NUCLEAR STRUCTURE

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1 Independent particles, correlations
2 Pauli principle correlations
3 The Hartree-Fock approximation
4 Treatments of correlations beyond the Hartree-Fock approximation

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1 - Independent particles, correlations

The concept of an independent particle state is of a statistical nature

For N particles $|\Psi_0> = \prod_{i=1,N} |\phi_i>$

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

Seen from the corresponding N-particle (purely spatial) wavefunction

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

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

Yet correlations 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 mathemetically 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

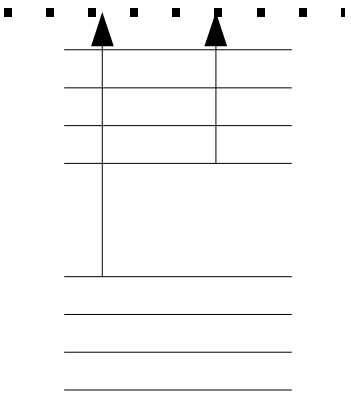
This is observed in atomic physics (for the ionisation potential) which does not come as a surprise

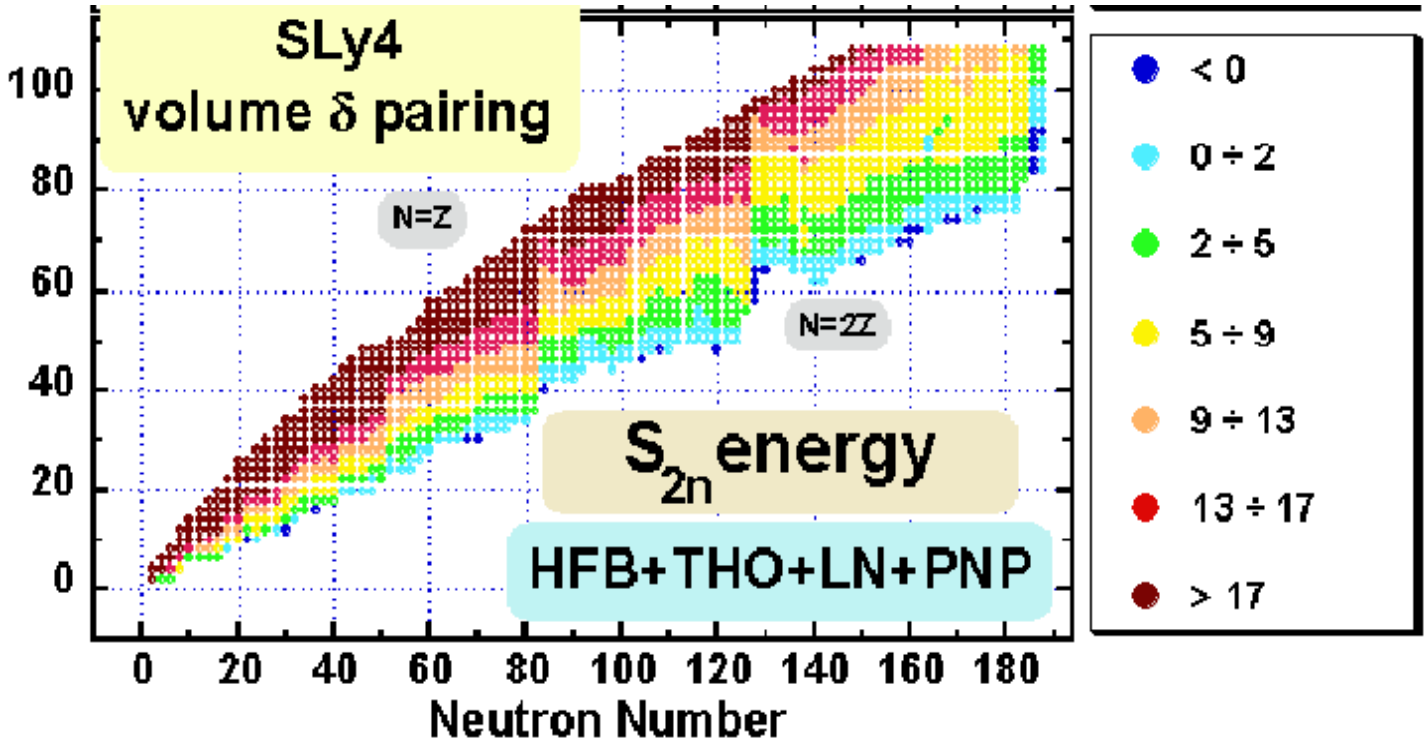
This is observed in nuclear physics which is more surprising :

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

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

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





J. Dobaczewski(U. Warsaw)

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

$$V(\vec{r}) = \int \rho(\vec{r}\,') \, v(\vec{r} - \vec{r}\,') d^3 r'$$

where v is a translationally invariant two-body interaction and ° the (un-normalized) probability density of presence of a nucleon

$$\rho(\vec{r}) = \sum_{i=1,A} |\phi_i(\vec{r})|^2$$

evaluated within the independent particle limit.

Beyond the spurious effect of self interaction and the neglection of the Pauli principle (the second correcting for the first incidentally) the very existence of such field in Nuclear Physics 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) one gets $\lambda \approx 1\ fm$ **which is of the order of the nucleonic size**

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

But, the Pauli principle, reducing the available phase-space quenches the effective interaction cross section to raise λ at a value ≥ the nuclear size

Then the problem is to define as best as possible, from first principles as much as possible, 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, one defines the hermitian idempotent (thus projector) operator A as

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

where sgn(P) is the signature of P.

This operator projects onto completely antisymetric states $|\Psi>$ i.e. such that

$P\,|\Psi> = sgn(P)\,|\Psi>$ for all P

These states form a subspace S_A of the space of the a priori physical space for systems of N particles

The Pauli principle postulates two things for N fermions states :

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

Then the naive independent wavefunction $|\Psi_0> = \prod_{i=1,N} |\phi_i>$
is not acceptable and instead one defines from it

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

It is normalized provided that $<\phi_i\,|\,\phi_j> = \delta_{ij}$
Its wavefunction

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

is called a Slater determinant, since

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

The above entails the so-called Pauli exclusion principle since, if one has in the state Ψ two individual states i and j (i ≠ j) such that

$$|\phi_i> \equiv |\phi_j>$$

then, calling T the transposition $i \leftarrow\rightarrow j$ **the state Ψ has a vanishing probability**

$$T\,|\Psi> = |\Psi> = -\,|\Psi> = 0$$

Considering the set $[\phi_i]$ **as forming 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 form an orthonormal basis of the physically acceptable states of N fermions.**

3 – The Hartree-Fock approximation

The Ritz theorem establishes that for non vanishing Ψ states, solving the variational problem

$$\delta\left[\frac{<\Psi \mid H \mid \Psi>}{<\Psi \mid \Psi>}\right] = 0$$

is equivalent to solving the Schrödinger stationary (eigenvalue) problem

$$H \mid \Psi> = E \mid \Psi>$$

The Hartree-Fock approximation consists in restricting the trial states in the above variation to be merely Slater determinants.

One shows that this is achieved by solving the stationary Schrödinger equation for individual states as

$$H_{HF} \mid \phi_j> = e_j \mid \phi_j>$$

to form with a set of N such individual solutions a Slater determinant Ψ.
In the above H_{HF} is the so-called one-body reduction of the hamiltonian H, defined if H includes a kinetic energy term K and a two body interaction v as

$$<\chi_i \mid H_{HF} \mid \chi_j> = <\chi_i \mid K \mid \chi_j> + <\chi_i \mid V_{HF} \mid \chi_j>$$

where the one-body potential V_{HF} is defined by

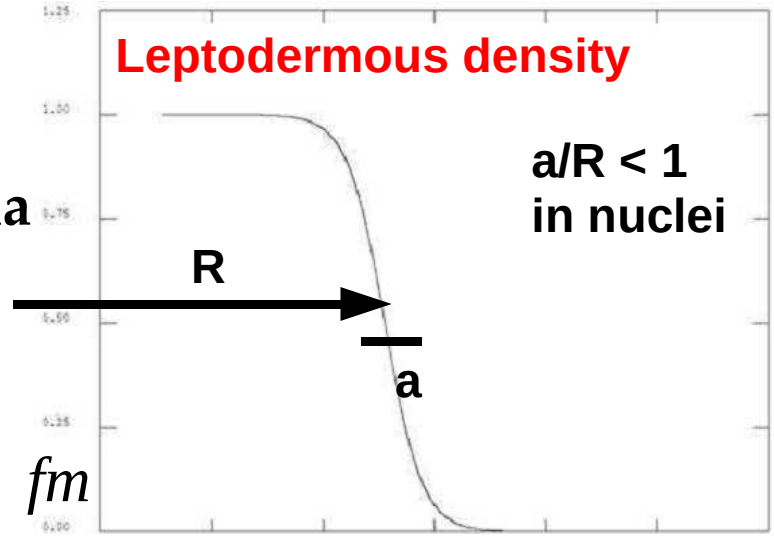
$$<\chi_i \mid V_{HF} \mid \chi_j> = \sum_{\alpha}^{occ.} <\chi_i\, \phi_\alpha \mid v \mid \widetilde{\chi_j\, \phi_\alpha}>$$

with $\mid \widetilde{m\ n}> = (1-T) \mid m\ n> = \mid m\ n> - \mid n\ m>$

Ignoring the transposition term (in T) in V_{HF} one retrieves the classical convolution potential (called the Hartree potential) previously guessed upon choosing $\mid \chi_i> \equiv \mid \vec{r}>$ and with a local two-body potential, namely such that $<\vec{r}_1\ \vec{r}_2 \mid v \mid \vec{r}_3\ \vec{r}_4> = \delta(\vec{r}_1 - \vec{r}_3)\, \delta(\vec{r}_2 - \vec{r}_4)\ v(\vec{r}_1 - \vec{r}_2)$ expanding the individual states ϕ on the r-basis $\mid \phi_m> = \int \phi_m(\vec{r}) \mid \vec{r}> d^3 r$ one finds

$$V_H(\vec{r}) = <\vec{r} \mid V_H \mid \vec{r}> = \int v(\vec{r} - \vec{r}\,')\, \rho(\vec{r}\,')\, d^3 r$$

From electron scattering one has confirmed the saturation (constant density) in the nuclear interna part and leptodermous (thin skin) properties.



The rough density profile is thus of the Fermi type $\rho(r) = \dfrac{\tilde{\rho}_0}{1 + e^{(r-R)/a}}$ $\dfrac{a}{R} < 1$ $Range \approx 0.8\ fm$

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

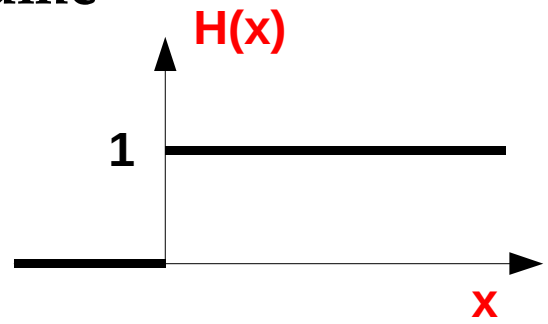
One may deform this model mean field by replacing R by a function of the two angles θ and ϕ defining a position in spherical coordinates

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

the first term being included to conserve the nuclear volume

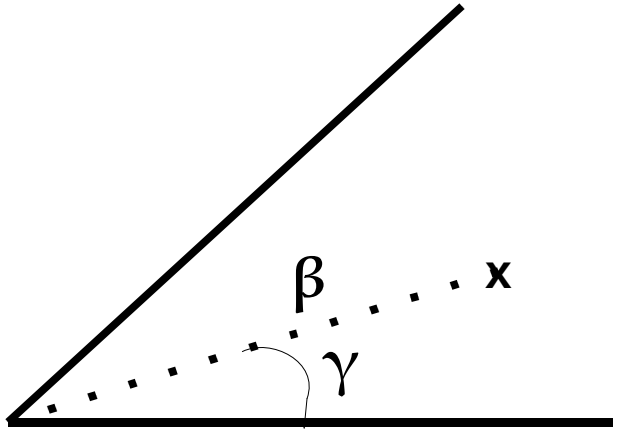
$$\rho(\vec{r}) \equiv \rho_0\, H[\,R(\theta,\phi) - r\,] \qquad (r_0 = 1.2\ \ fm)$$

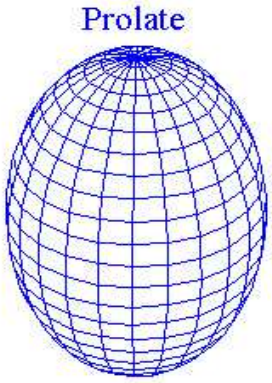
$$\iiint \rho(\vec{r})\;\; r^2 \sin(\theta)\, dr\, d\theta\, d\phi = A = \frac{4}{3\pi}\, r_0^3\, A\;\; \rho_0$$



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

$$\alpha_{20} = \beta\sin(\gamma) \quad \alpha_{2\mp2} = \beta/\sqrt{2}\cos(\gamma)$$
$$\alpha_{2\mp1} = 0$$



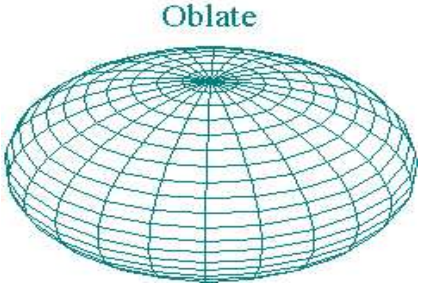


Axial quadrupole moment $Q_{20} = 2z^2 - (x^2 + y^2)$

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

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

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



The second term V_F in V_{HF} (involving the transposition T) is called the Fock term originating from the Pauli principle implying 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 strength 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 $\{|m>\}$

$|\phi_i> = \sum_n X_{m\,i}\,|n>$ one gets from $<m|\ [(K + V_{HF})\,|\phi_i>] = <m|\ [e_i\,|\phi_i>]$

$$\sum_n <m|\,K + V_{HF}\,|n>\,X_{n\,i} = e_i\,X_{m\,i} \qquad \text{with} \quad <m|\,n> = \delta_{m,n}$$

$$\sum_n \left(<m|\,K\,|n> + \sum_j^{occ.} \sum_{kl} X^*_{k\,j}\,X_{l\,j} <m\,k\,|v|\,\widetilde{n\,l}>\right) X_{n\,i} = e_i\,X_{m\,i}$$

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.

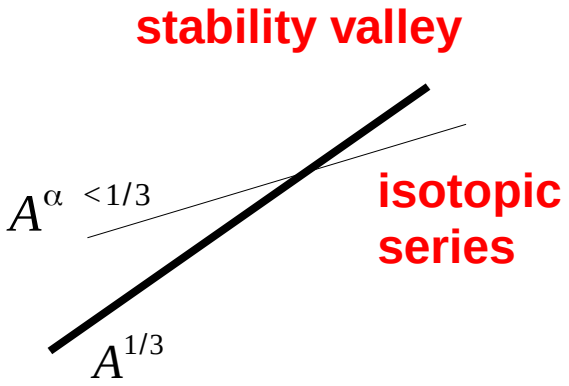
It then results that V_{HF} depends on the nucleus (even on the nuclear state),
so this entails that $V_{HF}(A+1) \neq V_{HF}(A)$
Now, approximating $|\Psi_{HF}(A+1)> \approx a^{\dagger}_{A+1}|\Psi_{HF}(A)> = |\Psi^{appr.}_{HF}(A+1)>$
One proves that

$$E^{appr.}_{HF}(A+1) = <\Psi^{appr.}_{HF}(A+1)|H|\Psi^{appr.}_{HF}(A+1)> = E_{HF}(A) + e_{A+1}$$

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.
Thus one may approximate the separation energy in the A+1 nucleus as

$$E^{sep.}(A+1) = |E(A+1) - E(A)| \approx |e_{A+1}|$$

This of course 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)
It is generally, however a good approximation for E_{A+1}



The energy of the Hartree-Fock solution is given by

$$E_{HF} = <\Psi \,|K+v|\, \Psi> = \sum_i^{occ.} \{<\phi_i \mid K \mid \phi_i> + (1/2) \sum_j^{occ.} <\phi_i\, \phi_j|\, v \mid \widetilde{\phi_i\, \phi_j}>\}$$

Since

$$e_i = \sum_i^{occ.} \{<\phi_i \mid K \mid \phi_i> + \sum_j^{occ.} <\phi_i\, \phi_j|\, v \mid \widetilde{\phi_i\, \phi_j}>\}$$

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

$$E_{HF} = (1/2) \sum_i^{occ.} (\, e_i + <\phi_i \mid K \mid \phi_i> \,) \neq \sum_i^{occ.} e_i$$

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 (with $w_{00} \propto r_1^2 r_2^2$) and a quadrupole term (with $w_{2\mu} \propto r_1^2 r_2^2$), further assumes the axial symmetry, one gets for the Hartree potential

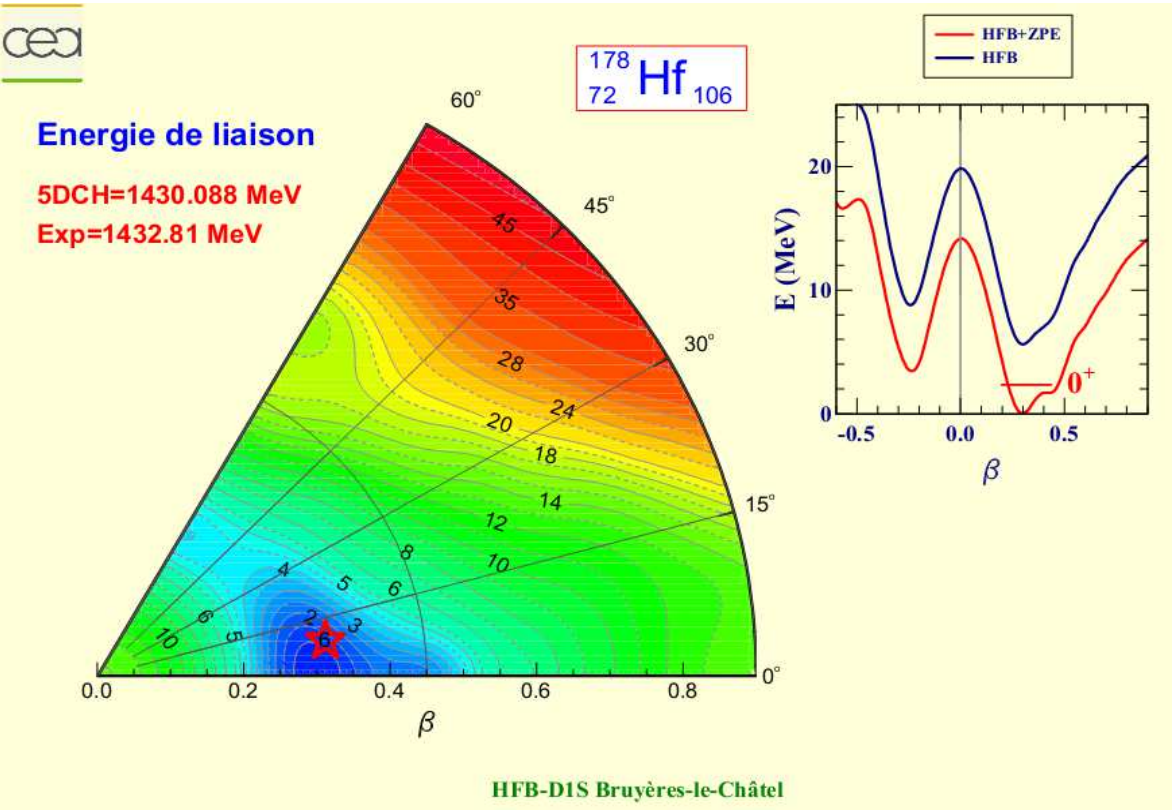
$$V_H(\vec{r}) \propto <\Psi_{HF} \mid r^2 \mid \Psi_{HF}> \; r^2 + \alpha <\Psi_{HF} \mid r^2 Y_{20}(\hat{r}) \mid \Psi_{HF}> \; r^2 Y_{20}(\hat{r})$$

which is the deformed harmonic oscillator of Å. Bohr and J. Rainwater yielding (with a spin-orbit and a $\vec{l}^2$ corrective term) the Nilsson model

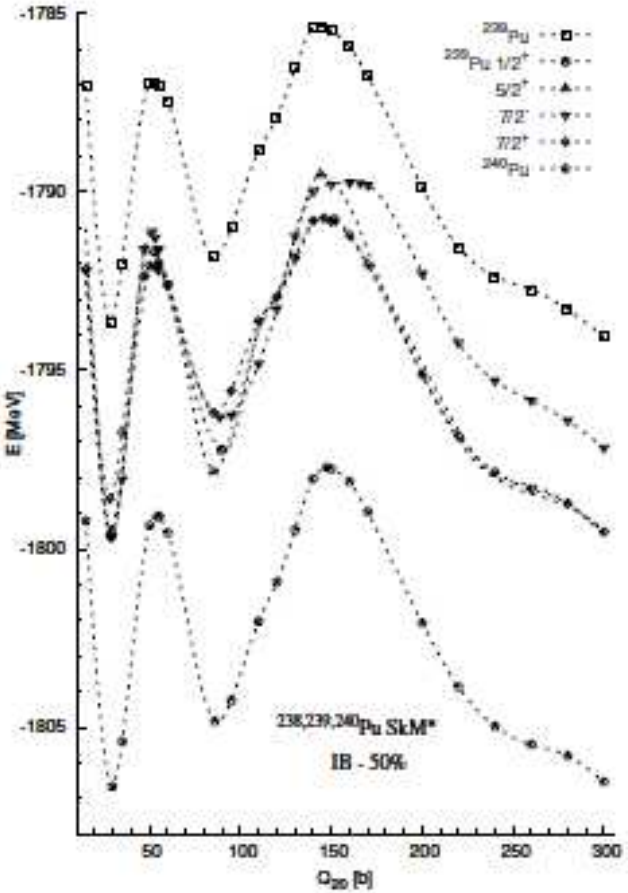
Solving the Hartree-Fock variational problem one gets a priori a local extremum, in practice for stability reasons, this is **a local minimum**.
Physical intuition and/or more or less educated guesses and trials lead to an **approximation of the ground state**.
One explores **non equilibrium solution 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 or fission barriers

M. Girod, J. Libert et al.

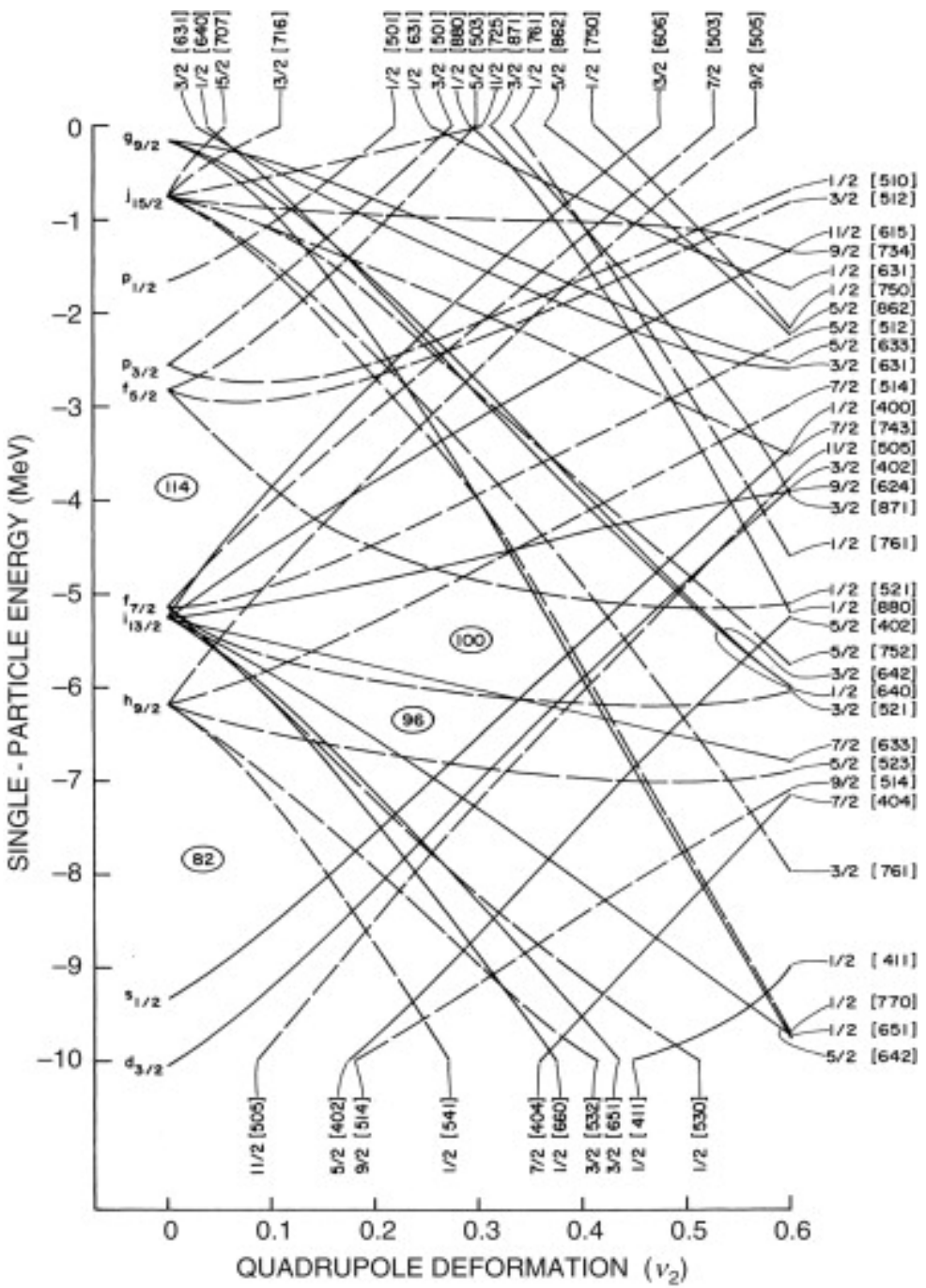


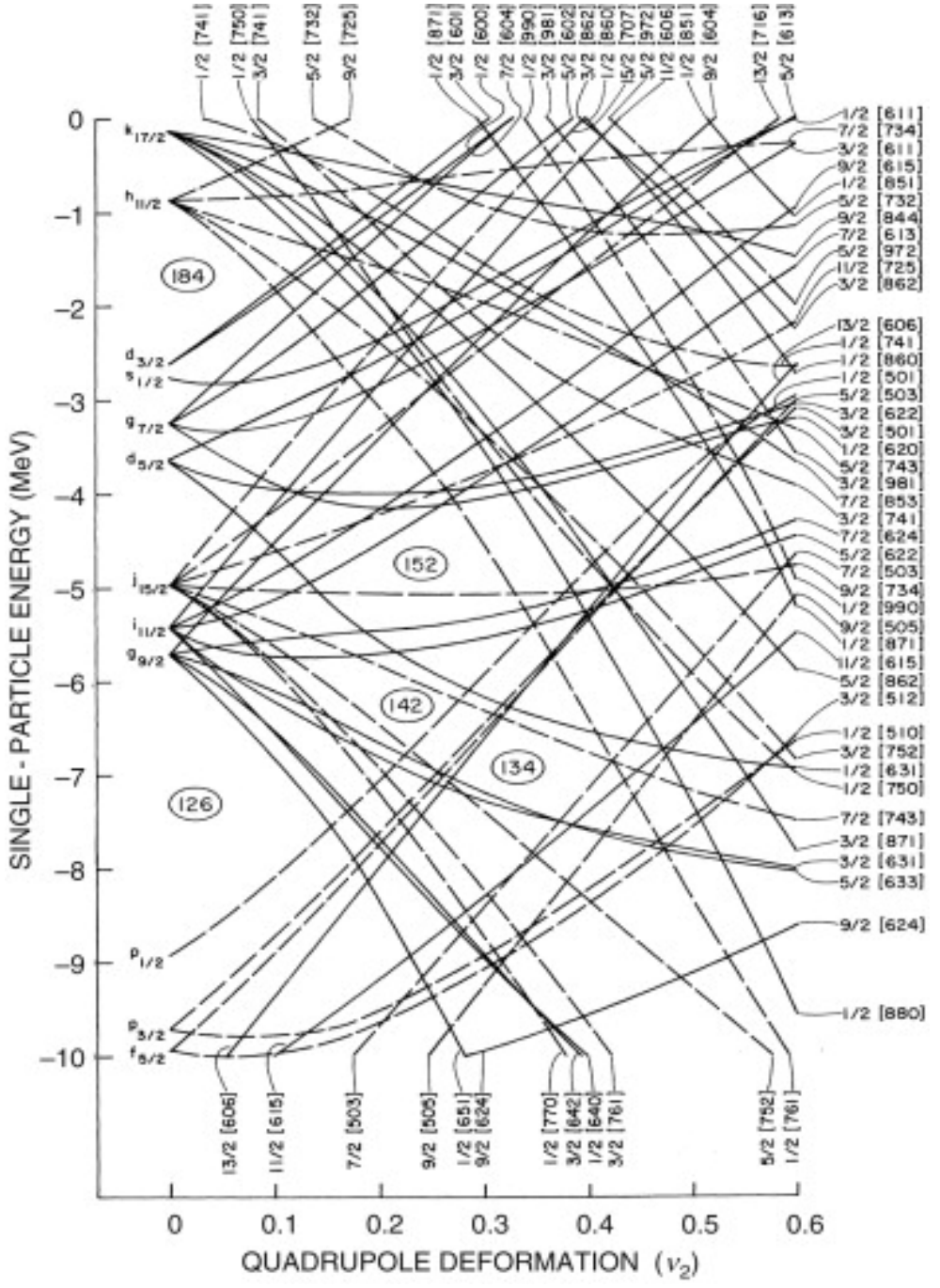
Koh Meng Hock, L. Bonneau, P. Quentin



R.D. Herzberg, P.T. Greenless

Nilsson diagrams





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 non vanishing norm states Ψ as

$$\delta\,[\int_{t_1}^{t_2} <\Psi \mid H - i\hbar \frac{\partial}{\partial t} \mid \Psi > dt\,] = 0 \quad \text{leading to} \quad H \mid \Psi > = i\hbar \frac{\partial}{\partial t} \mid \Psi >$$

The Hartree-Fock approximation consists here too to restrict the variation of Ψ to Slater determinants.The corresponding equations of motion (due to Dirac) for the individual states are written as

$$H_{HF} \mid \phi_j > = i\hbar \frac{\partial}{\partial t} \mid \phi_j >$$

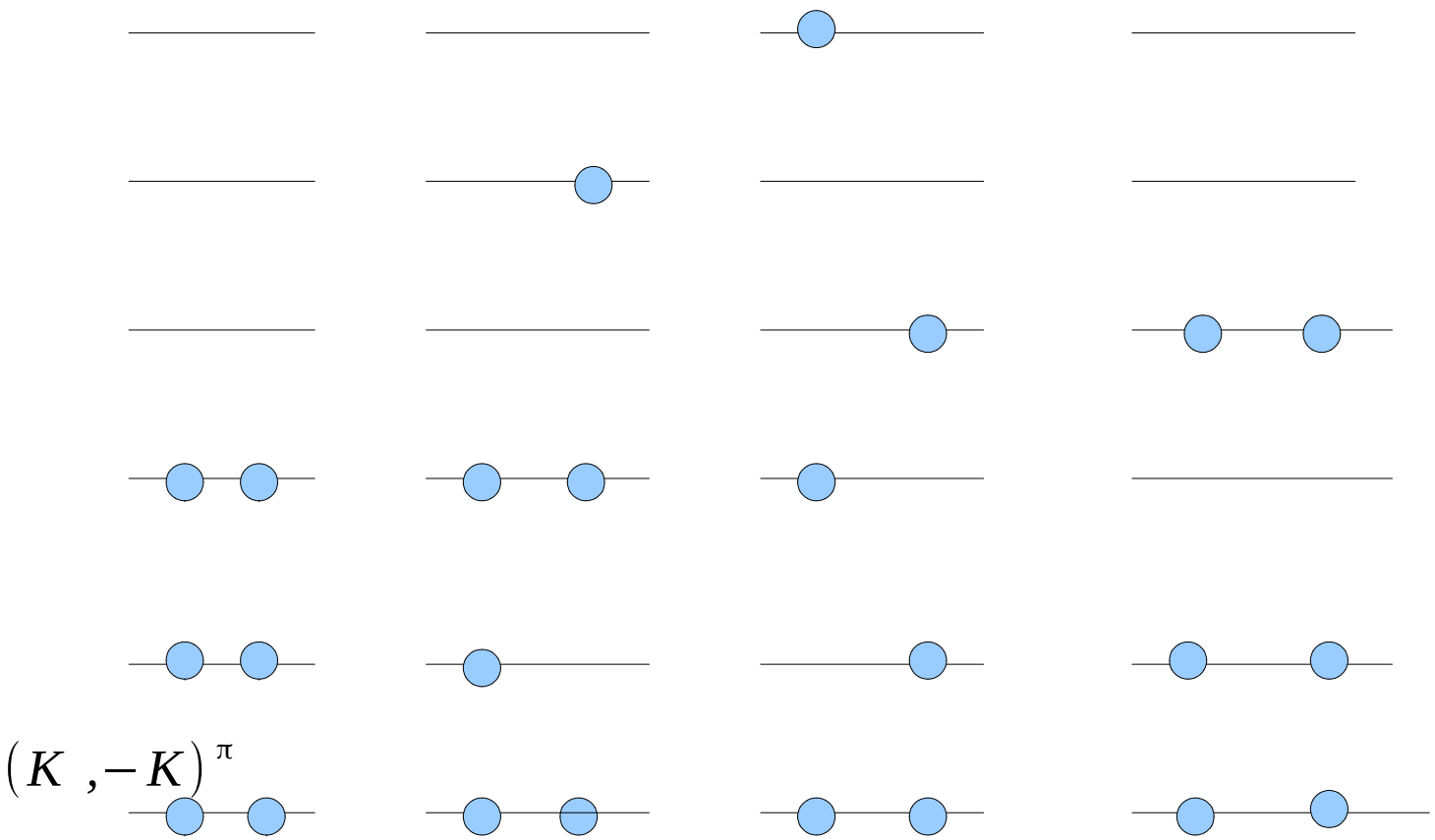
4 – Treatments of Correlations beyond the Hartree-Fock approximation

The Hartree-Fock approach may be viewed as replacing, to evaluate the stationary states, the exact hamiltonian H by its approximation H_{HF}.

To improve this description one should treat as best as possible the residual interaction

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

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



Symmetries

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 basis
to be truncated

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

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 $\delta(\vec{r}_1 - \vec{r}_2)$

- Note that such an interaction favours matrix elements of the type

$$< i\ \bar{i} \mid \delta^{(T=1)} \mid \widetilde{k\ \bar{k}} >$$

If the spin would be a good quantum number
(ie if single particle states would be eigenstates
of the projection of the spin on Oz with +1/2 or -1/2 as eigenvalues)
then the pair $[\ i\ ,\ \bar{i}\ ]$ **would correspond to two states**
with the same spatial structure but with opposite spins.

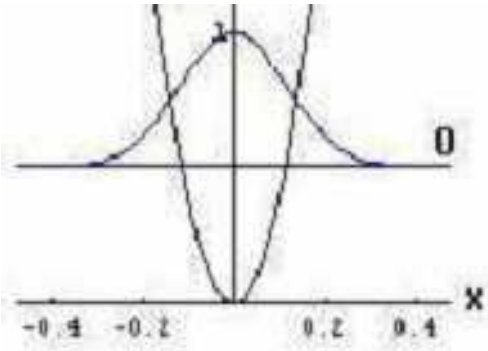
Then

$$< i\ \bar{i} \mid \delta^{(T=1)} \mid \widetilde{k\ \bar{k}} > = \iiint d^3 r\ |\phi_i(\vec{r})|^2\ |\phi_k(\vec{r})|^2 \quad \text{since} \quad \phi_{\bar{i}}(\vec{r}) = \phi_i(\vec{r})^*$$

Such pairs of wavefunctions are implied in a basis made of pair transfer states

To model the pairing correlations in simple terms
one often uses a delta interaction

Since, as above sketched, the matrix elements which are involved are single particle wavefunctions overlaps it appears that for 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 due to the Pauli principle).



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 (due to a standard approximation 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 residual interaction

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

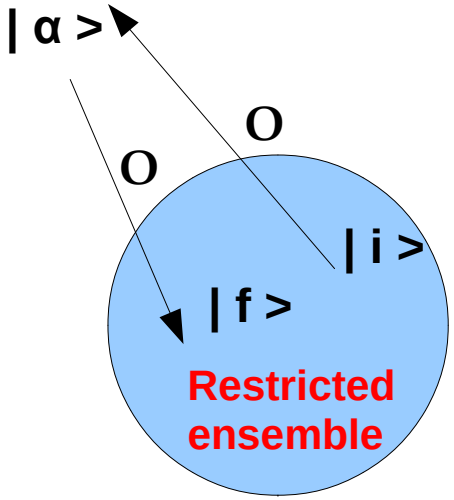
Of course modern calculations use more sophisticated forms of the residual interaction

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

- first for practical reasons (very difficult problem :
« *we are simply forced to simplify the force !*» B. Mottelson)
- second, because the interaction v is an « effective » interaction (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 (which becomes also « effective »)

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
and finally back to it



For Hartree-Fock calculations and more generally for approximate variational approaches,
the restricted ensemble is the one where the variation is made.
They are, e.g., Slater determinants for Hartree-Fock. One has thus, in this case, to include the effects of correlations not taken into account. Thus 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

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

They are many parametrisations for the interaction in use 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}

There are 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

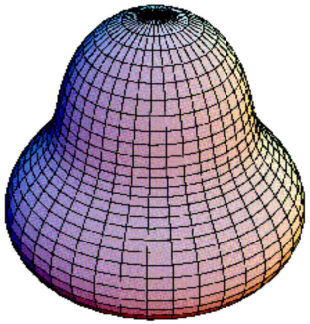
- Spurious symmetry breaking (rotational, translational symmetries, sometimes parity symmetry, particle number …) restored or not

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

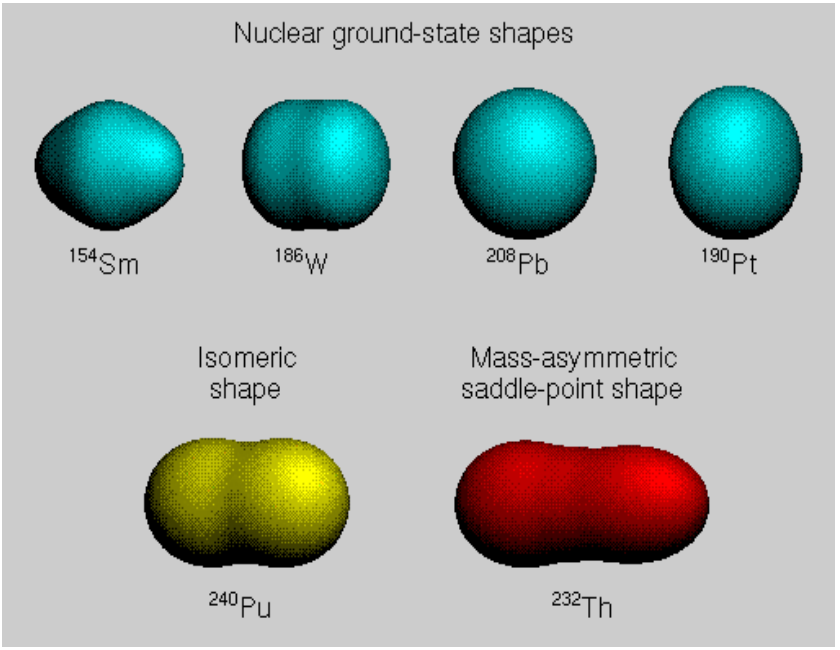
Symmetries broken in the Hartree-Fock approach

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

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



- parity symmetry (octupole intrinsic shapes)



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- particle number symmetry (BCS or similar calculations)

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

These spuriously broken symmetries must in principle be restored

Connexion between the symmetries of the density and of the V_{HF} potential :

The coherent symmetry theorem

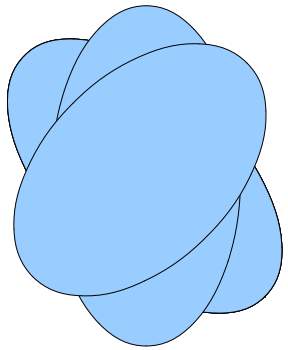
Given a symmetry generated by some operator S (e.g. a component of the angular momentum j_x for a rotation around the Ox axis)

Assume that [v , S] = 0
and that the subspace spanned by the occupied states $[|\phi_k>]$ is invariant under the application of S (invariant by rotation along Ox in our example)
Then V_{HF} constructed from the set $[|\phi_k>]$ is such that $[V_{HF}, S] = 0$

In simple terms the symmetry properties of V_{HF} depends on the symmetry properties of v and of the Hartree-Fock solution

To restore broken symmetries one reconstructs good symmetry states by adding solutions with appropriate weights (e.g. to make a spherical state from a deformed solution)

Superposing deformed ellipses



makes a spherical object

First example of treatment of correlations :

Including pairing correlations à la BCS

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

$$| BCS > = \prod_{pair\ \ i} \left(u_i + v_i \; a_i^{\dagger} \overline{a_i^{\dagger}} \right) | 0 >$$

where the products runs over a pair of states which are Kramers degenerate (if H is unchanged by time reversal symmetry its eigensolution comes by pair of states – a Kramers pair - having the same eigenvalue and 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 K (third component of the angular momentum) 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 unchanged by time reversal, one chooses

$$v_i > 0 \quad \text{and} \quad v_{-i} < 0 \; (if \;\; i > 0) \qquad |u_i| = |u_{-i}|$$
$$u_i > 0 \qquad\qquad (i > 0 \text{ or } < 0) \qquad |v_i| = |v_{-i}|$$

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, … particles, thus breaking the particle number symmetry
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 $\sqrt{<(N-<N>)^2>} = 3-4$

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

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

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

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

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

In the above the pairing gap is defined by

$$\Delta_i = -\sum_{j>0} <\phi_i\ \overline{\phi_i}\ |\ v_{res}\ |\ \widetilde{\phi_j\ \overline{\phi_j}}> u_j v_j$$

Secund example of treatment of correlations :

Including large amplitude collective correlations in the Generator coordinate (GCM) approach

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

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

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

Solving

$$\delta\,[\frac{<\Psi\,|\,H\,|\,\Psi>}{<\Psi\,|\,\Psi>}] = 0$$

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

$$\int <\Phi_q\,|\,H - E\,|\,\Phi_{q'}>\ f(q')\,dq' = 0$$

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

$$N_{qq'} = <\Phi_q | \Phi_{q'}>$$

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)

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