Electromagnetic properties of nuclei: from few- to many-body systems

Lecture 9

Many-body methods

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November 23rd, 2017

Lecture series for SFB 1245
TU Darmstadt

Many-body theory

In the few-body systems one can calculate with high accuracy

↓

Precision era

↓

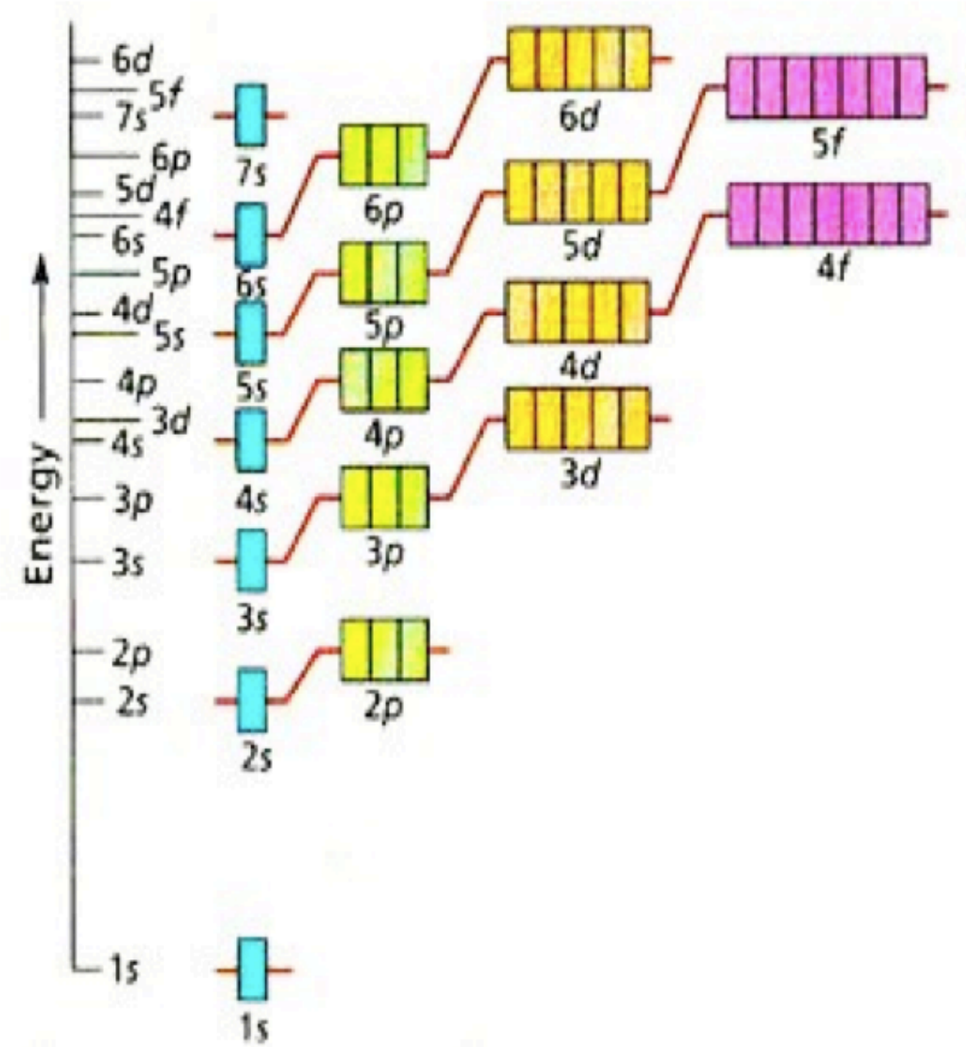
However, most of the nuclei are actually many-body systems

↓

Historical approach:
shell model in nuclei ⇒ ab- initio approaches

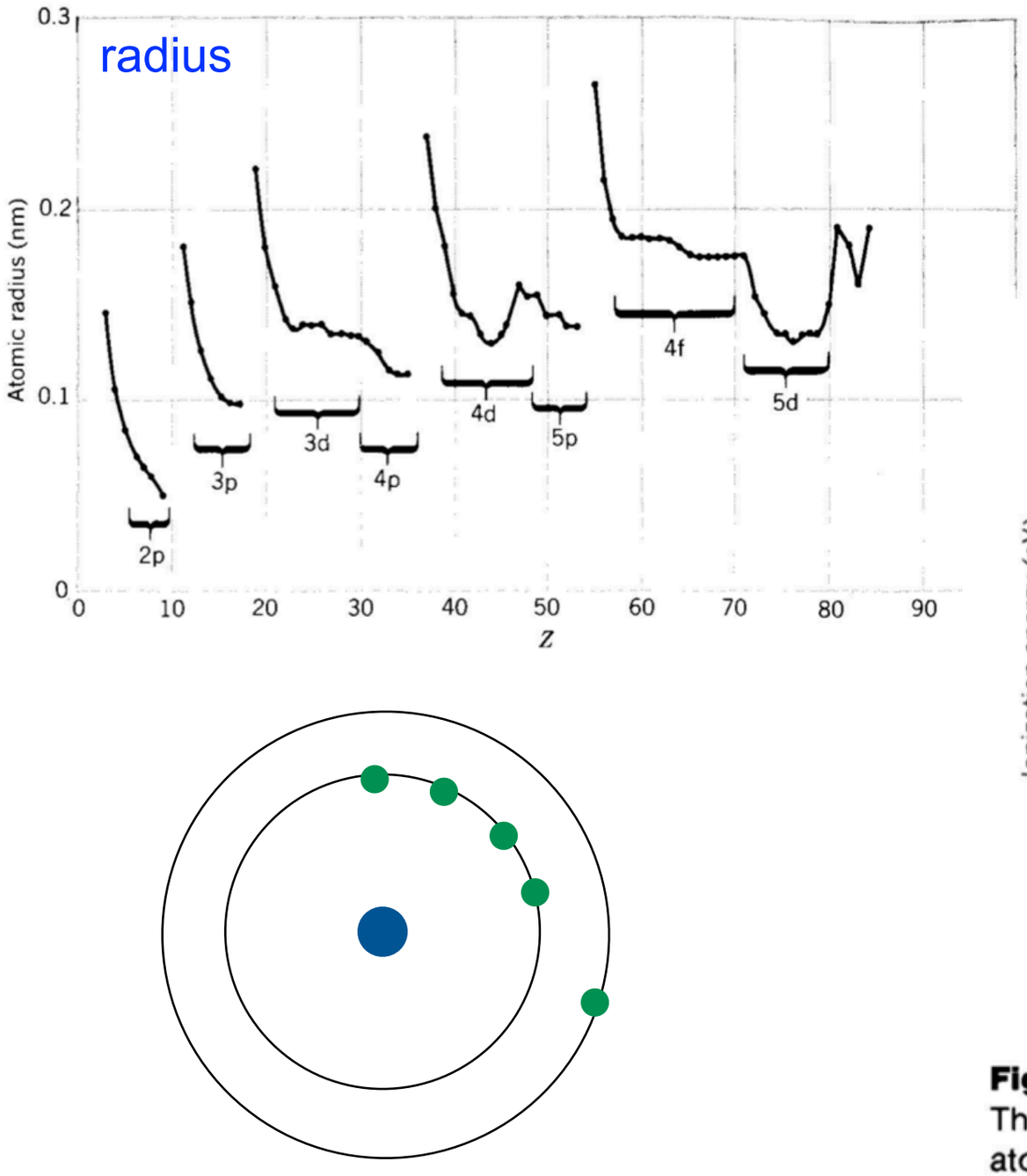
Shell Model in Atoms

Electrons in atoms occupy well defined shells of discrete, well separated energies.



Evidence of electron shells in atoms: sudden jumps in atomic properties as the shell gets filled up, such as atomic radius, ionization energy etc.

Shell Model in Atoms



From Krane
"*Introductory Nuclear Physics*"

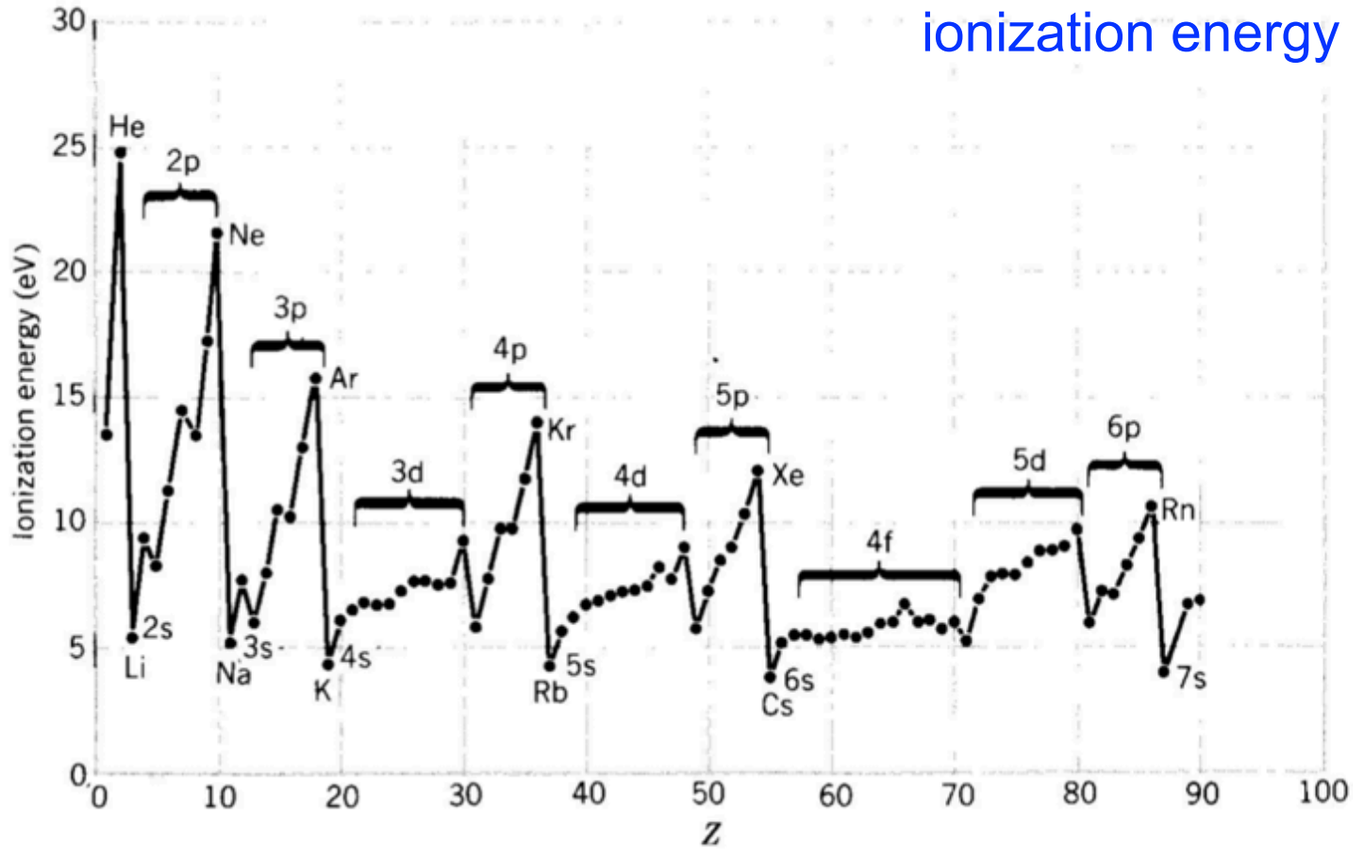


Figure 5.1 Atomic radius (top) and ionization energy (bottom) of the elements. The smooth variations in these properties correspond to the gradual filling of an atomic shell, and the sudden jumps show transitions to the next shell.

Do nucleons inside the nucleus do the same or not?

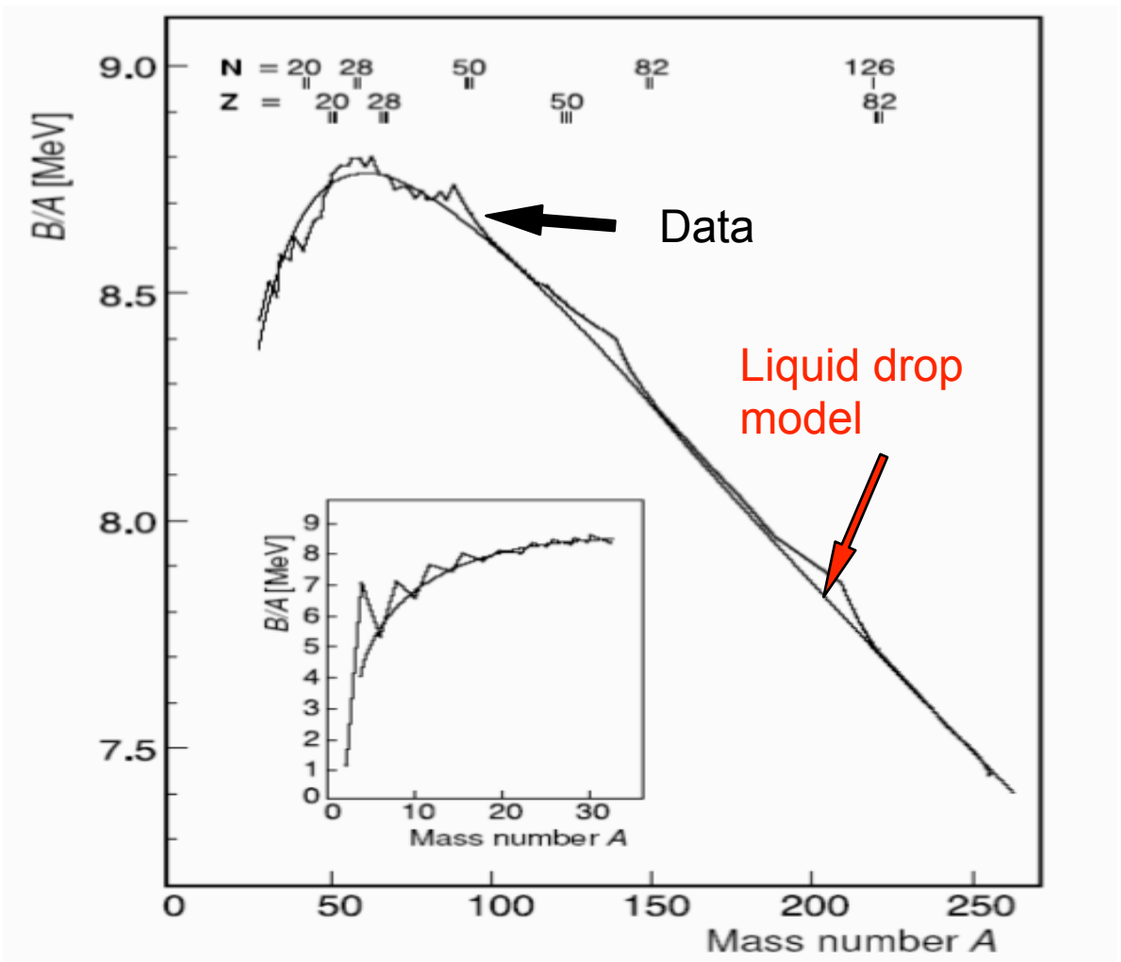
Shell Model in Nuclei?

Shell structure in the nucleus would mean that individual nucleons inhabit orbitals of well defined energy. Not evident a priory why this should be the case. Why?

- The liquid drop model (smooth) is very successful in describing the binging energy.

$$BE(A,Z) = a_v A - a_s A^{2/3} - a_c \frac{Z^2}{A^{1/3}} - a_a \frac{(N-Z)^2}{4A} - \frac{\delta}{A^{1/2}}$$

volume term — surface term — Coulomb term — (a)symmetry term — pairing term



Von Weizsaecker suggested the liquid drop model in 1935

Shell Model in Nuclei?

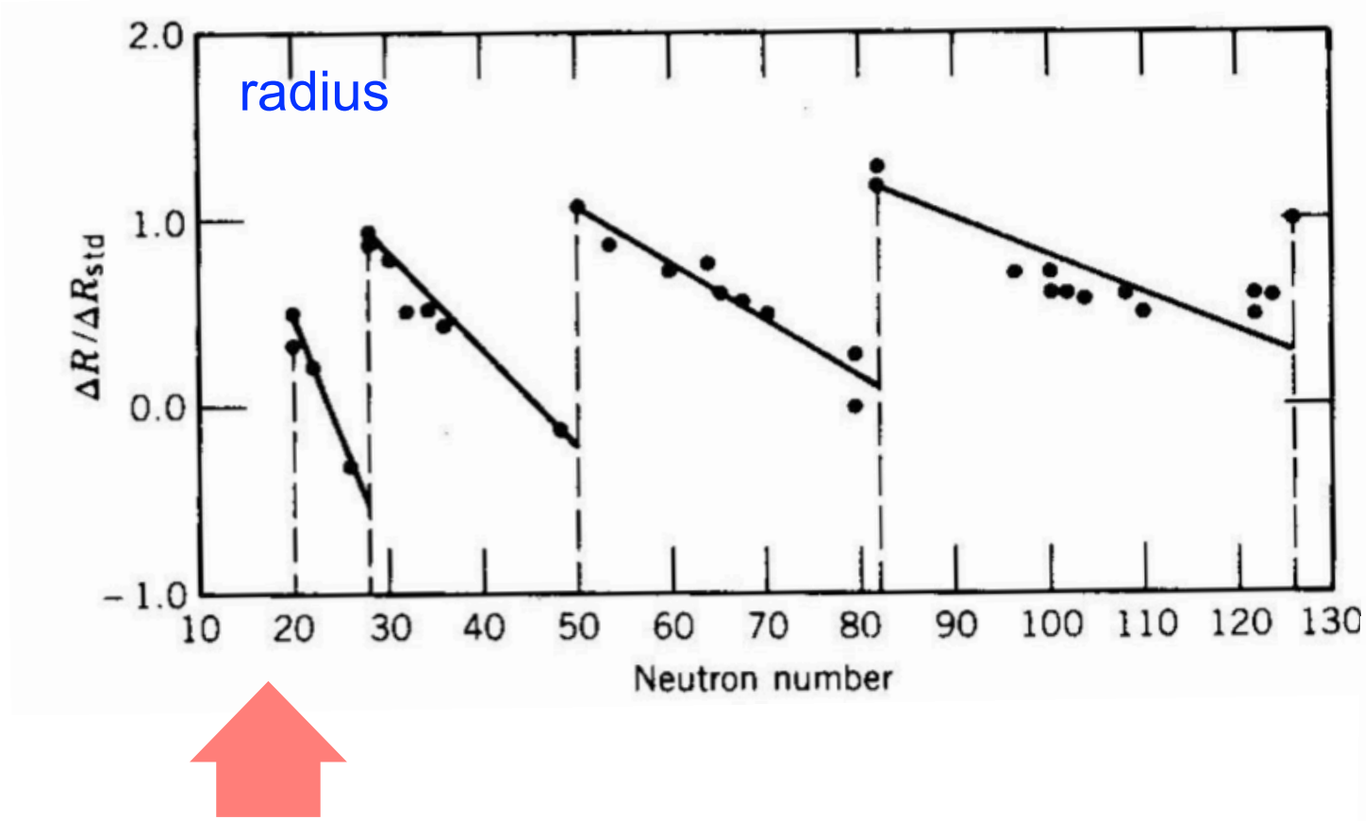
Shell structure in the nucleus would mean that individual nucleons inhabit orbitals of well defined energy. Not evident a priory why this should be the case. Why?

- The liquid drop model (smooth) is very successful in describing the binging energy.
- No obvious centre for nucleons to orbit around.
- No external potential in nuclei, that should be the equivalent of the Coulomb force in atoms.

But the experimental evidence seems to say otherwise!

Shell Model in Nuclei?

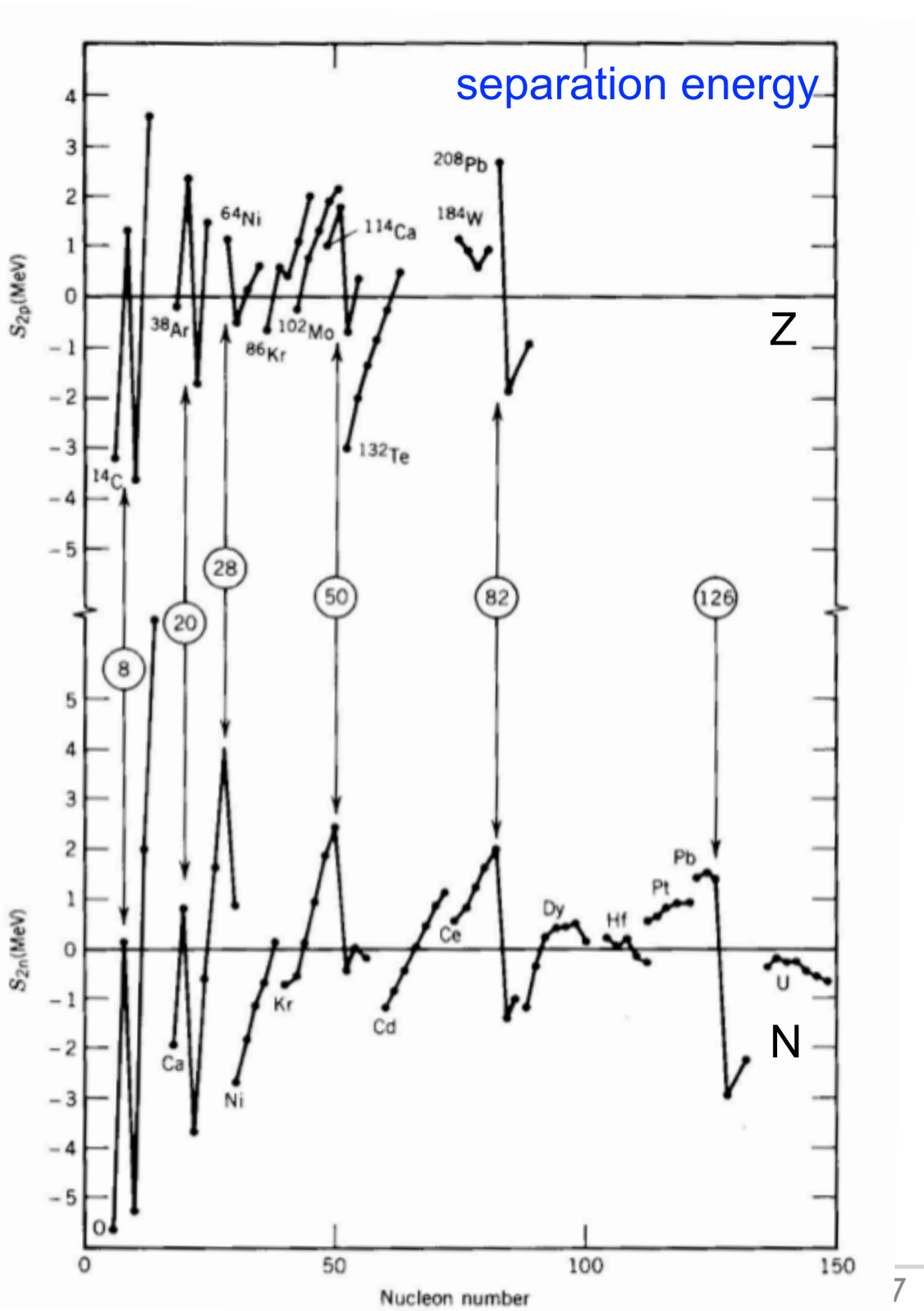
From Krane "*Introductory Nuclear Physics*"



Here the difference in radius has been divided by the standard ΔR_{std} expected from the $A^{1/3}$ dependence

Here difference between experiment and the prediction of the semi-empirical mass formula.

Jumps/Drops at neutron number: 2, 8, 20, 28, 50, 82, 126 ⇒ evidence of shell structure



Shell Model in Nuclei!

Nuclei exhibit a shell structure!
Experimental data indicate local maxima of the binding energy and local minima of radii in proximity of the neutron or proton
"magic numbers" 2, 8, 20,28, 50, 82, 126

only for neutrons

We are physicists, so we do not believe in magic!
Where do these magic numbers come from?
They have to be related to the way nucleons interact with each other.

The theory that explains this is called non interacting shell model or nuclear shell model. It is a simplified theory that accounts though for measured properties and can predict others. It is based on the assumption that the motion of the single nucleon is governed by a potential caused by all other nucleons.

In order to understand where the magic numbers come from and to explain the theory of the nuclear shell model, we need to open a parenthesis on:
- how to represent a many-body wave function
- what is an independent particle model

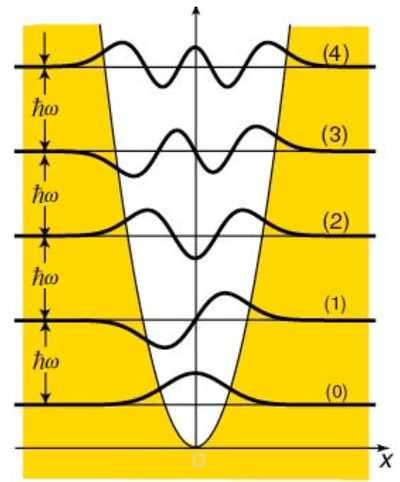
Many-body wave functions

- In order to construct a many-body wave function, one first has to start from a single particle (nucleon) wave function, which is separated in space/spin/isospin components

$$|\varphi_k\rangle = \left[|\varphi_k^{space}\rangle \otimes |\varphi_k^{spin}\rangle\right] \otimes |\varphi_k^{isospin}\rangle$$

This could be the solution of the single nucleon Schrödinger equation

$$h|\varphi_k\rangle = \varepsilon_k|\varphi_k\rangle \quad (\star)$$



$\{|\varphi_k\rangle\}$ Set of eigenstates of a single nucleon.
Different depending on what Hamiltonian h one uses.
Can assume for now that this is something we can solve analytically or also numerically. E.g., harmonic oscillator

- One can then use these single particle states to construct a many-body wave function. The many-body space is in general the product of many single particle Hilbert spaces

$$H^A = h_1 \otimes h_2 \otimes \cdots \otimes h_A$$

Each single particle Hilbert space is spanned by $\{|\varphi_k\rangle\}$ as solution of ($\star$)

Many-body wave functions

- We can construct a many-body wave function as the product of single particle wave functions that each live in their own single particle Hilbert space

$$|\psi^A\rangle = |\varphi_{k_1}\rangle \otimes |\varphi_{k_2}\rangle \otimes \cdots \otimes |\varphi_{k_A}\rangle$$

A-body

1-body

The symbol $\otimes$ is for an ordered product, which means if you exchange the index 1 with the index 2 you have a different w.f.

$$|\varphi_{k_1}\rangle \otimes |\varphi_{k_2}\rangle \neq |\varphi_{k_2}\rangle \otimes |\varphi_{k_1}\rangle,$$

The first position refers to the first particle, the second position refers to the second particle and so on...

Since we deal with identical particles which are fermions, we need to work with many-body states that are antisymmetrized with respect to the exchange of two particles

Many-body wave functions

- Antisymmetrized many-body wave function

$$|\psi^A\rangle = \mathcal{A}\left\{|\varphi_{k_1}\rangle \otimes |\varphi_{k_2}\rangle \otimes \cdots \otimes |\varphi_{k_A}\rangle\right\}$$

where the antisymmetrizer operator is

$$\mathcal{A} = \frac{1}{\sqrt{A!}} \sum_{\text{all perm P}} sign(P)\, P_P$$

mass number

where P_P is the permutation operator and

$sign(P) = (-1)^{n_p}$, n_p is the number of pair exchanges

Example A=2

Suppose we neglect spin-isospin now and use a coordinate representation of the single particle states, i.e., $\langle r|\varphi_k\rangle = \varphi_k(r)$

$$\langle r_1| \otimes \langle r_2|\, \mathcal{A}\left\{|\varphi_{k_1}\rangle \otimes |\varphi_{k_2}\rangle\right\} = \langle r_1| \otimes \langle r_2|\, \left(|\varphi_{k_1}\rangle \otimes |\varphi_{k_2}\rangle - |\varphi_{k_2}\rangle \otimes |\varphi_{k_1}\rangle\right)\frac{1}{\sqrt{2}}$$

$$= \frac{1}{\sqrt{2}}\left(\varphi_{k_1}(r_1)\varphi_{k_2}(r_2) - \varphi_{k_2}(r_1)\varphi_{k_1}(r_2)\right) = \frac{1}{\sqrt{2}}\det\begin{pmatrix} \varphi_{k_1}(r_1) & \varphi_{k_1}(r_2) \\ \varphi_{k_2}(r_1) & \varphi_{k_2}(r_2) \end{pmatrix}$$

Imposing antisymmetrization means respecting Pauli principle →
If we put two particle in the same state, when we permute, the antisymmetrizer will give zero.

Many-body wave functions

Case of A particles coordinate space representation

Slater Determinant

$$\langle r_1, r_2, ..., r_A | \psi^A \rangle = \frac{1}{\sqrt{A!}} \det \begin{pmatrix} \varphi_{k_1}(r_1) & \varphi_{k_1}(r_2) & \cdots & \varphi_{k_1}(r_A) \\ \vdots & \vdots & \ddots & \vdots \\ \varphi_{k_A}(r_1) & \varphi_{k_A}(r_2) & \cdots & \varphi_{k_A}(r_A) \end{pmatrix}$$

Determinant of an AxA matrix, with same particle in each column and same single particle state in each row.

It is a (simple) way to construct antisymmetrized states.

Independent particle model

In an independent particle model it is assumed that particles do not interact with each other.
They are only subject to the Pauli principle.

Formally this means that one can write the Hamiltonian for A particles as

$$H = \sum_{i}^{A} h_i, \qquad h_i : \text{single particle Hamiltonian}$$

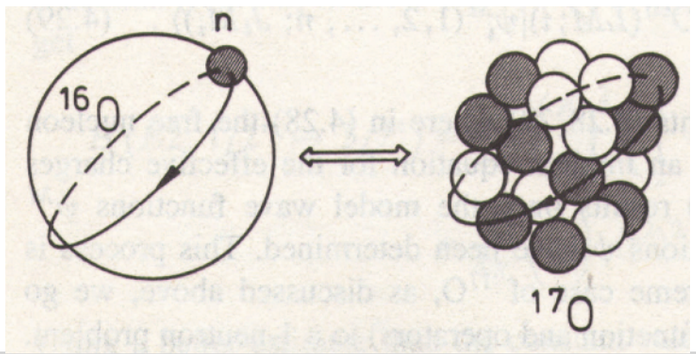
Note: there is nothing that connects particle i with particle j

Examples:

$h_i = \dfrac{p_i^2}{2m}$ only kinetic energy (Fermi gas models with SD of plane waves)

$h_i = \dfrac{p_i^2}{2m} + U_i$ U_i is the potential felt by particle i, which could be an external potential like the Coulomb force in atoms or an average potential given to *i* by the presence of all the other A-1 particles.

Assumption: The interaction of a nucleon with ALL the other particles is approximated by a “mean” potential



Independent particle model

$$H = \sum_i^A h_i$$

The solution of such Hamiltonian is obtained by solving the single particle Schrödinger equation

$$h_i|\varphi_k\rangle = \varepsilon_k|\varphi_k\rangle \implies h_i\varphi_k(r_i) = \varepsilon_k\varphi_k(r_i)$$ in coordinate space representation

Then the A-body states are just Slater Determinants of single particle states $\varphi_k(r_i)$

The solution of $H|\psi^A\rangle = E|\psi^A\rangle$ has the following energy

$$E = \sum_k^A \varepsilon_k \boxed{d_k} \longrightarrow$$ degeneracy: measures the occupancy of a single particle state

To convince yourself, prove that this is true for A=2

Independent particle model

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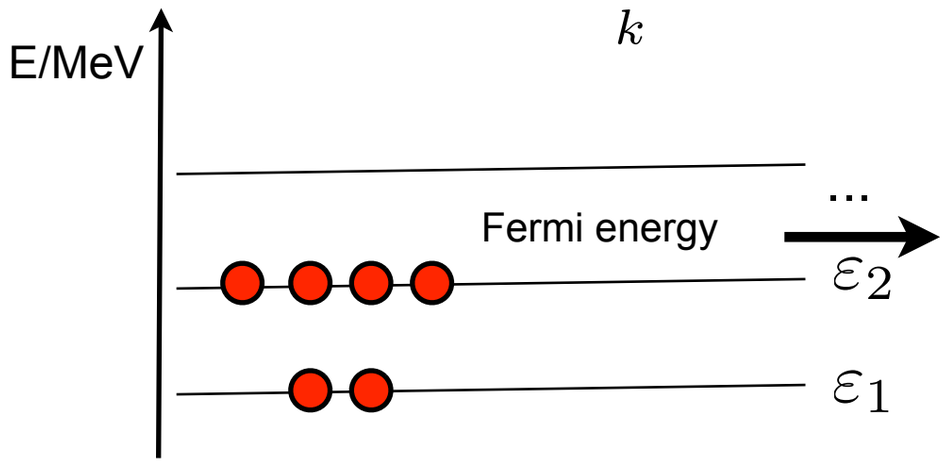
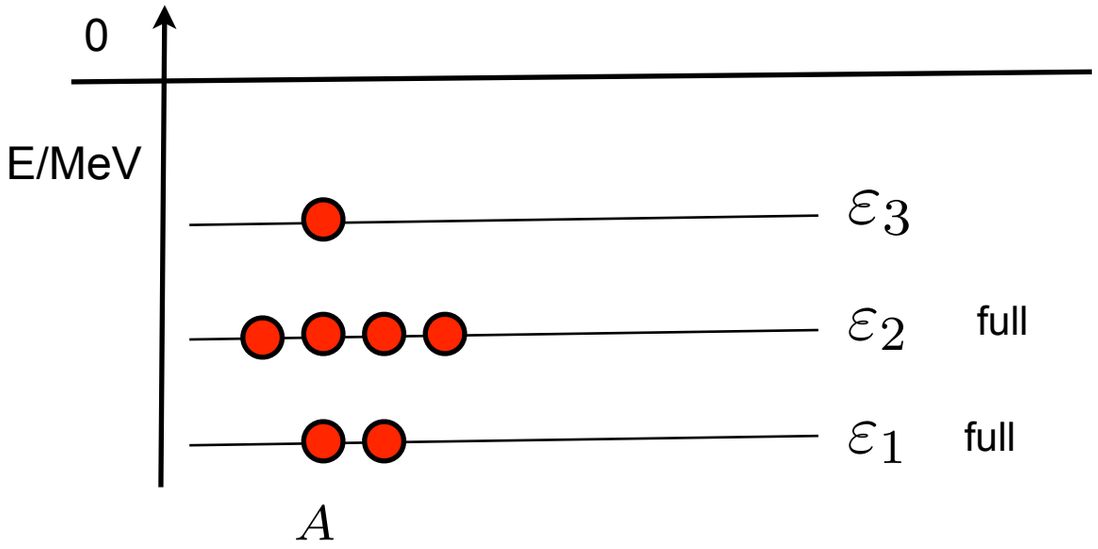


→ energy of the highest occupied state

Fill in the shells respecting Pauli principle (d_k) up to A particles

Magic numbers arise because the single particle spectrum is not smooth, but is made by discrete levels. Particles are grouped into shells with relatively large gaps between them.

Separation Energies

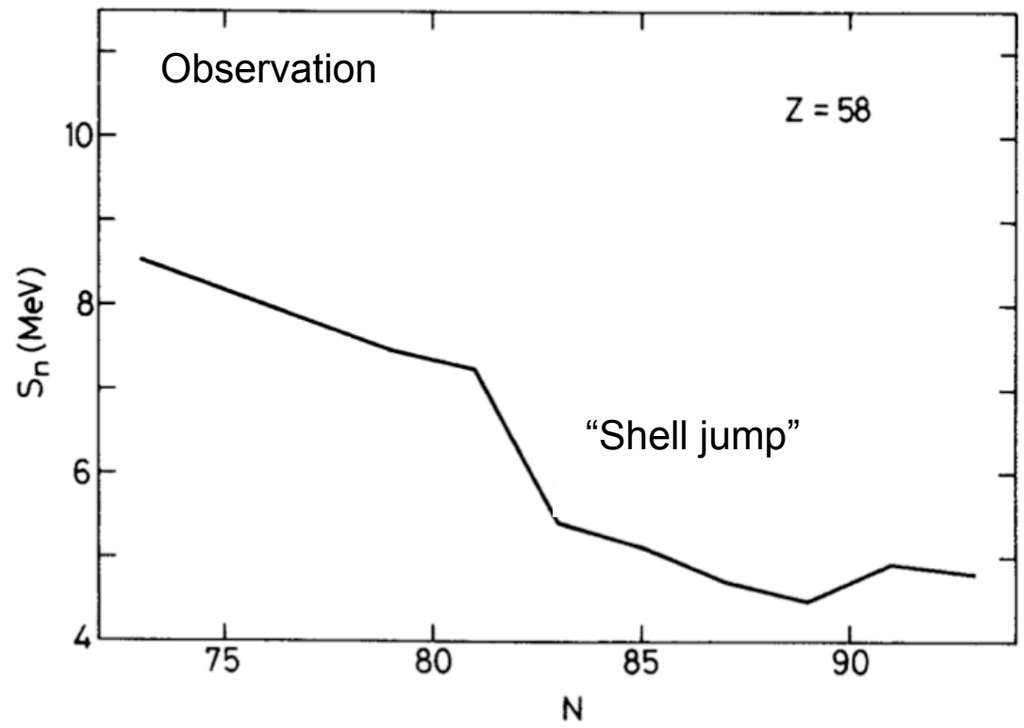


$$E_A = \sum_k \varepsilon_k d_k$$

g.s. energy (neg. number)

Energy of A-body system

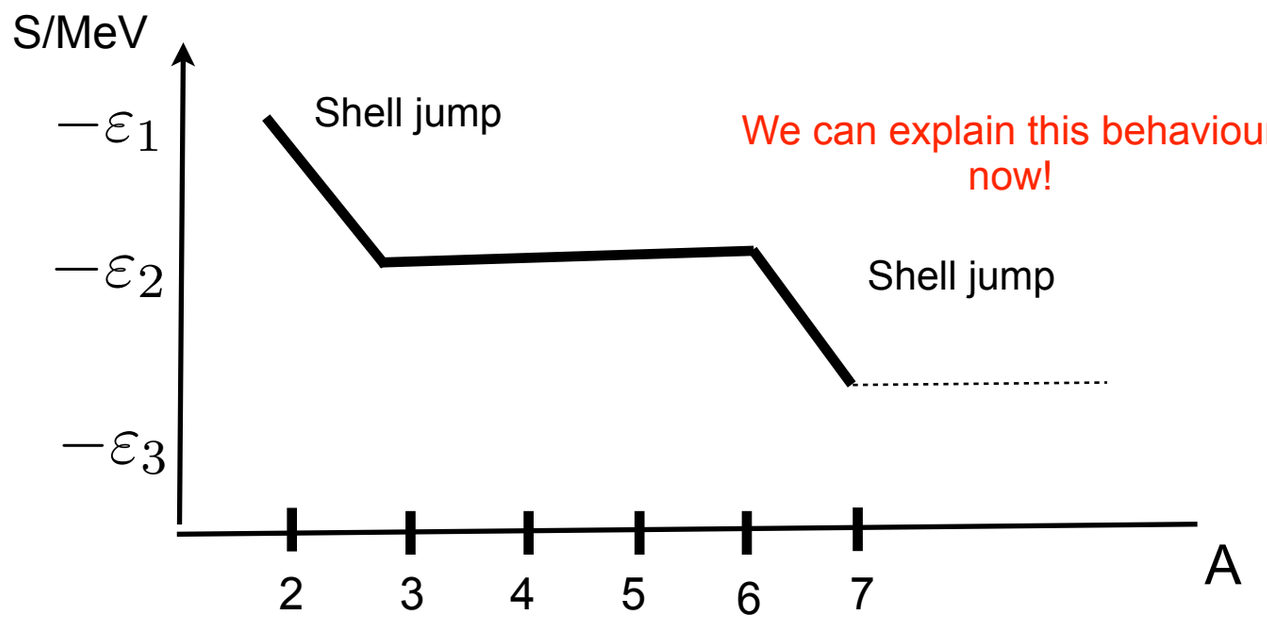
$$E_7 = 2\varepsilon_1 + 4\varepsilon_2 + \varepsilon_3$$
$$E_6 = 2\varepsilon_1 + 4\varepsilon_2$$
$$E_5 = 2\varepsilon_1 + 3\varepsilon_2$$
$$E_4 = 2\varepsilon_1 + 2\varepsilon_2$$
$$E_3 = 2\varepsilon_1 + \varepsilon_2$$
$$E_2 = 2\varepsilon_1$$
$$E_1 = \varepsilon_1$$



Separation energy

$$S^{(A)} = BE(A) - BE(A-1) = E_{A-1} - E_A$$

$$S^{(7)} = -\varepsilon_3$$
$$S^{(6)} = -\varepsilon_2$$
$$S^{(5)} = -\varepsilon_2$$
$$S^{(4)} = -\varepsilon_2$$
$$S^{(3)} = -\varepsilon_2$$
$$S^{(2)} = -\varepsilon_1$$



Nuclear shell model

Case of the spherical HO potential

$$U_i = \frac{1}{2} m\omega^2 r_i^2 \quad \Longrightarrow \quad h_i = \frac{p_i^2}{2m} + \frac{1}{2} m\omega^2 r_i^2$$

$$h_i \ \varphi(\vec{r}_i) = \varepsilon_k \ \varphi(\vec{r}_i)$$

HO in 3 dimensions

k bunch of quantum numbers $\qquad k = n\ell m$

For every particle (omit *i* index)

$$\varphi_{n\ell m}(\vec{r}\,) = R_{n\ell}(r) \ Y_{\ell m}(\hat{r})$$

analytical solution of the radial equation

spherical harmonics

n radial quantum number

ℓ, m quantum numbers related to angular momentum and its projection

$$\varepsilon_{n\ell} = \left(N + \frac{3}{2}\right) \hbar\omega = \left(\underbrace{2(n-1) + \ell}_{N} + \frac{3}{2}\right) \hbar\omega = \varepsilon_N$$

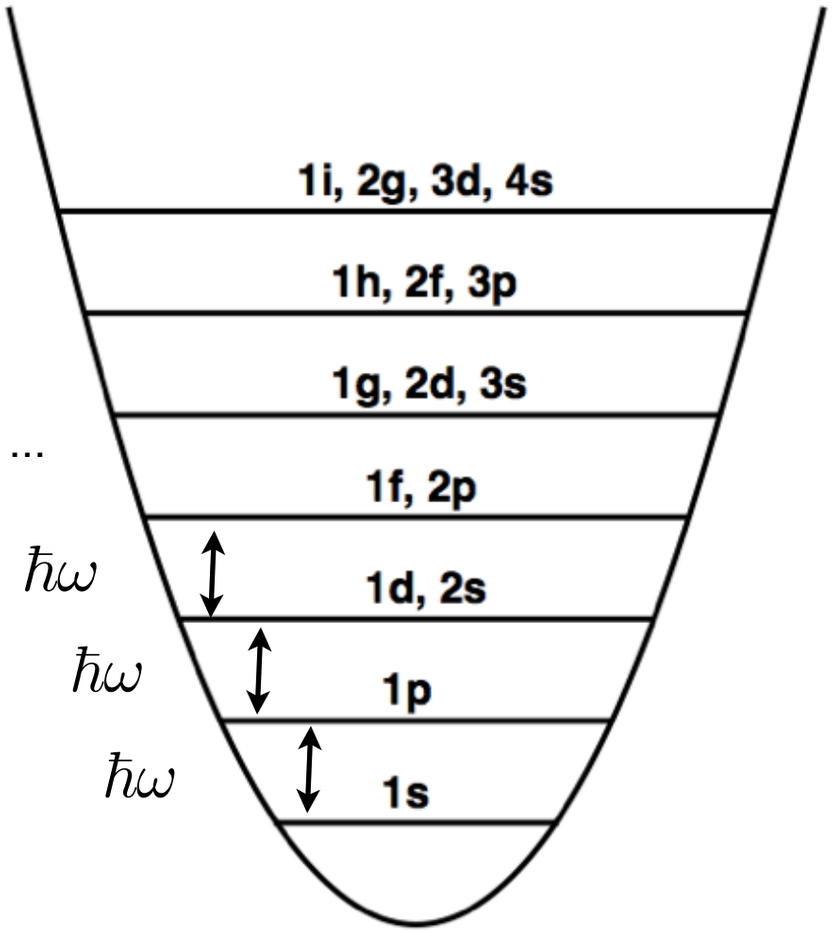
with degeneracy $\quad d_N = 2 \ \ (2\ell + 1)$

two possible spin projections

all possible values of m for a given

Nuclear shell model

Case of the spherical HO potential



The integrated degeneracy is related to the magic numbers

N	E_N	d_N	$\sum_N d_N$	$n(l)$	parity
0	$\frac{3}{2}\hbar\omega$	2	2	$1s$	+
1	$\frac{5}{2}\hbar\omega$	6	8	$1p$	-
2	$\frac{7}{2}\hbar\omega$	12	20	$1d, 2s$	+
3	$\frac{9}{2}\hbar\omega$	20	40	$1f, 2p$	-
4	$\frac{11}{2}\hbar\omega$	30	70	$1g, 2d, 3s$	+
5	$\frac{13}{2}\hbar\omega$	42	112	$1h, 2f, 3p$	-
6	$\frac{15}{2}\hbar\omega$	56	168	$1i, 2g, 3d, 4s$	+

The magic numbers are wrong after the first three!

Nuclear shell model

Does it depend on the “mean” potential we chose? We can do the same using a different U_i

infinite square well potential

harmonic oscillator potential

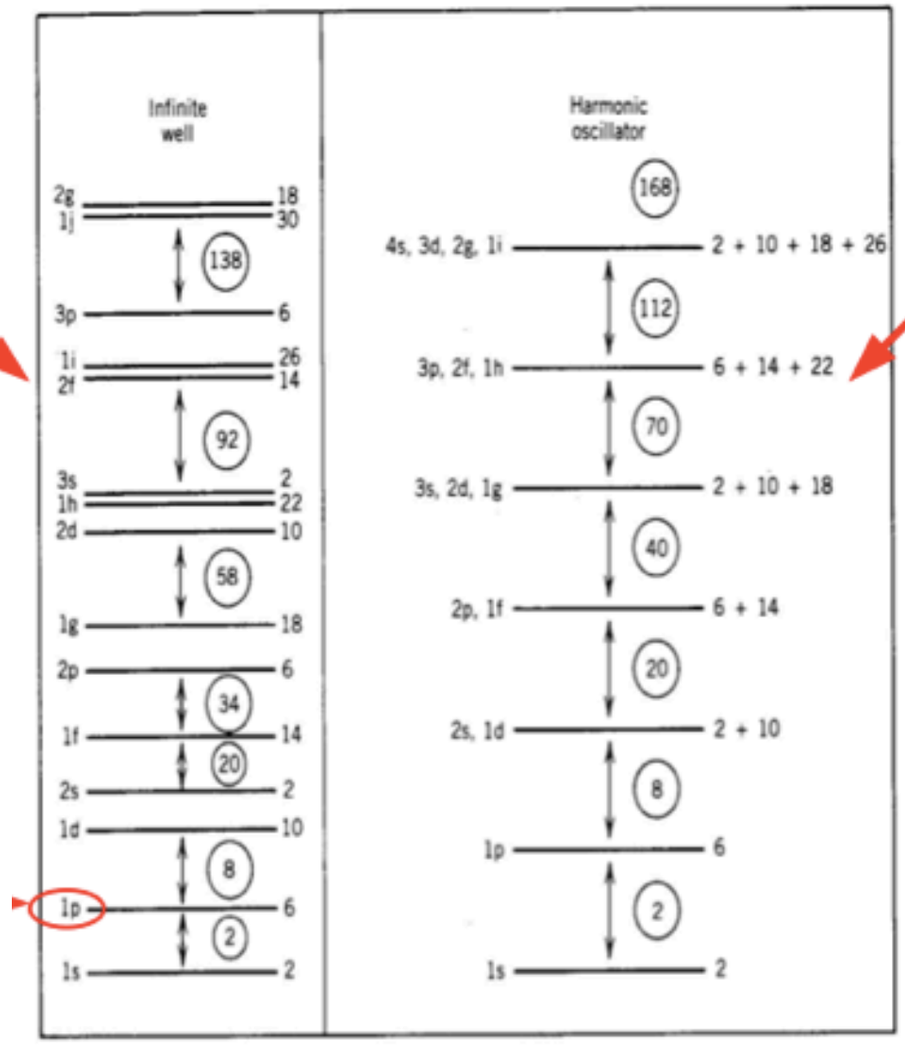
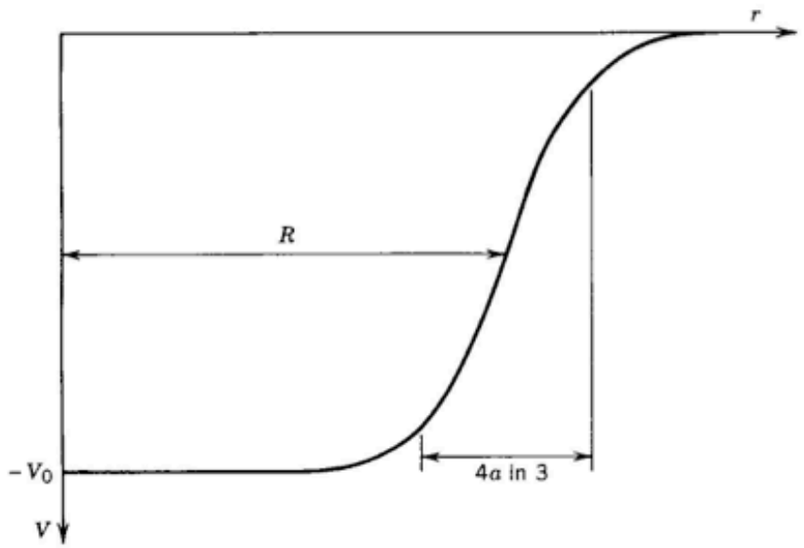


Figure 5.4 Shell structure obtained with infinite well and harmonic oscillator potentials. The capacity of each level is indicated to its right. Large gaps occur between the levels, which we associate with closed shells. The circled numbers indicate the total number of nucleons at each shell closure.

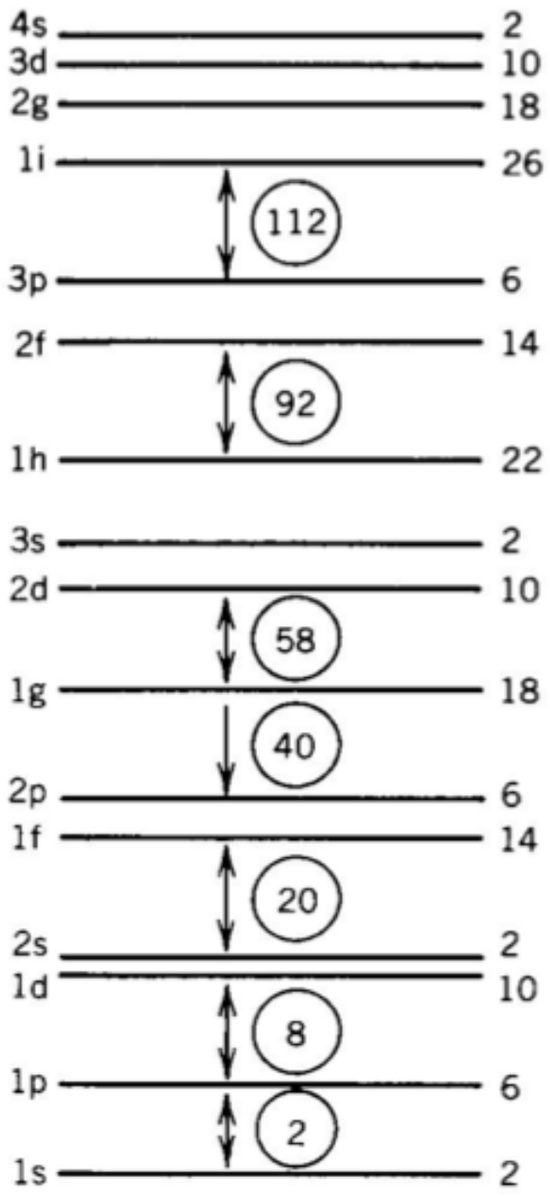
Krane, Introductory Nuclear Physics

Nuclear shell model

One can try to use a Wood-Saxton form for U_i



From Krane "*Introductory Nuclear Physics*"



Still the empirical magic number are not reproduced
2, 8, 20,28, 50, 82, 126

None of these single particle potentials seemed to work properly

Nuclear shell model

Is there a spin-orbit force?

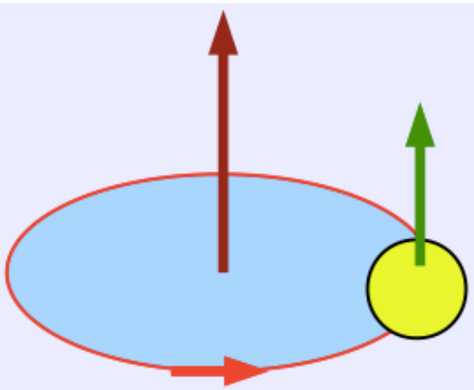
Mean field central potential plus an empirical spin-orbit term like

$$U(r) = V_0(r) + V_{\ell s}(r)\ \vec{\ell}\cdot\vec{s}$$

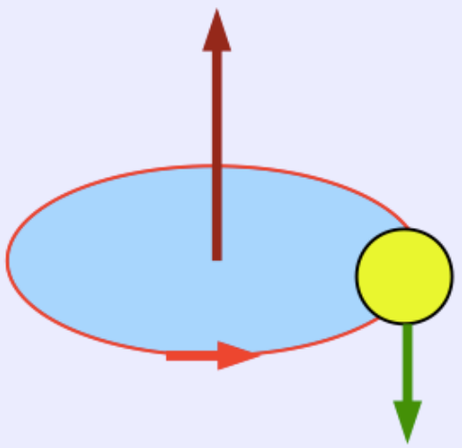
$\vec{\ell}$ orbital angular momentum

$\vec{s}$ spin (intrinsic) angular momentum

with $V_0(r), V_{\ell s}(r)$ being negative (attractive potentials)



L and S parallel
deeper attractive potential



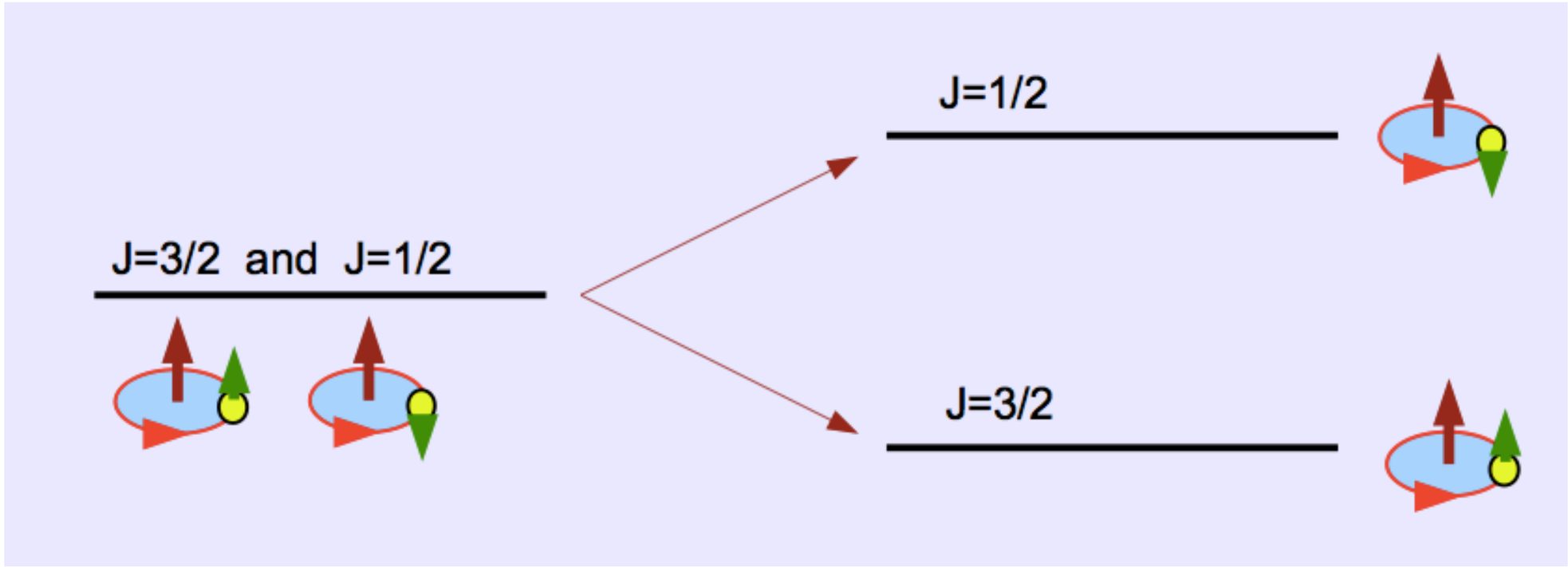
L and S anti-parallel
shallower attractive potential

Nuclear shell model

Spin-orbit splitting

Now the good quantum numbers is j, so we have to consider the angular momentum coupling

$$\vec{j} = \vec{\ell} + \vec{s} = \vec{\ell} + \frac{\vec{1}}{2} = \begin{cases} j = \frac{3}{2} \\ j = \frac{1}{2} \end{cases} \qquad \text{for } \ell = 1$$

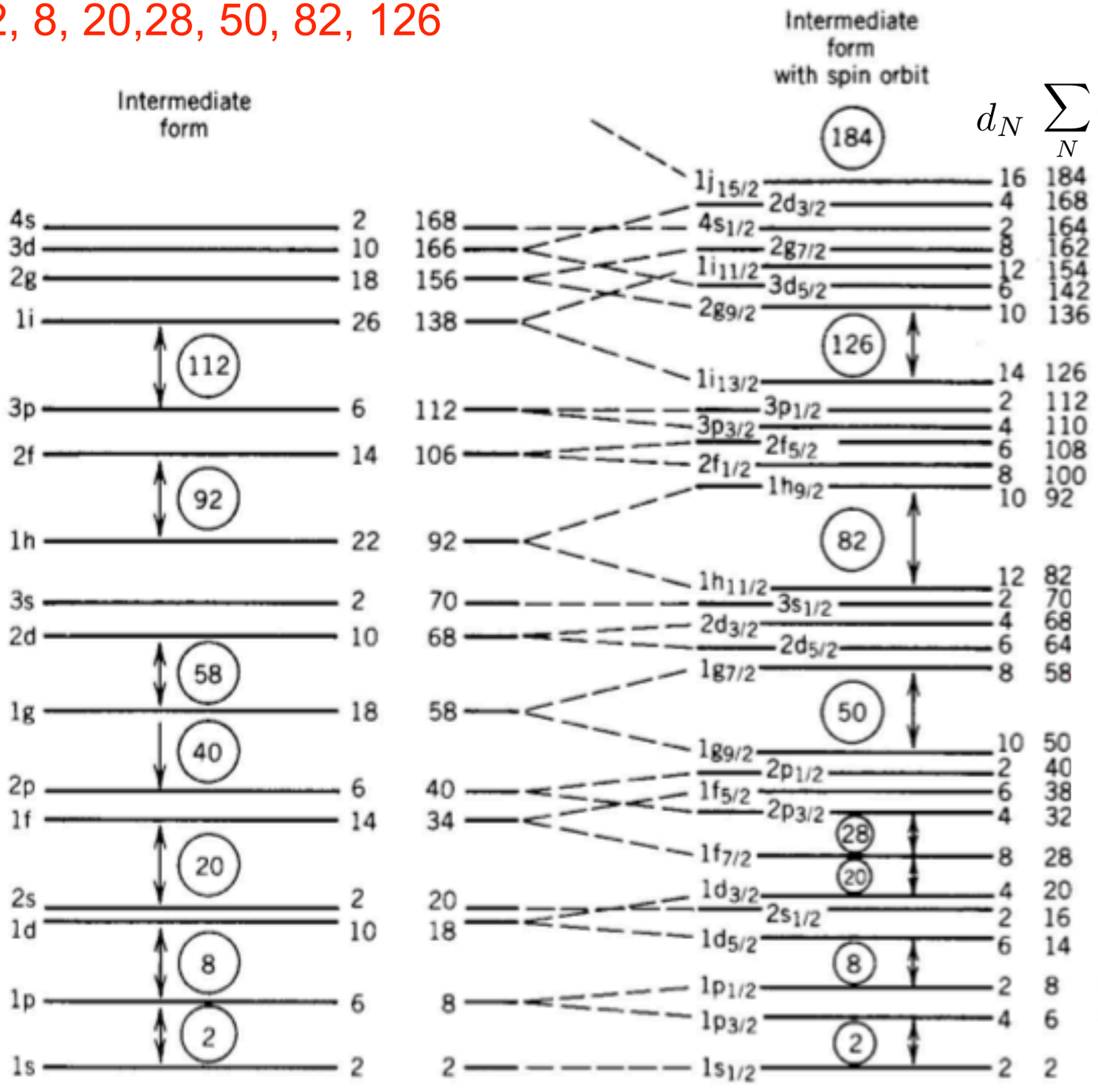


no spin-orbit force $\Longrightarrow$
degenerate levels

with spin-orbit $\Longrightarrow$
splitting of the levels

Nuclear shell model

With the addition of the spin-orbit, the magic numbers are reproduced
2, 8, 20,28, 50, 82, 126



Maria Goppert-Mayer and Hans Jensen
Nobel prize in 1963

Phys. Rev. **75**, 1969 (1949)

Degeneracy with spin-orbit force

$$d_N = (2j+1)$$

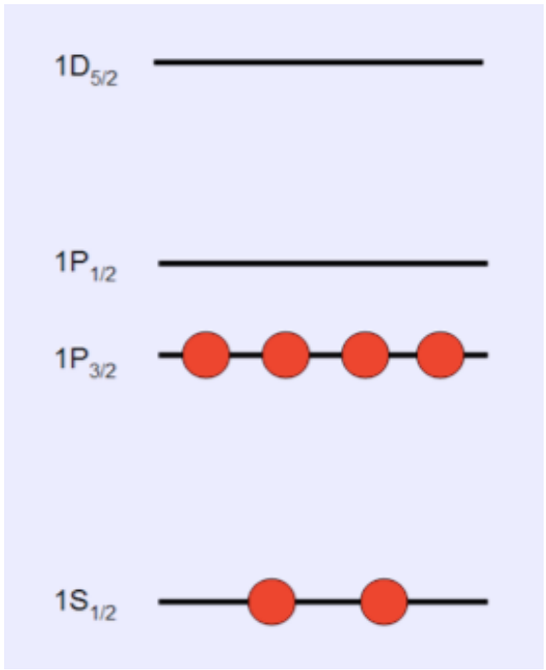
sub-shell
sub-shell
} P-shell

Interacting shell model

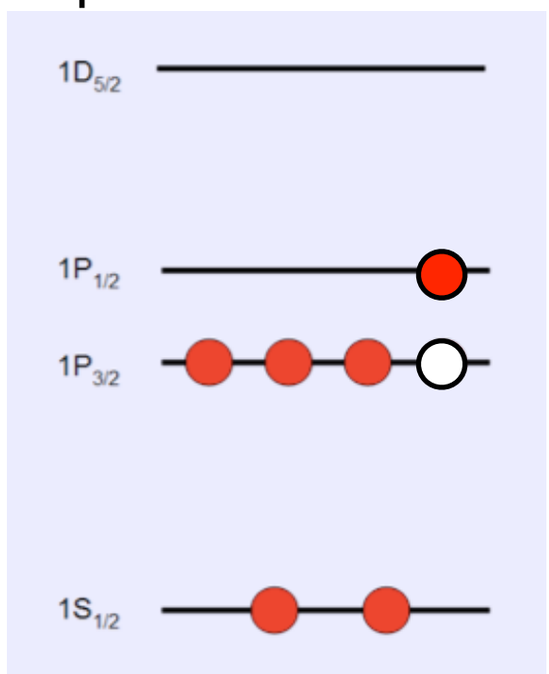
What we have described so far is known as non interacting shell model and we have discussed the ground state of nuclei.
However, in modern research what is used is the interacting shell model/shell model.

One can construct excited states or correlated ground states out of particle-hole excitations of the starting Slater determinant.

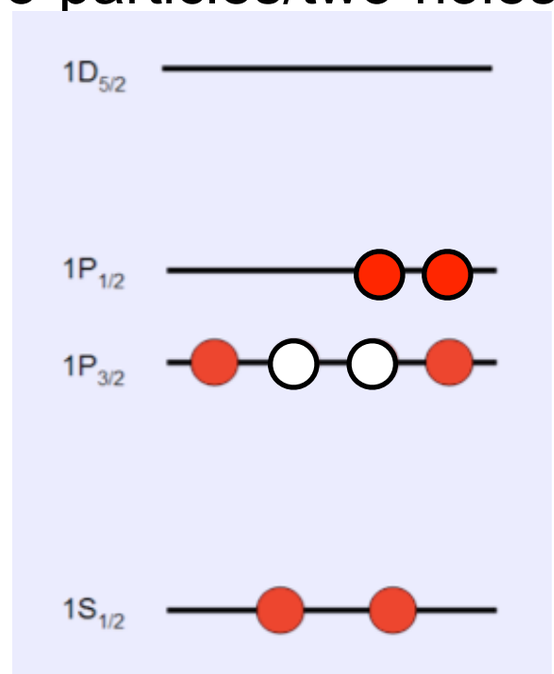
mean field/non interacting



one-particle/one-hole



two-particles/two-holes



In this way you construct many Slater determinants, that can form a many-body basis which one can use to expand the many-body wave function. This is also called configuration mixing or configuration interaction

$$|\Psi^A\rangle = \sum_i c_i |\psi_i^A\rangle$$

Interacting shell model

Hamiltonian with a two-body potential (now particles are interacting)

$$H = \sum_i^A \frac{p_i^2}{2m} + \sum_{i<j}^A V_{ij}$$

connects particle i with particle j

$$H = \sum_i^A \frac{p_i^2}{2m} + \sum_{i<j}^A V_{ij} + \underbrace{\sum_i^A U_i - \sum_i^A U_i}_{=0}$$

$$= \underbrace{\sum_i^A \frac{p_i^2}{2m} + \sum_i^A U_i}_{\text{non interacting Hamiltonian}} + \underbrace{\sum_{i<j}^A V_{ij} - \sum_i^A U_i}_{\text{residual interaction: total interaction minus the “mean”potential}}$$

$$= H^0 + W^{res}$$

If W_{res} is small, then mean field or perturbation around it are good.
If W_{res} is big, then you need to solve the problem non perturbatively by diagonalizing the whole H on the basis of eigenstates of H_0

→ Idea of interacting shell model

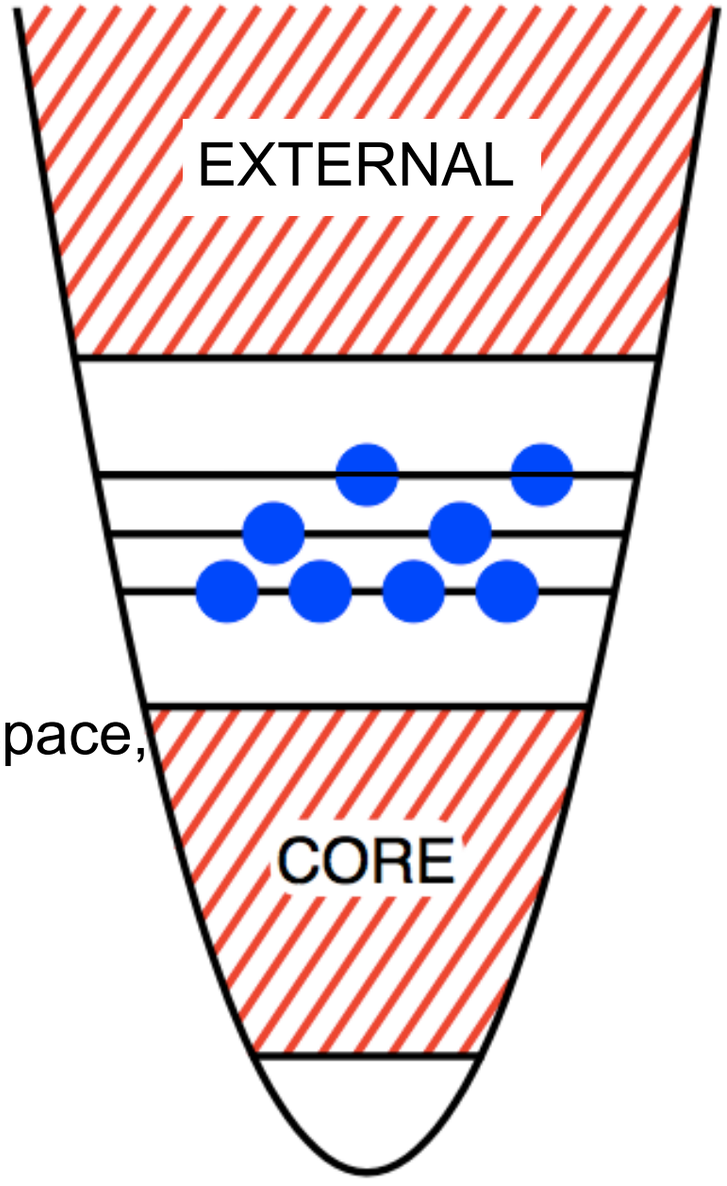
Interacting shell model

Construct orbitals from the HO potential $U_i = \frac{1}{2} m\omega^2 r_i^2 \qquad \hbar\omega \simeq 41 A^{-\frac{1}{3}}\ \mathrm{MeV}$

Ansatz:

For a given number on p and n, the mean field orbitals (ε_i) can be grouped in:

- inherent core:
  orbitals that are always full
- valence space:
  orbits that can have particle-hole excitations
- external space:
  all the remaining orbits that are always empty



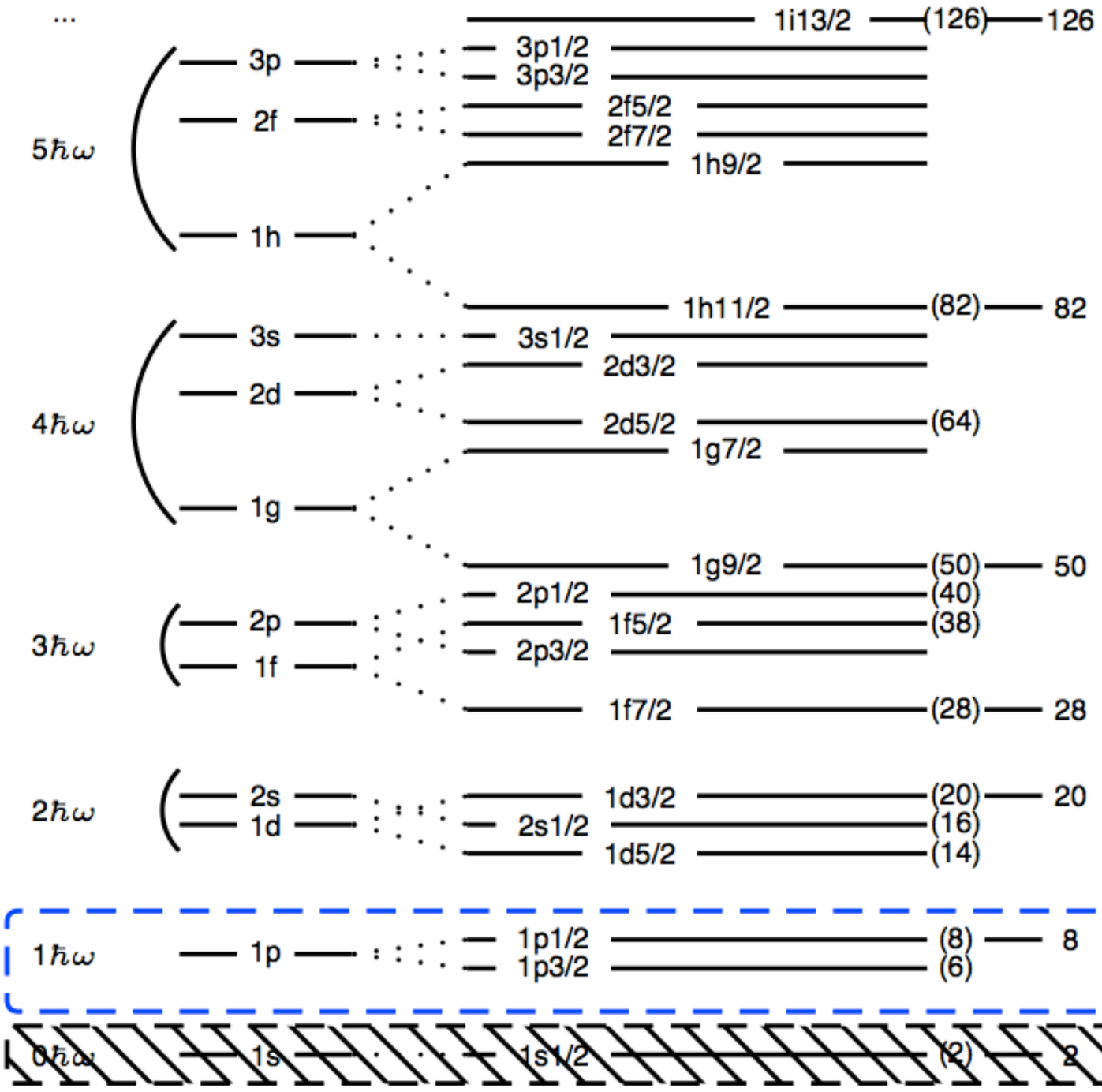
1. Starting from V_{ij} you construct a V^{eff}_{ij} that lives in the valence space, using phenomenology or many body perturbation theory

2. Solve H_0+W_{res} by **diagonalizing** a matrix with particle-hole excitations in your valence space

Effective Potentials

Phenomenological approach

The model space and the effective interaction are very much related. Typically, the effective interaction is a set of two-body matrix elements tuned to reproduce experimental data



p-shell nuclei

$$4 \leq A \leq 16$$

Cohen-Kurath interaction

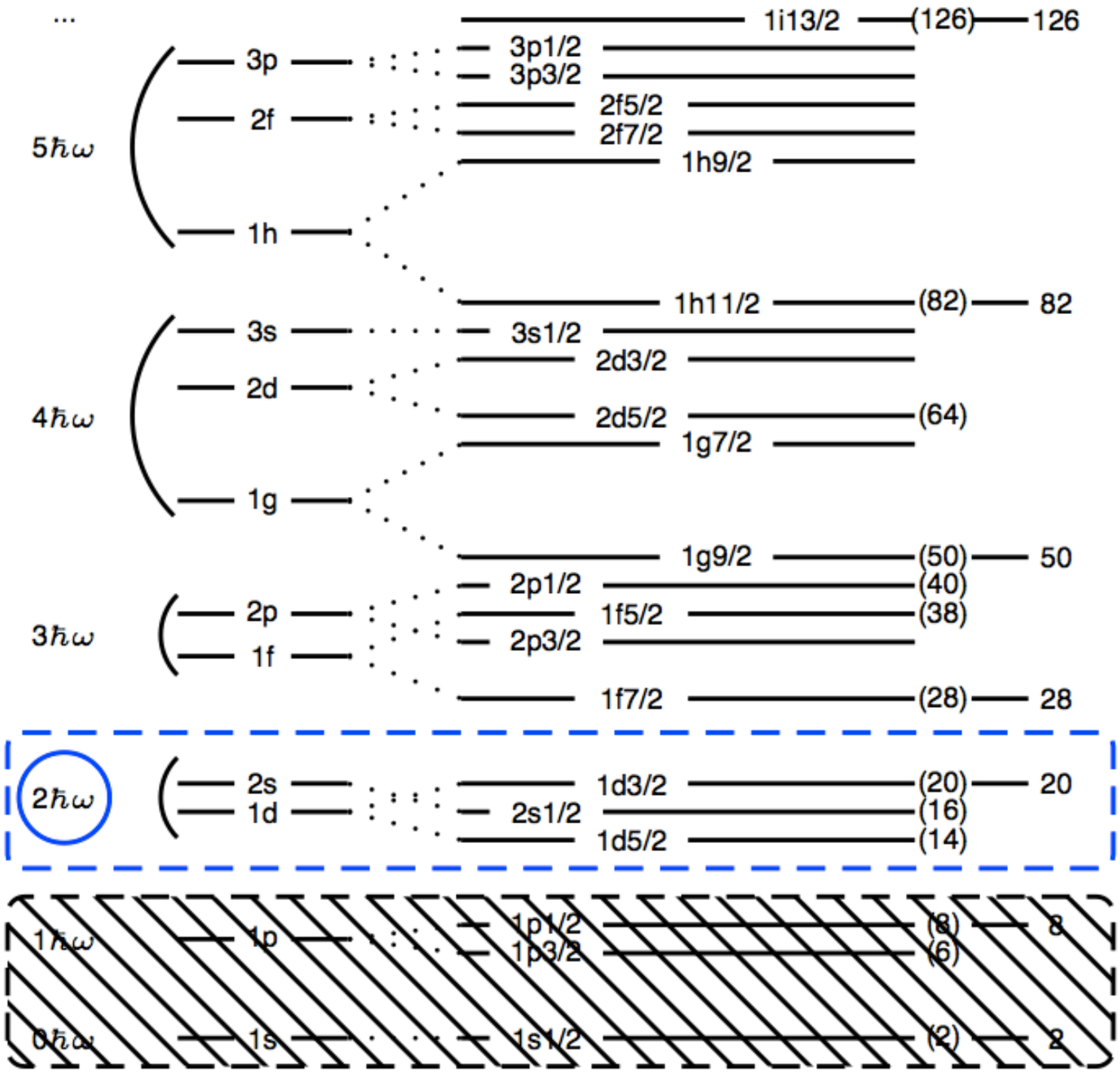
VALENCE SPACE

CORE

Effective Potentials

Phenomenological approach

The model space and the effective interaction are very much related. Typically, the effective interaction is a set of two-body matrix elements tuned to reproduce experimental data



sd-shell nuclei

$$16 \leq A \leq 40$$

USD interaction

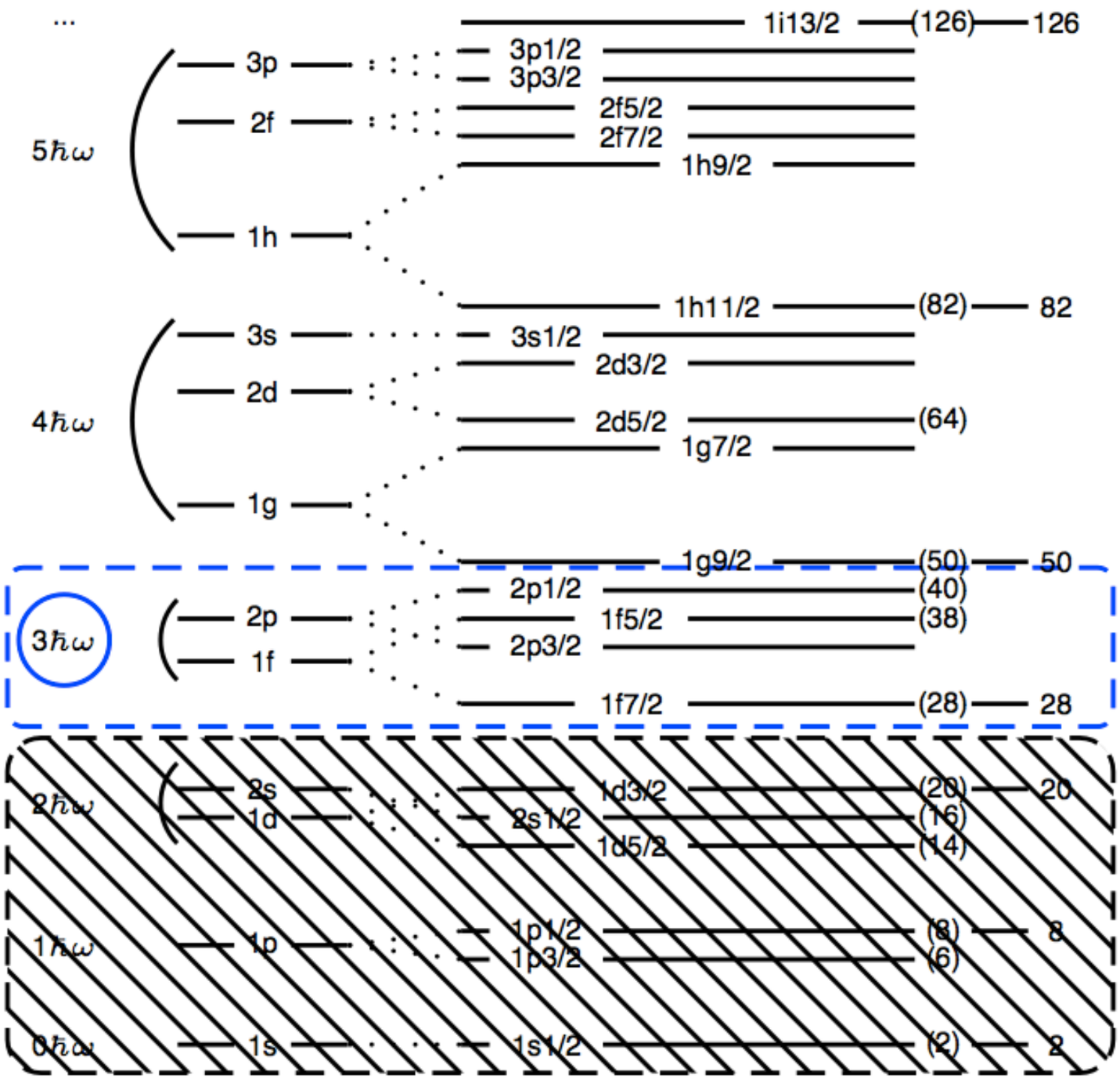
VALENCE SPACE

CORE

Effective Potentials

Phenomenological approach

The model space and the effective interaction are very much related. Typically, the effective interaction is a set of two-body matrix elements tuned to reproduce experimental data



pf-shell nuclei

$$40 \leq A \leq 80$$

GXPF1 interactions

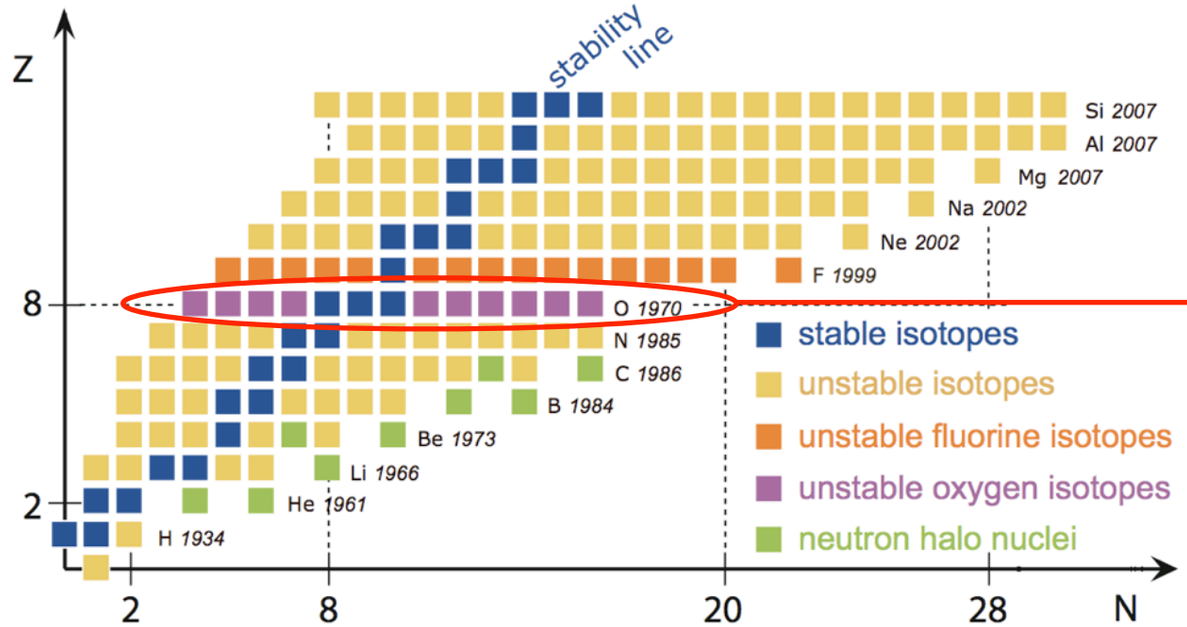
VALENCE SPACE

CORE

...

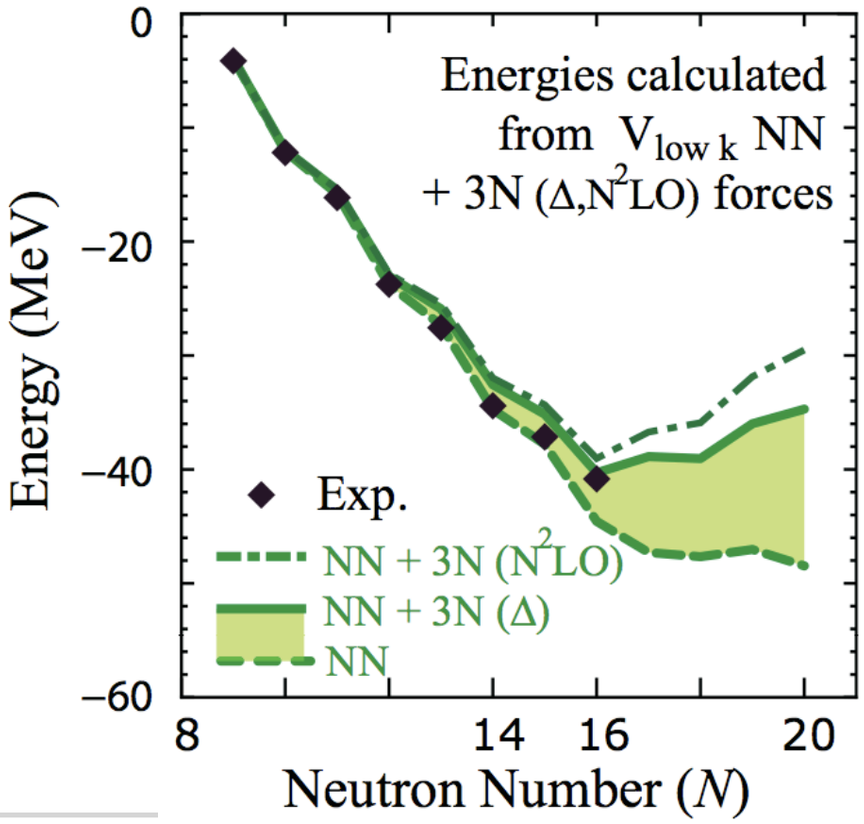
Effective potentials from MBPT

More fundamental approach



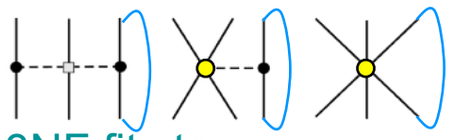
Shell Model: ^{16}O core

any SM calculation with realistic 2NF predicts bound $^{25\text{-}28}$O in contrast with experimental observation

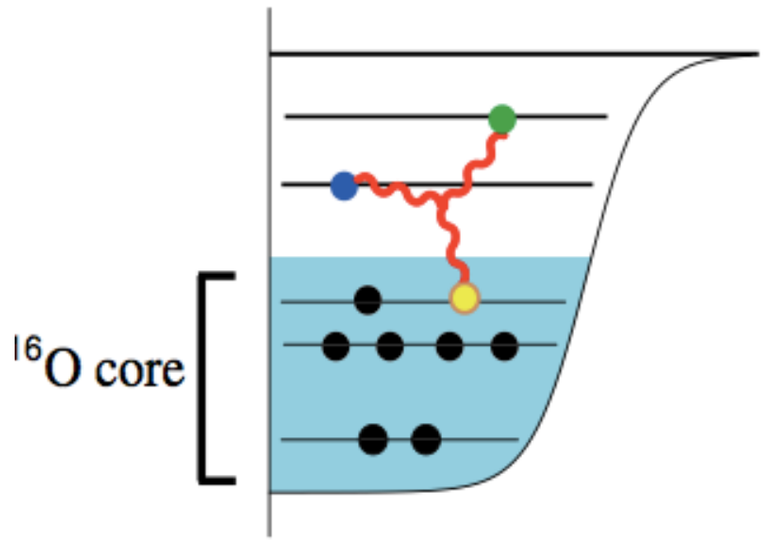


Otsuka et al. PRL 105, 032501 (2010)

First results with 3NF (effective 2NF)

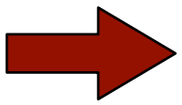


3NF fits to E(^{3}H) and ^{4}He rms



Ab-initio approach

To go beyond phenomenological potentials or the core approximations, using the more fundamental approach to nuclear interactions from chiral EFT



Solve the many-body problem with ab initio many-body methods