# Nuclear Theory II


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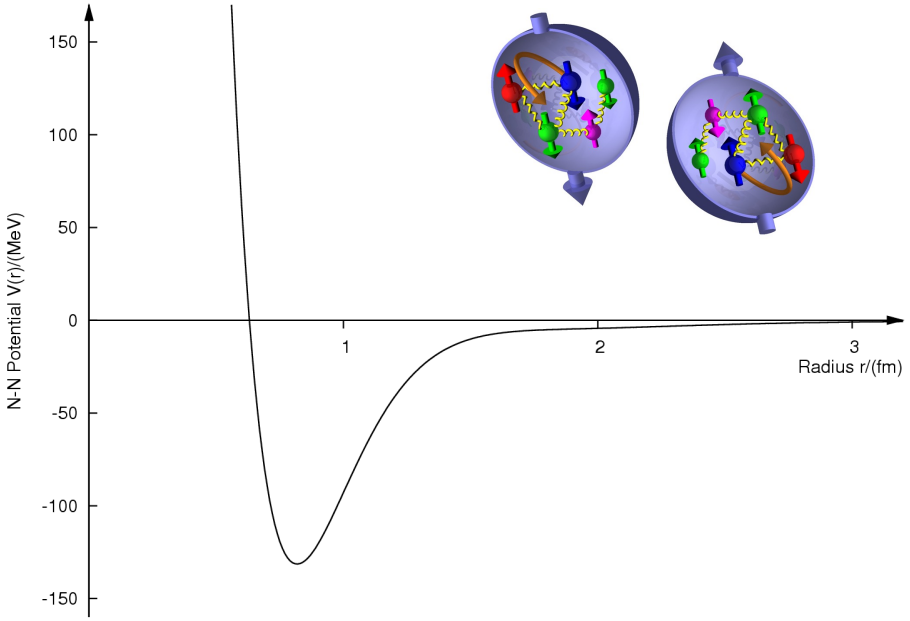
# The Nuclear Mean Field

# Introduction

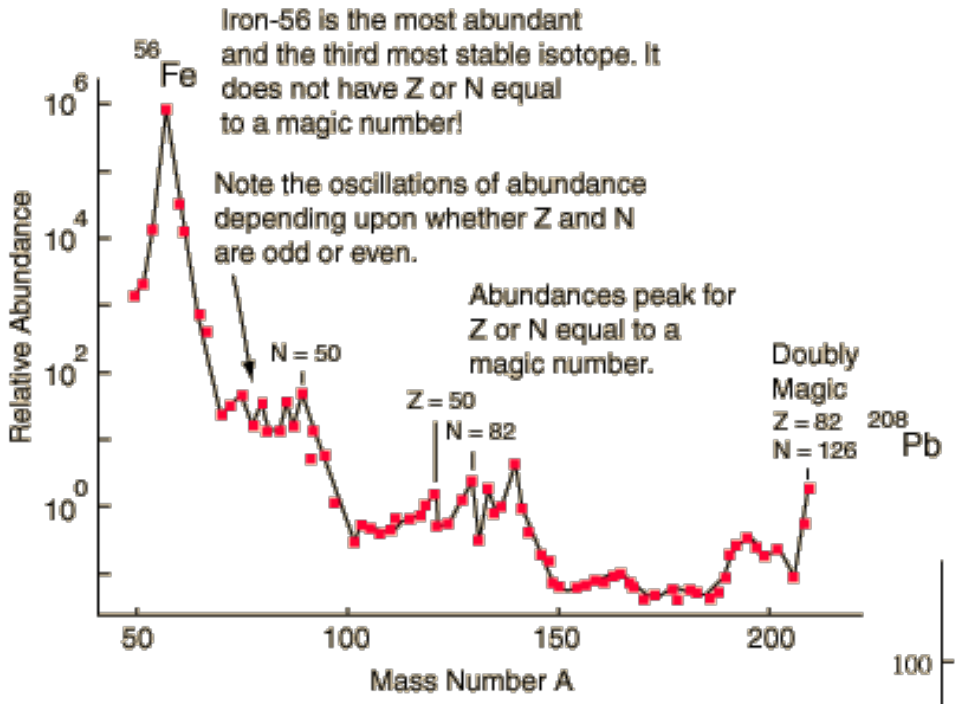
The basic assumption of the nuclear mean field is, to first order, the independent motion of each nucleon (proton or neutron) in an average nuclear potential.



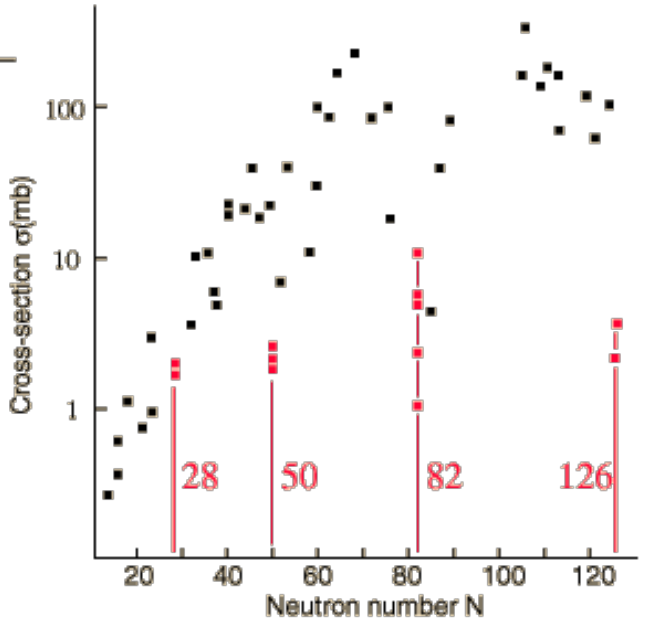

-how to describe the average field starting from the NN force between free nucleons?

-the many-body A-nucleon problem?

# Evidence for nuclear shell-structure:

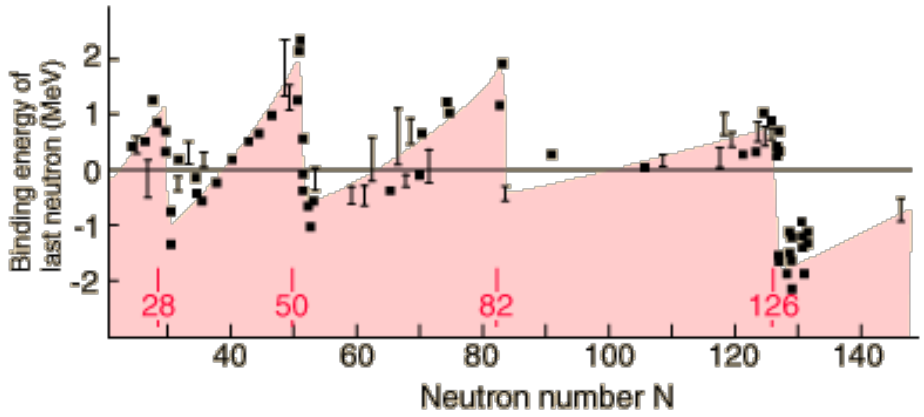



Enhanced abundances of elements for which Z or N is a magic number.

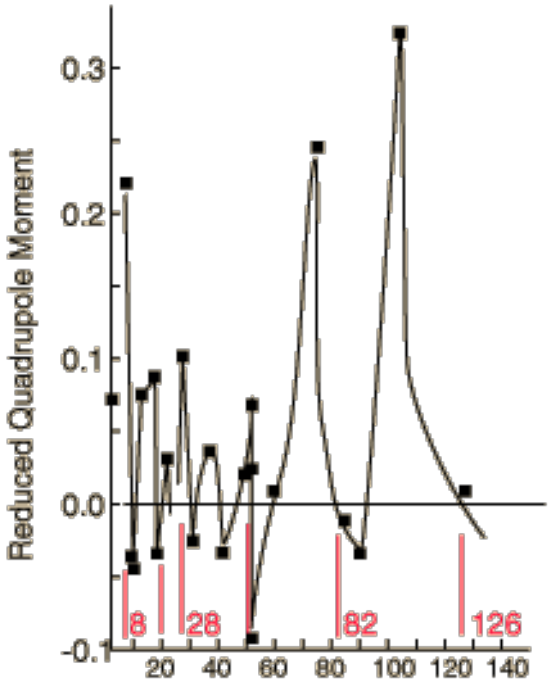



Nuclei with magic numbers of neutrons have neutron absorption cross-sections up to two orders of magnitude less than other nuclei with similar masses

The neutron-absorption cross-sections for isotopes for which N is a magic number are much lower than for the neighboring isotopes.

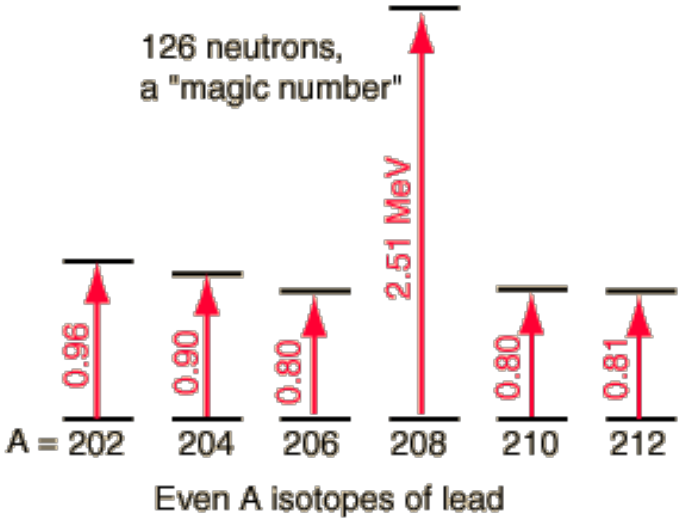



The binding energy of the last neutron relative to the Weizsäcker formula.




Quadrupole measurements for odd-A nuclei. The horizontal axis is either neutron number or proton number, whichever is odd.

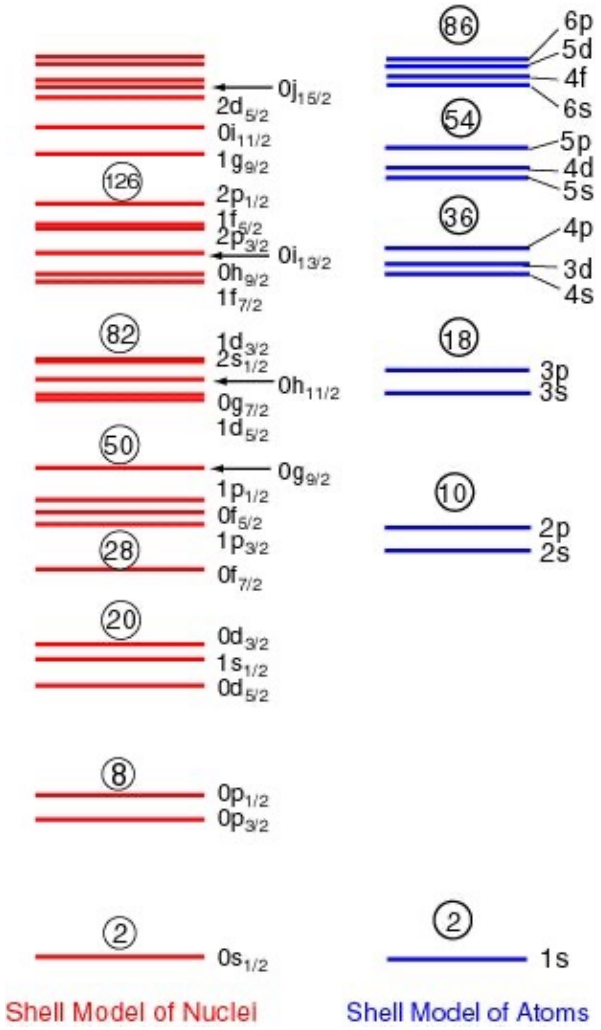
For a shell model, those nuclei with closed shells should be spherically symmetric and have no quadrupole moment.




Electric quadrupole moments are ≈ zero for magic number nuclei.

Excitation energies of first excited states.

# One-Particle Excitations




… one-body equation:

$$[T + U(r)]\,\phi_a(\vec{r}\,) = \epsilon_a \phi_a(\vec{r}\,)$$

average potential

$$\phi_a(\vec{r}\,) \quad (a \equiv n_a, l_a, j_a, m_a, \ldots)$$

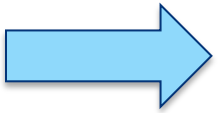
$$\vec{r} \equiv \vec{r}, \vec{\sigma}, \vec{\tau}, \ldots$$

-orthogonality:

$$\int \phi_a^*(\vec{r}\,)\phi_b(\vec{r}\,)\; d^3r = \delta_{ab}$$

… model Hamiltonian for A independent nucleons:

$$H_0 = \sum_{i=1}^{A} (T_i + U_i(r)) \equiv \sum_{i=1}^{A} h_0(i)$$



eigenfunctions: $\Psi_{a_1,a_2,\ldots a_A}(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_A) = \prod_{i=1}^{A} \phi_{a_i}(\vec{r}_i)$

eigenvalues: $E_0 = \sum_{i=1}^{A} \epsilon_{a_i}$

… antisymmetrization:

$$\Psi_{a_1,a_2}(\vec{r}_1, \vec{r}_2) = \frac{1}{\sqrt{2}} \left[\phi_{a_1}(\vec{r}_1)\phi_{a_2}(\vec{r}_2) - \phi_{a_1}(\vec{r}_2)\phi_{a_2}(\vec{r}_1)\right]$$

The average potential U(r) is not given explicitly. If one starts from a one- plus two-body Hamiltonian:

$$H = \sum_{i=1}^{A} T_i + \frac{1}{2} \sum_{i,j=1}^{A} V_{i,j}$$

$$H = \sum_{i=1}^{A} [T_i + U_i(r_i)] + \left( \frac{1}{2} \sum_{i,j=1}^{A} V_{i,j} - \sum_{i=1}^{A} U_i(r_i) \right) \equiv \sum_{i=1}^{A} h_0(i) + H_{RES}$$

The smaller the effect of $H_{RES}$, the better the assumption of an average, independent field for each nucleon.

## The radial equation and the single-particle spectrum

… start from a central, one-body potential => the total wave function:

$$\phi(\vec{r}\,) = R(r)Y(\theta,\phi) = \frac{u(r)}{r} Y(\theta,\phi)$$

… radial equation:

$$\frac{-\hbar^2}{2m}\frac{d^2u(r)}{dr^2} + \left[\frac{\hbar^2 l(l+1)}{2mr^2} + U(r)\right] u(r) = Eu(r)$$

Boundary conditions for bound states (E<0): $u(r) \lim_{r\to\infty} = 0 \qquad u(0) = 0$

… normalization:

$$\int_0^\infty R^2(r) r^2 dr = \int_0^\infty u^2(r) dr = 1$$

… solutions for the HO potential: $U(r) = \frac{1}{2} m\omega^2 r^2$

$$u_{kl}(r) = N_{kl}\, r^{l+1} e^{-\nu r^2} L_k^{l+1/2}(2\nu r^2) \qquad (\nu = m\omega/2\hbar)$$

Laguerre polynomials

$$E = \hbar\omega(2k + l + \frac{3}{2}) = \hbar\omega(N + \frac{3}{2})$$

| | |
|---|---|
| N = 0,1,2 … | major oscillator quantum number |
| l = N,N-2, … ,1 or 0 | orbital quantum number |
| k = (N-l) /2 | radial quantum number |

n = k+1 = (N-l+2)/2 number of nodes of the radial wave function in the interval [0,∞).

**Degeneracy:** -for a state with orbital angular mometum l: (2l+1)

… degeneracy of the oscillator shell N: $D_N = 2 \sum_{l=0 \text{or} 1}^{N} (2l+1) = (N+1)(N+2)$

spin projections

The total number of states in $N_{max}$ oscillator shells:

$$D_{\max} = \sum_{N=0}^{N_{max}} D_N = \frac{1}{3}(N_{max}+1)(N_{max}+2)(N_{max}+3)$$

$$N_{max} = 0, 1, 2, \ldots \quad \Rightarrow D_{\max} = 2, 8, 20, 40, 70, 112, 168, \ldots$$

For a given nucleus the HO frequency can be related to the nucleon number A. From the virial theorem => expectation value of the HO potential energy in the oscillator state ħωN:

$$\langle \frac{1}{2} m\omega^2 r^2 \rangle_N = \frac{1}{2}(N + \frac{3}{2})\hbar\omega$$

For a nucleus with N = Z = A/2:

$$\langle R^2 \rangle = \frac{2}{A} \sum_{N=0}^{N_{max}} D_N \langle r^2 \rangle_N = \frac{2}{A} \sum_{N=0}^{N_{max}} (N+1)(N+2)(N+\frac{3}{2}) \frac{\hbar}{m\omega}$$

… average over all occupied proton and neutron HO states.

In the limit of large $N_{max}$:

$$\langle R^2 \rangle = \frac{2}{A}\frac{\hbar}{m\omega}\frac{1}{4}(N_{max}+2)^4$$

$N_{max}$ is determined by the nucleon number:

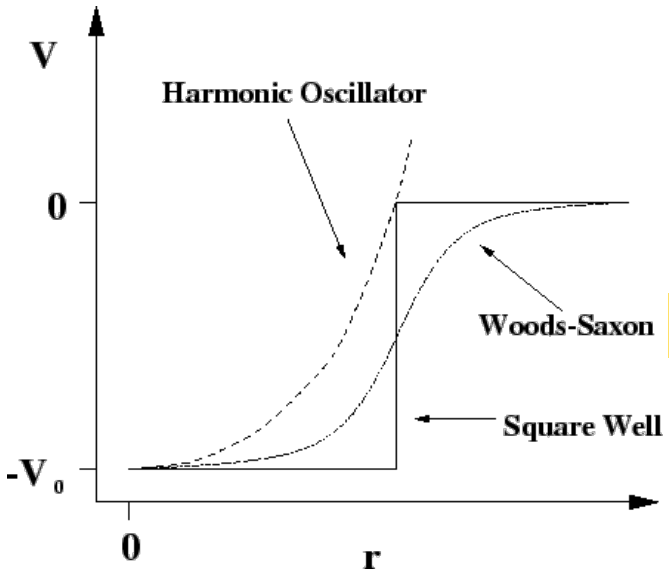
$$A = 2D_{\max} \approx \frac{2}{3}(N_{max}+2)^3$$

protons and neutrons

From: $\langle R^2 \rangle = \frac{3}{5}R_0^2 = \frac{3}{5}(r_0 A^{1/3})^2$

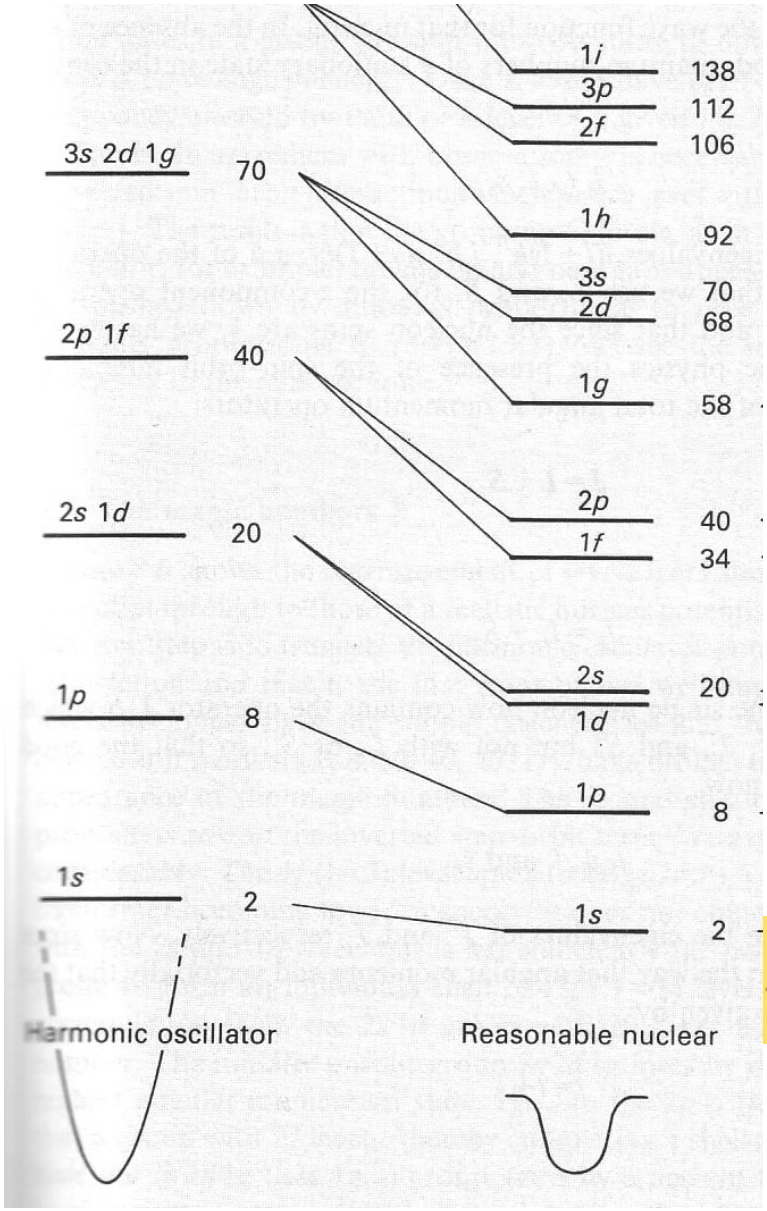
$$\hbar\omega = \frac{\hbar^2}{m\frac{3}{5}(r_0 A^{1/3})^2}\frac{3}{4}(\frac{3}{2}A)^{1/3} \approx 41A^{-1/3}\ \mathrm{MeV}$$

For A = 100: ħω = 8.8 MeV.




realistic nuclear single-particle potential

# The spin-orbit coupling




Mayer (1949,1950) and Haxel, Jensen, Suess (1949, 1950) – the average single-nucleon potential should contain a spin-orbit term:

$$h = h_0 + \zeta(r)\vec{l}\cdot\vec{s}$$

… an intrinsically relativistic effect. It is automatically included in the effective potential when the single – nucleon dynamics is described by the Dirac equation. When the nucleons are described as non-relativistic particles, the spin-orbit term must be added to the Schrödinger equation.

… the single-nucleon wave function:

$$< \vec{r}, \vec{\sigma} | nljm >= \frac{u_{nl}(r)}{r} \left[ Y_l(\theta, \phi) \otimes \chi_{1/2} \right]_{jm}$$

- the spin-orbit term is diagonal in this basis.

$$\varepsilon_{nlj} = \varepsilon^{(0)}_{nlj} + \Delta\varepsilon_{nlj}$$

$\varepsilon^{(0)}_{nlj} = \langle nljm|h_0|nljm\rangle$ does not depend on the spin quantum number.

From $\vec{l}\cdot\vec{s} = \frac{1}{2}(\vec{j}^{\,2} - \vec{l}^{\,2} - \vec{s}^{\,2})$ 

$$\Delta\varepsilon_{nlj} = \langle nljm|\zeta\vec{l}\cdot\vec{s}\,|nljm\rangle = \frac{D}{2}\left[j(j+1) - l(l+1) - \frac{3}{4}\right]$$

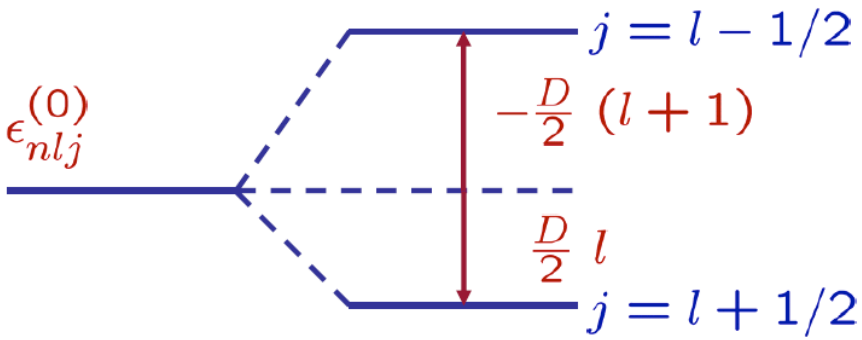
$D = \int u^2_{nl}(r)\zeta(r)\,dr \;<\; 0$ depends on the radial form of the potential.

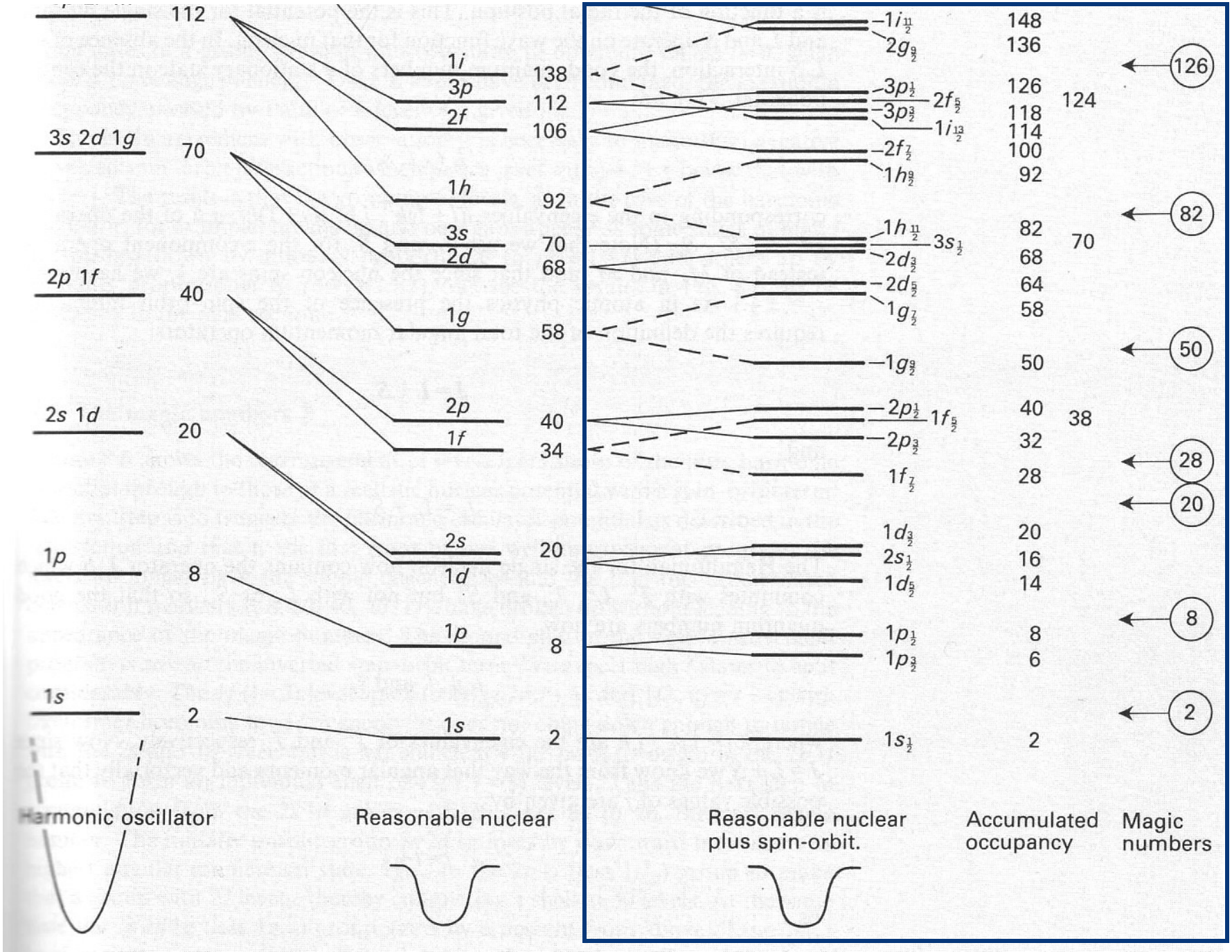
A much used form for ζ(r) is the derivative of the average potential: $\zeta(r) = V_{ls}r_0^2\frac{1}{r}\frac{\partial U(r)}{\partial r}$

Spin-orbit splitting:

$$\Delta\varepsilon_{nlj=l+1/2} = \frac{D}{2}l$$

$$\Delta\varepsilon_{nlj=l-1/2} = -\frac{D}{2}(l+1)$$




112
3s 2d 1g
70
2p 1f
40
2s 1d
20
1p
8
1s
2
Harmonic oscillator
1i
3p
2f
1h
3s
2d
1g
2p
1f
2s
1d
1p
1s
138
112
106
92
70
68
58
40
34
20
8
2
Reasonable nuclear
1i 11/2
2g 9/2
3p 1/2
2f 5/2
3p 3/2
1i 13/2
2f 7/2
1h 9/2
1h 11/2
3s 1/2
2d 3/2
2d 5/2
1g 7/2
1g 9/2
2p 1/2
1f 5/2
2p 3/2
1f 7/2
1d 3/2
2s 1/2
1d 5/2
1p 1/2
1p 3/2
1s 1/2
148
136
126
118
114
100
92
82
68
64
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50
40
32
28
20
16
14
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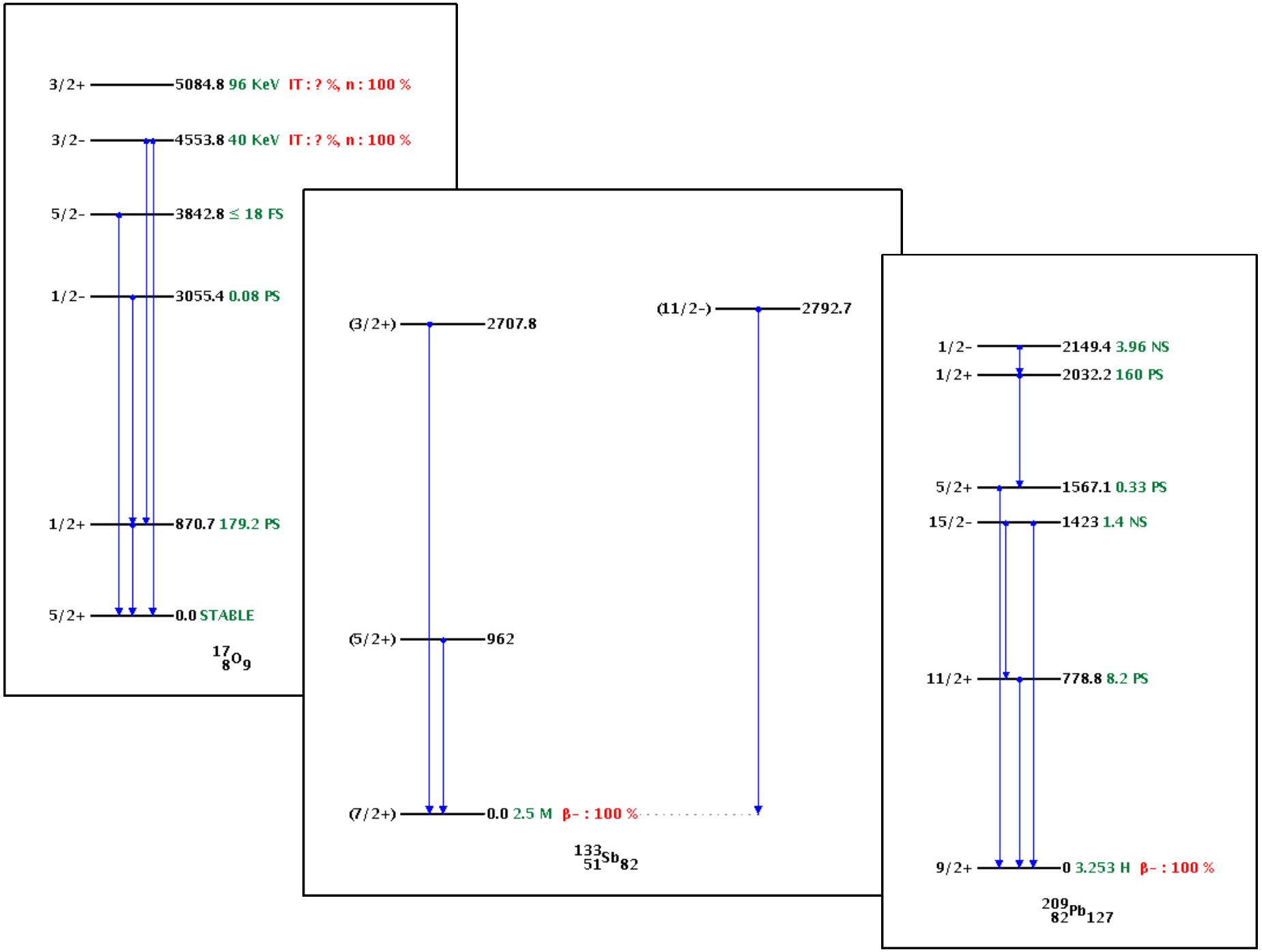
6
2
Reasonable nuclear plus spin-orbit.
126
124
82
70
50
38
28
20
8
2
Accumulated occupancy
Magic numbers

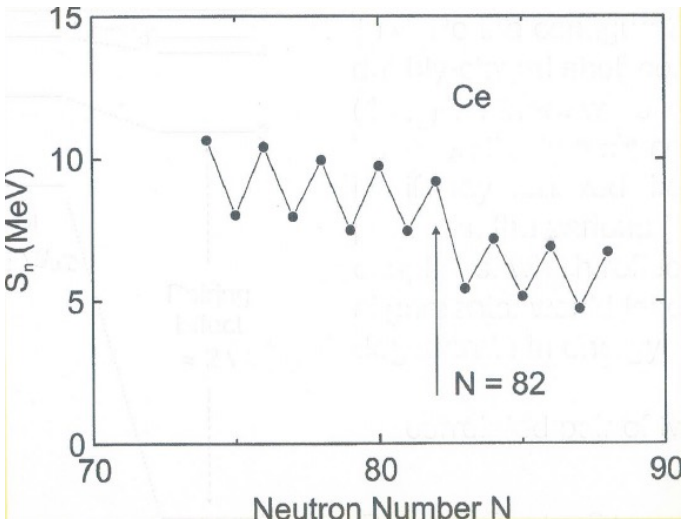

3/2+ 5084.8 96 KeV IT : ? %, n : 100 %
3/2- 4553.8 40 KeV IT : ? %, n : 100 %
5/2- 3842.8 ≤ 18 FS
1/2- 3055.4 0.08 PS
1/2+ 870.7 179.2 PS
5/2+ 0.0 STABLE
$^{17}_{8}O_{9}$
(3/2+) 2707.8
(11/2-) 2792.7
(5/2+) 962
(7/2+) 0.0 2.5 M β- : 100 %
$^{133}_{51}Sb_{82}$
1/2- 2149.4 3.96 NS
1/2+ 2032.2 160 PS
5/2+ 1567.1 0.33 PS
15/2- 1423 1.4 NS
11/2+ 778.8 8.2 PS
9/2+ 0 3.253 H β- : 100 %
$^{209}_{82}Pb_{127}$

# Pairing Correlations

# Empirical evidence for pairing correlations

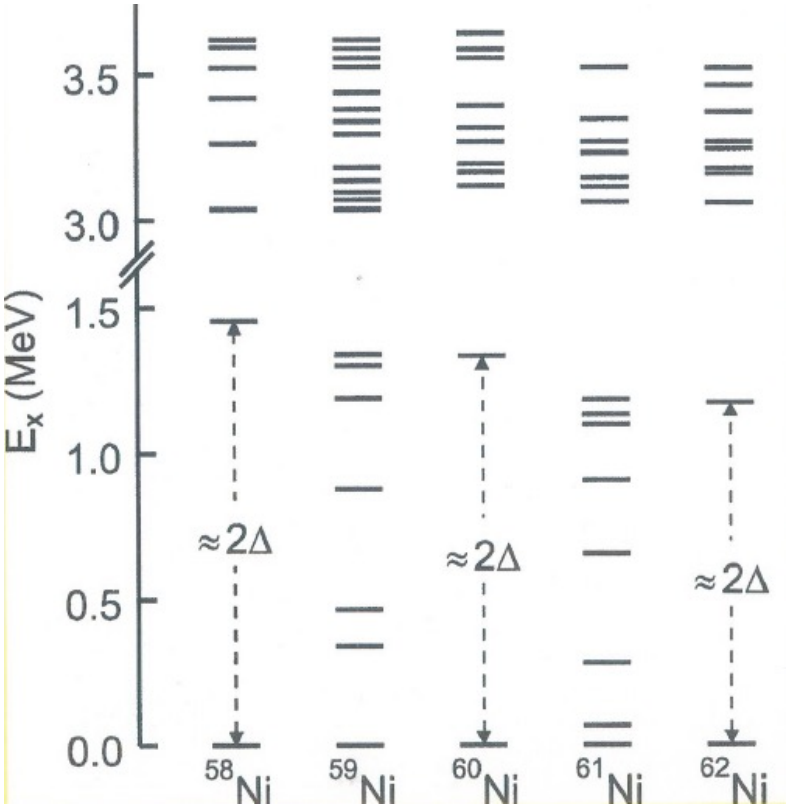
For even-even nuclei the ground-state has always zero angular momentum, i.e. the residual interaction lowers this particular state with respect to other ang. momentum combinations.

Odd-even effect: even-even nuclei are bound more tightly than neighboring odd-A nuclei.




One-neutron separation energies in Ce.

In even-even nuclei there is an energy gap of 1-2 MeV between the ground state and the lowest singe-particle excitations.



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# Possible Analogy between the Excitation Spectra of Nuclei and Those of the Superconducting Metallic State

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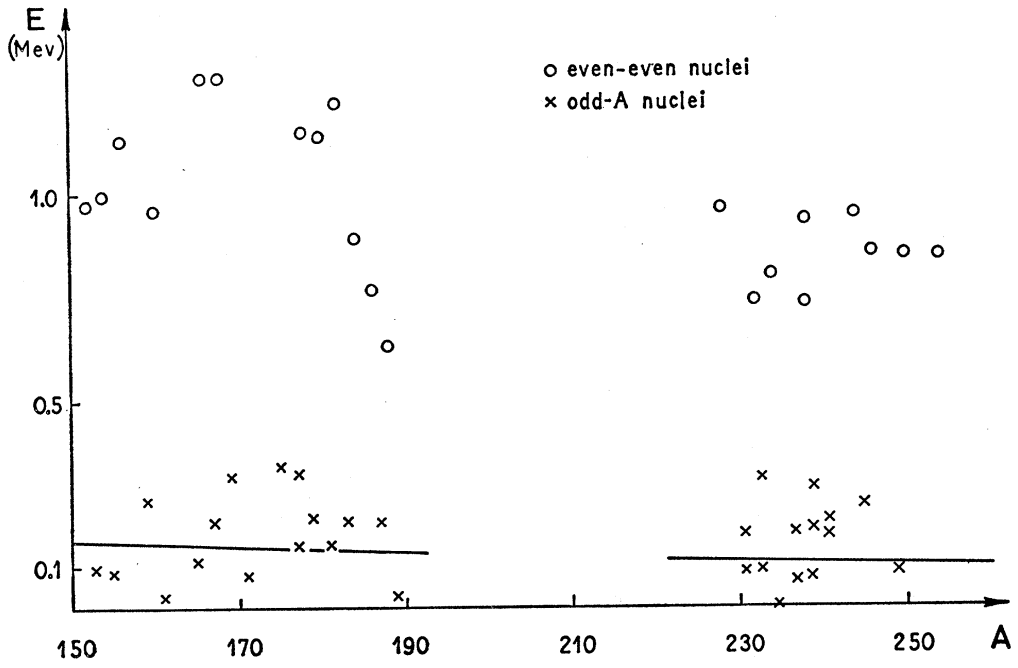
*Institute for Theoretical Physics, University of Copenhagen, Copenhagen, Denmark, and Nordisk Institut for Teoretisk Atomfysik, Copenhagen, Denmark*




Energies of first excited intrinsic states in deformed nuclei as a function of the mass number.

Pairing force between nucleons – in addition to the average shell-model potential there also acts a relatively short-range residual NN force.

Two nucleons in the same shell:

$$|nljj; J = 0M = 0\rangle = \sum_m < jmj - m|00 > |jm\rangle|j - m\rangle = \frac{1}{\sqrt{2j+1}} \sum_m (-)^{j-m} |jm\rangle|j - m\rangle$$

This state will have the lowest energy for a short-range interaction. In the state J=0 the nucleons are relatively close (the spatial overlap of the two nucleon densities is maximal), whereas they are not in higher angular momentum states.

For nuclei between closed shells, the nucleons (except the last one) will be paired off . This configuration will be most favorable energetically. To excite even-even nuclei, either a pair has to be lifted to a higher shell or it has to be broken. For odd nuclei, the odd unpaired nucleon can simply be lifted to higher orbits.

# Pairing in a degenerate single-j shell

… general two-body interaction: $$V(1,2) \rightarrow \frac{1}{4} \sum_{\alpha,\beta,\gamma,\delta} \langle \alpha\beta|V|\gamma\delta\rangle a^+_\alpha a^+_\beta a_\delta a_\gamma$$

PAIRING HAMILTONIAN:

$$H_P = -G \sum_{m,m'>0} a^+_{jm} a^+_{j-m} a_{j-m'} a_{jm'} (-)^{2j+m+m'}$$

a) Two particles in a single-j shell $2\Omega = 2j+1$ degenerate states.

The number of states occupied by 2 nucleons: $$N = \begin{pmatrix} 2j+1 \\ 2 \end{pmatrix}$$

Number of states of the form |m –m>: $$\Omega = \frac{2j+1}{2}$$

Example: $j = \frac{9}{2}$ $m = \frac{9}{2}, \frac{7}{2}, \frac{5}{2}, \frac{3}{2}, \frac{1}{2}, -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}, -\frac{7}{2}, -\frac{9}{2}$

In matrix representation the pairing Hamiltonian reads:

$$H_P = -G \begin{bmatrix} \overbrace{\begin{matrix} 1 & 1 & \dots & 1 \\ 1 & 1 & \dots & 1 \\ \dots & \dots & \dots & \dots \\ 1 & 1 & \dots & 1 \end{matrix}}^{\Omega} & \begin{matrix} 0 & \dots & 0 \\ 0 & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & 0 \end{matrix} \\ \begin{matrix} 0 & 0 & \dots & 0 \end{matrix} & \begin{matrix} 0 & \dots & 0 \end{matrix} \\ \begin{matrix} \dots & \dots & \dots & \dots \end{matrix} & \begin{matrix} \dots & \dots & \dots \end{matrix} \\ \begin{matrix} 0 & 0 & \dots & 0 \end{matrix} & \begin{matrix} 0 & \dots & 0 \end{matrix} \end{bmatrix}$$

with the two-nucleon basis arranged so that the first Ω states are those of the form $|m\ -m>$.

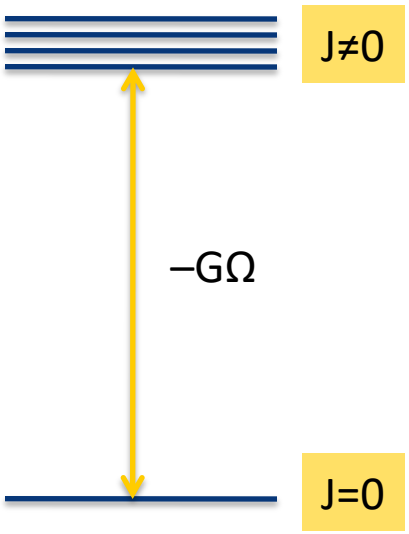
$$|\psi_0\rangle = \frac{1}{\sqrt{\Omega}} \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \frac{1}{\sqrt{\Omega}} \sum_{m>0} (-)^{j+m} a^+_{jm} a^+_{j-m} |0\rangle$$

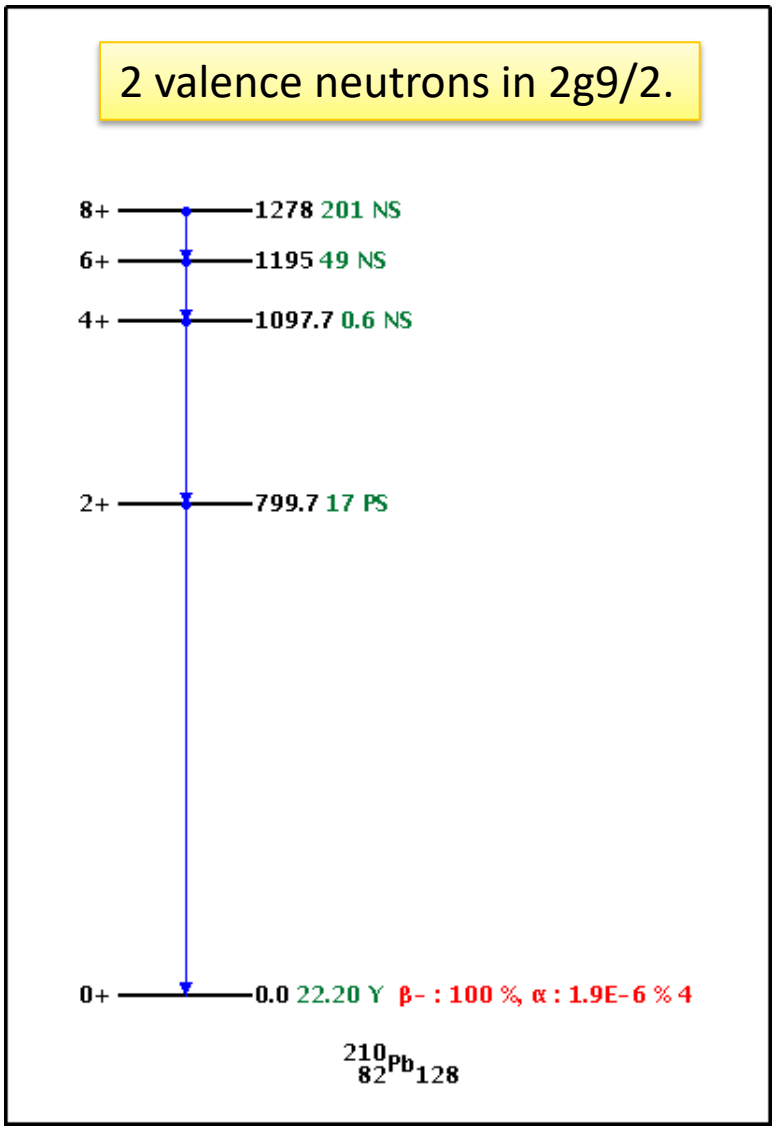
closed shell

is the lowest energy eigenstate of $H_P$ with $E_0 = -G\Omega$.

Since the eigenvalue of this state is equal to the trace of the matrix $H_P$, all other eigenstates of $H_P$ which are orthogonal to $|\psi_0\rangle$ must be degenerate with eigenvalue zero. This is because the sum of all eigenvalues equals the trace of the Hamiltonian matrix and because this particular matrix $H_P$ is negative definite.

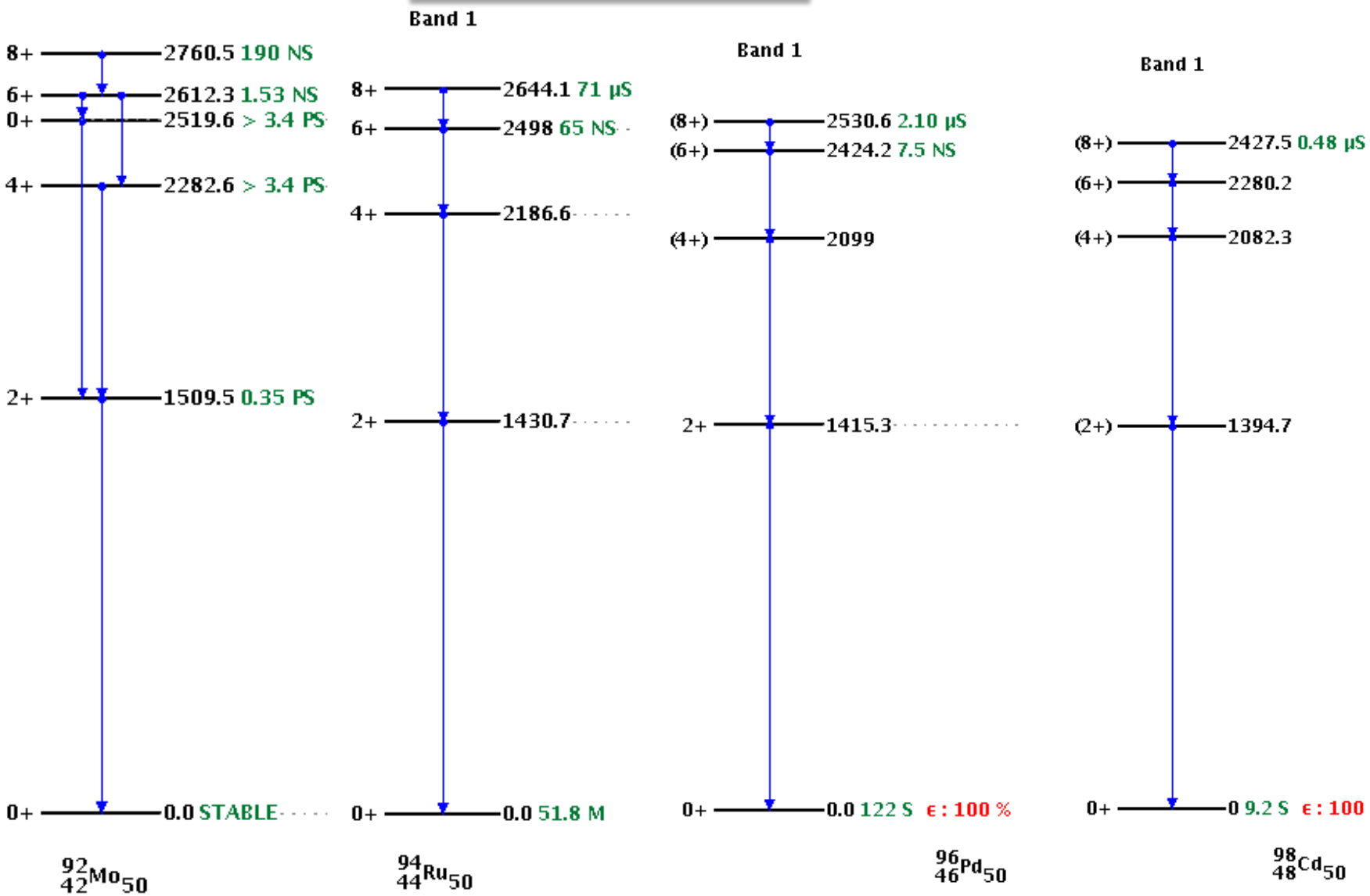
$|\psi_0\rangle$ is shifted downward in energy by $-G\Omega$.
All other states with $J\neq 0$ are not affected.



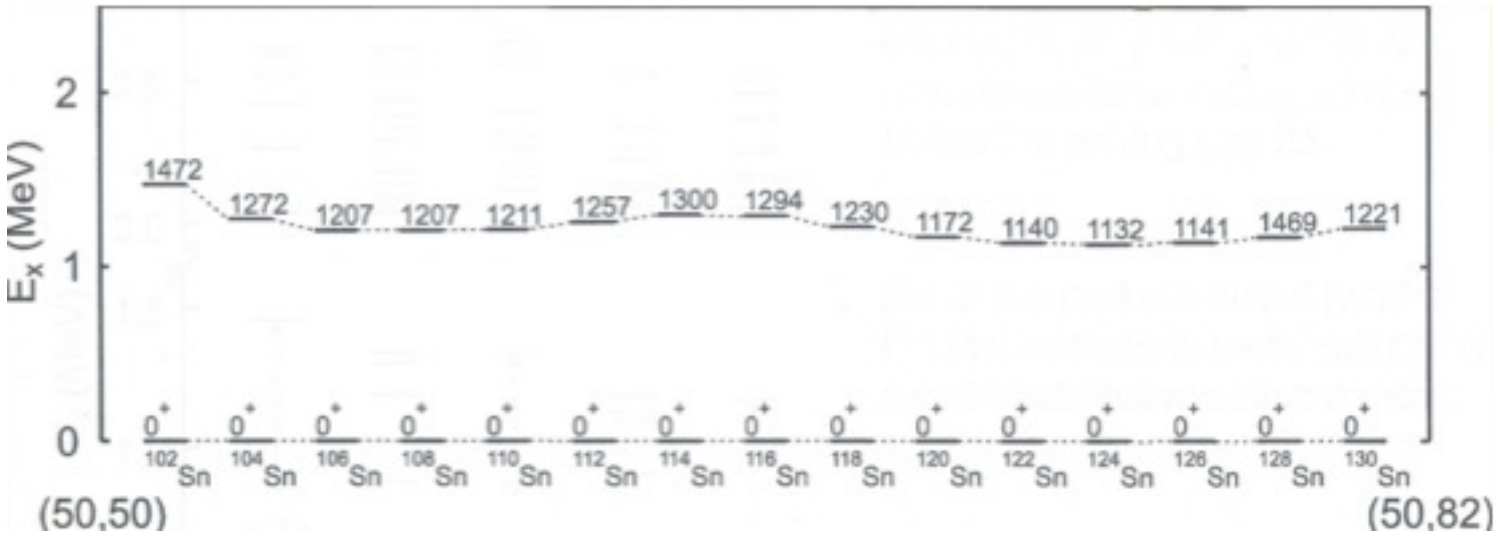
# b) n – particles in a single-j shell

Filling the 1g9/2 orbital.



# n-particles in non-degenerate shells: BCS

$2^{+}_{1}$ excitation energies in Sn isotopes:




… between 2 and 30 nucleons (1 to 15 pairs) are distributed over the available five neutron orbitals 2d5/2, 1g7/2, 1h11/2, 3s1/2, 2d3/2.

… consider a general trial wave function:

$$|\tilde{0}\rangle = \prod_{\nu>0} (u_\nu + v_\nu a_\nu^+ a_{\bar{\nu}}^+)|0\rangle$$

BCS ground state. Not an eigenstate of the number operator.

closed shell

… normalization: $\langle\tilde{0}|\tilde{0}\rangle = \prod_{\nu>0}(u_\nu^2 + v_\nu^2)$

… particle number: $\langle\tilde{0}|\hat{n}|\tilde{0}\rangle = \sum_{\nu>0} 2v_\nu^2$

… particle number uncertainty: $\Delta n^2 = \langle\tilde{0}|\hat{n}^2|\tilde{0}\rangle - \langle\tilde{0}|\hat{n}|\tilde{0}\rangle^2 = 4\sum_{\nu>0} u_\nu^2 v_\nu^2$

The uncertainty in the particle number arises from those single-particle states that are fractionally occupied, i.e. $u_\nu^2 \neq 0, 1 \qquad v_\nu^2 \neq 0, 1$

The coefficients $u_\upsilon$ and $v_\upsilon$ are determined from a constrained variational calculation:

$$\delta\langle\tilde{0}|\mathcal{H}|\tilde{0}\rangle = 0$$

$$\mathcal{H} = H - \lambda\hat{n} = \sum_{\nu>0}(\epsilon_\nu - \lambda)(a_\nu^+ a_\nu + a_{\bar{\nu}}^+ a_{\bar{\nu}}) - G\sum_{\mu,\nu>0} a_\mu^+ a_{\bar{\mu}}^+ a_{\bar{\nu}} a_\nu$$

The Lagrange multiplier is chosen such that the average particle number equals the actual number of valence particles:

$$\langle\tilde{0}|\hat{n}|\tilde{0}\rangle = n$$

From: $$\frac{\partial}{\partial n}\langle\tilde{0}|\mathcal{H}|\tilde{0}\rangle = 0 \Longrightarrow \lambda = \frac{\partial}{\partial n}\langle\tilde{0}|H|\tilde{0}\rangle$$

The BCS transformation from particle creation and annihilation operators to "quasiparticle" operators:

$$\begin{aligned} c_\nu^+ &= u_\nu a_\nu^+ - v_\nu a_{\bar{\nu}} \\ c_\nu &= u_\nu a_\nu - v_\nu a_{\bar{\nu}}^+ \end{aligned} \quad \Longrightarrow \quad \begin{aligned} a_\nu^+ &= u_\nu c_\nu^+ + v_\nu c_{\bar{\nu}} \\ a_\nu &= u_\nu c_\nu + v_\nu c_{\bar{\nu}}^+ \end{aligned}$$

inverse transformation

The BCS state is, by construction, the quasiparticle vacuum:

$$c_\nu|\tilde{0}\rangle = 0 \quad \forall\nu$$

Rewrite the Hamiltonian in terms of quasiparticle operators:

$$\mathcal{H} = U_0 + H_{11} + H_{20} + H_{02} + H_{\rm res}$$

$$\begin{aligned} H_{11} &\sim c^+c \\ H_{20} &\sim c^+c^+ \\ H_{\rm res} &\sim c^+c^+c^+c^+ + c^+c^+c^+c + c^+c^+cc + \text{h.c.} \end{aligned}$$

Because of the normal order of the operators, the expectation value of the interacting terms in the BCS state vanishes, and the ground-state energy:

$$\langle\tilde{0}|\mathcal{H}|\tilde{0}\rangle = U_0 = \sum_{\nu>0}\left[2(\epsilon_\nu - \lambda)v_\nu^2 - Gv_\nu^4\right] - G\left[\sum_{\nu>0} u_\nu v_\nu\right]^2$$

The variational problem: $\delta\langle\tilde{0}|\mathcal{H}|\tilde{0}\rangle = 0 \Longrightarrow \dfrac{d}{dv_\nu}U_0 = 0$

From: $v_\nu^2 + u_\nu^2 = 1$ ⟹ $\dfrac{d}{dv_\nu} = \dfrac{\partial}{\partial v_\nu} - \dfrac{v_\nu}{u_\nu}\dfrac{\partial}{\partial u_\nu}$

$$\frac{d}{dv_\nu}U_0 = 0 \quad \Longrightarrow \quad 2(\epsilon'_\nu - \lambda)u_\nu v_\nu = \Delta(u_\nu^2 - v_\nu^2) \quad \star$$

DEF. the pairing gap:

$$\Delta \equiv G\sum_{\nu>0} u_\nu v_\nu$$

$$\epsilon'_\nu \equiv \epsilon_\nu - Gv_\nu^2$$

includes the self-energy correction for a particle in a given orbital υ interacting, via the constant pairing force, with an extra pair of nucleons.

… solutions:

$$u_\nu^2 = \frac{1}{2}\left[1 + \frac{(\epsilon'_\nu - \lambda)}{\sqrt{(\epsilon'_\nu - \lambda)^2 + \Delta^2}}\right]$$

$$v_\nu^2 = \frac{1}{2}\left[1 - \frac{(\epsilon'_\nu - \lambda)}{\sqrt{(\epsilon'_\nu - \lambda)^2 + \Delta^2}}\right]$$

Two equations are needed to determine the chemical potential λ and the pairing gap Δ.

Insert the solutions for $u_\upsilon$ and $v_\upsilon$ into: $\Delta \equiv G \sum_{\nu>0} u_\nu v_\nu$

$$\frac{2}{G} = \sum_{\nu>0} \frac{1}{\sqrt{(\epsilon'_\nu - \lambda)^2 + \Delta^2}}$$

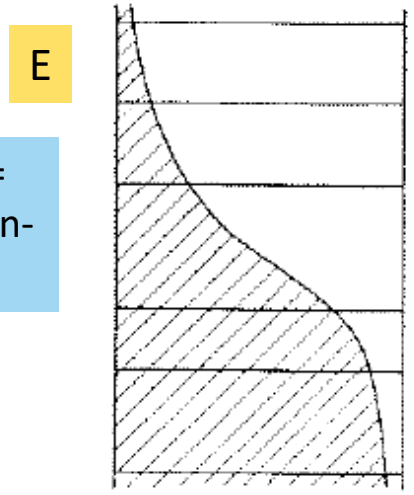
Gap equation

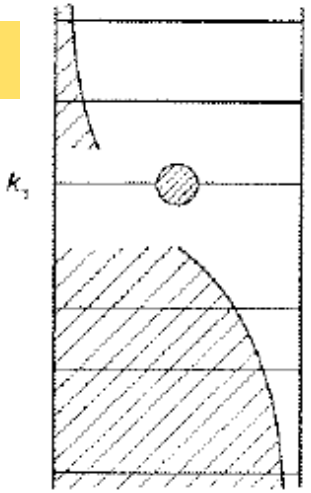
… plus the particle number condition:

$$n = \sum_{\nu>0} \left[ 1 - \frac{(\epsilon'_\nu - \lambda)}{\sqrt{(\epsilon'_\nu - \lambda)^2 + \Delta^2}} \right]$$

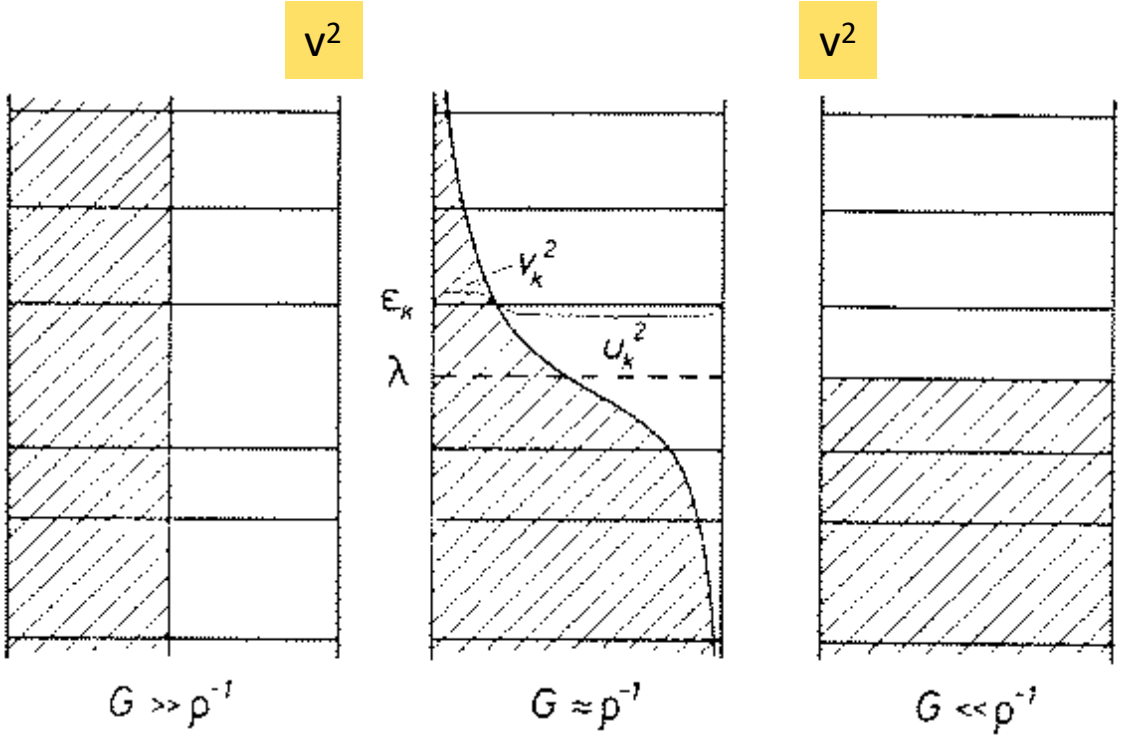
For a given set of single-particle energies, particle number n, and pairing strength G, these two coupled equations have to be solved simultaneously for the unknown quantities λ and Δ (solution by iteration).

Quasiparticle vacuum= ground state of an even-even nucleus.




One-quasiparticle state.




Population $v^2$ of pairs in single-particle levels for different ratios of the pairing strength to the average distance between single-particle levels.

The quasiparticle Hamiltonian:

$$H_{11} = \sum_{\nu>0} E_\nu (c_\nu^+ c_\nu + c_{\bar{\nu}}^+ c_{\bar{\nu}})$$

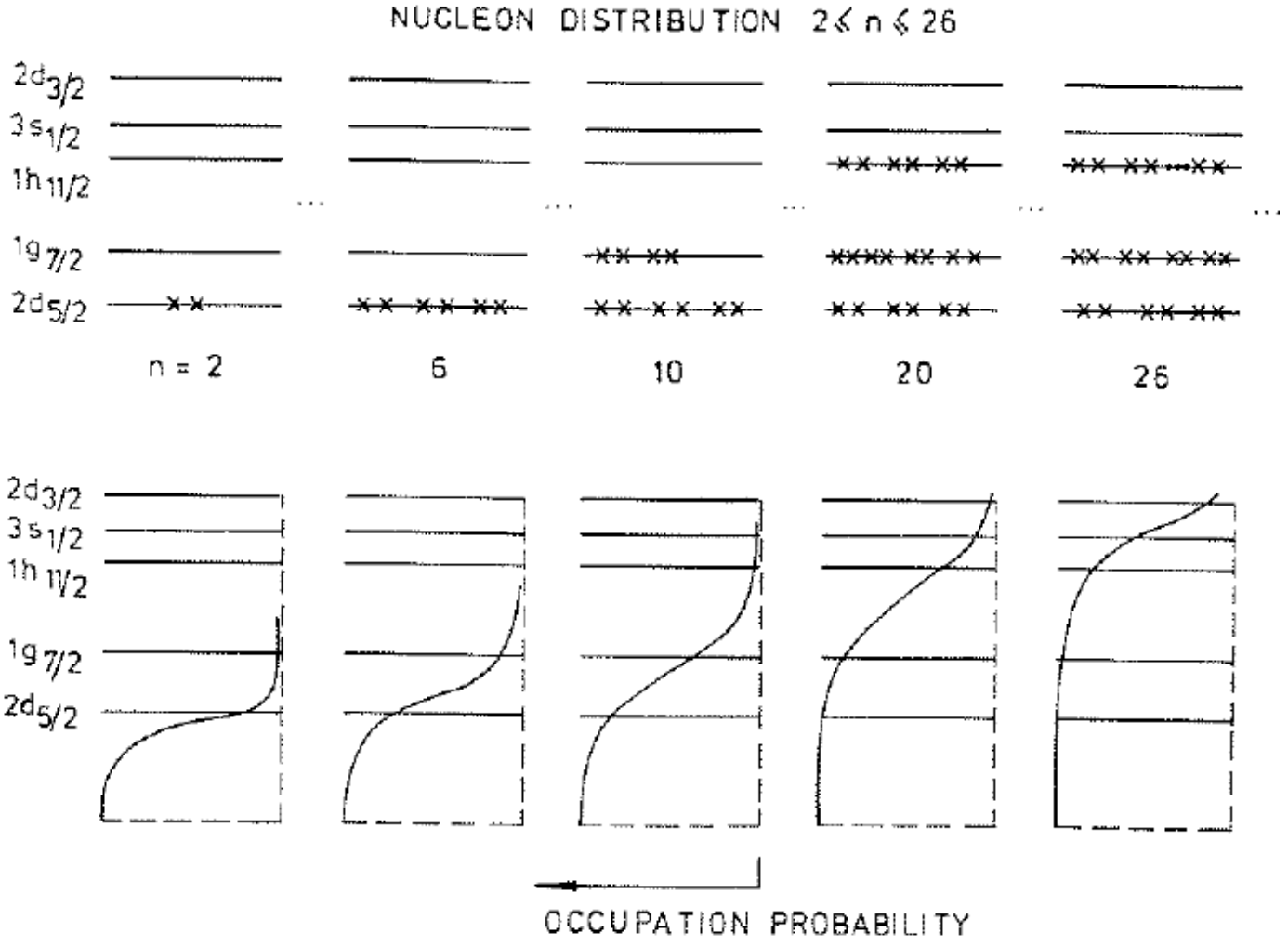
$$E_\nu \equiv \sqrt{(\epsilon'_\nu - \lambda)^2 + \Delta^2}$$ quasiparticle energy

$$H_{20} + H_{02} = \sum_{\nu>0} \underbrace{\left[2(\epsilon'_\nu - \lambda)u_\nu v_\nu - \Delta(u_\nu^2 - v_\nu^2)\right]}_{=0 \text{ from the variational condition.}} (c_\nu^+ c_{\bar{\nu}}^+ + c_{\bar{\nu}} c_\nu)$$

The quasiparticle transformation defines the representation in which the two-particle scattering processes across the Fermi level are absorbed in the definition of the new basis and the reference BCS-state.

The total Hamiltonian relative to $U_0$:

$$\mathcal{H} = \sum_{\nu>0} E_\nu (c_\nu^+ c_\nu + c_{\bar{\nu}}^+ c_{\bar{\nu}}) + \underbrace{H_{40} + H_{31} + H_{22} + \text{h.c.}}_{\text{quasiparticle residual interaction}}$$


NUCLEON DISTRIBUTION 2 ≤ n ≤ 26
2d3/2
3s1/2
1h11/2
1g7/2
2d5/2
n = 2
6
10
20
26
OCCUPATION PROBABILITY

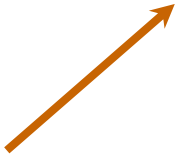
# Static Self-Consistent Mean-Field Approximations

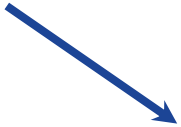
# Theories of Nuclear Structure

microscopic

**Ab initio** approaches - start from a given NN force
-GFMC
-no core shell model
-coupled cluster calculations
-unitary correlator method

**Microscopic models** based on effective interactions or effective energy-density functionals





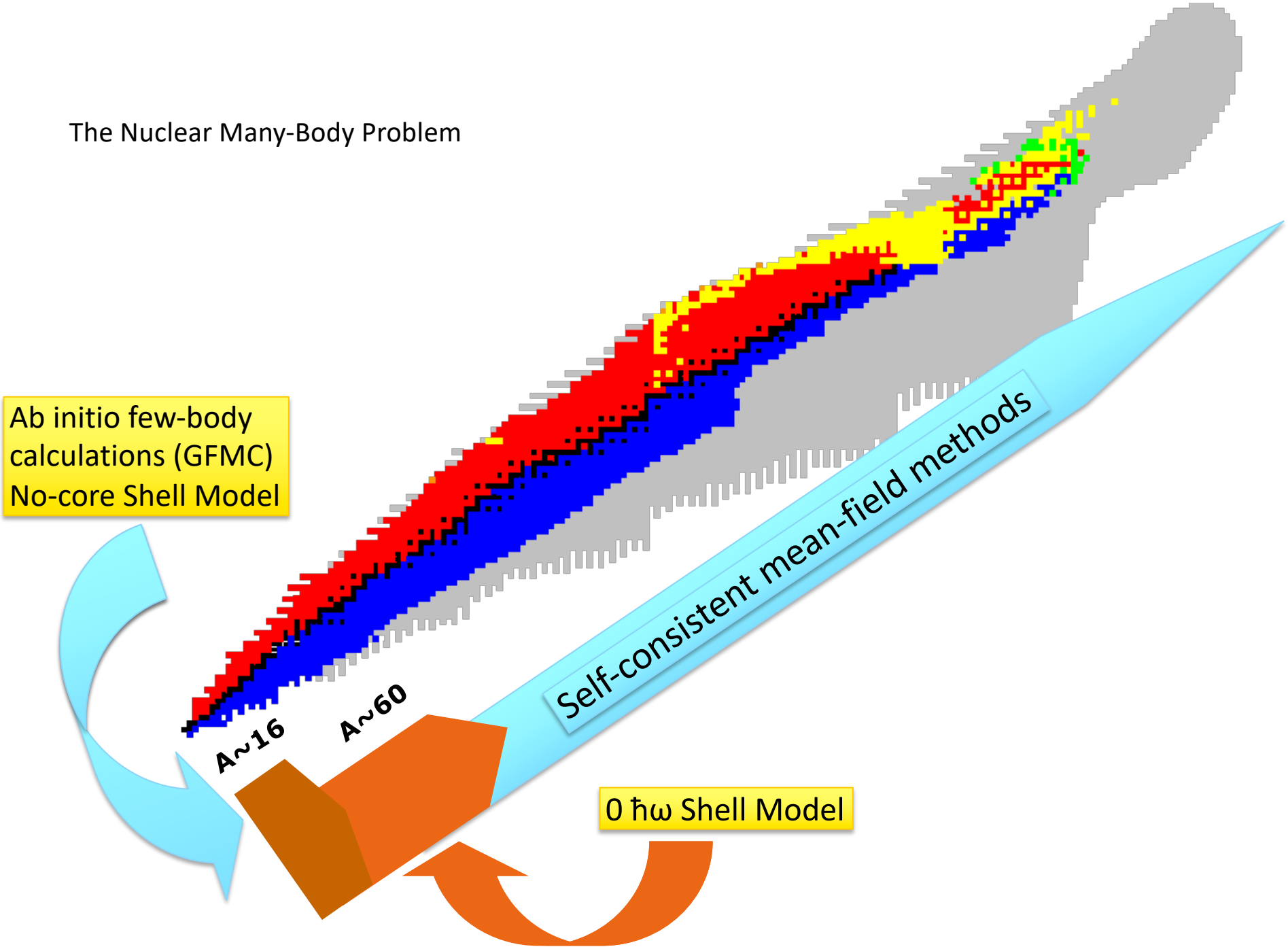
Large scale **Shell Model** calculations

Self-consistent mean-field models

**Mac-mic** approach
-liquid drop model plus shell corrections
-phenomenological input

phenomenological

The Nuclear Many-Body Problem



# Self-consistent mean-field models

**Mean-field approximation:** the dynamics of the nuclear many-body system is represented by independent nucleons moving in a self-consistent potential.

**Self-consistent potential:** corresponds to the actual density distribution for a given nucleus.

SCMF models approximate the exact energy-density functional with powers and gradients of ground-state nucleon densities. The density functional is not necessarily related to any given NN potential.

**Advantages of SCMF models (over the Shell Model approach):**

- global effective nuclear interactions (used for all nuclei!)
- description of arbitrarily heavy nuclei, including superheavy elements
- intuitive picture of intrinsic shapes

# The General Variational Principle

$$E[\Psi] = \frac{<\Psi|H|\Psi>}{<\Psi|\Psi>}$$

-any state which makes the functional E[Ψ] stationary, when |Ψ> is allowed to vary over the whole Hilbert space, is an eigenstate of the hamiltonian H with the eigenvalue E.

- variation: $<\Psi| \rightarrow <\Psi| + <\delta\Psi|$

$$\delta E[\Psi] = 0 \quad \Longrightarrow \quad <\delta\Psi|H - E|\Psi> = 0$$

- if this is satisfied for any variation ⇒ $H|\Psi> = E|\Psi>$

## Trial wave function:

- single Slater determinant ≡ **Hartree-Fock approximation**
- quasi-particle vacuum ≡ **Hartree-Fock-Bogoliubov approximation**
- linear combination of a finite number of Slater determinants ≡ **Shell Model**
- continuous superposition of Slater determinants ≡ **Hill-Wheeler equation**

# The Hartree-Fock Approximation

## 1. Basics of a mean-field description

The basic building block of any mean-field model is a set of single-nucleon wave functions:

$$\{\psi_i(\vec{x}), i = 1, \ldots, N_{\rm wf}\}\,, \quad \vec{x} = (\vec{r}, \sigma, \tau)$$

…the number of single-particle wave functions $N_{wf}$ is larger than the number of nucleons A

$$a_i^+ = \int d^3r \sum_{\sigma t} \psi_i(\vec{x})\; a_x^+$$

Creation operator for a nucleon in a single-particle state *i*

Creation operator for eigenstates of position

**HF approximation:** the state of a nucleus is described by a Slater determinant:

$$|\Phi\rangle \equiv \det\{\psi_i(\vec{x}), i=1, \ldots, A\}$$

$$\hat{a}_i^+|\Phi\rangle = 0 \qquad 1 \le i \le A \qquad\qquad \hat{a}_i|\Phi\rangle = 0 \qquad i > A$$

## 2. Single-particle density matrix

$$\rho_{ij} = < i|\rho|j > = < \Phi|a_j^+ a_i|\Phi >$$

…the density operator associated with the Slater determinant |Φ> can be expressed in terms of the single-nucleon orbitals:

$$\rho = \sum_i^A |\psi_i >< \psi_i| = \sum_i n_i |\psi_i >< \psi_i|$$

A completely antisymmetric state |Φ> is a Slater determinant only if the corresponding density matrix ρ is a projector onto the Hilbert space spanned by occupied single-particle orbitals:

$$\rho^2 = \rho$$

## 3. Hartree-Fock equations

…the hamiltonian of the system: sum of a kinetic energy and a two-body potential:

$$H = \sum_{ij} < i|T|j > a_i^+ a_j + \frac{1}{4} \sum_{ijkl} < ij|V|kl > a_i^+ a_j^+ a_l a_k$$

…the expectation value in a Slater determinant $|\Phi>$:

$$E[\rho] =< \Phi|H|\Phi >= \sum_{ij} < i|T|j > \rho_{ji} + \frac{1}{2} \sum_{ijkl} < ij|V|kl > \rho_{ki}\rho_{lj}$$

defines the energy E as a functional of the single-particle density matrix ρ associated with the state $|\Phi>$.

the variational equation:

$$\delta\{E[\rho] - \mathrm{tr}\Lambda(\rho^2 - \rho)\} = 0$$

**The Hartree-Fock hamiltonian:**

…hermitian operator acting in the space of single-particle states

$$h_{ij} \equiv < i|h|j >= \frac{\partial E[\rho]}{\partial \rho_{ji}}$$

…from the variational equation:

$$[h, \rho] \equiv h\rho - \rho h = 0$$

Hartree-Fock equation

The solution of the Hartre-Fock equation is a single-particle basis in which both h and ρ are diagonal.

$$h|\lambda_\nu >= e_\nu|\lambda_\nu >$$ HF orbitals

---

$$h = h[\rho]$$ → The HF equation is non-linear!

Iterative solution:

1) initial guess for the HF orbitals $|\lambda_\nu >$ $\Longrightarrow$ $\rho = \sum_{\nu=1}^{A} |\lambda_\nu >< \lambda_\nu|$

2) with this density matrix ρ construct the HF hamiltonian h

3) Diagonalize h: new set of HF orbitals $|\lambda'_\nu >$

Repeat steps 2) and 3) until two successive calculations give the same HF orbitals to a desired accuracy: **self-consistent HF Hamiltonian.**

# The Hartree-Fock-Bogoliubov Approximation

Pure Slater determinants → occupation numbers n={0,1}. This is strictly valid only for doubly magic nuclei. All the others have partially occupied shells with a high density of almost degenerate states that are mixed by the residual two-body interaction: **nuclear pairing scheme.**

## 1. Pairing correlations

…concept of independent quasi-particles defined by the Bogoliubov transformation:

$$b_n^+ = \sum_i (U_{in}\, a_i^+ + V_{in}\, a_i)$$

which relates single-particle states to quasiparticle states. In compact notation:

$$\begin{pmatrix} b \\ b^+ \end{pmatrix} = \mathcal{W}^+ \begin{pmatrix} a \\ a^+ \end{pmatrix}, \quad \mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}$$

→ the transformation matrix is unitary.

The ground state of the system is given then by the condition to be the quasi-particle vacuum:

$$b_n|\Phi\rangle = 0 \qquad \forall n$$

…quasi-particle wave functions in coordinate space:

$$\phi_n = \begin{pmatrix} \phi_n^{(U)}(\vec{x}) \\ \phi_n^{(V)}(\vec{x}) \end{pmatrix} = \begin{pmatrix} \sum_i U_{in}\psi_i(\vec{x}) \\ \sum_i V_{in}\psi_i(\vec{x}) \end{pmatrix}$$

The single-particle density: $\rho_{ij} = \langle\Phi|a_j^+ a_i|\Phi\rangle = (V^* V^T)_{ij} = \rho_{ji}^*$

The pair tensor: $\kappa_{ij} = \langle\Phi|a_j a_i|\Phi\rangle = (V^* U^T)_{ij} = -\kappa_{ji}$

The completely antisymmetric state $|\Phi>$ is a quasiparticle vacuum only if the associated **generalized density matrix:**

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

satisfies the relations: $\mathcal{R}^2 = \mathcal{R} \qquad \mathcal{R}^+ = \mathcal{R}$

## 2. Hartree-Fock-Bogoliubov equations

…derived from the variational principle by using a quasiparticle vacuum as the trial wave function.

The qp vacuum is not an eigenstate of the particle number operator → additional constraint: the average number of particles = number of particles in the system.

$$< \Phi|N|\Phi >=< \Phi|\sum_i a_i^+ a_i|\Phi >= \mathrm{tr}\rho = \bar{N}$$

…minimize the expectation value of the hamiltonian:

$$\begin{aligned} \hat{H} &= H - \mu N \\ &= \sum_{ij} < i|T-\mu|j > a_i^+ a_j + \frac{1}{4}\sum_{ijkl} < ij|V|kl > a_i^+ a_j^+ a_l a_k \end{aligned}$$

$$E[\rho,\kappa] \equiv < \Phi|\hat{H}|\Phi > \equiv E[\mathcal{R}]$$

$$\delta E[\rho,\kappa,\kappa^*] = \sum_{ij}\frac{\partial E}{\partial \rho_{ij}}\delta\rho_{ij} + \frac{1}{2}\sum_{ij}\left[\frac{\partial E}{\partial \kappa_{ij}^*}\delta\kappa_{ij}^* + \frac{\partial E}{\partial \kappa_{ij}}\delta\kappa_{ij}\right]$$

Hartree-Fock hamiltonian

$$h_{ij} = \frac{\partial E[\mathcal{R}]}{\partial \rho_{ji}} = h^*_{ji}$$

Pairing field

$$\Delta_{ij} = \frac{\partial E[\mathcal{R}]}{\partial \kappa^*_{ij}} = -\Delta_{ji}$$

$$h_{ij} = < i|T - \mu|j > + \sum_{kl} < ik|V|jl > \rho_{lk}$$

$$\Delta_{ij} = \frac{1}{2} \sum_{kl} < ij|V|kl > \kappa_{kl}$$

The quasiparticle hamiltonian: $\mathcal{H} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix}$

…the variational equation: $\delta\{E[\mathcal{R}] - \mathrm{tr}\Lambda(\mathcal{R}^2 - \mathcal{R})\} = 0$

Hartree-Fock-Bogoliubov equation

$$[\mathcal{H}, \mathcal{R}] = 0$$

$$\begin{pmatrix} h & \Delta \\ -\Delta & -h^* \end{pmatrix} \begin{pmatrix} U_n \\ V_n \end{pmatrix} = e_n \begin{pmatrix} U_n \\ V_n \end{pmatrix}$$

$\mathcal{H} = \mathcal{H}[\mathcal{R}]$ ⟹ the HFB equation is nonlinear. Solution by **iteration**.

1) initial guess for the density and pair matrices ρ and κ

2) calculate the Hartree-Fock hamiltonian h and pairing field Δ

3) solve the eigenvalue HFB equation

4) from the eigenvectors evaluate the new density and pair matrices. The trace of the density matrix will not, in general, be equal to the number of particles in the system -> change the chemical potential $\mu \rightarrow \mu + \delta\mu$ until the trace equals the desired number of particles.

5) repeat steps 2) → 4) until two successive calculations give the same density and pair matrices to a desired accuracy.

The stationary value of the energy functional:

$$E = < \Phi | H | \Phi > = \mu \bar{N} + \mathrm{tr}(h\rho - \kappa^* \Delta) - < \Phi | V | \Phi >$$

1. Quasiparticle basis $\phi_n$ → diagonalizes the generalized one-body matrix R
2. Canonical basis $\psi_i$ → diagonalizes the one-body density ρ
3. Hartee-Fock basis → diagonalizes the mean-field Hamiltonian h

## 3. Symmetries and constraints

- symmetries related to the shape of the nucleus – spherical, axial quadrupole, triaxial quadrupole, octupole
- time reversal symmetry – for even-even nonrotating nuclei. The creation of a quasiparticle or the rotation of the nucleus breaks time-reversal symmetry.

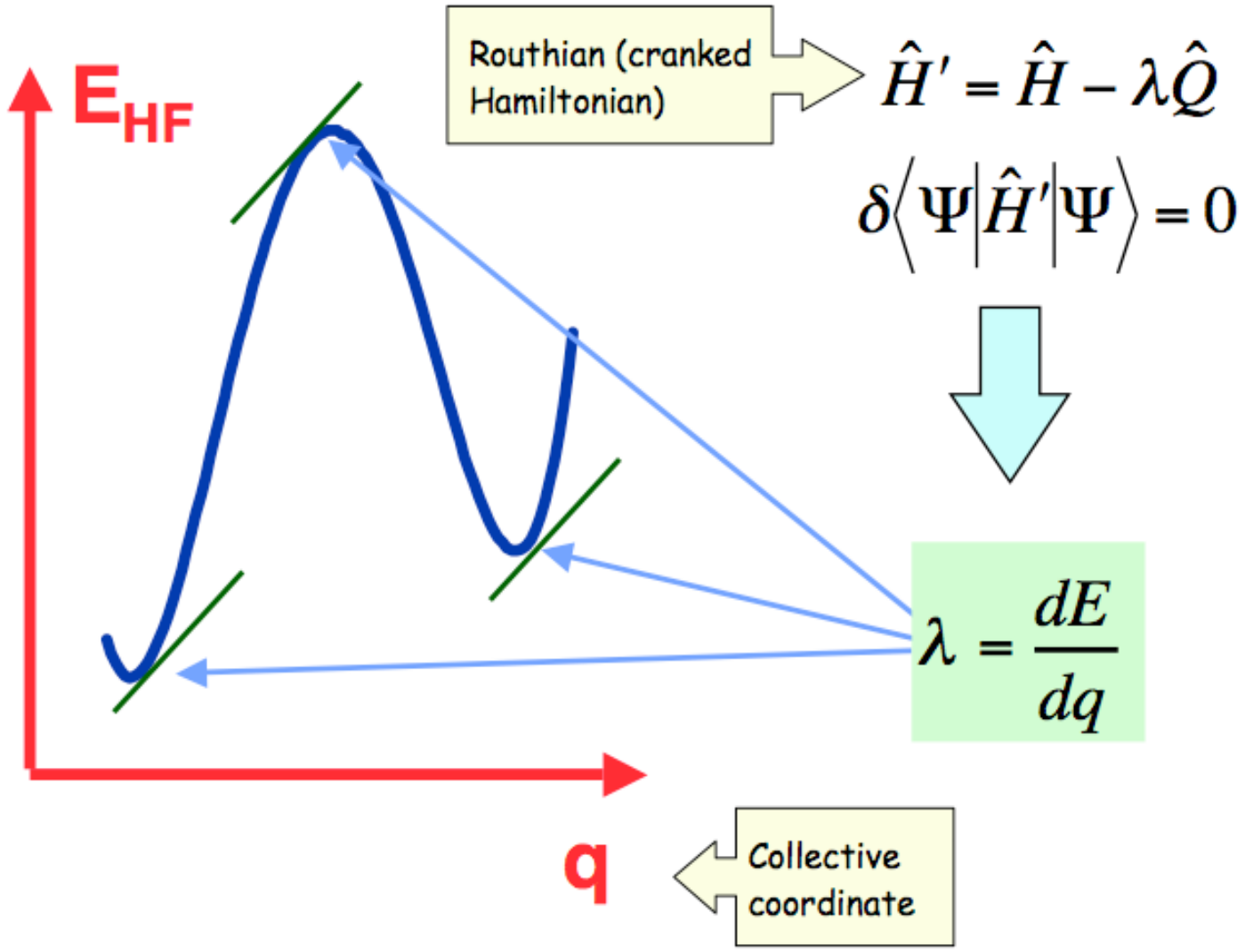
The landscape of the energy as a function of a shape degree of freedom is explored with the help of constraints.

The equations of motion are obtained by minimization of a Routhian:

$$E = \langle \hat{H} \rangle - \sum_{q=p,n} \lambda_q \langle \hat{N}_q \rangle - \sum_{\alpha} \lambda_\alpha \langle \hat{Q}_\alpha \rangle$$

with a constraint on the expectation value:

$$\langle \hat{Q}_\alpha \rangle \equiv \langle \Phi | \hat{Q}_\alpha | \Phi \rangle = Q_\alpha$$


Routhian (cranked Hamiltonian)
$\hat{H}' = \hat{H} - \lambda\hat{Q}$
$\delta\langle\Psi|\hat{H}'|\Psi\rangle = 0$
$E_{HF}$
$\lambda = \frac{dE}{dq}$
q
Collective coordinate

# 4. The BCS approximation

…well defined only in the case of time-reversal invariance -> Kramers degeneracy of single-particle states: $\epsilon_n = \epsilon_{\bar{n}}$ for time-conjugate partners $\phi_n, \phi_{\bar{n}}$

The BCS approximation: forces the pairing potential to be diagonal in the basis of the eigenstates of the mean-field potential:

$$\Delta = \begin{pmatrix} 0 & d \\ -d^T & 0 \end{pmatrix}$$

$$d_{n\bar{m}} = \delta_{nm} d_{n\bar{m}}, \quad h\varphi_n = \epsilon_n \varphi_n$$

The pairing problem reduces to the determination of occupation amplitudes by solving the gap equation:

$$(\varepsilon_n - \mu)(u_n^2 - v_n^2) + 2d_{n\bar{n}} u_n v_n = 0$$

The two-component wave functions become simply:

$$\phi_n^{(U)} = u_n \varphi_n \qquad \phi_n^{(V)} = v_n \varphi_n$$

## 5. Local densities and currents

The full density matrix can be decomposed into four separate spin-isospin terms:

$$\begin{aligned}\rho(\mathbf{r}\sigma\tau,\mathbf{r}'\sigma'\tau') \\ = \quad & \frac{1}{4}\Big\{\Big[\rho_{00}(\mathbf{r},\mathbf{r}')\,\delta_{\sigma\sigma'}+\mathbf{s}_{00}(\mathbf{r},\mathbf{r}')\cdot\boldsymbol{\sigma}_{\sigma'\sigma}\Big]\,\delta_{\tau\tau'} \\ & +\sum_{\alpha=-1}^{+1}\Big[\rho_{1\alpha}(\mathbf{r},\mathbf{r}')\,\delta_{\sigma\sigma'}+\mathbf{s}_{1\alpha}(\mathbf{r},\mathbf{r}')\cdot\boldsymbol{\sigma}_{\sigma'\sigma}\Big](\tau_{\tau'\tau})_\alpha\Big\}\end{aligned}$$

where: $\boldsymbol{\sigma}_{\sigma'\sigma}=(\sigma'|\hat{\boldsymbol{\sigma}}|\sigma)\quad,\quad\boldsymbol{\tau}_{\tau'\tau}=(\tau'|\hat{\boldsymbol{\tau}}|\tau)$

For pure proton and neutron states only the α = 0 components of the isovector densities contribute.

There are six local densities and currents that can be derived from the full density matrix. We omit the second index in the densities, and with T=0 or 1:

## Local densities and currents:

T=0 density:

$$\rho_0(\mathbf{r}) = \rho_0(\mathbf{r},\mathbf{r}) = \sum_{\sigma\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma\tau)$$

T=1 density:

$$\rho_1(\mathbf{r}) = \rho_1(\mathbf{r},\mathbf{r}) = \sum_{\sigma\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma\tau)\,\tau$$

T=0 spin density:

$$\mathbf{s}_0(\mathbf{r}) = \mathbf{s}_0(\mathbf{r},\mathbf{r}) = \sum_{\sigma\sigma'\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma'\tau)\,\boldsymbol{\sigma}_{\sigma'\sigma}$$

T=1 spin density:

$$\mathbf{s}_1(\mathbf{r}) = \mathbf{s}_1(\mathbf{r},\mathbf{r}) = \sum_{\sigma\sigma'\tau} \rho(\mathbf{r}\sigma\tau;\mathbf{r}\sigma'\tau)\,\boldsymbol{\sigma}_{\sigma'\sigma}\,\tau$$

Current:

$$\mathbf{j}_T(\mathbf{r}) = \tfrac{i}{2}(\nabla' - \nabla)\,\rho_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Spin-current tensor:

$$\mathcal{J}_T(\mathbf{r}) = \tfrac{i}{2}(\nabla' - \nabla) \otimes \mathbf{s}_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Kinetic density:

$$\tau_T(\mathbf{r}) = \nabla\cdot\nabla'\,\rho_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

Kinetic spin-density:

$$\mathbf{T}_T(\mathbf{r}) = \nabla\cdot\nabla'\,\mathbf{s}_T(\mathbf{r},\mathbf{r}')\big|_{\mathbf{r}=\mathbf{r}'}$$

# Choices for the effective interaction

## 1. MEAN-FIELD EFFECTIVE INTERACTIONS

**Gogny interaction**: sum of two Gaussians with space, spin and isospin exchange mixtures. In addition, a density-dependent interaction plus a spin-orbit term.

$$\begin{aligned}\hat{v}_{\text{Gogny}}(\mathbf{r}_{12}) = & \sum_{j=1}^{2} e^{-(\mathbf{r}_{12}/\mu_j)^2}\left(W_j + B_j\hat{P}_\sigma - H_j\hat{P}_\tau - M_j\hat{P}_\sigma\hat{P}_\tau\right) \\ & + t_3\left(1 + x_0\hat{P}_\sigma\right)\delta(\mathbf{r}_{12})\,\rho^\alpha\left(\tfrac{\mathbf{r}_1+\mathbf{r}_2}{2}\right) \\ & + \mathrm{i}W_{ls}(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2)\cdot\hat{\mathbf{k}}^\dagger \times \delta(\mathbf{r}_{12})\,\hat{\mathbf{k}}\end{aligned}$$

Exchange operators: $\hat{P}_\sigma = \frac{1}{2}(1 + \hat{\boldsymbol{\sigma}}_1\cdot\hat{\boldsymbol{\sigma}}_2)$ $\quad$ $\hat{P}_\tau = \frac{1}{2}(1 + \hat{\tau}_1\cdot\hat{\tau}_2)$

$\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$ $\quad$ $\hat{\mathbf{k}} = -\frac{\mathrm{i}}{2}(\nabla_1 - \nabla_2)$

The Gogny interaction is used both in the mean-field and pairing channels.

## Skyrme interactions

In the Skyrme Hartree-Fock approach, the total binding energy is given by the sum of the kinetic energy, the Skyrme energy functional that models the effective interaction between nucleons, the Coulomb energy, the pair energy, and corrections for spurious motions:

$$E = E_{\rm kin} + \int d^3r\, \mathcal{E}_{\rm Sk} + E_{\rm Coul} + E_{\rm pair} - E_{\rm corr}$$

The Skyrme energy functional:

$$\mathcal{E}_{\rm Sk} = \sum_{T=0,1} \left( \mathcal{E}_T^{\rm even} + \mathcal{E}_T^{\rm odd} \right)$$

Contains only time-even dens.

Dependence on time-odd currents

Density-dependent coefficients

$$\mathcal{E}_T^{\rm even} = C_T^{\rho}\rho_T^2 + C_T^{\Delta\rho}\,\rho_T\Delta\rho_T + C_T^{\tau}\,\rho_T\tau_T + C_T^{J}\mathcal{J}_T^2 + C_T^{\nabla J}\,\rho_T\,\nabla\cdot\mathbf{J}_T$$

$$\mathcal{E}_T^{\rm odd} = C_T^{s}\,\mathbf{s}_T^2 + C_T^{\Delta s}\,\mathbf{s}_T\cdot\Delta\mathbf{s}_T + C_T^{sT}\,\mathbf{s}_T\cdot\mathbf{T}_T + C_T^{\nabla s}\,(\nabla\cdot\mathbf{s}_T)^2 + C_T^{j}\,\mathbf{j}_T^2 + C_T^{\nabla j}\,\mathbf{s}_T\cdot\nabla\times\mathbf{j}_T$$

does not contribute for even-even nuclei!

## Single-particle hamiltonian:

The contribution from the Skyrme interaction to the single-particle Hamiltonian:

$$\hat{h}_q = U_q - \nabla \cdot B_q \nabla - \tfrac{\mathrm{i}}{2}\{\mathcal{W}_q, \nabla\sigma\} + \mathbf{S}_q \cdot \hat{\boldsymbol{\sigma}} - \nabla \cdot (\hat{\boldsymbol{\sigma}} \cdot \mathbf{C}_q)\nabla - \tfrac{\mathrm{i}}{2}\{\mathbf{A}_q, \nabla\}$$

where:

$$\{\mathcal{W}_q, \nabla\sigma\} = \sum_{ij} \{W_{ij}, \nabla_i \hat{\sigma}_j\} \qquad (q = p, n)$$

…the local potentials are calculated from:

time-even:

$$U_q = \frac{\delta E}{\delta \rho_q}, \quad B_q = \frac{\delta E}{\delta \tau_q}, \quad \mathcal{W}_q = \frac{\delta E}{\delta \mathcal{J}_q}$$

time-odd:

$$\mathbf{A}_q = \frac{\delta E}{\delta \mathbf{j}_q}, \quad \mathbf{S}_q = \frac{\delta E}{\delta \mathbf{s}_q}, \quad \mathbf{C}_q = \frac{\delta E}{\delta \mathbf{T}_q}$$

The time-odd fields A, C, and S contribute to the single-particle Hamiltonian only in situations where the intrinsic time-reversal symmetry is broken and the Kramers degeneracy of single-particle levels is removed.

## 2. PAIRING CORRELATIONS

…pairing-energy functional: $$E_{\rm pair} = \sum_{q=p,n} \frac{V_q}{4} \int d^3r \left[1 - \left(\frac{\rho(\mathbf{r})}{\rho_c}\right)^\beta\right] \tilde{\rho}_q^2(\mathbf{r})$$

corresponds to the density-dependent two-body zero-range local pairing force:

$$v_{\rm pair} = \frac{V_0}{2}(1 - \hat{P}_\sigma)\left[1 - \left(\frac{\rho(\mathbf{r}_1)}{\rho_c}\right)^\beta\right]\delta(\mathbf{r}_1 - \mathbf{r}_2)$$

Volume pairing
$\rho_c \to \infty$

Surface pairing
$\rho_c \approx \rho_{nm}$

The pairing strengths $V_{p,n}$ are adjusted phenomenologically to reproduce the odd-even staggering of energies in selected chains of nuclei.

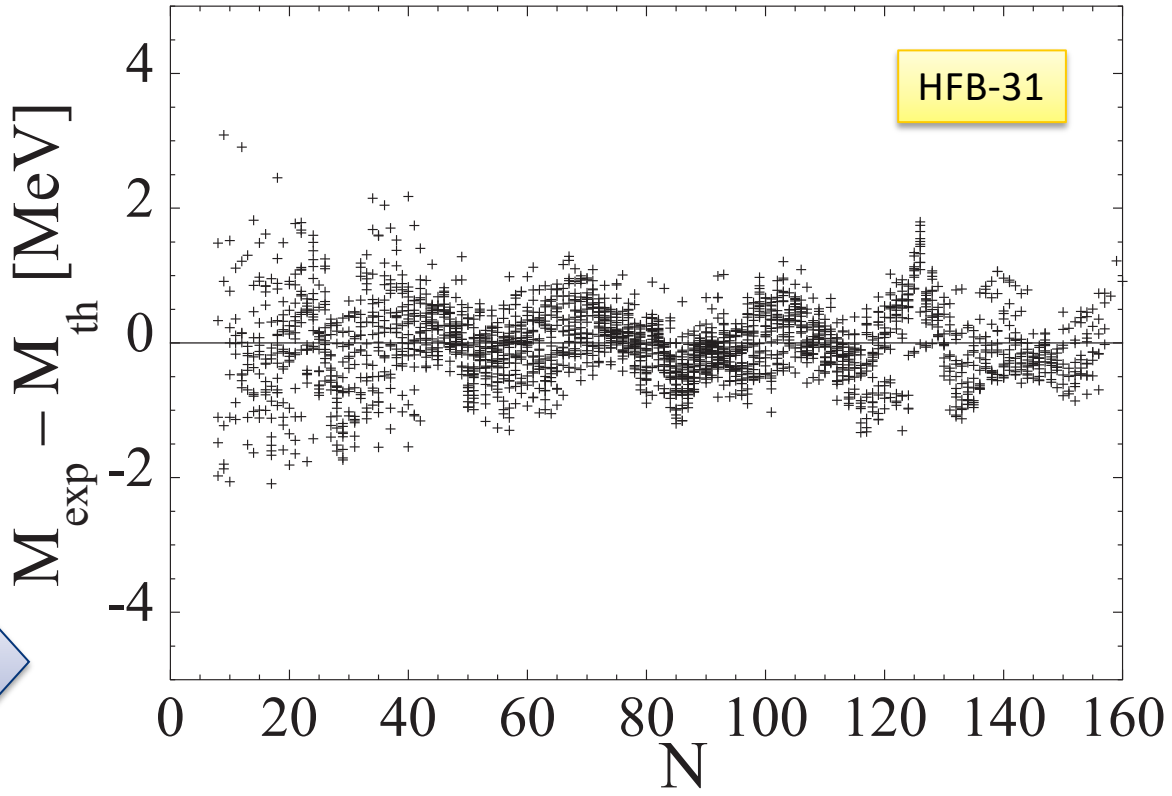
# Applications: ground-state properties

## 1. Binding Energies

Microscopic Skyrme-Hartree-Fock-Bogoliubov mass tables:

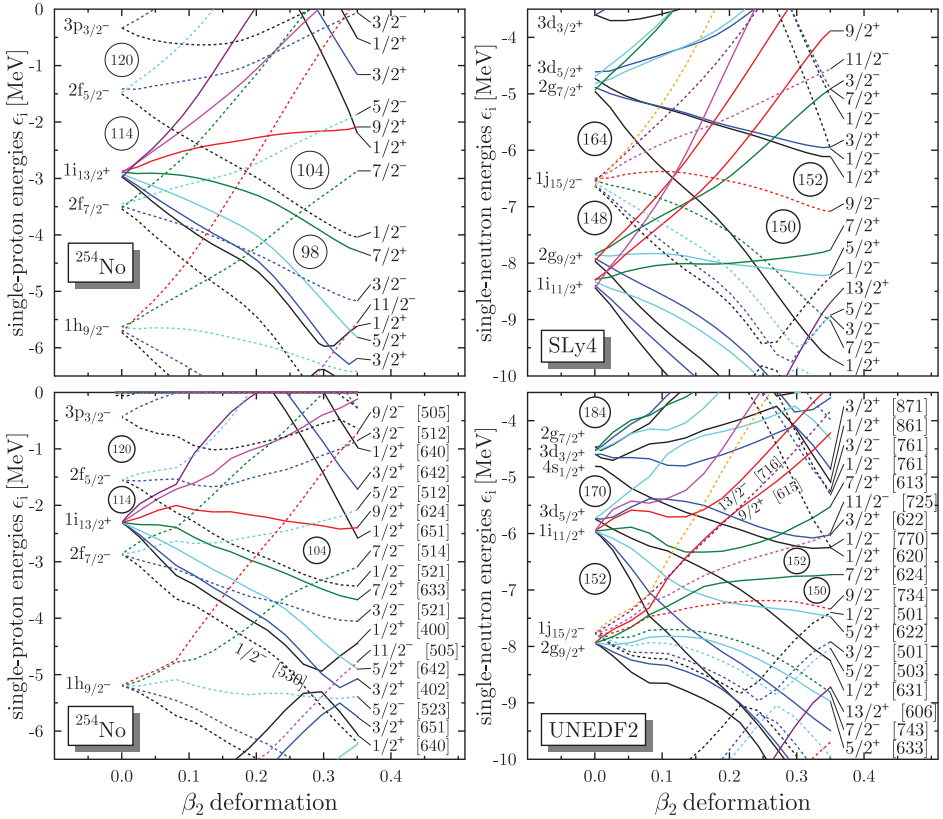
Differences between experimental and calculated masses as a function of the neutron number.

**Root Mean Square Deviation: 0.56 MeV** with respect to the 2353 measured masses of nuclei with N and $Z \geq 8$.

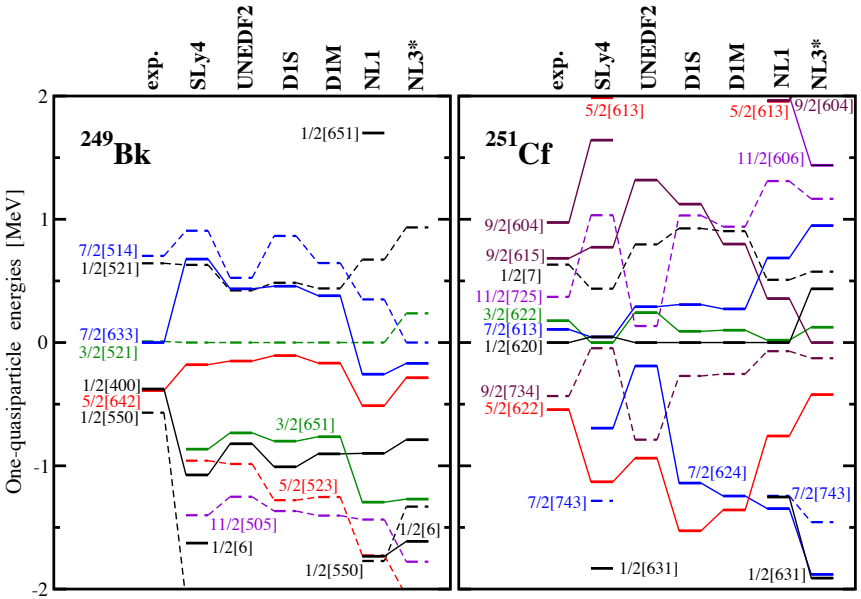



PHYSICAL REVIEW C **93**, 034337 (2016)

# 2. Shell structure



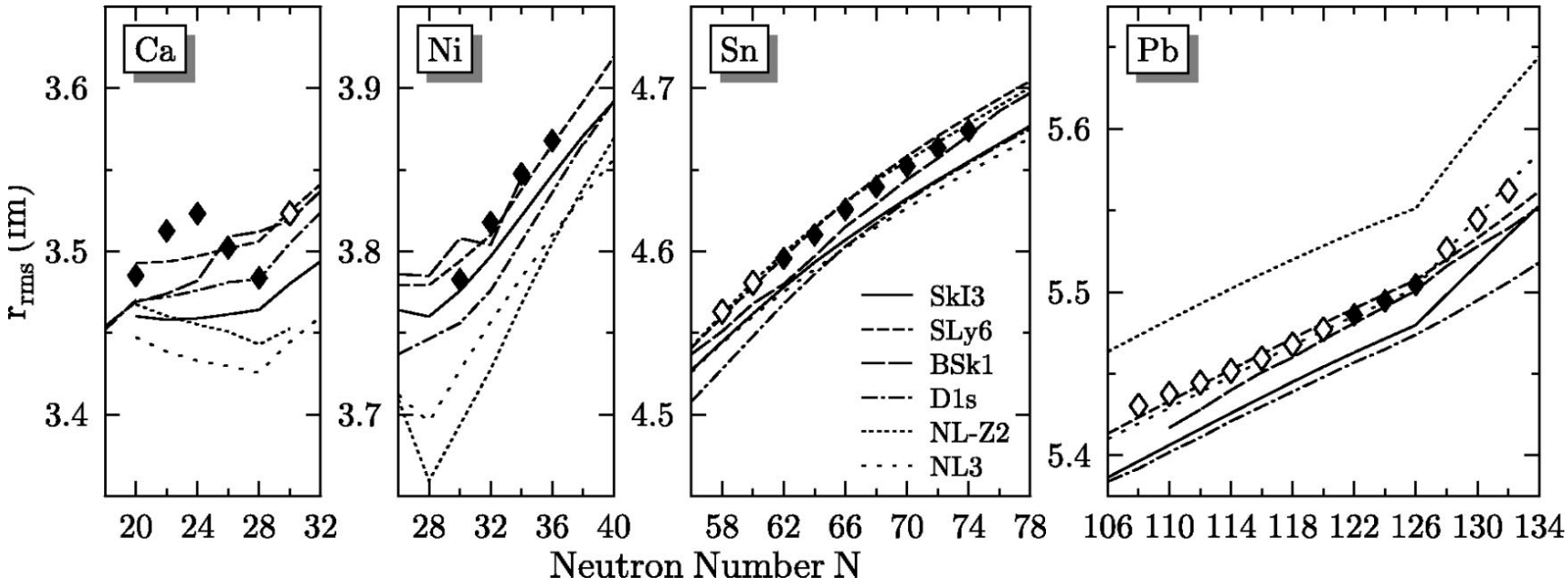

Proton and neutron Nilsson diagrams of $^{254}$No calculated with the Skyrme EDF SLy4 and UNEDF2 functionals.




Experimental and calculated quasiparticle spectra in $^{249}$Bk and $^{251}$Cf.

Nucl. Phys. A 944, 388 (2015).

# 3. Observables of the Density Distribution




Comparison of r.m.s. radii of the charge distributions from spherical mean-field calculations. Filled diamonds: direct radius measurements; open diamonds: measurements of isotopic shifts.

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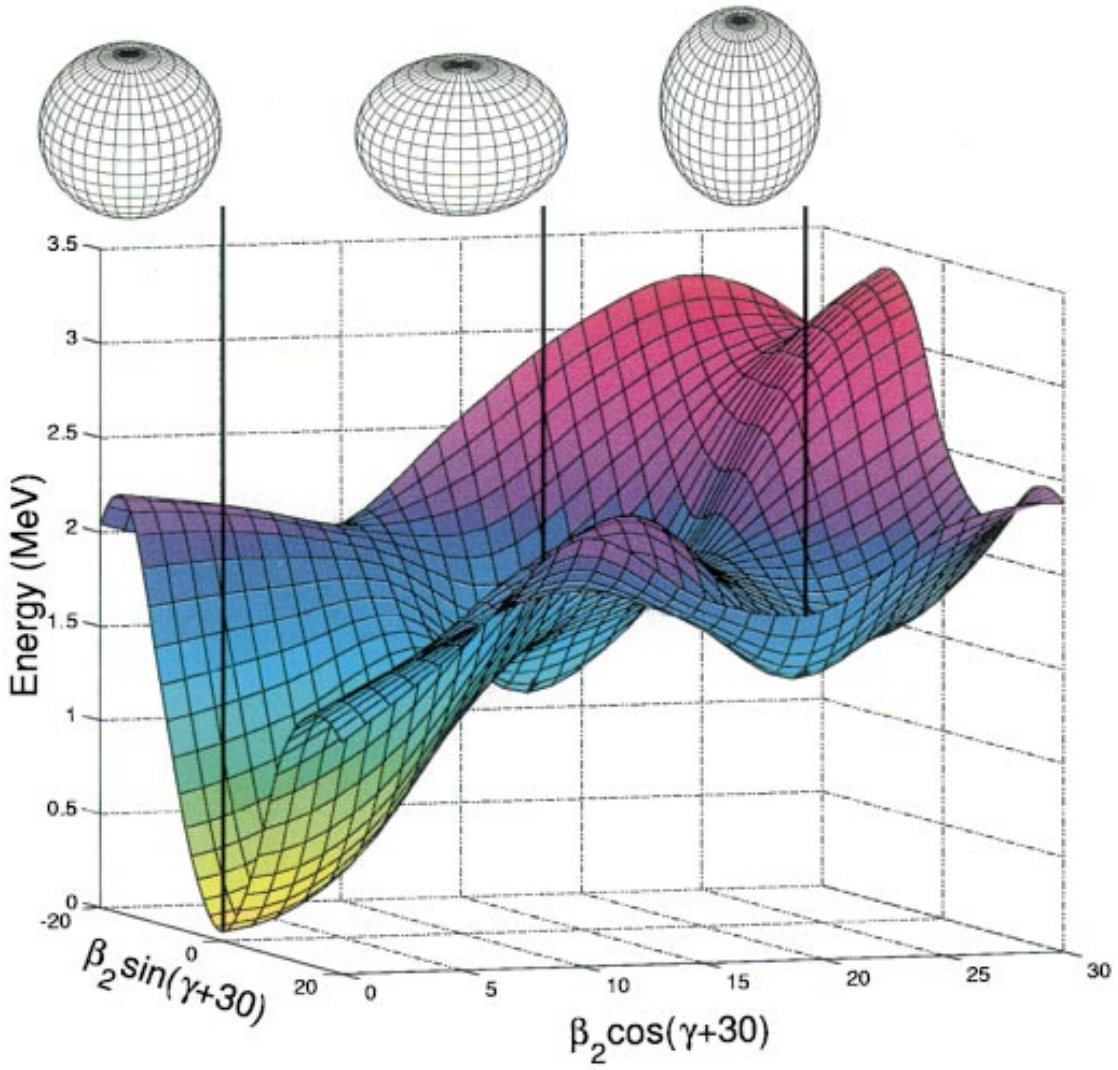
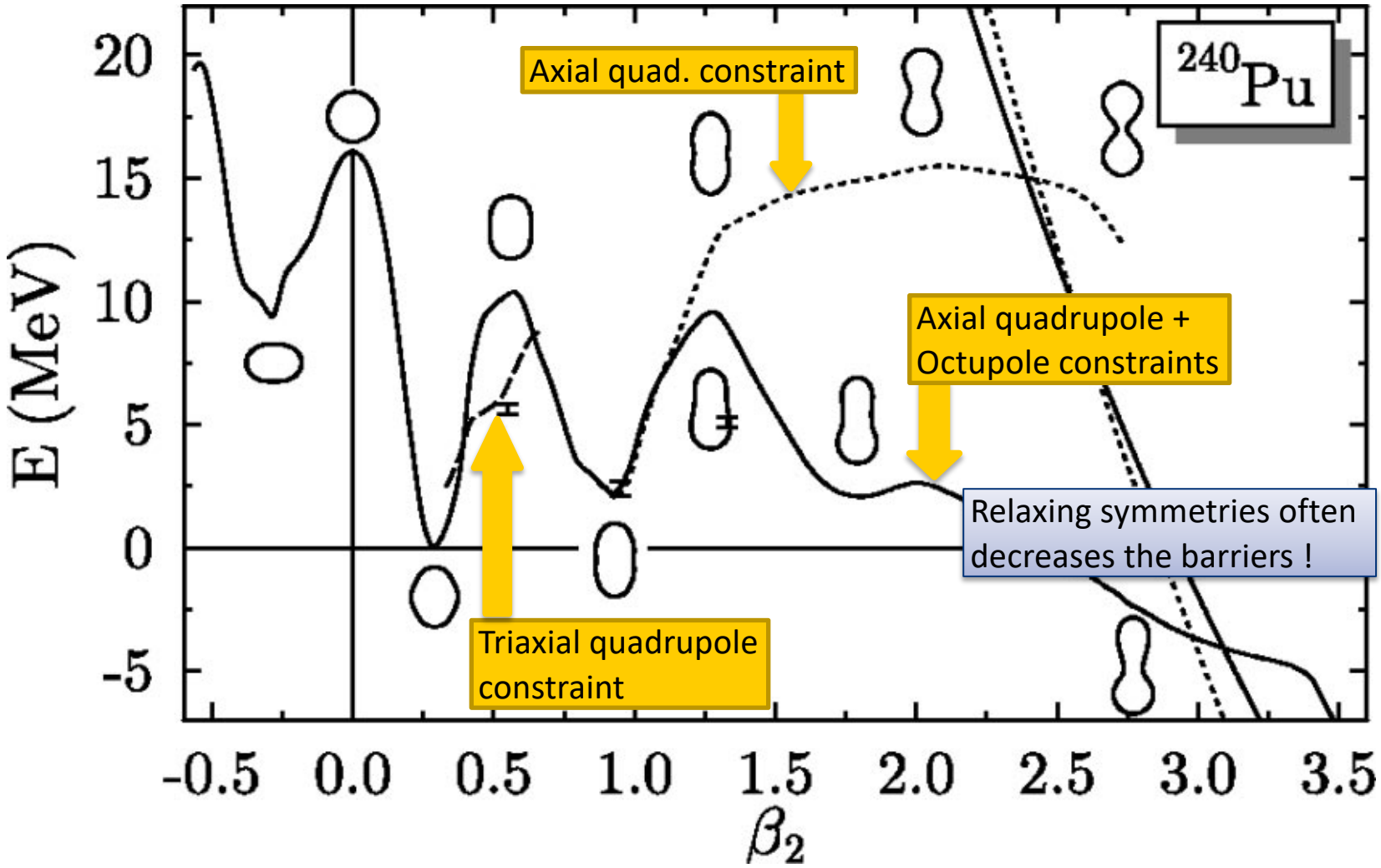



Calculated potential energy surface of $^{186}$Pb. Spherical, oblate and prolate minima are indicated by thick vertical black lines. Calculations are performed on a cartesian mesh. The $\beta_2$ parameter expresses the elongation of the nucleus along the symmetry axis, while the γ parameter relates to the degree of triaxiality in the deformation. The γ parameter is defined such that γ=0 corresponds to a prolate shape and γ=60 to an oblate shape.

# 5. Fission barriers




Paths in the deformation energy landscape of $^{240}$Pu calculated with the SkI4 force. The solid line corresponds to axial quadrupole and octupole (reflexion asymmetric) constraints, the dashed line to triaxial quadrupole constraints, the dotted line to axial quadrupole constraint only.

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