Chapter 3

Nuclear Shell Model

March 30, 2017

Checklist

- Review what will learned so far
- Single particle Hamiltonian: Harmonic Oscillator and Woods-Saxon
- Discussion on evidences of nuclear shell effects: Try to propose an alternate picture
- Evolution of shell structure in unstable nuclei
- Shell model from a perturbation perspective
- Homeworks and projects

Key concepts we learned in the first section

- Nuclear binding energy and separation energy
- Hermitian operator
- Commutation relation and representation
- Parity
- Angular momentum coupling
- One-particle Hamiltonian (in one dimension)
- Unbound states

Given two operators and their eigenstates as

$$\hat{A}|\alpha\rangle = a|\alpha\rangle \quad \text{and} \quad \hat{B}|\beta\rangle = b|\beta\rangle \tag{1.86}$$

and assuming that they commute, i. e. $[\hat{A}, \hat{B}] = 0$, then they have common eigenvalues (see Homework problems 1), i. e.,

$$\hat{A}|\alpha\beta\rangle = a|\alpha\beta\rangle, \quad \hat{B}|\alpha\beta\rangle = b|\alpha\beta\rangle \tag{1.87}$$

Single particle model (Independent-particle model)

$$H^{(0)}\phi(\boldsymbol{r}) = E^{(0)}\phi(\boldsymbol{r}).$$

Spherical coordinates

$$H^{(0)} = \frac{\boldsymbol{p}^2}{2m} + V(r) = \frac{\hat{\boldsymbol{l}}^2}{2mr^2} - \frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + V(r)$$

$$\hat{\boldsymbol{l}}^2 Y_{lm}(\theta\varphi) = \hbar^2 l(l+1)Y_{lm}(\theta\varphi)$$

$$\phi_{nlm}(\boldsymbol{r}) = R_{nl}(r)Y_{lm}(\theta\varphi),$$

It is convenient to replace the radial eigenfunction $R_{nl}(r)$ by the function $u_{nl}(r)$ defined as

$$R_{nl}(r) = u_{nl}(r)/r$$

and the eigenvalue problem acquires the simpler, one dimensional, form,

$$-\frac{\hbar^2}{2\mu}\frac{\mathrm{d}^2}{\mathrm{d}r^2}u_{nl}(r) + \left[\frac{l(l+1)\hbar^2}{2\mu r^2} + V(r)\right]u_{nl}(r) = E_{nl}u_{nl}(r)$$

Quantum Harmonic Oscillator

$$V(r) = m\omega^2 r^2/2.$$

The eigenvalues corresponding to this potential are

$$E_{nl} = (2n + l + \frac{3}{2})\hbar\omega$$

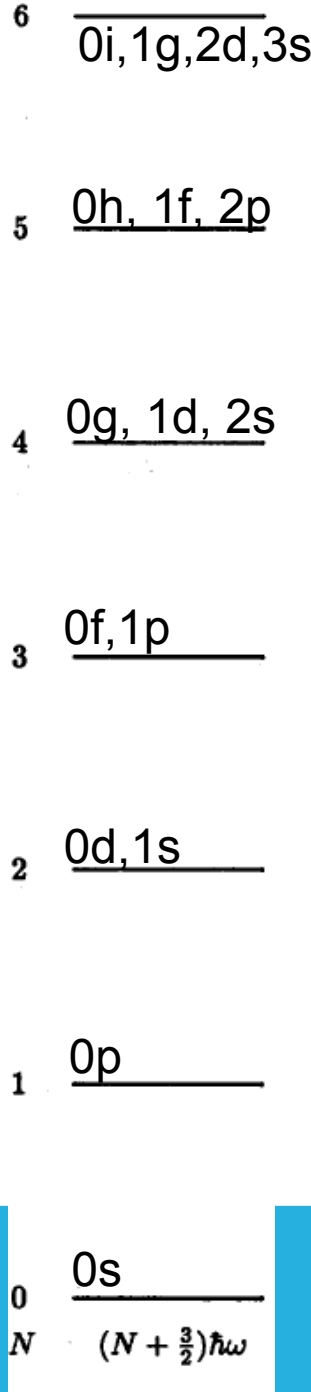
principal quantum number

$$N = 2n + l$$

Popular description
http://en.wikipedia.org/wiki/Quantum_harmonic_oscillator

Energy levels corresponding to an Harmonic oscillator potential

N	n	l	$E_{nl}(\hbar\omega)$	
0	0	0	3/2	0s
1	0	1	1+3/2	0p
2	0	2	2+3/2	0d
	1	0	2+3/2	1s
2	0	3	3+3/2	0f
	1	1	3+3/2	1p
2	0	4	4+3/2	0g
	1	2	4+3/2	1d
	2	0	4+3/2	2s



Empirical formula for $\hbar\omega$

$$\hbar\omega = 45A^{-1/3} - 25A^{-2/3},$$

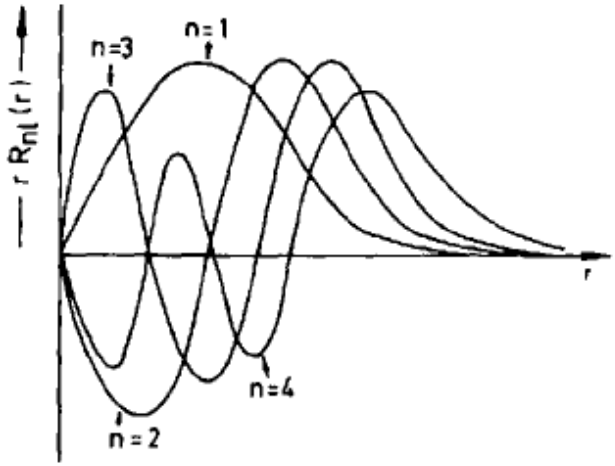
It is in the order of 10MeV

Radial wave function

l, orbital angular momentum
n, number of nodes

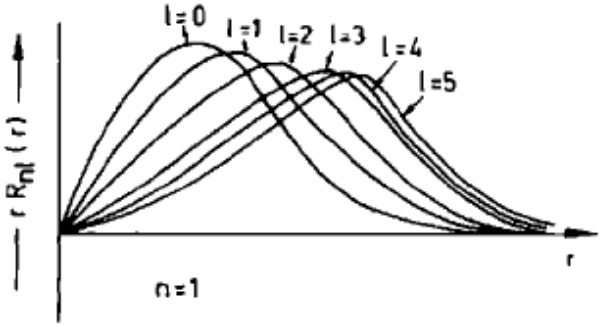
$$R_{nl}(r) = N_{nl}\,\alpha^{3/2} e^{-\alpha^2 r^2/2} (\alpha r)^l f(r^2)$$

$$\alpha = \sqrt{\frac{m\omega}{\hbar}}$$



The normalization factor N_{nl} is given by

$$N_{nl} = \left\{ \frac{2^{n+l+2}}{\sqrt{\pi}(2n+2l+1)!!} \right\}^{1/2},$$



such that

$$\int_0^\infty |R_{nl}(r)|^2 r^2 dr = 1.$$

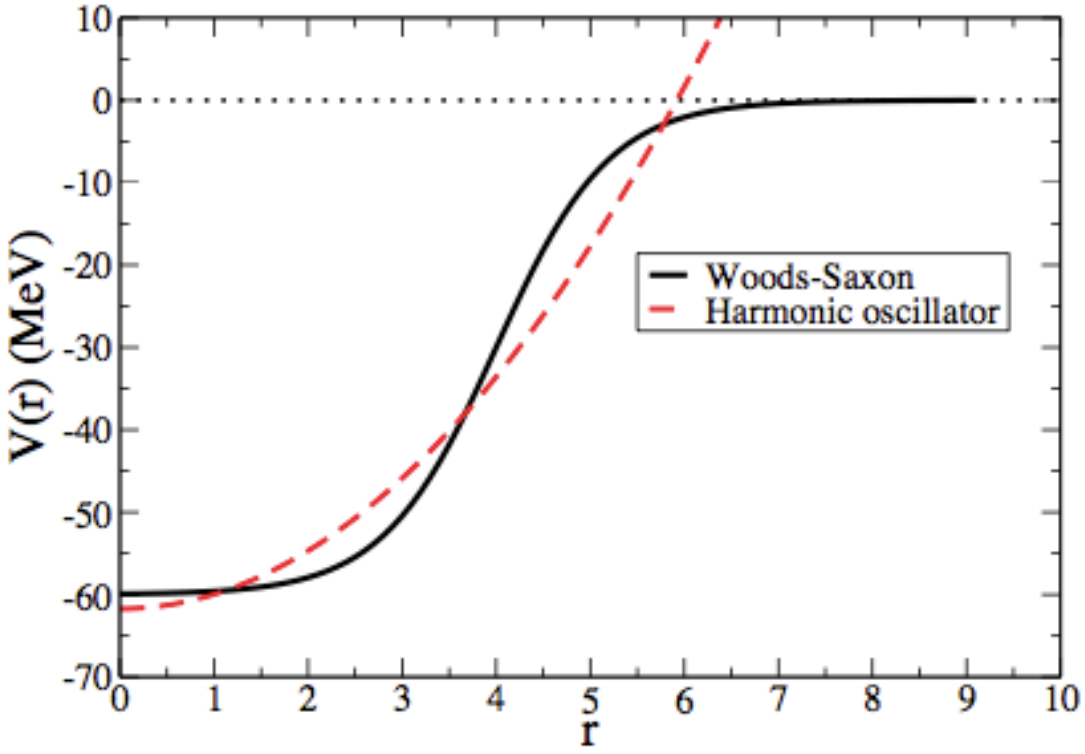
The double folding factor is defined as

$$n!! = n(n-2)(n-4)\cdot\ldots\,(2 \text{ or } 1)$$

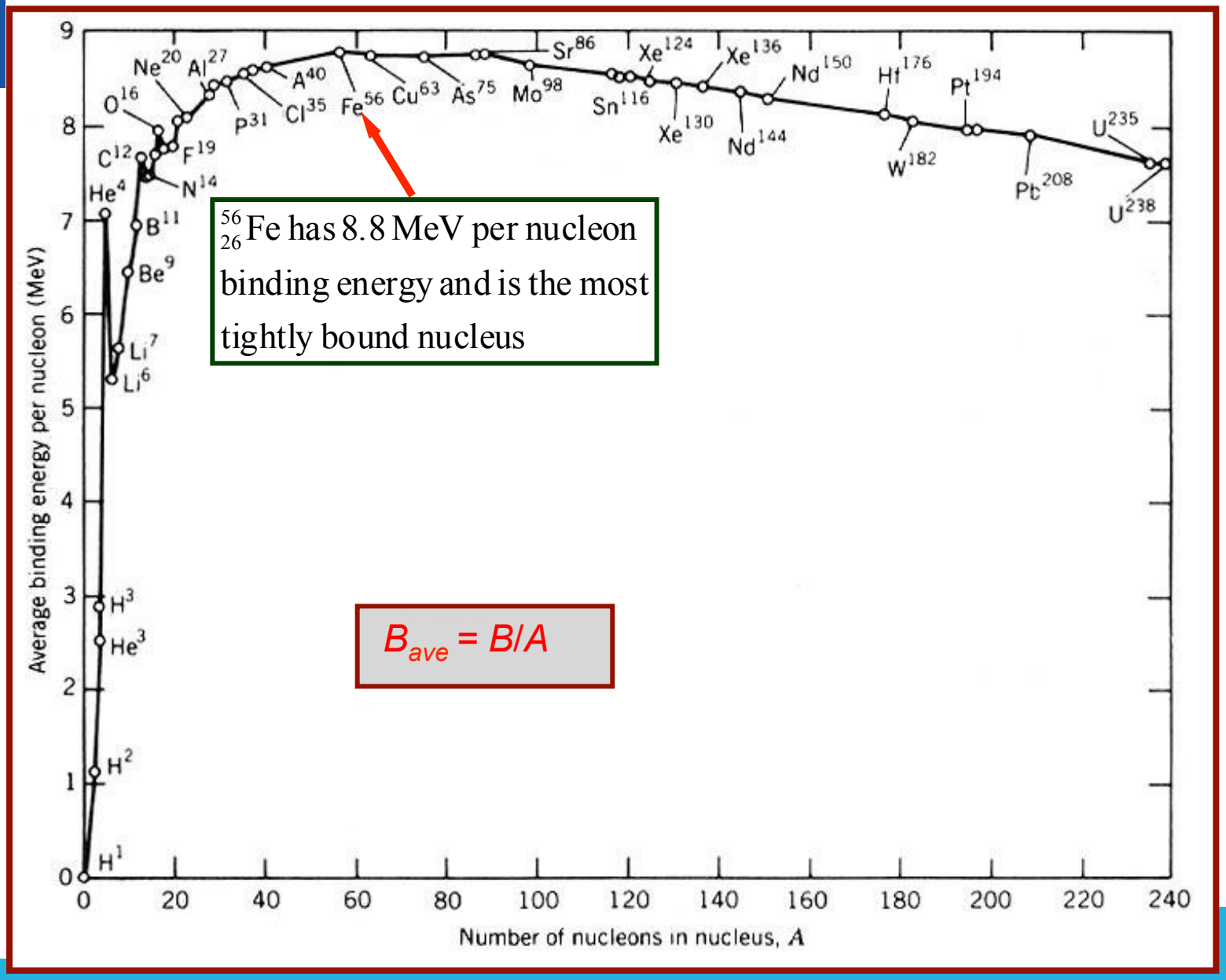
Table 3.1: Energy levels corresponding to an Harmonic oscillator potential of frequency ω. The states are labelled by $N = 2n + l$. The energies E_{nl} are in units of $\hbar\omega$. D_l is the degeneracy of the state (n, l).

N	n	l	E_{nl}	$\|nl\rangle$	parity	$D_l = 2(2l+1)$	$\sum D_l$
0	0	0	3/2	0s	+	2	2
1	0	1	1+3/2	0p	-	6	8
2	0	2	2+3/2	0d	+	10	20
	1	0	2+3/2	1s	+	2	
3	0	3	3+3/2	0f	-	14	40
	1	1	3+3/2	1p	-	6	
4	0	4	4+3/2	0g	+	18	70
	1	2	4+3/2	1d	+	10	
	2	0	4+3/2	2s	+	2	

$$\hbar\omega = 45A^{-1/3} - 25A^{-2/3},$$



The average binding energy per nucleon versus mass number *A*



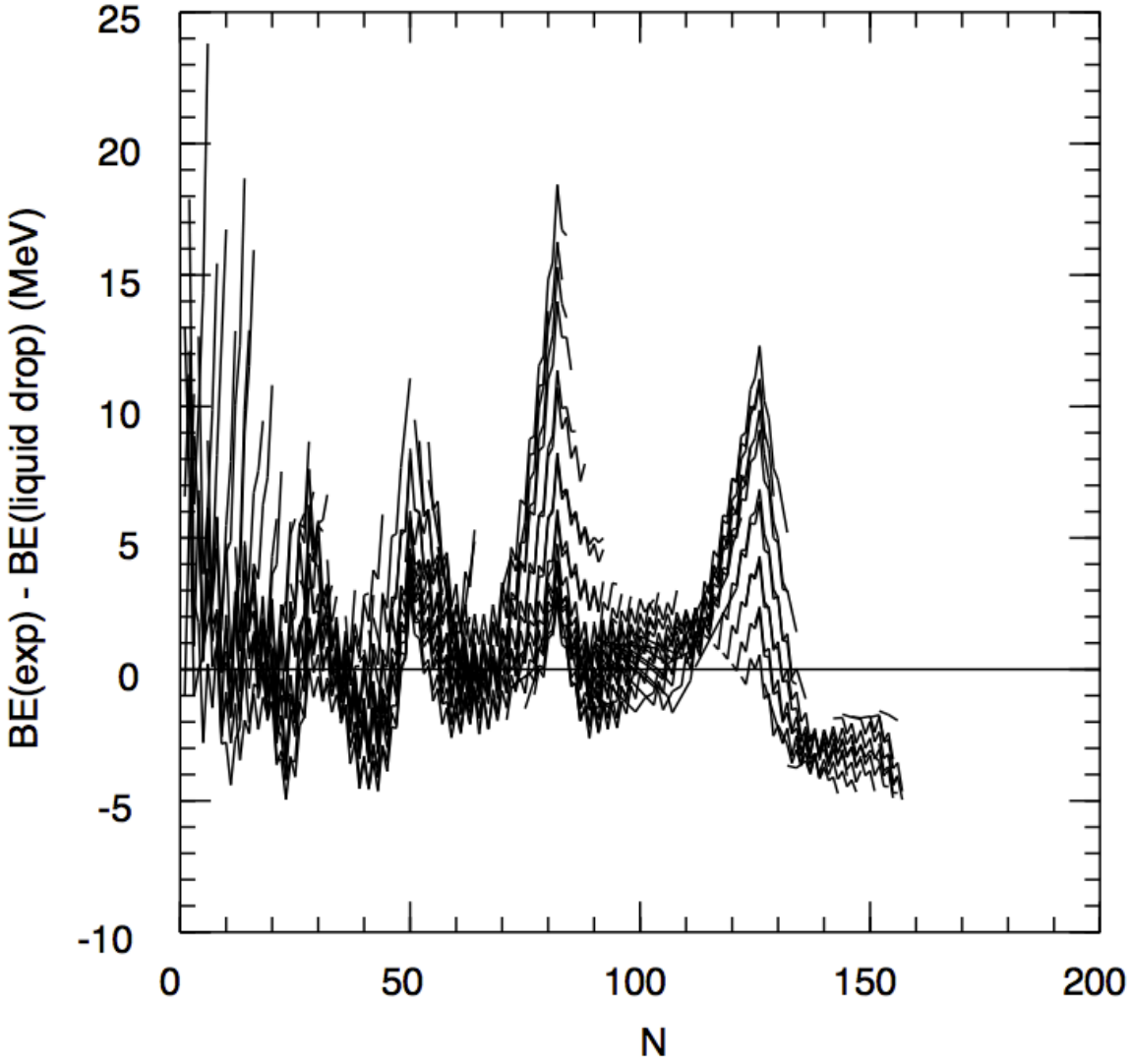
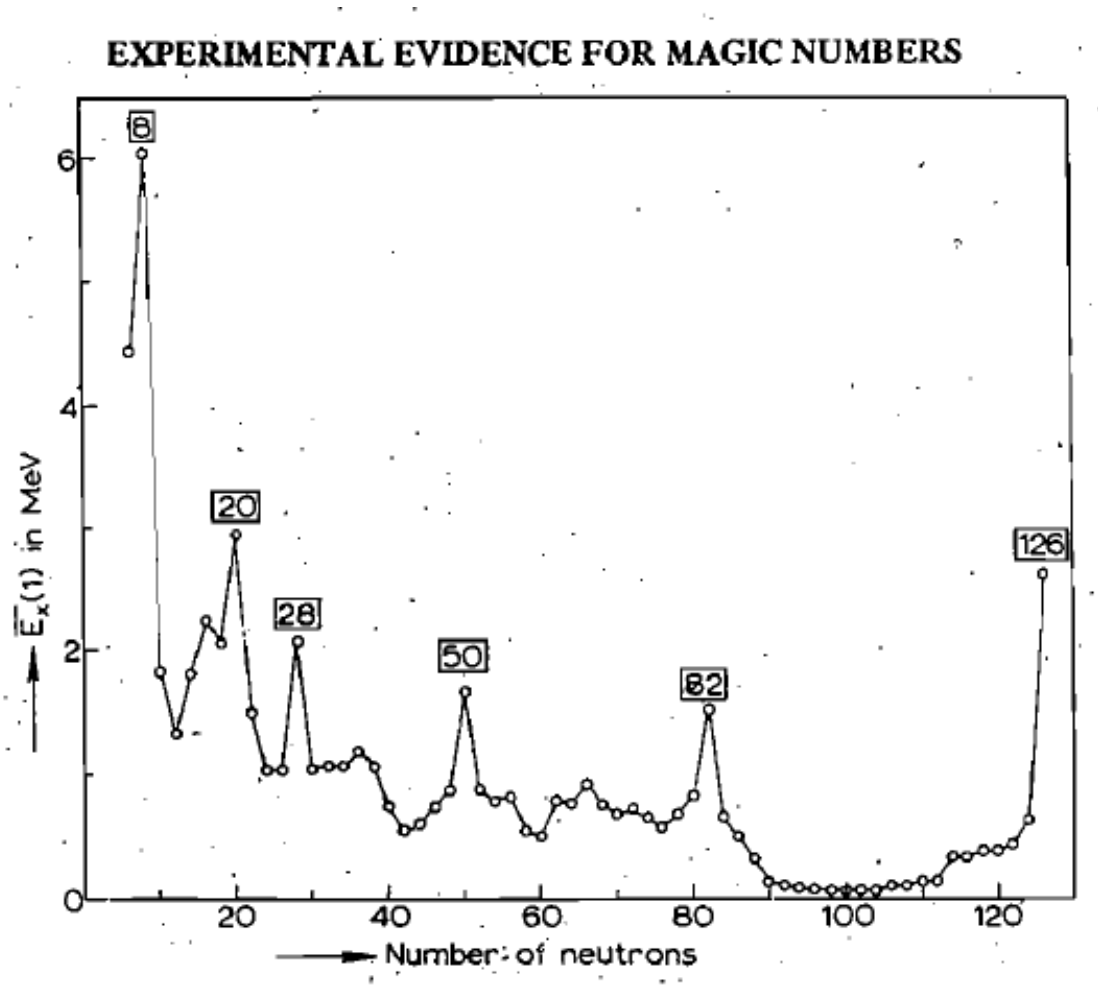


Figure 17: The difference between the experimental and liquid-drop binding energies as a function of N. The dashed lines show the magic numbers 28, 50, 82 and 126.

1. The binding energies of magic-number nuclei is much larger than in the neighboring nuclei. Thus larger energy is required to separate a single nucleon from magic nuclei.
2. The number of stable nuclei with magic values of Z or N is much larger than the corresponding number in neighboring nuclei.
3. Naturally occurring isotopes with magic Z or N have greater relative abundances.
4. The first excited states in nuclei with magic numbers of neutrons or protons lie at higher energies than the same states in neighboring nuclei.
5. Electric quadrupole moments of magic-number nuclei is zero as expected in closed shell nuclei, since they should be spherically symmetric.
6. The energy of alpha or beta particles emitted by magic-number radioactive nuclei is larger than that from other nuclei.



Average excitation energy of the first excited states in doubly even nuclei

The neutron separation energies

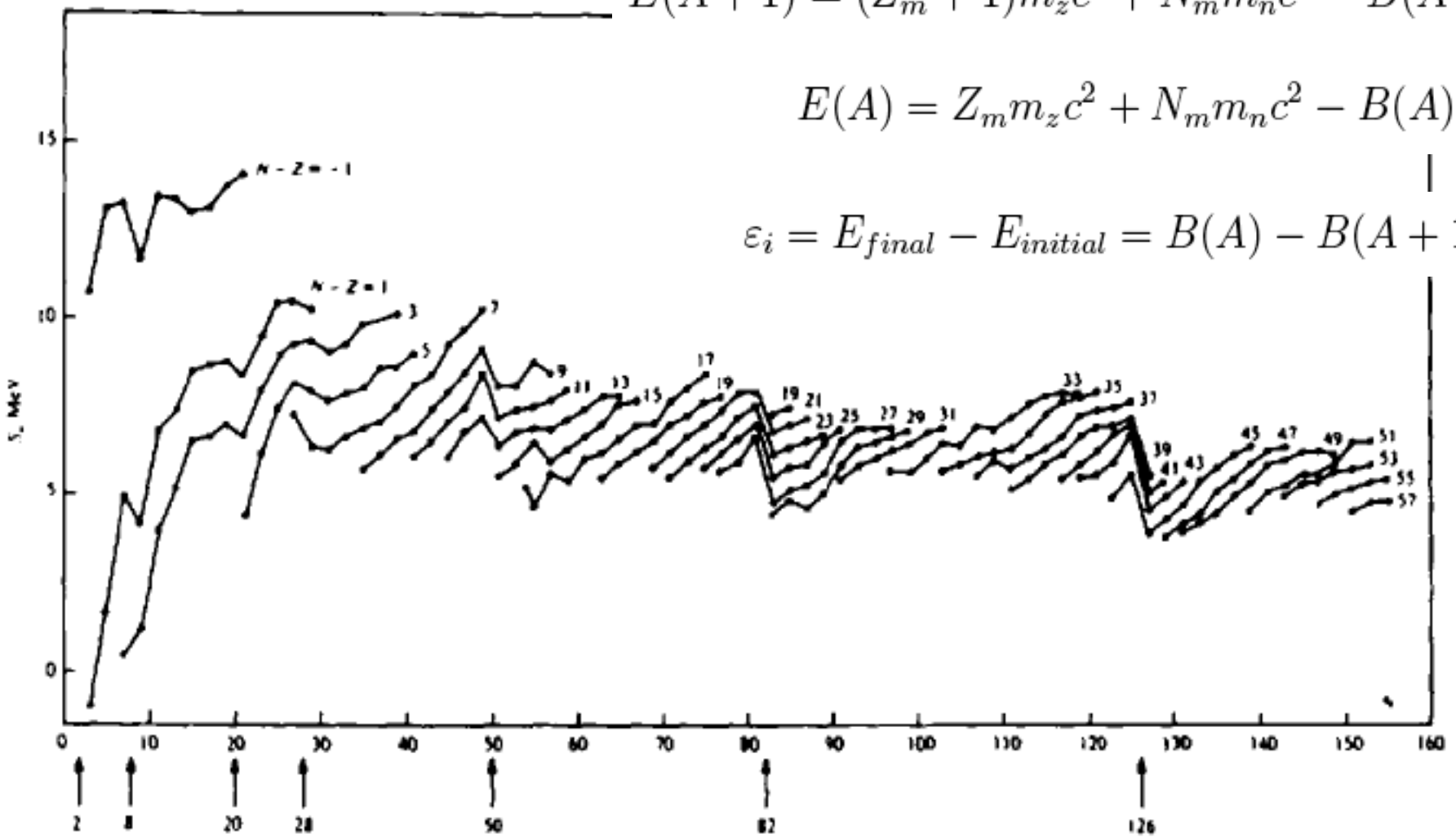
The energy ε_i is the one needed to separate the particle

$$ {}^{A+1}_{Z_m+1}X_{N_m} \longrightarrow \text{proton} + {}^{A}_{Z_m}Y_{N_m} $$

$$ E(A+1) = (Z_m+1)m_z c^2 + N_m m_n c^2 - B(A+1) $$

$$ E(A) = Z_m m_z c^2 + N_m m_n c^2 - B(A) $$

$$ \varepsilon_i = E_{final} - E_{initial} = B(A) - B(A+1) $$



Spin-orbit interaction

Maria Goeppert Mayer, On Closed Shells in Nuclei, Phys. Rev. 75, 1969 (1949)

Thanks are due to Enrico Fermi for the remark, "Is there any indication of spin-orbit coupling?" which was the origin of this paper.

The spin-orbit potential has the form

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2 + V_{so}(r)\, \boldsymbol{l} \cdot \boldsymbol{s}$$

It is found experimentally that V_{ls} is negative, which means that the state with $j = l + 1/2$ is always energetically below the $j = l - 1/2$ level.

Osc. No.	Square well	Spect. term	Spin term	No. of states	Shells	Total No.
0	$1s$	$1s$	$1s_{1/2}$	2	2	2
			$1p_{1/2}$	4		
1	$1p$	$2p$	$1p_{3/2}$	2	6	8
	$1d$	$3d$	$1d_{5/2}$	6		
2			$1d_{3/2}$	4	12	
	$2s$	$2s$	$2s_{1/2}$	2		20
			$1f_{7/2}$	8	8?	28?
	$1f$	$4f$	$1f_{5/2}$	6		
3			$2p_{3/2}$	4	22	
	$2p$	$3p$	$2p_{1/2}$	2		
			$1g_{9/2}$	10		50
	$1g$	$5g$				
			$1g_{7/2}$	8		
4			$2d_{5/2}$	6		
	$2d$	$4d$	$2d_{3/2}$	4	32	
	$3s$	$3s$	$3s_{1/2}$	2		
			$1h_{11/2}$	12		82
	$1h$	$6h$				
			$1h_{9/2}$	10		
5			$2f_{7/2}$	8		
	2	$5f$	$2f_{5/2}$	6	44	
			$3p_{3/2}$	4		
	$3p$	$4p$	$3p_{1/2}$	2		
			$1i_{13/2}$	14		126
	$1i$	$7i$				
			$1i_{11/2}$			
6	$2g$	$6g$				
	$3d$	$5d$				
	$4s$	$4s$				

The Nobel Prize in Physics 1963

Eugene Wigner, Maria Goeppert-Mayer, J. Hans D. Jensen

The Nobel Prize in Physics 1963

Eugene Wigner

Maria Goeppert-Mayer

J. Hans D. Jensen

Eugene Paul Wigner

Maria Goeppert-Mayer

J. Hans D. Jensen

The Nobel Prize in Physics 1963 was divided, one half awarded to Eugene Paul Wigner "for his contributions to the theory of the atomic nucleus and the elementary particles, particularly through the discovery and application of fundamental symmetry principles",the other half jointly to Maria Goeppert-Mayer and J. Hans D. Jensen "for their discoveries concerning nuclear shell structure".

http://nobelprize.org/nobel_prizes/physics/laureates/1963/

$$H = \frac{\boldsymbol{p}^2}{2m} + \frac{1}{2}m\omega^2 r^2 + V_{so}(r)\,\boldsymbol{l}\cdot\boldsymbol{s}$$

$$\boldsymbol{j}^2 = \boldsymbol{l}^2 + \boldsymbol{s}^2 + 2\,\boldsymbol{l}\cdot\boldsymbol{s}$$

$$\boldsymbol{l}\cdot\boldsymbol{s} = (\boldsymbol{j}^2 - \boldsymbol{l}^2 - \boldsymbol{s}^2)/2$$

with the basis $|nlsjm\rangle$

$$\boldsymbol{l}\cdot\boldsymbol{s}|nlsjm\rangle = \frac{\hbar^2}{2}\big[j(j+1) - l(l+1) - s(s+1)\big]|nlsjm\rangle$$

the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2}u_{nl}(r) + \left\{\frac{l(l+1)\hbar^2}{2mr^2} + \frac{1}{2}m\omega^2 r^2 + \right.$$
$$\left. + \frac{\hbar^2}{2}\big[j(j+1) - l(l+1) - 3/4\big]V_{so}(r)\right\}u_{nl}(r) = E_{nl}u_{nl}(r)$$

$$|l_1 m_1 l_2 m_2\rangle \quad \text{or} \quad |l_1 l_2 l m\rangle \tag{1.91}$$

and, therefore, the standard projectors are

$$\sum_{l_1 m_1 l_2 m_2} |l_1 m_1 l_2 m_2\rangle\langle l_1 m_1 l_2 m_2| = \hat{I} \quad \text{or} \quad \sum_{l_1 l_2 l m} |l_1 l_2 l m\rangle\langle l_1 l_2 l m| = \hat{I} \tag{1.92}$$

One can write the vector in one representation in terms of the other representation, for instance

$$|l_1 m_1 l_2 m_2\rangle = \sum_{l m} |l_1 l_2 l m\rangle\langle l_1 l_2 l m|l_1 m_1 l_2 m_2\rangle, \tag{1.93}$$

and

$$|l_1 m_1 l_2 m_2\rangle = \sum_{l m} \langle l_1 m_1 l_2 m_2|l m\rangle|l_1 l_2 l m\rangle \tag{1.94}$$

The number $\langle l_1 m_1 l_2 m_2|l m\rangle = \langle l_1 l_2 l m|l_1 m_1 l_2 m_2\rangle$ is real and is called Clebsch-Gordan coefficient. Due to the orthonormality of the basis elements

$$|l_1 l_2 l m\rangle = \sum_{m_1 m_2} \langle l_1 m_1 l_2 m_2|l m\rangle|l_1 m_1 l_2 m_2\rangle \tag{1.95}$$

The Clebsch-Gordan coefficient can best be written in terms of the 3-j symbol defined as

$$\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & -m \end{pmatrix} = \frac{(-1)^{l_1-l_2+m}}{\sqrt{2l+1}} \langle l_1 m_1 l_2 m_2 | l m \rangle \tag{1.96}$$

with the properties that

1. $\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & m \end{pmatrix} = \begin{pmatrix} l_2 & l & l_1 \\ m_2 & m & m_1 \end{pmatrix} = \begin{pmatrix} l & l_1 & l_2 \\ m & m_1 & m_2 \end{pmatrix}$
2. $\begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & m \end{pmatrix} = (-1)^{l_1+l_2+l} \begin{pmatrix} l_2 & l_1 & l \\ m_2 & m_1 & m \end{pmatrix}$
3. $\begin{pmatrix} l_1 & l_2 & l \\ -m_1 & -m_2 & -m \end{pmatrix} = (-1)^{l_1+l_2+l} \begin{pmatrix} l_1 & l_2 & l \\ m_1 & m_2 & m \end{pmatrix}$
4. $m_1 + m_2 - m = 0$

Consider a problem with *two* angular momenta $\hat{\mathbf{L}}$ and $\hat{\mathbf{S}}$,
They each have a set of eigenstates

$$\hat{\mathbf{L}}^2|lm_l\rangle = l(l+1)|lm_l\rangle \quad ; \; \hat{\mathbf{S}}^2|sm_s\rangle = s(s+1)|sm_s\rangle$$
$$\hat{L}_3|lm_l\rangle = m_l|lm_l\rangle \quad ; \; \hat{S}_3|sm_s\rangle = m_s|sm_s\rangle$$

The two angular momenta are then described in the *direct-product space*

$$|lm_l sm_s\rangle \equiv |lm_l\rangle|sm_s\rangle \quad ; \text{ direct-product space}$$

Since they act in different spaces, the operators $\mathbf{L}$ and $\mathbf{S}$ commute with each other

$$[\hat{L}_i, \hat{S}_j] = 0 \quad ; \text{ different spaces}$$

Thus the operators $\{\hat{\mathbf{L}}^2, \hat{L}_3, \hat{\mathbf{S}}^2, \hat{S}_3\}$ all commute with each other

$$\{\hat{\mathbf{L}}^2, \hat{L}_3, \hat{\mathbf{S}}^2, \hat{S}_3\} \quad ; \text{ mutually commuting}$$

The direct-product states are evidently eigenstates of these mutually commuting hermitian operators

$$\begin{aligned}
\hat{\mathbf{L}}^2|lm_l sm_s\rangle &= l(l+1)|lm_l sm_s\rangle \quad ; \hat{L}_3|lm_l sm_s\rangle = m_l|lm_l sm_s\rangle \\
\hat{\mathbf{S}}^2|lm_l sm_s\rangle &= s(s+1)|lm_l sm_s\rangle \quad ; \hat{S}_3|lm_l sm_s\rangle = m_s|lm_l sm_s\rangle
\end{aligned} \tag{3.67}$$

There are $(2l+1)\times(2s+1)$ states in this direct-product basis.

Now introduce the *total angular momentum*

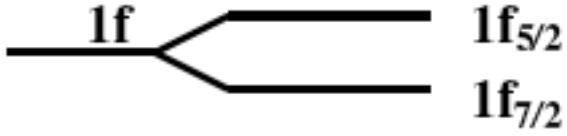
$$\hat{\mathbf{J}} \equiv \hat{\mathbf{L}} + \hat{\mathbf{S}} \tag{3.68}$$

one may assume $V_{so}(r) = -V_0$.

$$\left[j(j+1) - l(l+1) - 3/4\right] V_{so}(r) = -V_0 \begin{cases} l; & j = l + 1/2 \\ -l-1; & j = l - 1/2 \end{cases}$$

The total angular momentum quantum number $j = l \pm 1/2$ of the nucleon is denoted by an extra index j: $\mathrm{nl_j}$

e.g. the 1f state splits into a $1f_{7/2}$ and a $1f_{5/2}$ state



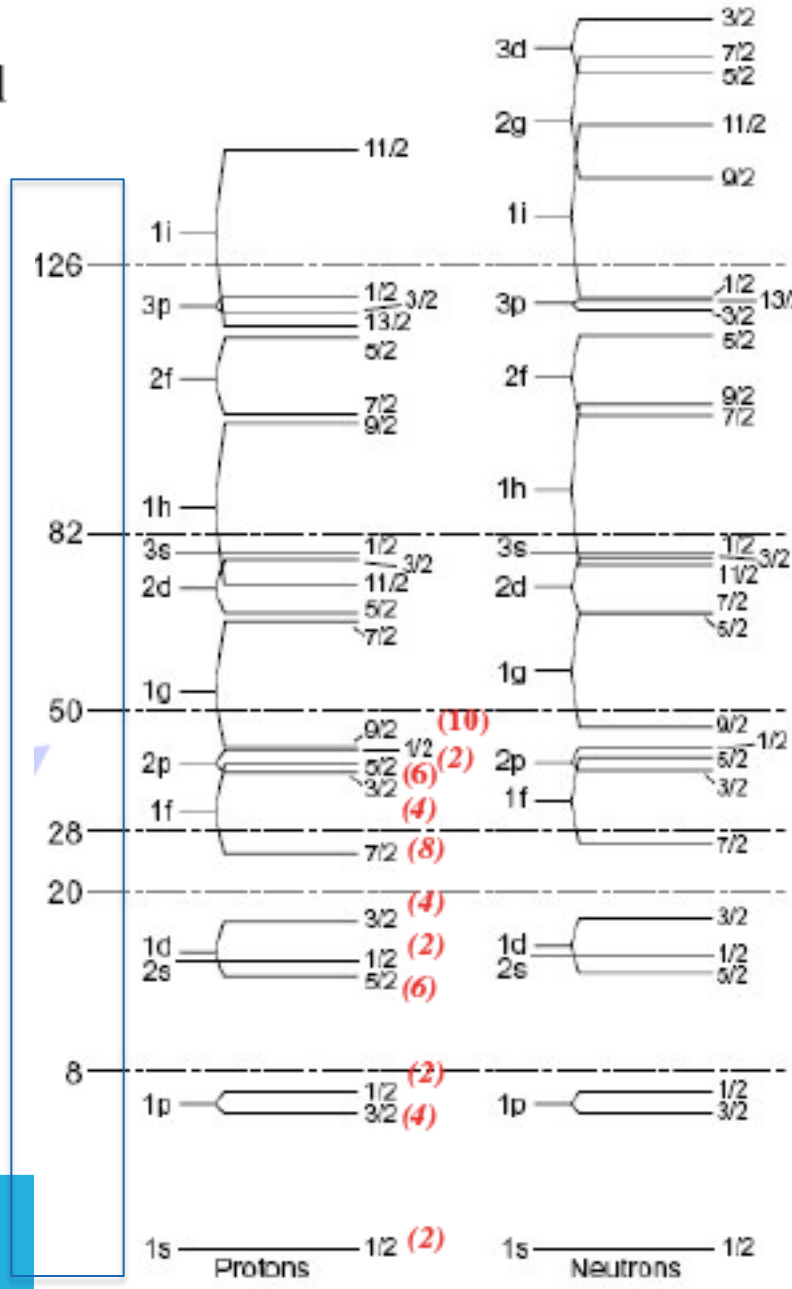
The *nlj* level is (2*j* + 1) times degenerate

Single particle energy levels:

➔ **Spin-orbit interaction** leads to a **sizeable splitting of the energy states** which are indeed comparable with the gaps between the *nl* shells themselves.

Magic numbers appear when the gaps between successive energy shells are particularly large.

2, 8, 20, 28, 50, 82, 126



As always

$$\hat{\mathbf{J}}^2 = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2 \tag{3.69}$$

The commutation relations for $\hat{\mathbf{J}}$ follow immediately from the above

$$\begin{aligned} [\hat{J}_i\,, \hat{J}_j] &= i\epsilon_{ijk}\hat{J}_k \\ [\hat{\mathbf{J}}^2\,, \hat{J}_i] &= 0 \end{aligned} \tag{3.70}$$

The square of the total angular momentum is now also given by

$$\hat{\mathbf{J}}^2 = \hat{\mathbf{L}}^2 + \hat{\mathbf{S}}^2 + 2\hat{\mathbf{L}}\cdot\hat{\mathbf{S}} \tag{3.71}$$

Since the square of an angular momentum commutes with all of its components, the operators $\{\hat{\mathbf{L}}^2, \hat{\mathbf{S}}^2, \hat{\mathbf{J}}^2, \hat{J}_3\}$ all commute with each other

$$\{\hat{\mathbf{L}}^2, \hat{\mathbf{S}}^2, \hat{\mathbf{J}}^2, \hat{J}_3\} \qquad ;\ \text{mutually commuting} \tag{3.72}$$

We make some comments on this result:

- The spectrum of eigenvalues of the total angular momentum follows from our general analysis in the previous section;
- The eigenvalues of $(\hat{\mathbf{S}}^2, \hat{\mathbf{L}}^2)$ must remain the same due to the orthogonality of the eigenstates of hermitian operators;
- The goal now is to express the eigenstates of total angular momentum in terms of the direct product basis in Eqs. (3.64)

$$|lsjm_j\rangle = \sum_{m_l, m_s} \langle lm_l sm_s | lsjm_j \rangle \, |lm_l sm_s\rangle \quad ; \text{C-G coefficients} \quad (3.74)$$

The numerical transformation coefficients $\langle lm_l sm_s | lsjm_j \rangle$ in this expression are known as the *Clebsch-Gordan (C-G) coefficients.*

The commutation relations

$$[l_x, l_y] \equiv l_x l_y - l_y l_x = \mathrm{i} l_z \,,$$

$$[s_x, s_y] = \mathrm{i}\, s_z$$

$$[j_x, j_y] = \mathrm{i}\, j_z$$

$$[l^2, l_k] = 0 \quad \text{for} \quad k = x,y,z$$

$$[s^2, s_k] = 0 \quad \text{for} \quad k = x,y,z \,.$$

$$[l, s] = 0 \,.$$

$$l^2 \psi_{l\frac{1}{2}jm} = l(l+1)\, \psi_{l\frac{1}{2}jm} \,,$$

$$s^2 \psi_{l\frac{1}{2}jm} = \tfrac{1}{2}(\tfrac{1}{2}+1)\, \psi_{l\frac{1}{2}jm} = \tfrac{3}{4} \psi_{l\frac{1}{2}jm} \,,$$

$$j^2 \psi_{l\frac{1}{2}jm} = j(j+1)\, \psi_{l\frac{1}{2}jm}$$

$$j_z \psi_{l\frac{1}{2}jm} = m \psi_{l\frac{1}{2}jm}$$

$$m = -j, -j+1, \ldots, j-1, j$$

Since we assume that the nucleon-core potential is spherically symmetric the quantum numbers $l.j, m$ are conserved (as discussed in the previous Chapter). This potential will also be assumed to be invariant under reflections, and therefore the parity π of the state $|nljm>$ will also be conserved. To find the value of the parity one has to analyze the Spherical Harmonics $Y_{lm_l}(\theta\varphi)$ which, for $m_l \geqslant 0$, is given by

$$Y_{lm_l}(\theta\varphi) = \sqrt{\frac{2l+1}{4\pi}}\sqrt{\frac{(l-m_l)!}{(l+m_l)!}}(-1)^{m_l}\mathrm{e}^{\mathrm{i}m_l\varphi}P_l^{m_l}(\cos\theta) \tag{3.32}$$

where

$$P_l^{m_l}(\xi) = \frac{(-1)^{m_l}}{2^l l!}\frac{(l+m_l)!}{(l-m_l)!}(1-\xi^2)\frac{\mathrm{d}^{l-m_l}}{\mathrm{d}\xi^{l-m_l}}(\xi^2-1)^l \tag{3.33}$$

For $m_l < 0$ it is,

$$Y_{lm_l}(\theta\varphi) = (-1)^{m_l}Y^*_{l-m_l}(\theta\varphi) \tag{3.34}$$

The parity transformation corresponds to $\boldsymbol{r} \longrightarrow -\boldsymbol{r}$, that is $(r, \theta, \varphi) \longrightarrow (r, \pi - \theta, \varphi + \pi)$, and since for spherically symmetric potentials the value of r is the same for all values of the angles, only the transformation of the Spherical Harmonics has to be considered. Therefore one finds,

$$\Psi_{nljm}(-\boldsymbol{r}) \quad \longrightarrow \quad (-1)^l \Psi_{nljm}(\boldsymbol{r}) \tag{3.35}$$

We have seen that the parity associated to this wave function is $(-1)^l$ and since $N = 2n + l$ the parity also is $(-1)^N$. That is, all the states in a band corresponding to the quantum number N has the same parity.

Symmetries

For a given state, n, l, j, s, j_z(m), parity are good quantum numbers

$[\boldsymbol{l}, \boldsymbol{s}] = 0$.

The spherical harmonics all possess definite parity

$\boldsymbol{r} \to -\boldsymbol{r}, \quad ; r \to r, \theta \to \pi - \theta, \phi \to \pi + \phi$

$$\Pi^{\mathrm{op}} Y_{lm}(\theta, \phi) = Y_{lm}(\pi - \theta, \pi + \phi) = (-1)^l Y_{lm}(\theta, \phi) .$$

$$\Pi^{\mathrm{op}} f(\boldsymbol{r}) = f(-\boldsymbol{r}) = \Pi f(\boldsymbol{r})$$

Parity for the system

$$\pi = \prod_{i=1}^{A} (-1)^{\ell_i}$$

Angular momentum of the system

$$\vec{J} = \sum_{i=1}^{n} \vec{j}_i$$

$$\chi_{1/2} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad m_s = +\tfrac{1}{2} \text{ (spin up)} \qquad \text{and}$$

$$\chi_{-1/2} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \qquad m_s = -\tfrac{1}{2} \text{ (spin down)}$$

The eigenvalues of s_x and s_y are also $\frac{1}{2}$ and $-\frac{1}{2}$. The s_x and s_y matrices cannot be diagonal if s_z is diagonal. This follows from the commutation relations satisfied by the components (3.17), namely

$$\boxed{[s_x, s_y] = is_z \qquad [s_z, s_x] = is_y \qquad [s_y, s_z] = is_x} \tag{3.19}$$

$$s_x = \tfrac{1}{2}\sigma_x = \tfrac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$s_y = \tfrac{1}{2}\sigma_y = \tfrac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$s_z = \tfrac{1}{2}\sigma_z = \tfrac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\psi_{nlj=l+1/2,m} = \begin{pmatrix} \sqrt{\frac{l+\frac{1}{2}+m}{2l+1}}\phi_{nlm-1/2} \\ \sqrt{\frac{l+\frac{1}{2}-m}{2l+1}}\phi_{nlm+1/2} \end{pmatrix}$$

$$= \sqrt{\frac{l+\frac{1}{2}+m}{2l+1}}\phi_{nlm-1/2}\chi_{1/2} + \sqrt{\frac{l+\frac{1}{2}-m}{2l+1}}\phi_{nlm+1/2}\chi_{-1/2}$$

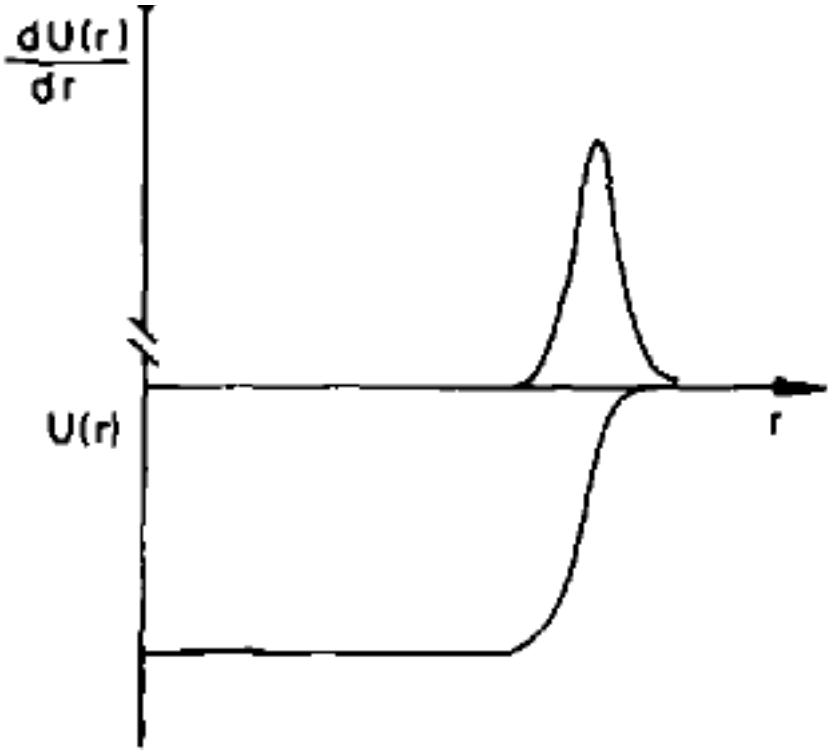
$$\psi_{nlj=l-1/2,m} = \begin{pmatrix} \sqrt{\frac{l+\frac{1}{2}-m}{2l+1}}\phi_{nlm-1/2} \\ -\sqrt{\frac{l+\frac{1}{2}+m}{2l+1}}\phi_{nlm+1/2} \end{pmatrix}$$

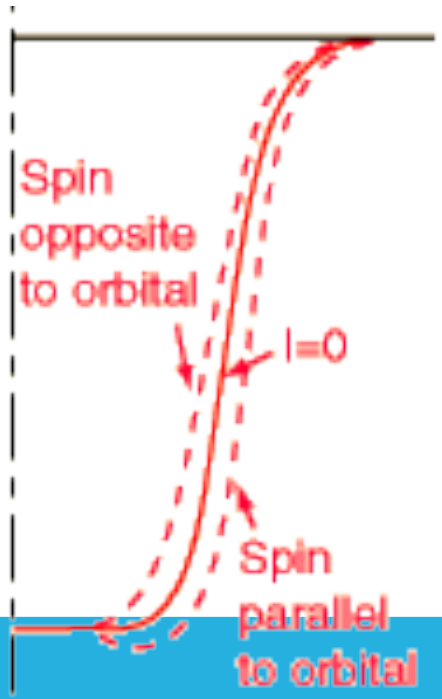
$$= \sqrt{\frac{l+\frac{1}{2}-m}{2l+1}}\phi_{nlm-1/2}\chi_{1/2}$$

$$- \sqrt{\frac{l+\frac{1}{2}+m}{2l+1}}\phi_{nlm+1/2}\chi_{-1/2}$$

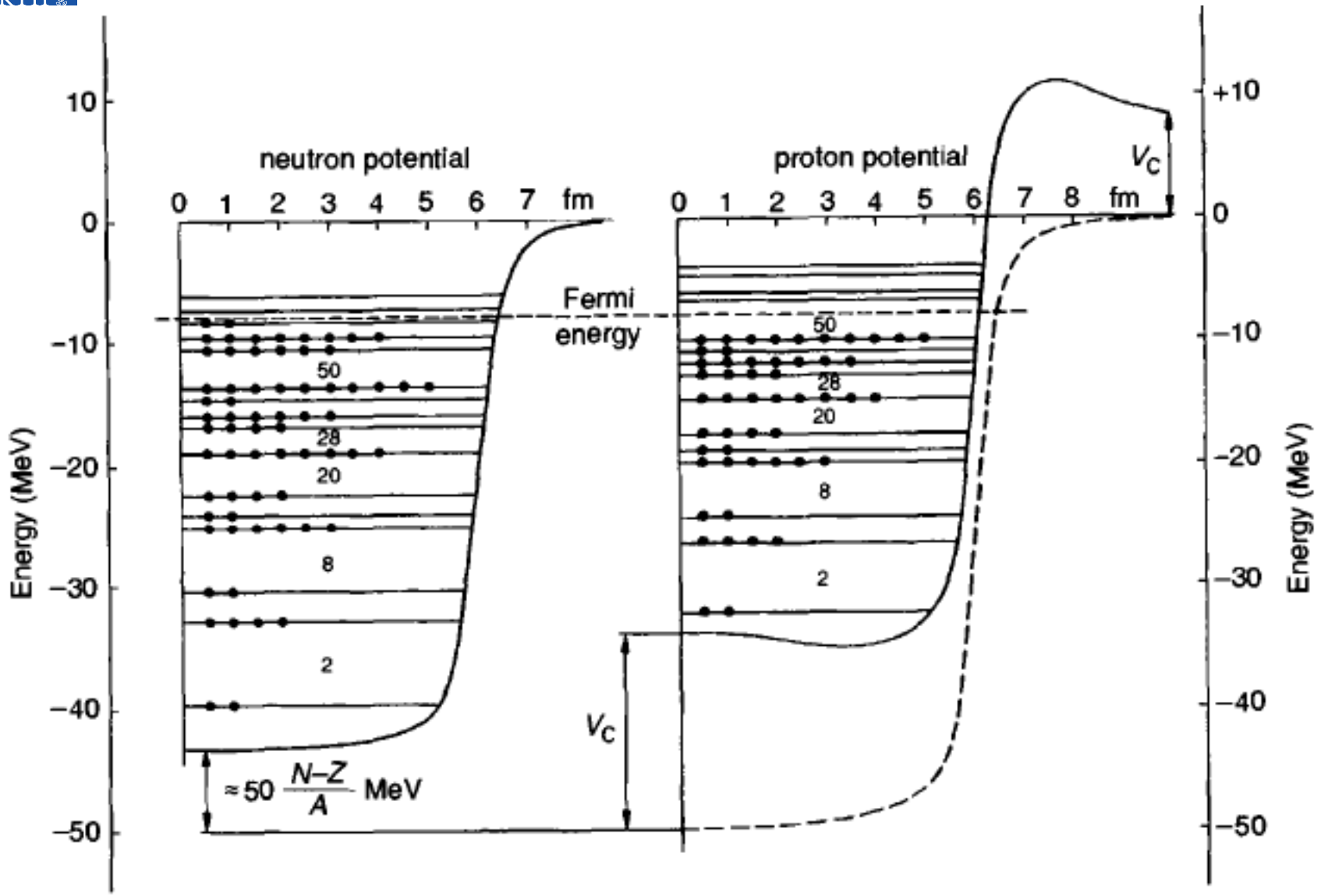
The spin orbit turns out to be mainly a surface effect, being a function of r and connected to the average potential through a relation of the form

$$V_{so}(r) = -V_{so}\frac{1}{r}\frac{dV(r)}{dr}$$





Coulomb effect



The spectra of proton and neutron are similar to each other

Average nuclear potential well: Woods-Saxon

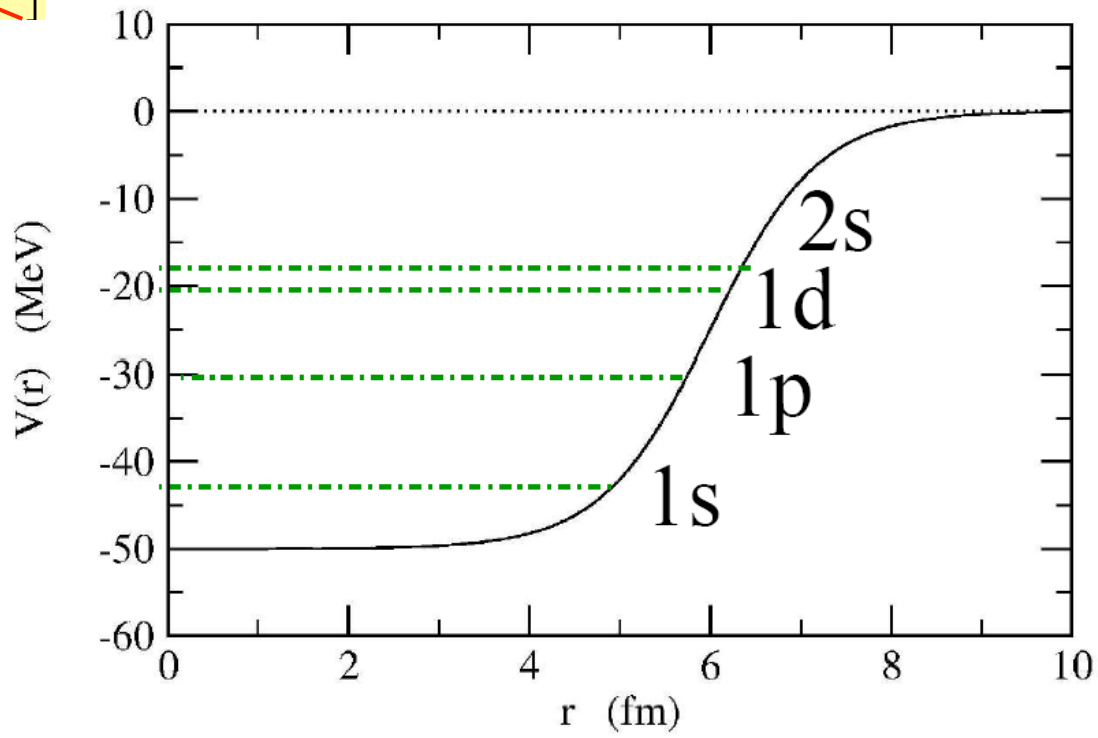
$$\hat{H} = \sum_{i=1}^{A} \frac{\hat{p}_i^2}{2m_i} + \sum_{i<j}^{A} \hat{V}(r_i, r_j)$$

$$\hat{H} = \sum_{i=1}^{A} \left[\frac{\hat{p}_i^2}{2m_i} + \hat{V}(r_i) \right] + \left[\sum_{i<j}^{A} \hat{V}(r_i, r_j) - \sum_{i=1}^{A} \hat{V}(r_i) \right]$$

$$\left[-\frac{\hbar^2}{2 \cdot m} \nabla^2 + V(r) - \varepsilon \right] \Psi(r) = 0$$

$$\Psi(r) = \frac{u_\ell(r)}{r} \cdot Y_{\ell m}(\vartheta, \varphi) \cdot X_{m_s}$$

$$V(r) = -V_0 / \left\{ 1 + \exp\left[(r - R_0)/a \right] \right\}$$

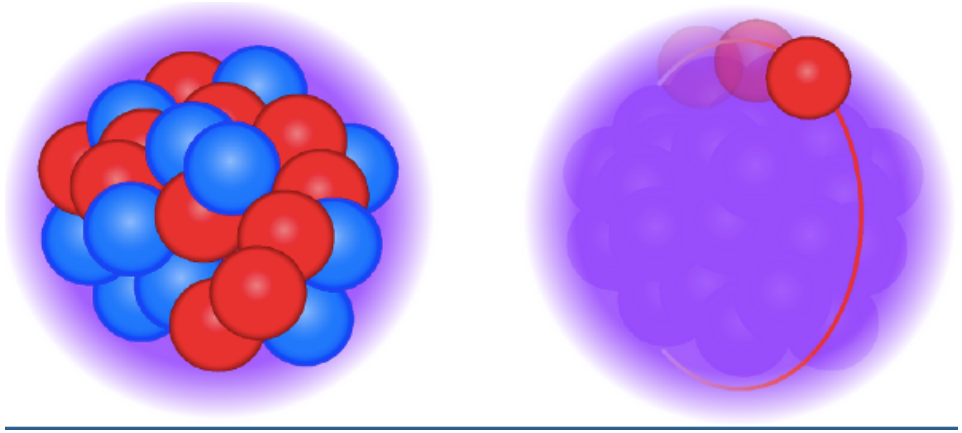


We can re-write the Hamiltonian by adding and subtracting a one-body potential U(r) as

$$\hat{H} = \sum_{i=1}^{A}\left[-\frac{\hbar^2}{2m}\Delta_i + U(i)\right] + \sum_{i<j=1}^{A} W(i,j) - \sum_{i=1}^{A} U(i) = \hat{H}^{(0)} + \hat{V}\,,$$

$H^{(0)}$ is the single particle Hamiltonian describing an ensemble of independent particles moving in an effective average potential. V is called the residual interaction. In some cases it is also denoted as $H^{(1)}$ (recall the perturbation theory).

$$H := H^{(0)} + H^{(1)}\,.$$



The very notion of a mean field is fulfilled when $H^{(1)}$ is small.

The total Hamiltonian is a summation of all single-particle Hamiltonians

$$H_0 = \sum_{i=1}^{A} H_0(i) \tag{3.6}$$

the eigenvectors $|\varphi_{n_i}>$ and eigenvalues ϵ_{n_i} of $H_0(i)$ satisfy

$$H_0(i) < \mathbf{r_i}|\varphi_{\mathbf{n}} >= (\frac{\mathbf{p_i^2}}{\mathbf{2m_i}} + \mathbf{U(r_i)}) < \mathbf{r_i}|\varphi_{\mathbf{n_i}} >= \epsilon_{\mathbf{n_i}} < \mathbf{r_i}|\varphi_{\mathbf{n}} > \tag{3.7}$$

Since the Hamiltonian H_0, with eigenvalues given by

$$H_0|\Psi_\alpha >= E_\alpha|\Psi_\alpha > \ , \tag{3.8}$$

is a sum of the Hamiltonians $H_0(i)$ and the degrees of freedom of different particles are

The total wave function is a product of single particle wave functions

$$\Psi(1,2,\ldots,A) = \prod_{i=1}^{A} \varphi(i)$$

$$< n_1\mathbf{r}_1, n_2\mathbf{r}_2 \ldots . n_A\mathbf{r}_A | \Psi_\alpha >= \Psi_\alpha(n_1\mathbf{r}_1, n_2\mathbf{r}_2, \ldots n_A\mathbf{r}_A) = \varphi_{n_1}(\mathbf{r}_1)\varphi_{n_2}(\mathbf{r}_2)\ldots\varphi_{n_A}(\mathbf{r}_A) \quad (3.9)$$

and the eigenvalues are

$$E_\alpha = \epsilon_{n_1} + \epsilon_{n_2} + \ldots + \epsilon_{n_A} \quad (3.10)$$

From $< \varphi_i | \varphi_j >= \delta_{ij}$, it follows that $< \Psi_\alpha | \Psi_\beta > = \delta_{\alpha\beta}$.

"Quite apart from the problem of the nature of the nuclear constituents themselves, which is not of direct importance for the present discussion, it is, at any rate, clear that the nuclear models hitherto treated in detail are unsuited to account for the typical properties of nuclei for which, as we have seen, energy exchanges between the individual nuclear particles is a decisive factor. In fact, in these models it is, for the sake of simplicity, assumed that the state of motion of each particle in the nucleus can, in the first approximation, be treated as taking place in a conservative field of force, and can therefore be characterized by quantum numbers in a similar way to the motion of an electron in an ordinary atom. In the atom and in the nucleus we have indeed to do with two extreme cases of mechanical many-body problems for which a procedure of approximation resting on a combination of one-body problems, so effective in the former case, loses any validity in the latter ...."

Niels Bohr (1936)

Bohr's criticism had a profound effect on the development of the nuclear shell model. His strong objections discouraged theoretical physicists from using it. Giulio Racah who started to work on nuclear spectroscopy was convinced that the shell model was indeed not valid for nuclei. He then applied the methods he developed to atomic spectroscopy. Calculations of nuclear energies were still carried out by Wigner and Feenberg, Hund, Jahn and some others. Most of their

In r-representation it is,

$$\langle \boldsymbol{r}|nlsjm\rangle = R_{nlj}(r)\left[Y_l(\theta\varphi)\chi_{1/2}\right]_{jm}, \quad R_{nlj}(r) = u_{nlj}(r)/r \tag{3.28}$$

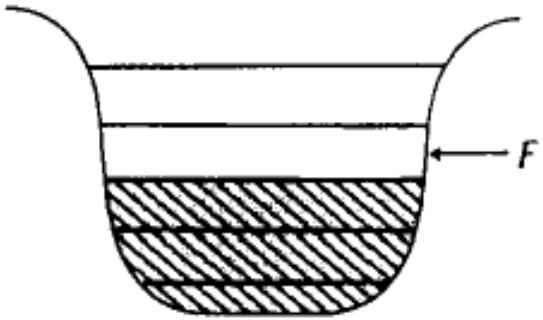
and the Schrödinger equation becomes

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2}u_{nl}(r) + \left\{\frac{l(l+1)\hbar^2}{2mr^2} + \frac{1}{2}m\omega^2 r^2 + \right.$$
$$\left. + \frac{\hbar^2}{2}\left[j(j+1) - l(l+1) - 3/4\right]V_{so}(r)\right\}u_{nl}(r) = E_{nl}u_{nl}(r). \tag{3.29}$$

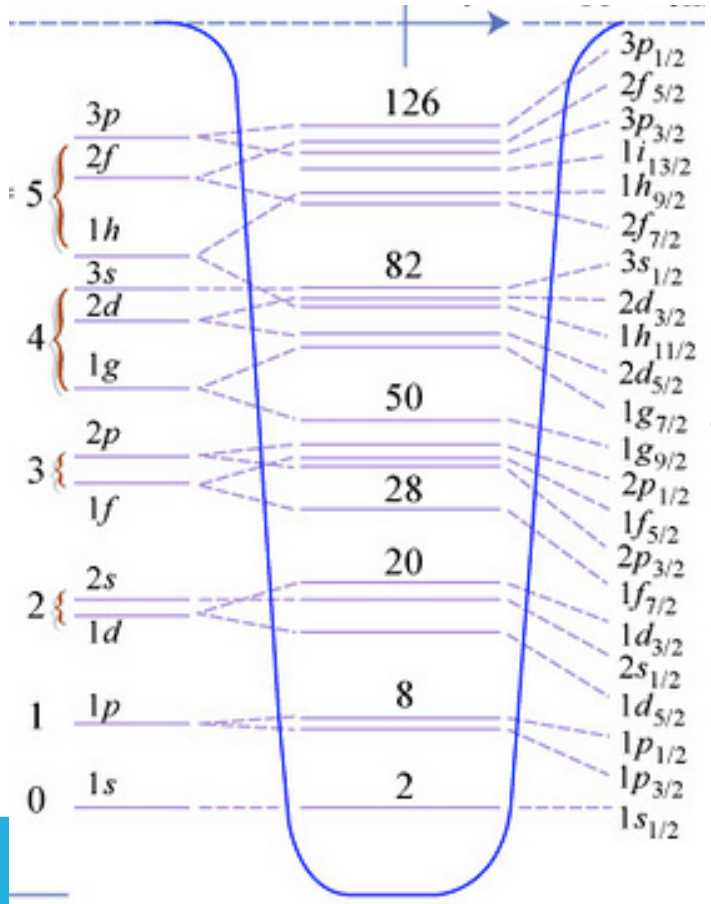
Filling scheme

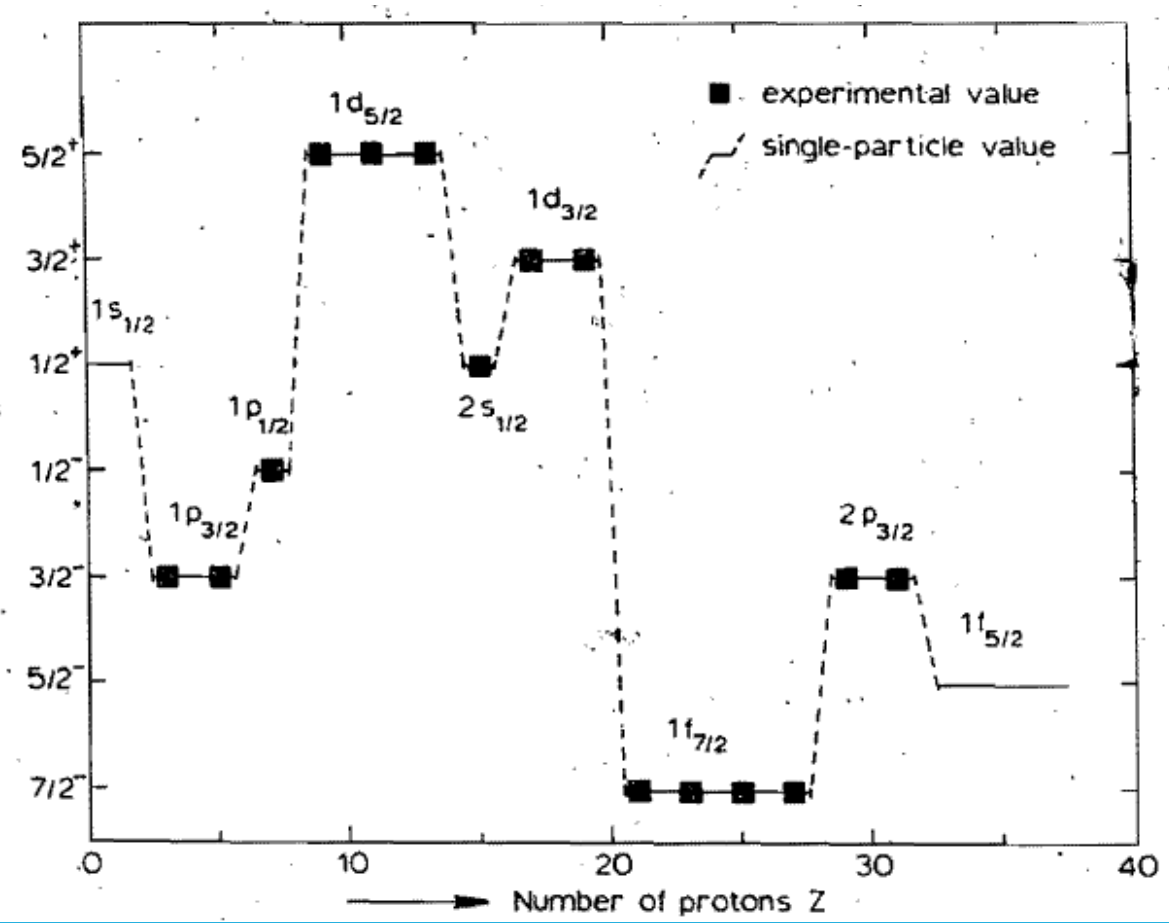
The single-particle states will be characterized by the good quantum numbers

$$|\alpha\rangle \quad = \quad |nlsjm_j\rangle$$



Single-particle levels filled up to F.





Spin-parity

Single-particle model can be used to make predictions about the spins of ground states

Filled sub-shells have zero nuclear spin and positive parity (observed experimentally)

All even-even nuclei have **J=0**, even when the sub-shell is not filled. (Pairing hypothesis)

Last neutron/proton determines the net nuclear spin-parity.

-In odd-A there is only one unpaired nucleon. Net spin can be determined precisely

-In even-A odd-Z/odd-N nuclides we have an unpaired p and an unpaired n. Hence the nuclear spin will lie in the range |jp-jn| to (jp+jn). For the parity $P_{nucleus} = P_{last\_p} \times P_{last\_n}$

According to Eq. (3.10) the energy of the core is

$$E_{core} = \sum_{i=1}^{A} \epsilon_{h_i} \tag{3.36}$$

and the energy of $A+1$ nucleus in the state p_k is

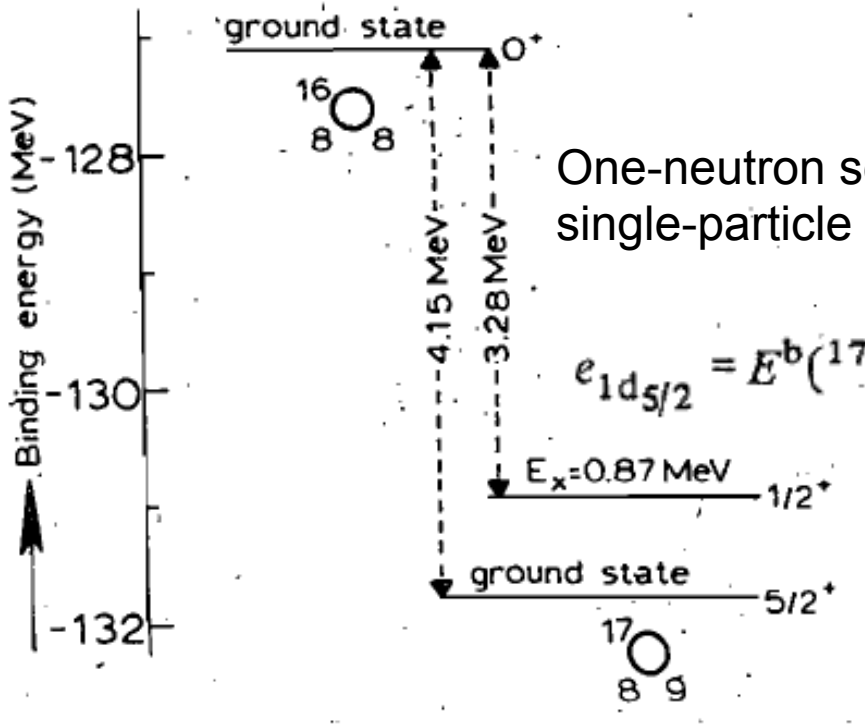
$$E_{A+1}(p_k) = E_{core} + \epsilon_{p_k} \tag{3.37}$$

from where one gets,

$$\epsilon_{p_k} = E_{A+1}(p_k) - E_{core} \tag{3.38}$$

Since all single-particle energies are negative one finds that

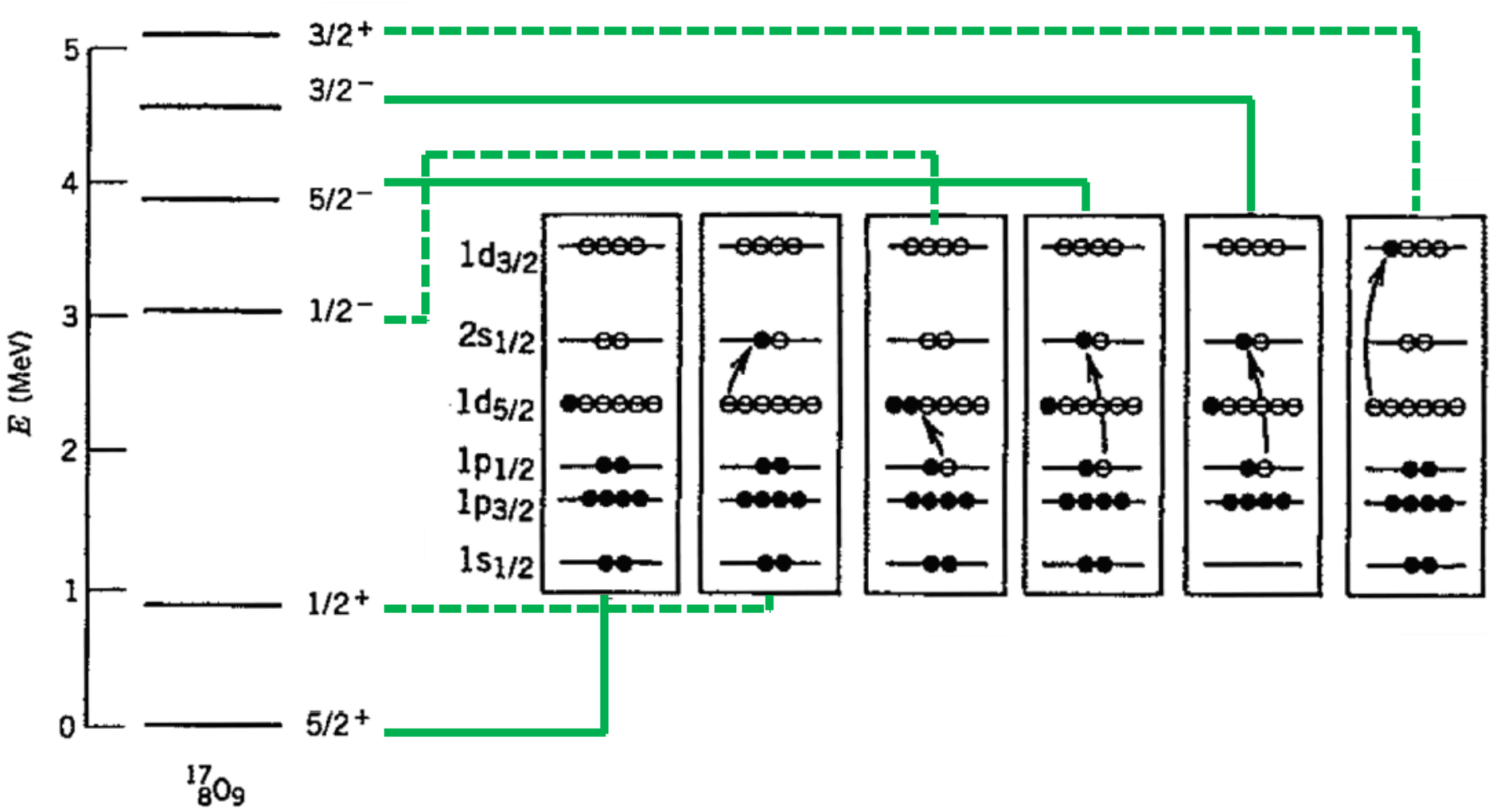
$$E_{A+1}(p_k) < E_{core} \tag{3.39}$$



One-neutron separation energy (opposite of single-particle energy)

$$e_{1d_{5/2}} = E^b(^{17}O) - E^b(^{16}O)$$

protons: $(1s_{1/2})^2\ (1p_{3/2})^4\ (1p_{1/2})^2$
neutrons: $(1s_{1/2})^2\ (1p_{3/2})^4\ (1p_{1/2})^2\ (1d_{5/2})^1$



Single-particle states observed in odd-A nuclei (in particular, one nucleon + doubly magic nuclei like ^{4}He, ^{16}O, ^{40}Ca) characterizes single-particle energies of the shell-model picture.

Success of the extreme single-particle model

Z	Isotope	Observed J^π	Shell model nlj
3	^{9}Li	$(3/2^-)$	$1p_{3/2}$
5	^{13}B	$3/2^-$	$1p_{3/2}$
7	^{17}N	$1/2^-$	$1p_{1/2}$
9	^{21}F	$5/2^+$	$1d_{5/2}$
11	^{25}Na	$5/2^+$	$1d_{5/2}$
13	^{29}Al	$5/2^+$	$1d_{5/2}$
15	^{33}P	$1/2^+$	$2s_{1/2}$
17	^{37}Cl	$3/2^+$	$1d_{3/2}$
19	^{41}K	$3/2^+$	$1d_{3/2}$
21	^{45}Sc	$7/2^-$	$1f_{7/2}$
23	^{49}Va	$7/2^-$	$1f_{7/2}$
25	^{53}Mn	$7/2^-$	$1f_{7/2}$
27	^{57}Co	$7/2^-$	$1f_{7/2}$
29	^{61}Cu	$3/2^-$	$2p_{3/2}$
31	^{65}Ga	$3/2^-$	$2p_{3/2}$
33	^{69}As	$(5/2^-)$	$1f_{5/2}$
35	^{73}Br	$(3/2^-)$	$1f_{5/2}$

- Ground state spin and parity:

  Every orbit has 2j+1 magnetic sub-states, fully occupied orbitals have spin J=0, they do not contribute to the nuclear spin.

  For a nucleus with one nucleon outside a completely occupied orbit the nuclear spin is given by the single nucleon.

$$n\ \ell\ j \rightarrow J$$
$$(-)^{\ell} = \pi$$

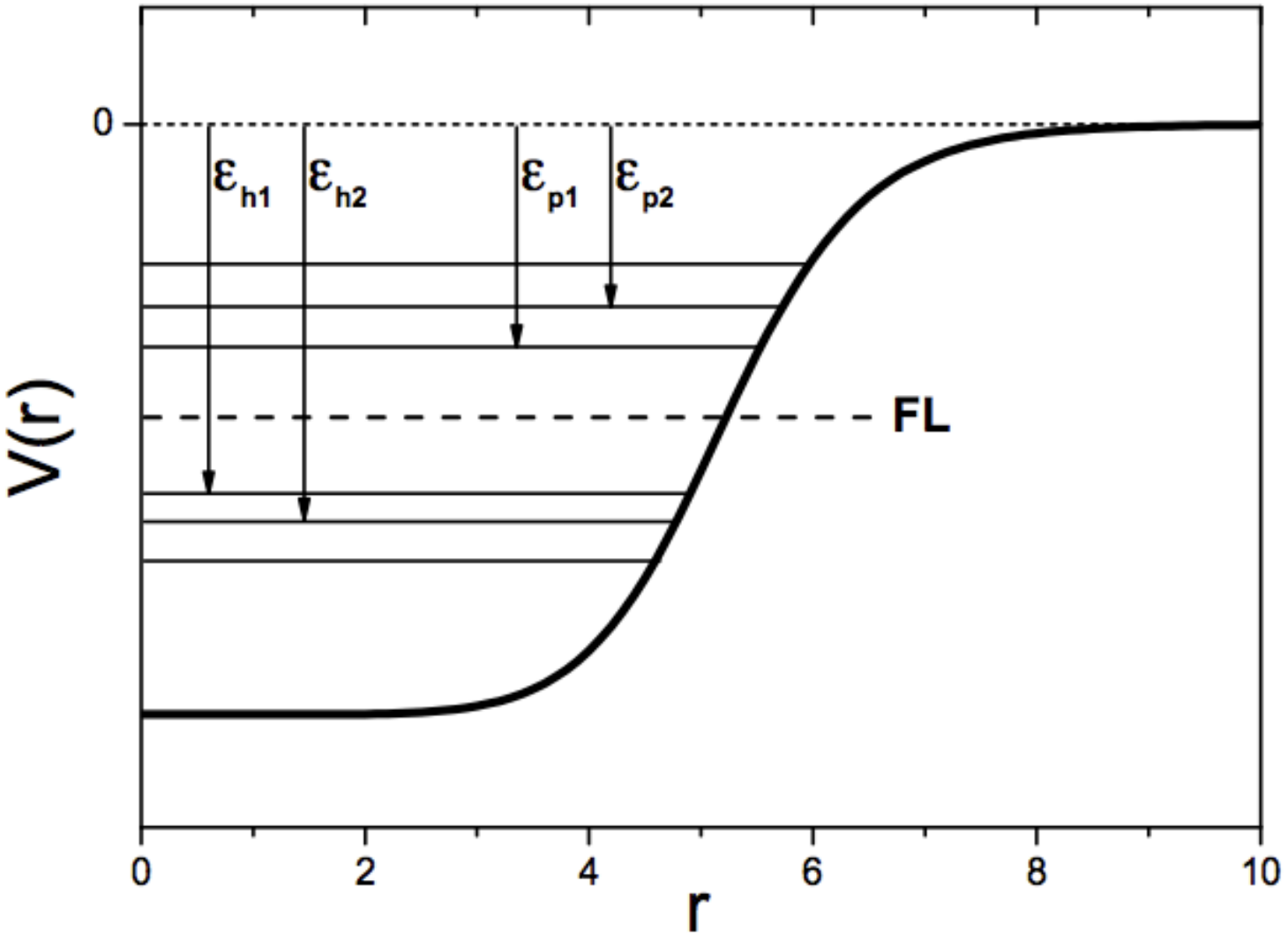
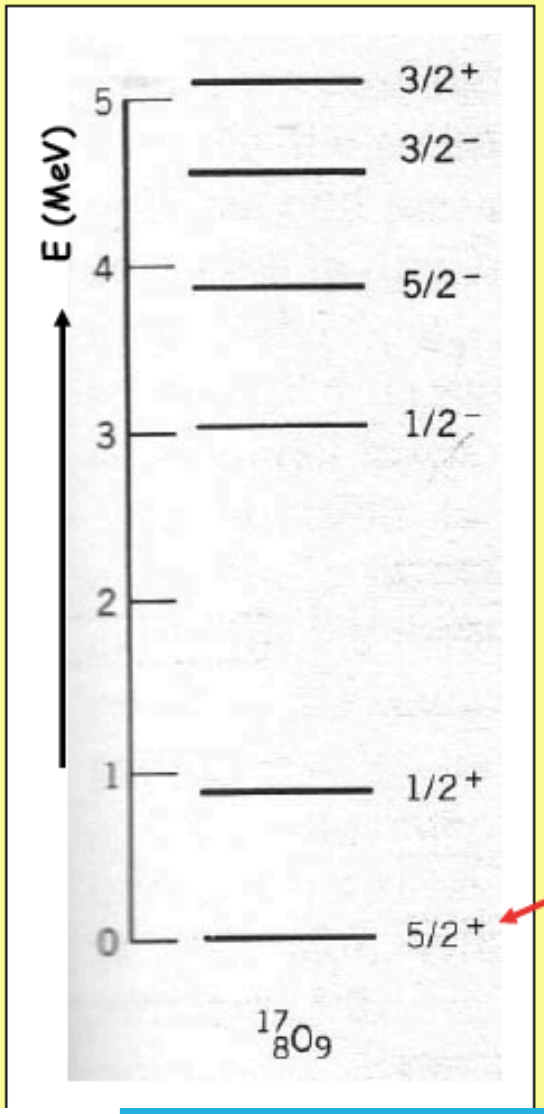
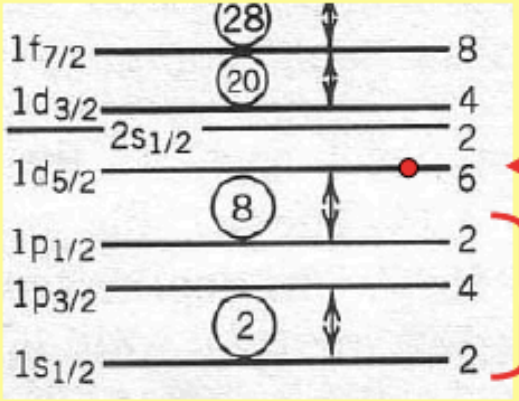


Figure 3.3: Single particle states in the shell model potential. The energies ϵ are measured from the continuum threshold. The Fermi level is indicated as FL.



There are 8 protons and 9 neutrons, so we only need the low lying states in the shell model spectrum to understand the energy levels:



valence n

Ground state: full to here plus one neutron

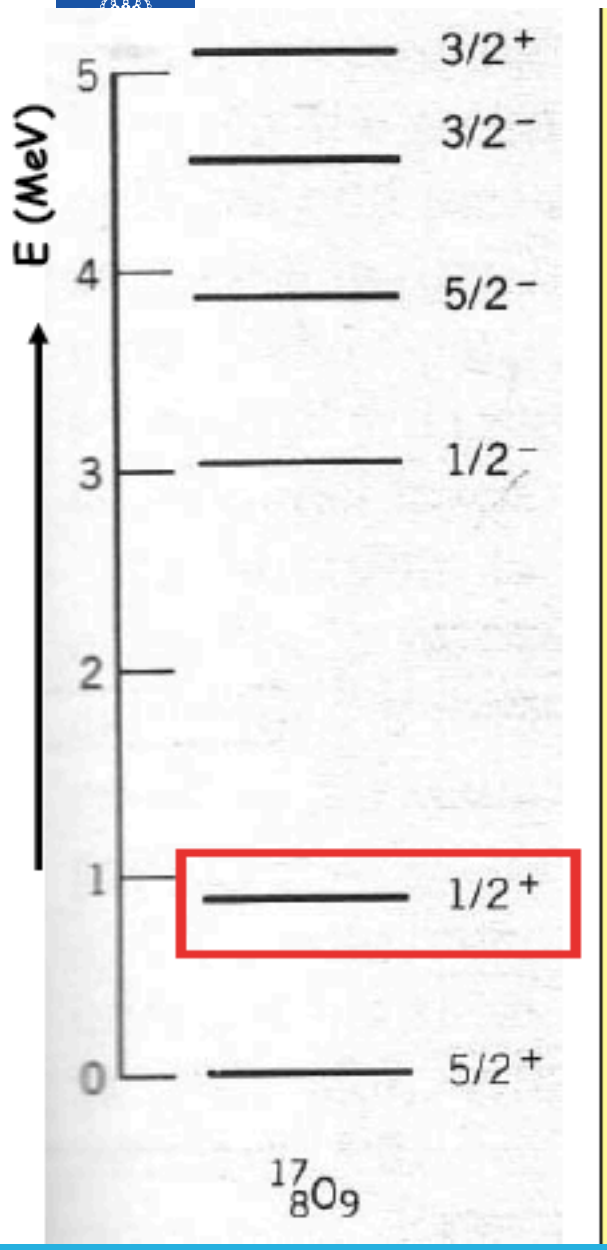
Ground state quantum numbers should be those of the valence neutron in the $1d_{5/2}$ state:

$J^{\pi} = 5/2^{+}$

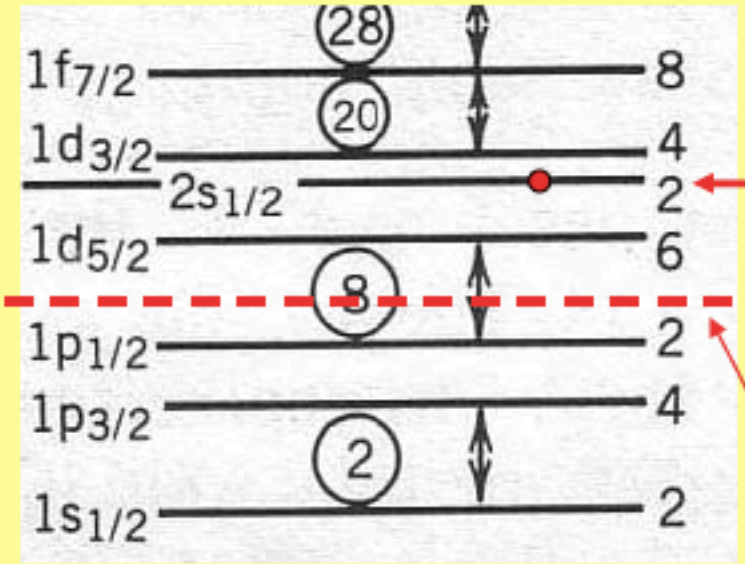
Magnetic moment prediction: $j = l + \frac{1}{2}$, odd neutron

→ $\mu = \mu_{neutron} = -1.91\ \mu_N$

measured value: $-1.89\ \mu_N$

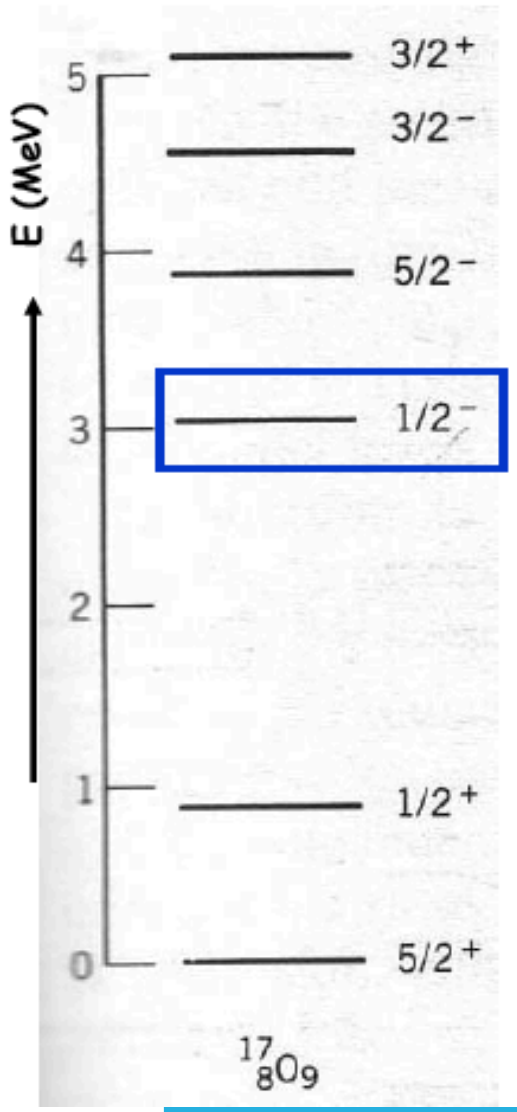


First excited state: $J^\pi = \frac{1}{2}^+$



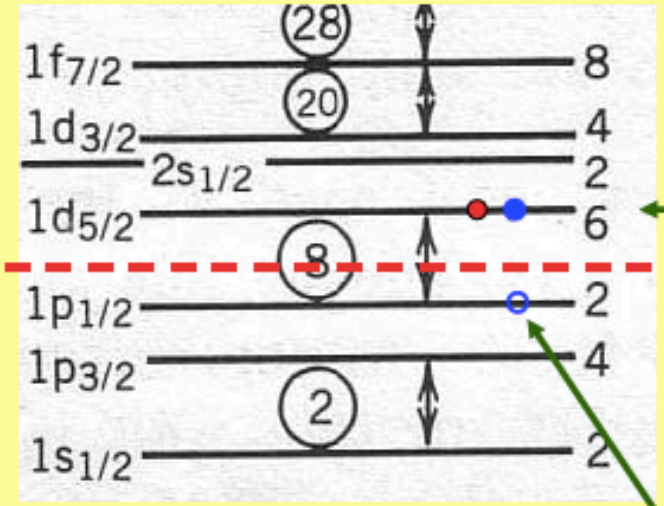
$\frac{1}{2}^+$ state

ground state full to here



Next excited state: $J^{\pi} = \frac{1}{2}^{-}$

→ explained by promoting a neutron from the filled 1 $p_{1/2}$ level to the $1d_{5/2}$ level



0+ pair

$\frac{1}{2}^{-}$ neutron hole

Nucleus	E_{level}(keV)	Jπ	$T_{1/2}$	
13O	0.0	(3/2-)	8.58 ms *5*	$0p_{3/2}$
15O	0.0	1/2-	122.24 s *16*	$0p_{1/2}$
17O	0.0	5/2+	STABLE	$0d_{5/2}$
17O	870.73 *10*	1/2+	179.2 ps *18*	$1s_{1/2}$
19O	0.0	5/2+	26.88 s *5*	$0d_{5/2}$
19O	96.0 *5*	3/2+	1.39 ns *5*	
19O	1471.7 *4*	1/2+	0.88 ps *12*	$1s_{1/2}$
21O	0.0	(5/2+)	3.42 s *10*	$0d_{5/2}$
21O	1218 *4*	(1/2+)		$1s_{1/2}$
23O	0	1/2+	82 ms *+45-28*	$1s_{1/2}$

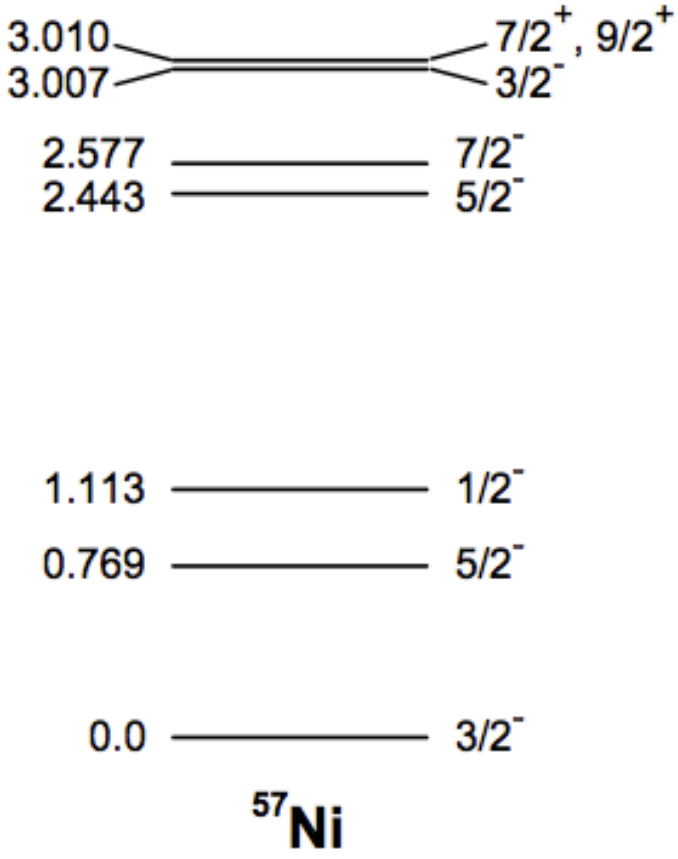
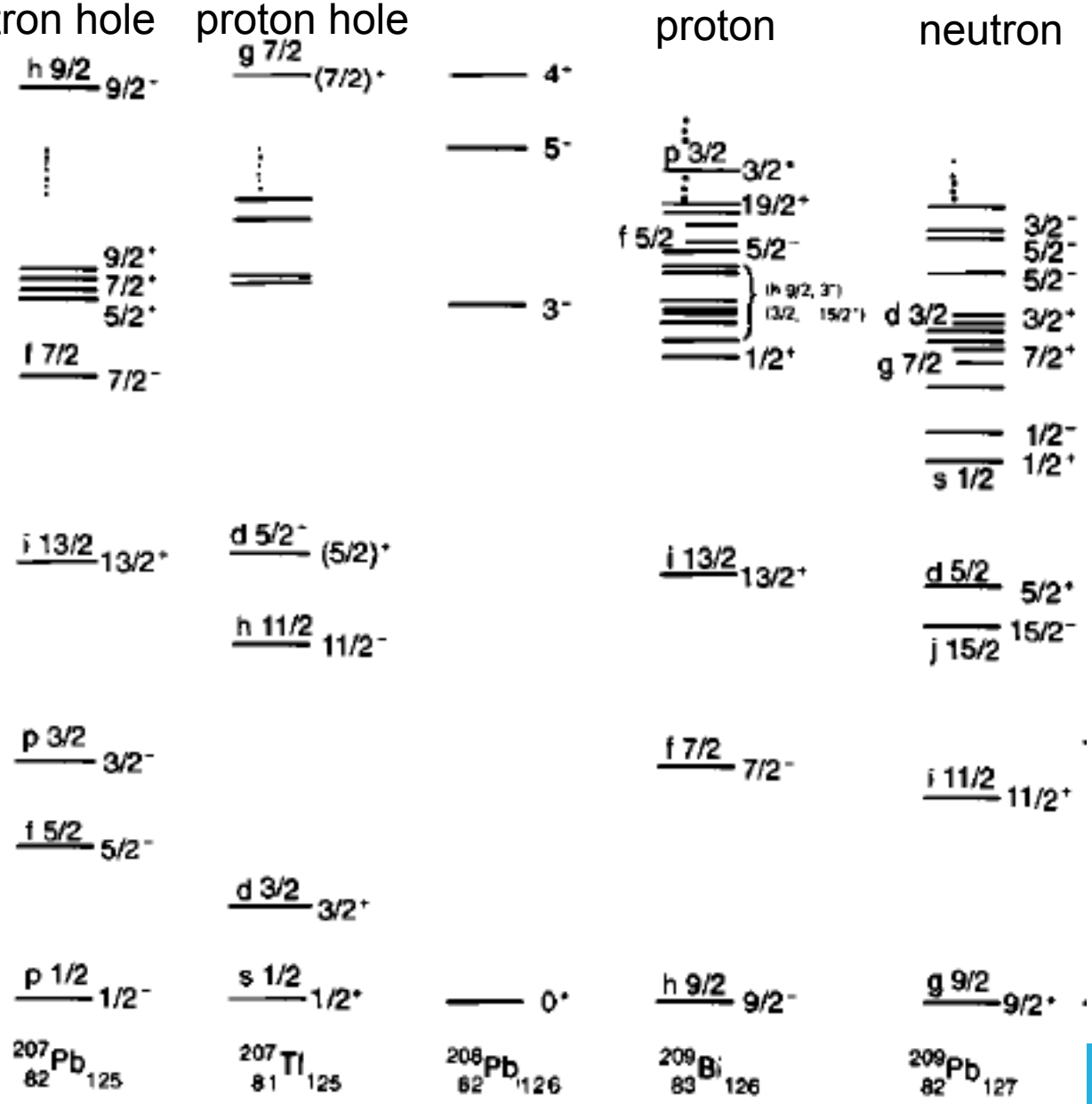


Figure 3.4: Experimental spectrum of the nucleus $^{57}Ni_{29}$ taken from the Internet site mentioned in the text. Energies are in MeV. The level at 3.010 MeV has not been completely determined yet. It can be $7/2^+$ as well as $9/2^+$.

The experimental energies in the spectrum are given relative to the ground state of the nucleus, as seen in Fig. 3.4. To obtain the corresponding values of ϵ one has to evaluate the binding energies $B(Z,N)$. In the Internet site mentioned above are given the values of $B(Z,N)/A$. For our case we need the binding energies of ^{56}Ni (the core) and of ^{57}Ni (see Eq. (3.38)), It is $B(28,28)/56 = 8.643$ MeV and $B(28,29)/57 = 8.671$ MeV, i. e. $\epsilon_{1p_{3/2}}$ = - 10.239 MeV. This is the lowest state. It corresponds to the state labelled p_1 in Fig. 6.15. The state $0f_{5/2}$, at 0.769 MeV, corresponds to p_2 (is less negative). Therefore one gets $\epsilon_{0f_{5/2}}$ = (- 10.239 + 0.769) MeV = - 9.470 MeV. In the same fashion it is $\epsilon_{1p_{1/2}}$ = -9.126 MeV and $\epsilon_{0g_{9/2}}$ = - 7.229 MeV.

The evaluation of the single-particle energies follows this procedure in all cases.



Doubly magic

The energy of the nucleus referred to the core is now (see Eq. (3.38))

$$E_{A-1}(h_1) - E_{core} = -\epsilon_{h_1} \tag{3.40}$$

which is a *positive* number. This implies that a state which is more bound than h_1, for instance the one labeled h_2 in Fig. 3.5, lies at higher energy than h_1 since $|\epsilon_{h_2}| > |\epsilon_{h_1}|$.

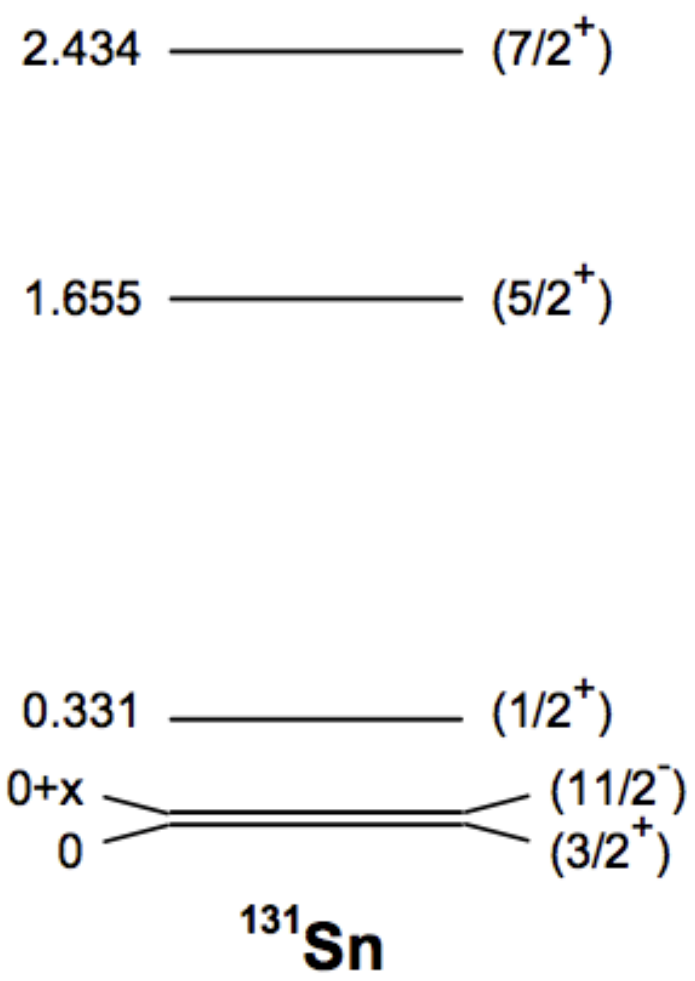
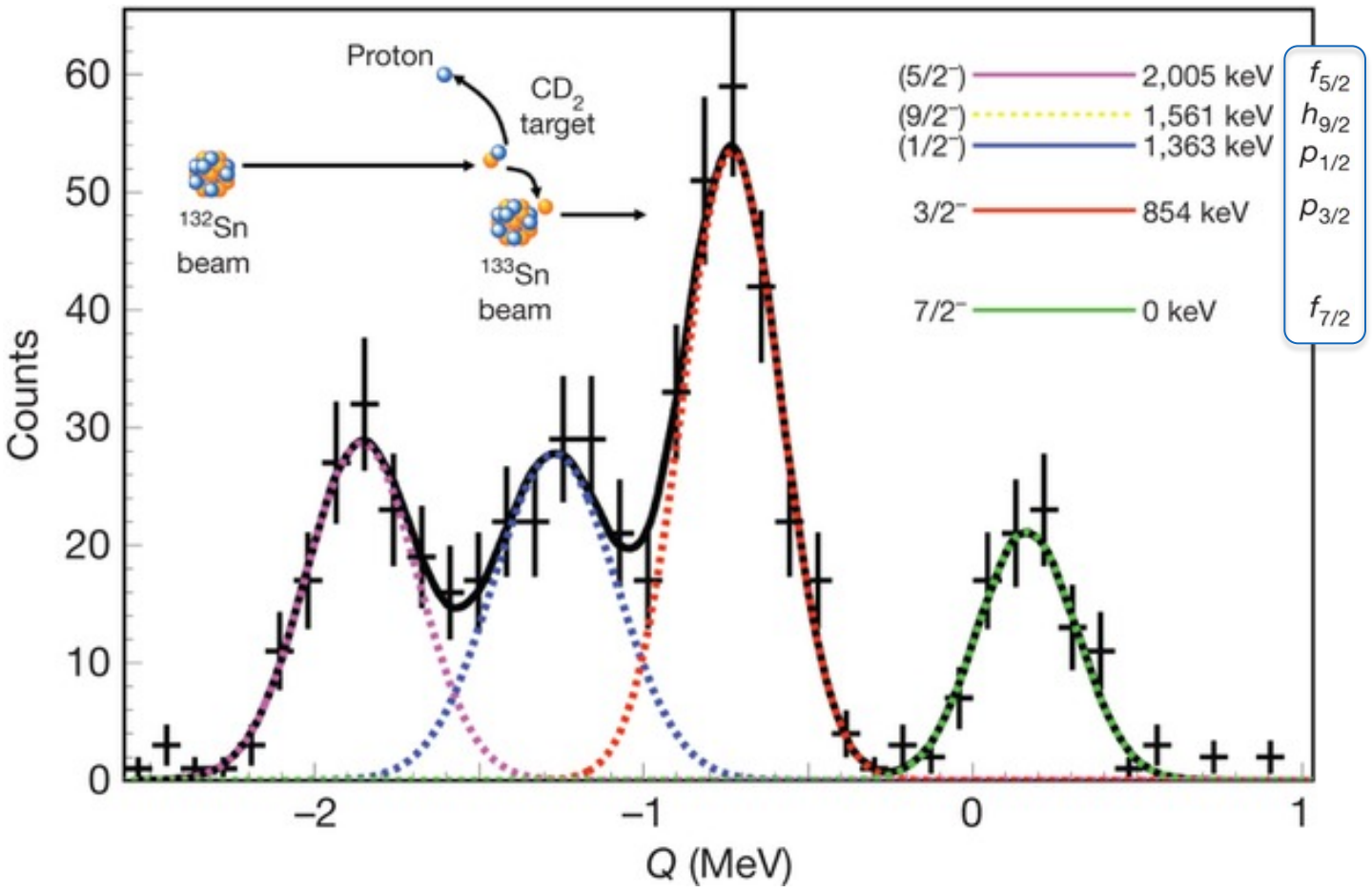


Figure 3.6: Experimental spectrum of the nucleus $^{131}_{50}Sn_{81}$. The levels are in parenthesis, meaning that they are not completely determined yet. The level $11/2^-$ is at 0.0+x MeV, implying that it is only slightly above the $3/2^+$ ground state.

The ground state single-particle energy is, according to Eq. (3.40), $\epsilon_{h_1} = E_{core} - E_{A-1}(h_1)$, where h_1 is the hole state $1d_{3/2}$ and the core is ^{132}Sn(gs) (*gs* means ground state). The binding energies of interest are $B(50,81)/131 = 8.363$ MeV and $B(50,82)/132 = 8.355$ MeV. Therefore it is E_{core} = -$B(50,82)$ = -1102.860 Mev and $E_{A-1}(h_1)$ = -$B(50,81)$ = -1095.553 MeV, from where one gets $\epsilon_{1d_{3/2}}$ = -7.307 MeV. For the other states it is $\epsilon_{0h_{11/2}}$ = -7.307 MeV also, $\epsilon_{2s_{1/2}}$ = (-7.307 - 0.332) MeV = -7.639 MeV, $\epsilon_{1d_{5/2}}$ = -8.962 MeV and $\epsilon_{0g_{7/2}}$ = -9.741 MeV.

Single-particle states in 133Sn: Doubly magic nature of 132Sn

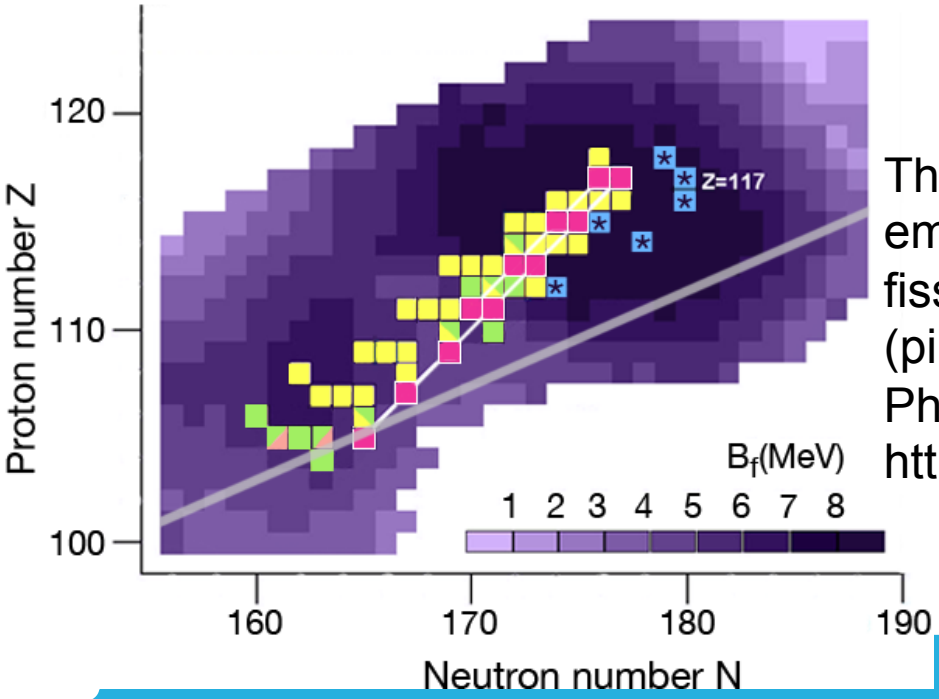


Paul Cottle, Nature 465, 430–431 (2010)
K. L. Jones et al., Nature 465, 454–457 (2010)

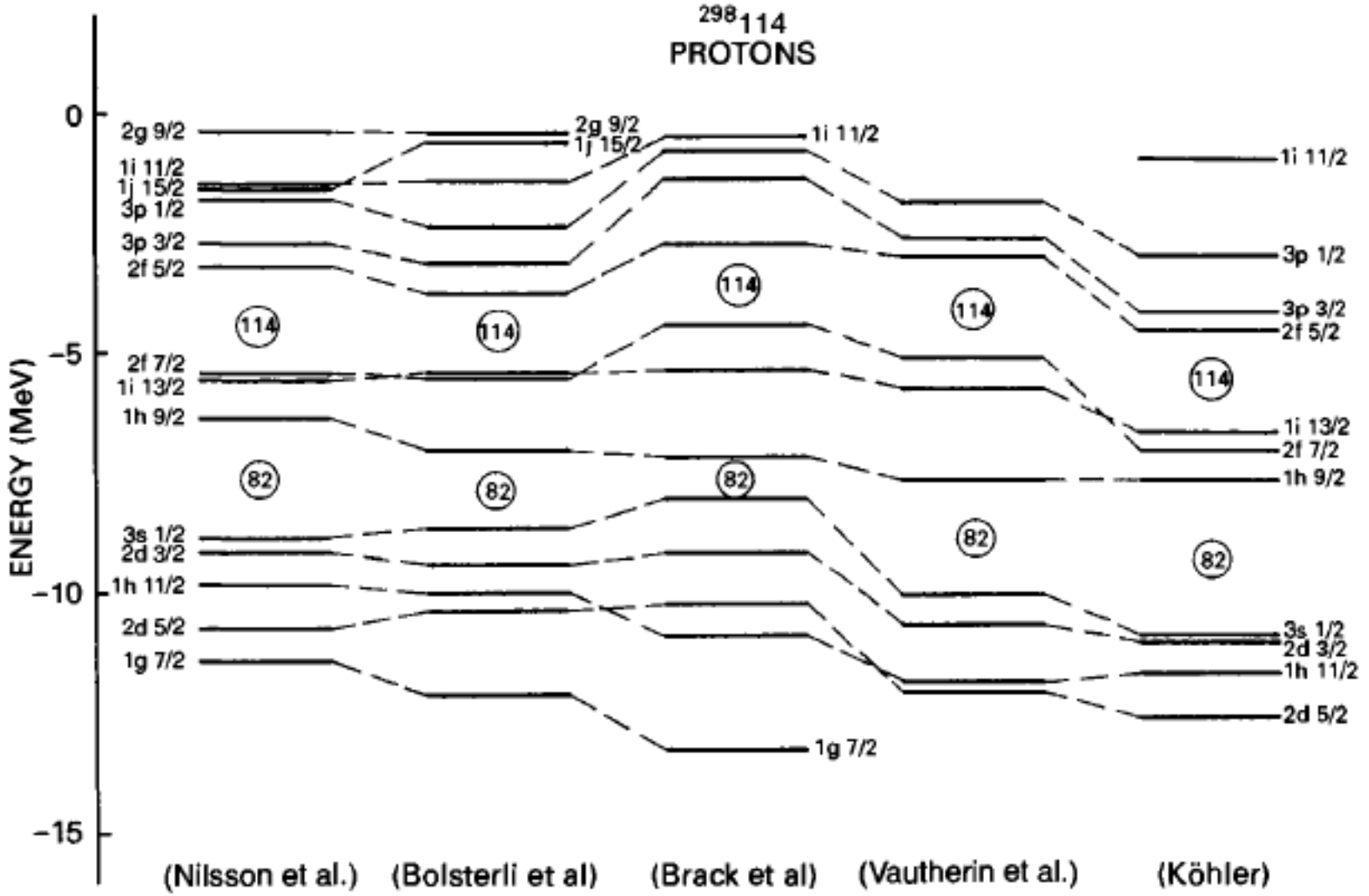
Shell closure in superheavy nuclei (an open problem)

Synthesis of a New Element with Atomic Number Z=117, PRL 104, 142502 (2010)

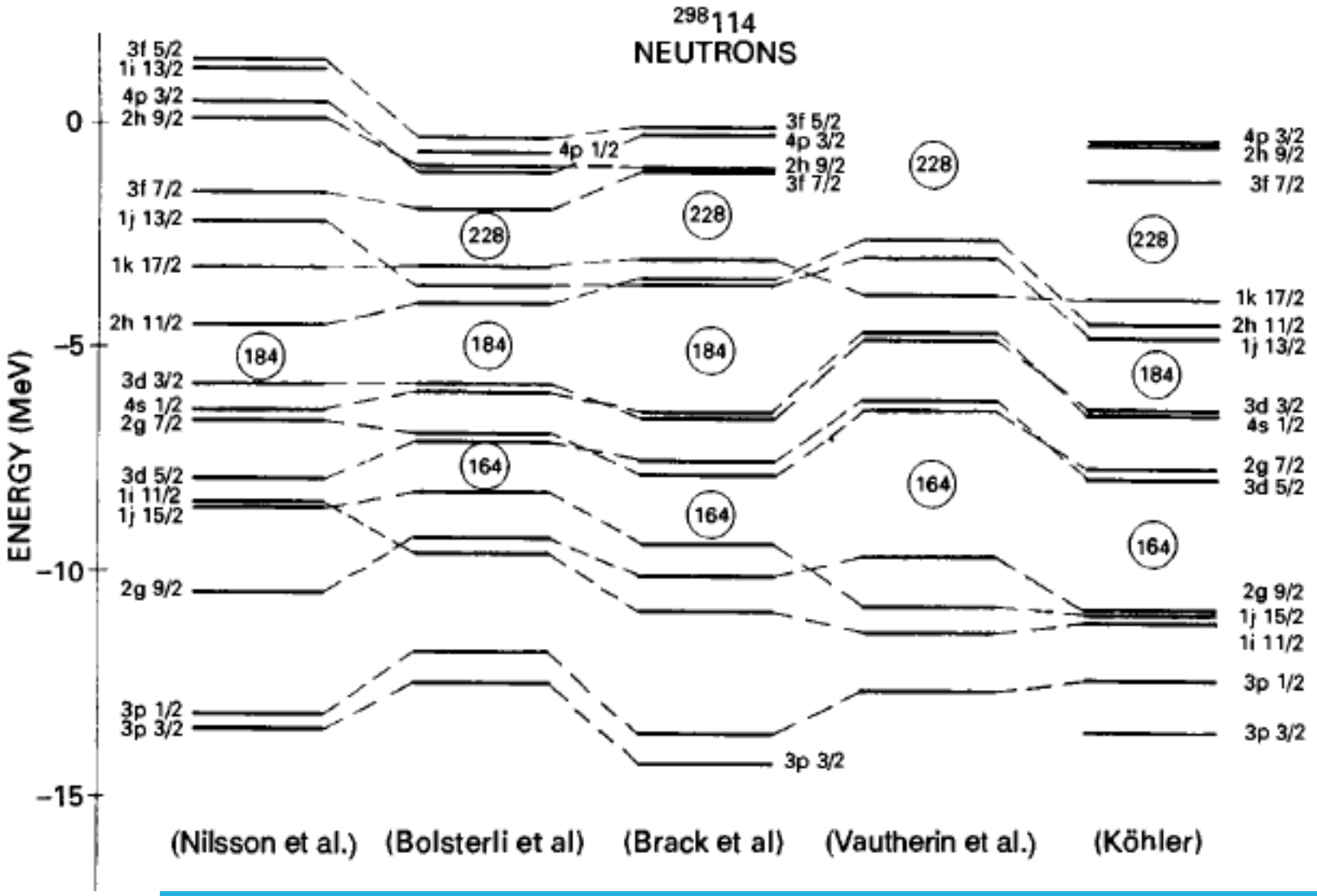
According to classical physics, elements with Z >104 should not exist due to the large Coulomb repulsion. The occurrence of superheavy elements with Z>104 is entirely due to nuclear shell effects.



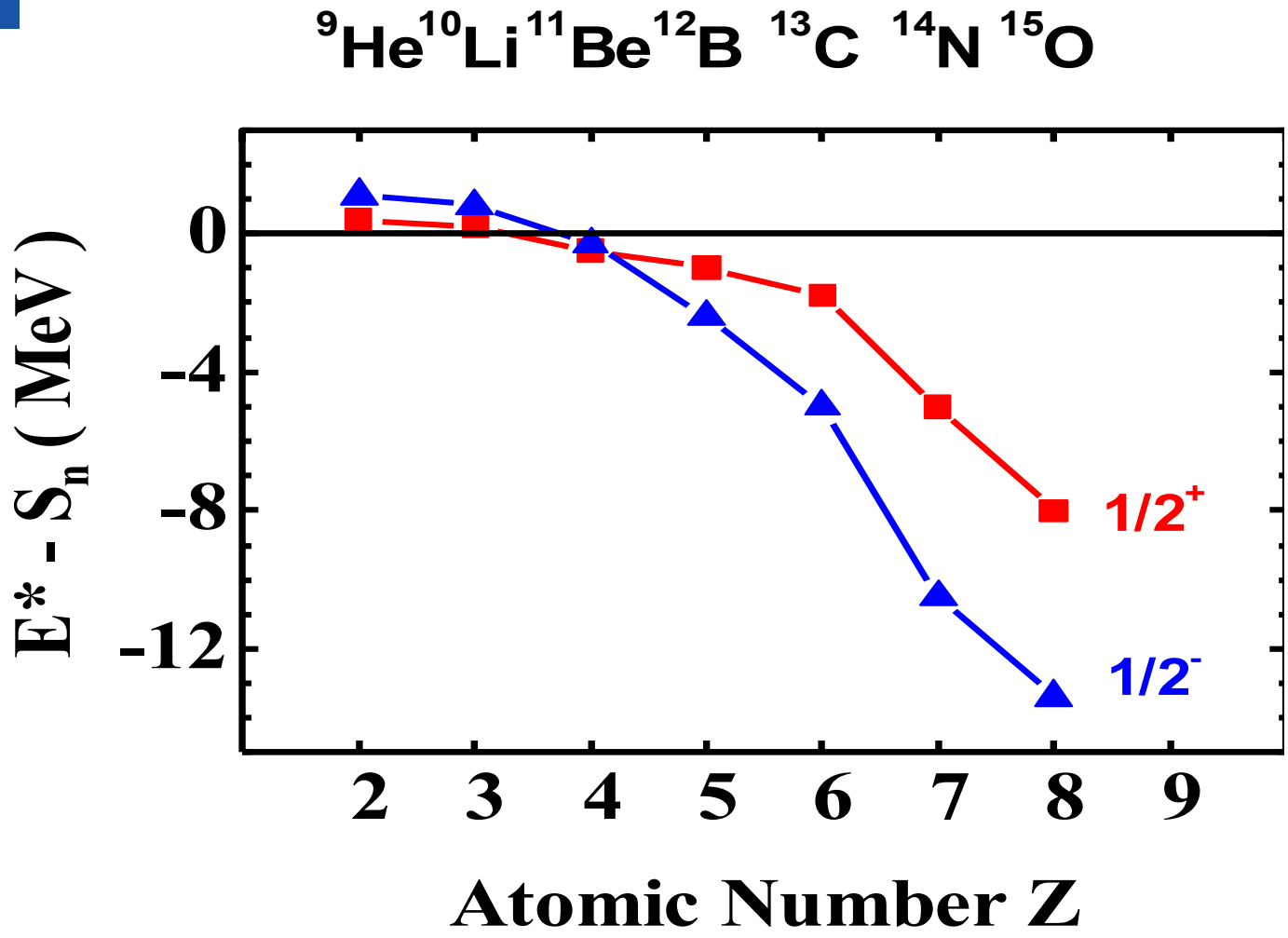
The nuclei in the chart decay by α emission (yellow), spontaneous fission (green), and β+ emission (pink).
Physics 3, 31 (2010)
http://physics.aps.org/articles/v3/31



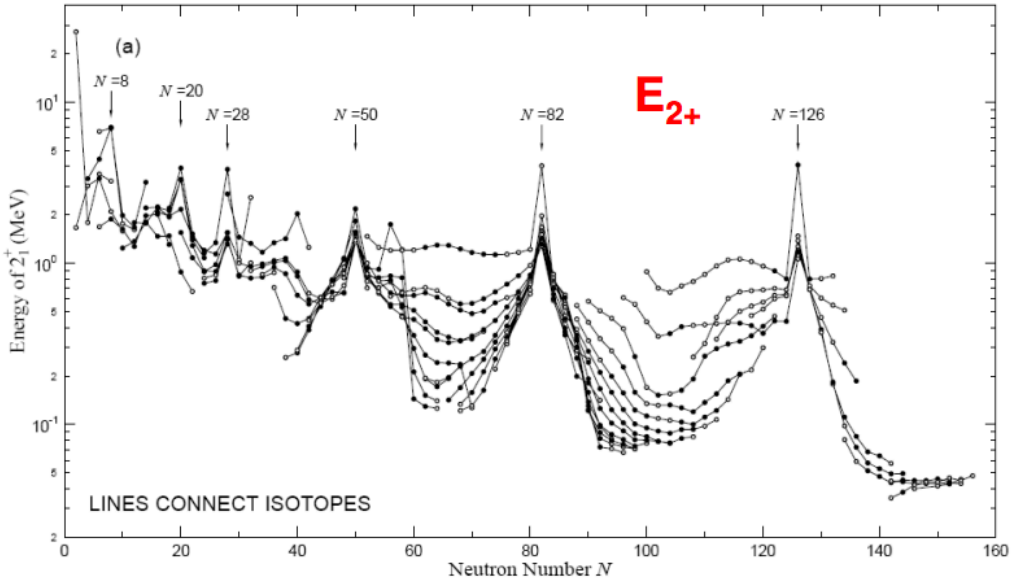
S.G. Nilsson and I. Ragnarsson: Shapes and Shells in Nuclear Structure, Cambridge Press, 1995

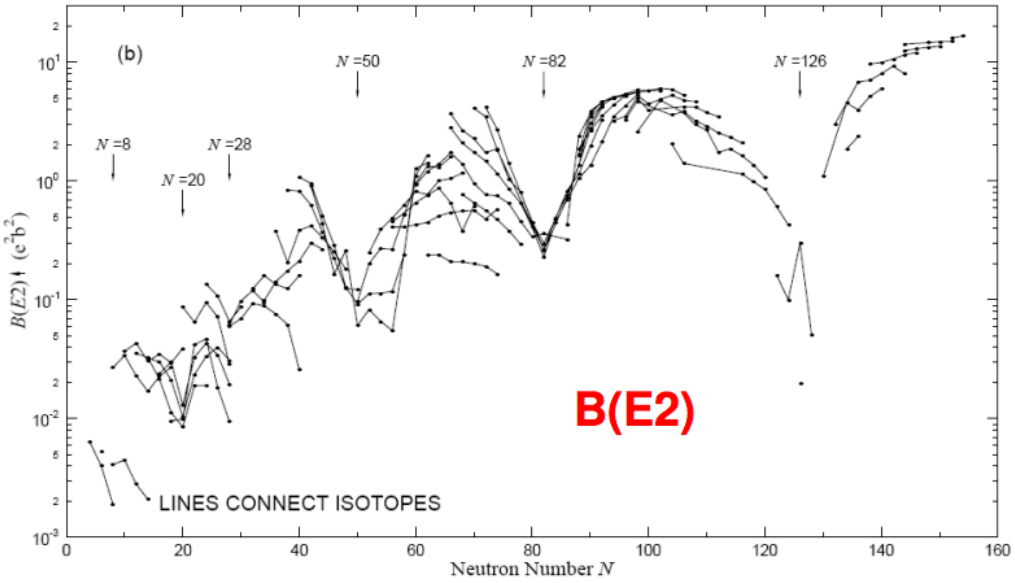

^{298}114
NEUTRONS
ENERGY (MeV)
0
−5
−10
−15
3f 5/2
1i 13/2
4p 3/2
2h 9/2
3f 7/2
1j 13/2
1k 17/2
2h 11/2
3d 3/2
4s 1/2
2g 7/2
3d 5/2
1i 11/2
1j 15/2
2g 9/2
3p 1/2
3p 3/2
4p 1/2
228
184
164
(Nilsson et al.)
(Bolsterli et al)
(Brack et al)
(Vautherin et al.)
(Köhler)

Island of Inversion



Shell structure: B(E2) and E_{2^+}



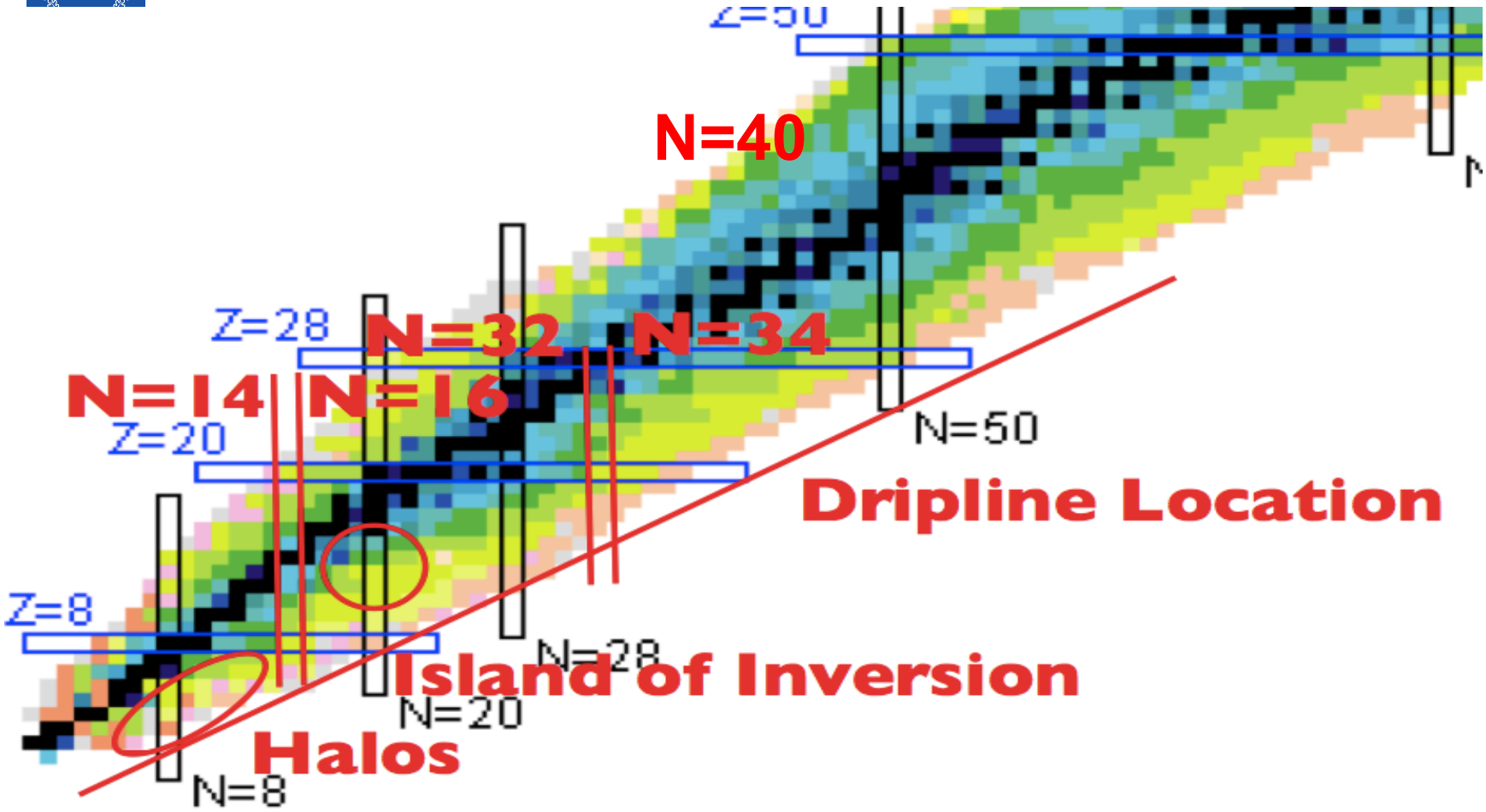


Nuclei with magic N

- Relatively high-lying first 2^+ exited state
- Relatively low B(E2) transition strength

S. Raman et al, Atomic Data and Nuclear Data Tables 78 (2001) 1.

Shell evolution at drip lines



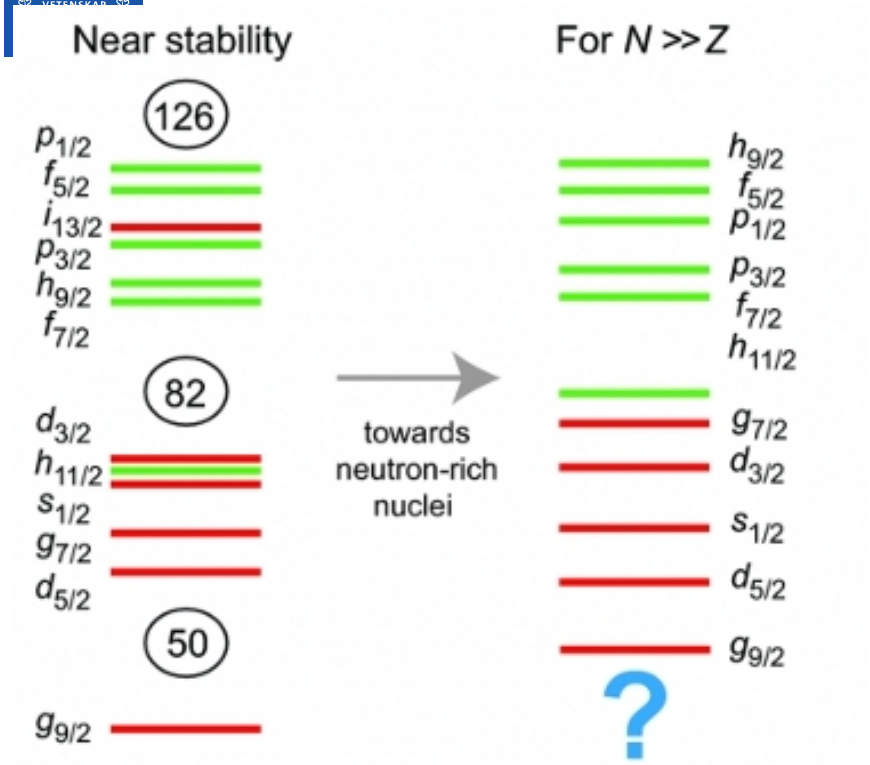
- A comprehensive review can be found in:
O. Sorlin, M.-G. Porquet, Prog. Part. Nucl. Phys. 61, 602 (2008).

Shell evolution and its indication on the isospin dependence of the spin-orbit splitting

Zhen-Xiang Xu and Chong Qi*
KTH (Royal Institute of Technology), Alba Nova University Center, SE-10691 Stockholm, Sweden
(Dated: September 3, 2012)

http://arxiv.org/pdf/1208.6461v1.pdf

Shell structure at the drip lines



- Mean field near stability
- Strong spin-orbit term

- Mean field for $N >> Z$?
- Reduced spin-orbit
- Diffuse density
- Tensor force

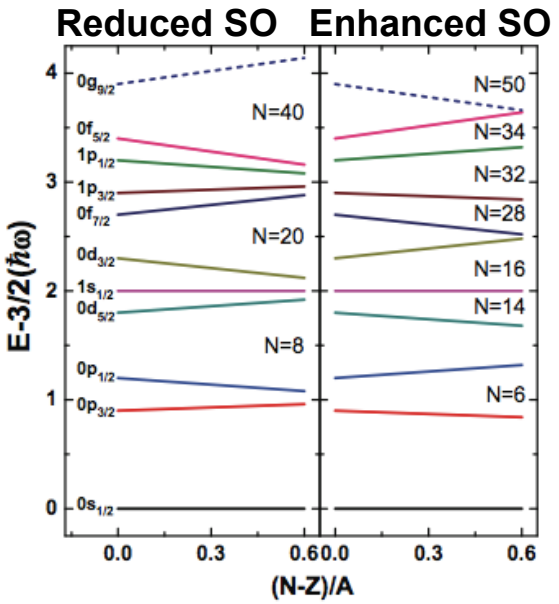


FIG. 1. (Color online) The evolution of the shell structure as a function of $(N-Z)/A$ with the HO potential plus SO coupling of the form $\lambda(1+\kappa_{SO}\frac{N-Z}{A})\hbar\omega \mathbf{l}\cdot\mathbf{s}$. We take $\lambda = 0.2$ and $\kappa_{SO} = -1$ (left) and 1 (right). The $0g_{9/2}$ orbital is shifted upwards by $0.3\hbar\omega$ for a clearer presentation.

Mean-field for dripline nuclei

➢Orbitals with higher *l* loses its energy faster when going towards the dripline I. Hamamoto, Phys. Rev. C 85, 064329 (2012).

This naturally explains the disappearing of N=14 subshell in C and N isotopes [It is due to a complicated interplay between NN and NP interactions from a shell-model point of view, C.X. Yuan, C. Qi, F.R. Xu, Nucl. Phys. A 883, 25 (2012).].

➢Choice of the Central and SO potential

$$V = V_0(1 + \frac{4\kappa}{A}\mathbf{t}\cdot\mathbf{T}_d),$$

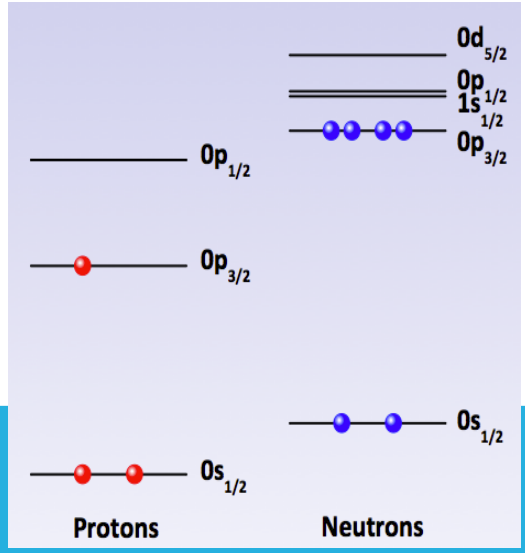
and

$$V_{SO} = \lambda V_0(1 + \frac{4\kappa_{SO}}{A}\mathbf{t}\cdot\mathbf{T}_d),$$

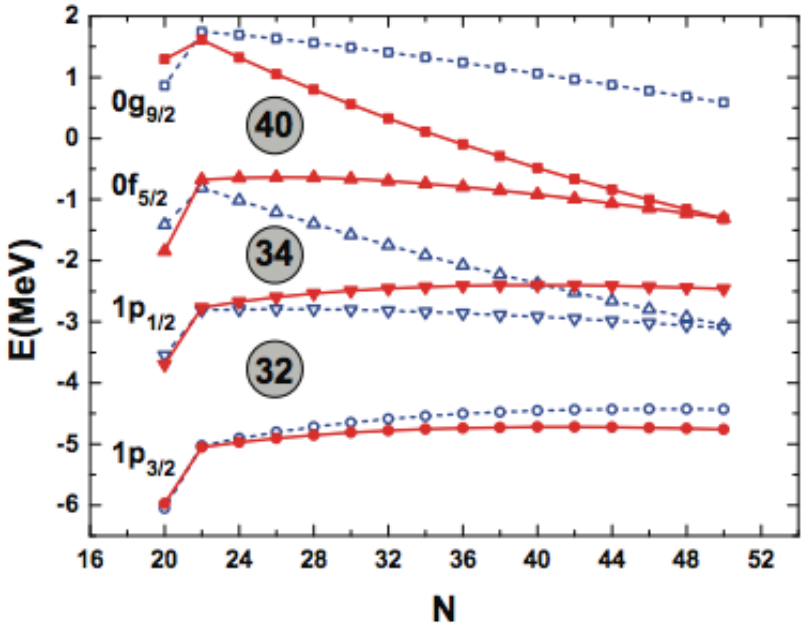
The standard WS potential

A. Bohr and B.R. Mottelson, Nuclear Structure (Benjamin, New York, 1969), Vol. I.

$$\kappa = \kappa_{SO} = -\frac{33}{51},$$



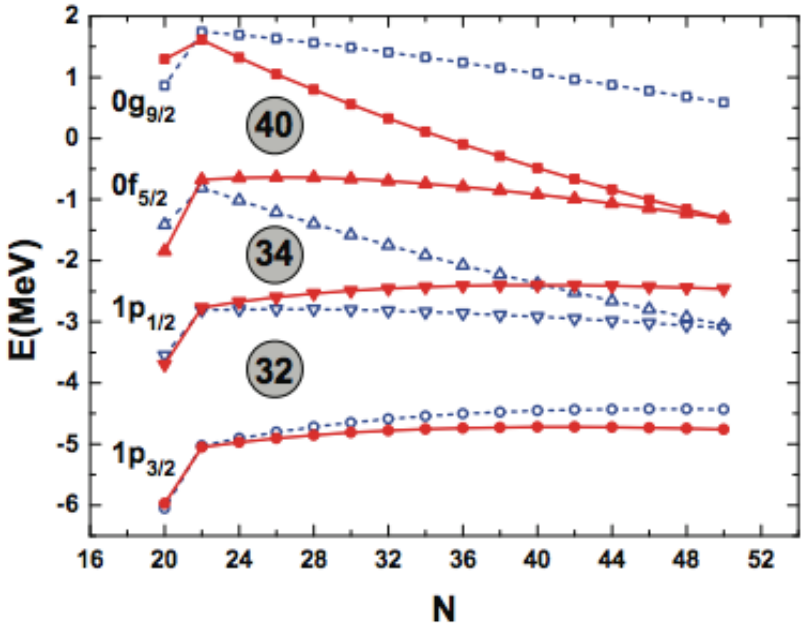
Single-particle structure of Ca isotopes



Simple rules of shell evolution

- HO magic numbers like N=8, 20 disappear;
- New SO magic numbers like N = 6, 14, 16, 32 and 34 will appear;
- The traditional SO magic numbers N = 28 and 50 and the magic number N = 14 will be eroded somehow but are more robust than the HO magic numbers;
- Pseudospin symmetry breaks, resulting in new shell closures like N = 56 and 90;
- HO shell closures like N = 40 and 70 will not emerge.

Single-particle structure of Ca isotopes



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Chapter 4

Magnetic resonances in nuclei

Magnetic Effects on Atomic Spectra—The Normal Zeeman Effect

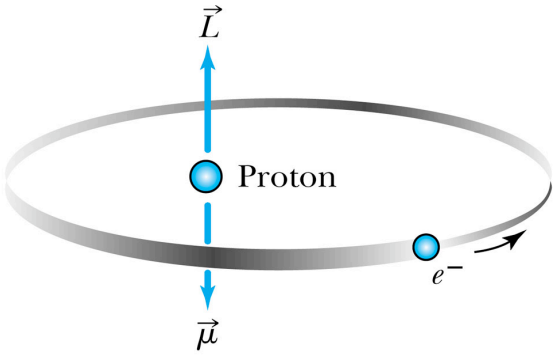
Consider the atom to behave like a small magnet.

Think of an electron as an orbiting circular current loop of $I = dq / dt$ around the nucleus.

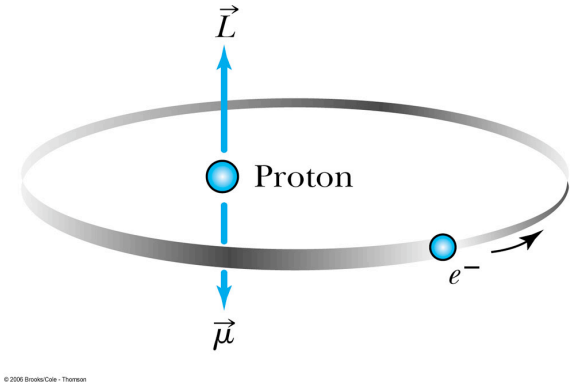
The current loop has a magnetic moment $\mu = IA$ and the period $T = 2\pi r / v$.

$$\vec{\mu} = -\frac{e}{2m}\vec{L}$$

where $L = mvr$ is the magnitude of the orbital angular momentum.



The Normal Zeeman Effect



- Since there is no magnetic field to align them, $\vec{\mu}$ point in random directions. The dipole has a potential energy

$$V_B = -\vec{\mu} \cdot \vec{B}$$

The angular momentum is aligned with the magnetic moment, and the torque between $\vec{\mu}$ and $\vec{B}$ causes a precession of $\vec{\mu}$.

$$\mu_z = \frac{e\hbar}{2m} m_\ell = -\mu_B m_\ell$$

Where $\mu_B = e\hbar / 2m$ is called a **Bohr magneton**.

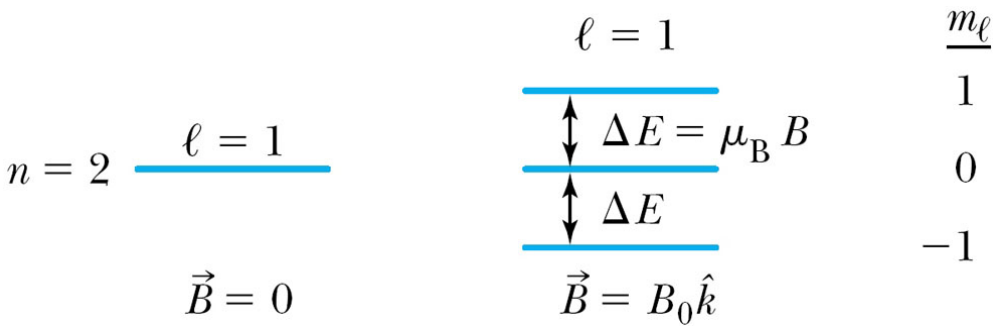
The Normal Zeeman Effect

The potential energy is quantized due to the magnetic quantum number m_ℓ.

$$V_B = -\mu_z B = +\mu_B m_\ell B$$

When a magnetic field is applied, the 2*p* level of atomic hydrogen is split into ***three*** different energy states with energy difference of $\Delta E = \mu_B B\, \Delta m_\ell$.

m_ℓ	Energy
1	$E_0 + \mu_B B$
0	E_0
−1	$E_0 - \mu_B B$



4.1 Charge particles in a magnetic field

Assume a nucleon in the presence of a magnetic field carrying only its intrinsic angular momentum, i. e. its 1/2-spin. This would happen is the nucleon is trapped within the region where the experiment is performed. For instance, a proton in some molecules forming a crystal, or a proton in a molecule of human tissue, which is largely composed of water with two hydrogen atoms (where the nucleus is the proton itself) in each H_2O (water) molecule.

Assuming also that the magnetic field applied externally has the form

$$\boldsymbol{B} = B_0 \boldsymbol{k} \tag{4.1}$$

where B_0 is constant and $\boldsymbol{k}$ is the unit vector in the z-direction, the Hamiltonian is

$$H = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -\mu_z B_0 \tag{4.2}$$

where the magnetic moment is defined by,

$$\boldsymbol{\mu} = \frac{gq}{2mc} \boldsymbol{s} \tag{4.3}$$

Since only the intrinsic spin of the particle is considered, the g-factor in Eq. (4.3) is as the g_s factor above, but for clarity of presentation we give them again here. In the cases of interest in the applications the g-factors are

$$g = \begin{cases} 2.00 & \text{electron} \\ 5.58 & \text{proton} \\ -3.82 & \text{neutron} \end{cases} \tag{4.4}$$

As before, q is the charge of the particle ($q = -e$ for electron) and $\boldsymbol{s} = (s_x, s_y, s_z)$ are the Pauli matrices given by,

$$s_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad s_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}; \quad s_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.5}$$

The Hamiltonian becomes,

$$H = -\boldsymbol{\mu} \cdot \boldsymbol{B} = -\frac{gq}{2mc} B_0 \boldsymbol{s} \cdot \boldsymbol{k} = \omega_0 s_z = \frac{\omega_0 \hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.6}$$

where

$$\omega_0 = -\frac{gq}{2mc} B_0 \tag{4.7}$$

and the eigenvalues are,

$$H \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\omega_0 \hbar}{2} \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad H \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\omega_0 \hbar}{2} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{4.8}$$

There are two stationary (i.e. time independent) states with energies

$$E_\pm = \pm \frac{\omega_0 \hbar}{2} \tag{4.9}$$

If the particle is in the state +, it will not decay unless a perturbation disturbs it. When it decays a photon with energy $E_+ - E_- = \hbar\omega_0$ will be emitted which can be measured with great precision, thus allowing one to determine precisely quantities like the g-factor.

A convenient way to perturb the system is by applying a weak and time-dependent magnetic field in the x-direction. Rabi chose for this purpose the form $B_1 \cos\omega t\, \boldsymbol{i}_x$. The perturbation will then vary from $-B_1$ to $+B_1$ as the time increases. The hope is that at a certain value of ω the transition will take place. Notice that B_1 has to be very small in comparison to B_0 in order not to destroy the spectrum determined by B_0 (i.e. the levels $E_\pm$). The problem is then to solve the Hamiltonian

$$H = \omega_0 s_z - \frac{gqB_1}{2mc} \cos\omega t s_x \tag{4.10}$$

with $\omega_1 = -\dfrac{gqB_1}{2mc}$, one gets

$$H = \frac{\omega_0\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \frac{\omega_1\hbar}{2}\cos\omega t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1\cos\omega t \\ \omega_1\cos\omega t & -\omega_0 \end{pmatrix} \tag{4.11}$$

where $|\omega_1| \ll |\omega_0|$. One has to use the time-dependent Schrödinger equation, i.e.

$$H\Psi(t) = \mathrm{i}\hbar\frac{\mathrm{d}\Psi(t)}{\mathrm{d}t} \tag{4.12}$$

Time-dependent perturbation treatment

Since B_1 is very small the solution $\Psi(t)$ should not be very different from the solution corresponding to $B_1 = 0$. We will therefore solve first the case $B_1 = 0$, i. e.

$$\frac{\hbar}{2}\begin{pmatrix} \omega_0 & 0 \\ 0 & -\omega_0 \end{pmatrix}\begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \mathrm{i}\hbar\begin{pmatrix} \dot{a}(t) \\ \dot{b}(t) \end{pmatrix} \tag{4.13}$$

where $\dot{a}(t) = \dfrac{\mathrm{d}a(t)}{\mathrm{d}t}$. One thus has

$$\begin{cases} \dfrac{\hbar}{2}\omega_0 a(t) &= \mathrm{i}\hbar\dfrac{\mathrm{d}a(t)}{\mathrm{d}t} \\ -\dfrac{\hbar}{2}\omega_0 b(t) &= \mathrm{i}\hbar\dfrac{\mathrm{d}b(t)}{\mathrm{d}t} \end{cases} \Longrightarrow \begin{cases} a(t) &= a(0)\,\mathrm{e}^{-\mathrm{i}\omega_0 t/2} \\ b(t) &= b(0)\,\mathrm{e}^{\mathrm{i}\omega_0 t/2} \end{cases} \tag{4.14}$$

The general case is

$$\frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1\cos\omega t \\ \omega_1\cos\omega t & -\omega_0 \end{pmatrix}\begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \mathrm{i}\hbar\begin{pmatrix} \dot{a}(t) \\ \dot{b}(t) \end{pmatrix} \tag{4.15}$$

since $|\omega_1| \ll |\omega_0|$, one proposes as solution

$$\begin{pmatrix} a(t) \\ b(t) \end{pmatrix} = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\omega_0 t/2}\, c(t) \\ \mathrm{e}^{\mathrm{i}\omega_0 t/2}\, d(t) \end{pmatrix} \tag{4.16}$$

which contains the main term explicitly.

The Schrödinger equation becomes

$$\frac{\hbar}{2}\begin{pmatrix} \omega_0 & \omega_1\cos\omega t \\ \omega_1\cos\omega t & -\omega_0 \end{pmatrix}\begin{pmatrix} \mathrm{e}^{-\mathrm{i}\omega_0 t/2}\, c(t) \\ \mathrm{e}^{\mathrm{i}\omega_0 t/2}\, d(t) \end{pmatrix} = \mathrm{i}\hbar\begin{pmatrix} -\mathrm{i}\frac{\omega_0}{2}\mathrm{e}^{-\mathrm{i}\omega_0 t/2}c(t) + \mathrm{e}^{-\mathrm{i}\omega_0 t/2}\dot{c}(t) \\ \mathrm{i}\frac{\omega_0}{2}\mathrm{e}^{\mathrm{i}\omega_0 t/2}d(t) + \mathrm{e}^{\mathrm{i}\omega_0 t/2}\dot{d}(t) \end{pmatrix} \tag{4.17}$$

with $\cos\omega t = \left(\mathrm{e}^{\mathrm{i}\omega t/2} + \mathrm{e}^{-\mathrm{i}\omega t/2}\right)/2$,

$$\mathrm{i}\begin{pmatrix}\dot{c}(t)\\ \dot{d}(t)\end{pmatrix}=\frac{\omega_1}{4}\begin{pmatrix}\left[\mathrm{e}^{\mathrm{i}(\omega_0+\omega)t}+\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}\right]d(t)\\ \left[\mathrm{e}^{-\mathrm{i}(\omega_0-\omega)t}+\mathrm{e}^{-\mathrm{i}(\omega_0+\omega)t}\right]c(t)\end{pmatrix} \tag{4.18}$$

The idea is to change ω in the perturbation term $B_1\cos\omega t$ such that $\hbar\omega_0\approx\hbar\omega$. Since ω_0 is large, the highly oscillating functions $\mathrm{e}^{\pm\mathrm{i}(\omega_0+\omega)t}$ can be neglected. One thus gets

$$\begin{cases}\mathrm{i}\dot{c}(t)=\dfrac{\omega_1}{4}\,\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}d(t)\\ \mathrm{i}\dot{d}(t)=\dfrac{\omega_1}{4}\,\mathrm{e}^{-\mathrm{i}(\omega_0-\omega)t}c(t)\end{cases} \tag{4.19}$$

which is a coupled set of two first order differential equations. To solve it one transforms it in a second order differential equation as follows.

$$\begin{cases}\mathrm{i}\ddot{c}(t)=\dfrac{\omega_1}{4}\,\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}\Big[\mathrm{i}(\omega_0-\omega)d(t)+\dot{d}(t)\Big]\\ \mathrm{i}\ddot{d}(t)=\dfrac{\omega_1}{4}\,\mathrm{e}^{-\mathrm{i}(\omega_0-\omega)t}\Big[-\mathrm{i}(\omega_0-\omega)c(t)+\dot{c}(t)\Big]\end{cases} \tag{4.20}$$

and replacing $c(t)$ and $\dot{c}(t)$ from Eq. (4.19)

$$\begin{aligned} \mathrm{i}\ddot{d}(t) &= \frac{\omega_1}{4}\,\mathrm{e}^{-\mathrm{i}(\omega_0-\omega)t}\Big[-\mathrm{i}(\omega_0-\omega)\,\frac{4\mathrm{i}}{\omega_1}\,\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}\dot{d}(t)+\frac{\omega_1}{4\mathrm{i}}\,\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t}d(t)\Big] \\ &= (\omega_0-\omega)\dot{d}(t)-\mathrm{i}\left(\frac{\omega_1}{4}\right)^2 d(t) \end{aligned}$$

$$\ddot{d}(t)+\mathrm{i}(\omega_0-\omega)\dot{d}(t)+\left(\frac{\omega_1}{4}\right)^2 d(t)=0 \tag{4.21}$$

which has the solution

$$d(t)=A\mathrm{e}^{-\mathrm{i}(\omega_0-\omega)t/2}\sin\Omega t,\quad \Omega=\frac{1}{2}\sqrt{(\omega_0-\omega)^2+(\omega_1/2)^2} \tag{4.22}$$

where A is a constant which is determined by the normalization condition, i.e.,

$$\left(c^*(t),d^*(t)\right)\begin{pmatrix}c(t)\\ d(t)\end{pmatrix}=\left|c(t)\right|^2+\left|d(t)\right|^2=1 \tag{4.23}$$

One proceeds in the same fashion with $c(t)$ to obtain

$$c(t) = 2A\,\frac{\omega_0 - \omega_1}{\omega_1}\,\mathrm{e}^{\mathrm{i}(\omega_0-\omega)t/2}\left(-\sin\Omega t - \mathrm{i}\sqrt{1+\frac{\omega_1^2}{4(\omega_0-\omega)^2}}\cos\Omega t\right)$$

Rabi formula

We have assumed that before the perturbation the system is in the state $(+)$, i.e.

$$c(0) = 1; \quad d(0) = 0 \tag{4.25}$$

$$\left|c(0)\right|^2 + \left|d(0)\right|^2 = \left|c(0)\right|^2 = 1 \tag{4.26}$$

From $\left|c(0)\right|^2 = 1$, and after some algebra, one gets,

$$\left|A\right|^2 = \frac{(\omega_1/2)^2}{(\omega_0 - \omega)^2 + (\omega_1/2)^2} \tag{4.27}$$

and the probability that the transition takes place, i.e. that the system is in the state $(-)$ is

$$\left|d(t)\right|^2 = \frac{(\omega_1/2)^2}{(\omega_0 - \omega)^2 + (\omega_1/2)^2} \sin^2 \Omega t \tag{4.28}$$

and a resonance occurs when $\omega = \omega_0$. Eq. (4.28) is the Rabi's formula.

Nuclear magnetic resonance was first described and measured in molecular beams by Isidor Isaac Rabi in 1938. In 1944, Rabi was awarded the Nobel Prize in physics for this work.

`http://www.nobelprize.org/nobel_prizes/physics/laureates/1944/`

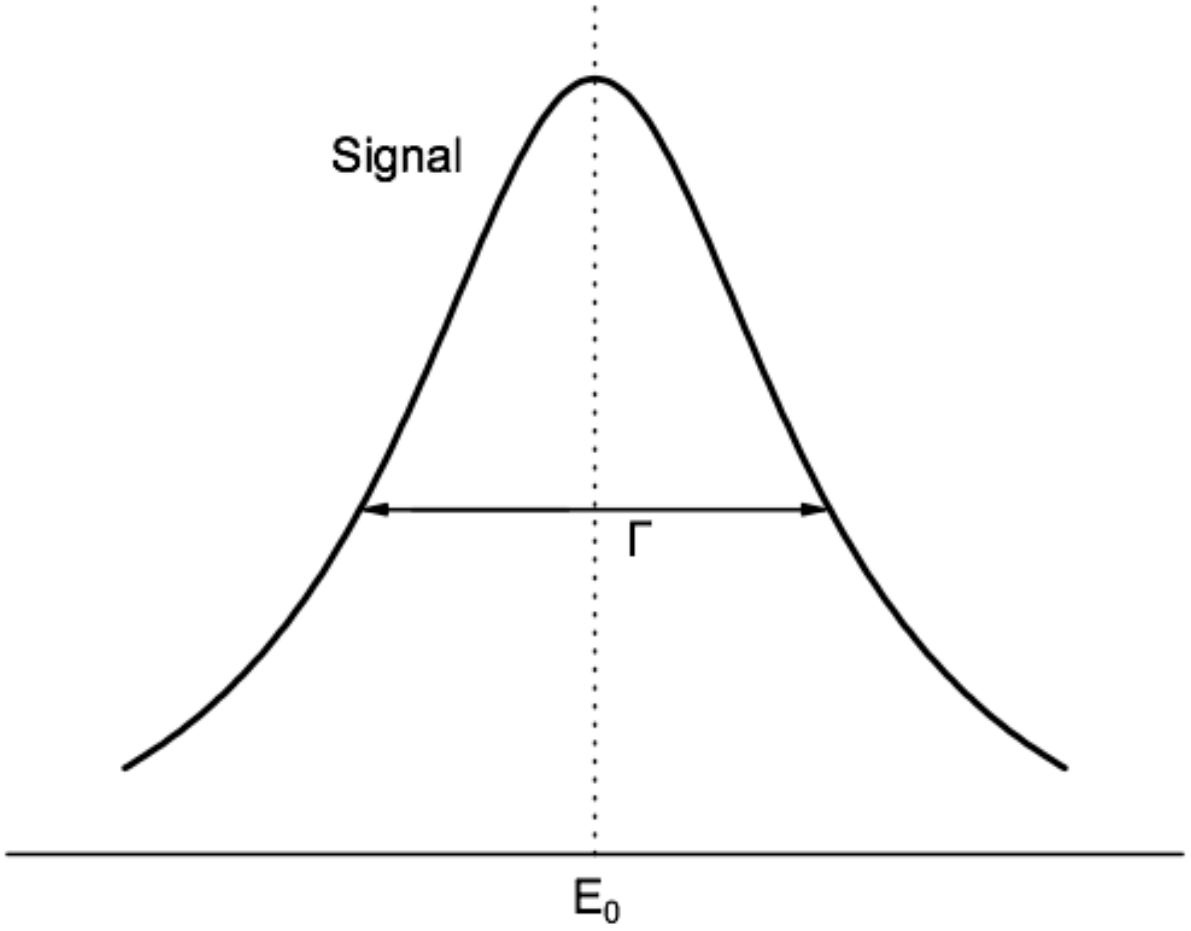


Figure 4.1: The resonant form of the signal as the energy E, corresponding to the weak magnetic field $\mathbf{B}_1$, approaches the energy E_0 induced by $\mathbf{B}_0$. The width of the resonance is Γ.

The wave function of a resonance with a peak at energy E_0 and a width Γ can be factorized as

$$\Phi(E, \mathbf{r}) = \sqrt{\frac{\Gamma/2}{\pi\left[(E - E_0)^2 + (\Gamma/2)^2\right]}}\,\Psi(\mathbf{r}), \tag{2.4}$$

where $\Psi(\mathbf{r}) = \sqrt{\pi\Gamma/2}\,\Phi(E_0, \mathbf{r})$. Through the Fourier transform, we obtain the time evolution of the resonance

$$\Phi(t, \mathbf{r}) = \int_{-\infty}^{\infty} \Phi(E, \mathbf{r}) e^{-iEt/\hbar} dE = \Psi(\mathbf{r}) e^{-i\tilde{E}t/\hbar}, \tag{2.5}$$

which gives us the resonance in the form of a stationary state, but with a complex energy

$$\tilde{E} = E_0 - i\frac{\Gamma}{2}. \tag{2.6}$$

The probability of measuring the system at t is given by

$$|\Phi(t, \mathbf{r})|^2 = |\Psi(\mathbf{r})|^2 e^{-\Gamma t/\hbar}. \tag{2.7}$$

4.3 Nuclear magnetic resonance (NMR)

Nuclear magnetic resonance (NMR) is a physical phenomenon in which magnetic nuclei in a magnetic field absorb and re-emit electromagnetic radiation. This energy is at a specific resonance frequency which depends on the strength of the magnetic field and the magnetic properties of the isotope of the atoms.

One sees that A shows a form similar to that of the Breit-Wigner formula

$$\frac{(\omega_1/2)^2}{(\omega_0-\omega)^2+(\omega_1/2)^2}\frac{\hbar^2}{\hbar^2}=\frac{(\Gamma_1/2)^2}{(E_0-E)^2+(\Gamma_1/2)^2} \tag{4.29}$$

from which one can define $E=\hbar\omega_0$ as the magnetic resonance energy and $\Gamma_1=\hbar\omega_1$ as the the width.

In Fig. 4.1 the form of the signal resulting from this expression is shown. The signal-energy plot shown in Fig. 4.1 has been used to investigate the inner structure of materials. Many scientific techniques exploit NMR phenomena to study molecular physics, crystals, and non-crystalline materials through NMR spectroscopy. NMR allows the observation of specific quantum mechanical magnetic properties of the atomic nucleus. In particular, it is used in Medicine to image nuclei of atoms inside the body (magnetic resonance imaging (MRI)).

In all applications of MRI one uses SI units and introduces the Bohr magneton

$$\mu_B=\frac{q\hbar}{2mc} \tag{4.30}$$

In these units the frequency becomes

$$\omega_0 = \frac{gqB_0}{2mc} = \frac{g\mu_B B_0}{\hbar} = \gamma B_0 \tag{4.31}$$

This is known as the Larmor Equation. As already mentioned, for electrons it is $g = 2.00$ and $\mu_B = 5.79 \times 10^{-5}\text{eV/T}$, where the unit Tesla is $1\text{T} = 10^4\text{gauss}$. Remember $\hbar c \approx 200\text{MeVfm}$. The precise value of $\hbar$ is $\hbar = 6.58 \times 10^{-22}\text{MeVsec}$. For protons $g = 5.58$ (as also already mentioned) and $\mu_N = 3.15 \times 10^{-8}\text{eV/T}$. In practical applications, the frequency is similar to VHF and UHF television broadcasts (60−1000 MHz).

4.4 Magnetic fields and magnetic moments

A nucleon moving in a single-particle state outside a central potential, as discussed above, will be affected by the presence of an external magnetic field. The corresponding Hamiltonian is,

$$H = -\frac{q}{2mc}\boldsymbol{\mu} \cdot \boldsymbol{B} \tag{4.32}$$

where q is the effective charge of the nucleon, $\boldsymbol{B}$ is the magnetic field and $\boldsymbol{\mu}$ is the dimensionless nuclear dipole moment defined as,

$$\boldsymbol{\mu} = g_l \hat{l} + g_s \hat{s} \tag{4.33}$$

The effective charge should be $q = 1.0\ e$ (e is the absolute value of the electron charge) for protons and 0 for neutrons. However, its value is taken to be about 1.5 e for protons and about 1.0 e for neutrons (these are illustrative values that can vary in different nuclear regions, i. e. for different values of N and Z). The reason why the effective charge was introduced is that the odd nucleon affects the core and it has been shown that its influence can be taken into account by the effective charge.

The magnetic moments can be measured with great precision, thus providing precise value for the g-factors also. These are given by,

$$g_l = \begin{cases} 1 & \text{proton} \\ 0 & \text{neutron} \end{cases} \qquad g_s = \begin{cases} 5.58 & \text{proton} \\ -3.82 & \text{neutron} \end{cases} \tag{4.34}$$

Dipole magnetic moments in nuclei

When the magnetic field is applied the energies observed experimentally are quantized according to the allowed angular momenta in Eq. (4.33). To measure the dipole magnetic moment μ one chooses the maximum splitting of the levels. One sees from Eq. (4.32) that the maximum effect of the magnetic field would be induced by the maximum alignment of $\boldsymbol{\mu}$ and $\boldsymbol{B}$. This is what one chooses experimentally. Classically this occurs when $j_z = j$ (since $\boldsymbol{B}$ is in the z-direction). In Quantum Mechanics one has to choose the projection m of the total angular momentum such that $m = j$. Therefore one defines the dipole magnetic moment as

$$\mu = \langle jm = j | g_l \hat{l}_z + g_s \hat{s}_z | jj \rangle \tag{4.35}$$

notice that μ is just a number without dimensions.

Since $\boldsymbol{l} = \boldsymbol{j} - \boldsymbol{s}$ one can write

$$\mu = \langle jj | g_l \hat{j}_z + (g_s - g_l) \hat{s}_z | jj \rangle \tag{4.36}$$

To calculate the values obtained by the application of the operator $\hat{s}_z$ upon the state $|jj\rangle$, we expand this state in terms of the eigenvectors of $\hat{s}_z$, i. e.

$$|jm\rangle = \sum_{m_l m_s} \langle l m_l 1/2 m_s | jm \rangle | l m_l 1/2 m_s \rangle \tag{4.37}$$

It is $m_l = j - m_s$ and $m_s = \pm 1/2$, $m_l = j \mp 1/2$. Therefore

$$\begin{aligned}\mu &= \left\langle l, j-\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| jj \right\rangle^2 \left[g_l j + \frac{g_s - g_l}{2} \right] \\ &+ \left\langle l, j+\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \middle| jj \right\rangle^2 \left[g_l j - \frac{g_s - g_l}{2} \right]\end{aligned}$$

a) $j = l - 1/2$

$$\left\langle j+\frac{1}{2}, j-\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| jj \right\rangle^2 = \frac{1}{2(j+1)}$$
$$\left\langle j+\frac{1}{2}, j+\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \middle| jj \right\rangle^2 = \frac{2j+1}{2(j+1)}$$

$$\mu = g_l j - (g_s - g_l)\frac{j}{2(j+1)} \tag{4.39}$$

b) $j = l + 1/2$

$$\left\langle j-\frac{1}{2}, j-\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \middle| jj \right\rangle^2 = 1$$
$$\left\langle j-\frac{1}{2}, j+\frac{1}{2}, \frac{1}{2}, -\frac{1}{2} \middle| jj \right\rangle^2 = 0$$

$$\mu = g_l j + (g_s - g_l)/2 \tag{4.40}$$

Magnetic moments

$\mu = g_j j \mu_N$,
μ_N – nuclear magneton, g_j – Lande g-factor

$$g_j = \frac{j(j+1)+l(l+1)-s(s+1)}{2j(j+1)} g_l + \frac{j(j+1)-l(l+1)+s(s+1)}{2j(j+1)} g_s$$

IF $j = l \pm 1/2$

$$jg_j = g_l l + g_s/2 \qquad \text{for } j = l + 1/2$$

$$jg_j = g_l j\left(1+\frac{1}{2l+1}\right) - g_s j\left(\frac{1}{2l+1}\right) \qquad \text{for } j = l - 1/2$$

$g_l = 1$ for p and $g_l = 0$ for n, $g_s \approx +5.6$ for p and $g_s \approx -3.8$ for n

$$jg_{proton} = l + 5.6 \times \frac{1}{2} = j + 2.8 \qquad \text{for } j = l + 1/2$$

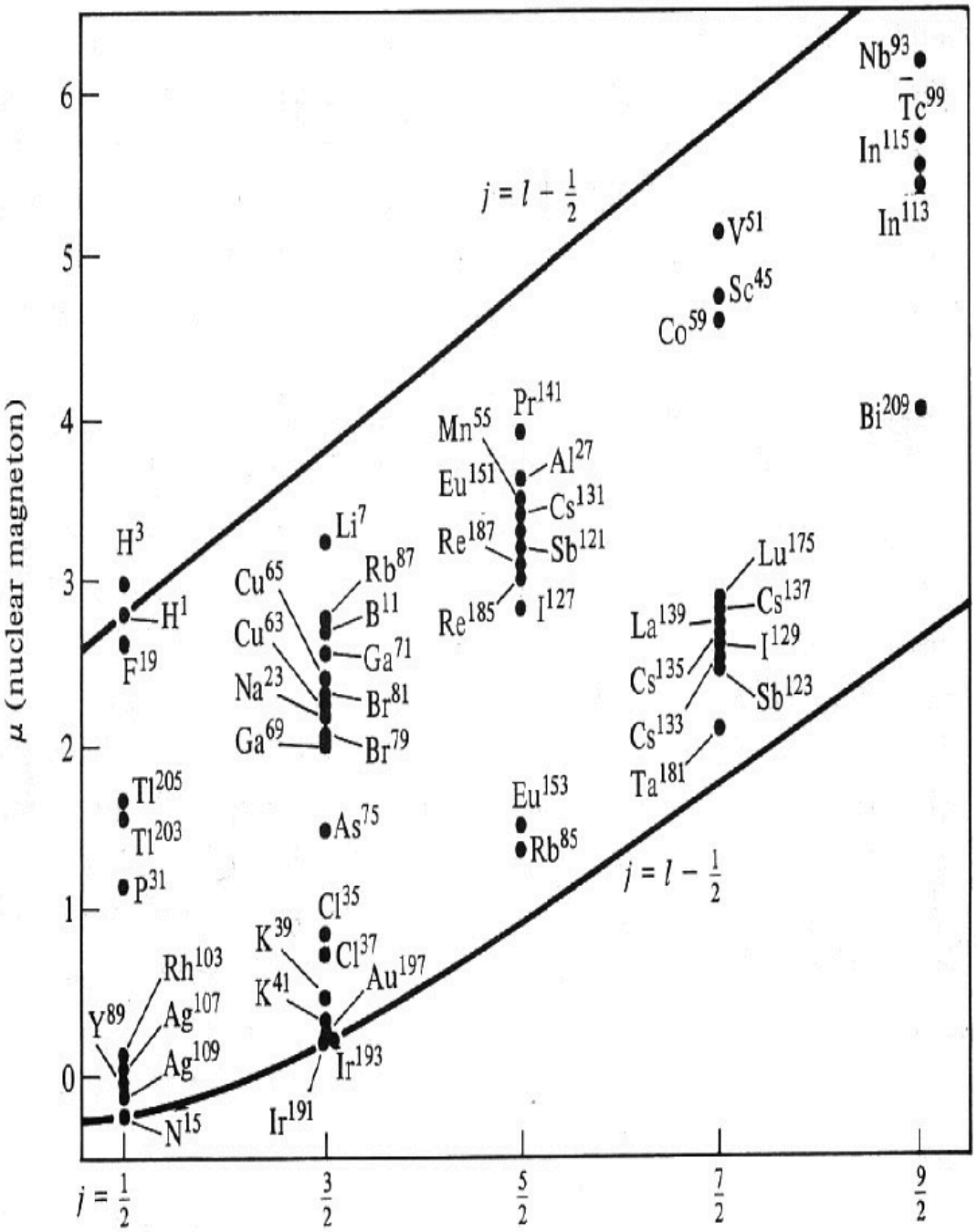
$$jg_{proton} = j\left(1 + \frac{1}{2l+1}\right) - 5.6 \times j\left(\frac{1}{2l+1}\right) = 1 - \frac{2.3}{j+1} \qquad \text{for } j = l - 1/2$$

$$jg_{neutron} = -3.8 \times \frac{1}{2} = -1.9 \qquad \text{for } j = l + 1/2$$

$$jg_{neutron} = 3.8 \times j\left(\frac{1}{2l+1}\right) = \frac{1.9j}{j+1} \qquad \text{for } j = l - 1/2$$

For a given j the measured moments lie between $j = l\text{-}1/2$ and $j = l\text{+}1/2$

Magnetic moments for odd-proton nuclei



Thank you!