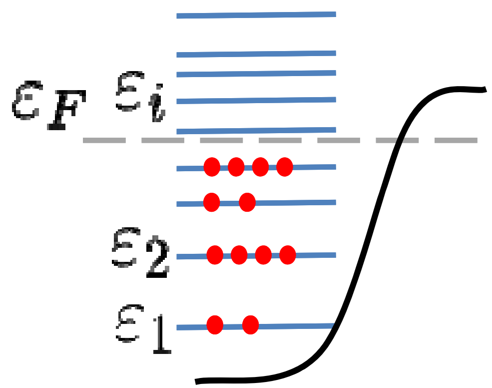
Hartree-Fock equations

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

(A set of coupled Schrodinger equations)

Hartree-Fock potential

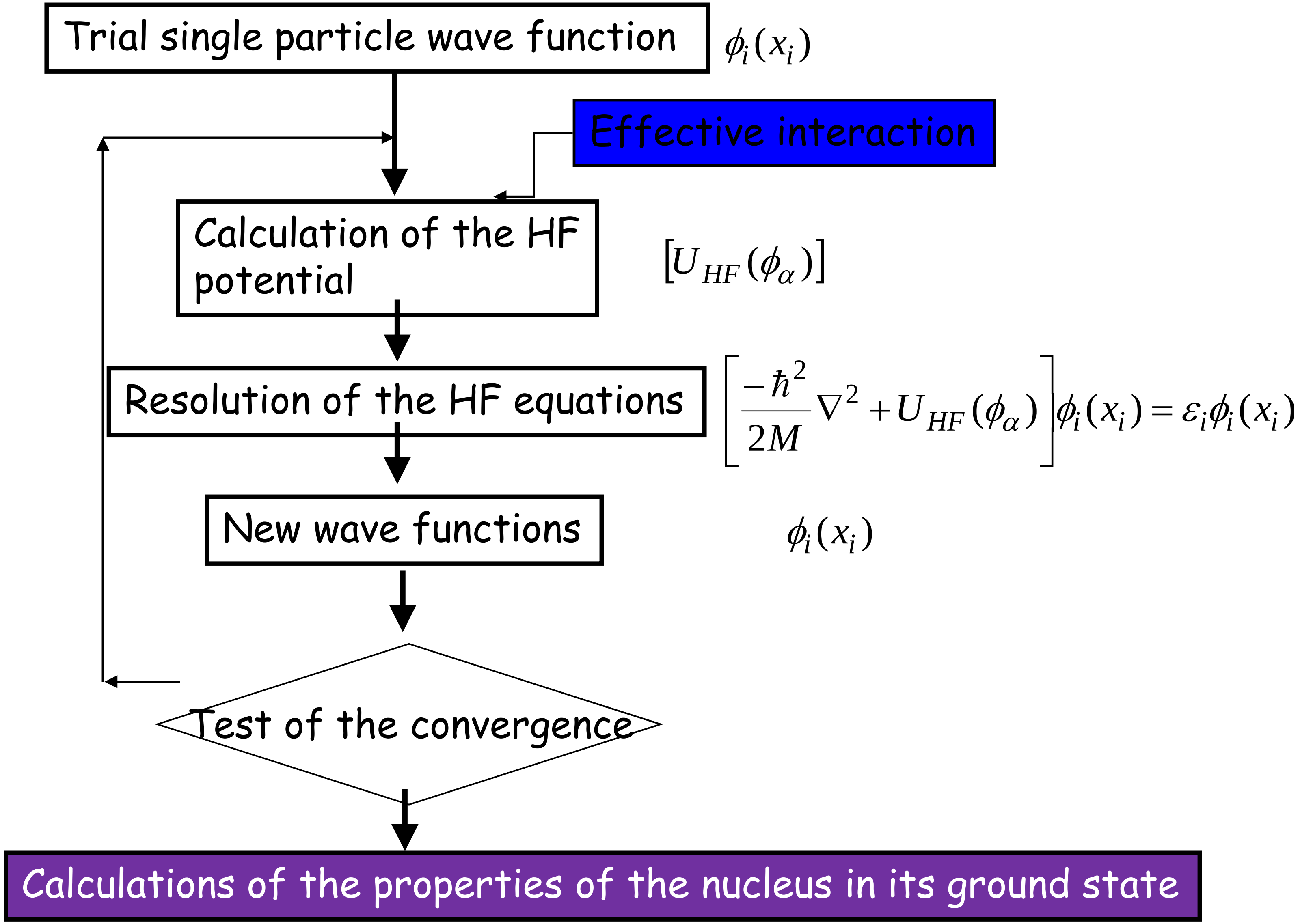
Single particle wave functions



Self consistent mean field :
the Hartree Fock potential depends on the solutions (the single particle wave functions)

-> Resolution by iteration

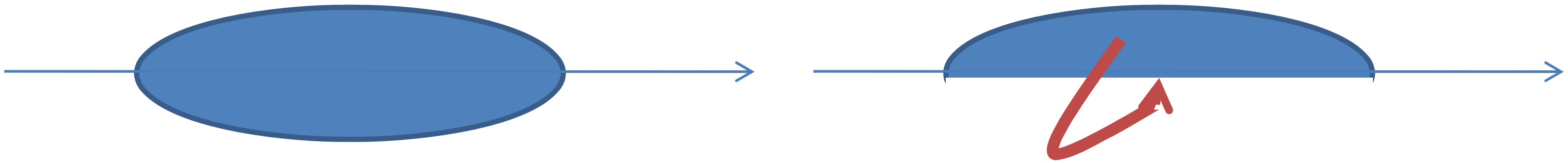
Resolution of the Hartree Fock equations



•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 $\frac{1}{4}$
triaxial shapes but parity enforced : $\frac{1}{2}$

- 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

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

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.

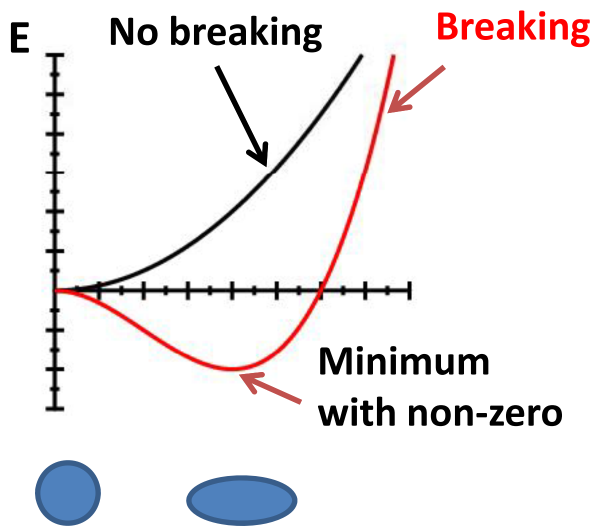
The stronger the correlations, the better such an approximation.

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 breaking



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

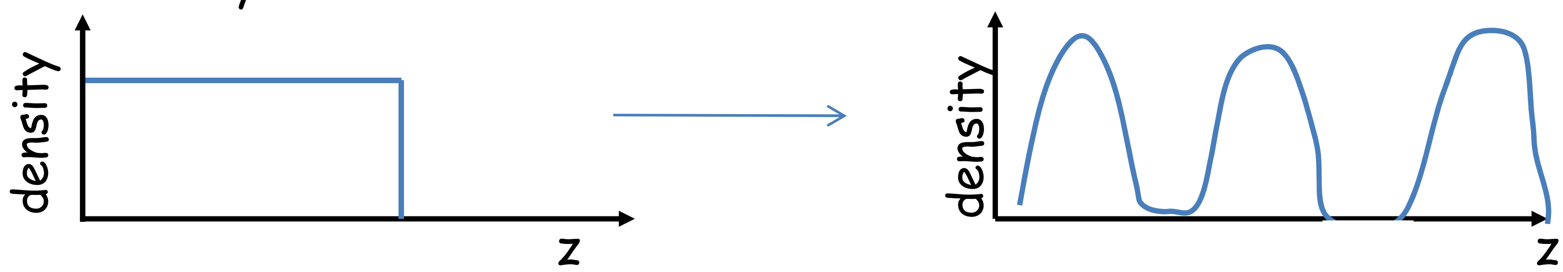
Symmetry violation and phase transition 2/2
Why a phase transition ?

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

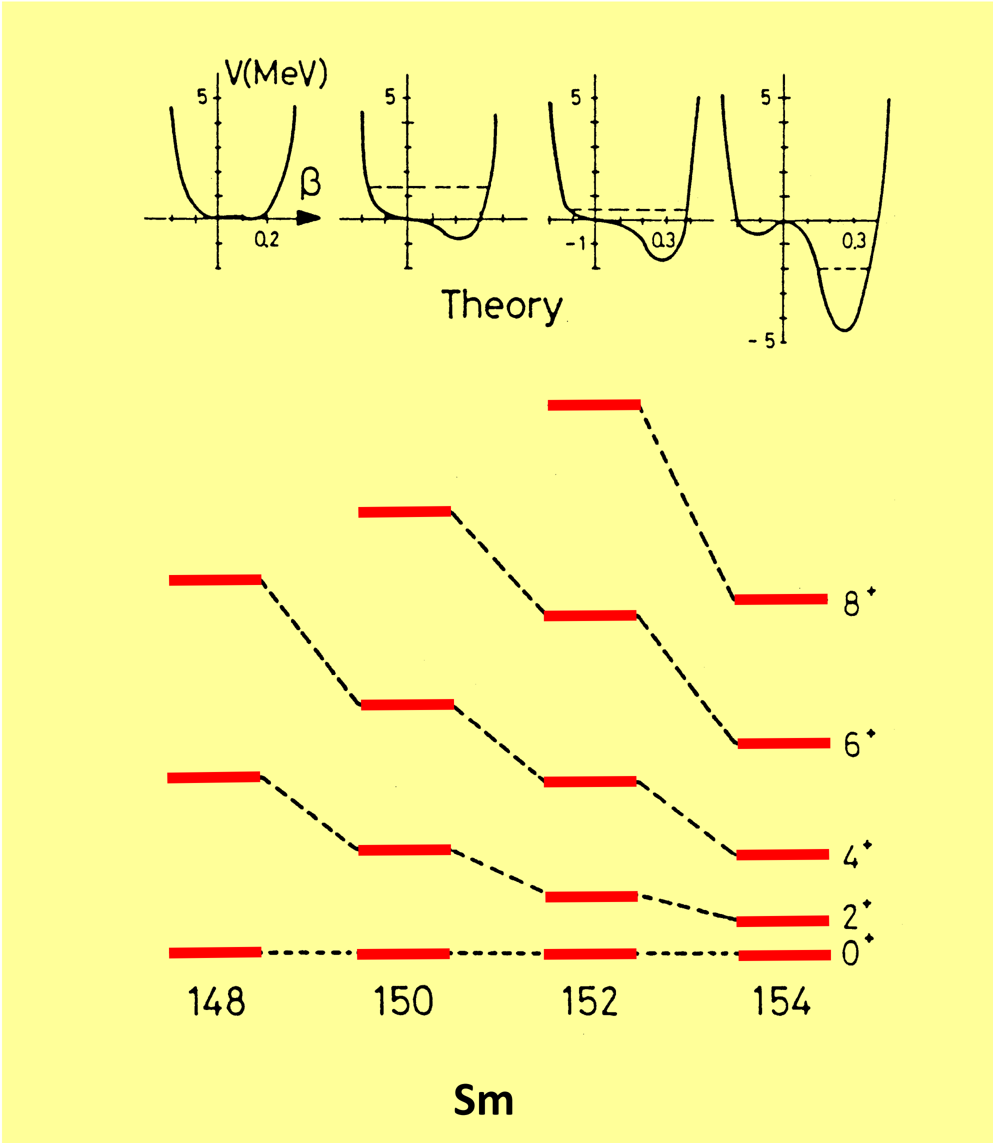
* Breaking of the rotational invariance related to the spherical-deformed transition due to quadrupole vibration

* 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* :

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

With J the moment of inertia

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

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

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

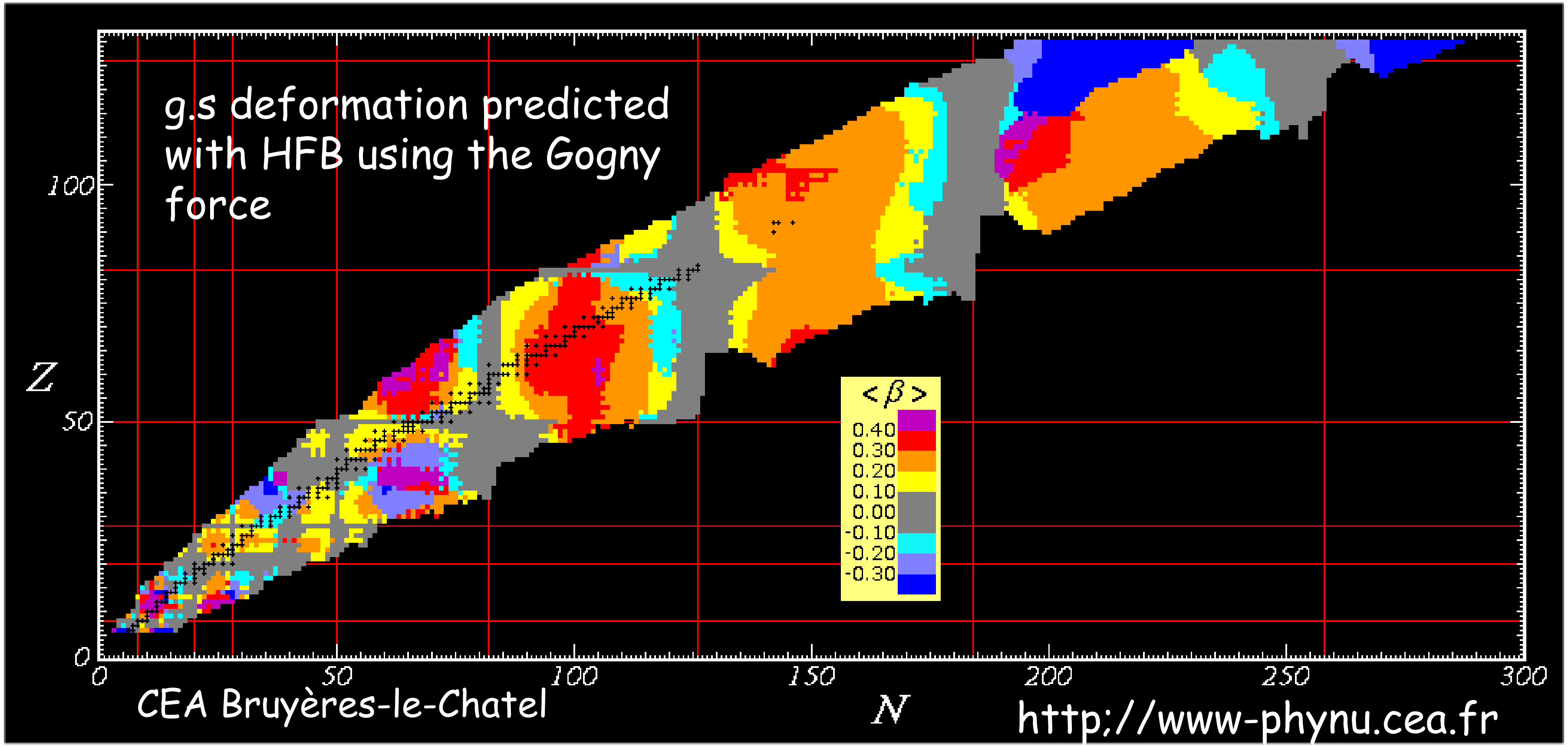
To compare with a wash machine: 1300 tpm

* <u>Mécanique quantique</u> 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



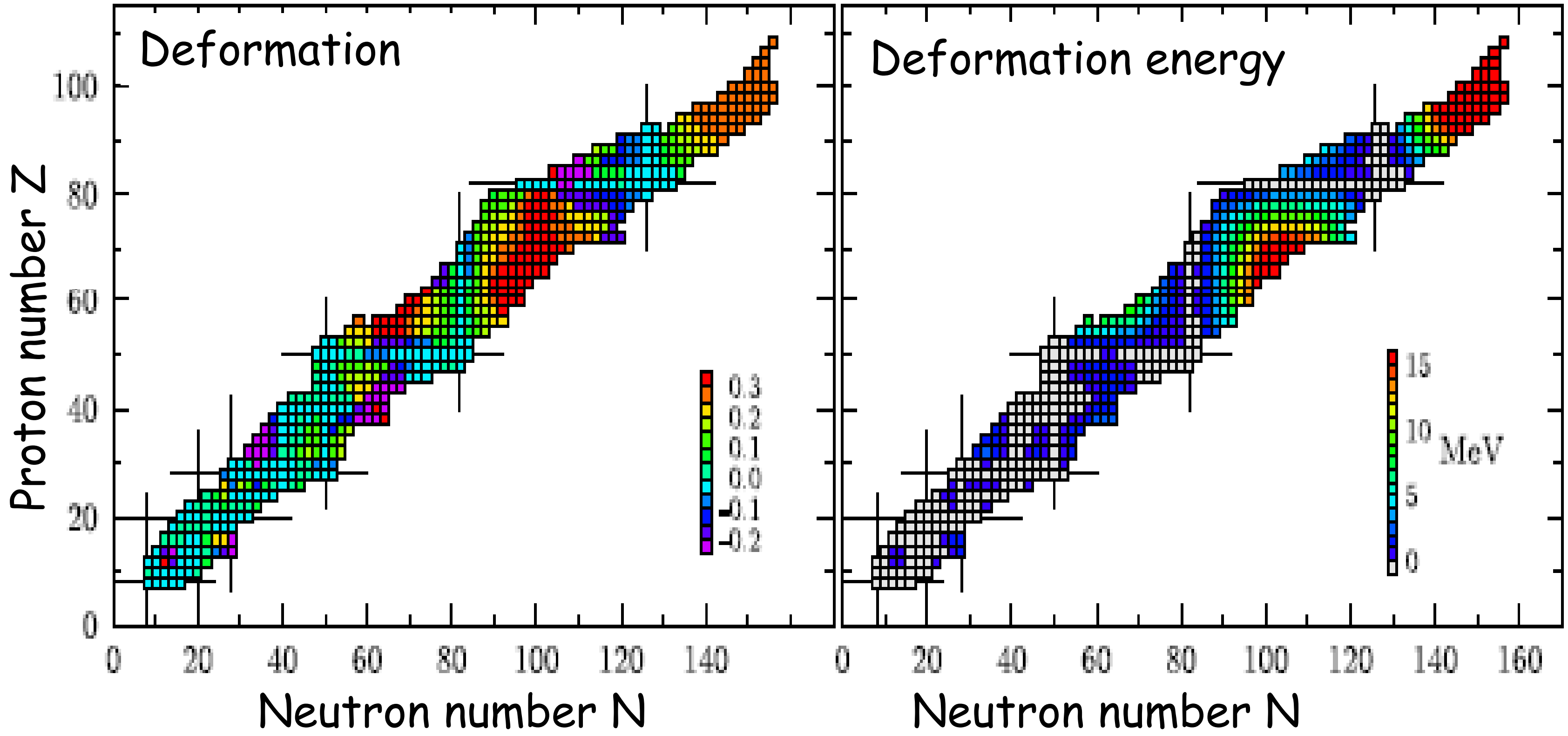
with β characterizing the axial quadrupole deformation

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

Static deformation energy from HFB (1/2)

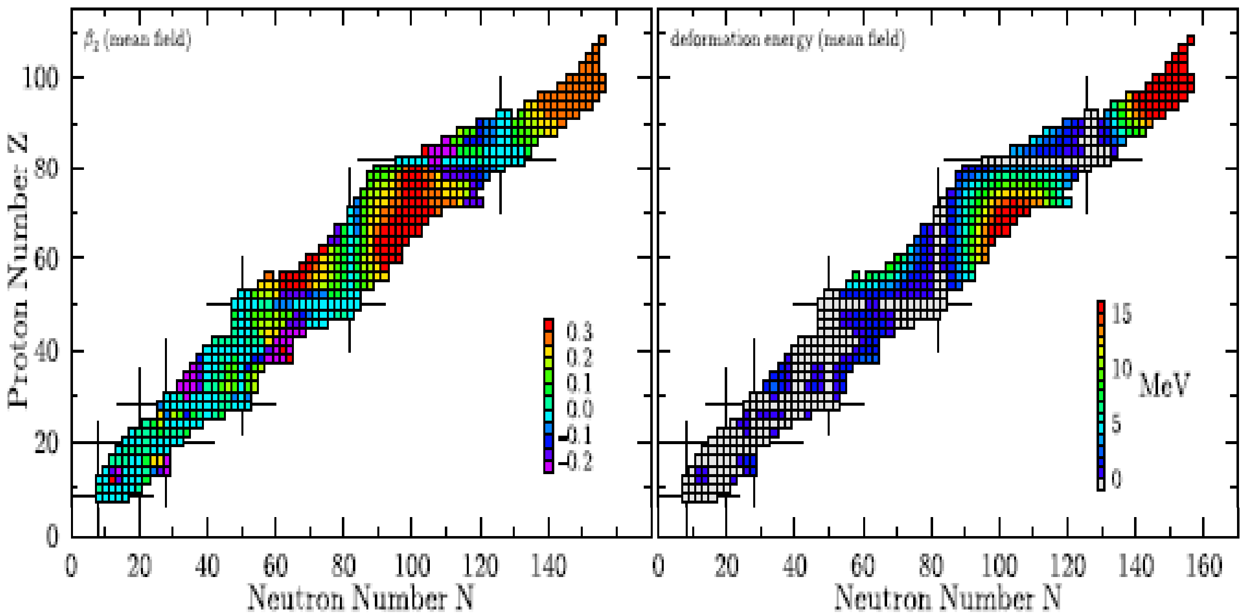
The energy gained by static deformation is :

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



"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>

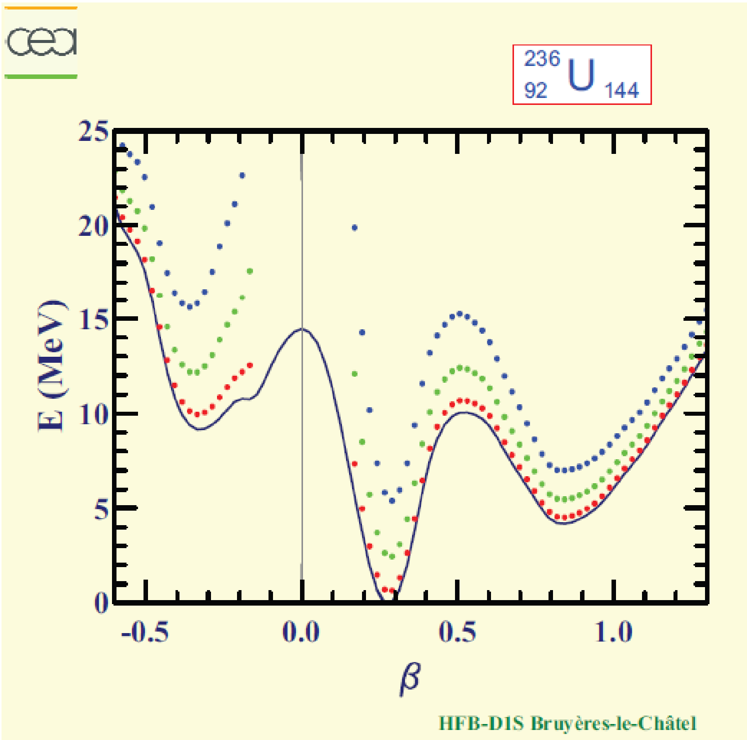
* above Z=50 three regions of well-deformed prolate nuclei : mid shell nuclei

* up to a 15 MeV energy gain

In many nuclei, the minimum of the energy is found for $\beta \neq 0$.

The deformed ground state solution violates the rotational invariance

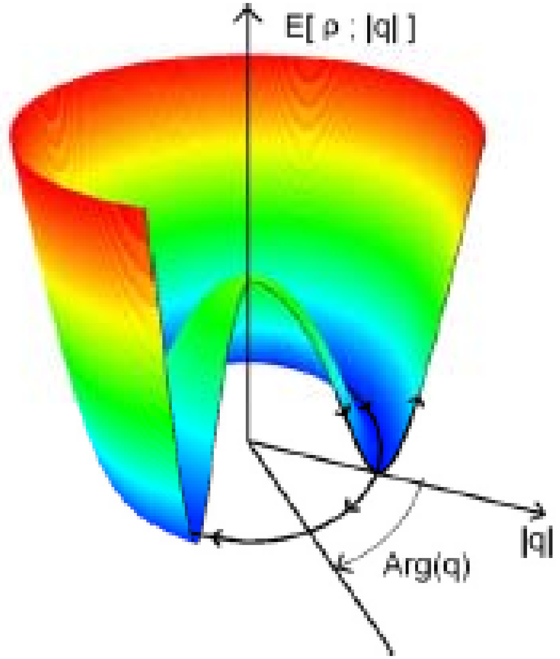
$$\left[H_{HF}, \hat{J} \right] \neq 0$$



Order parameter

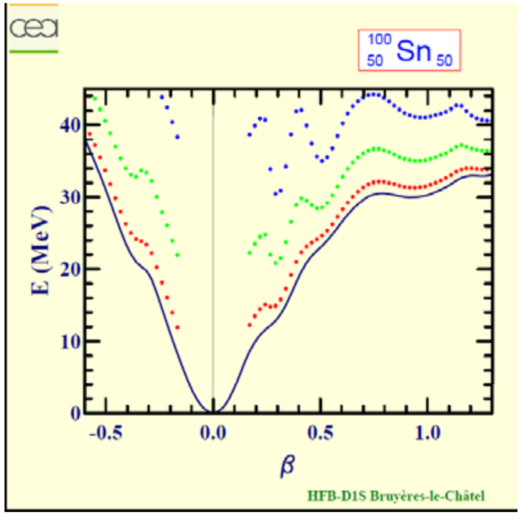
-> the breaking of the symmetry is monitored by the magnitude (and the phase) of an order parameter q.

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

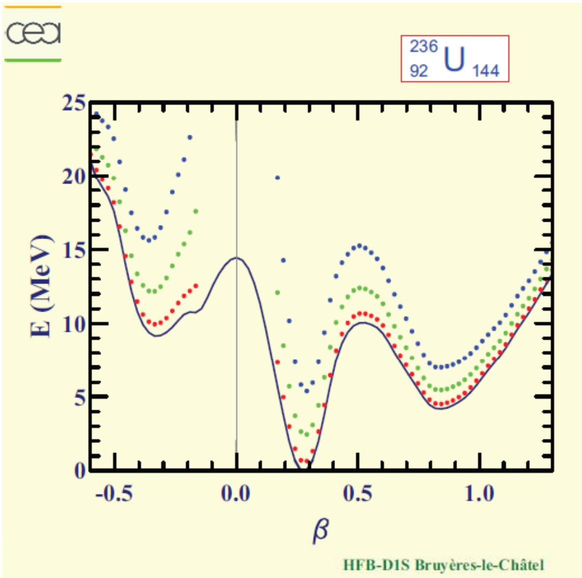


For the spherical-deformed phase transition the order parameter q is the deformation

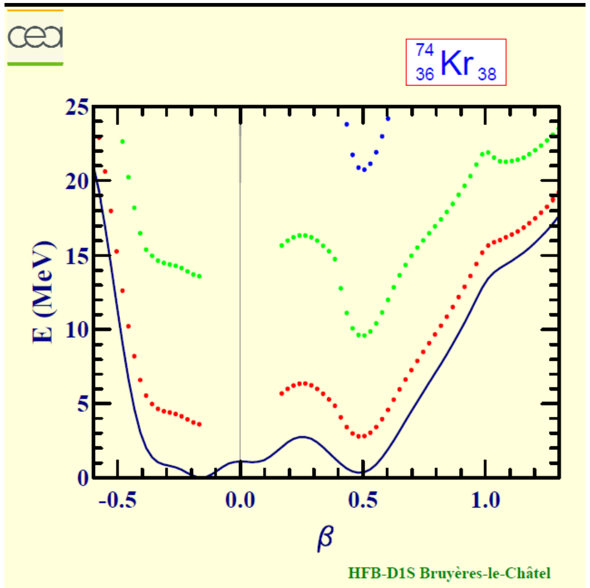
Typical cases of symmetry violations



Rigid spherical:
So symmetry violation



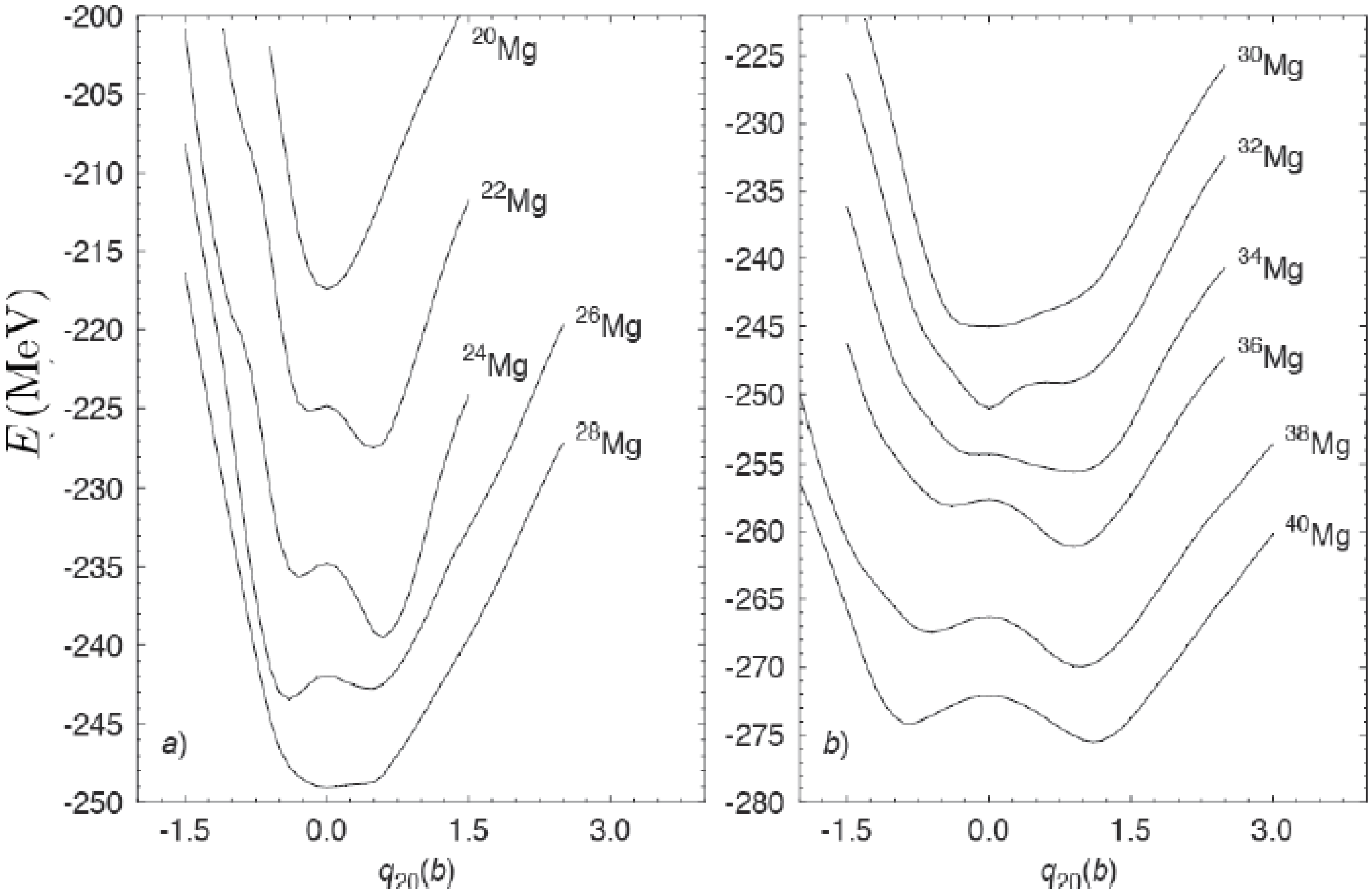
Well-deformed



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

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

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

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

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

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

Restoration of the translational symmetry breaking (2/2)

-> Intrinsic Hamiltonian

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

* 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 !!!!!!

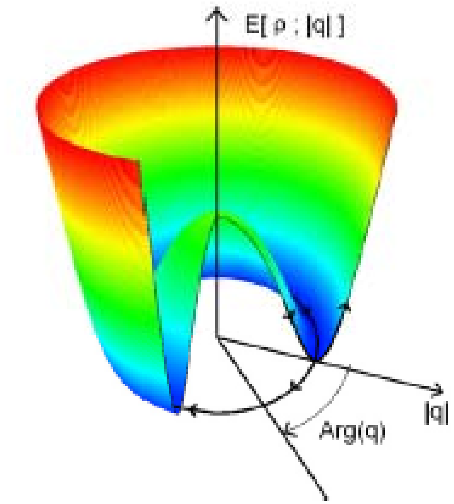
Except for translation, the transformation to the intrinsic system and the construction of a collective Hamiltonian are difficult.

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	$I=0^+$ $T=T_0,T_0\pm2$, …

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

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

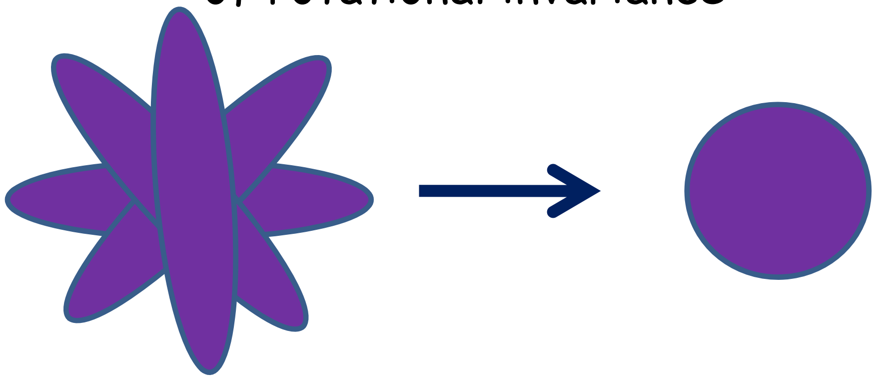
And apply the elements R(Ω) of the group onto $|\phi\rangle$

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

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

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

Schematic illustration of the restoration of rotational invariance

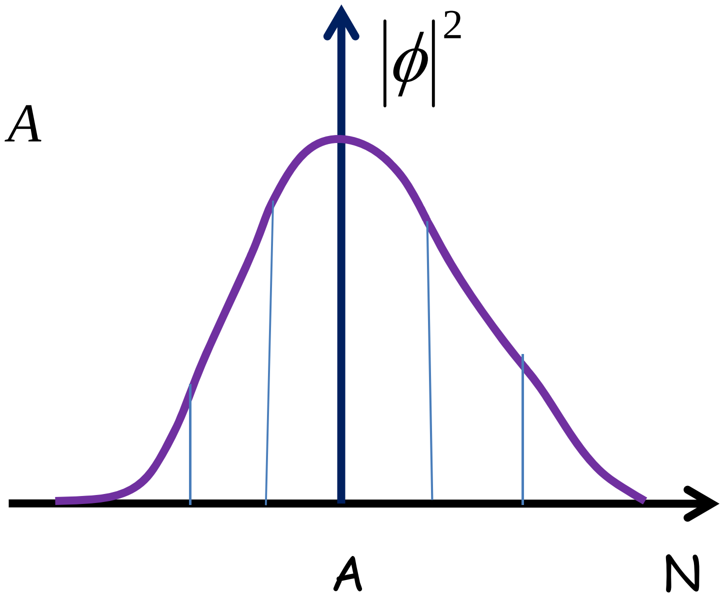


Projection methods (2/2)
Example of particle number projection

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 $f_n=0\ \forall 2n \neq A$

State of the art calculations example 1

"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 J^2, J_z N and Z

$$\left| JMKN_0 Z_0 q \right\rangle = P^J_{MK} P_{N_0} P_{Z_0} \left| \Phi_q \right\rangle$$

Angular-momentum projection

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

Particle number projection

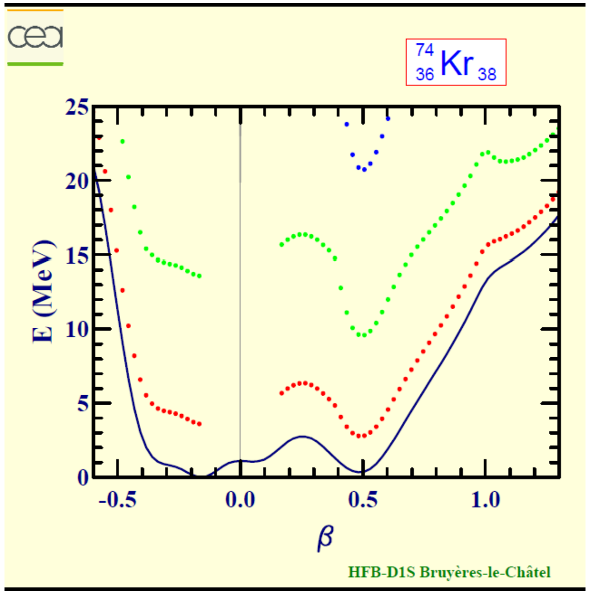
HFB state, (deformation q)

+

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

$$\left| JMKN_0 Z_0 k \right\rangle = \sum_q f_{Jk}(q) \left| JMKN_0 Z_0 q \right\rangle$$

Configuration mixing : why ?

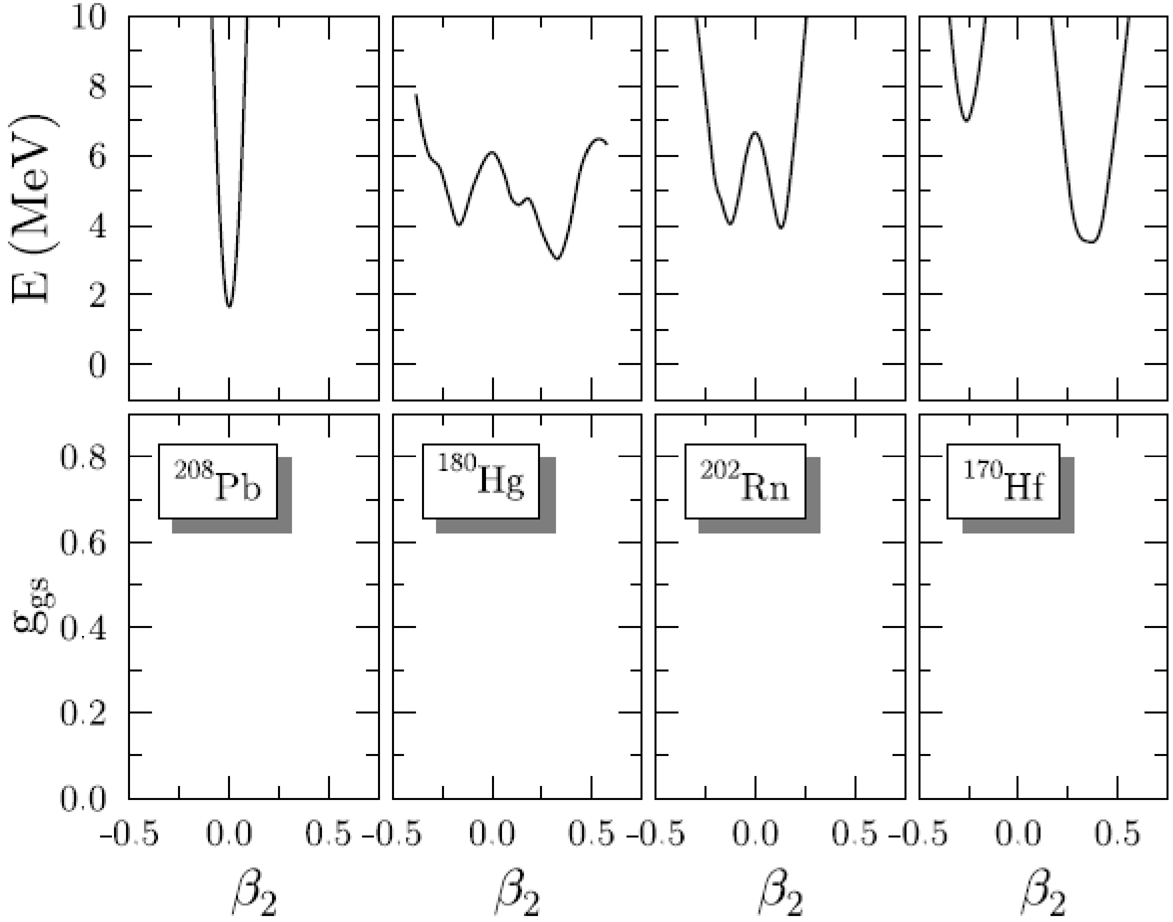


Why ?

-Take into account more correlations

- give access to ground state and excited states

Typical situations



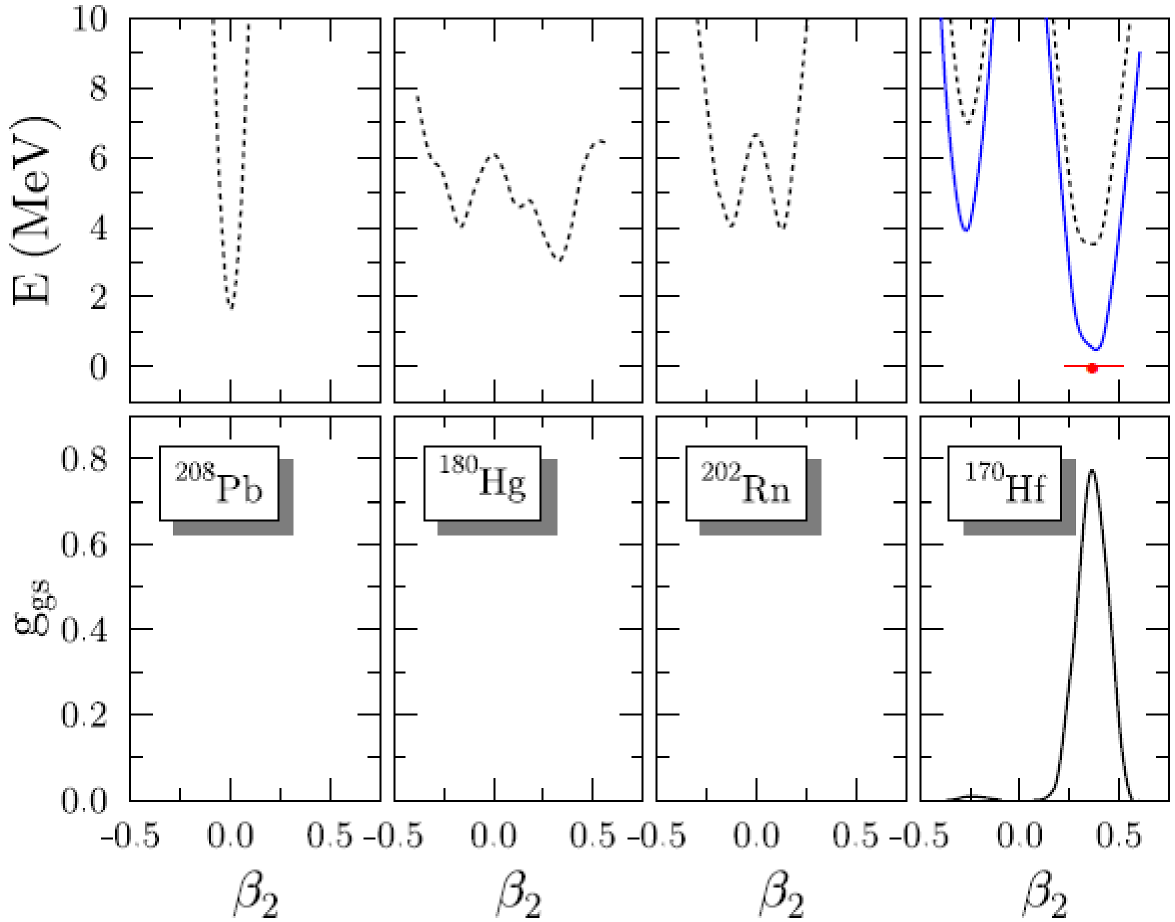
HFB results projected on N and Z

+ projection on J

+ configuration mixing

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

Typical situations



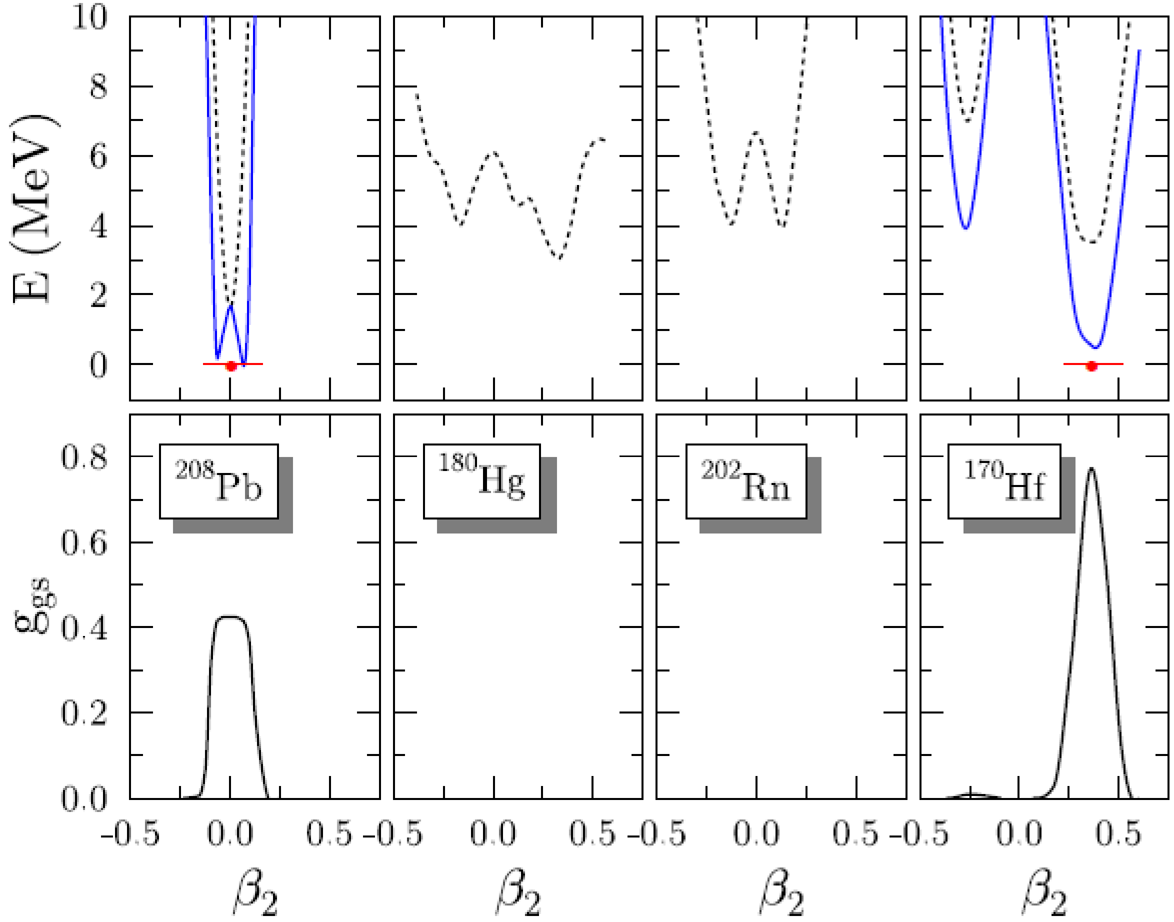
HFB results projected on N and Z

+ projection on J

+ configuration mixing

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

Typical situations



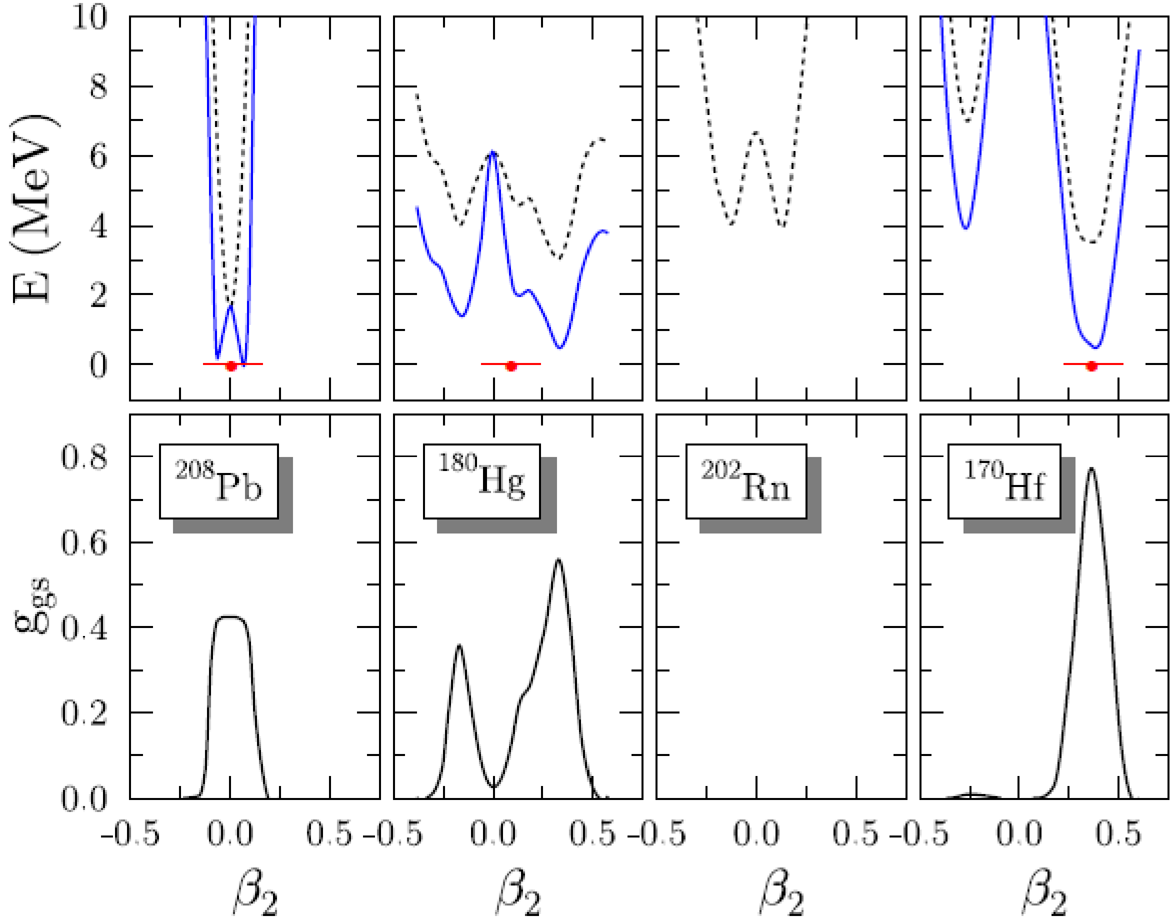
HFB results projected on N and Z

+ projection on J

+ configuration mixing

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

Typical situations



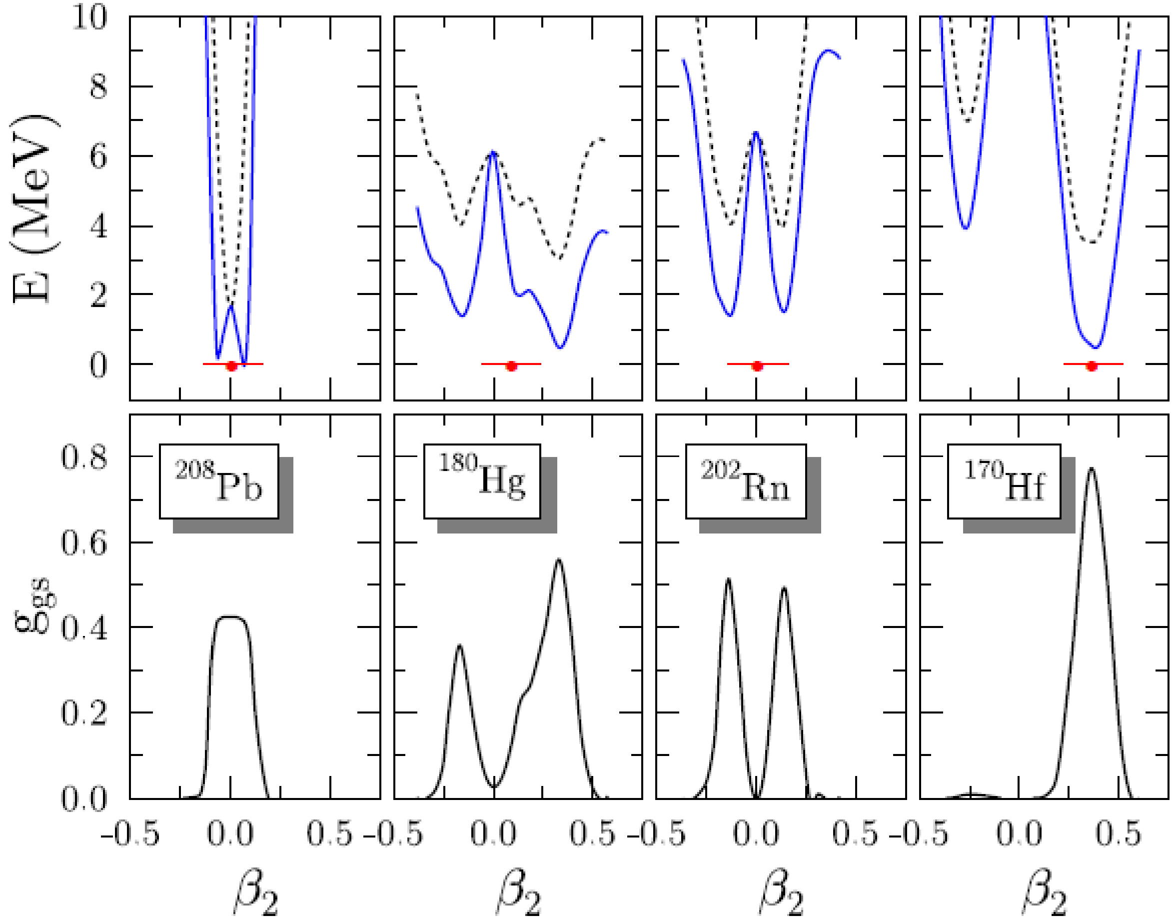
HFB results projected on N and Z

+ projection on J

+ configuration mixing

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

Typical situations



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

Orders of magnitude

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. Bertsch, P.-H. Heenen, Phys. Rev. C. 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

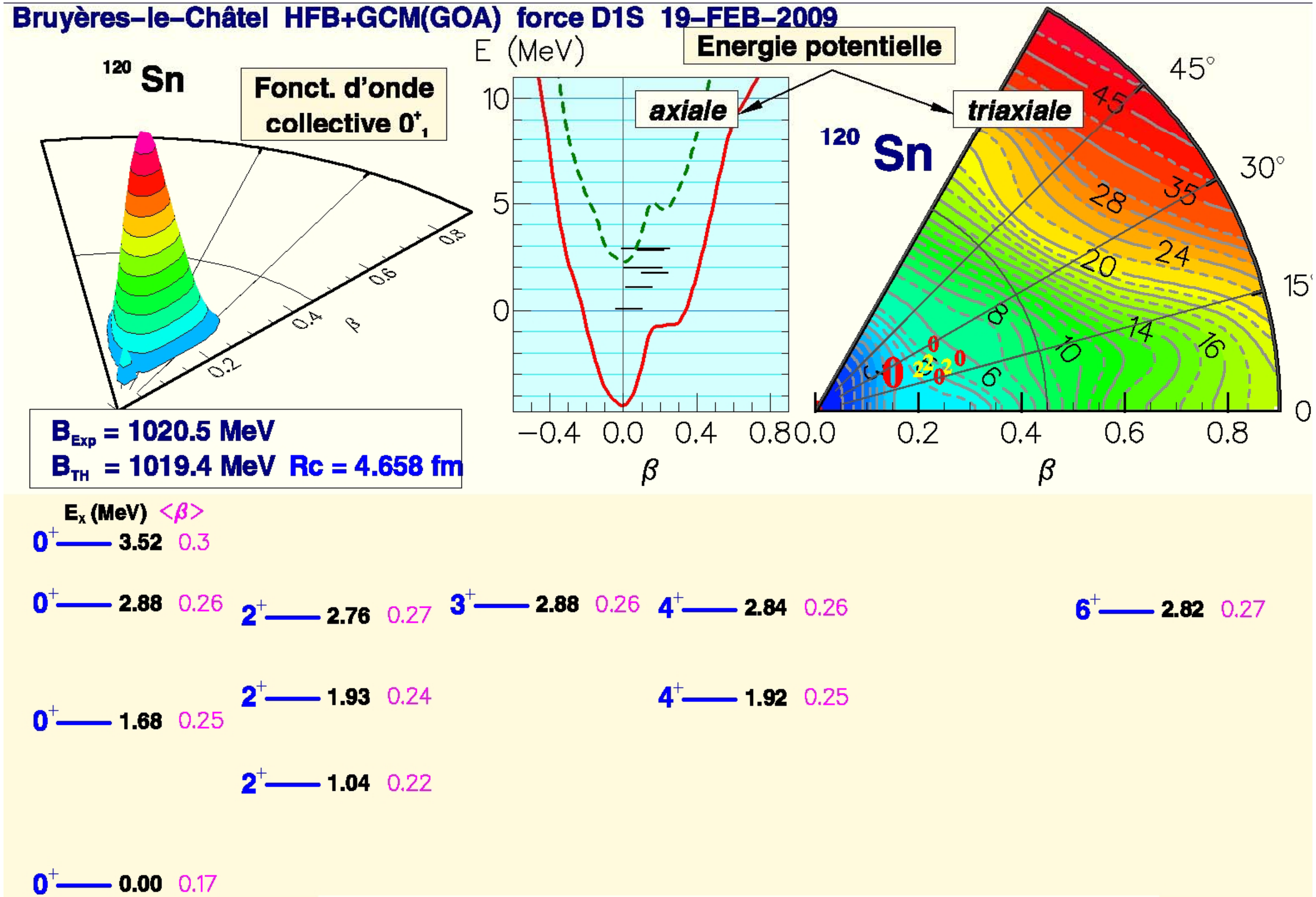
Results for nuclei with Z=10 -110 and N < 200

* Ground state : r_c, S_{2n}, S_{2p}
  -> E_{cor}, Q_{20}

* Y-rast band 0^+_1, 2^+_1, 4^+_1, 6^+_1 energy, transition probabilities, quadrupole deformation

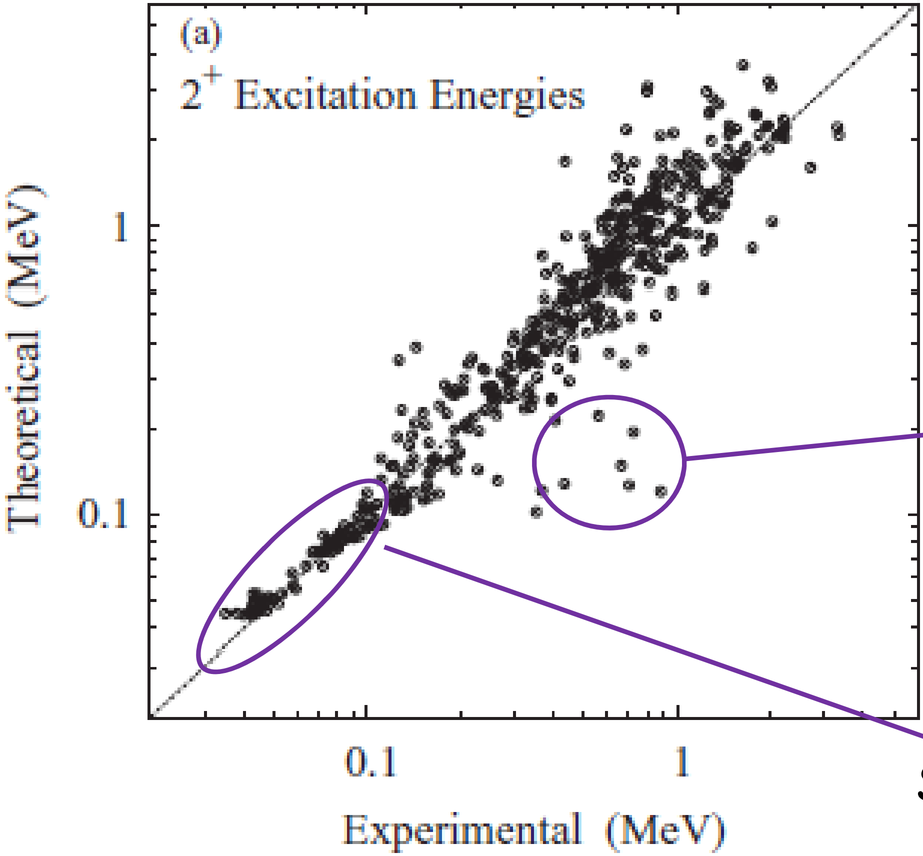
* Y-rare states 0^+_2, 2^+_2, 2^+_3

-> **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



Premiers états collectifs

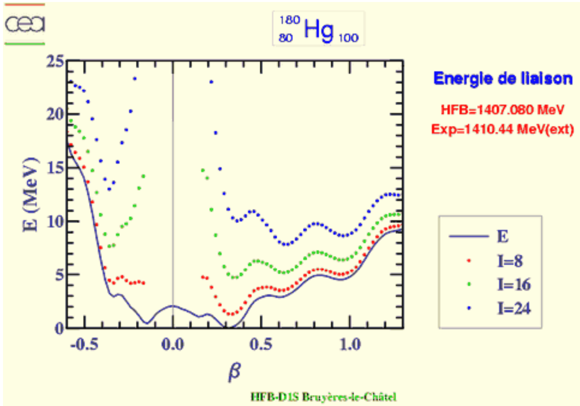
First 2^+ state: Excitation energy

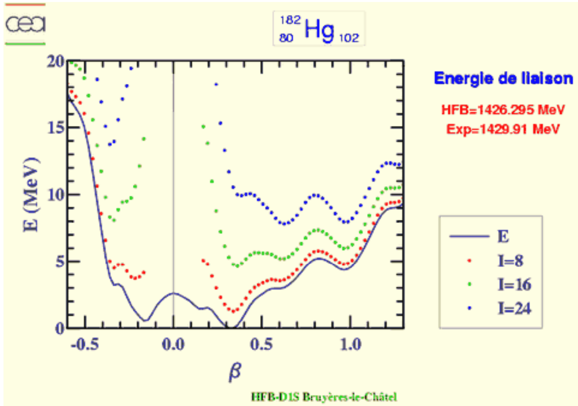


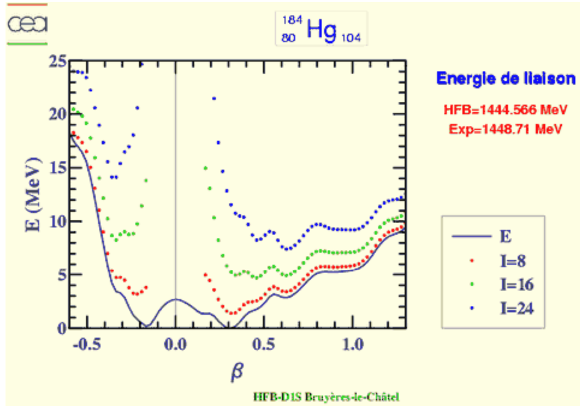
Z = 80 – 82 , N = 104

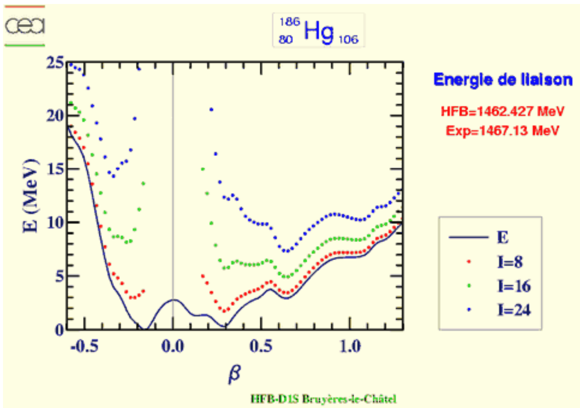
Strongly deformed actinides

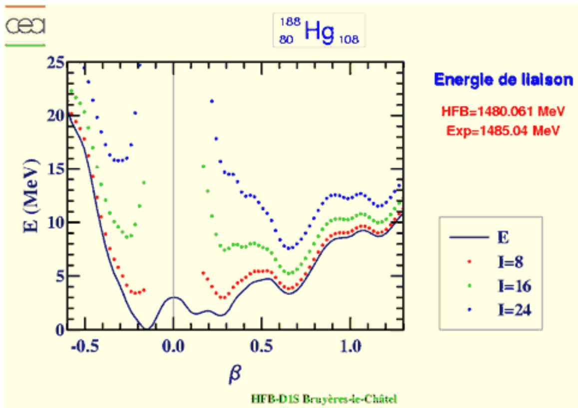
Shape coexistence in N ~ 104 Hg and Pb isotopes

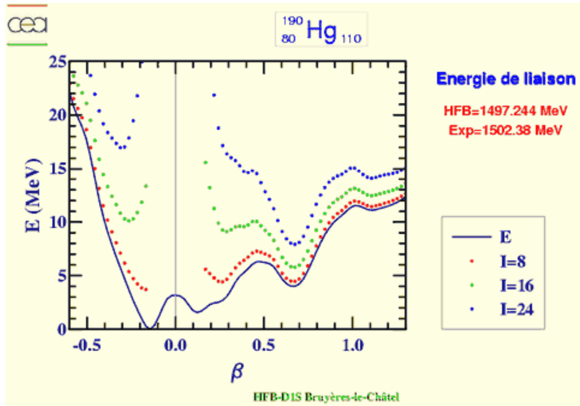












See also J.P. Delaroche *et al.*, PRC (1994)

Search for β-vibrations

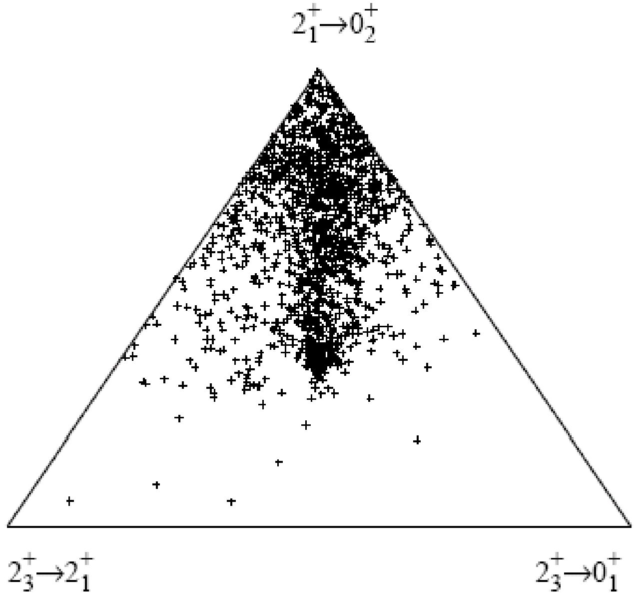
If the spectrum truly exhibits a β-vibrational band, the quadrupole transitions between it and the g.s. should be governed by a single parameter, the quadrupole operator between the two intrinsic states.

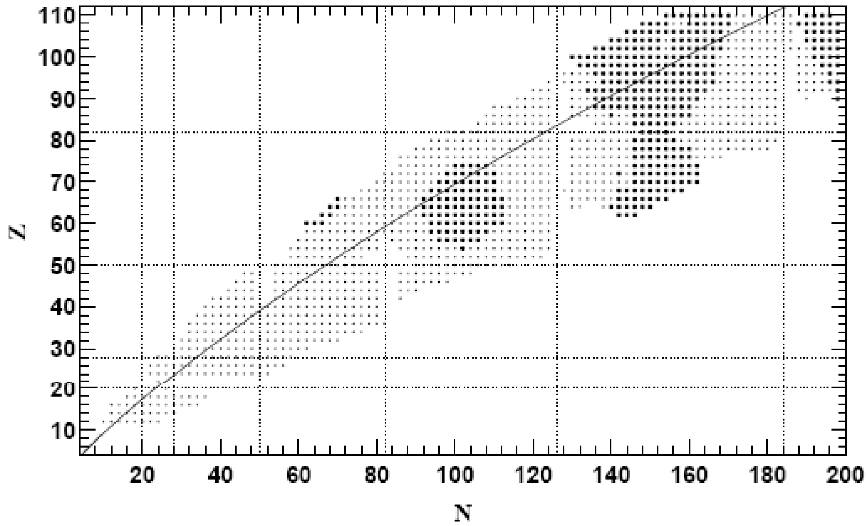
$$\left\langle \beta\, J_\beta \left\| M(E2) \right\| g\, J_g \right\rangle = (2J_g + 1)^{1/2} (J_g\, 020 | J_\beta 0) \langle \beta | M(E2) | g \rangle$$

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

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 β-vibrations





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 β-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)

----

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

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

$$\downarrow$$

2) Projection

$$P|\phi\rangle$$

Advantages:

simple …

Drawbacks:

violates the variational principle

Variation after projection

1) Projection

$$P|\phi\rangle$$

$$\downarrow$$

2) Variation

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

Advantages:

* proper variational principle

Drawbacks:

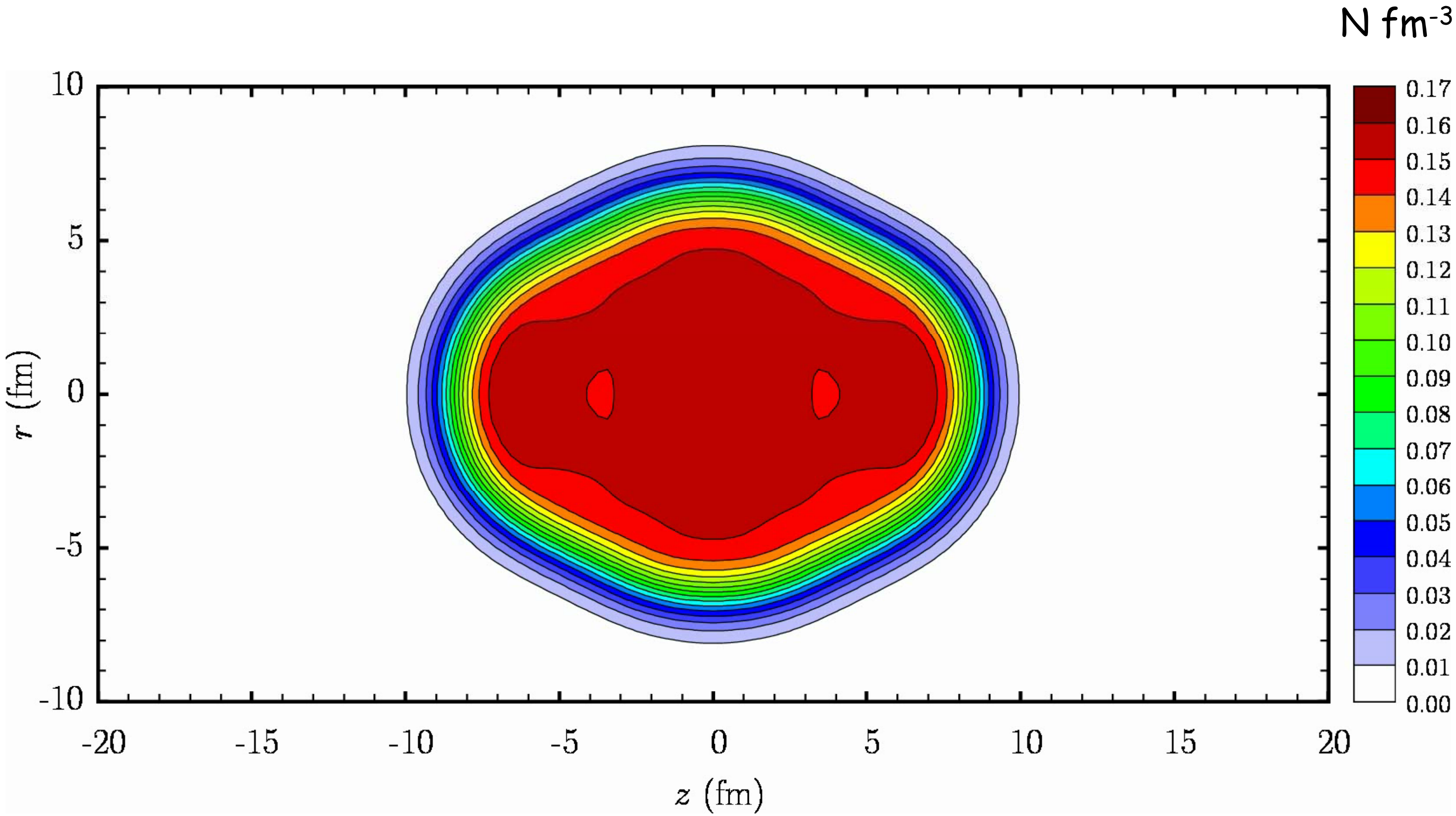
* more complicated

(repeat the variation for all I or N)

* PHP is a multi-body operator …

Nucleon density

$^{240}Pu \rightarrow {}^{134}Sn + {}^{106}Ru$



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

Bibliography

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

* Breaking and restoring symmetries within the nuclear energy density functional method.
T. Duguet and J. Sadoudi
J. Phys. G: Nucl. Part. Phys. 37, 064009 (2010).

* P. Ring and P. Schuck, The Nuclear Many-Body Problem (Springer Verlag, New York, Heidelberg, Berlon, 1980).