Microscopic description of atomic nuclei

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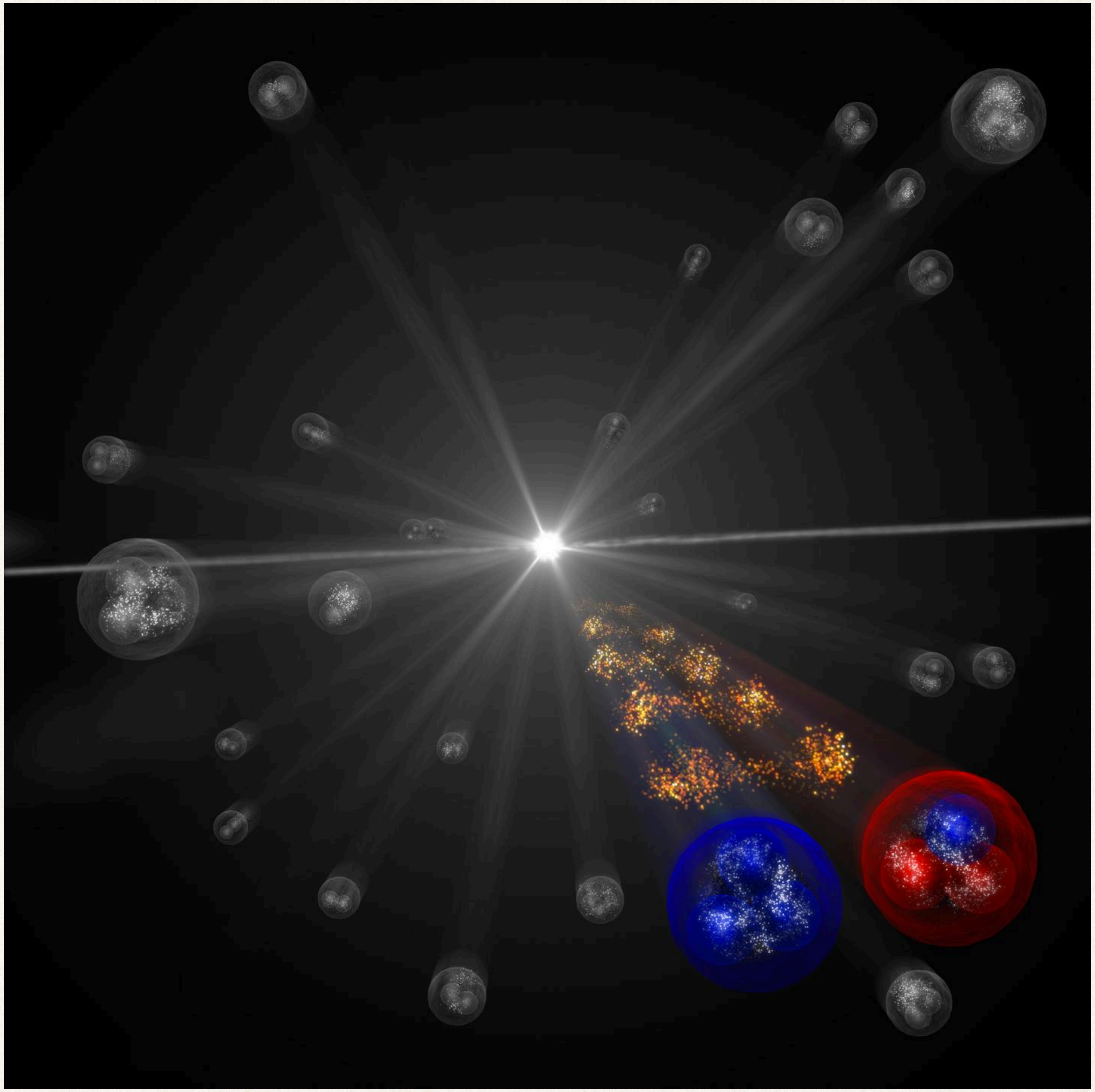
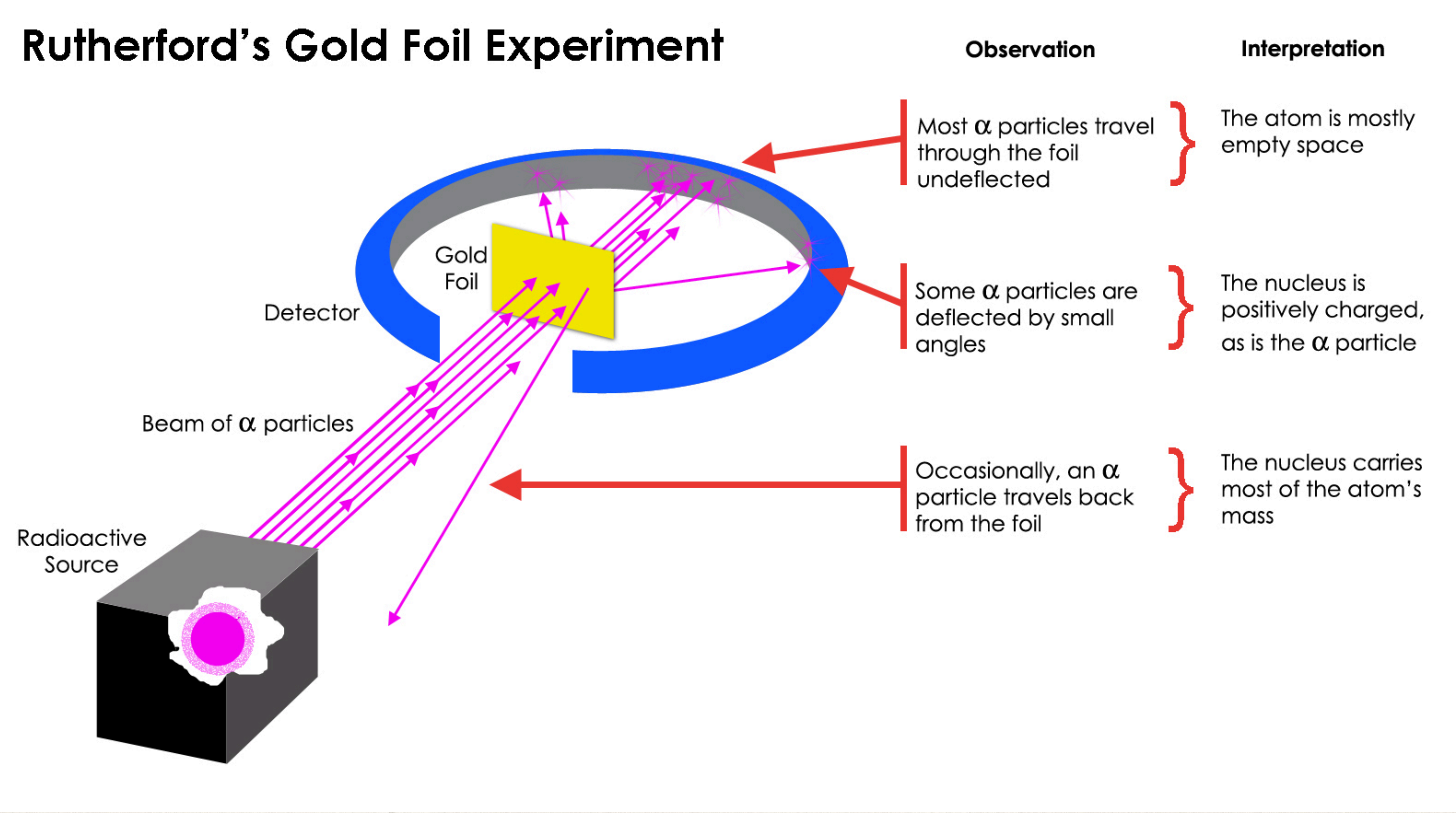


The discovery of the nucleus

The structure of the atom was first probed by the Rutherford experiment in 1909.

A beam of particles generated by the radioactive decay of radium was directed onto a sheet of a very thin gold foil



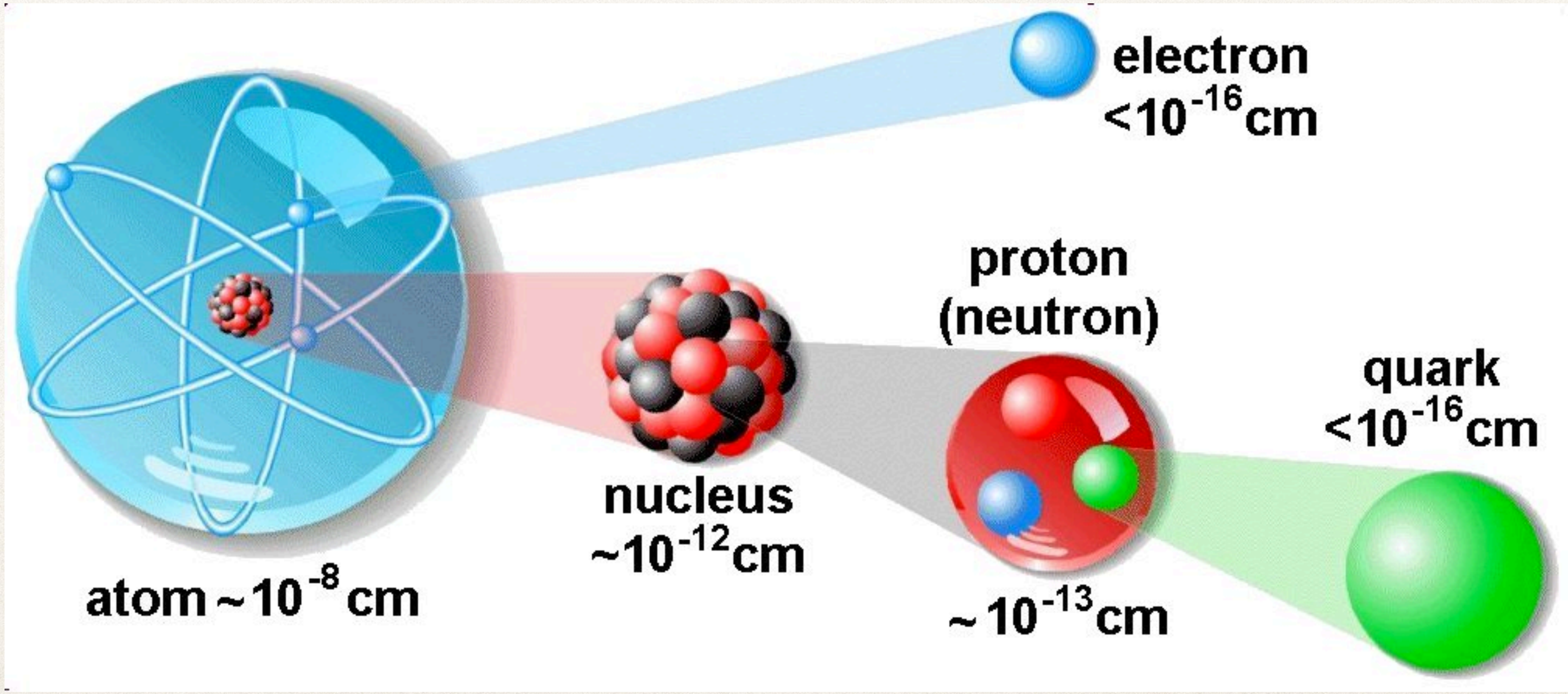
What is the nucleus of the atom?

- The nucleus contains A nucleons: A = Z protons + N neutrons

Protons (uud) are positive charged particles 2000 times heavier (M_pc^2 = 938.272 MeV) than electrons (M_ec^2= 0.511MeV).

Neutrons (udd) are electric neutral particles with mass (M_nc^2 = 939.565 MeV) comparable to the proton one.

- A nucleus is characterized by its mass number A and its atomic number Z. ${}^{A}_{Z}X$.
- The nucleus is a quantum object.
- Nucleons are hadron particles (particles governed by the strong interaction)
- Nucleons are baryons (made of 3 quarks)
- Nucleons are fermions (like electrons)

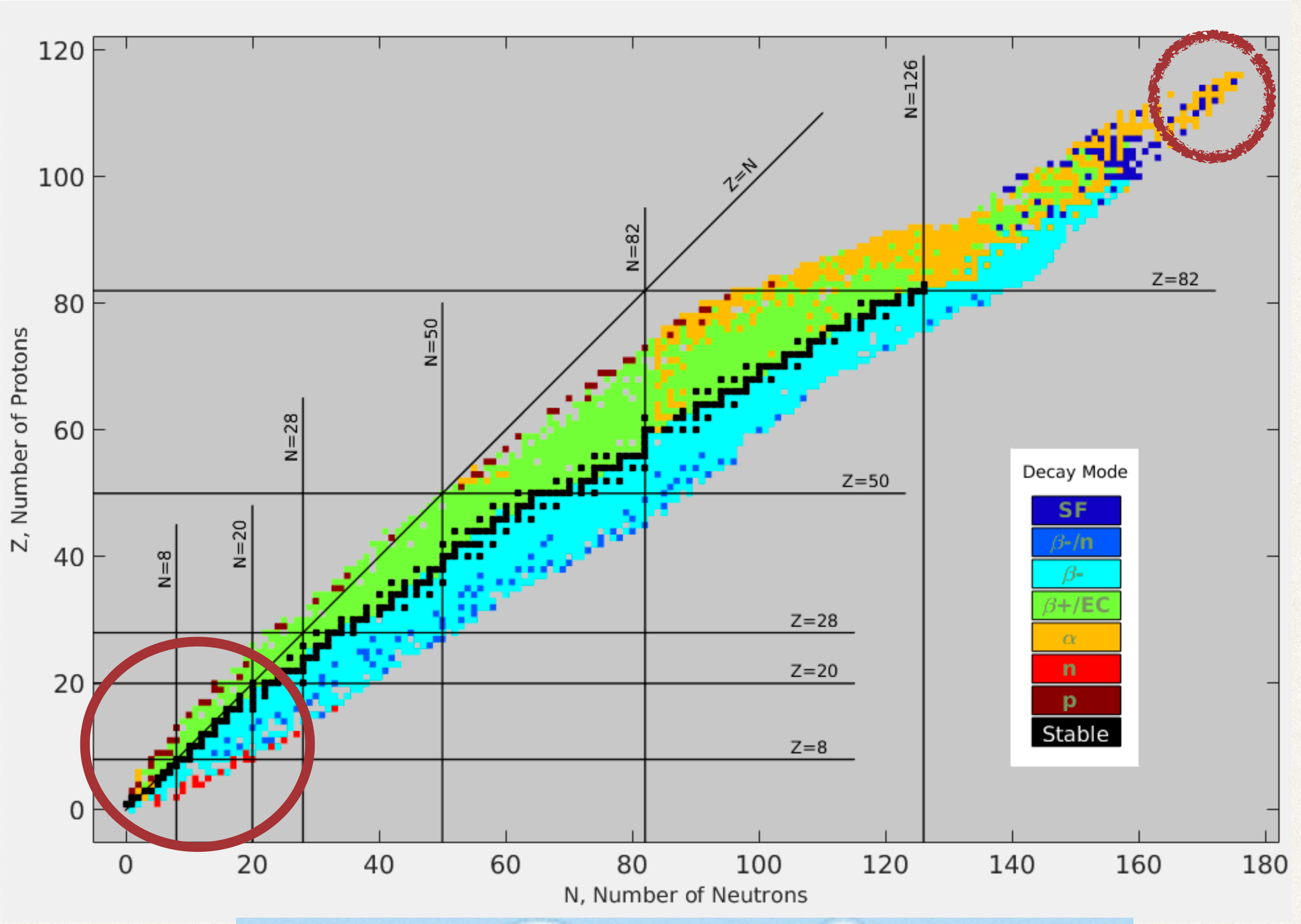


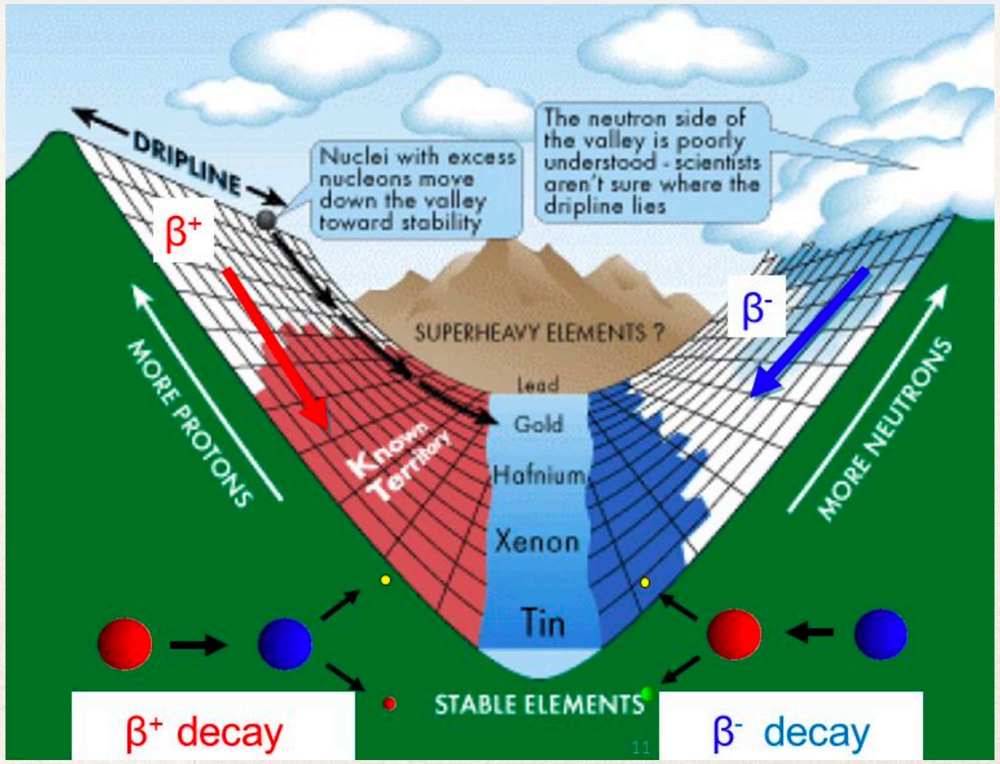
A nucleus is almost 100.000 times smaller than an atom

Chart of nuclides

Physicists map the inventory of known nuclei on a "**chart of nuclides**"

- The **lowest part** of the valley corresponding to the region of **most stable nuclei.**
- The **region of stable nuclei** is roughly found on a diagonal line where N/Z~1, known as the **line of beta stability**.
- The **sides of the valley** correspond to increasing instability to beta decay (β^- or β^+). The decay of a nuclide becomes more energetically favorable the further it is from the line of beta stability.
- The **boundaries of the valley** correspond to the **nuclear drip lines.** Below this diagonal is a jagged line called **the "neutron dripline"**. Above this diagonal is another jagged line called the "**proton dripline**". Nuclei found above the proton dripline and below the neutron dripline tend to be highly unstable and undergo radioactive decay.



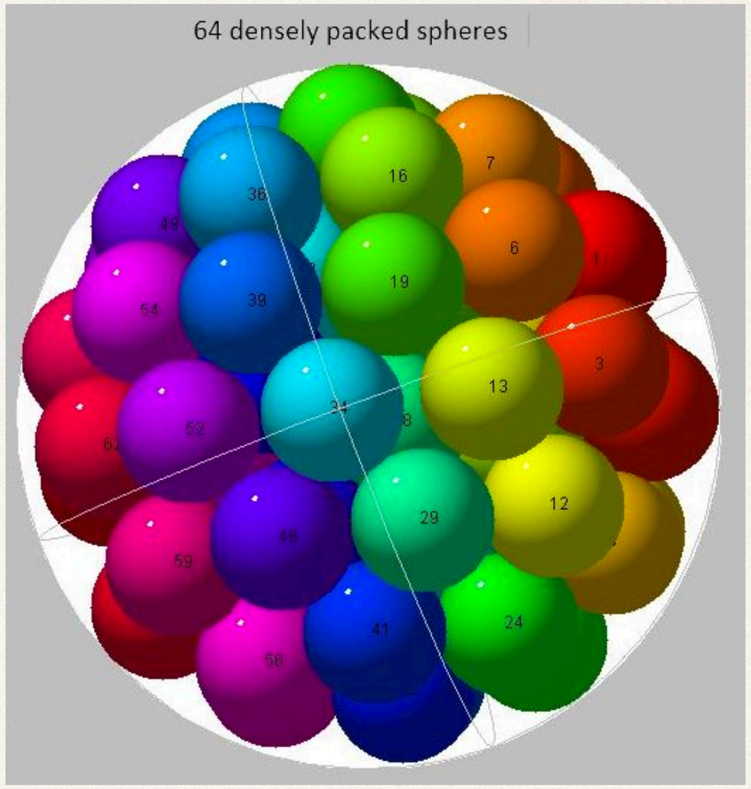


Island of stability

Long-lived superheavy isotopes outside of the valley of stability. They are expected to have particular configurations of "magic" atomic and neutron numbers.

Nuclear properties: size and density

Experiments have shown that the "volume" of a nucleus is proportional to the number of nucleons that make up the nucleus.



Protons and neutrons are each ~ 1.4×10^{-15} m in diameter.

^{56}**Fe** (Z=26, N=30) has a diameter of about **4 proton diameters**.

^{235}**U** (Z=92, N=143) has a diameter just over **6 proton diameters across.** (check: a bag containing 235 similar marbles is about six marble diameters across)

The **size of a nucleus** is essentially the size of a ball of these particles.

The volume of the nucleus is directly proportional to the total number of nucleons, assuming a spherical shape:

$$\frac{4}{3}\pi R^3 = const \times A \Rightarrow R^3 \propto A \rightarrow R \propto A^{1/3} \Rightarrow$$

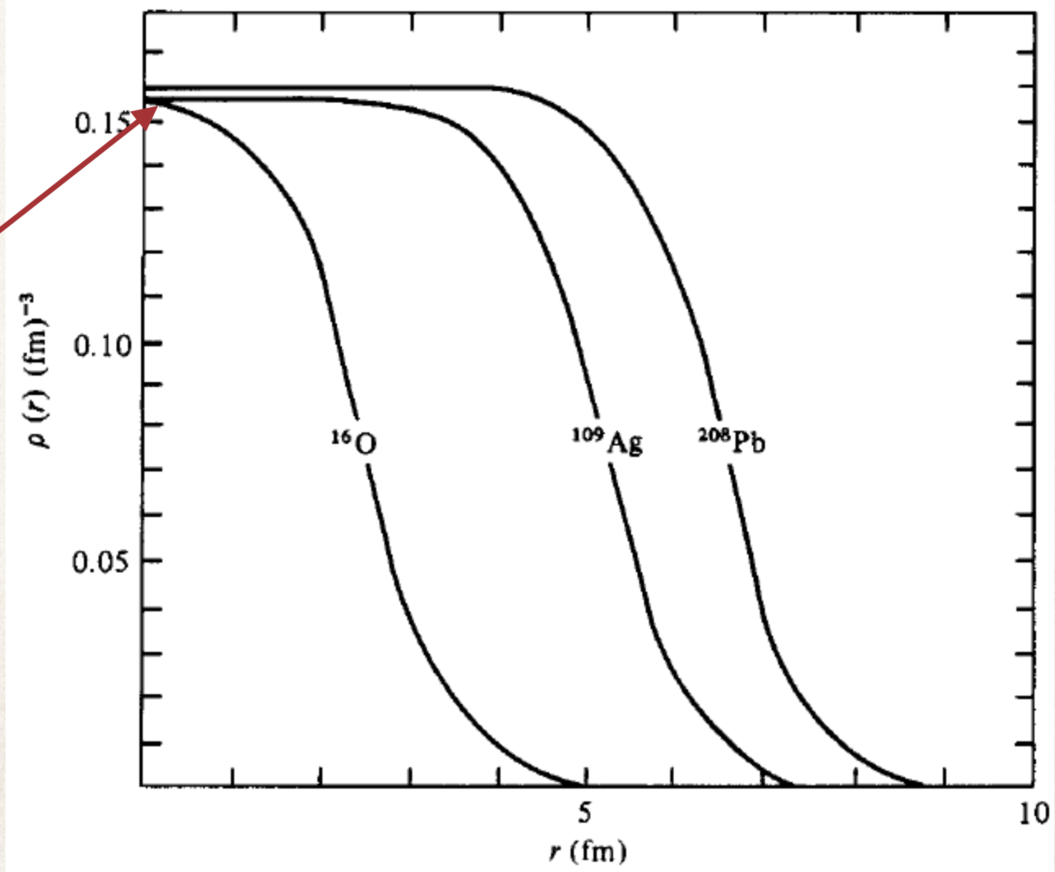
$$R = 1.25 \times A^{1/3}\,(\mathrm{fm})$$

All nuclei have nearly the same density.

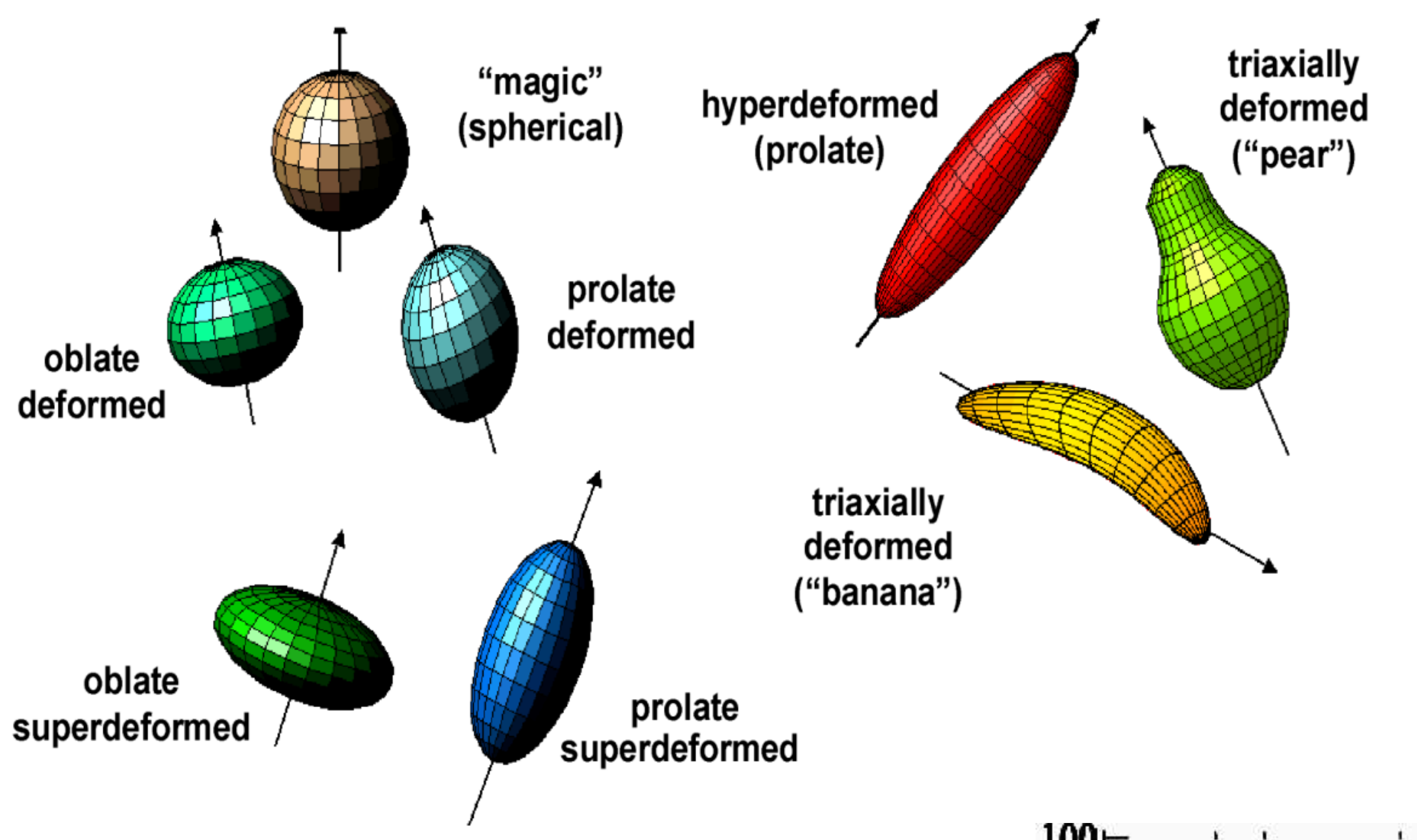
ρ_0 = 0.16 nucleons / fm^3 ~ 2×10^{17} kg/m^3

(density of water 1000 kg/m^3)

Nucleons combine to form a nucleus as though they were tightly packed spheres.



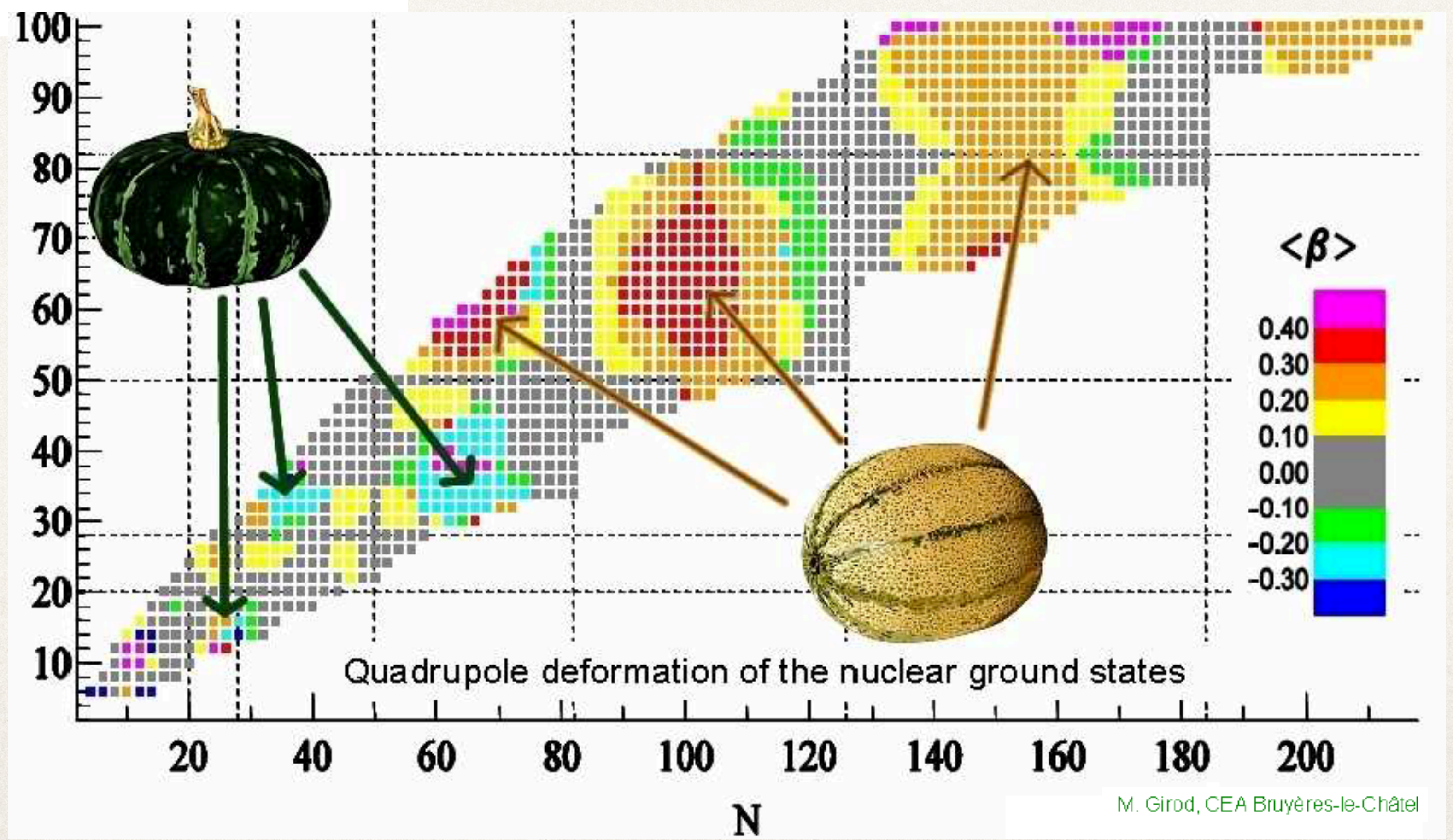
Nuclear properties: shape



The shape of atomic nuclei depends on the residual interaction of the valence nucleons outside closed shells that can polarize the nuclear core.

Nuclei can be:
Spherical,
Prolate(rugby ball-shaped),
Oblate (discus-shaped),
Triaxial (a combination of oblate and prolate deformation)

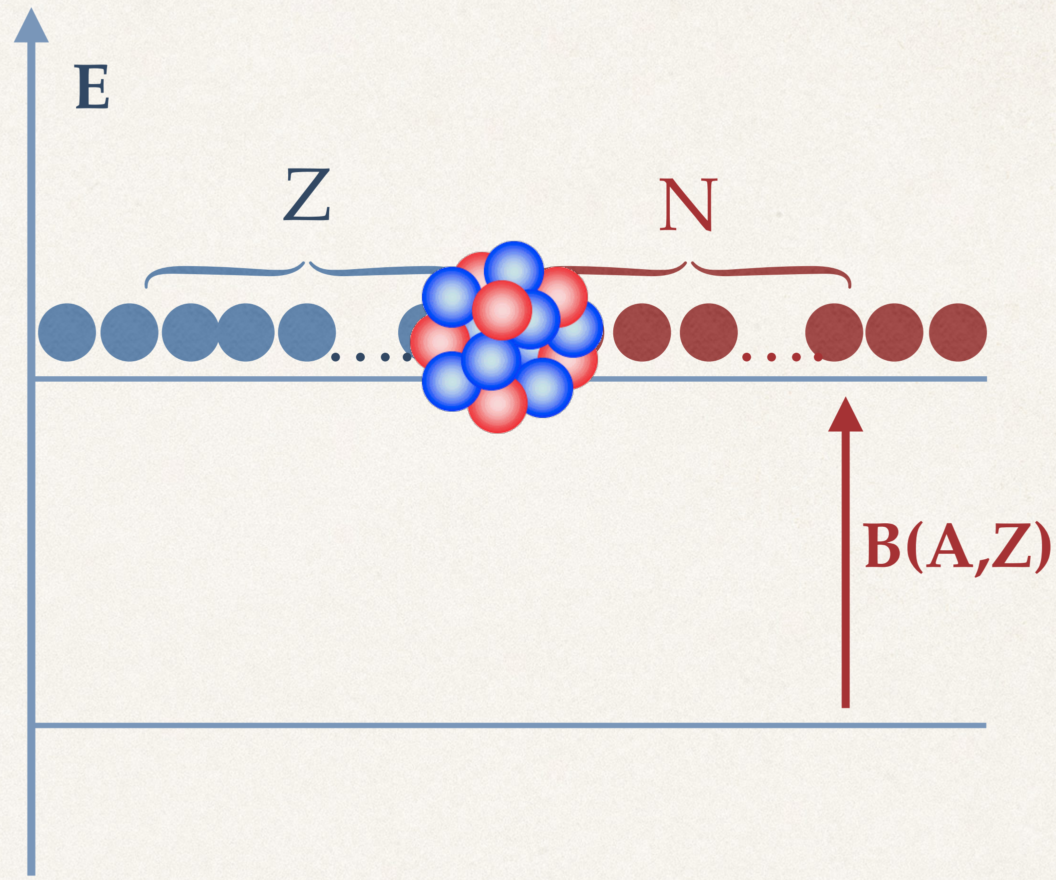
Ground–state nuclear deformation predicted with the Hartree-Fock-Bogoliubov approach



Nuclear properties: binding energy

The best way to see the competition between the ***attractive nuclear force*** and the ***electric repulsive force*** inside atomic nuclei is to look at nuclear binding energies.

The nucleus is a bound system: its mass is lower than the mass of its components.



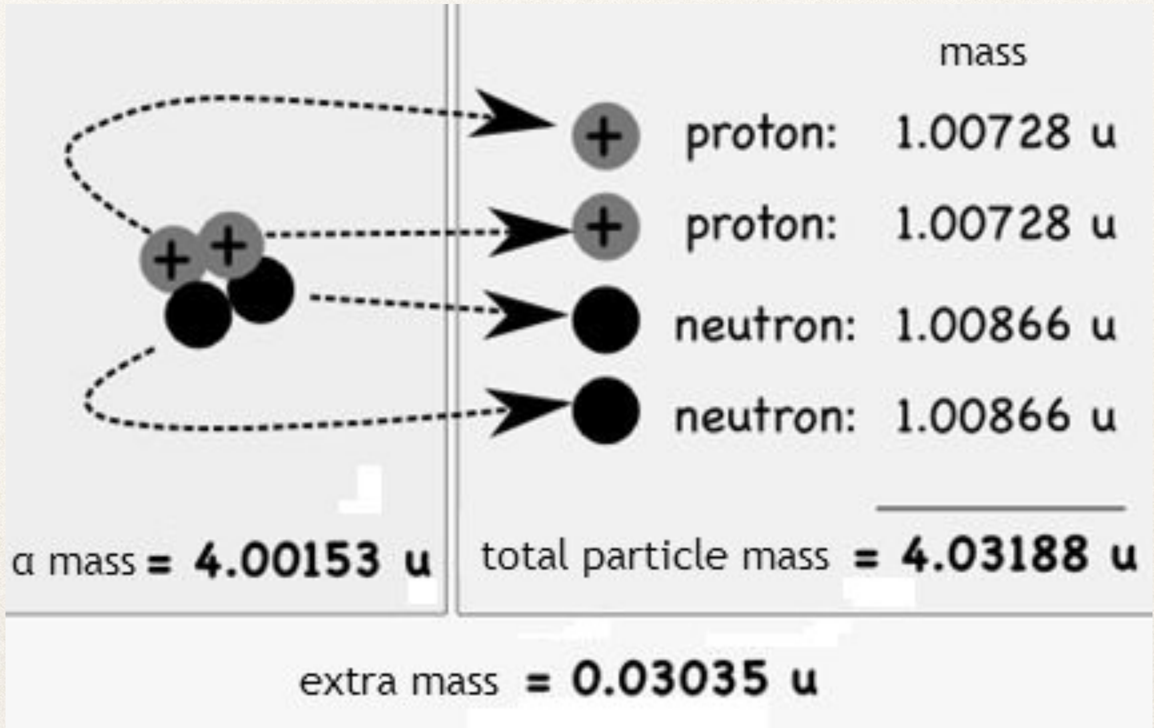
The **binding energy** represents **how much energy we would have to supply to pull the nucleus apart into separate free nucleons**. The nuclear force tries to hold the nucleus together and therefore increases the binding energy. The electrostatic force, which pushes the protons apart, decreases the binding energy.

The binding energy is defined as the the total mass energy of constituent nucleons minus the mass energy of the nucleus:

$$\mathbf{B(A,Z) = \Sigma m(free\ nucleons) - M(A,Z)}$$

$$\mathbf{B(A,Z) = N\, M_n + Z\, M_p - M(A,Z)}$$

Stable bound system for B > 0

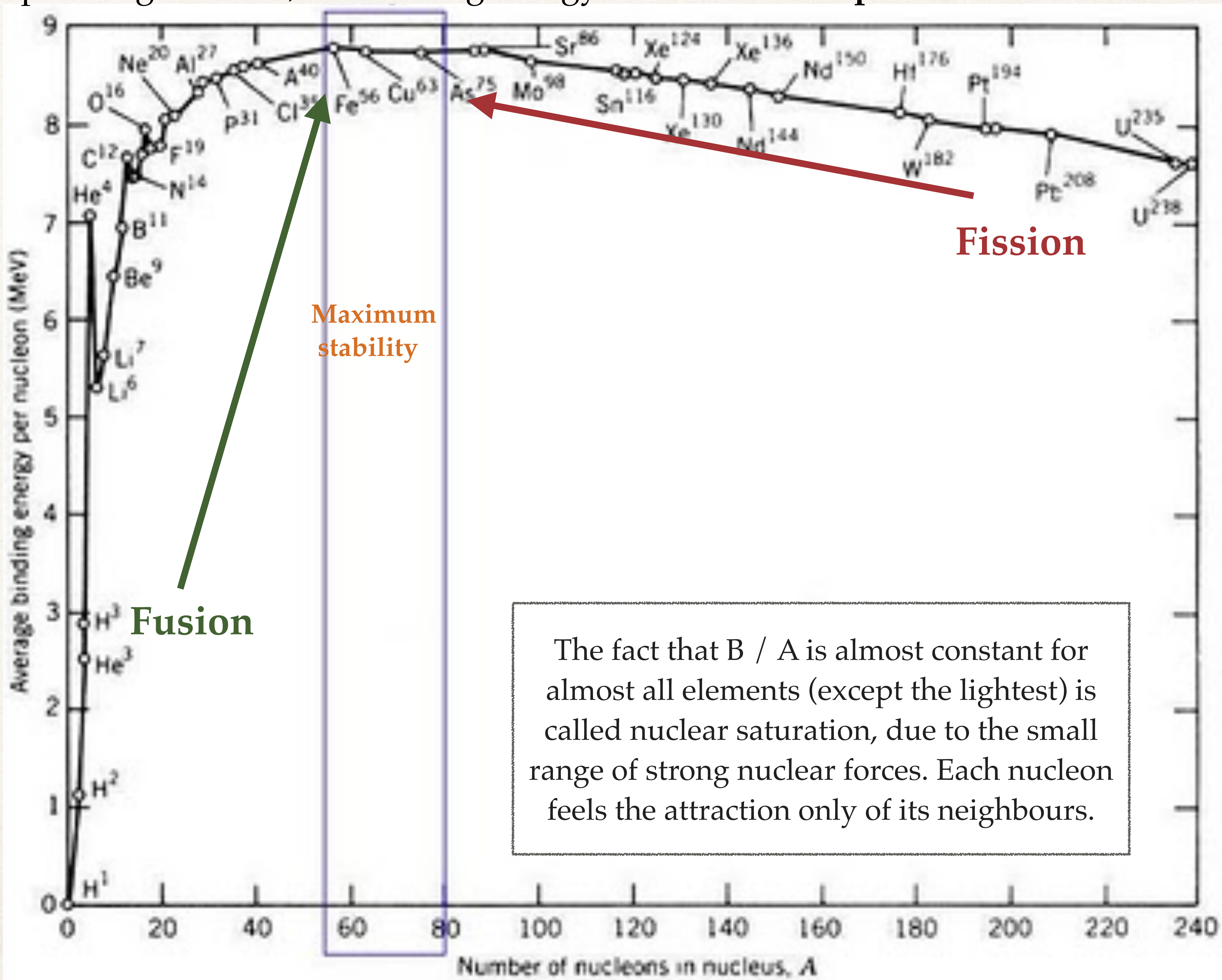


Nuclear properties: binding energy

The binding energy, per nucleon, of the most stable nucleus for each element.

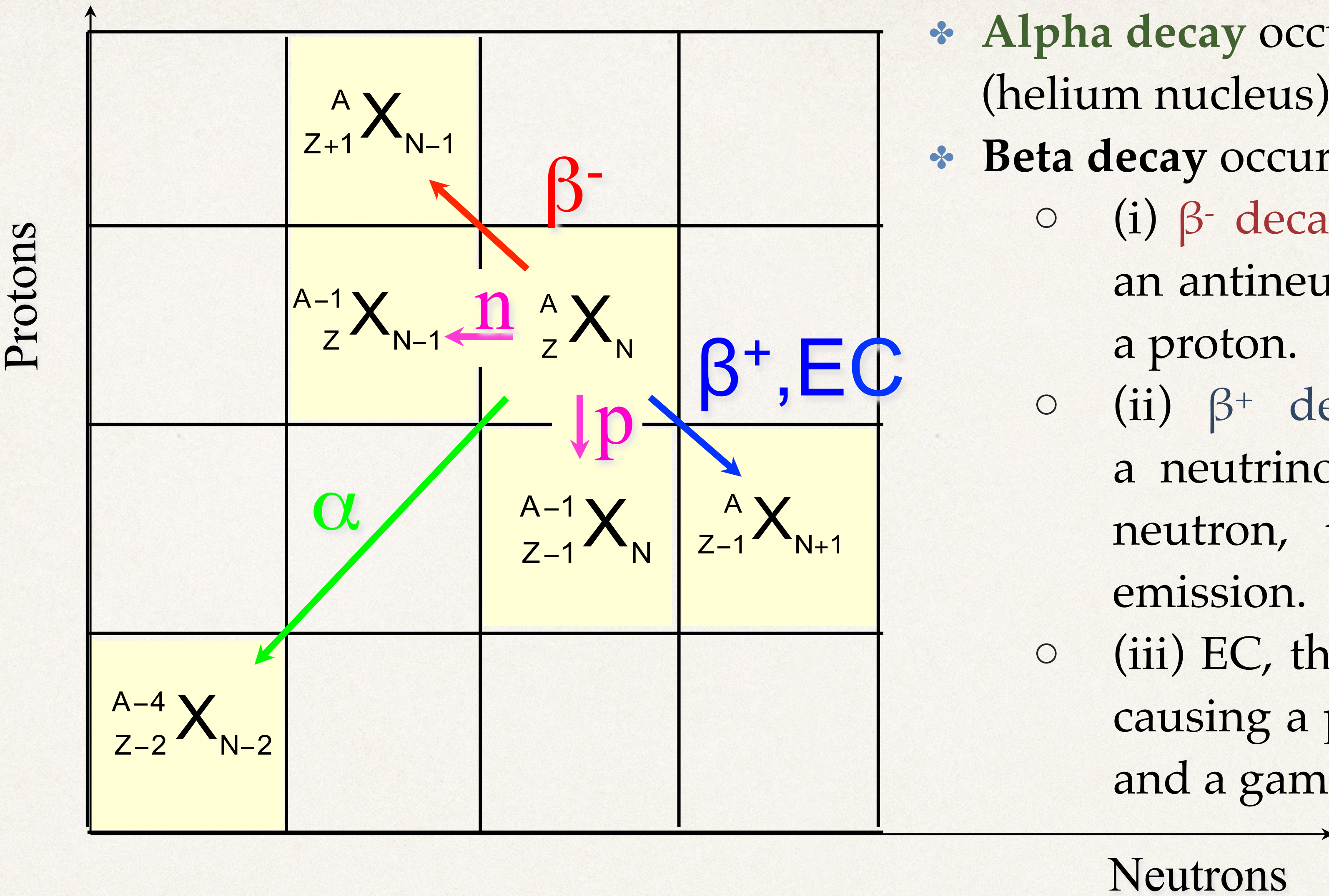
The peak of that curve is at the ^{56}**Fe** no other nucleus is more tightly bound.

Except for light nuclei, the binding energy is about **8 MeV per nucleon**

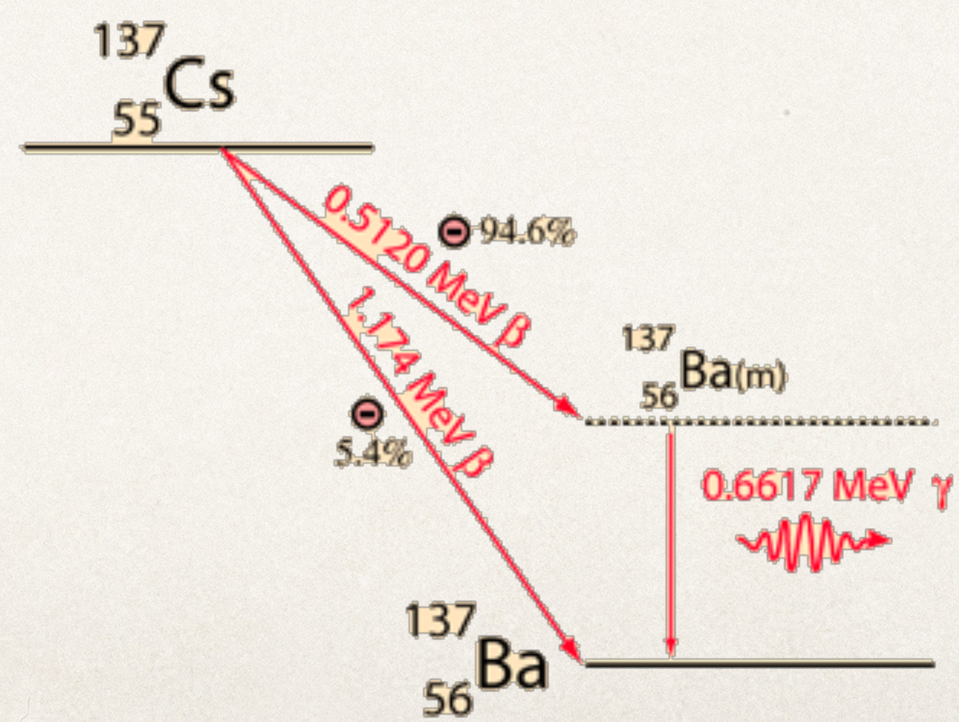


The fact that B / A is almost constant for almost all elements (except the lightest) is called nuclear saturation, due to the small range of strong nuclear forces. Each nucleon feels the attraction only of its neighbours.

Radioactivity



- **Alpha decay** occurs when the nucleus ejects an alpha particle (helium nucleus).
- **Beta decay** occurs in two ways;
  - (i) β^- decay, when the nucleus emits an electron and an antineutrino in a process that changes a neutron to a proton.
  - (ii) β^+ decay, the nucleus emits a positron and a neutrino in a process that changes a proton to a neutron, this process is also known as positron emission.
  - (iii) EC, the nucleus may capture an orbiting electron, causing a proton to convert into a neutron. A neutrino and a gamma ray are subsequently emitted.



- **Gamma decay** a radioactive nucleus first decays by the emission of an alpha or beta particle. The daughter nucleus that results is usually left in an excited state and it can decay to a lower energy state by emitting a gamma ray photon.
- other decay modes: **neutron emission, cluster decay and nuclear fission**

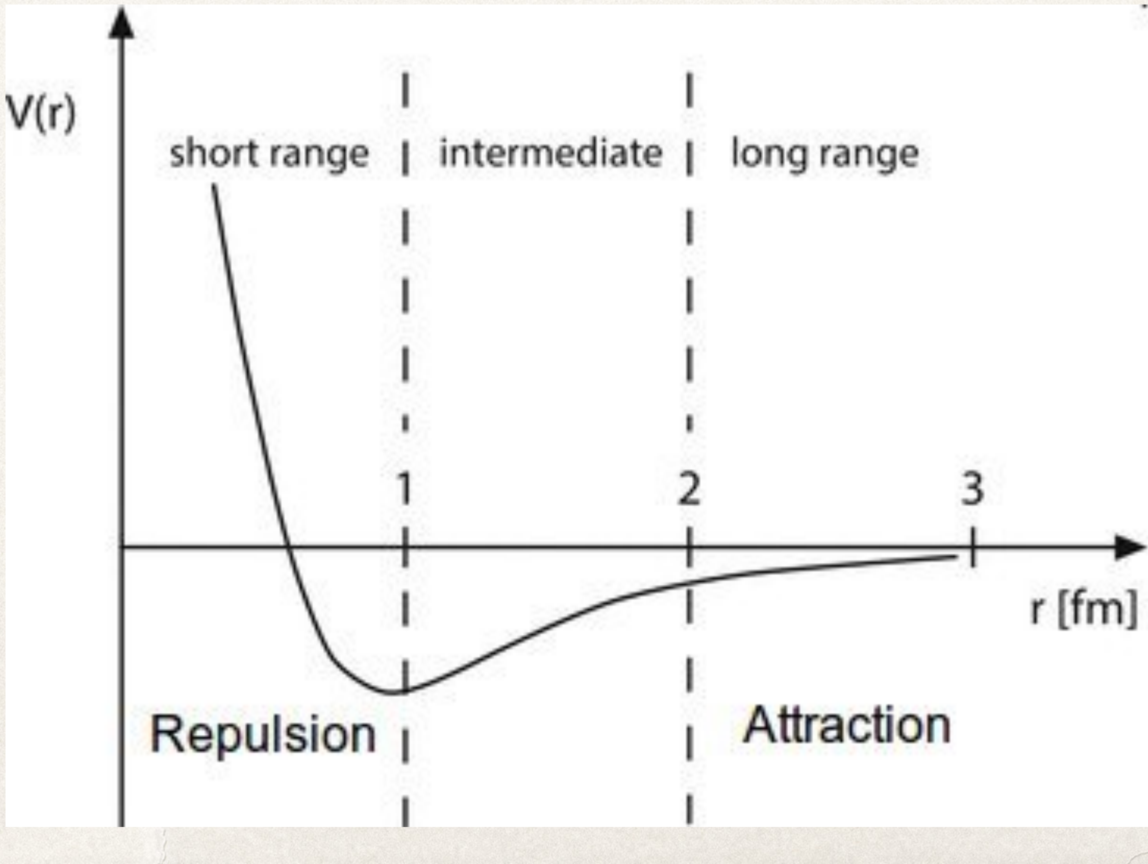
The Nucleon Nucleon interaction

A traditional goal of nuclear physics has been the understanding of the properties of atomic nuclei in terms of the "bare" interaction between pairs of nucleons. However, the underlying theory of strong interactions, QCD, shows that the NN interaction is not fundamental.

The nucleon-nucleon interaction is still unknown nowadays!

The properties of the nuclear force can be deduced from the properties of the structures it creates, namely **the atomic nuclei.**

- **Short range:** ~1 fm (10^{-15}m), resulting from particle scattering.
- **Attractive**: strongly attractive to nucleons whose centers are at a distance of about 1 fm, but weakens abruptly to extinction at distances beyond 2.5 fm. If we try to **pull two nucleons apart**, **the attractive nuclear force holds them together,** next to each other.
- **Repulsive**: at very short distances, below 0.7 fm (repulsive core). This determines the size of the nuclei. If **we try to squeeze** two nucleons into each other, we encounter a **very strong repulsion**, giving the nucleons essentially a **solid core**.
- **Saturated**: Each nucleon feels the attraction only of its neighbors, otherwise the binding energy would increase by A (A-1). But it increases with A (B/A ~ 8 MeV).
- **Charge independent**: Vpp=Vnn=Vnp
- Depends on whether the spins of the nucleons are parallel or anti-parallel
- It has **a non-central or tensor component**. This part does not conserve the orbital momentum, which under the regime of central forces is a constant of motion.



The Nucleon Nucleon interaction

In most microscopic approaches, **the degrees of freedom are those of the nucleons**, namely their **position, spin and isospin**.

$$\vec{r}_i, \quad \vec{p}_i, \quad \vec{s}_i, \quad \vec{t}_i \quad (i = 1, \dots A)$$

The wave function of the NN system: $\Psi_{NN} = \psi_{\text{space}} \chi_S^{m_s} \phi_T^{T_z}$

If one takes as the starting point the hamiltonian of this quantum system, one should in principle write very generally

$$H = \sum_{i=1}^{A} t_i + \frac{1}{2} \sum_{i,j} v(i,j)$$

where t_i is the kinetic energy of nucleon i and v(i,j) the nucleon-nucleon potential energies.

An appropriate functional form for the NN potential is parameterized in such a way that it **reproduces** as closely as possible **the data on NN scattering** and **deuteron properties**. There are two classes of such potentials: local and nonlocal.

- Higher order terms as **3-body forces** are usually **neglected**.
- One of the inherent difficulties in nuclear physics is the **lack of precise knowledge of the interactions v(i, j).** BUT, we can restrict the form of the nucleon-nucleon interaction by **symmetry considerations.**

The Nucleon Nucleon interaction: symmetry requirements

One postulates a certain number of restrictions for the nucleon-nucleon interaction

$$V(1,2) = V(\vec{r_1}, \vec{p_1}, \vec{\sigma_1}, \vec{\tau_1}, \vec{r_2}, \vec{p_2}, \vec{\sigma_2}, \vec{\tau_2})$$

Eisenbud and Wigner (1941)

- **Invariance with respect to exchange of coordinates**:

$$V(1,2) = V(2,1)$$

- **Translational invariance**: the potential shall depend only on the relative distance of the particles $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$:

$$V(1,2) = V(\vec{r}, \vec{p_1}, \vec{\sigma_1}, \vec{\tau_1}, \vec{p_2}, \vec{\sigma_2}, \vec{\tau_2})$$

- **Galilean invariance**: the potential is unchanged under a transformation to a system travelling at constant speed, and therefore it should depend only on the relative momentum $\vec{p} = \frac{1}{2}(\vec{p_1} - \vec{p_2})$

$$V(1,2) = V(\vec{r}, \vec{p}, \vec{\sigma_1}, \vec{\tau_1}, \vec{\sigma_2}, \vec{\tau_2})$$

- **Rotation invariance in ordinary space**: the potential must be scalar.
- **Invariance with respect to rotation in iso-space.**

Okubo and Marshak (1958)

- **Hermiticity**.
- **Invariance with respect to space reflexions (parity)**:

$$V(\vec{r}, \vec{p}, \vec{\sigma_1}, \vec{\tau_1}, \vec{\sigma_2}, \vec{\tau_2}) = V(-\vec{r}, -\vec{p}, \vec{\sigma_1}, \vec{\tau_1}, \vec{\sigma_2}, \vec{\tau_2})$$

- **Invariance with respect to time-reversal** (guarantees that the equations of motion do not depend on the direction of time-evolution):

$$V(\vec{r}, \vec{p}, \vec{\sigma_1}, \vec{\tau_1}, \vec{\sigma_2}, \vec{\tau_2}) = V(\vec{r}, -\vec{p}, -\vec{\sigma_1}, \vec{\tau_1}, -\vec{\sigma_2}, \vec{\tau_2})$$

The Nucleon Nucleon interaction

The most general form of the NN potential that preserves invariance under particle exchange, translation, Galilean transformation, rotation, parity, and time-reversal:

$$V(1,2) = V_C + V_S(\vec{\sigma}_1 \cdot \vec{\sigma}_2) + V_T S_{12}(\vec{r}) + V_{T'} S_{12}(\vec{p}) + V_{LS} \vec{L} \cdot \vec{S} + V_Q (\vec{L} \cdot \vec{S})^2$$

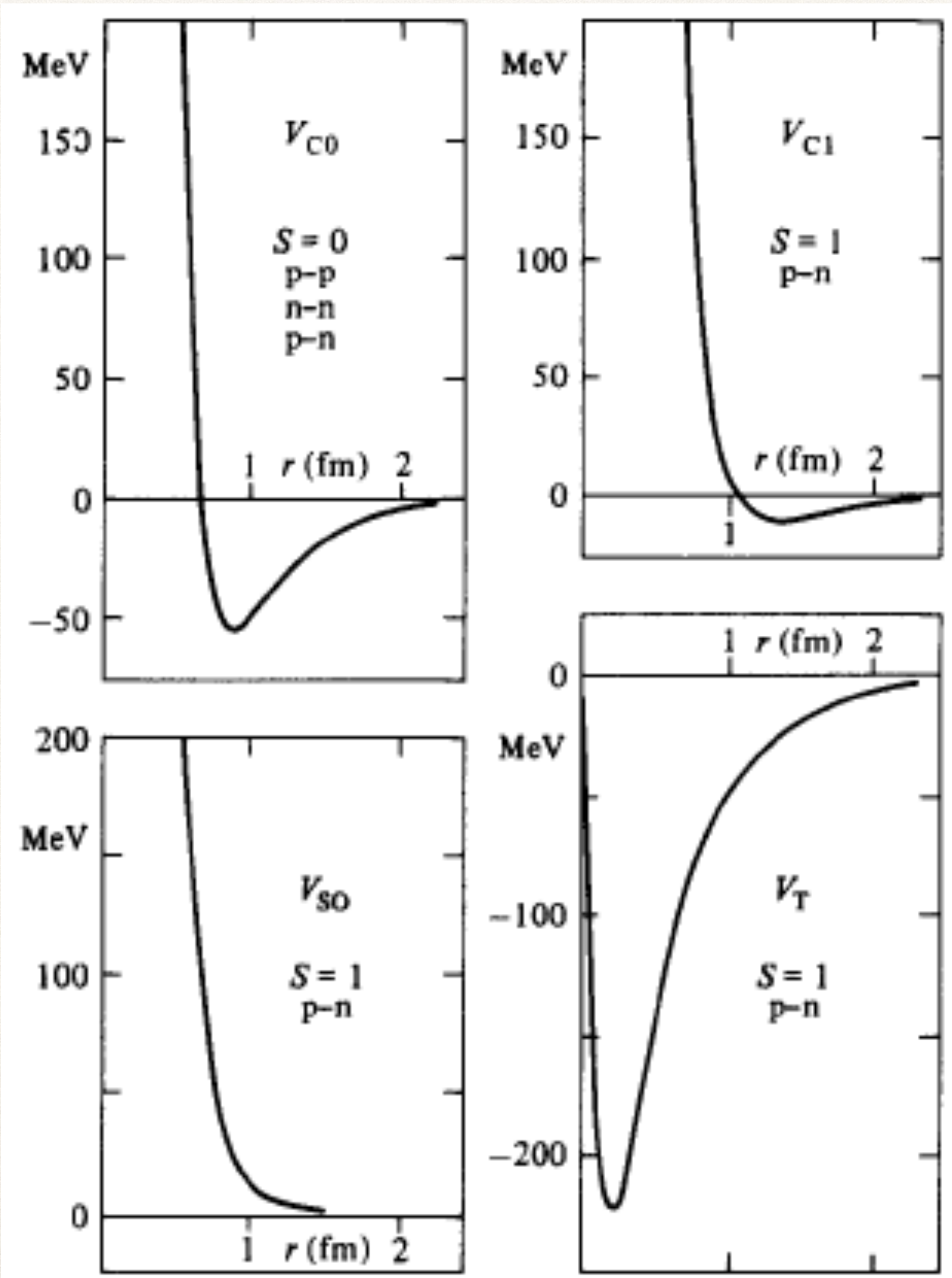
… the spin-orbit operator: $\vec{L} \cdot \vec{S} = \frac{1}{2}(\vec{r} \times \vec{p}) \cdot (\vec{\sigma}_1 + \vec{\sigma}_2)$

… the tensor operator $S_{12} = 3\left(\vec{\sigma}_1 \cdot \frac{\vec{r}}{r}\right)\left(\vec{\sigma}_2 \cdot \frac{\vec{r}}{r}\right) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2)$

… scalar functions: $V_\alpha = V_\alpha(r^2, p^2, L^2) \qquad \alpha = \{C, S, T, T', LS, Q\}$

The Nucleon Nucleon interaction

Paris potential



Includes:

- expression for the **antisymmetric S = 0** (states of two protons or two neutrons or a neutron proton). For total S = 0, the nucleons "feel" only a central potential
- expression for the symmetric **S = 1 states** (possible only in the proton-neutron system). For total S = 1, there are four potential contributions (central, tensor and 2 spin-orbit coupling terms):
- $$V(r) = V_{C1}(r) + V_T(r)\Omega_T + V_{SO}(r)\Omega_{SO} + V_{SO2}(r)\Omega_{SO2}$$

$$\Omega_T = 3\frac{(\boldsymbol{\sigma}_1 \cdot \mathbf{r})(\boldsymbol{\sigma}_2 \cdot \mathbf{r})}{r^2} - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

$$\hbar\Omega_{SO} = (\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2) \cdot \mathbf{L}$$

$$\hbar^2\Omega_{SO2} = (\boldsymbol{\sigma}_1 \cdot \mathbf{L})(\boldsymbol{\sigma}_2 \cdot \mathbf{L}) + (\boldsymbol{\sigma}_2 \cdot \mathbf{L})(\boldsymbol{\sigma}_1 \cdot \mathbf{L}).$$

The Nucleon Nucleon interaction

Meson-exchange potentials

In 1935 Yukawa made an analogy between the strong, short-ranged nuclear force and the electromagnetic force between charged particles. If the Coulomb force is due to the exchange of a virtual quantum – photon, perhaps the nuclear force is likewise due to a virtual particle, necessarily of integral spin, exchanged between nucleons.

The stationary Klein-Gordon equation for the pion field:

$$\left(\nabla^2 - \frac{m_\pi^2 c^2}{\hbar^2}\right)\phi = -g\delta(\vec{r})$$

⇨ solution: $$\phi = g\frac{e^{-\mu r}}{r} \qquad \mu \equiv \frac{m_\pi c}{\hbar}$$

The potential between two nucleons is proportional to the wave function of the pion, i.e. to the probability amplitude that the emitted pion finds itself close to the other nucleon.

⇨ YUKAWA POTENTIAL: $$V = g^2\frac{e^{-\mu r}}{r}$$

The Nucleon Nucleon interaction

The Yukawa potential function,

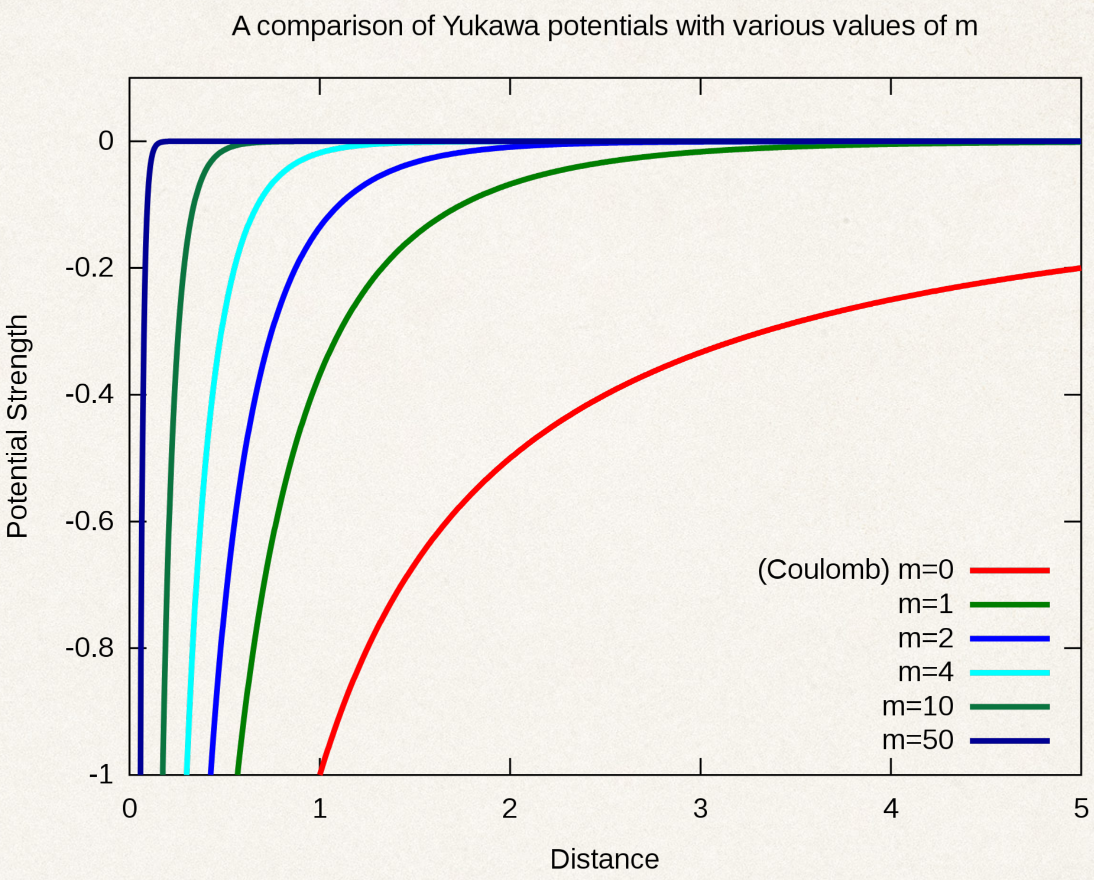
$$V_{\text{Yukawa}}(r) = -g^2 \frac{e^{-kmr}}{r},$$

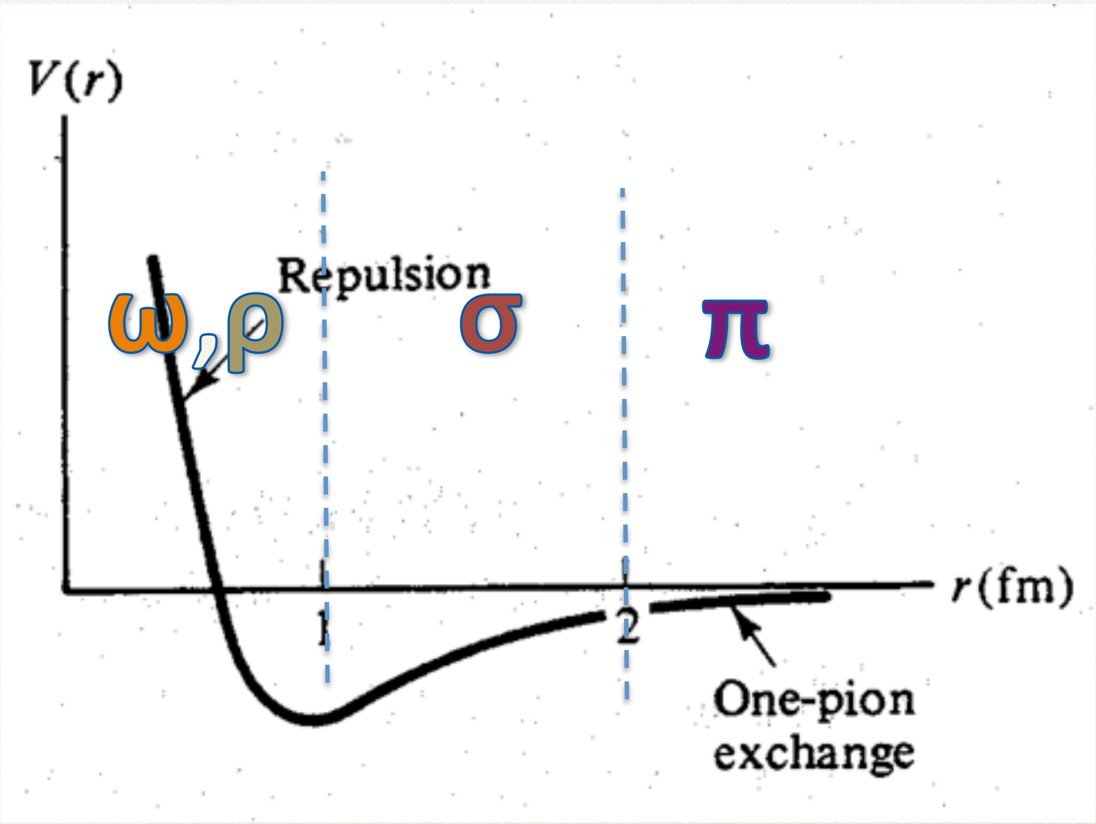
$V_{\text{Yukawa}}(r) \rightarrow -\infty$ as $r \rightarrow 0$ (same as the Coulomb potential).

This “unnatural” behavior of the infinitely attractive force is corrected by the addition of a potential of an impenetrable hard sphere (i.e. an infinitely repulsive force), the existence of which has been ascertained by scattering experiments p - p and p - n.

Thus, the N-N potential takes the form:

$$V(r) = +\infty, \ \gamma\iota\alpha \ r < r_C$$
$$V(r) = V_{\text{Yukawa}}(r), \ \gamma\iota\alpha \ r > r_C$$



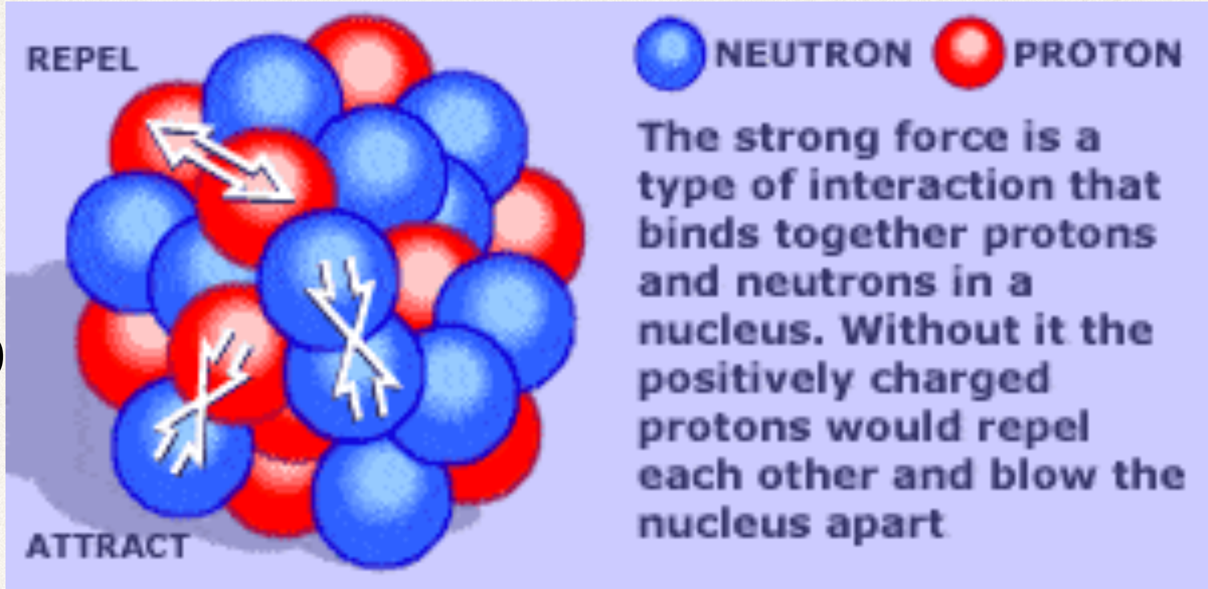


Nuclear models

Nucleus = ***A* nucleons that interact**

We face two challenges

- **Nuclear Interaction inside the nuclei (unknown)**
- **N body formalism**



- **The liquid drop model:** global view of the nucleus associated to a quantum liquid.

- **The Shell Model:** each nucleon is independent in an attractive potential.

- **Microscopic methods, Hartree-Fock, BCS, Hartree-Fock-Bogoliubov:** The nuclear structure is described within the assumption that each nucleon is interacting with an average field generated by all the other nucleons.

The liquid drop

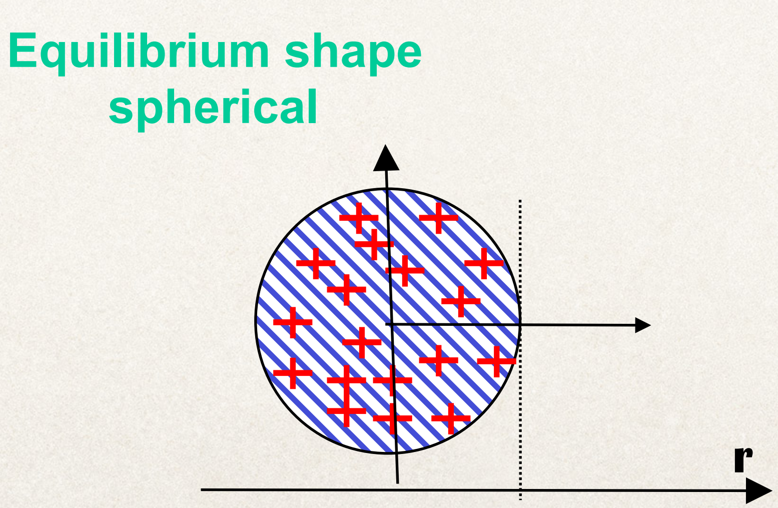
Model developed by Von Weizsacker and N. Bohr (1937)

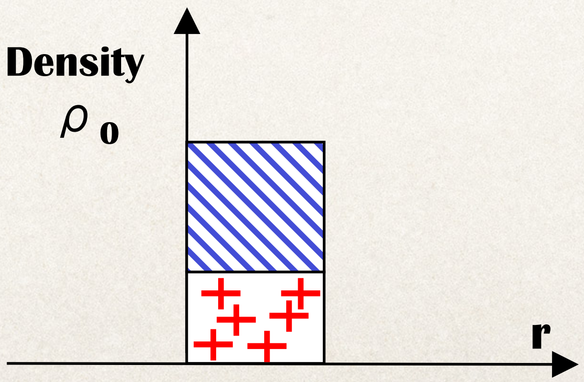
The model was based on the resemblance of the nucleus to a liquid drop. It is a rough model that omits secondary nuclear characteristics, and emphasizes to the strong attraction between nucleons. It has been first developed to describe the nuclear fission.

- The core is spherical, consisting of incompressible matter, so that: $R \sim A^{1/3}$.
- The NN interaction is identical for all nucleons, whether they are protons or neutrons: Vpn = Vpp = Vnn
- The NN interaction is saturated (that is, each nucleon only senses its neighbors).

The model has been used to predict the main properties of the nuclei such as: nuclear radii, nuclear masses and binding energies, decay, fission.

The binding energy of the nuclei is described by the Bethe-Weiszaker formula





Volume ≈ A
$R = r_0 A^{1/3}$

The liquid drop

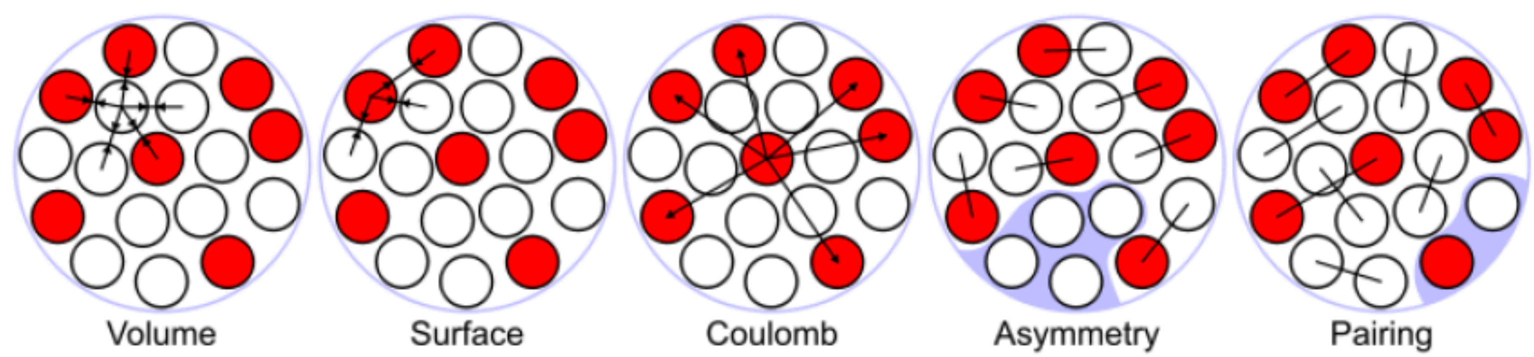
The semi-empirical Bethe-Weiszaker formula

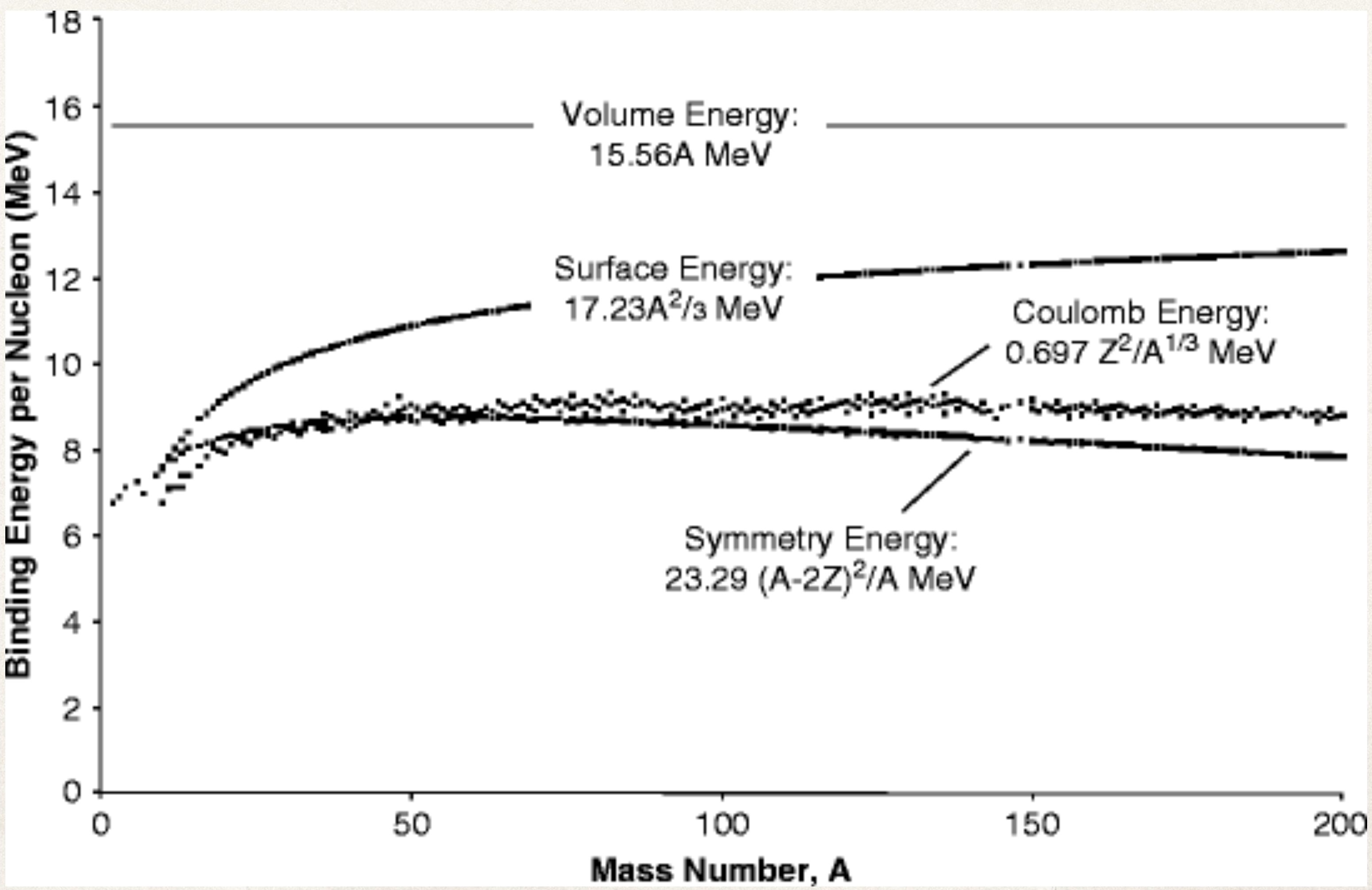
$$B(A,Z) = a_V A - a_S A^{2/3} - a_C \frac{Z^2}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} \pm \delta$$

+ even-even

- odd-odd

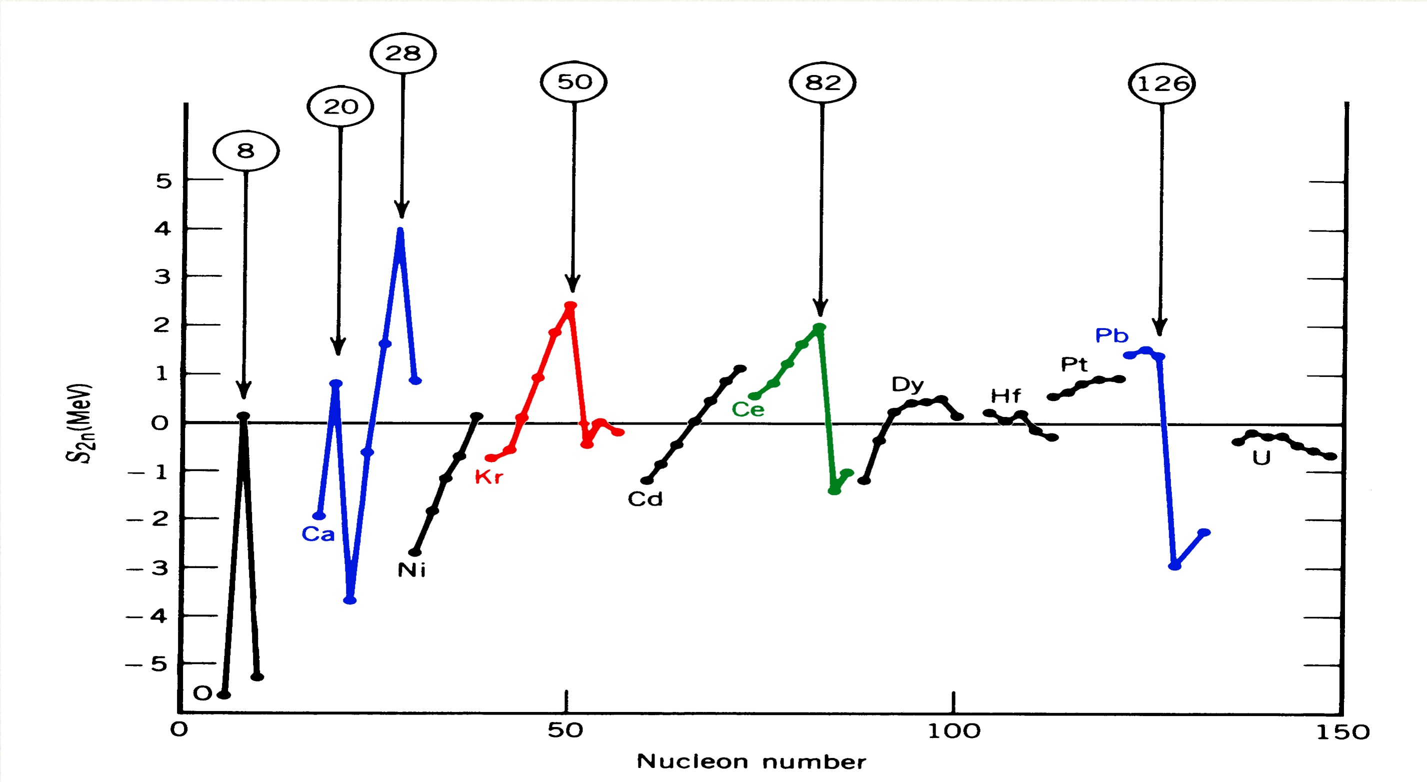
0 for odd-even, even-odd

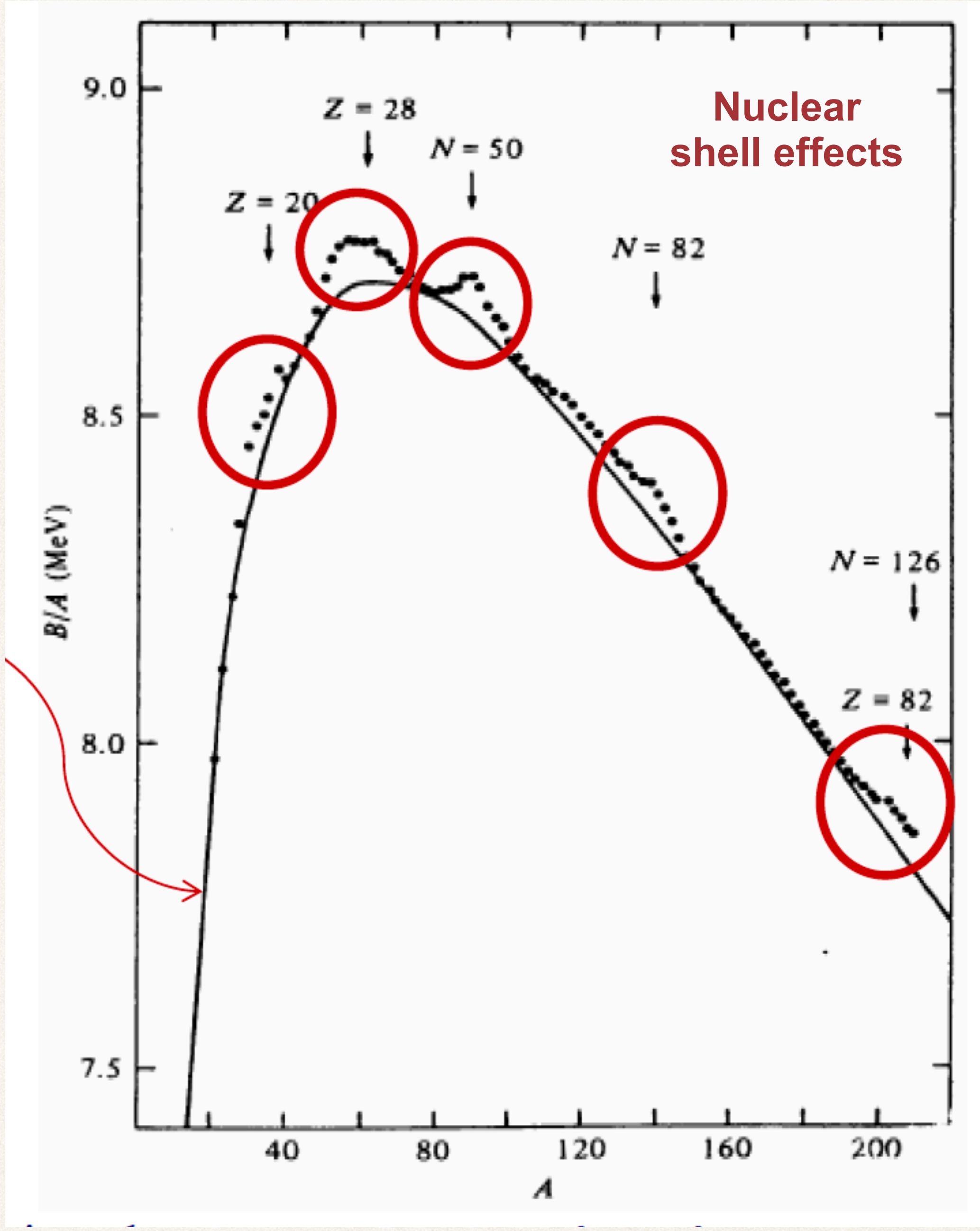




Liquid drop model - Problems

1. Fission fragments: only symmetric fission
2. Nuclear radii: some nuclei away for the $A^{1/3}$
3. Nuclear masses: difference in MeV between experimental masses and masses calculated with the liquid drop formula as a function of the neutron number. **Nuclear shell effects!**
4. **Two neutron separation energy S_{2n},** energy needed to remove 2 neutrons from a given nucleus (N,Z) **S_{2n}=B(N,Z)-B(N-2,Z).**





For most nuclei, the 2n separation energies are smooth functions of particle numbers apart from discontinuities for magic nuclei

Magic nuclei have increased particle stability and require a larger energy to extract particles.

Microscopic description of the atomic nucleus

There are many «***structure effects***» in nuclei, that **can not be reproduced by macroscopic approaches** like the liquid drop model.
Need for **microscopic approaches**, for which the fundamental ingredients are the nucleons and the interaction between them

Nucleus = A nucleons in strong interaction

The many-body problem
Can be solved exactly for $A < 4$
For $A >> 10$: approximations

Nucleon-Nucleon force
unknown
Different effective forces used depending on the method chosen to solve the many-body problem

Shell Model
only a small number of particles are active

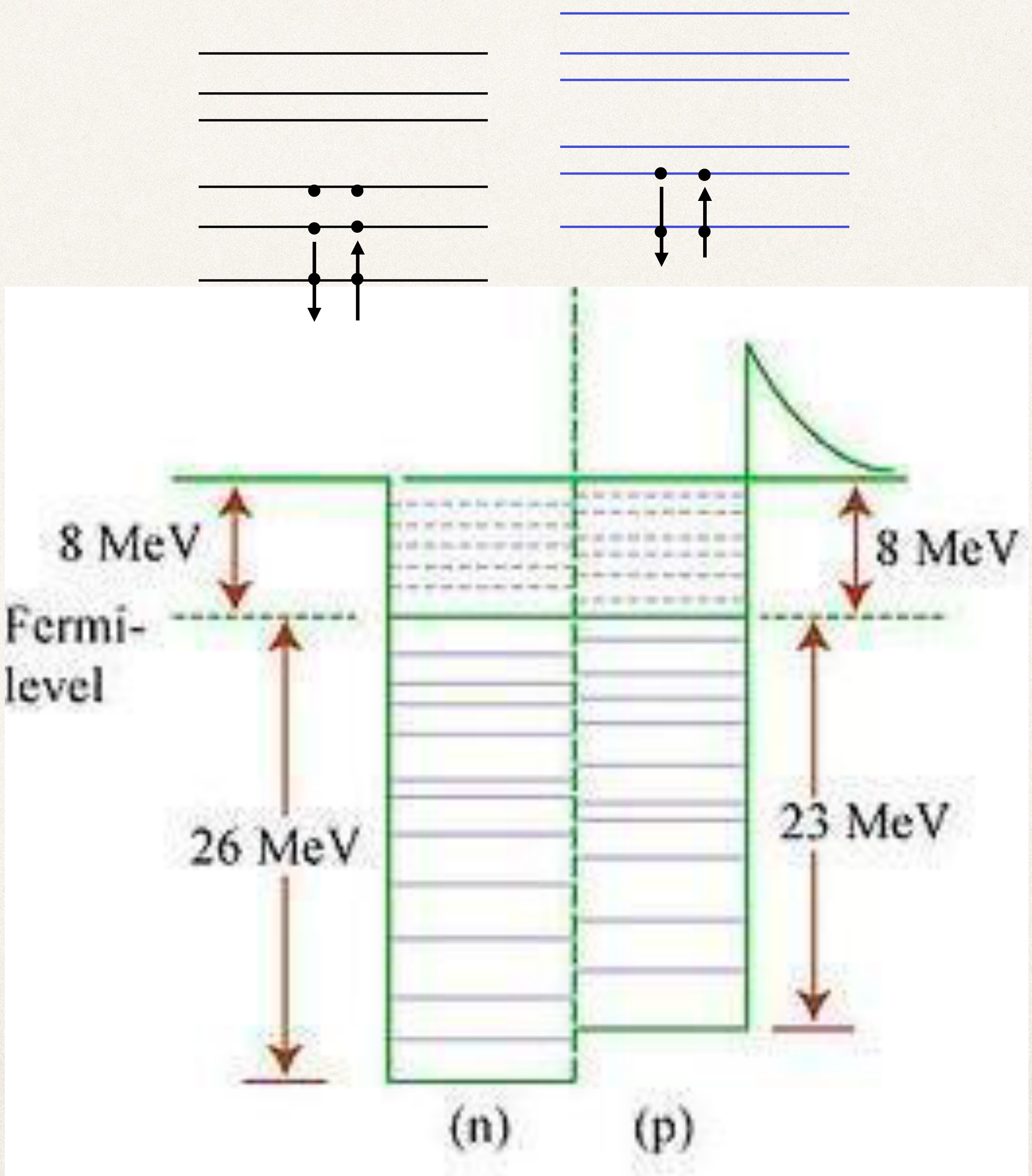
Mean Field models

- no inert core
- not all the correlations between particles are taken into account

Shell Model

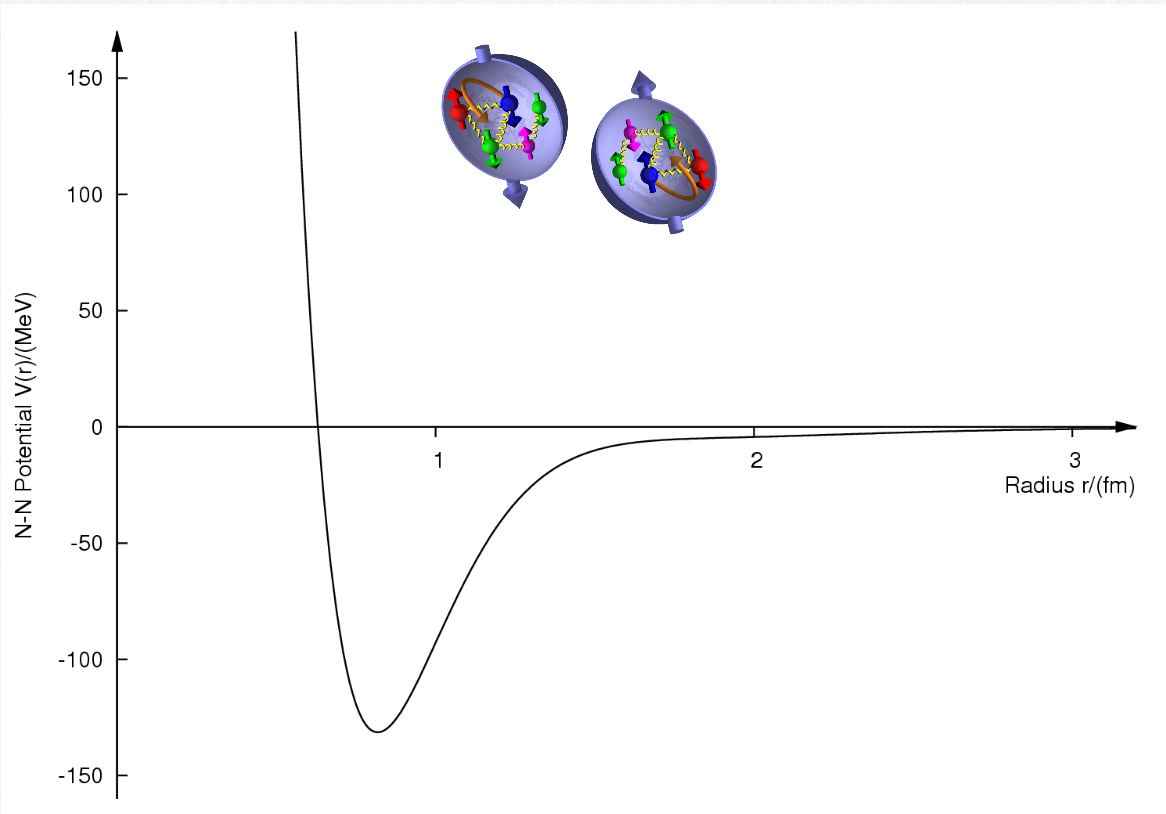
The shell model of the nucleus describes the **nucleons** in the nucleus
in the same way as electrons in the atom
In analogy with atomic structure one may postulate that in the nucleus the nucleons move fairly independently in individual orbits in an average potential …"
M. Goeppert Mayer, Nobel Conference 1963el developed by M. Goeppert Mayer in 1948

- **Nucleons are quantum objects**: only some values of the energy are available, a **discrete number of states**
- **Nucleons are fermions**: two nucleons can not occupy the same quantum state: the Pauli principle. **The energy levels of the nucleons are filled from the lowest to the highest** as nucleons are added to the nucleus.
- There are **separate energy levels for protons and neutrons.**
- Nucleons **fill every energy level in orbitals with a definite angular momentum**.
- As in atoms, **many nuclear properties** (angular momentum, magnetic moment, shape, etc.) **are determined by the last occupied or unoccupied level**.



Shell Model

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



… 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:

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

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

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

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

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

Shell Model

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): $u(r)\lim_{r\to\infty} = 0$ $\quad u(0) = 0$

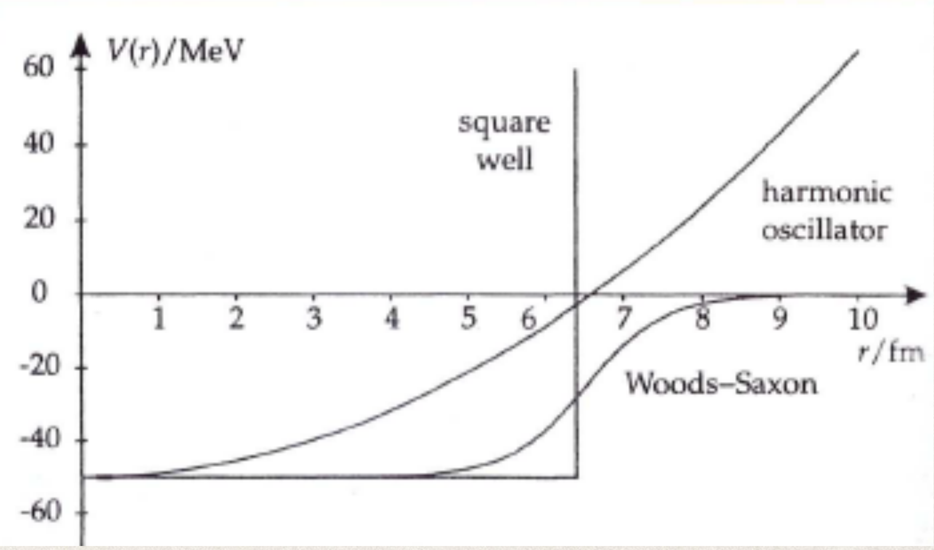
… normalization: $$\int_0^\infty R^2(r)r^2dr = \int_0^\infty u^2(r)dr = 1$$

Nuclear potential deduced from data:

Wood Saxon potential: $V(r) = -\frac{V_0}{1+\exp[(r-R)/a]}$

Square well: $V(r) = -V_0\,(r \leqslant R)$ and $V(r) = 0\,(r > R)$

harmonic oscillator: $V(r) = \frac{1}{2}m\omega^2r^2$



Shell Model

… 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 momentum 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

Shell Model

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 energy: $\varepsilon_{nlj} = \varepsilon^{(0)}_{nlj} + \Delta\varepsilon_{nlj}$ with $\varepsilon^{(0)}_{nlj} = \langle nljm | h_0 | nljm \rangle$

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

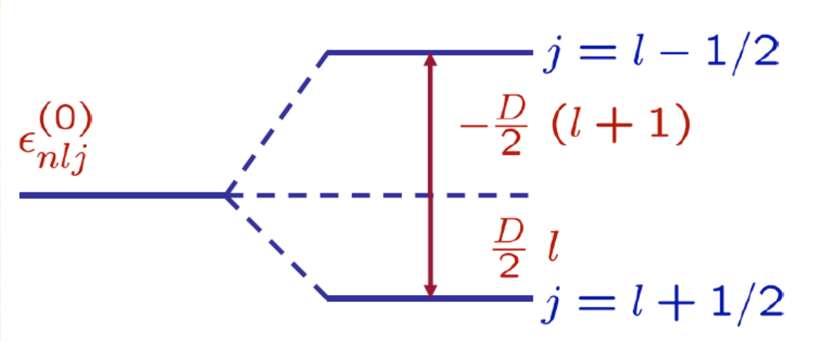
$$\Delta\varepsilon_{nlj} = \langle nljm | \zeta \vec{l} \cdot \vec{s} \, | nljm \rangle = \frac{D}{2} \left[j(j+1) - l(l+1) - \frac{3}{4} \right]$$

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

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

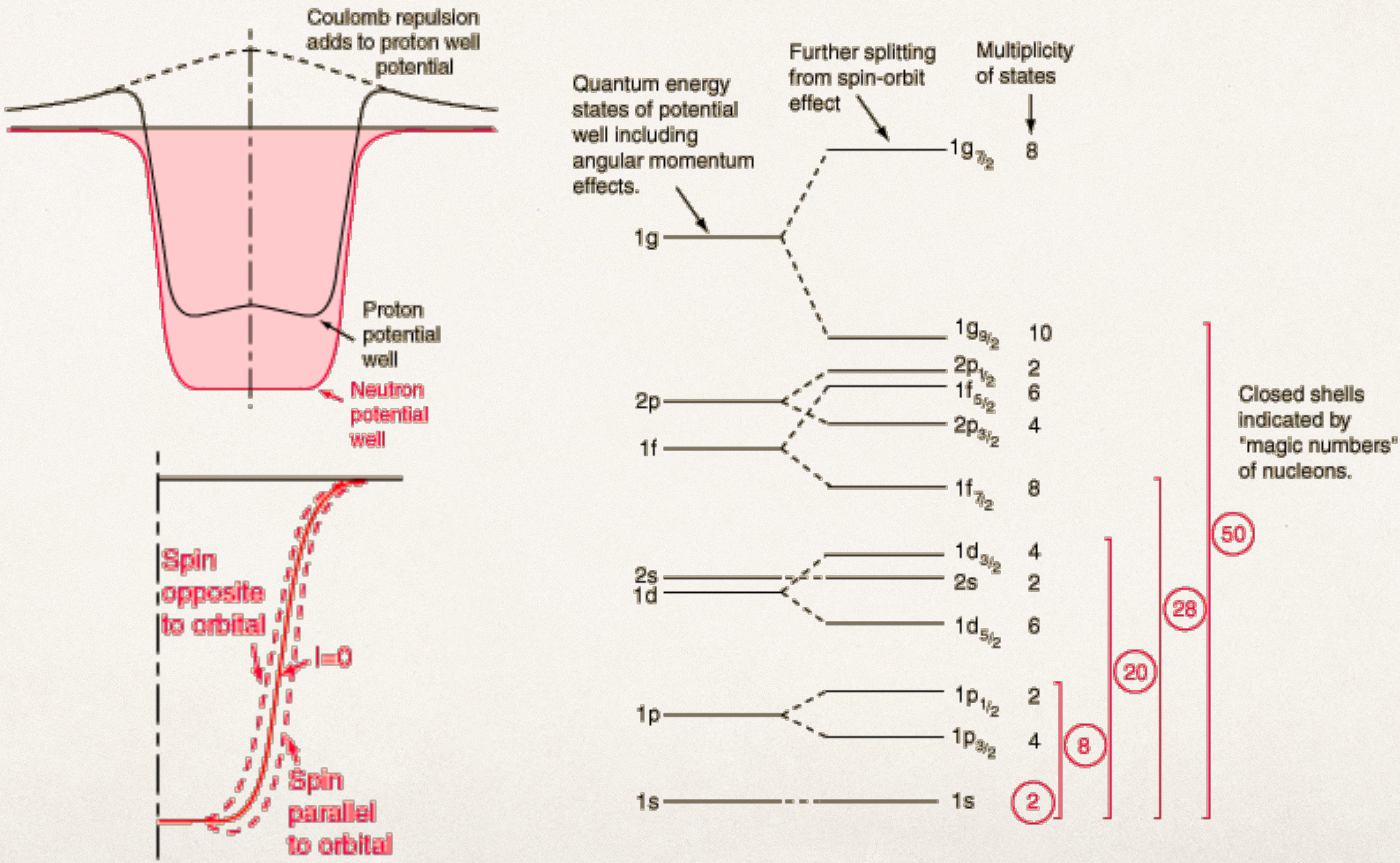
$$\Delta\varepsilon_{nlj=l+1/2} = \frac{D}{2} l$$

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



Shell Model

The spin-orbit coupling



Shell Model

Advantages

- Satisfying results for magic nuclei: ground state and low lying excited states
- The ability to describe simultaneously all spectroscopic properties of low-lying states with very different structure within a nucleus.
- Effective interactions connected with both two- and three-nucleon bare forces.
- A description of collective properties in the laboratory frame.

Problems:

- The effective interactions strongly **depend on the choice of the configuration space** (active shells and the truncation scheme): there is **no universal effective SM interaction** that can be used for all nuclei!
- The effective interactions **are adjusted** starting from microscopic two-body forces. 3-nucleon effects?
- A **large number of two-body matrix elements** (10^2 – 10^3?) **have to be adjusted to the data** => the effective interactions cannot be unique! **Extrapolations to nuclei far from stability not reliable**!
- **Nuclei very far from stability will require calculations with matrix dimension > 10^{10}** => far beyond the limits of current Shell Model variants!

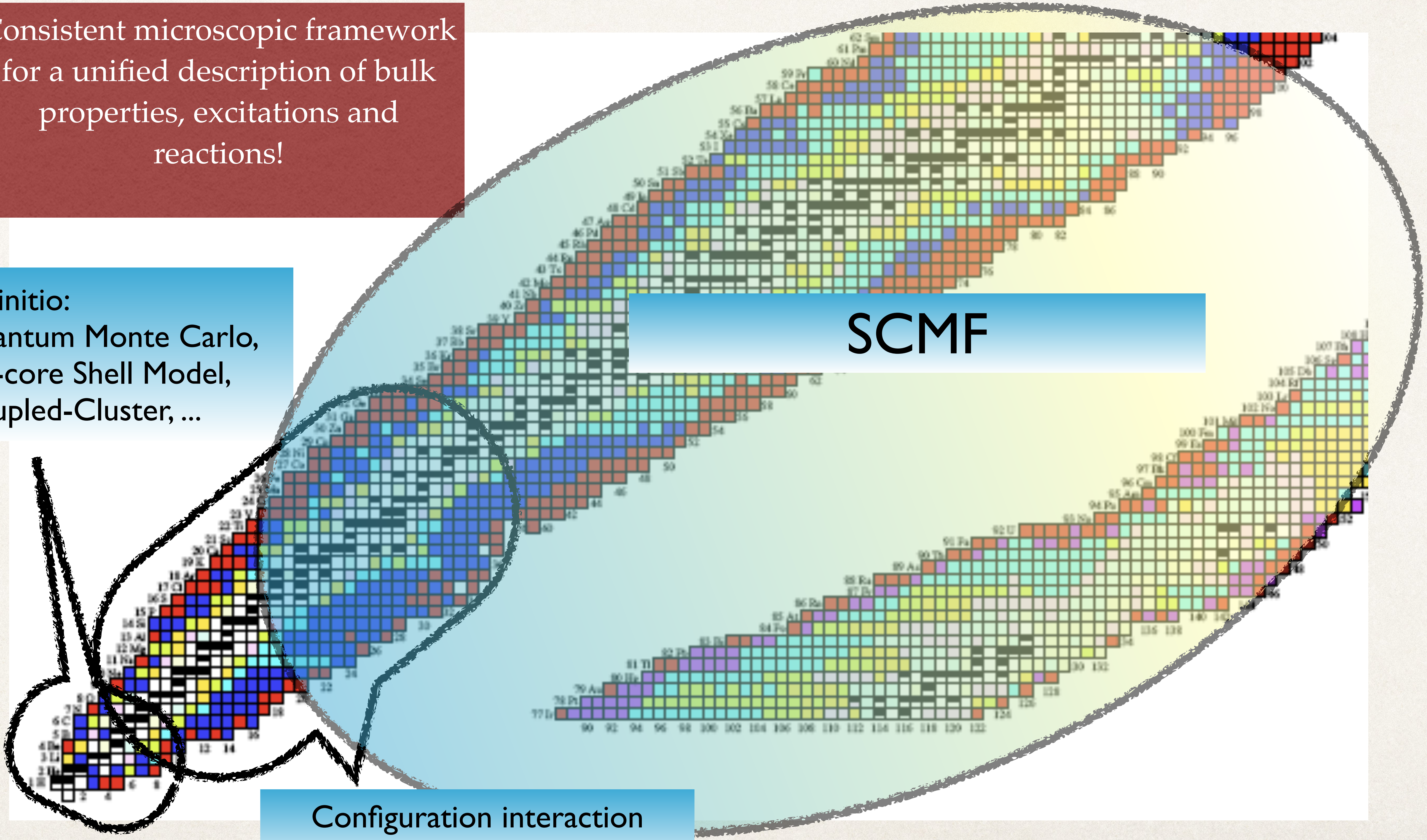
Improved shell model (currently used):

The particles are not independent: due to their interactions with the other particles they do not occupy a given orbital but a sum of configurations having a different probability.

-> definition of a valence space where the particles are active

Self-Consistent Mean-Field Approximations

Consistent microscopic framework for a unified description of bulk properties, excitations and reactions!



Ab initio:
Quantum Monte Carlo,
No-core Shell Model,
Coupled-Cluster, ...

SCMF

Configuration interaction
(Interacting Shell-Model)

Self-Consistent Mean-Field Approximations

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

Self-Consistent Mean-Field Approximations

The General Variational Principle

Any state which makes the functional $E[\Psi]$ stationary,

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

when $|\Psi>$ is allowed to vary over the whole Hilbert space is an eigenstate of the hamiltonian H with the eigenvalue E.

$$H|\Psi>= E|\Psi>$$

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**

Any trial wave function will have an energy expectation value that is greater than or equal to the true ground-state wave function corresponding to the given Hamiltonian

Self-Consistent Mean-Field Approximations

The Hartree-Fock Approximation

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

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

…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:

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

Self-Consistent Mean-Field Approximations

The Hartree-Fock Approximation

...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 Hartree-Fock hamiltonian: $h_{ij} \equiv< i|h|j >= \dfrac{\partial E[\rho]}{\partial \rho_{ji}}$

...from the variational equation: $\delta\{E[\rho] - \mathrm{tr}\Lambda(\rho^2 - \rho)\} = 0$

Hartree-Fock equation $\boxed{[h, \rho] \equiv h\rho - \rho h = 0}$

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

Self-Consistent Mean-Field Approximations

The Hartree-Fock Approximation

$$h = h[\rho]$$ ⇒ the HF equation is non-linear!

Iterative solution:

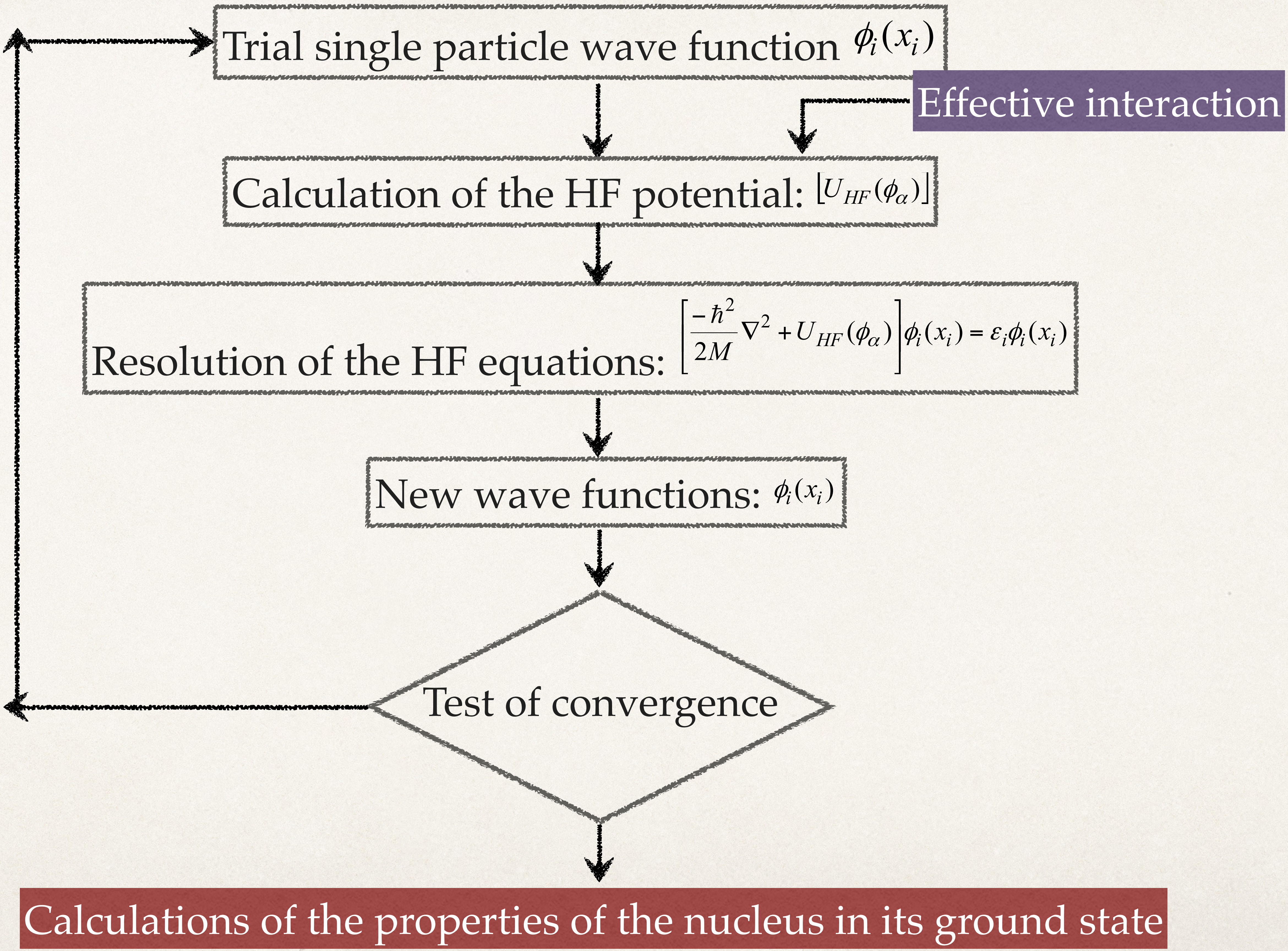
1) initial guess for the HF orbitals $|\lambda_\nu> \quad \Longrightarrow \quad \rho = \sum_{\nu=1}^{A} |\lambda_\nu><\lambda_\nu|$

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.**

Self-Consistent Mean-Field Approximations



Self-Consistent Mean-Field Approximations

The Hartree-Fock-Bogoliubov Approximation

The HF approximation is strictly valid only for **doubly magic nuclei**. All the others have partially occupied shells (open-shell) with a high density of almost degenerate states that are mixed by the residual two-body interaction: **nuclear pairing scheme**.

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.

Self-Consistent Mean-Field Approximations

The Hartree-Fock-Bogoliubov Approximation

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

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

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

The paring 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** if and only if the associated **generalised density matrix**:

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

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

Self-Consistent Mean-Field Approximations

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

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

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

Self-Consistent Mean-Field Approximations

$\mathcal{H} = \mathcal{H}[\mathcal{R}]$ → 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.

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

Self-Consistent Mean-Field Approximations

- 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.

In order to find a constrained minimum of energy one has to find a minimum of the Routhian

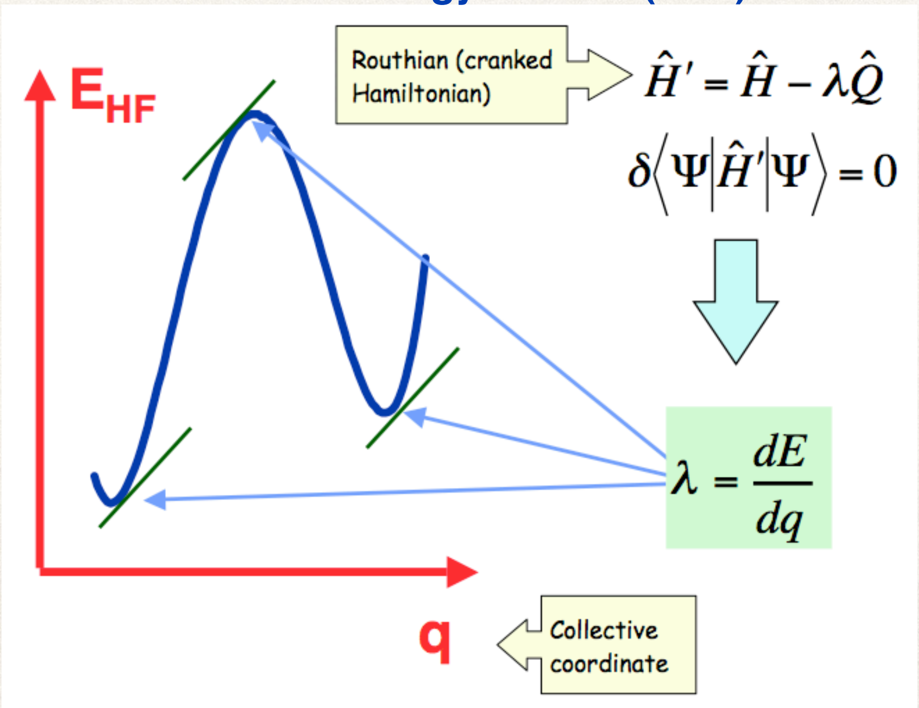
$$E = \langle \hat{H} \rangle - \sum_{q=p,n} \lambda_q \langle \hat{N}_q \rangle - \sum_{\alpha} \lambda_\alpha \langle \hat{Q}_\alpha \rangle$$

with a constraint on the expectation value:

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

mass multipole operator

Potential energy surface (PES)



Self-Consistent Mean-Field Approximations

Choices for the effective interaction

Gogny interaction

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

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

Exchange operators:

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

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

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

Self-Consistent Mean-Field Approximations

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:

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

The Skyrme energy functional:

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

Contains only time-even dens.

Dependence on time-odd currents

Density-dependent coefficients

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

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

does not contribute for even-even nuclei!

Self-Consistent Mean-Field Approximations

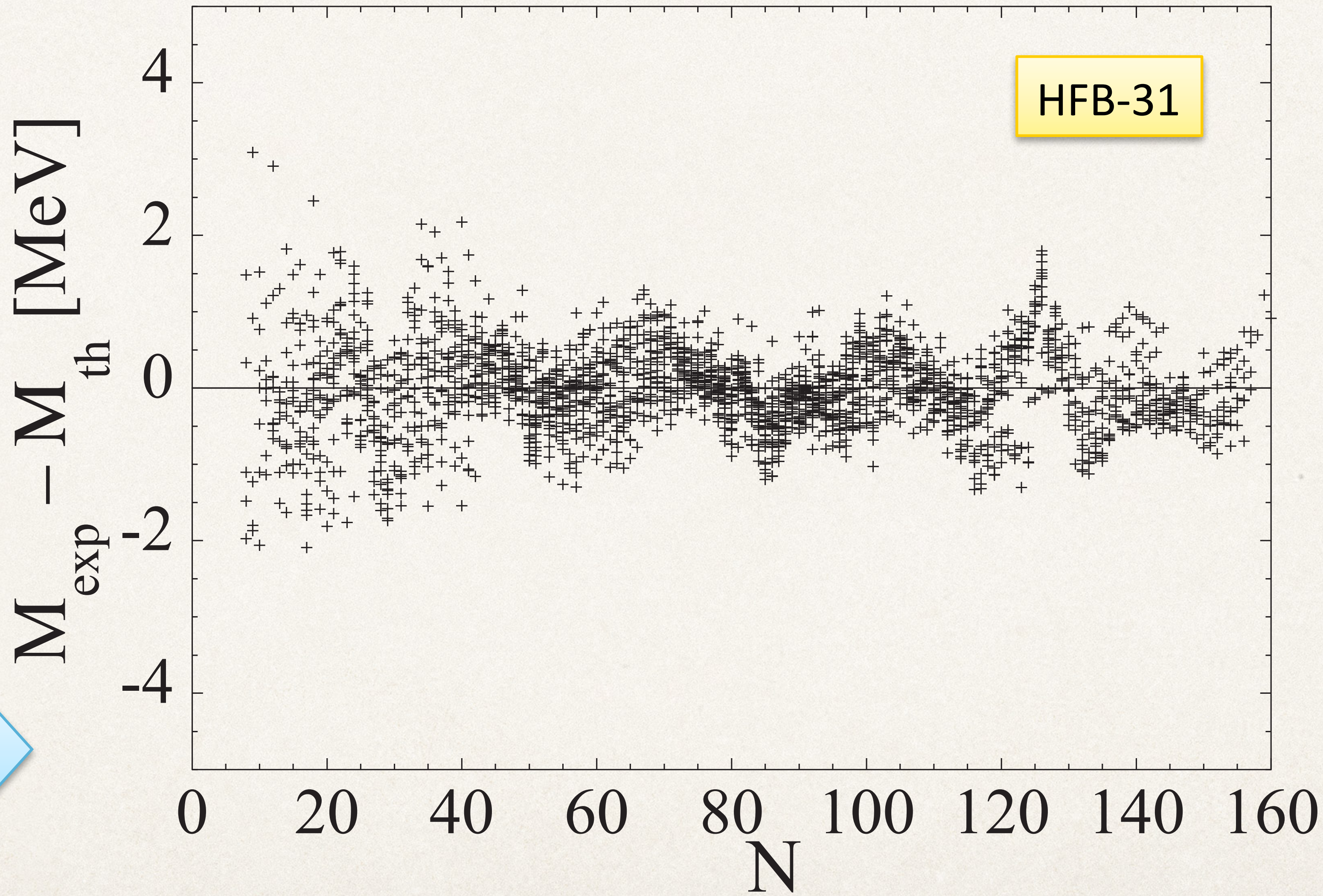
Applications: ground-state properties

1. Binding Energies

Microscopic Skyrme-Hartree-Fock-Bogoliubov mass tables:

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

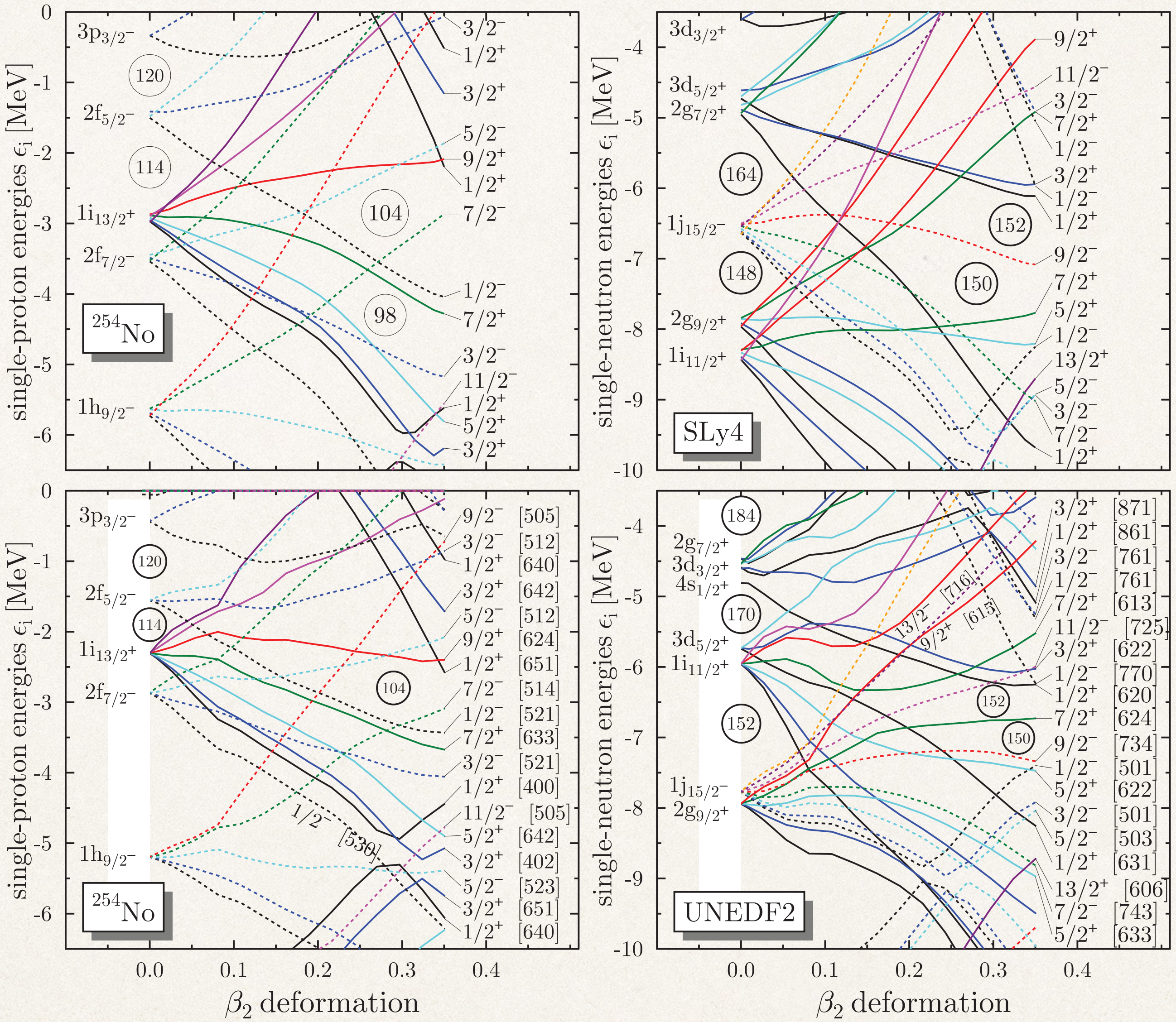
Root Mean Square Deviation: 0.56 MeV with respect to the 2353 measured masses of nuclei with N and Z ≥ 8.



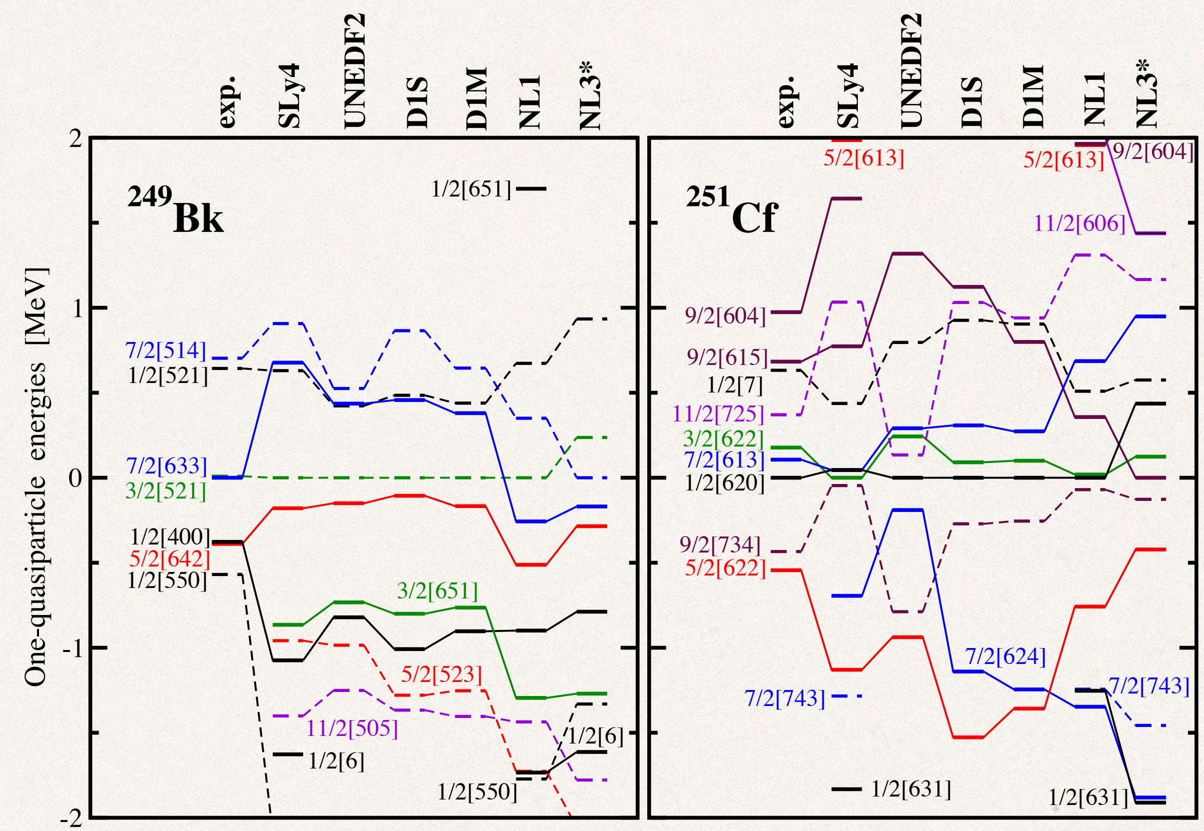
PHYSICAL REVIEW C **93**, 034337 (2016)

Self-Consistent Mean-Field Approximations

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).

Self-Consistent Mean-Field Approximations

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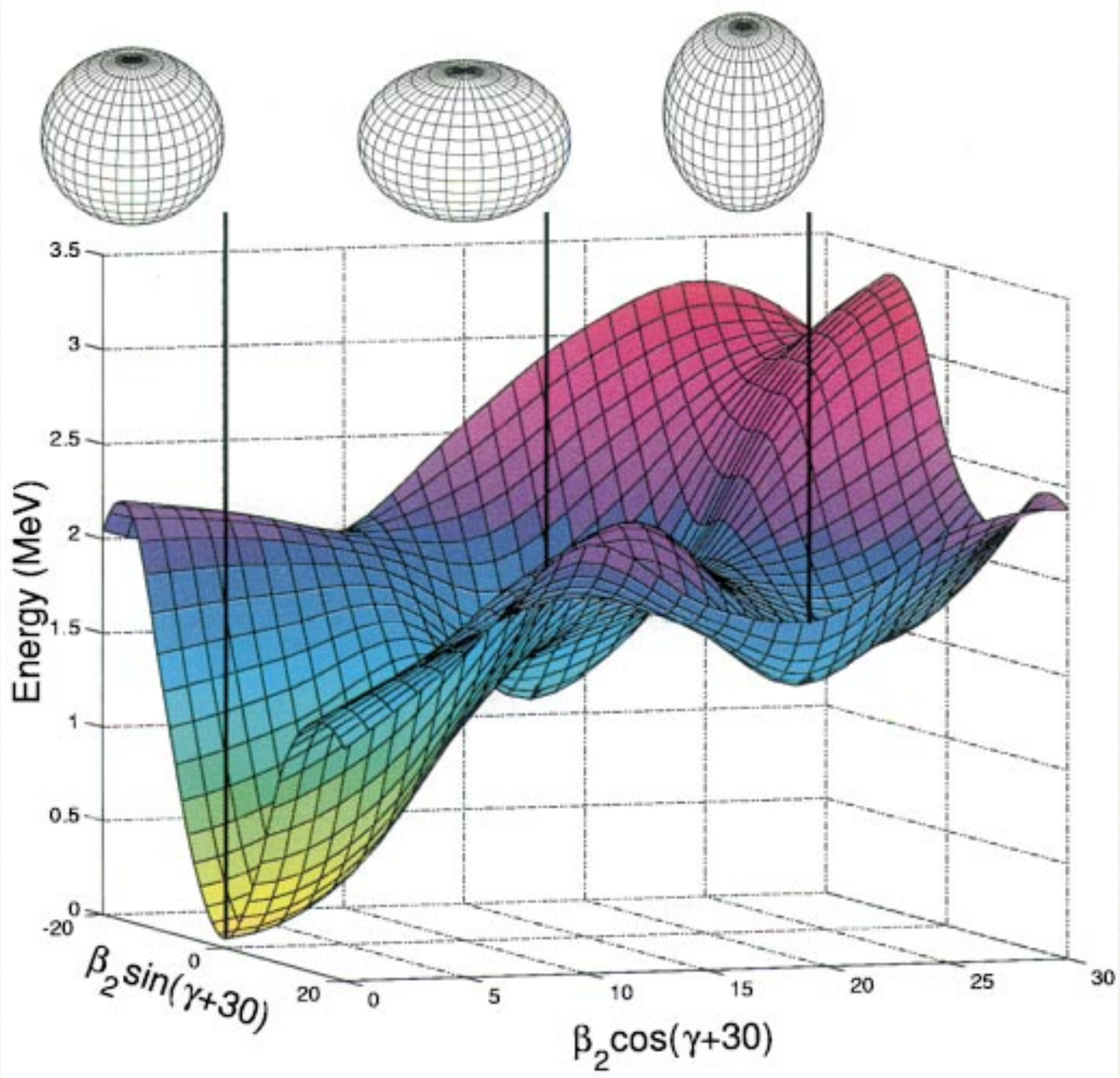
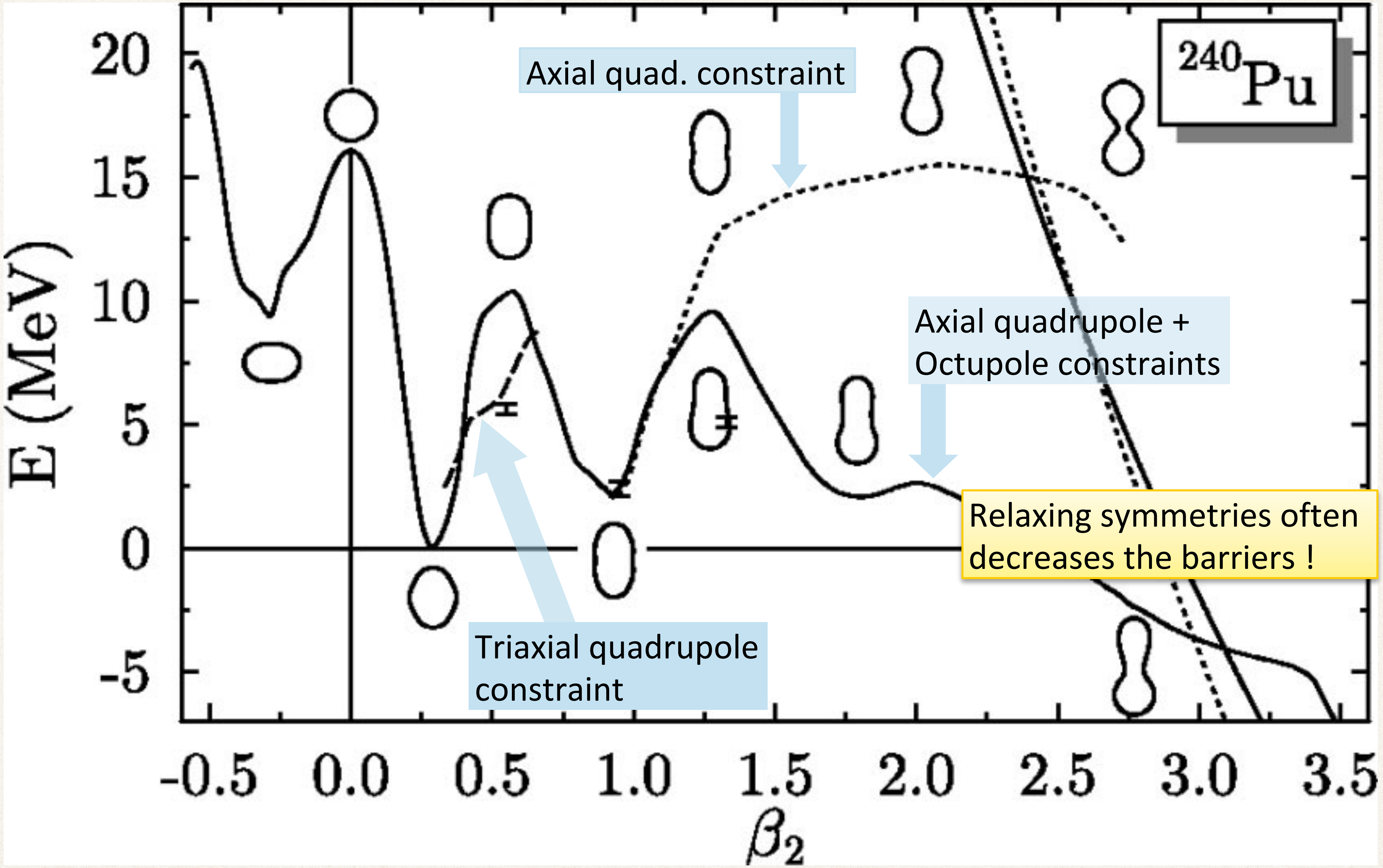


Calculated potential energy surface of ^{186}Pb. Spherical, oblate and prolate minima are indicated by thick vertical black lines. Calculations are performed on a cartesian mesh. The β_2 parameter expresses the elongation of the nucleus along the symmetry axis, while the γ parameter relates to the degree of triaxiality in the deformation. The γ parameter is defined such that $\gamma=0$ corresponds to a prolate shape and $\gamma=60$ to an oblate shape.

Self-Consistent Mean-Field Approximations

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.

Bender, Heenen, and Reinhard

Rev. Mod. Phys., Vol. 75

Self-Consistent Mean-Field Approximations

Relativistic Hartree-Bogoliubov Theory

The Dirac equation provides an economical and natural description of bulk nuclear properties and the nucleon single-particle spectrum, with **the correct spin-orbit force arising automatically**.

Kinematical relativistic effects are small in nuclei, but the different behavior of the large Lorentz scalar and vector potentials leads to large dynamical relativistic interaction effects in the nuclear matter energy density (**natural saturation mechanism!**)

A covariant formulation in terms of hadron degrees of freedom **incorporates the basic symmetries of QCD** (Lorentz invariance, parity conservation, isospin symmetry, spontaneously broken chiral symmetry).

The self-consistent relativistic mean-field framework presents a particular **realization of the relativistic Kohn-Sham density functional theory**.

Self-Consistent Mean-Field Approximations

Relativistic Hartree-Bogoliubov Theory

- Analysis of **open-shell nuclei** (correlations in the self-consistent RMF).

- Unified treatment of the nuclear MF (particle-hole (ph)) and pairing (particle-particle (pp)) correlations. Crucial for an accurate description of ground states and properties of excited states in weakly bound nuclei.

$$E_{RMF}[\hat{\rho}, \hat{k}, \phi_m] = E_{RMF}[\hat{\rho}, \phi_m] + E_{pair}\hat{k}], E_{pair}[\hat{k}] = \frac{1}{4} Tr[\hat{k}^* V^{pp} \hat{k}]$$

- Separable pairing interaction $< k|V^{^1S_0}|k' >= -Gp(k)p(k')$
- It reduces the number of "unknowns" to just the density and the pairing tensor. Once these 2 objects are known (by solving the HFB equation), you can in principle calculate any observable.

Self-Consistent Mean-Field Approximations

Relativistic effective lagrangian density

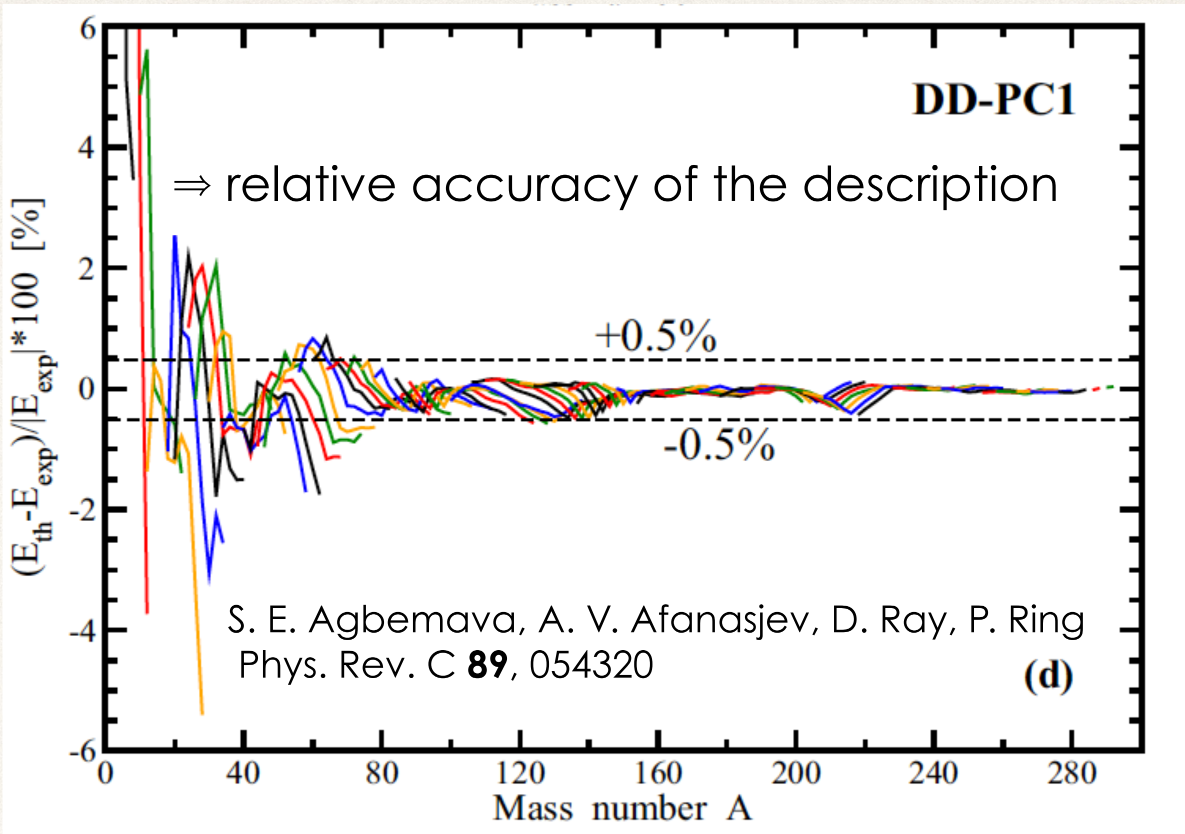
- In conventional QHD a nucleus is described as a system of Dirac nucleons coupled to exchange mesons through an effective Lagrangian. In MF approximation the meson-field operators are replaced by their ***expectation values in the nuclear ground state***.
- In analogy to the meson-exchange RMF phenomenology, an effective Lagrangian that includes the **isoscalar-scalar, isoscalar vector and isovector-vector four-fermion interactions**, reads

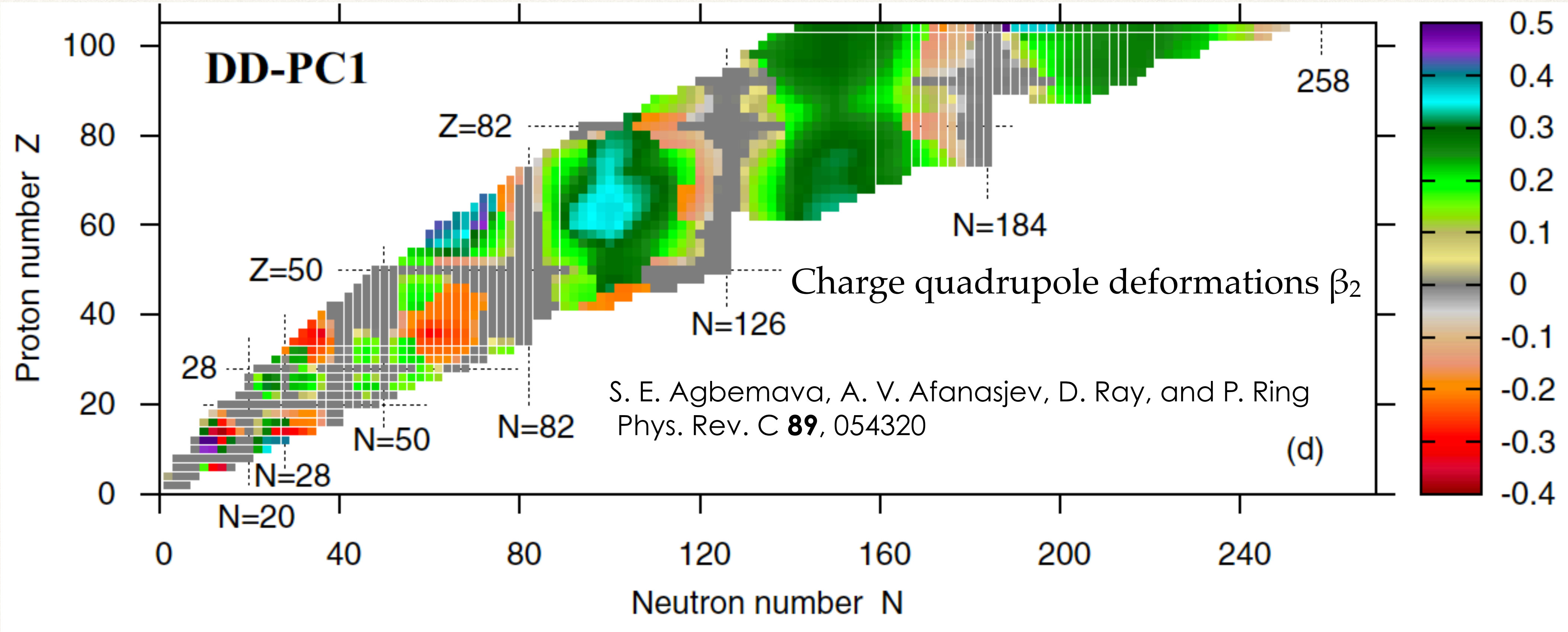
$$\begin{aligned}\mathcal{L} \;=\;& \bar{\psi}(i\gamma\partial - m)\psi - \frac{1}{2}\alpha_S(\hat{\rho})(\bar{\psi}\psi)(\bar{\psi}\psi) - \frac{1}{2}\alpha_V(\hat{\rho})(\bar{\psi}\gamma^\mu\psi)(\bar{\psi}\gamma_\mu\psi)\\ & - \frac{1}{2}\alpha_{TV}(\hat{\rho})(\bar{\psi}\vec{\tau}\gamma^\mu\psi)(\bar{\psi}\vec{\tau}\gamma_\mu\psi) - \frac{1}{2}\delta_S(\partial_\nu\bar{\psi}\psi)(\partial^\nu\bar{\psi}\psi) - e\bar{\psi}\gamma A\frac{(1-\tau_3)}{2}\psi\end{aligned}$$

- Free nucleon Lagrangian, point-coupling interaction terms and coupling of the protons to the electromagnetic field. Derivative terms accounts for the leading effects of finite-range interactions.

Self-Consistent Mean-Field Approximations

The HFB equation gives the ground-state energy of a nucleus, hence its mass; You can calculate, e.g., the r.m.s. radius of the system, or its (intrinsic) quadrupole moment.





Self-Consistent Mean-Field Approximations

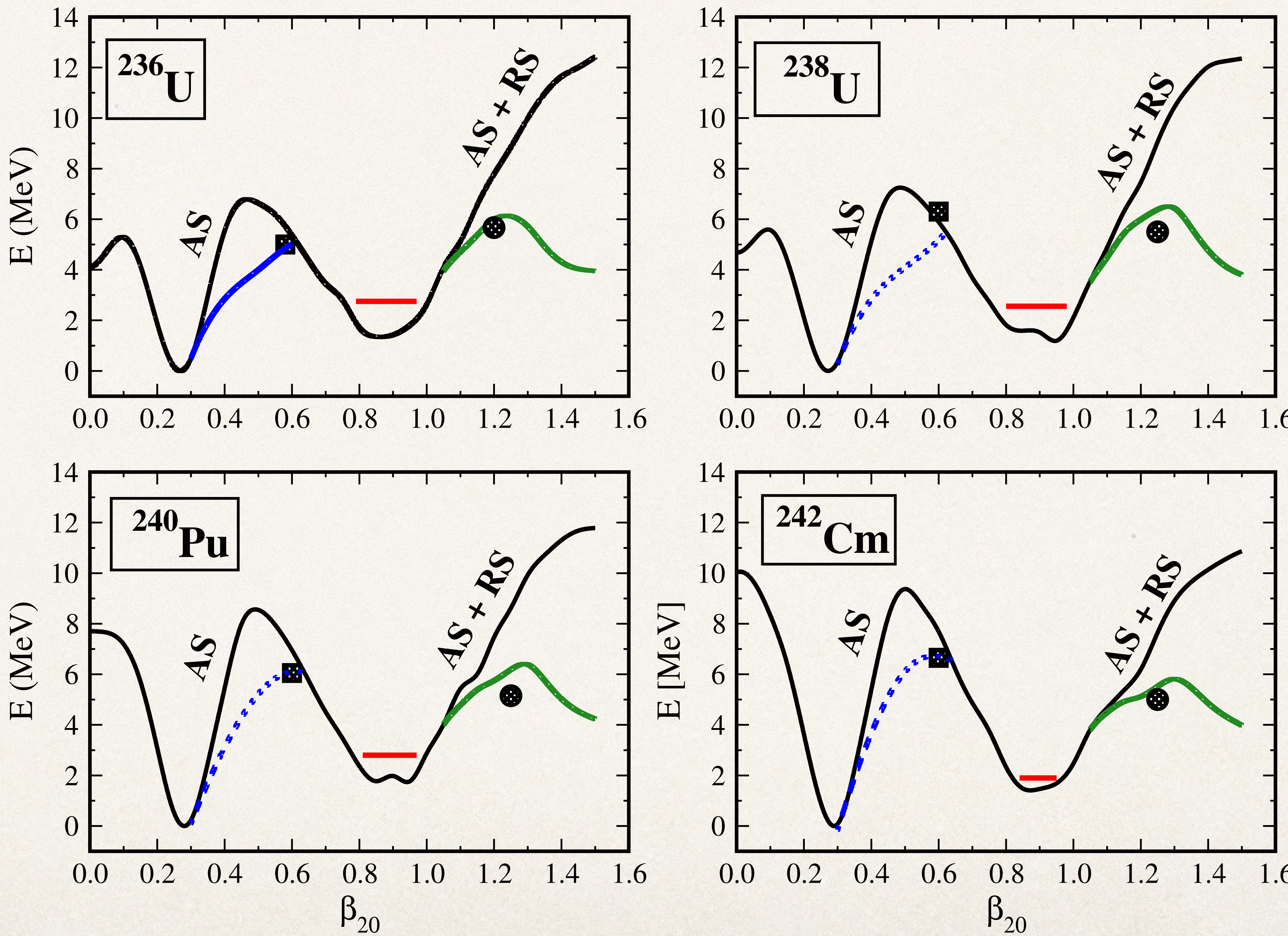
Test: "double-humped" fission barriers of actinides

Potential energy surfaces of actinides

Black: Axial symmetric calculations

Blue: Triaxial calculations. Decrease of the first barrier

Green: Axial symmetric calculations including reflection asymmetry (octupole). Decrease of the second barrier.



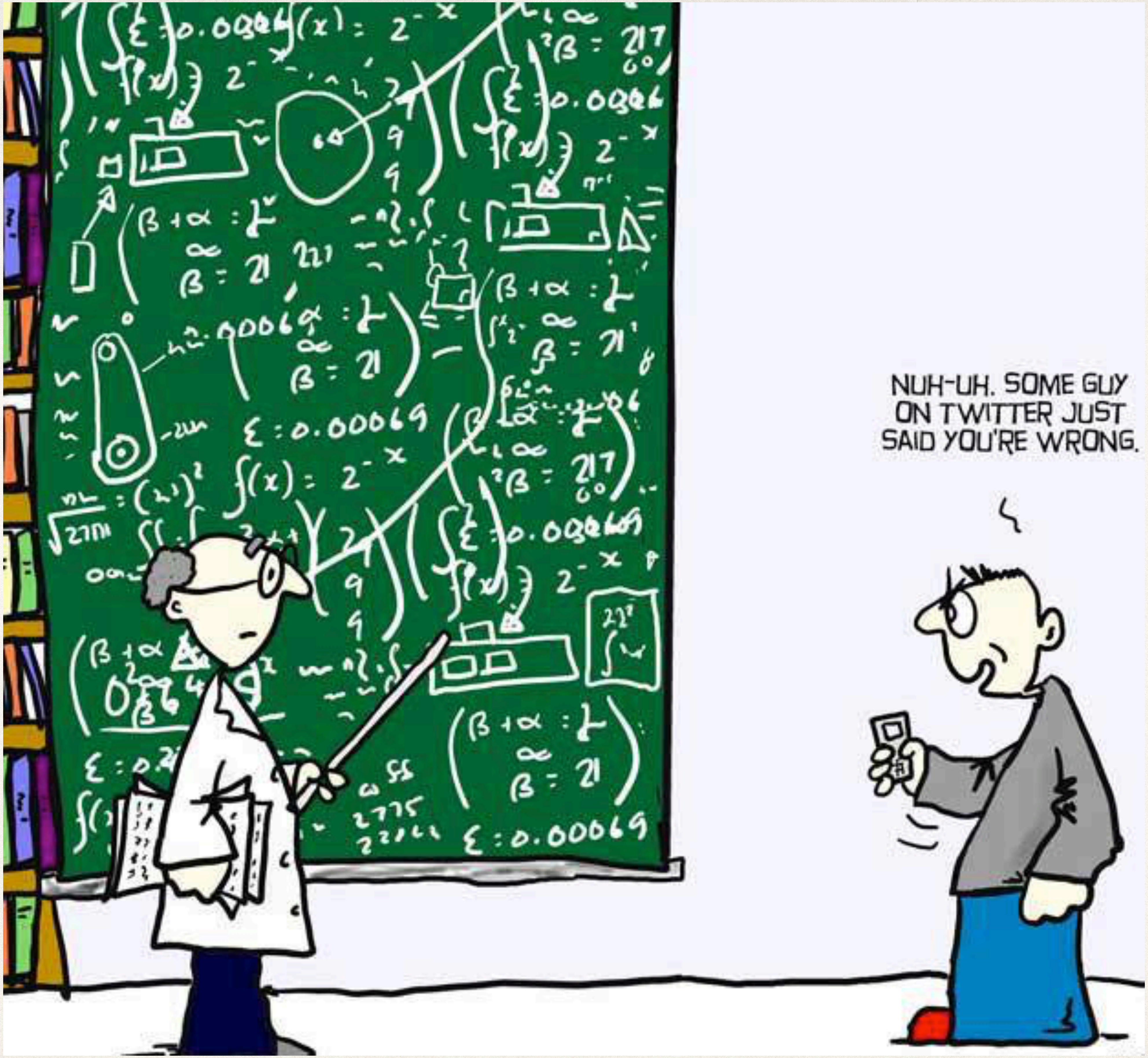
Self-Consistent Mean-Field Approximations

VIRTUES:

- an intuitive interpretation of mean-field results in terms of **intrinsic shapes** and shells with **single-particle states.**
- the **full model space** of occupied states can be used; no distinction between core and valence particles, and **no need for effective charges.**
- the use of **universal effective interactions**; universal in the sense that they can be applied to all nuclei throughout the periodic chart.

PROBLEMS:

- an independent particle-description establishes a **body-fixed intrinsic frame** of the nucleus. The relation of mean-field results to spectroscopic observables in the laboratory frame depends on additional assumptions.
- by construction, **a mean-field state breaks** necessarily several **symmetries** of the nuclear Hamiltonian (translational, rotational).
- the mean-field approach becomes **ill-defined** when the binding energy changes slowly with a collective degree of freedom (transitional nuclei).



Thank you for your attention!