3   Nuclear Shell Models I

In order to apply quantum mechanics calculation to describe nuclear structure. Check point can be done from nuclear spectroscopy, decay processes, and nuclear reaction.

3.1   Evidence of nuclear shell structure

As early as 1917 Harkins pointed out that nuclei with even numbers of protons or neutrons are more stable than those with odd numbers. Elsasser (1933) found that special numbers of protons or neutrons form particularly stable configurations. We shall list here a series of facts which indicate that we obtain especially stable nuclei when either the number of protons Z or the number of neutrons N = A – Z is equal to one of the following numbers (Mayer 1948):

$$2, 8, 14, 20, 28, 50, 82, 126$$

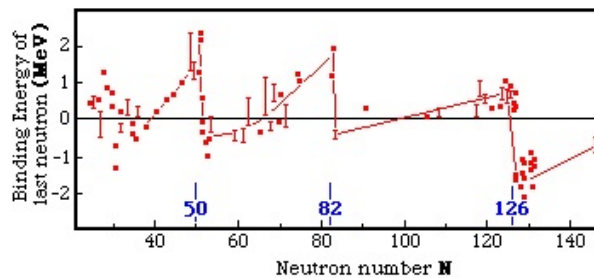These values are commonly referred to as *magic numbers*.

Figure 1:

3.2 Single-particle in spherical potential well

Schrodinger's equation

$$-\frac{1}{2\mu}\nabla^2\varphi(r) + V(r)\varphi(r) = E\varphi(r) \tag{1}$$

$$\nabla^2\varphi(r) + \frac{2\mu}{\hbar^2}(E - V(r))\varphi(r) = 0 \tag{2}$$

Working in spherical coordinate system

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2\hbar^2}\hat{L}^2$$

Separate the variable

$$\varphi(r, \theta, \phi) = R_{El}(r)Y_{lm}(\theta, \phi)$$

Using the fact that

$$\hat{L}^2 Y_{lm}(\theta, \phi) = l(l+1)\hbar^2 Y_{lm}(\theta, \phi)$$

From (3), we get the radial equation

$$\frac{d^2 R_{El}}{dr^2} + \frac{2}{r}\frac{dR_{El}}{dr} + \left(\frac{2\mu}{\hbar^2}(E - V(r)) - \frac{l(l+1)}{r^2}\right)R_{El} = 0 \tag{3}$$

3.3 Rigid sphere

Rigid spherical potential well of radius a

$$V(r) = \begin{cases} 0, & 0 \leq r \leq a \\ \infty, & r > a \end{cases} \tag{4}$$

Radial equation inside the sphere

$$\frac{d^2 R_{El}}{dr^2} + \frac{2}{r}\frac{dR_{El}}{dr} + \left(k^2 - \frac{l(l+1)}{r^2}\right)R_{El} = 0, \quad k^2 = \frac{2\mu E}{\hbar^2} \tag{5}$$

Substituting $u_{El}(r) = rR_{El}(r)$, we will have

$$R_{El} = \frac{u_{El}}{r} \rightarrow \frac{d^2 R_{El}}{d^2 r} + \frac{2}{r}\frac{dR_{El}}{dr} = \frac{1}{r}\frac{d^2 u_{El}}{dr^2}$$

From equation (5) we have

$$\frac{d^2 u_{El}}{dr^2} + \left(k^2 - \frac{l(l+1)}{r^2} \right) u_{El} = 0 \qquad (6)$$

$$\rho = kr \rightarrow u_{El}(r) = u_{El}(\rho), \quad u''_{El}(\rho) + \left(1 - \frac{l(l+1)}{\rho^2} \right) u_{El}(\rho) = 0 \qquad (7)$$

This is known in the name of *spherical Bessel differential equation.* [See https://mathworld.wolfram.com/SphericalBesselDifferentialEquation.html] Its solutions appear in term of *spherical Bessel functions of the first and second kinds,* respectively, as

$$u_{El}(\rho) = A_l j_l(\rho) + B_l y_l(\rho) \qquad (8)$$
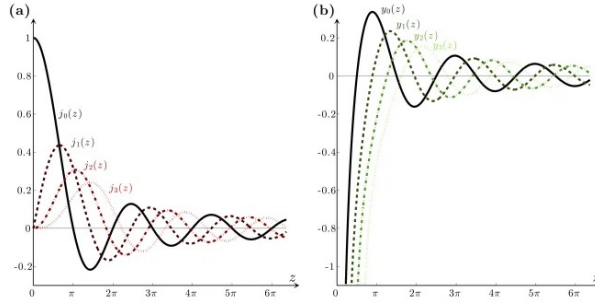
See figure (1).

Figure 2:

Since $y_l(\rho)$ is not finite at origin, we set the integration constant $B_l = 0$. Then we have

$$u_{El}(\rho) = A_l j_l(\rho) \qquad (9)$$

as our solution, with A_l as the normalization constant. Note that the radial solution vanishes at the boundary

$$j_l(\rho) = 0 \rightarrow \rho = ka = \beta_{nl} \qquad (10)$$

$$E = \frac{\hbar^2 k^2}{2\mu} \rightarrow E_{nl} = \frac{\hbar^2 \beta_{nl}^2}{2\mu a^2} \qquad (11)$$

Note that β_{nl} is called *zero points of Bessel functions.*

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$$j_0(kr) = \frac{\sin kr}{kr}$$

$$j_1(kr) = \frac{\sin kr}{(kr)^2} - \frac{\cos kr}{kr}$$

$$j_2(kr) = \frac{3\sin kr}{(kr)^3} - \frac{3\cos kr}{(kr)^2} - \frac{\sin kr}{kr}$$

β_{nl}	$n=1$	$n=2$	$n=3$	$n=4$
$l=0$	3.142	6.283	9.425	12.566
$l=1$	4.493	7.725	10.904	14.066
$l=2$	5.763	9.095	12.323	15.515
$l=3$	6.988	10.417	13.698	16.924
$l=4$	8.183	11.705	15.040	18.301

Figure 3:

Spectroscopic notation of nuclear energy levels, similar to atomic levels,

$$n - shell, \ l - orbital = (0, 1, 2, 3, ...) \rightarrow (s, p, d, f, ...)$$

List of levels inside rigid spherical well:

$$1s, 1p, 1d, 2s, 1f, 2p, ...$$

3.4   Isotropic harmonic potential

The isotropic harmonic potential well

$$V(r) = \frac{1}{2}\mu\omega r^2 = \frac{1}{2}\mu\omega^2(x^2 + y^2 + z^2) \tag{12}$$

From (3), we will have radial equation in the form

$$\frac{d^2 R_{El}}{dr^2} + \frac{2}{r}\frac{dR_{El}}{dr} + \left(\frac{2\mu E}{\hbar^2} - \frac{\mu^2\omega^2}{\hbar^2}r^2 - \frac{l(l+1)}{r^2}\right) R_{El} = 0 \tag{13}$$

Using the fact that the energy level of the system will be the same as we have derived from Cartesian coordinate coordinate calculation, i.e.,

$$E = E_N = \hbar\omega(N + 3/2)$$

Then we have from (13)

$$\frac{d^2 R_{Nl}}{dr^2} + \frac{2}{r}\frac{dR_{nl}}{dr} + \left((2N+3)\frac{\mu\omega}{\hbar} - \frac{\mu^2\omega^2}{\hbar^2}r^2 - \frac{l(l+1)}{r^2}\right) R_{Nl} = 0 \tag{14}$$

Let us define

$$\alpha^2 = \frac{\hbar}{\mu\omega}, \ \rho = r/\alpha, \ u_{Nl}(\rho) = \rho R_{Nl}(\rho)$$

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We get from (14)

$$\frac{d^2 u_{Nl}}{d\rho^2} + \left((2N+3) - \rho^2 - \frac{l(l+1)}{\rho^2}\right) u_{Nl} = 0 \qquad (15)$$

Let us define

$$u_{Nl}(\rho) = f(\rho)e^{-\rho^2/2}\rho^l \qquad (16)$$

$$(15) \rightarrow \rho\frac{d^2 f}{d\rho^2} + (2(l+1) - 2\rho^2)\frac{df}{d\rho} + 2\rho((N-l)f = 0 \qquad (17)$$

$$\eta = \rho^2, f = f(\eta) \rightarrow \eta\frac{d^2 f}{d\eta^2} + \left(l + \frac{1}{2} + 1 - \eta\right)\frac{df}{d\eta} + \frac{N-l}{2}f = 0 \qquad (18)$$

We derive the *associated Laguerre equation* for $f(\eta)$, its solution exist for $(N-l)/2 = n - 1 \geq 0$, in form of *associated Laguerre polynomial*

$$L_{n-1}^{l+1/2}(\eta), \ n = (N-l)/2 + 1 = 1, 2, 3, ... \rightarrow N = 2(n-1) + l$$

We finally have

$$R_{nl}(r) = N_{nl}r^l e^{-\mu\omega r^2/2\hbar} L_{n-1}^{l+1/2}(\mu\omega r^2/\hbar) \qquad (19)$$

$$E_{nl} = (2n + l - 1/2)\hbar\omega \qquad (20)$$

List of some nuclear levels

n	l	Orbitals	Energy
1	0	1s	$\frac{3}{2}\hbar\omega$
1	1	1p	$\frac{5}{2}\hbar\omega$
2,1	0,2	2s,1d	$\frac{7}{2}\hbar\omega$

3.5 Wood-Saxon potential

The wood-Saxon potential well

$$V_{WS}(r) = -\frac{V_0}{1 + e^{(r-R)/a}} \qquad (21)$$

where $R = r_0 A^{1/3}$ is the nuclear radius, with $r_0 = 1.27fm$, $a \simeq 0.67fm$ *skin thickness*, and $V_0 \simeq 50 - 33(N-Z)/A$ in MeV, see figure (6).

An analytic solution of radial Schrodinger's equation of Wood-Saxon potential can be found in the book by F. Flugge (Practical Quantum Mechanics, Springer). The energy levels are derived by graphical method, as always done for finite potential well problem. Comparison with the previous two model potentials is shown in figure (3.5).
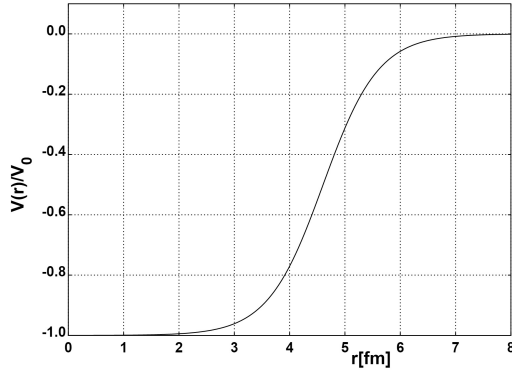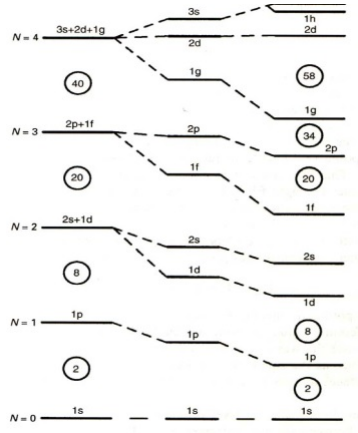
Figure 4:

Figure 5:

3.6 Spin-orbit coupling

Mayer and Jansen (1949) included (strong) spin-orbit potential, in order to explain the magic number, in the form

$$V(r) = V_{central}(r) + V_{SO}(r)\vec{L} \cdot \vec{S}$$

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The spin-orbit interaction splits the l-level into two j-levels, i.e., $j = l \pm 1/2$, and the splitting are determined from

$$\vec{L} \cdot \vec{S} = \frac{1}{2} \left[J^2 - L^2 - S^2 \right] \tag{22}$$

$$\langle lm | \vec{L} \cdot \vec{S} | lm \rangle = \frac{\hbar^2}{2} \left[j(j+1) - l(l+1) - \frac{3}{4} \right] \tag{23}$$

$$= \frac{\hbar^2}{2} \begin{cases} -l, & j = l + 1/2 \\ (l+1), & j = l - 1/2 \end{cases} \tag{24}$$

Normally we will take $V_{SO}(r) \to \alpha$ a model parameter, for comparison with experiment. The spin-orbit coupling shift is shown in figure (3.6).
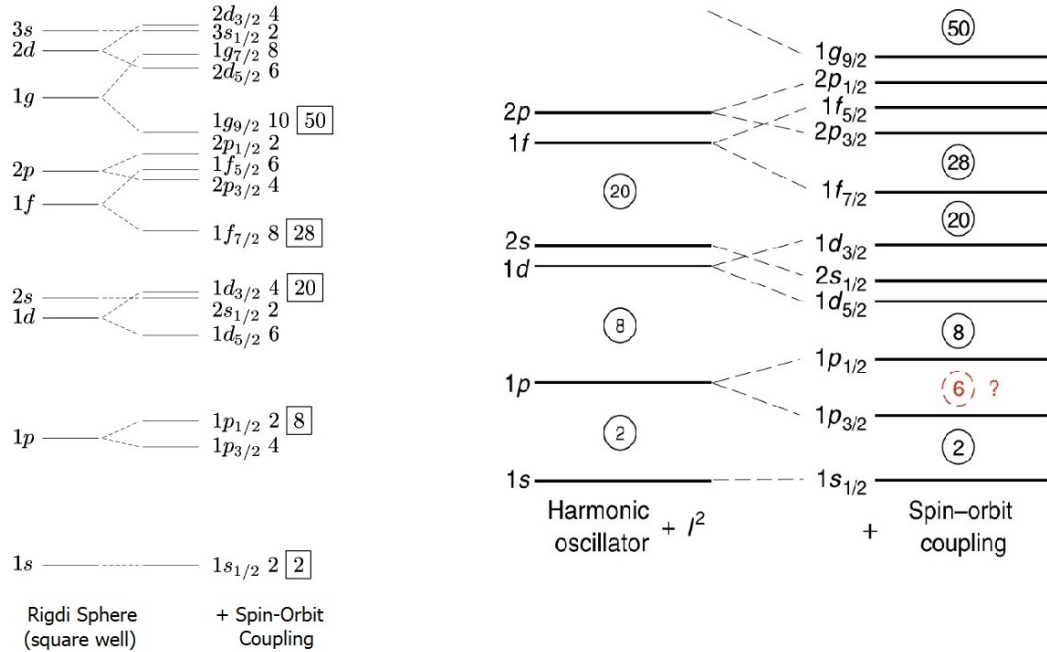

Figure 6:

3.7 Multinucleon configurations

We already have shell structure of one-nucleon, i.e., isotropic harmonic oscillator + LS coupling (with correct set of magic numbers). For multinucleon nuclei, the occupation into the nuclear levels are determined to follow:

- Pauli's exclusion principle

- Hund's rule of maximal spin alignment within the same orbital

- the fact that it is better for neutron and proton to occupy different potential wells
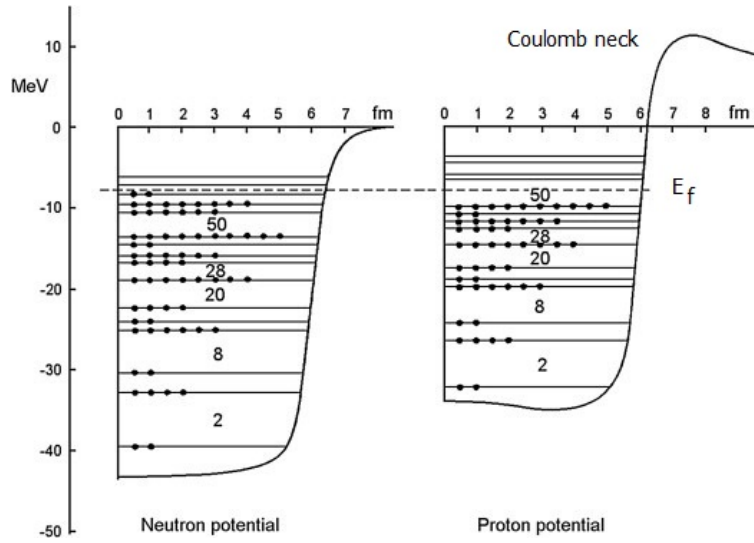

Figure 7: Neutron and proton potential wells.

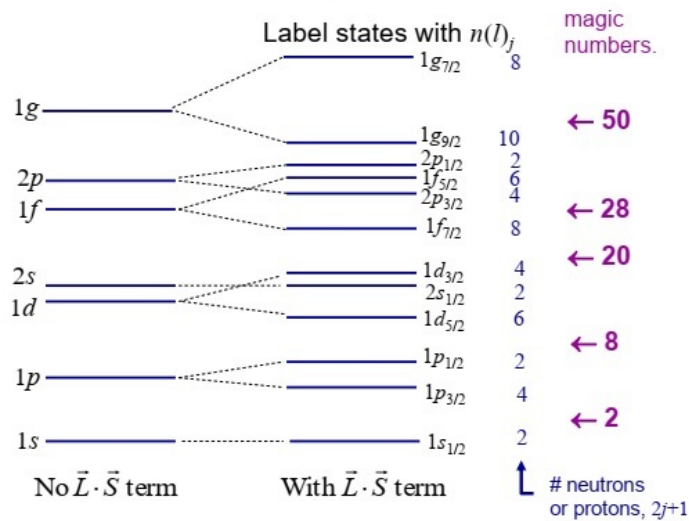A list of nuclear orbitals(nlj) (with LS-coupling) with occupation numbers ($2j + 1$):

Figure 8: A list of nuclear orbitals (nlj).
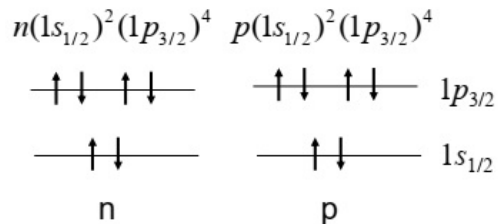
Ground state configuration of ^{12}C:

Figure 9: Ground state configuration of ^{12}C.

Ground state configuration of ^{13}C:

$$n(1s_{1/2})^2(1p_{3/2})^4(1p_{1/2})^1 \quad p(1s_{1/2})^2(1p_{3/2})^4$$
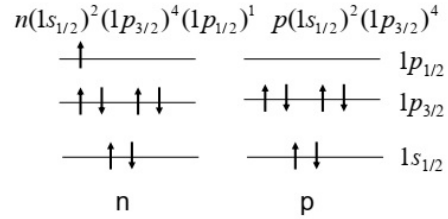
Figure 10: Ground state configuration of ^{13}C.

The first excited state configuration of ^{12}C, assume an excitation of a neutron, it leaves *hole state* at the lower level.

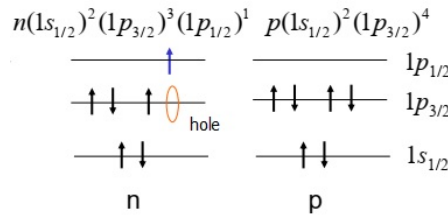$$n(1s_{1/2})^2(1p_{3/2})^3(1p_{1/2})^1 \quad p(1s_{1/2})^2(1p_{3/2})^4$$

Figure 11: First excited state configuration of ^{12}C with hole.

3.8   Spin and parity

3.8.1   Nuclear spin

According to Hund's rule of nucleon occupation, the nuclear spin is determined from the summation of spins of all unpaired nucleons.

Element	^{1}H	^{2}H	^{12}C	^{13}C	^{14}N	^{16}O	^{31}P	^{32}S
Nuclear spin quantum number (I)	1/2	1	0	1/2	1	0	1/2	0
Number of spin states	2	3	1	2	3	1	2	1

Figure 12: Nuclear spin.

3.8.2 Nuclear parity

- Parity of single nucleon orbital (nlj) is defined to be

$$\pi = (-1)^l$$

  The parity of this state is denoted by j^π.

- Parity of multi-nucleon nuclei is determined from the product of all one nucleon parity

$$\pi = \Pi_{i,A}(-1)^{l_i}$$

  Note that

  - for odd A nuclei (even/odd or odd/even of n/p), there is always one un-pair nucleon in the ground state. Therefore the parity of the odd A nuclei ground state is determined from parity of the un-paired nucleon orbital.

  - for nuclear orbital (nlj), there are $2j+1$ occupation number, this corresponds to

$$m_j = -j, -(j-1), ..., +(j-1), +j$$

    This represents the orientations of $\vec{J}$. So that for filled orbital the total $j = 0$. For example of ^{12}, its ground state parity is $j^\pi = 0^+$

  - in case of ^{13}C, its ground state parity is $j^\pi = \frac{1}{2}^-$

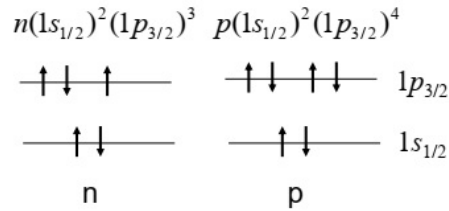 - in case of ^{11}C, its ground state parity is $j^\pi = \frac{3}{2}^-$

Figure 13: Ground state configuration of ^{11}C.

- the parity of first excited state of ^{12}C is determined from j of excited neutron and created hole:

$$\vec{J} = \vec{J}_n + \vec{J}_{hole} \rightarrow j = j_n + j_h, ..., |j_n - j_h| \quad (25)$$

$$j_n = 1/2, j_h = 3/2 \rightarrow j = 2, 1 \quad (26)$$

$$\rightarrow \pi = \pi(p_{1/2})\pi(p_{3/2}) = (-1)(-1) = +1 \rightarrow j^\pi = 1^+ \text{ or } 2^+ \quad (27)$$

$$\text{Observed } j^\pi = 2^+ \quad (28)$$