

NUCLEAR STRUCTURE

SELF-CONSISTENT MEAN FIELDS

Philippe QUENTIN

CENBG (Université de Bordeaux and IN2P3/CNRS)

- 1 Independent particles, correlations
- 2 Pauli principle correlations
- 3 The Hartree-Fock approximation
- 4 Correlations beyond the Hartree-Fock approximation
- 5 Symmetries
- 6 Examples of correlations treatment

Caveat emptor

We will treat **the many-body problem**
within **a non-relativistic quantal hamiltonian approach**
(merely nucleonic degrees of freedom)

As opposed to relativistic mean field approaches

Using Lagrangian (nucleonic and mesonic degrees of freedom)

In a nucleus

$$E_k = (\gamma-1) mc^2 \sim \frac{1}{2} m\beta^2 c^2 = 30 \text{ MeV (Fermi motion)}$$

$$E_0 = mc^2 \sim 940 \text{ MeV}$$

Thus, $\beta^2 \sim 0.06$ **a non relativistic treatment is reasonable**

The de Broglie wavelength $\lambda = h/\gamma mv \sim hc/(2E_0 E_k)^{1/2} \sim 4 \text{ fm}$
(since β is small, $\gamma \sim 1$ and $E_k \sim mv^2/2$)

The size of the nucleon is $\sim 1 \text{ fm}$

Thus **a quantum mechanical treatment is needed**

1 - Independent particles, correlations

The concept of an independent N-particle state is of a **statistical nature**

It is defined for N particles from a set of N single particle states $[|\phi_i\rangle]$ as

$$|\Psi_0\rangle = \prod_{i=1, N} |\phi_i\rangle$$

A particular case $|\vec{r}_i\rangle = \prod_{i=1, N} |\vec{r}_i\rangle$

From the corresponding N-particle (purely spatial, no spin) wavefunction, one gets **the probability of presence** at $[\vec{r}_i]$

$$\Psi([\vec{r}_i]) = \langle [\vec{r}_i] | \Psi_0 \rangle = \prod_{i=1, N} \langle \vec{r}_i | \phi_i \rangle$$

$$\text{Prob}(1 \text{ in } \vec{r}_1, 2 \text{ in } \vec{r}_2, \dots) = \prod_{i=1, N} \text{Prob}(i \text{ in } \vec{r}_i)$$

Yet correlations do exist

- of dynamical nature (pairing correlations, quantal fluctuations around some classical equilibrium solution, etc.)
- due to symmetries

Examples of the latter : geometrical (e.g. planar reflexion), global spin symmetry for a system of two distant particles like in the EPR problem, etc.)

One-body, two-body observables, ... :

$$Op^{(1)} = \sum_{i=1, N} O(q_i, p_i)$$

$$Op^{(2)} = \frac{1}{2!} \sum_{i=1, N ; j \neq i} O(q_i, q_j, p_i, p_j)$$

hermitian, commuting with any permutation P of N objects

- same mathematical form for any i or (i,j)

- $O(q_i, q_j, p_i, p_j) = O(q_j, q_i, p_j, p_i)$ etc.

Examples of one-body potentials :

Kinetic energy, Coulomb electron-nucleus interaction

Examples of two-body potentials :

Electron-electron coulomb, nucleon-nucleon strong interactions

Independent particle states are **mathematically acceptable** stationary solutions of the Schrödinger equation for a **one-body Hamiltonian**

In atomic physics neglecting the residual interaction, the dynamics is reasonably approximated by such a one-body Hamiltonian

In nuclear physics this is of course a priori different

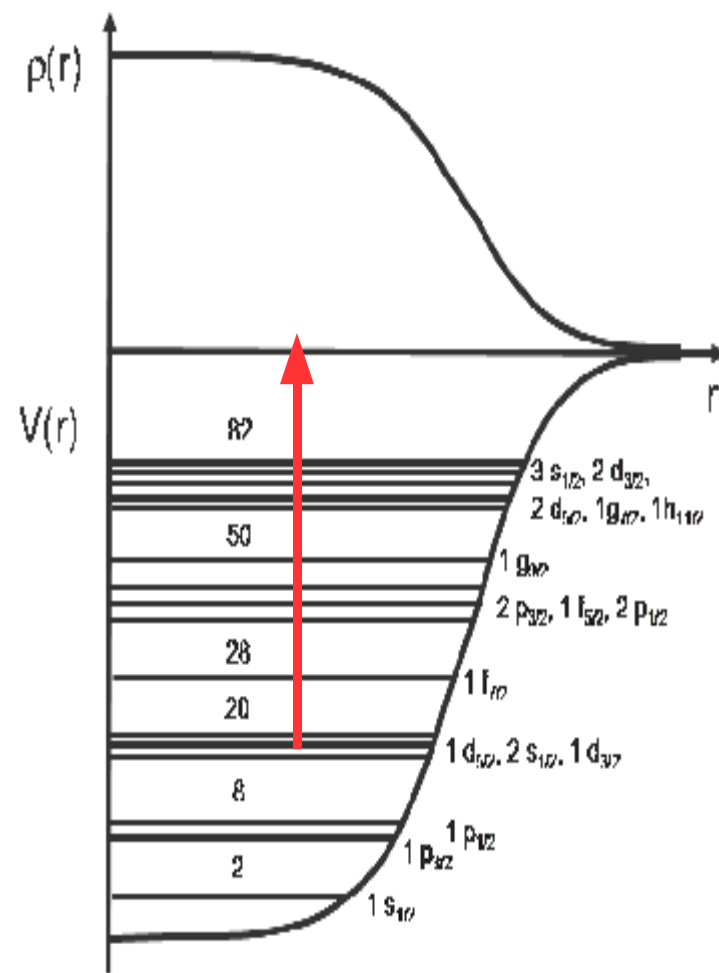
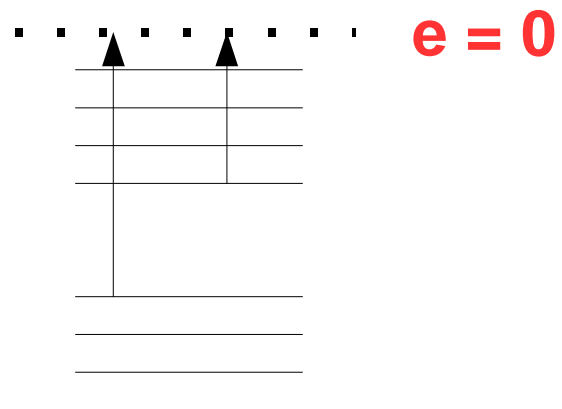
For a one body potential binding fermions in a restricted part of the space, **shell effects** have been observed (bunching of the single particle states)

When one such shell is filled the **separation energy** (positive quantity) is suddenly decreased

For a one-body Hamiltonian

$$E = \sum_{i=1, Z} e_i$$

$$E_{sep} = |E(Z) - E(Z-1)| = |e_{last}|$$

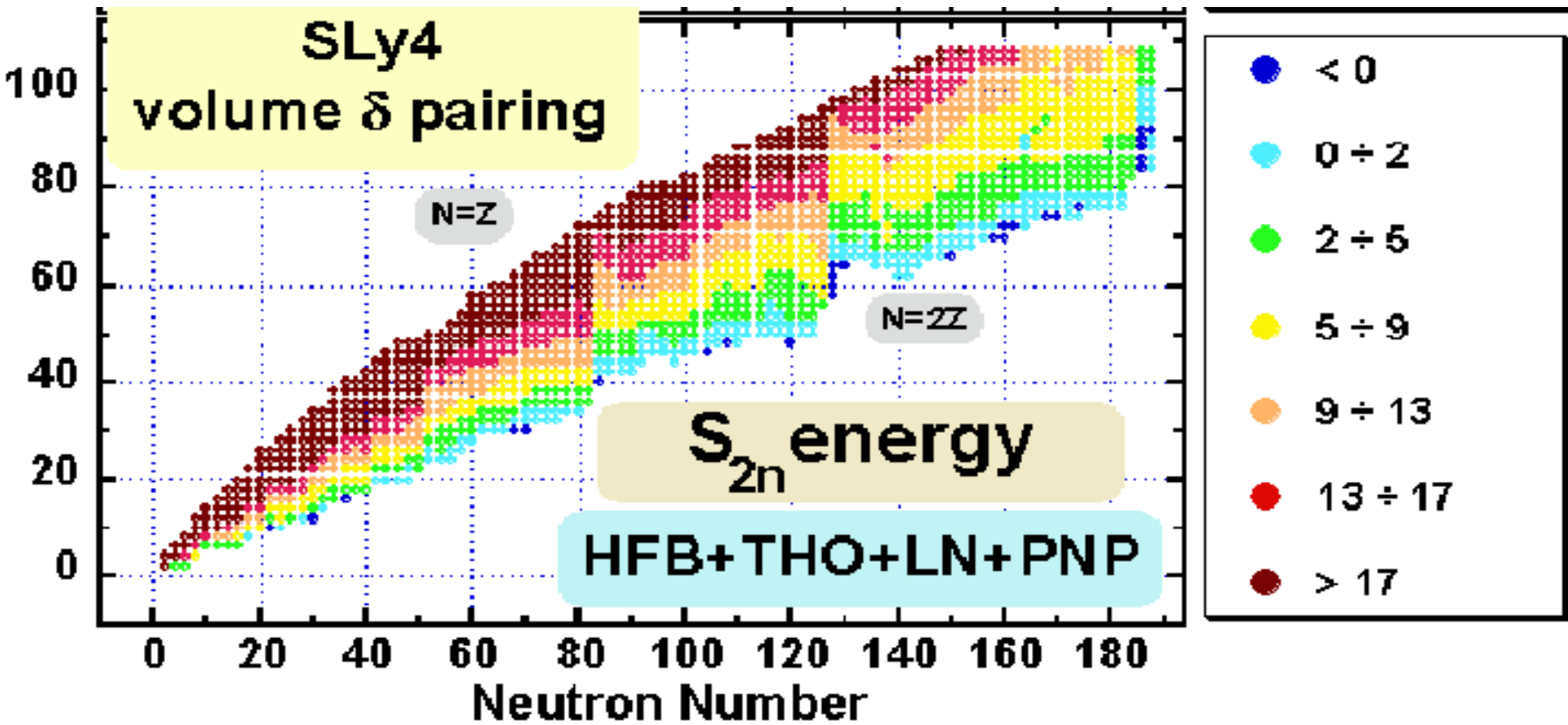


This is observed in atomic physics (for the **ionisation potential**) which does not come as a surprise due to the mostly one-body character of H

But this is **observed in nuclear physics** which is more surprising :
 The Hamiltonian is not a one-body potential

$$H = \sum_{i=1}^A \frac{\vec{p}^2}{2m} + \frac{1}{2} \sum_{i=1}^A \sum_{j<i} v(i, j) + \dots$$

Should a mean (i.e. averaged) potential exist in the nucleus ?



In some **classical** fashion one might expect (Hartree 1928) that this mean field V would be obtained by the following **convolution product** :

$$V(\vec{r}) = \sum_{i=1}^A \int |\phi_i(\vec{r}')|^2 v(\vec{r} - \vec{r}') d^3 r'$$

Where the two-body interaction $v(\vec{r} - \vec{r}')$ is translationally invariant and $|\phi_i(\vec{r}')|^2$ is the probability density of presence of the i -nucleon in r' evaluated within the independent particle limit.

Thus

$$V(\vec{r}) = \int \rho(\vec{r}') v(\vec{r} - \vec{r}') d^3 r' \quad \text{with} \quad \rho(\vec{r}') = \sum_{i=1}^A |\phi_i(\vec{r}')|^2$$

Beyond the spurious effect of self interaction and the neglect of the Pauli principle (the second correcting for the first incidentally)

the very **existence of such a mean field** seems a priori to be questioned :

Evaluating roughly **the mean free path** as

$$\lambda = 1/(\sigma \rho)$$

with the saturation nuclear density

and an average value of the free N-N cross section

(at an energy typical of the nucleonic zero point motion ~ 30 MeV) one gets

$$\lambda \approx 1 \text{ fm}$$

which is **of the order of the nucleonic size** (radius $R \approx 1.2 A^{1/3}$ fm)

This is, of course, not consistent with the very **concept of a nucleonic motion in an average field**.

A given nucleon does not feel the presence of the $A - 1$ other nucleons but merely those immediately close to it

The Pauli principle, reducing the available phase-space for scattering quenches the effective interaction cross section to raise λ at a value larger or equal to the nuclear size

Therefore **the practical problem** given the Hamiltonian

$$H = \sum_{i=1}^A \frac{\vec{p}^2}{2m} + \frac{1}{2} \sum_{i=1}^A \sum_{j<i} v(i, j) + \dots$$

is to define as best as possible, from first principles, this mean field, in particular taking into account the Pauli principle which proves to be essential.

2 – Pauli principle correlations

From the complete set of $N!$ non hermitian permutation operators P of N objects one defines the hermitian idempotent (thus projector) operator A as

$$A = \frac{1}{N!} \sum_{\{P\}} \text{sgn}(P) P$$

where $\text{sgn}(P)$ is the signature of P .

Any permutation is equal to a product of $m(P)$ transpositions, whose number is defined up to an arbitrary number $2n$ and one defines

$$\text{sgn}(P) = -1^{m(P)}$$

One proves that the operator A

a) is hermitian

b) satisfies $\forall P ; A P = P A = \text{sgn}(P) A$

Thus it is idempotent $A^2 = \frac{1}{N!} \sum_{\{P\}} \text{sgn}(P) P A = \frac{1}{N!} \sum_{\{P\}} A = A$

A being hermitian and idempotent is therefore a projector

One defines completely antisymmetric states $|\Psi\rangle$ by

$$\forall P ; P |\Psi\rangle = \text{sgn}(P) |\Psi\rangle$$

Thus the operator A projects onto **completely antisymmetric states** $A |\Psi\rangle$ since

$$P A |\Psi\rangle = \text{sgn}(P) A |\Psi\rangle$$

These completely antisymmetric states form a subspace S_A of the space of systems of N particles

The **Pauli principle postulates** two things for the states of N **identical fermions**

- A symmetry principle for the Hamiltonian : $[H,P] = 0$ for all P
- A choice principle : acceptable physical states belong to the subspace S_A

Notation

The permutation P is defined as $\{ i \} \xrightarrow{P} \{ P(i) \}$

Then **the naive independent particle wavefunction**

$$|\Psi_0\rangle = \prod_{i=1,N} |\phi_i\rangle$$

is not acceptable

Instead one defines from it

$$|\Psi\rangle = \frac{1}{\sqrt{N!}} A |\Psi_0\rangle = \frac{1}{\sqrt{N!}} \sum_{[P]} \text{sgn}(P) \prod_{i=1,N} |\phi_{P(i)}\rangle$$

It is normalized provided that the individual wavefunctions are such

$$\langle \phi_i | \phi_j \rangle = \delta_{ij}$$

Its wavefunction

$$\Psi([\vec{r}_i]) = \frac{1}{\sqrt{N!}} \sum_{[P]} \text{sgn}(P) \prod_{i=1,N} \langle \vec{r}_i | \phi_{P(i)} \rangle$$

is called **a Slater determinant**, since the determinant of a matrix $[M_{i,j}]$ is

$$\det [M_{i,j}] = \sum_{[P]} \text{sgn}(P) \prod_{i=1,N} M_{i,P(i)}$$

where here

$$M_{i,j} = \langle \vec{r}_i | \phi_j \rangle \quad \text{with} \quad j \equiv P(i)$$

The above entails the so-called **Pauli exclusion principle** stating that two identical fermions within a given system cannot be in the same (single particle) state

If one has in the state $|\Psi_0\rangle$ or equivalently $|\Psi\rangle$ two identical fermions in two individual states labeled i and j ($i \neq j$) such that

$$|\phi_i\rangle \equiv |\phi_j\rangle$$

then, calling $T_{i,j}$ the transposition

$$\forall k \neq i \text{ and } j ; P(k) = k \quad \text{while} \quad P(i) = j , \quad P(j) = i$$

the state $|\Psi\rangle$ has a vanishing probability, since

$$T_{i,j} |\Psi\rangle = |\Psi\rangle = -|\Psi\rangle = 0$$

If the set $[|\phi_i\rangle]$ constitutes an orthonormal (complete) basis of the one-particle physical space,

the ensemble of above defined **Slater determinants**

built from N different such individual particle basis state constitutes **an orthonormal basis**

of the physically acceptable states of N identical fermions.

3 – The Hartree-Fock approximation

The Ritz theorem establishes that solving the variational problem for normalized states $|\Psi\rangle$

$$\delta [\langle \Psi | H | \Psi \rangle] = 0$$

is equivalent to solving the Schrödinger stationary (eigenvalue) problem

$$H | \Psi \rangle = E | \Psi \rangle$$

The Hartree-Fock approximation consists in restricting the trial states in the above variation to be **merely Slater determinants** $|\Psi\rangle$.

Varying $|\Psi\rangle$ is performed by varying the single particle states $|\phi_i\rangle$ leading to

$$\forall i \quad ; \quad \frac{\delta [\langle \Psi | H | \Psi \rangle - e_i \langle \phi_i | \phi_i \rangle]}{\delta \phi_i(\vec{r}')} = 0$$

where one has defined **the functional derivative** as a function of \vec{r} such that

$$\frac{\delta E[f(\vec{r}')] }{\delta f(\vec{r}')} = \lim_{\epsilon \rightarrow 0} \frac{\delta \{ E[f(\vec{r}') + \epsilon \delta(\vec{r}' - \vec{r})] - E[f(\vec{r}')] \}}{\epsilon}$$

and where $\langle \Psi | H | \Psi \rangle - e_i \langle \phi_i | \phi_i \rangle$ is considered as a functional of $\phi_i(\vec{r}')$ with e_i being a Lagrange multiplier to conserve the norm of $|\phi_i\rangle$

NB One must make independent variations of $\phi_i(\vec{r}')$ and $\phi_i(\vec{r}')^*$

This leads to a set of **stationary Schrödinger equations** for the states $|\phi_i\rangle$

$$H_{HF} |\phi_i\rangle = e_i |\phi_i\rangle$$

where one has introduced a one-body hamiltonian, called the **Hartree-Fock Hamiltonian**

$$H_{HF} = K + V_{HF}$$

composed of a kinetic energy K and a one-body « Hartree-Fock » potential V_{HF}

The latter is defined if H includes a two body interaction v from the Hartree-Fock solution

which is a Slater determinant built from a set $\{|\phi_\alpha\rangle\}$

of N solutions of the above one-body Schrödinger equations, as

$$\forall \chi_i, \chi_j \quad ; \quad \langle \chi_i | V_{HF} | \chi_j \rangle = \sum_{\alpha} \langle \chi_i \phi_{\alpha} | v | \widetilde{\chi_j \phi_{\alpha}} \rangle$$

where one defines a (not-normalized) antisymmetrized ket

$$|\widetilde{m n}\rangle = (1 - T) |m n\rangle = |m n\rangle - |n m\rangle$$

The first term of V_{HF} i.e. ignoring the Pauli principle (or the transposition operator T) is called **the Hartree potential**

It is exactly equal to the classical mean field considered above

Hartree potentials in position representation

**Assuming the two-body potential to be local
(plus translational and rotational invariant) i.e.**

$$\langle \vec{r}_1 \vec{r}_2 | v | \vec{r}_3 \vec{r}_4 \rangle = \delta(\vec{r}_1 - \vec{r}_3) \delta(\vec{r}_2 - \vec{r}_4) v(|\vec{r}_1 - \vec{r}_2|)$$

From the definition of the Hartree potential

$$\langle \chi_i | V_H | \chi_j \rangle = \sum_{\alpha} \langle \chi_i \phi_{\alpha} | v | \chi_j \phi_{\alpha} \rangle$$

choosing

$$|\chi_i\rangle \equiv |\vec{r}\rangle, \quad |\chi_j\rangle \equiv |\vec{r}'\rangle$$

one gets upon developing the single particle states in the $\{|\vec{r}\rangle\}$ basis

$$|\phi_m\rangle = \int \phi_m(\vec{r}) |\vec{r}\rangle d^3 r$$

$$\langle \vec{r} | V_H | \vec{r}' \rangle = \sum_{\alpha} \iint d^3 r_0 d^3 r_0' \phi_{\alpha}^*(\vec{r}_0) \phi_{\alpha}(\vec{r}_0') \langle \vec{r} \vec{r}_0 | v | \vec{r}' \vec{r}_0' \rangle$$

and thus

$$V_H(r) = \langle \vec{r} | V_H | \vec{r}' \rangle = \delta(\vec{r} - \vec{r}') \int d^3 r_0 v(|\vec{r} - \vec{r}_0|) \rho(\vec{r}_0) d^3 r_0$$

Expressing the local character of the Hartree potential

Microscopic foundation of two usual phenomenological Hartree fields

A) the Woods Saxon potential

From electron scattering experiment one shows for heavier enough nuclei, their geometrical **saturation property** (constant density in the nuclear internal part thus volume $\propto A$ and radius $\propto A^{1/3}$) and its **leptodermous** (thin skin) character

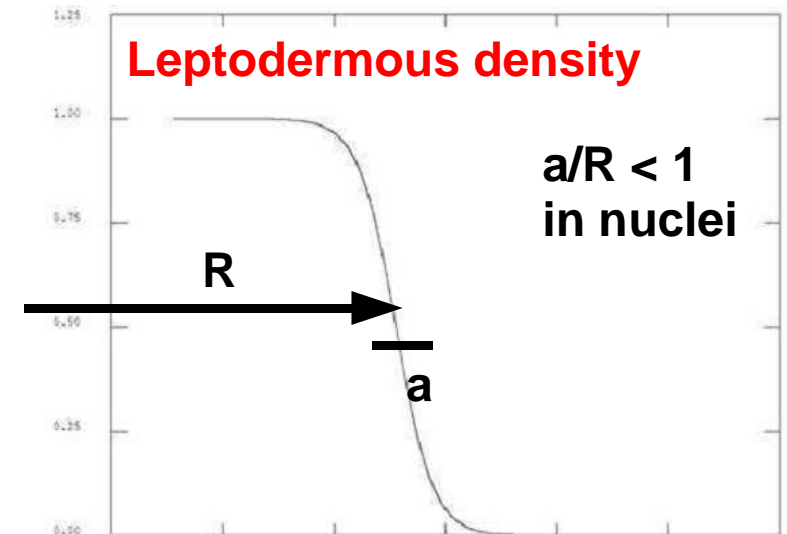
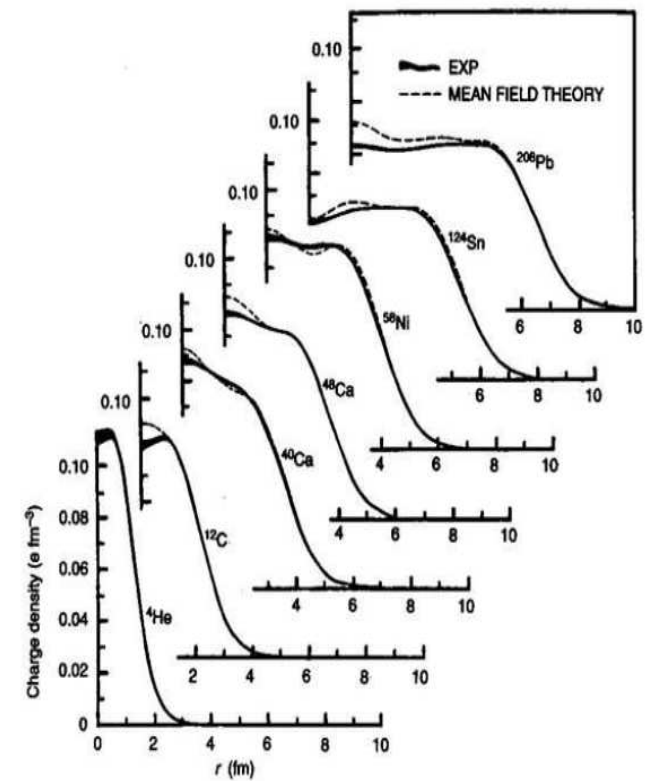
Roughly the density profile is thus of the Fermi type

$$\rho(r) = \frac{\tilde{\rho}_0}{1 + e^{(r-R)/a}} \quad \frac{a}{R} < 1 \quad a \approx 1 \text{ fm}$$

Convoluting ρ with an interaction v whose range is much shorter (~ 0.8 fm) than R ,* one yields a Fermi type V_H potential which is **the Woods-Saxon ansatz**

$$W_{WS}(r) = \frac{V_0}{1 + e^{(r-R)/a}}$$

* In the case of a $\delta(\vec{r} - \vec{r}')$ interaction one has exactly $V_{HF}(\vec{r}) \propto \rho(\vec{r})$



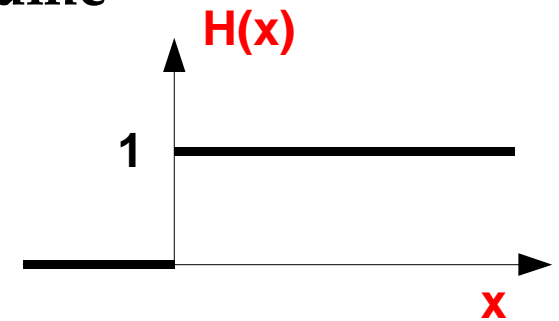
One may **deform this model mean field** by replacing R by a function of the two angles θ and ϕ defining a position in spherical coordinates

$$R \rightarrow R(\theta, \phi) = \mathring{R}(\{\alpha_{\lambda, \mu}\}) \left(1 + \sum_{\lambda} \sum_{\mu=-\lambda}^{\mu=+\lambda} \alpha_{\lambda, \mu} Y_{\lambda, \mu}(\theta, \phi)\right)$$

the first term being included to conserve the nuclear volume

$$\iiint \rho(\vec{r}) r^2 \sin(\theta) dr d\theta d\phi = A = \frac{4\pi}{3} r_0^3 A \rho_0$$

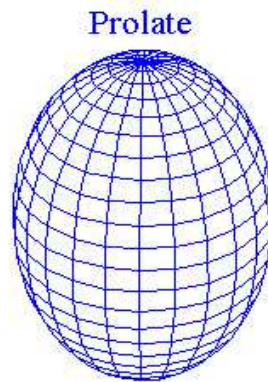
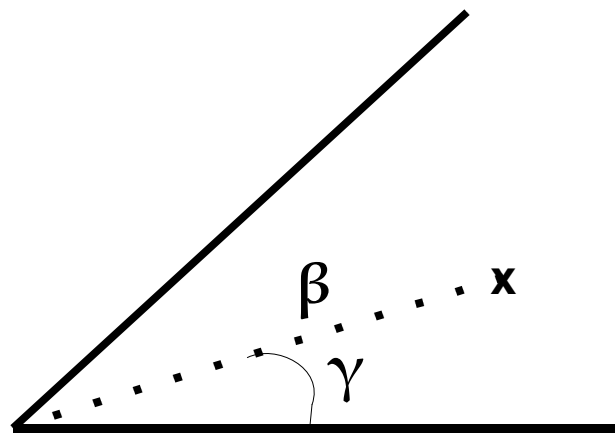
$$\rho(\vec{r}) \equiv \rho_0 H[R(\theta, \phi) - r] \quad (r_0 \approx 1.2 \text{ fm})$$



Restricting to the quadrupole ($\lambda=2$) term one gets the two parameters (β, γ) collective \AA . Bohr model such that (in the intrinsic frame)

$$\alpha_{20} = \beta \sin(\gamma) \quad \alpha_{2\pm 2} = \beta / \sqrt{2} \cos(\gamma)$$

$$\alpha_{2\mp 1} = 0$$

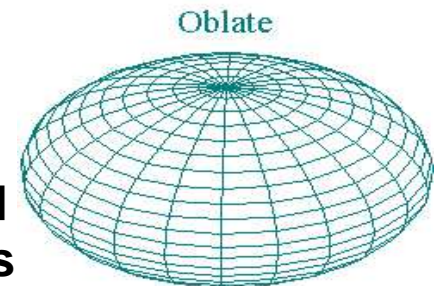


Axial quadrupole moment $Q_{20} = 2z^2 - (x^2 + y^2)$

$$Q = \int \rho(\vec{r}) Q_{20} d^3 r$$

Prolate ($Q > 0$): rugby ball
at low deformation
Axially symmetric ellipsoid
Symmetry axis = large axis

Oblate ($Q < 0$): pancake
at low deformation
Axially symmetric ellipsoid
Symmetry axis = small axis



B) The Nilsson model

One may expand the two body interaction in multipoles

$$v(|\vec{r}_1 - \vec{r}_2|) = \sum_{\lambda} \sum_{\mu=-\lambda}^{\mu=+\lambda} w_{\lambda\mu}(r_1, r_2) Y_{\lambda\mu}(\hat{r}_1)^* Y_{\lambda\mu}(\hat{r}_2)$$

If one truncates the expansion to include

only a monopole term $\lambda = 0$ (with $w_{00} \propto r_1 r_2$)

and a quadrupole term $\lambda = 2$ (with $w_{2\mu} \propto r_1 r_2$)

further assumes the axial symmetry

one gets for the Hartree potential

$$V_H(\vec{r}) = \alpha \langle \Psi_{HF} | r^2 | \Psi_{HF} \rangle (x^2 + y^2 + z^2) + \\ \beta \langle \Psi_{HF} | r^2 Y_{20}(\hat{r}) | \Psi_{HF} \rangle (2z^2 - x^2 - y^2)$$

which is the axially **deformed harmonic oscillator** of **Å. Bohr** and **J. Rainwater**

Adding a spin-orbit and a \vec{l}^2 corrective term, one gets
the Nilsson model

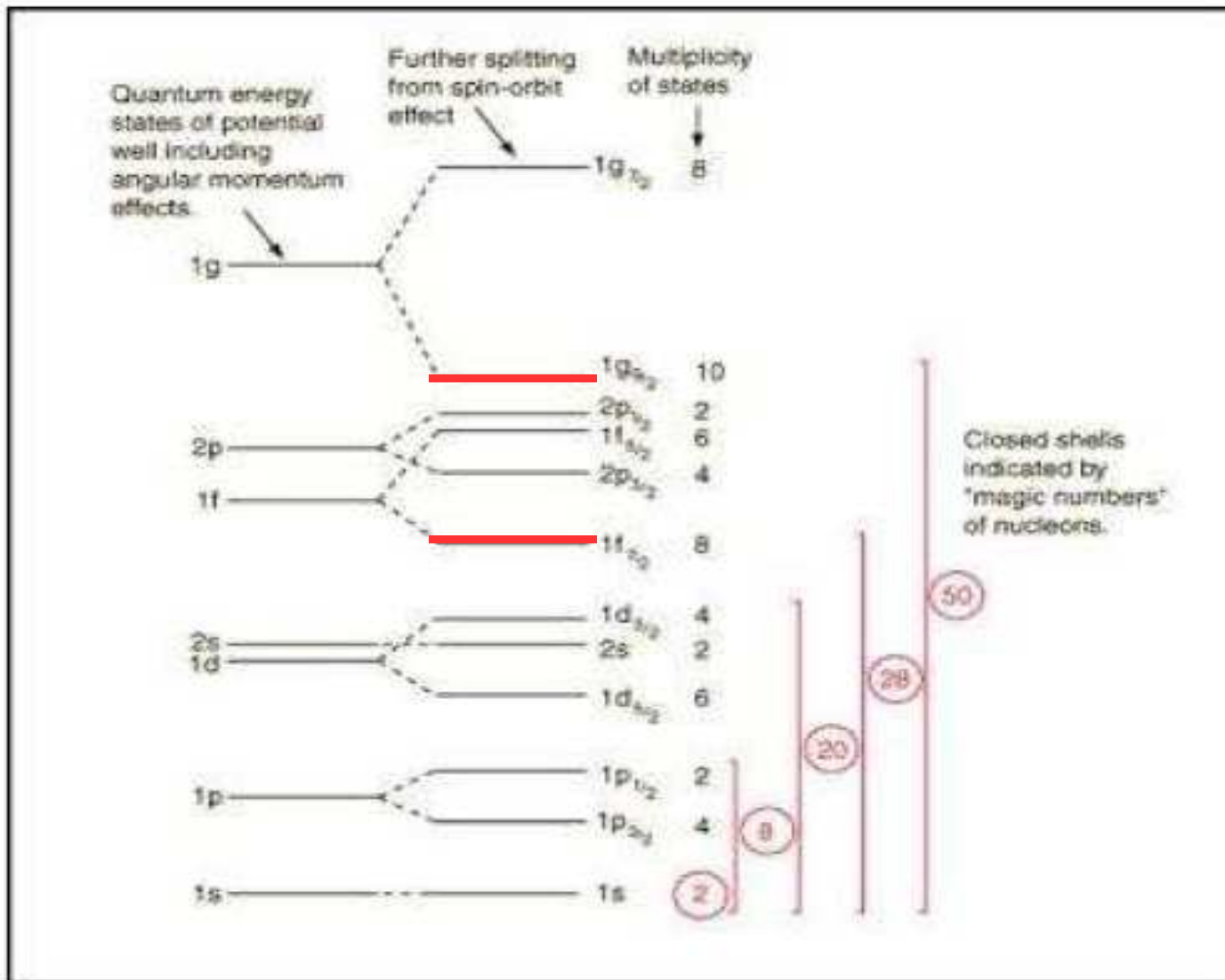
Spin-orbit term $\vec{l} \cdot \vec{s}$

In Atomic Physics (for the Coulomb interaction) :
its origin lies in the Pauli **non-relativistic approximate reduction** of the relativistic Dirac equation
(it is due to the Thomas coupling of the two spinor components)

In Nuclear Physics (for the strong interaction
a similar effect is much too small to explain the magicity)
The true origin of the main part of the spin orbit potential is
here due to the relativistic treatment of **exchange of some vector mesons** (ω, ρ)

Phenomenological corrective term \vec{l}^2

Its role is to correct from the HO parabolic wall
into one closer to a Fermi-like pattern (as a Woods Saxon)
Incidentally it lifts the degeneracy within a major shell



Intruder states

within a major shell
of opposite parity
states

Spin orbit

$$\alpha \vec{l} \cdot \vec{s}$$

with $\alpha < 0$

Perturbative energy corrections to single particle energies

$$\begin{aligned} \langle nlj | \alpha \vec{l} \cdot \vec{s} | nlj \rangle &= \frac{\alpha l}{2} && \text{for } j = l + 1/2 && \text{lowered} \\ &= -\frac{\alpha(l+1)}{2} && \text{for } j = l - 1/2 && \text{raised} \end{aligned}$$

The Fock term

The second term V_F in V_{HF} (involving the transposition T) is the Fock term.

It is originating from **the Pauli principle** which implies to project on S_A .

In the nuclear medium, the absolute value of its contribution to the average potential is typically **one order of magnitude smaller** than the one of V_H

(both for the Coulomb pp and the strong interaction NN parts).

The negative signature of T makes V_F to quench the attraction of V_H .

An important feature of the Hartree-Fock equations is their **non linear character**.

Decomposing the solutions ϕ for individual states on a basis $\{|m\rangle\}$

$$|\phi_i\rangle = \sum_m X_{mi} |m\rangle \quad \text{one gets}$$

$$\sum_{mn} \langle m | K + V_{HF} | n \rangle X_{ni} = e_i \sum_m X_{mi}$$

$$\sum_{mn} \left(\langle m | K | n \rangle + \sum_j^{occ.} \sum_{kl} X_{kj}^* X_{lj} \langle m k | v | \widetilde{n l} \rangle \right) X_{ni} = e_i \sum_m X_{mi}$$

This is generally **solved by iterations**, hoping for a convergence:

- guess some set of ϕ for the occupied individual states
- get from them a V_{HF} potential
- diagonalize H_{HF} and deduce a new set of occupied states ϕ , etc.

When convergence is reached, there is a consistency between the mean field and the eigensolutions of the associated one-body Hamiltonian. One calls this a self-consistent solution.

It then results that V_{HF} depends on the nucleus (even the nuclear state), so this entails that $V_{HF}(A+1) \neq V_{HF}(A)$

Now, approximating $|\Psi_{HF}(A+1)\rangle \approx |\Psi_{HF}^{appr.}(A+1)\rangle = a_{A+1}^\dagger |\Psi_{HF}(A)\rangle$

One proves that

$$E_{HF}^{appr.}(A+1) = \langle \Psi_{HF}^{appr.}(A+1) | H | \Psi_{HF}^{appr.}(A+1) \rangle = E_{HF}(A) + e_{A+1}$$

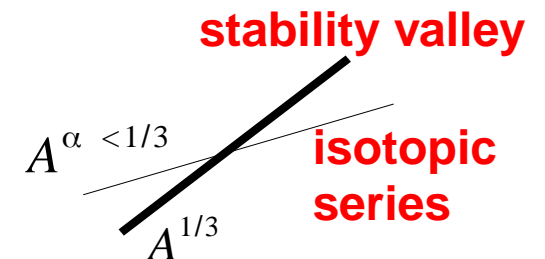
where $E_{HF}(A)$ is the energy of the Hartree-Fock of the solution for A nucleons and e_{A+1} is the energy of the lowest unoccupied state of the mean field associated to this solution for A nucleons.

Thus one approximates the separation energy in the A+1 nucleus as

$$S_N(A+1) = |E(A+1) - E(A)| \approx e_{A+1}$$

This is a reasonable approximation, yet it does not take into account the polarization effects (as e.g. the size scaling in $A^{1/3}$ in the bulk, due to the nuclear saturation)

For instance, see N. Smirnova lectures, $e_n(1d_{5/2})$ is only approximated as the binding energy differences of ^{17}O and ^{16}O



The energy of the Hartree-Fock solution is given by

$$E_{HF} = \langle \Psi | K + v | \Psi \rangle = \sum_i^{occ.} \{ \langle \phi_i | K | \phi_i \rangle + (1/2) \sum_j^{occ.} \langle \phi_i \phi_j | v | \overline{\phi_i \phi_j} \rangle \}$$

Since

$$e_i = \sum_j^{occ.} \{ \langle \phi_i | K | \phi_i \rangle + \sum_j^{occ.} \langle \phi_i \phi_j | v | \overline{\phi_i \phi_j} \rangle \}$$

the Hartree-Fock (total) energy is not given as the sum of the individual energies of the occupied states

$$E_{HF} = (1/2) \sum_i^{occ.} (e_i + \langle \phi_i | K | \phi_i \rangle) \neq \sum_i^{occ.} e_i$$

If one approximates roughly the Hartree-Fock field as a harmonic oscillator using a usual virial theorem for eigenstates of this Hamiltonian

$$\langle \phi_j | K | \phi_j \rangle = \langle \phi_j | V_{HO} | \phi_j \rangle$$

then

$$E_{HF} \approx \frac{3}{4} \sum_i^{occ.} e_i$$

The same harmonic oscillator approximation provides a nuclear energy scale as a function of the nucleon number A

In a Harmonic Oscillator

due to the virial theorem for each s.p. state

$$e_{\text{pot}} = e_{\text{kin}} = e_{\text{tot}}/2 \propto N\omega$$

Thus $e_{\text{tot}} \propto \omega^2 \langle r^2 \rangle \propto N\omega$ thus $\omega \langle r^2 \rangle \propto N$

and the maximum size is reached for the last shell

there are $\sim N^3$ states in shells filled up to the N phonon states

$$\text{thus } A \sim N^3 \text{ and } \omega \langle r^2 \rangle_N \propto A^{1/3}$$

(assuming a 4-fold spin-isospin degeneracy)

Since as we have seen the linear size scale as $A^{1/3}$

$$\langle r^2 \rangle_N \propto A^{2/3}$$

Therefore $\hbar\omega \propto A^{-1/3}$

Solving the Hartree-Fock variational problem one gets a **local extremum**,
 in practice for stability reasons, this is a **local minimum**.

Physical intuition and/or more or less educated guesses and trials lead to an
 approximation of **the ground state** (minimum minimorum).

One explores non equilibrium solution by solving a constrained variational
 problem (constraining e.g. some multipole moment $Q_{\lambda\mu}$) $\delta(H - \chi Q_{\lambda\mu}) = 0$

One so obtains e.g. **shape coexistence energy patterns, fission barriers ...**

M. Girod, J. Libert et al.

L. Bonneau, P. Quentin, D. Samsoen

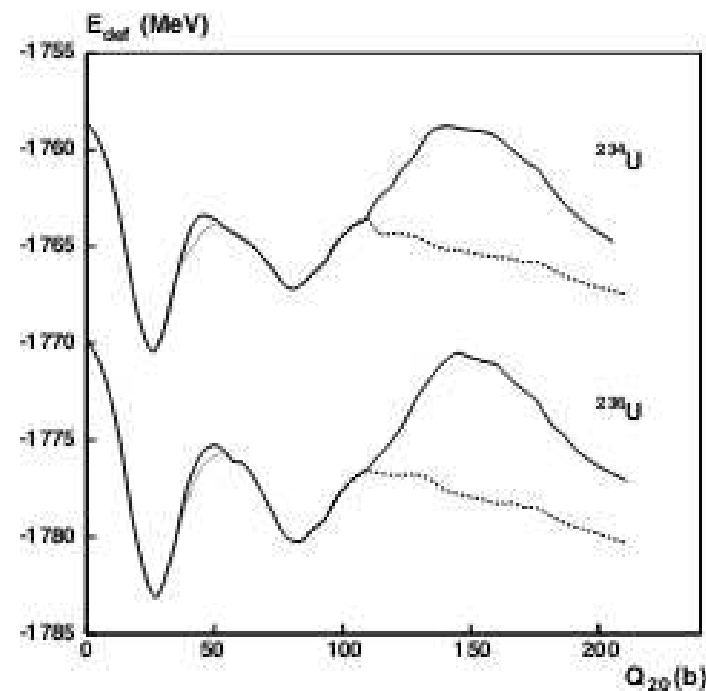
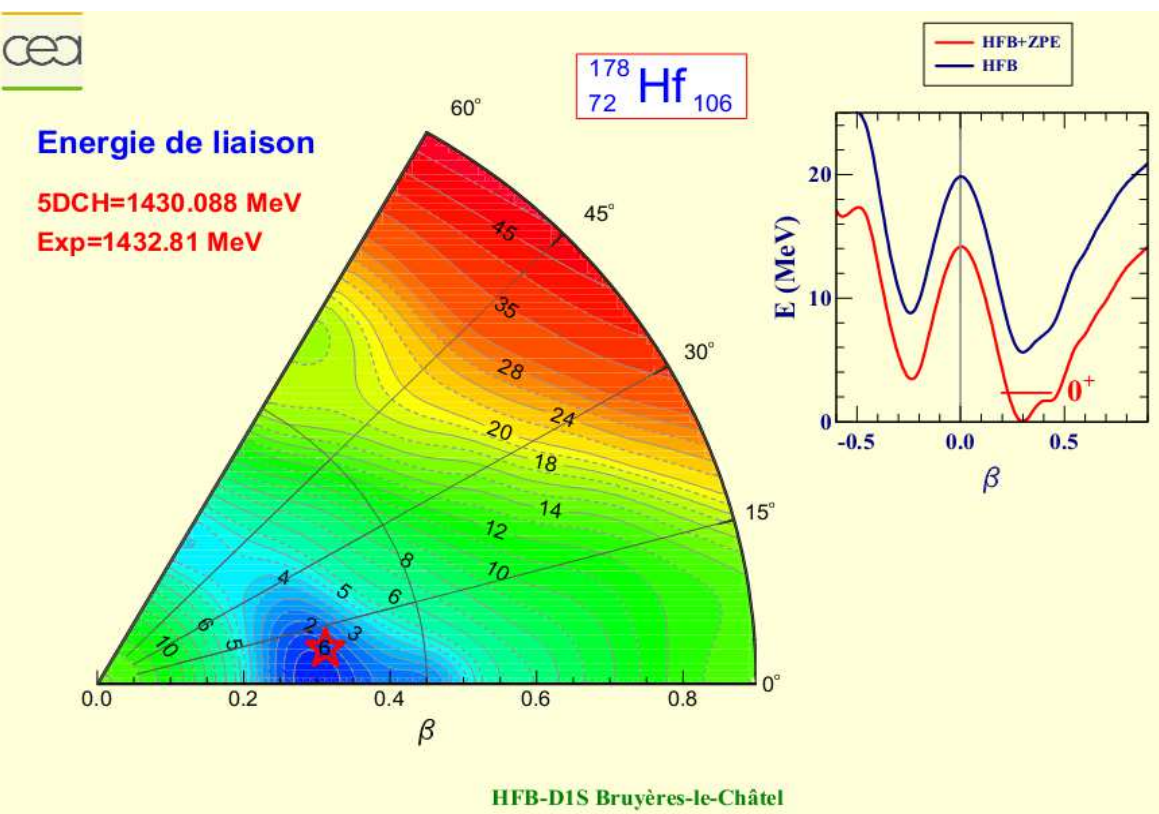
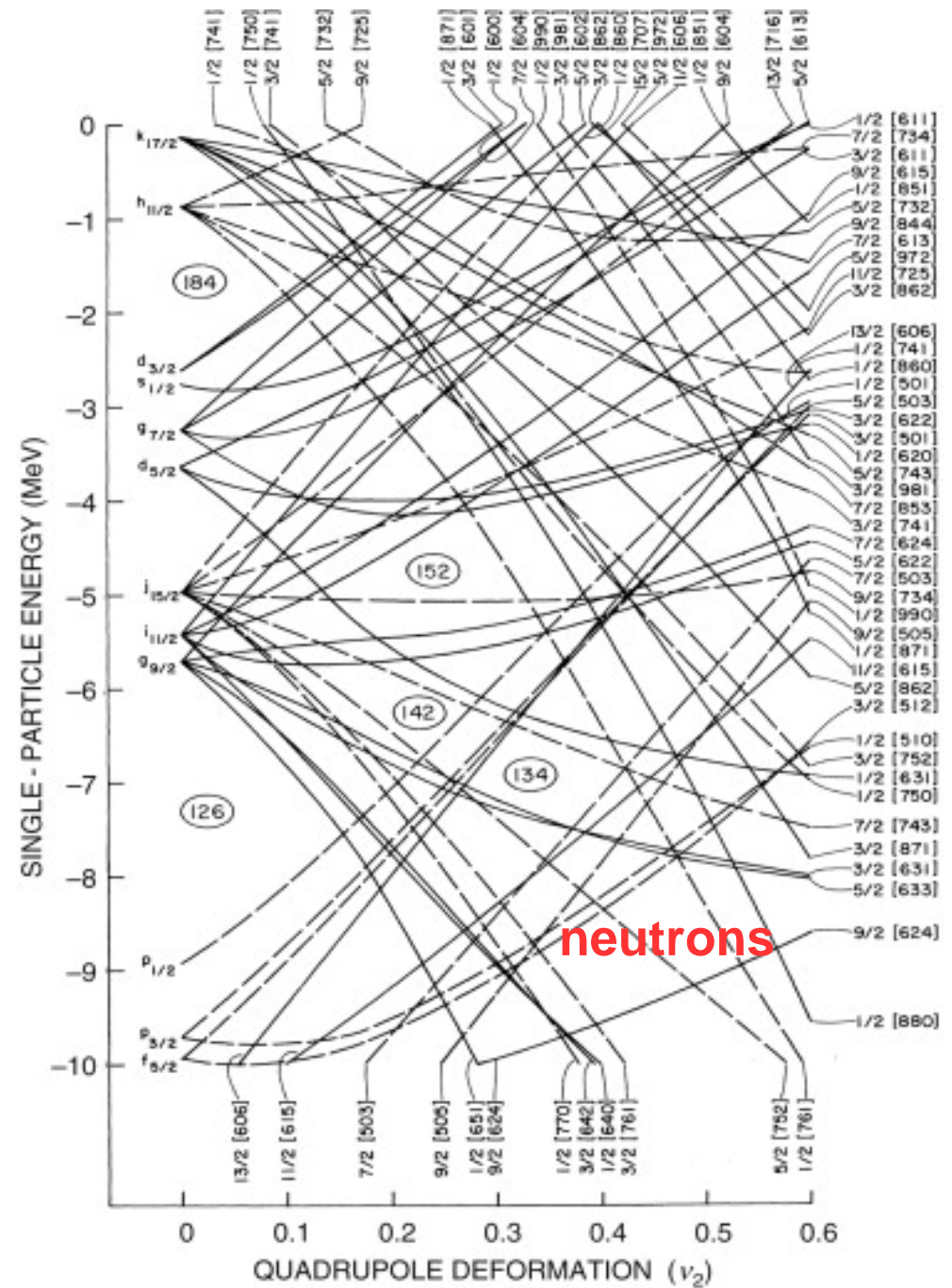
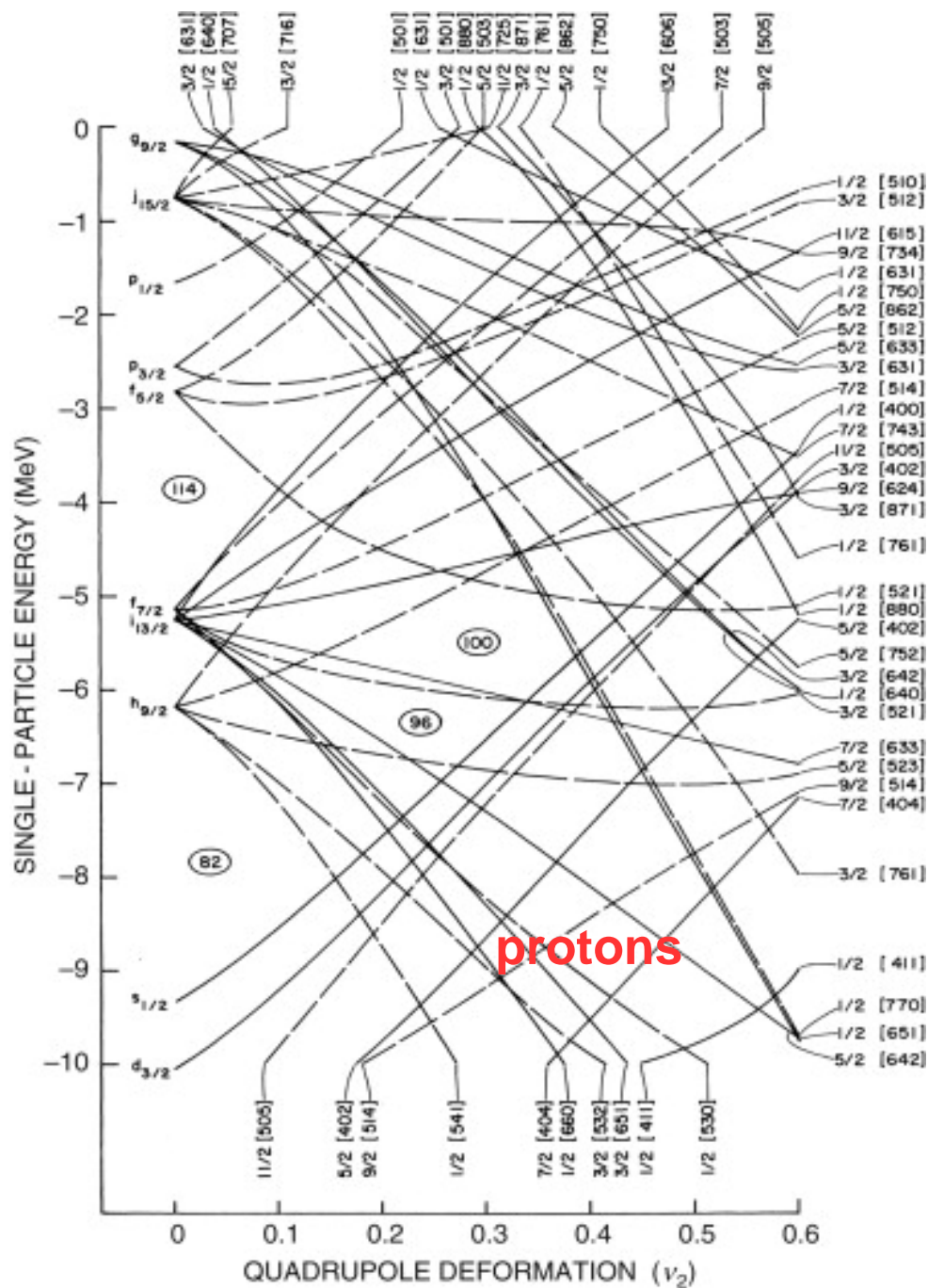


Fig. 15. Deformation energy curves (without rotational correction) of ²³⁴U and ²³⁶U within HF + BCS(G) approach. The triaxial and reflection asymmetric effects are shown with dotted and dashed lines, respectively.



Shape coexistence

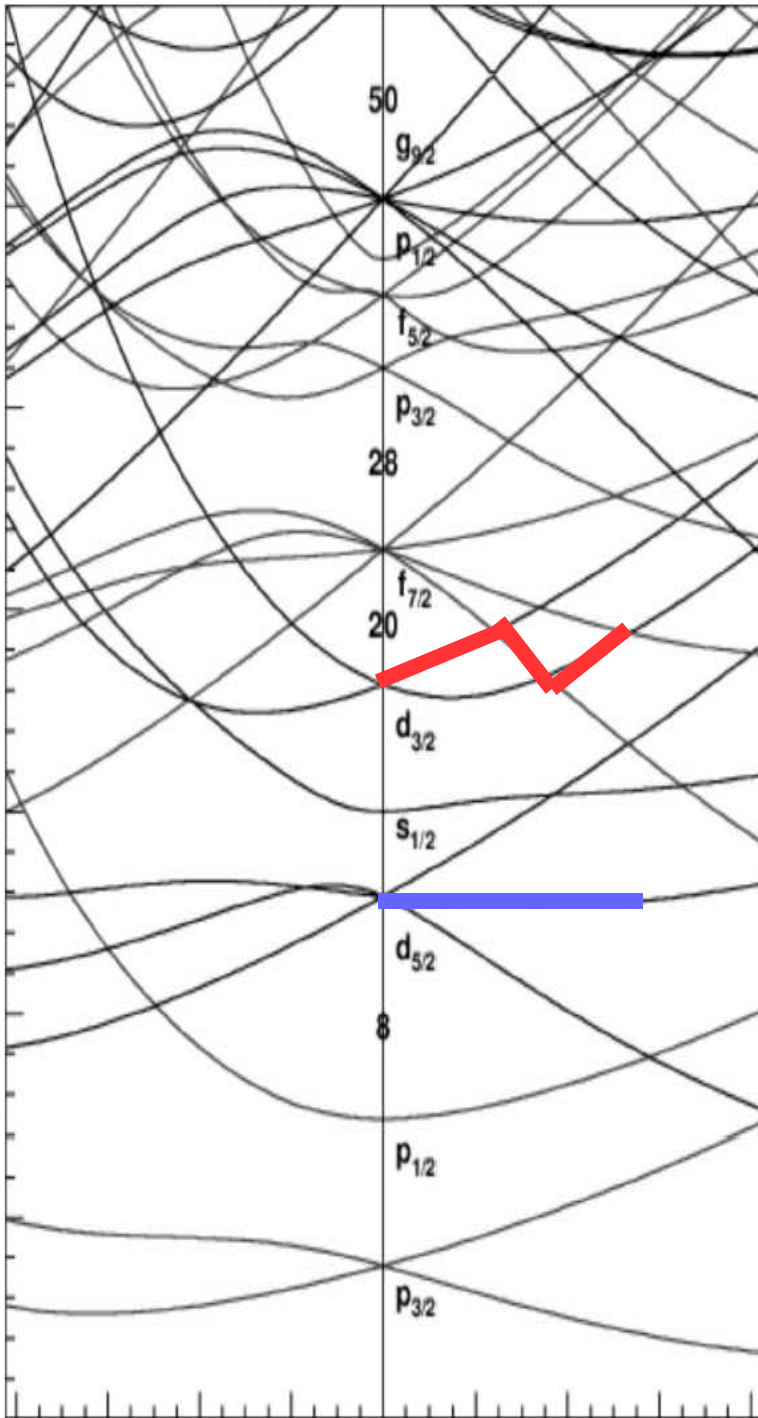
Consider the ^{31}Na nucleus

$Z = 11$, $N = 20$

Upon deforming the odd proton stays on the same orbit $K^\pi = 3/2^+$ stemming from the $1d_{5/2}$ subshell with a slight tendency to deformation (spherical mid sub-shell)

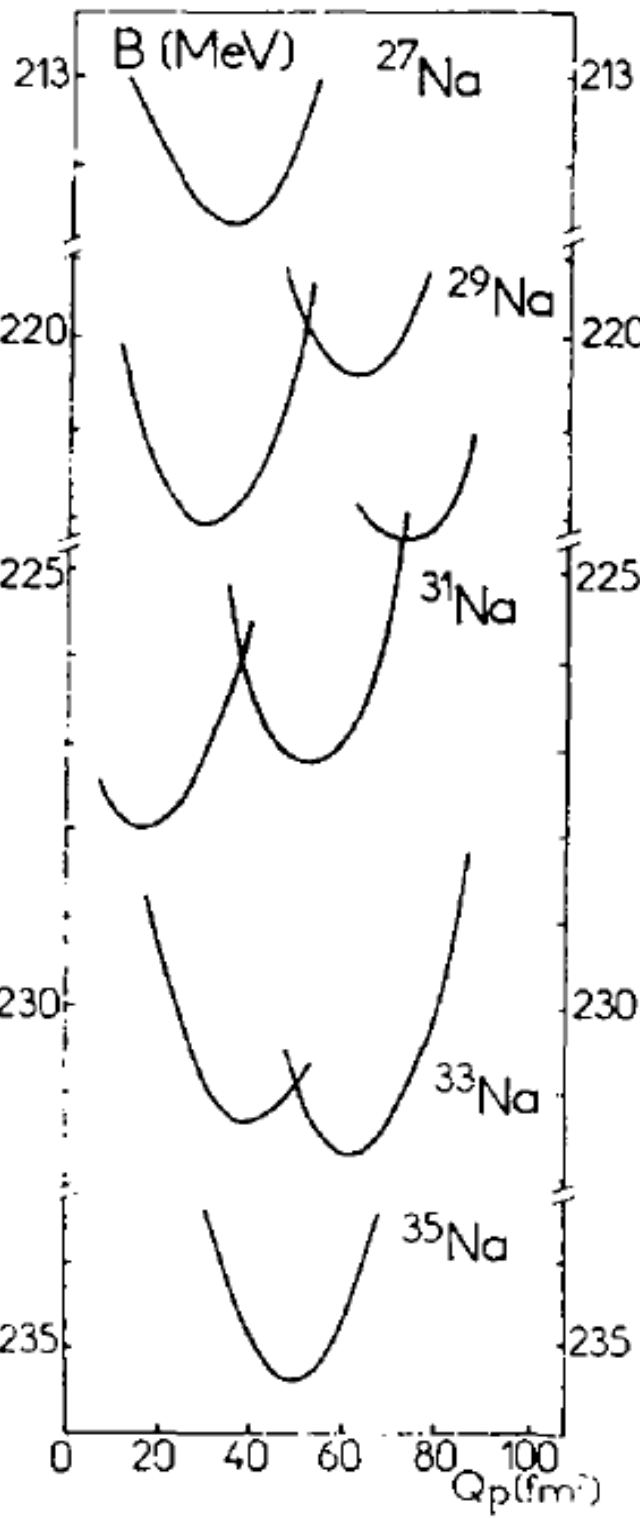
While the last two neutrons jump from a state $K^\pi = 3/2^+$ (from $1d_{3/2}$) onto a state $K^\pi = 1/2^-$ (from intruding $1f_{7/2}$)

The downsloping character of the $1/2^-$ state plus core polarisation effects induce an **other local minimum which is deformed**



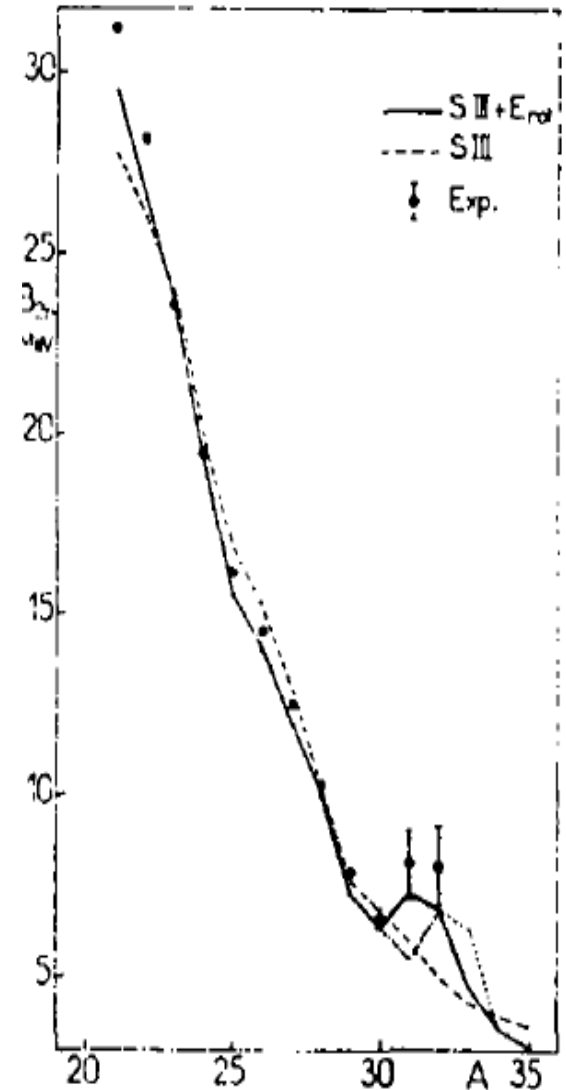
Constrained Hartree-Fock deformation energy curves of some sodium isotopes

(X. Campi et al. Nucl. Phys. A251 (1975) 193)



Around $N = 20$ on a deformed minimum is established and becomes the ground state for $N = 22$

An experimental signature : a discontinuity in the 2-neutron separation energy between $N = 18$ and $N = 20$



The Hartree-Fock approximation may be **extended to the non-stationary case**. The Schrödinger equation may be formally cast into the form of a variational problem for normalized states $|\Psi\rangle$ of the following functional

$$\delta \left[\int_{t_1}^{t_2} \langle \Psi | H - i\hbar \frac{\partial}{\partial t} | \Psi \rangle dt \right] = 0$$

The Hartree-Fock approximation consists here too to **restrict the variation of $|\Psi\rangle$ to Slater determinants**.

The corresponding equations of motion (due to Dirac) for the individual states are written as

$$H_{HF} |\phi_j\rangle = i\hbar \frac{\partial |\phi_j\rangle}{\partial t}$$

4 – Treatments of Correlations beyond the Hartree-Fock approximation

The Hartree-Fock approach to determine the stationary states, results in the replacement of the « exact » hamiltonian H by its one-body approximation H_{HF}

What is left out is called **the residual interaction**

$$V_{res} = H - H_{HF} = v - V_{HF}$$

Whereas shell model calculations pay less attention to the determination of a mean field encompassing as much physics as possible and place the emphasis on treating well V_{res} Self-consistent variational approaches producing complicated 1-body states are forced to **treat approximately the residual interaction**

The latter including a 2-body interaction yields a mixing of Slater determinants (**configuration mixing**) and as a consequence produces **correlations**

One way to treat the residual interaction is to diagonalize it in a restricted basis corresponding to limited particle-hole excitations

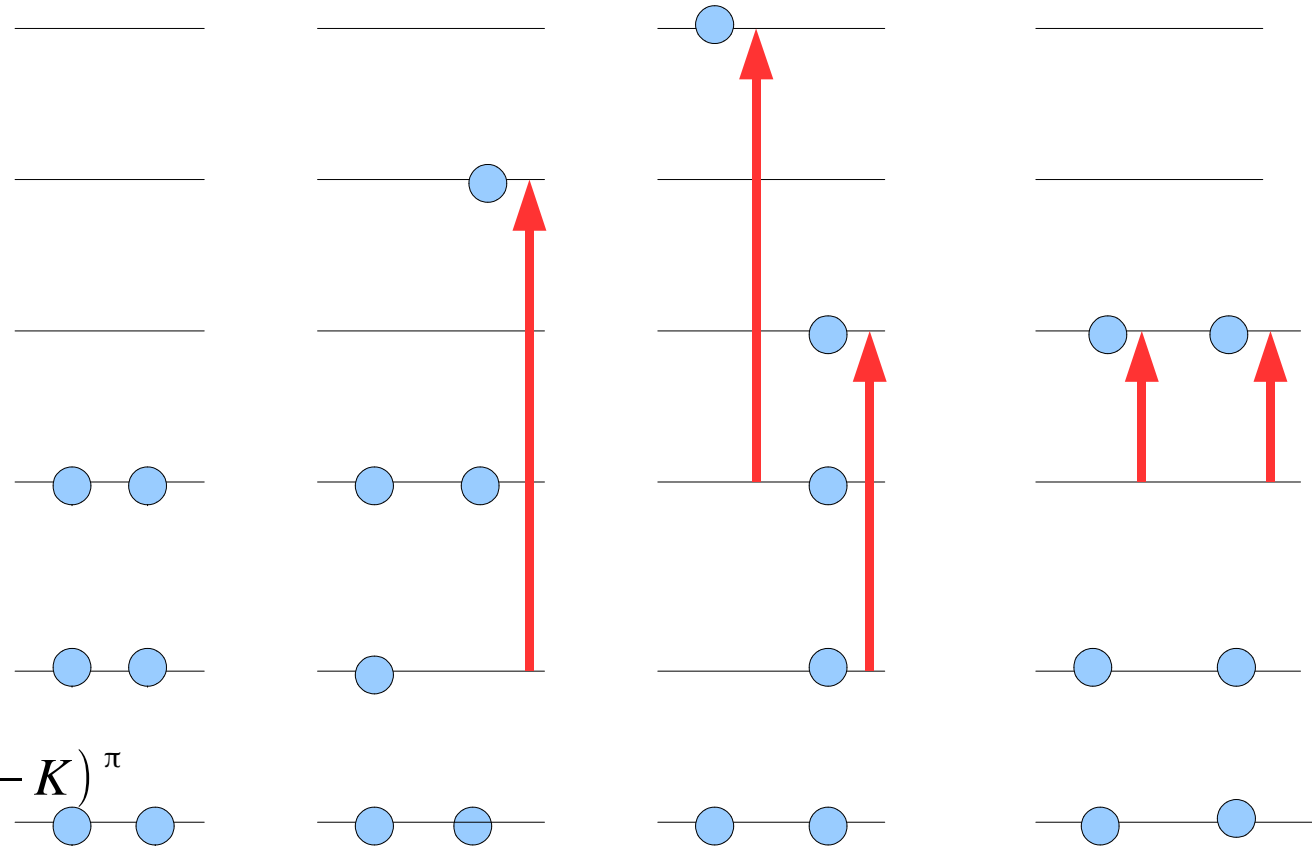
Symmetries
(assumed here)

Kramers degeneracy
Necessary condition:
even nucleus

and e.g. axial and
parity symmetries
K and π conserved
→ strong reduction of
states as (2), (3) ...

**These states form
a N-body basis
to be truncated**

**States of type (4) for
g.s. of even nuclei
are numerically and
dynamically favored**



(1) vacuum
 $|\Phi_0\rangle$

(2) 1p 1h
 $a_p^\dagger a_h |\Phi_0\rangle$

(3) 2p 2h
 $a_{p'}^\dagger a_p^\dagger a_h a_h |\Phi_0\rangle$

(4) one-pair
transfer
 $a_p^\dagger a_{T(p)}^\dagger a_h a_{T(h)} |\Phi_0\rangle$

$(K, -K)^\pi$

This is due to **the binding character of pairing correlations.**

The latter is due to some specific part of the residual interaction.

- Start from the multipole expansion

- Note that the higher multipole part may be well described by a zero range interaction $\delta(\vec{r}_1 - \vec{r}_2)$

- We will show that such an interaction favours matrix elements of the type

$$\langle \phi_i \phi_{T(i)} | \delta^{(T=1, S=0)} | \overline{\phi_k \phi_{T(k)}} \rangle \quad \begin{array}{c} \swarrow \nearrow \\ \delta \\ \swarrow \nearrow \end{array}$$

These terms are implied in a basis made of 1-pair transfer states

Notation : for axial symmetry, in cylindrical coordinates

$$\langle \vec{r} \sigma | \phi_K \rangle \propto f^\sigma(\rho, z) e^{i\Lambda\theta} \delta(K, \Lambda + \sigma) | \chi_\sigma \rangle$$

Let us compute

$$\langle \phi_i \phi_j | \delta^{(T=1, S=0)} | \overline{\phi_k \phi_l} \rangle$$

Due to the $S = 0$ character of the interaction the ket (similarly for the bra) to consider is

$$\frac{1}{\sqrt{2}} [| \phi_k^+ \phi_l^- \rangle - | \phi_k^- \phi_l^+ \rangle] \quad \text{where} \quad | \phi_k^{+/-} \rangle$$

are the kets for the space degrees of freedom associated with the spinors $| \chi_{+/-} \rangle$

Developing the 4 terms of the matrix element of $\delta^{(T=1, S=0)}$

one gets performing the trivial integration on θ and the spinor scalar products, a term

$$[(f_i^+)^*(f_j^-)^* f_k^+ f_l^-] + [(f_i^-)^*(f_j^+)^* f_k^- f_l^+] - [(f_i^+)^*(f_j^-)^* f_l^+ f_k^-] - [(f_i^-)^*(f_j^+)^* f_l^- f_k^+]$$

and thus

$$[(f_i^+)^*(f_j^-)^* - (f_i^-)^*(f_j^+)^*] [f_k^+ f_l^- - f_l^- f_k^+]$$

Owing to

$$f_{T(i)}^+ = (f_i^+)^* = -f_i^- \quad \text{and} \quad f_{T(i)}^- = (f_i^-)^* = f_i^+$$

if one takes **the state j** (and l resp.)

as the time reversed of the state i (and k resp.) one gets for the integrand

$$[|f_i^+|^2 + |f_i^-|^2] [|f_k^+|^2 + |f_k^-|^2] = 1$$

which maximizes, for real **f-factors**

$$[(f_i^+)^*(f_j^-)^* - (f_i^-)^*(f_j^+)^*] \quad \text{and} \quad [f_k^+ f_l^- - f_l^- f_k^+]$$

and thus **maximizes the absolute value of the matrix element**

The couple of states $|\phi_i\rangle$ and $|\phi_{T(i)}\rangle$ is called a **Cooper pair**

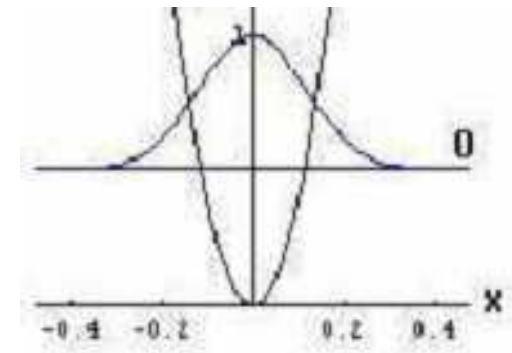
A particular case of the above is realized **in spherical symmetry** where one considers the pairs of states $|nljm\rangle$ and $|nlj-m\rangle$

As a consequence to model the pairing correlations in simple terms one often uses a **delta interaction**.

Since, with such an interaction, the matrix elements are single particle wavefunctions overlaps

in nuclei with N significantly far from Z , **n-n or p-p correlations are prevalent over n-p correlations** ($|T_z|=1$ thus $T=1$ thus $S=0$ interaction).

In this approach what is left in the residual interaction are therefore **low multiple interactions** responsible in particular for quantal fluctuations (zero point motion) around a classical equilibrium point.



These correlations are usually called **RPA correlations** (name due to one of the standard approximations to evaluate them).

First microscopic calculations (Copenhagen, ~1960) took stock on these simplifications of the residual interaction to mock it up as a **pairing plus quadrupole interaction**

$$v_{res}(\vec{r}_1 - \vec{r}_2) = -V \delta(\vec{r}_1 - \vec{r}_2) + \chi \sum_{\mu=-2}^{\mu=+2} Q_{2\mu}^*(\vec{r}_1) \cdot Q_{2\mu}(\vec{r}_2)$$

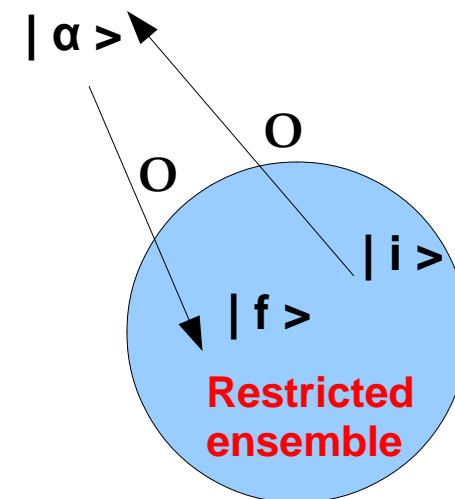
Of course modern calculations use more sophisticated forms of the residual

In principle, the residual interaction is fixed whenever the interaction v and the Hartree-Fock potential V_{HF} are given. In practice, this is not so clear:

- first for **practical reasons** (a very difficult handling: « *we are simply forced to simplify the force !* » B. Mottelson)
- second, because the interaction v is an « **effective** » force (see below)
- third, because to include the effects of the residual interaction one uses **a restricted basis** either in a diagonalisation procedure or in its Ritz theorem equivalent within a variational procedure. This entails a much significant renormalisation of the residual interaction (a further cause of effectiveness)

The concept of effective interaction

One labels an operator O as effective when to compute its matrix elements between two states belonging to a restricted ensemble, one includes in some more or less approximate way, higher order effects including the interaction with states outside the retained ensemble coming finally back to it



For Hartree-Fock calculations and in general for approximate variational approaches, the restricted ensemble is the one where the variation is made (Slater determinants for Hartree-Fock).

One must then include effects of correlations not taken into account.

The interaction in use there is **not the N-N interaction between free nucleons**.

These corrections are in particular corrections due to the presence of other particles mocked up by **a density dependence**. This is generally done as

$$v_{DD}(\vec{r}_1, \vec{r}_2) = \rho((\vec{r}_1 + \vec{r}_2)/2)^\alpha \delta(\vec{r}_1 - \vec{r}_2)$$

They are many parametrisations of the interaction in Hartree-Fock calculations among which **the most popular** are (beyond the p-p Coulomb interaction) :

- **the Skyrme forces** made of a **zero range scalar term** plus gradient corrections, a zero range spin orbit interaction and the above v_{DD}

- **the Gogny forces** made of **two (finite range) gaussian scalar terms** plus gradient corrections, a zero range spin orbit interaction and the above v_{DD}

PARTIAL CONCLUSION: Two main routes to treat the residual interactions

Shell Model calculations

- Crude (simple) spherical model wave functions + ad hoc individual energies

$$H_{MF} = \sum_i e_i a_i^\dagger a_i$$

- Restricted number of 1-body states to define n- particle n-hole states

- Complete many body basis given this restriction

- Elaborated residual interaction (theoretical or deduced from relevant experimental matrix elements)

- Good symmetries (rotational symmetry, parity, particle number)

To sum up : poor mean field excellent treatment of the residual interaction

Self-Consistent Mean Field plus Correlations Approach

- Elaborated mean field carrying most of the physics relevant to 1-body properties

- Effective interactions phenomenologically determined

- Approximate and partial treatment of the residual interaction

- Spurious symmetry breaking (rotational, translational symmetries, sometimes parity symmetry, particle number ...) restored or not

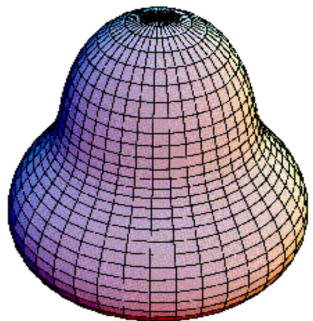
To sum up : excellent mean field poor treatment of the residual interaction

5 – Symmetries

Symmetries spuriously broken
in the Hartree-Fock approach

- **translational**, the average potential is located
at a well defined place

- **rotational** whenever the shape of the intrinsic
density (or of the (Hartree potential)) is non
spherically symmetric

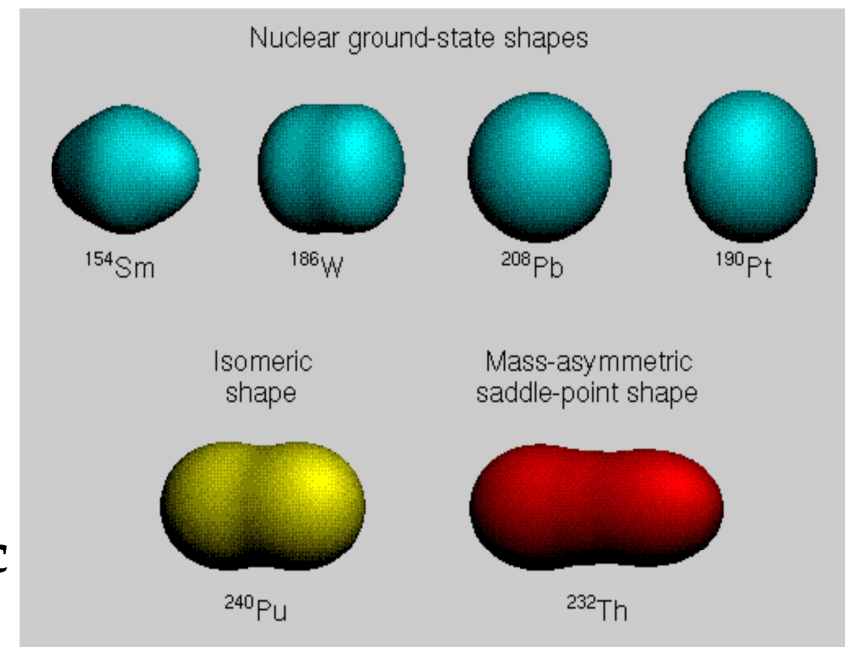


- **parity symmetry** (octupole intrinsic shapes)

- **particle number symmetry** (BCS or similar calculations)

NB **The rotational symmetry in isospin space** is broken, this is due to
i) a physical effect (due the p-p Coulomb interaction and -to a very small
extent- to a piece of the strong interaction)

ii) a spurious effect (V_{HF} depending differently on ρ_n and ρ_p)



P. Möller, T2 LANL

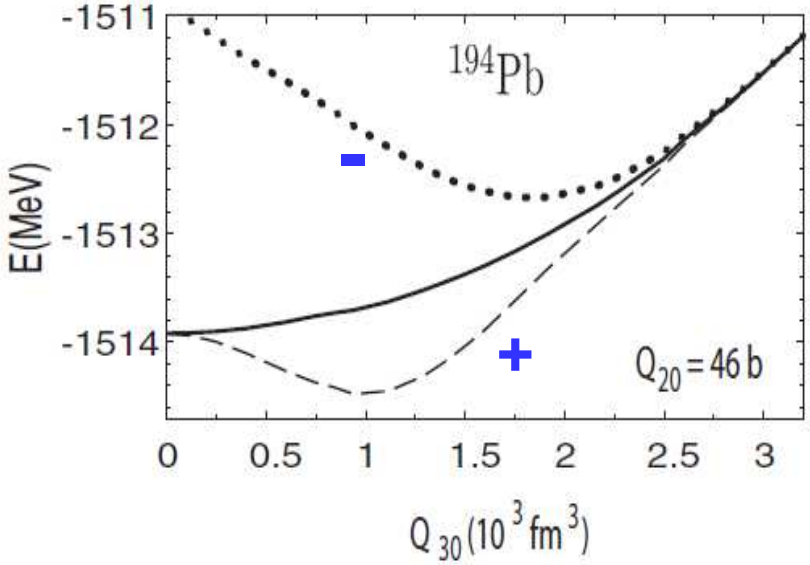
These spuriously broken symmetries **must in principle be restored**

To do so one reconstructs good symmetry states by adding solutions with appropriate weights

Intrinsic parity : involution operator P

$$|\Phi^{(p)}\rangle = \frac{|\Psi\rangle + p P |\Psi\rangle}{\sqrt{2(1 + p \langle \Psi | P | \Psi \rangle)}} \quad \text{leading to}$$

$$E^{(p)} = \frac{\langle \Psi | H | \Psi \rangle + \langle \Psi | PHP | \Psi \rangle + p (\langle \Psi | PH | \Psi \rangle + \langle \Psi | HP | \Psi \rangle)}{2(1 + p \langle \Psi | P | \Psi \rangle)}$$

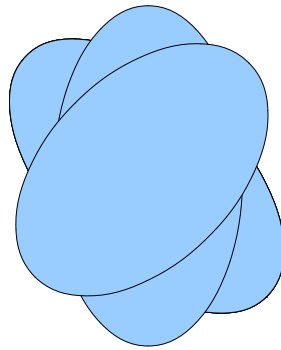


Rotations : unitary rotation operator R(Ω)

$$|\Phi_{IM}\rangle \propto \int d\omega [D_{MK}^I(\omega)]^* R(\omega) |\Psi_K\rangle$$

with $R(\omega) = \exp(i\alpha j_x) \exp(i\beta j_y) \exp(i\gamma j_z)$

Superposing deformed ellipses



makes a spherical object

Given a solution e.g. axially symmetrical $|\Psi_K\rangle$

One has a perfect angular information on the angle of the axis of symmetry

Heisenberg principle :

the canonically conjugated variable, the angular momentum, is distributed

Upon projecting on normalized states $|\Phi_{IK}\rangle$ of good angular momentum I

$$|\Psi_K\rangle = \sum_I a_I |\Phi_{IK}\rangle$$

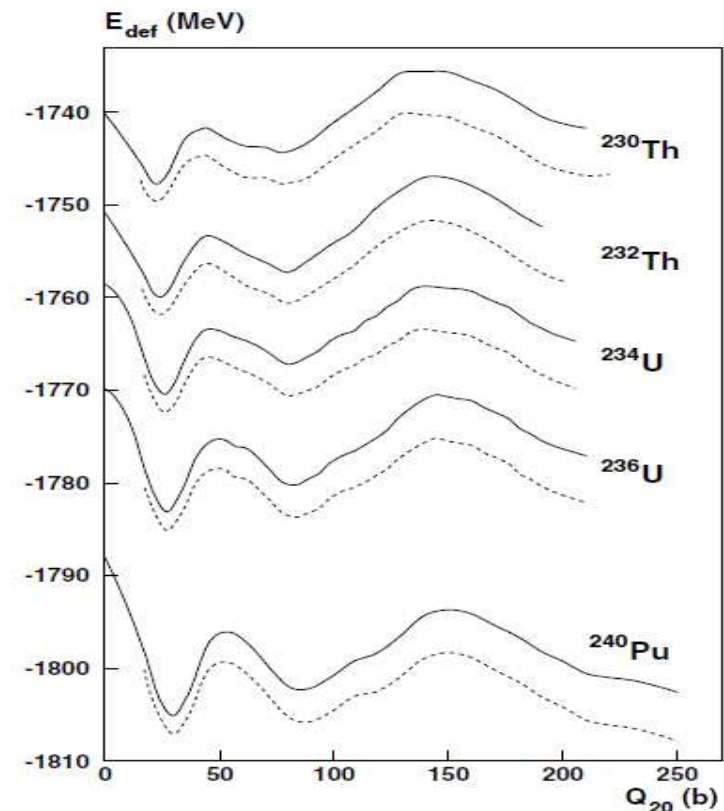
One assumes for well deformed solutions $|\Psi_K\rangle$ of an even-even nucleus that the energies of the projected states follow a pure rotor law

$$E_I = \langle \Phi_{IK} | H | \Phi_{IK} \rangle = E_0 + \frac{\hbar^2 I(I+1)}{2J_{in.}}$$

Then the true ground state energy E_0 is given by

$$E_0 = \langle \Psi_K | H | \Psi_K \rangle - \frac{\langle \Psi_K | \vec{J}^2 | \Psi_K \rangle}{2J_{in.}}$$

(Lipkin approximate projection energy formula)



Connexion between the symmetries of the density and of the V_{HF} potential :
the symmetry properties of V_{HF} depends on the symmetry properties of v and
of the Hartree-Fock solution

The consistent symmetry theorem

Given a symmetry generated by some hermitian operator S
(e.g. the angular momentum component j_z for a rotation around the Oz axis)

Assume that $[v, S] = 0$

and that the subspace spanned by the occupied states $[|\alpha\rangle]$ is invariant
under the application of S (invariant by rotation along Oz in our example)

Then V_{HF} constructed from the set $[|\alpha\rangle]$ is such that $[V_{\text{HF}}, S] = 0$

One defines from S a unitary linear operator

$$U = \exp(i\theta S)$$

From $[S, v] = 0$ one gets $[U, v] = 0$

Calling $\tilde{v} = v(1 - T)$ and with

$$U^+|i\rangle \equiv |U^+(i)\rangle \quad \text{and thus} \quad \langle U^+(i)| \equiv \langle i|U$$

$$U^+|j U(\alpha)\rangle \equiv |U^+(j) \alpha\rangle \quad \text{and thus} \quad \langle U^+(i) \alpha| \equiv \langle i U(\alpha)|U$$

One has

$$\begin{aligned} \forall i, j ; \quad \langle i|U V_{HF} U^+|j\rangle &= \sum_{\alpha} \langle U^+(i) \alpha| \tilde{v} |U^+(j) \alpha\rangle \\ &= \sum_{\alpha} \langle i U(\alpha)| U \tilde{v} U^+ |j U(\alpha)\rangle \\ &= \sum_{\alpha} \langle i U(\alpha)| \tilde{v} |j U(\alpha)\rangle \\ &= \sum_{\alpha\beta\gamma} (X_{\beta\alpha})^* X_{\gamma\alpha} \langle i \beta| \tilde{v} |j \gamma\rangle \end{aligned}$$

$$\text{since} \quad \sum_{\alpha} (X_{\beta\alpha})^* X_{\gamma\alpha} = \delta_{\beta,\gamma}$$

$$\forall i, j ; \quad \langle i|U V_{HF} U^+|j\rangle = \sum_{\beta} \langle i \beta| \tilde{v} |j \beta\rangle = \langle i|V_{HF}|j\rangle$$

$$\text{thus} \quad [V_{HF}, U] = 0 \quad \text{and this} \quad \forall \theta \quad \text{thus} \quad [V_{HF}, S] = 0$$

PRACTICAL CONSEQUENCES OF SYMMETRIES

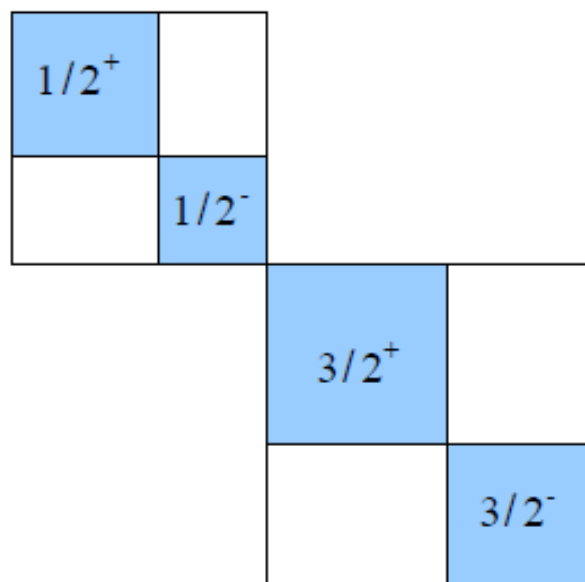
When solving the HF by projection on a sp basis one has to diagonalize a matrix diagonal by blocks since due to the symmetry whose operator is noted \hat{S} one has

$$[\hat{H}_{HF}, \hat{S}] = 0$$

and thus $\langle i | \hat{H}_{HF} | j \rangle = 0$

if the two eigenstates $|i\rangle, |j\rangle$ do not share the same symmetries

The more symmetries, the smaller the block dimensions, making calculations faster



Example

Axial symmetry + intrinsic parity

One has blocks $1/2^+, 1/2^-, \dots$

If only axial symmetry

One has larger blocks $1/2, 3/2, \dots$

6 – Examples of correlations treatment

Pairing correlations à la BCS

One desires to mock up a state including 0- 1- 2- ... **Cooper pairs** within the Bardeen Cooper Schrieffer ansatz for an even nucleus

$$|BCS\rangle = \prod_{\text{pair } i} (u_i + v_i a_i^\dagger \bar{a}_i^\dagger) |0\rangle$$

where the products runs over a pair of states which are Kramers degenerate (if H_{HF} is unchanged by time reversal symmetry its one-body eigenstates come by pairs of states – **Kramers pairs** - having the same eigenenergy which are conjugated by time reversal one from the other).

We define positive i states as such (e.g. as in the axial symmetry case) that their third component of the angular momentum K is positive.

Their time reversed pair companion would then correspond to a negative i .

We define the u 's and the v 's to be real

For the BCS state to be time reversal invariant, one chooses

$$\begin{array}{ll} v_i > 0 \quad \text{and} \quad v_{-i} < 0 \quad (\text{if } i > 0) & |u_i| = |u_{-i}| \\ u_i > 0 & (\text{for all signs of } i) \quad |v_i| = |v_{-i}| \end{array}$$

For the BCS state to be normalized (the one body states i being normalized) one has $u_i^2 + v_i^2 = 1$ for all i . The v_i^2 parameter corresponds to the occupation probability of the state i (and also of its time reversed)

The BCS wavefunction is a sum of Slater determinants having 0, 2, 4, ..., N-2, N, N+2, ... particles

This is of course a serious drawback of this approximation

One fixes the mean value of the number of fermions to a given value N by using a Lagrange parameter λ (called the chemical potential) in a variational process described below.

Typically for deformed heavy nuclei one has for each charge state

$$\sqrt{\langle (N - \langle N \rangle)^2 \rangle} = 3 - 4$$

The variational solution of the BCS problem is obtained by making the variation with respect to the sets $[|\phi_i\rangle]$ and $[v_i^2]$ as

$$\delta [H - \lambda_n N_n - \lambda_p N_p] = 0$$

yielding the set $[|\phi_i\rangle]$ and

$$v_i^2 = \frac{1}{2} \left[1 - \frac{(e_i - \lambda)}{\sqrt{\Delta_i^2 + (e_i - \lambda)^2}} \right]$$

$$u_i^2 = \frac{1}{2} \left[1 + \frac{(e_i - \lambda)}{\sqrt{\Delta_i^2 + (e_i - \lambda)^2}} \right]$$

In the above the pairing gap is defined by

$$\Delta_i = - \sum_{j>0} \langle \phi_i \phi_{T(i)} | v_{res} | \overline{\phi_j \phi_{T(j)}} \rangle u_j v_j$$

**Large amplitude collective correlations
in the Generator Coordinate Method (GCM) approach**

One performs a variational calculation for a trial wave function which corresponds to **a mixing of states**

$$| \Psi \rangle = \int f(q) | \Phi_q \rangle dq$$

where the $[| \Phi_q \rangle]$ are solutions of e.g. variational calculations under a constraint on a operator Q whose eigenvalue is noted q

Imposing

$$\delta \left[\frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \right] = 0$$

one has to solve the following eigenvalue problem to get the $f(q)$ solutions

$$\int \langle \Phi_q | H - E | \Phi_{q'} \rangle f(q') dq' = 0$$

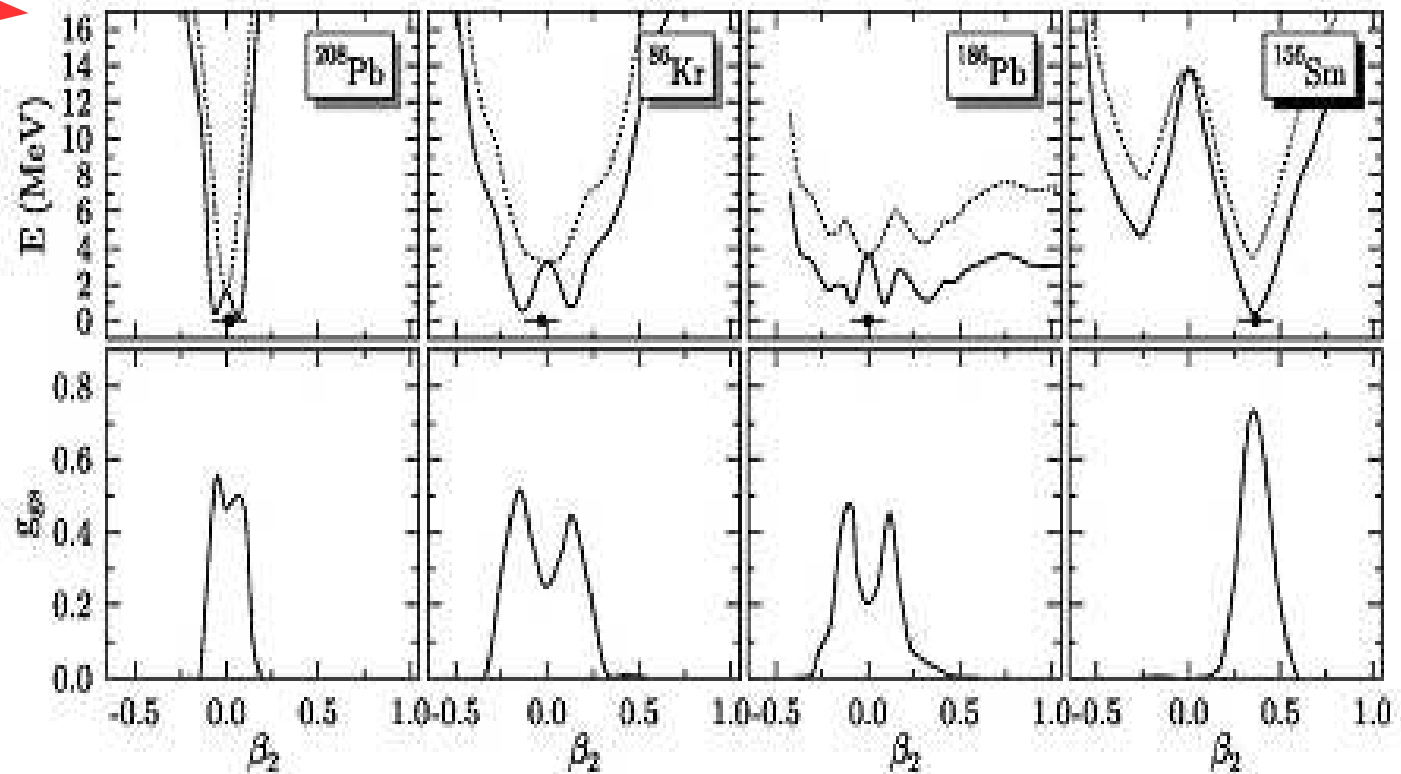
In practice, one has to be careful to remove from the space spanned by the set $[|\Phi_q\rangle]$ states corresponding to **zero eigenvalues of the norm matrix**

$$N_{qq'} = \langle \Phi_q | \Phi_{q'} \rangle$$

This approach might also be used **to restore symmetries** (in that case the $f(q)$ might be known by theoretical arguments beforehand (one has « just » to perform the integration on the relevant q 's)

M. BENDER, G. F. BERTSCH, AND P.-H. HEENEN

An example of complicated **multiple GCM calculations** : projection on spin 0 followed by a mixing of different quadrupole deformation states



Epilogue : some attempt to bridge self-consistent mean-field calculations and shell model calculations :

The Highly Truncated Diagonalization Approach (HTDA)

The basic idea is that if some physics is included in the mean field a mixing involving a relatively moderate number of Slater determinants (thousands or tens of thousand states) could be enough to describe ground state correlations and may be low energy excited states

Moreover this presents two advantages

a) preserve by construction the particle number and the Pauli principle (as opposed to BCS or RPA approaches)

b) make more transparent the calculational output

For instance, one should identify directly Cooper pair excitations as opposed to their being dissiminated over hundred thousand components

In practice

- 1) One defines an « as good as possible » **mean field** V_0 (typically through self-consistent plus BCS calculations)
- 2) Consider the Slater determinant $|\Psi_0\rangle$ solution of the eigenvalue problem associated with the one body hamiltonian $H_0 = K + V_0$ as a **vacuum** for a many-body basis composed of n particles - n holes (n p - n h) states excited above $|\Psi_0\rangle$
- 3) Choose a **suitable truncation of the many body basis** in two ways
 - considering only valence single particle states around the Fermi level λ allowed to generate particle - hole excitations (typically in the $[\lambda - 6, \lambda + 6]$ (MeV) interval for a description of pairing correlations in heavy nuclei)
 - truncate the size of the many body basis either in terms of a maximum order n for n p - n h states and/or in terms of unperturbed energies of n p - n h states

$$\langle np-nh | H_0 | np-nh \rangle = \sum_{i=1}^n e_i^{(p)} - \sum_{j=1}^n e_j^{(h)}$$

3) Approximate **the residual interaction** with respect to the physical problem in accordance with the choice made for the truncated basis

- a delta force for instance for studying pairing correlations

- a low-l multipole-multipole interaction for studying RPA correlations

- a combination of them whereby using e.g. a long-range interaction ...

The rationale for that may be schematized as

$$H = H_{1b} + H_{res.} \equiv [K + V_{1b} + C] + [v - V_{1b} - C]$$

one chooses $V_{1b} \equiv V_{HF}^{\Psi_0}$ and $C = - \langle \Psi_0 | v | \Psi_0 \rangle$

thus $\langle \Psi_0 | H_{1b} | \Psi_0 \rangle = \langle \Psi_0 | H | \Psi_0 \rangle$

$$\langle \Psi_0 | H_{res.} | \Psi_0 \rangle = 0$$

replace in H_{1b} v by e.g. a δ interaction so that

$$H_{res.} \approx \delta - \delta_{HF}^{\Psi_0} + \langle \Psi_0 | \delta | \Psi_0 \rangle$$

This formalism has mostly been used **to describe pairing correlations in even-even nuclei**

It has been extended to describe **rotations** (within a Routhian HTDA frame)

or **time - odd systems** (high K-isomers, odd nuclei) which in both cases

imply a low pairing correlations regime where BCS is at fault

Example of results

N. Pillet, P. Quentin, J. Libert, Nucl. Phys. A697, 141 (2002)

Ground and isomeric states in ^{178}Hf (SIII plus δ residual interactions)

Effects on the correlation energy ($E_{\text{corr.}}$ in MeV) of the inclusion of various np – nh components in the correlated wave-function for both charge states

Ground state correlation energies

Distribution	$n = 2$ (pair transfer only)	$n = 1, 2$	$n = 1, 2, 3$
Neutrons	–1.105	–1.173	–1.177
Protons	–1.956	–2.024	–2.032

Isomeric energies

Comparison of calculated and experimental excitation energies of the considered isomeric states of ^{178}Hf

State	th.	exp.	State	th.	exp.
$8^-(n)$	1.17	1.15*	16^+	2.59	2.45
$8^-(p)$	1.42		14^-	2.83	2.57
$6^+(n)$	1.41	1.54*	15^+	2.90	
$6^+(p)$	2.25				