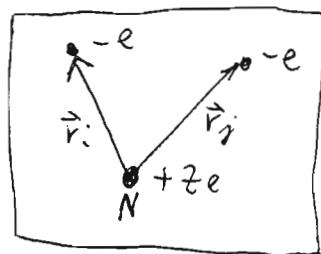


Section 3.1: single-particle motion

- Topics:
- spherical shell model (1949-55)
 - deformed shell model (Nilsson model, 1955)

Interlude: "Magic" numbers in atomic shell model

When one studies the properties of atoms, one finds that certain "magic" elements with atomic number $Z = 2, 10, 18, 36, 54$, and 86 show unusually high electron ionization energies, and these atoms do not readily form molecules, like most other atoms. These elements are called the inert (noble) gases. Explanation via atomic shell model:

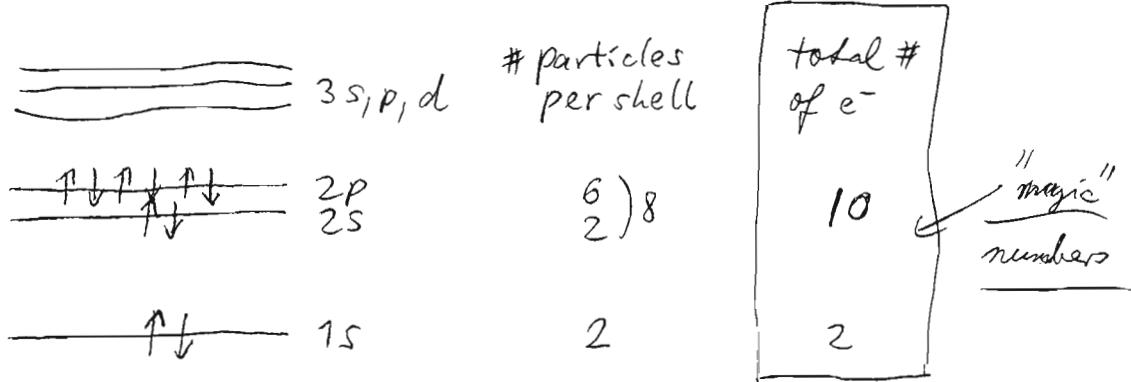


$$\left\{ \begin{array}{l} H = \sum_{i=1}^Z \left(-\frac{\hbar^2}{2m_e} \nabla_i^2 - \frac{Ze^2}{r_i} \right) + \frac{1}{2} \sum_{i,j=1}^Z \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \\ \qquad \qquad \qquad \text{electron-nucleus} \qquad \qquad \qquad \text{electron-electron} \\ + \text{spin-orbit term} + \dots \\ \qquad \qquad \qquad \uparrow \\ \qquad \qquad \qquad (\text{small, perturb. theory}) \end{array} \right.$$

If we neglect the 2-body e^-e^- interaction, we have a one-body operator and can immediately write down the answer

$$E_{\text{tot}} \approx \sum_{i=1}^Z E_i \quad \text{with } E_i \equiv E_n \sim \frac{1}{n^2}.$$

The degeneracy of the s.p. levels ~~there~~ explains the lowest "magic" numbers of atomic physics; high ionization energies are due to "shell gaps".



However, to explain the higher "magic numbers" of the noble gases quantitatively ($Z=18, 36, \dots$) one needs to take the e^-e^- int. into account → atomic Hartree-Fock theory (1928-30).

Indirect exp. evidence for nuclear shell structure

- ① "large" binding energy (relative to smooth liquid drop formula) at certain magic numbers:

for protons: $Z = \underbrace{2, 8, 20, 28, 50, 82, 114, \dots}$
exp. confirmed

for neutrons: $N = \underbrace{2, 8, 20, 28, 50, 82, 126, 184, \dots}$
exp. confirmed

- ② large p/n separation energies at these magic numbers

NOTE: similar to atomic ionization energies!

- ③ ground-state quadrupole moments vanish at magic numbers.
→ nuclei are spherical.

- ④ First excited collective states have unusually high energy at magic p/n numbers, in particular for "doubly magic" nuclei:

${}_{\text{8}}^{\text{16}} \text{O}$: 6.8 MeV $(N=8, Z=8)$	${}_{\text{20}}^{\text{40}} \text{Ca}$: 3.8 MeV $(N=20, Z=20)$	${}_{\text{82}}^{\text{208}} \text{Pb}$: 2.6 MeV $(Z=82, N=126)$
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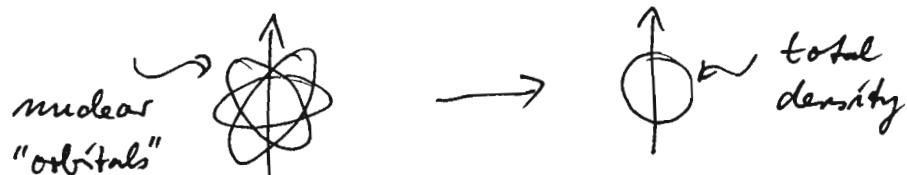
These properties hint at nuclear shell model:

properties ① and ② are due to "shell gaps".

③ can be explained by filled shell: $|nljm_j\rangle$.

If all magnetic substates $m_j = -j, \dots, +j$ are filled,

the nuclear matter distribution is spherical:



④ can be understood as follows: at magic numbers, shells are completely filled. For excited states, nucleons must be transferred to next higher shell (shell gap, ΔE large).

Spherical shell model

Ref: Ring & Schuck,
Chapter 2.

Basic idea: The motion of all nucleons ($V^{(2)}, V^{(3)}$) cause a one-body mean field ($V^{(1)}$) in which a given nucleon moves. To obtain the correct magic p/n numbers, one needs to add a spin-orbit interaction of high strength.

- Discuss slides 1 and 2 of this section.

Phenomenological Hamiltonian:

$$H = \sum_{i=1}^A h_i(x_i) \quad (x = \vec{r}, \sigma_z, t_z)$$

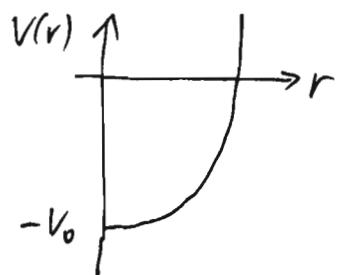
↓
one-body!

S.p. Hamiltonian:

$$h(\vec{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V(r) + V_{es}(r)$$

↓
spherical ↓
 spin-orbit

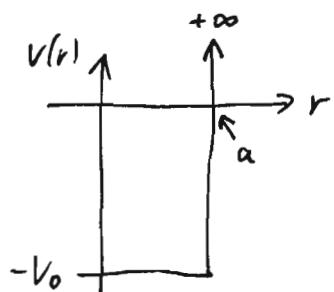
model potentials:



a) 3-D spherical harmonic oscillator

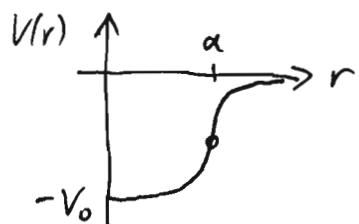
$$V(r) = -V_0 + \frac{1}{2} m \omega^2 r^2$$

$$\approx -50/-70 \text{ MeV}$$



b) spherical infinite square well

$$V(r) = \begin{cases} -V_0 & ; r \leq a \\ +\infty & ; r > a \end{cases}$$



c) ~~Woods~~ "Woods-Saxon" potential

$$V(r) = -V_0 \left[1 + \exp\left(\frac{r-a}{b}\right) \right]^{-1}$$

↑ requires numerical solution
of 1-D radial eqn.

I. Nuclear shell model without $\vec{l} \cdot \vec{s}$ term

Cartesian $(x, y, z) \rightarrow$ spherical coord. (r, θ, ϕ)

$$h(\vec{r}) = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \right) + \frac{\vec{l}^2(\theta, \phi)}{2mr^2} + V(r)$$

Observe that h commutes with \vec{l}^2 and L_z and parity Π . Good quantum #'s:

$$\begin{array}{cccc} h & \vec{l}^2 & L_z & \Pi \\ \downarrow & \downarrow & \downarrow & \downarrow \\ E & l & m_e & (-1)^l \end{array}$$

Form simultaneous eigenstates (leave out parity):

$$\left. \begin{aligned} h |E, l, m_e\rangle &= E |E, l, m_e\rangle \\ \vec{l}^2 |E, l, m_e\rangle &= \hbar^2 l(l+1) |E, l, m_e\rangle \\ L_z |E, l, m_e\rangle &= \hbar m_e |E, l, m_e\rangle \end{aligned} \right\}$$

Use separation ansatz

$$\begin{aligned} \Psi_{E, l, m_e}(r, \theta, \phi) &= \langle r, \theta, \phi | E, l, m_e \rangle = \langle r | E_l \rangle \langle \theta, \phi | l_m \rangle \\ &\equiv R_{El}(r) Y_{lm}(\theta, \phi) \end{aligned}$$

resulting in the 1-D (radial) Schrödinger eq (see e.g. Shankar, QM):

$$\left. \left\{ \frac{d^2}{dr^2} + \frac{2m}{\hbar^2} [E - V_{\text{eff}}(r)] \right\} U_{El}(r) = 0 \right\}$$

$$\text{with } U_{El}(r) \stackrel{\text{def}}{=} r \cdot R_{El}(r)$$

$$\text{and } V_{\text{eff}}(r) = V(r) + \frac{\hbar^2 l(l+1)}{2mr^2}$$

\uparrow \uparrow
 Shell-model centrifugal pot.

Solution for 3-D harmonic oscillator:

$$E_{nl} = -V_0 + \hbar\omega(N + \frac{3}{2})$$

with

$$\begin{cases} N = 2(n-1) + l & \text{principal quantum \#} \\ n = 1, 2, 3, \dots \\ l = 0, 1, 2, \dots \end{cases}$$

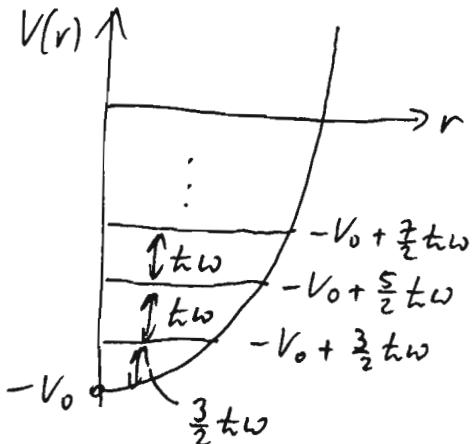
\Rightarrow energy degeneracy: E depends on N

$$(2l+1) \cdot 2$$

N	combinations (n, l)	state	# nucleons in shell	total # nucleons
0	$n=1, l=0$	1s	2	2
1	$n=1, l=1$	1p	6	8
2	$n=2, l=0$ $n=1, l=2$	2s 1d	$2 \begin{pmatrix} 10 \end{pmatrix} 12$	20
:	:	:		

This reproduces the 3 lowest "magic numbers" for p/n,
but not the higher ones \Rightarrow need $\vec{l} \cdot \vec{s}$ term.

S.p. energies in H.O. model



The shell spacing, $\hbar\omega$, can be obtained by calculating the mean square radius in the shell model

$$\langle R^2 \rangle = \frac{1}{A} \sum_{i=1}^A \langle \varphi_i | r^2 | \varphi_i \rangle$$

and relating it to the empirical radius $R = r_0 A^{1/3}$. In this way one finds

$$\hbar\omega = 41 \cdot A^{-1/3} \quad [\text{MeV}]$$

II. Include spin-orbit term

$$h(\vec{r}) = -\frac{\hbar^2}{2m} \nabla^2 + V(r) - \frac{2\alpha}{\hbar^2} \vec{l} \cdot \vec{s}$$

where α is a constant to be fitted to exp. data.

Let's express $\vec{l} \cdot \vec{s}$ in the usual form

$$\vec{l} + \vec{s} = \vec{j} \quad \Rightarrow \quad (\vec{l} + \vec{s})^2 = \vec{j}^2 \quad \Rightarrow \quad \boxed{\vec{l} \cdot \vec{s} = \frac{1}{2} (\vec{j}^2 - \vec{l}^2 - \vec{s}^2)}$$

We observe: h commutes with $\vec{j}^2, \vec{l}^2, \vec{s}^2, j_z$ and π'
associated quantum #'s $j \downarrow l \downarrow s=\frac{1}{2} \downarrow m_j \downarrow \pi=(-1)^l$

Ansatz for s.p. W.F.'s in "coupled repr." (= total- j basis);

Note: W.F. is a 2-component spinor:

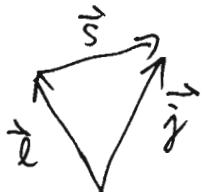
$$\Psi_{n,l,s=\frac{1}{2},j,m_j}(r, \theta, \varphi) = R_{nlj}(r) \cdot S_{l,s=\frac{1}{2},j,m_j}(\theta, \varphi)$$

with the "spherical spinors"

$$S_{l,s=\frac{1}{2},j,m_j}(\theta, \varphi) = \sum_{m_e, m_s} \langle l m_e, s=\frac{1}{2} m_s | j m_j \rangle Y_{lm_e}(\theta, \varphi) \chi_{\frac{1}{2}, m_s}$$

Clebsch-Gordan coeff. Spin-vector

Angular momentum
coupling in general



Special case here ($s=\frac{1}{2}$)

$$\begin{array}{c} \frac{1}{2} \\ \uparrow \\ l \\ \uparrow \\ j = l + \frac{1}{2} \end{array} \quad \text{or} \quad \begin{array}{c} \downarrow \frac{1}{2} \\ \uparrow \\ l \\ \uparrow \\ j = l - \frac{1}{2} \end{array}$$

If we apply the simple spin-orbit term to this WF, we can replace the operators by their eigenvalues:

$$\hat{\vec{l}} \cdot \hat{\vec{s}} |n, l, s=\frac{1}{2}, j, m_j\rangle = \frac{\hbar^2}{2} [j(j+1) - l(l+1) - s(s+1)] |...>$$

For the 2 possible cases $j = l \pm \frac{1}{2}$ one finds

$$\hat{\vec{l}} \cdot \hat{\vec{s}} |...> = \frac{\hbar^2}{2} \left\{ \begin{array}{l} l \\ -(l+1) \end{array} \right. ; \begin{array}{l} \text{for } j = l + \frac{1}{2} \\ \text{for } j = l - \frac{1}{2}, l \neq 0 \end{array} \left\} |...>$$

Therefore, the spin-orbit int. yields an odd. energy

$$\begin{aligned} \Delta E_{ls} &= -\frac{2\alpha}{\hbar^2} \langle n l \frac{1}{2} j m_j | \hat{\vec{l}} \cdot \hat{\vec{s}} | n l \frac{1}{2} j m_j \rangle = \\ &= -\alpha \left\{ \begin{array}{l} l \\ -(l+1) \end{array} \right\} \end{aligned}$$

Putting everything together, the s.p. energies are

$$E_{nj} = -V_0 + \hbar \omega \underbrace{\left(N + \frac{3}{2} \right)}_{N=2(n-1)+l} + \alpha \left\{ \begin{array}{l} -l ; \text{ for } j = l + \frac{1}{2} \\ +(l+1) ; \text{ for } j = l - \frac{1}{2}, l \neq 0 \end{array} \right\}$$

From fit to exp. data one finds

$$\alpha \approx 0.5 \text{ MeV}$$

Discuss spin-orbit splitting of levels E_{nj} :

- 1) The $l=0$ (s) levels are not affected by the ls term.
- 2) The states with $j = l - \frac{1}{2}$ (i.e. \hat{l} and \hat{s} are antiparallel) are shifted to higher energies, and those with $j = l + \frac{1}{2}$ (i.e. \hat{l} and \hat{s} are parallel) are shifted to lower energies.

Note: in atomic physics, it is the other way around!

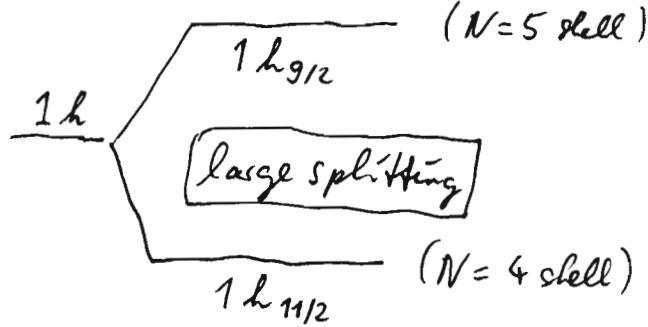
3) The level splitting affects mostly the high- l states:

$l=1 (p)$



Small splitting

$l=5 (h)$

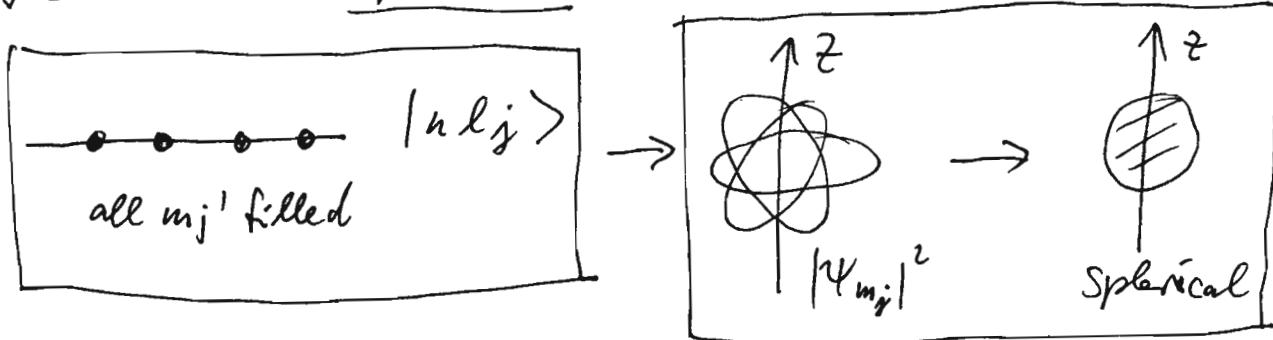


Discuss remaining slides in this section:

- level spectrum, "orbital" plot, measured neutron s.p. levels in $^{209}_{82}\text{Pb}$.
 - Fermi levels for stable and n -rich nuclei
 - shell gap disappearance (theory) near the n -drip-line
-

Ground state total angular momentum and parity (J^π) in spherical shell model

Consider the shell model state $|nlj\rangle$. If all magnetic substates are filled ($m_j = -j, -j+1, \dots, +j$) this shell has a spherical matter distribution ($J=0$).



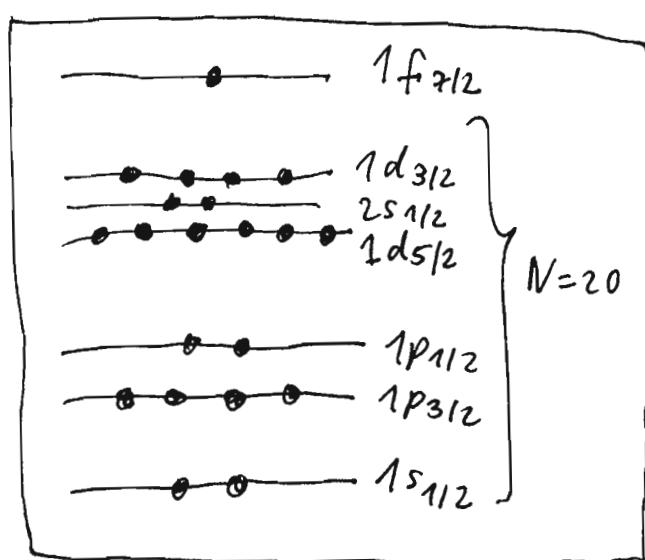
Indeed, one finds that all nuclei with filled j -shells in both protons and neutrons have total ang. mom. $J=0$.

Another case of interest is to add a single nucleon outside a closed-shell nucleus, e.g. $^{41}_{20}\text{Ca}$ with 20 protons and 21 neutrons. In this case, ~~the~~ all levels including $1d_{3/2}$

are filled with neutrons, and the last neutron ~~is~~ has to be put into the $1f_{7/2}$ level.

Since $^{40}_{20}\text{Ca}$ is spherical with $J=0$, we expect $^{41}_{20}\text{Ca}$ to have a. g.s. total angular momentum

$$J = j = \frac{7}{2}$$



Furthermore, the parity of the $^{40}_{20}\text{Ca}$ "core" is (+1), and the additional neutron in the $1f_{7/2}$ level has parity $(-1)^l = (-1)^3 = -1$ for the "f" level ($l=3$).

\Rightarrow spherical shell model predicts $J'' = \frac{7}{2}^-$
for g.s. of $^{41}_{20}\text{Ca}$.

Indeed, the level schemes on the NNDC Website confirm this!

Other examples: homework!

If we add 2 nucleons outside a closed shell, things get more complicated: From angular momentum coupling

rules (\rightarrow Clebsch-Gordan coefficients!) one obtains:

$$|j_1 - j_2| \leq J \leq j_1 + j_2$$
$$\Rightarrow |j - j| \leq J \leq 2j \Rightarrow J = 0, 1, 2, \dots, 2j$$

For example, in $^{42}_{20}\text{Ca}$, the g.s. could have angular momenta

$$J = 0, 1, 2, \dots, 7$$
$$2j = 2 \cdot \frac{7}{2} = 7$$

In the simple shell model, all s.p. states in the $1f_{7/2}$ shell have the same energy, so we usually cannot determine the J -value of the ground state. In reality, the degeneracy is broken by the "residual interaction"

$$V_{\text{res}} = \underbrace{V^{(2)} + V^{(3)}} - \underbrace{V^{(1)}}_{\text{true Hamiltonian}} \quad \text{shell model}$$

The short-range part of V_{res} gives rise to pairing forces, and we will see later in Section 4 that, according to the BCS pairing theory, the g.s. angular momentum of all even-even nuclei is $J=0$.

Electric multipole moments Q_{em} of nuclei

From classical EM theory (e.g. Jackson) we have

$$Q_{\text{em}} = \int d^3r \rho_c(\vec{r}) r^\ell Y_{\ell m}^*(\theta, \phi)$$

For the charge distribution $\rho_c(\vec{r})$ of the nucleons modelled as point particles we have

$$\rho_c(\vec{r}) = \sum_{i=1}^A e \underbrace{\left(\frac{1}{z} + t_z^{(ii)} \right)}_{= q_i} \delta(\vec{r} - \vec{r}_i)$$

resulting in the El-multipole operator

$$\hat{Q}_{\text{em}} = \sum_{i=1}^A e \left(\frac{1}{z} + t_z^{(ii)} \right) r_i^\ell Y_{\ell m}^*(\theta_i, \phi_i) = \sum_{i=1}^A \hat{Q}_{\text{em}}^{(i)}$$

↑
isospin

which shows that \hat{Q}_{em} is a one-body operator.

The observables, i.e. nuclear multipole moments, are

defined as the expectation values of \hat{Q}_{em} in the many-body quantum state $|J, M\rangle$:

$$\overline{Q}_{\text{em}} = \langle J, M | \hat{Q}_{\text{em}} | J, M \rangle.$$

Specifically, the quadrupole moment is defined as

$$\overline{Q} \stackrel{\text{def}}{=} \langle J, M=+J | \underbrace{\sqrt{\frac{16\pi}{5}} \hat{Q}_{20}}_{= Q_{zz}} | J, M=+J \rangle$$

i.e. the matrix element is evaluated for the magnetic substate $M=+J$ with the highest ang. mom. projection.

In general, it is difficult to calculate \overline{Q} for an arbitrary many-body WF (this requires "second quantization" ~~techniques~~ techniques, see Section 4).

However, the simple shell model can make a prediction for a single nucleon in a j -shell, with all of the other shells completely filled. In this case, the quadrupole moment of the nucleus should equal that of the single particle, i.e.

$$\overline{Q} = \overline{Q}_{\text{core}} + \overline{Q}_{j\text{-shell}} = \overline{Q}_{j\text{-shell}}.$$

For the latter, we obtain from the shell model for a proton ($q=+e$):

$$\overline{Q}_{j\text{-shell}} = \langle n, l, j, m_j = +j | \sqrt{\frac{16\pi}{5}} e r^2 Y_{20}(\Omega) | n, l, j, m_j = +j \rangle$$

Using the single-particle WF's of the spherical shell model, one finds, after some considerable algebra [e.g. textbook

by Greiner & Maruhn, p. 246-247]:

$$\bar{Q}_{j\text{-shell}} = (-e) \langle r^2 \rangle_{nj} \frac{2j-1}{2j+1} \quad (*)$$

where $\langle r^2 \rangle_{nj}$ is the mean square radius of a nucleon in the s.p. quantum state (nlj) . The expression (*) makes a very interesting prediction:

$\bar{Q}_{j\text{-shell}} = 0$ for a $j = \frac{1}{2}$ shell, and $\bar{Q}_{j\text{-shell}} < 0$ otherwise, i.e. the quadrupole moment is negative (oblate charge distribution) for $j > \frac{1}{2}$.

Experimentally, this is true only near major closed shells.

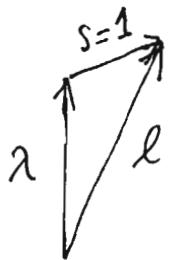
In general, electric quadrupole moments predicted by the simple spherical shell model are much too small (up to a factor of 100), and most exp. \bar{Q} 's are positive (prolate shape). Reason: collective motion of many nucleons. More in the following sections.

γ -decay: electric multipole transitions

$$\begin{array}{c} \hline \\ \hline \end{array} \quad \left(J_i, M_i \right) \\ \gamma \quad \left(E \ell \right) \\ \hline \quad \left(J_f, M_f \right) \quad \begin{array}{c} \hline \\ \hline \end{array}$$

Another important exp. observable are $E \ell$ -photon transitions in nuclei. The total ang. momentum ℓ of the photon arises from the

coupling of the photon spin, $S=1$, to its orbital angular momentum $\lambda=0, 1, 2, \dots \rightarrow$ Electric multipole radiation



- with $\ell = 1$ (dipole)
 $\ell = 2$ (quadrupole)
 $\ell = 3$ (octupole)
 $\ell = 4$ (hexadecapole)

We have already discussed the radioactive decay law in Section 2. The γ -decay rate, λ_γ , is

$$N(t) = N_0 e^{-\lambda_\gamma t}$$

can be calculated from the quantum theory of El multipole radiation. One finds [e.g. Greiner & Maruhn textbook, p. 75-98]

$$\lambda_\gamma = \frac{8\pi (\ell+1)}{\ell [(2\ell+1)!!]^2} \frac{1}{t} \left(\frac{E_\gamma}{\hbar c} \right)^{2\ell+1} B(E\ell, J_i \rightarrow J_f)$$

with $(2\ell+1)!! = 1 \cdot 3 \cdot 5 \cdots (2\ell+1)$

and $E_\gamma = E_i - E_f = \text{photon energy}$

and $B(E\ell, J_i \rightarrow J_f) = \text{"reduced transition probability"} \\ = \text{"BE}\ell\text{-value".}$

Important conclusions

1) λ_γ is proportional to $E_\gamma^{2\ell+1}$

2) the nuclear structure information is contained in the BE ℓ -value defined as

$$B(E\ell, J_i \rightarrow J_f) = \frac{1}{2J_i + 1} \sum_{M_i, M_f} \left| \langle J_f M_f | \hat{Q}_{em} | J_i M_i \rangle \right|^2$$

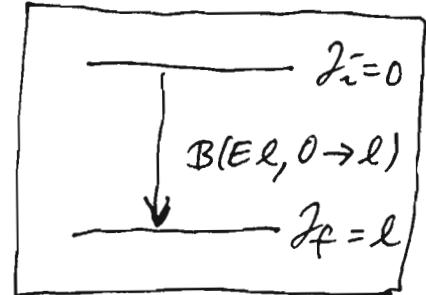
El-multipole operator, see p. 12.

Nuclear experimentalists can measure the photon transition rate λ_p and the photon energy E_p which determines $B(E\ell, J_i \rightarrow J_f)$.

The $B(E\ell)$ -value from exp. can be compared to theor. calculations. This is a severe test of the many-body wave functions ψ_i and ψ_f .

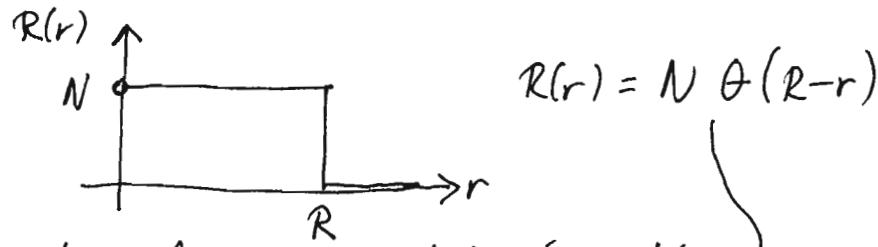
Single-particle estimate of $B(E\ell)$ -value: "Weisskopf unit"

Weisskopf, a professor at MIT, derived a simple estimate for the $B(E\ell)$ -value for a single proton transition using a simplified shell-model wave function



$$\psi_{em}(\vec{r}) = R(r) Y_{lm}(l) \quad (\text{spin is left out!})$$

Use radial WF which is constant inside the nuclear radius R



From normalization of WF one determines N :

$$I = \langle \psi | \psi \rangle = \int_0^{\infty} dr r^2 R^2(r) \underbrace{\int dR Y_{lm}^* Y_{lm}}_{=1} = N^2 \int_0^R dr r^2$$
$$= N^2 \frac{R^3}{3} \quad \leadsto \quad N^2 = \frac{3}{R^3}$$

$$\text{Calculate } B(E\ell, 0 \rightarrow \ell) = \frac{1}{2\ell+1} \sum_{m=-\ell}^{+\ell} |\langle \ell m | Q_{\ell m} | 00 \rangle|^2 \quad (1)$$

Consider the matrix element

$$\begin{aligned} \langle \ell m | Q_{\ell m} | 00 \rangle &= \int_0^{\infty} r^2 dr \int d\Omega Y_{\ell m}^*(\hat{r}) Q_{\ell m} Y_{00}(\hat{r}) = \\ &= \underbrace{\int_0^R r^2 dr \int d\Omega [N Y_{\ell m}^*(\ell)] [e^{-r^2} Y_{\ell m}(\ell)] [N \cdot Y_{00}]}_{\substack{\text{R} \\ "1/\sqrt{4\pi}"}} = \\ &= \frac{N^2 e}{\sqrt{4\pi}} \int_0^R r^{\ell+2} dr \underbrace{\int d\Omega Y_{\ell m}^* Y_{\ell m}}_{=1} = \frac{N^2 e}{\sqrt{4\pi}} \frac{R^{\ell+3}}{\ell+3} = \frac{3e}{\sqrt{4\pi}} \frac{R^\ell}{\ell+3} \end{aligned} \quad (2)$$

$N^2 = 3/R^3$

Therefore, the $B(E\ell)$ -value becomes

$$B(E\ell, 0 \rightarrow \ell) \stackrel{(1)}{=} \sum_{m=-\ell}^{+\ell} \underbrace{\frac{e^2}{4\pi} \left(\frac{3R^\ell}{\ell+3} \right)^2}_{= 2\ell+1} = (2\ell+1) \frac{e^2}{4\pi} \left(\frac{3R^\ell}{\ell+3} \right)^2$$

In summary:

$$B(E\ell, 0 \rightarrow \ell)_{\text{Weisskopf}} = e^2 \left(\frac{2\ell+1}{4\pi} \right) \left(\frac{3R^\ell}{\ell+3} \right)^2 \quad \text{"Weisskopf unit"}$$

The $B(E\ell)$'s are usually quoted in units of

$$[e^2 \cdot \text{fm}^{2\ell}]$$

or, more commonly in units of

$$[e^2 \cdot \text{barn}^\ell]$$

where

$$1 \text{ barn} = 1 \text{ b} = 100 \text{ fm}^2$$