The Shell Model

1. Similarities and differences between modeling the atomic electrons and the nucleons

   - Both electrons and nucleons are fermions
   - Electrons are negatively charged, while nucleons can be positively charged or neutral
   - Occupancy of electrons and nucleons is governed by the Pauli Exclusion principle
   - Interactions are electromagnetic and strong (in the nucleus)

2. Simple → complex atoms

   hydrogen-like → many electrons

   Screening of the nuclear charge → more complicated QM problem to solve.

Figure 5.1 Atomic Energy Levels for $n = 1$ to 4 in (a) a Hydrogen-Like Atom and (b) a Many-Electron Atom

Note that the energy axis is not to scale.

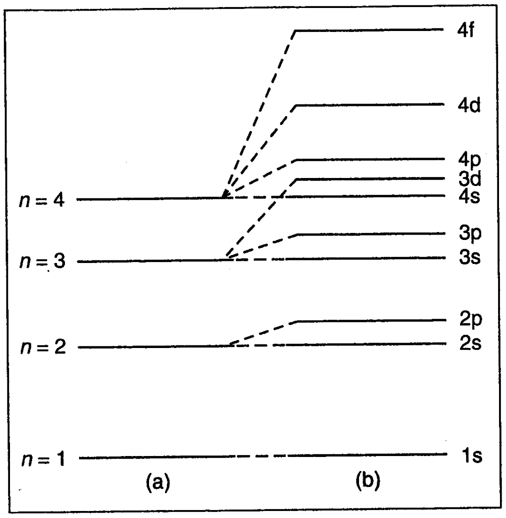
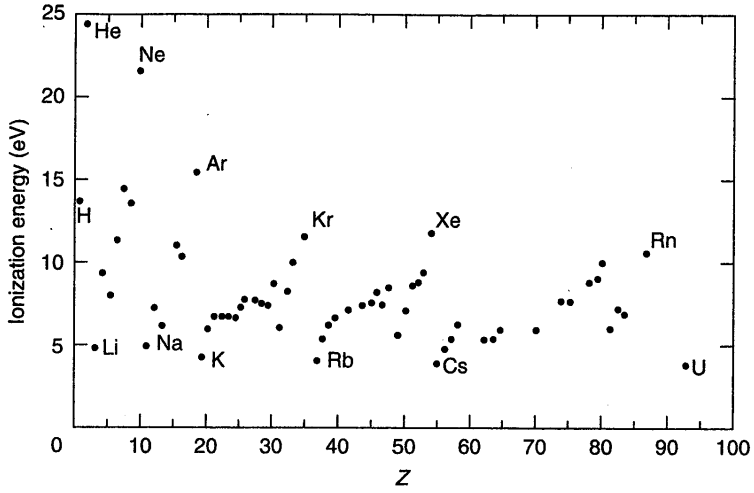


Table 5.2 Occupancy of Atomic Energy Levels in Order of Increasing Energy

Shell	n	l	Notation	Degeneracy $2(2l+1)$	Accumulated Occupancy
K	1	0	1s	2	2
L	2	0	2s	2	4
L	2	1	2p	6	10
M	3	0	3s	2	12
M	3	1	3p	6	18
N	4	0	4s	2	20
N	3	2	3d	10	30
N	4	1	4p	6	36
O	5	0	5s	2	38
O	4	2	4d	10	48
O	5	1	5p	6	54
P	6	0	6s	2	56
P	4	3	4f	14	70
P	5	2	5d	10	80
P	6	1	6p	6	86

Magic Numbers for the electrons

Figure 5.2 | Electron Ionization Energies as a Function of *Z*



What is the evidence for Nuclear Shell Structure?

1. We studied binding energies in the previous chapter when we constructed the semiemperical mass formula. Is it possible to see unusual binding energies as a function of N or Z in the nucleus, similar to the deviations of binding energies observed in complex atoms?

Figure 5.3 | Differences Between the Measured Binding Energy per Nucleon and the Value Predicted by the Liquid Drop Model as a Function of *A*

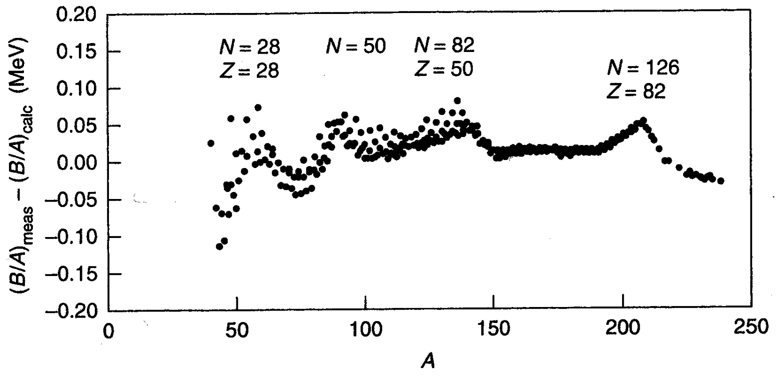
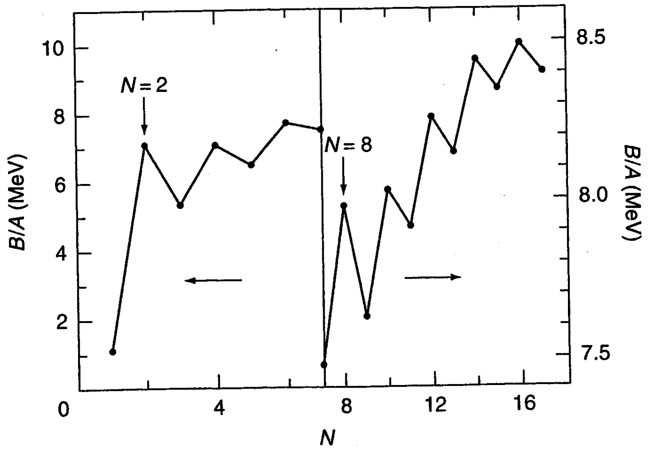
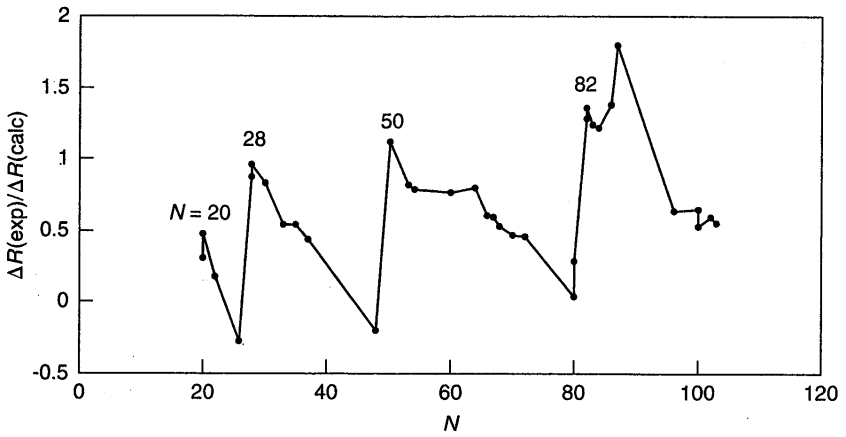


Figure 5.4 | Binding Energy per Nucleon for Light Nuclei with $N = Z$



Further Evidence for a Nuclear Shell Model

Figure 5.5 Change in the Measured Nuclear Radius for a Change in Neutron Number $\Delta N = 2$ Normalized to the Change Predicted by Equation (3.23)



Data from E. B. Shera *et al., Phys. Rev. C14* (1976), 731. Copyright 1976 by the American Physical Society.

Further Evidence for a Nuclear Shell Model

Figure 5.6 | Number of Stable Isotones as a Function of *N* (Even)

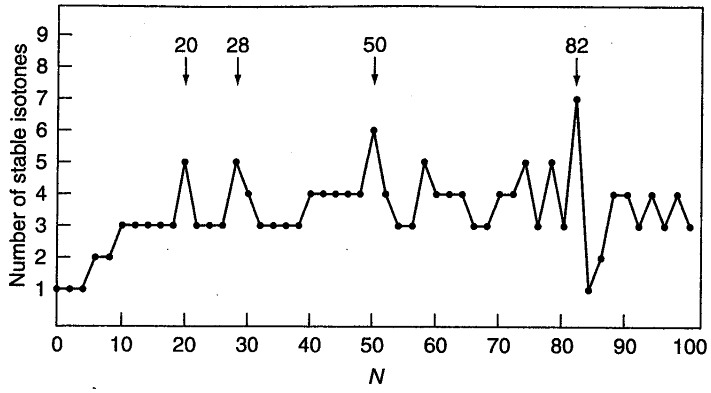
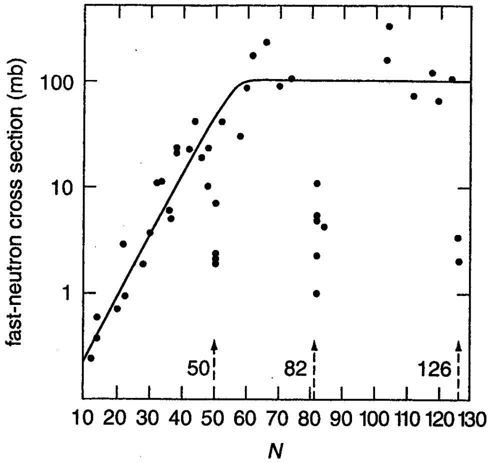


Figure 5.7 | Absorption Cross Sections for 1 MeV Neutrons

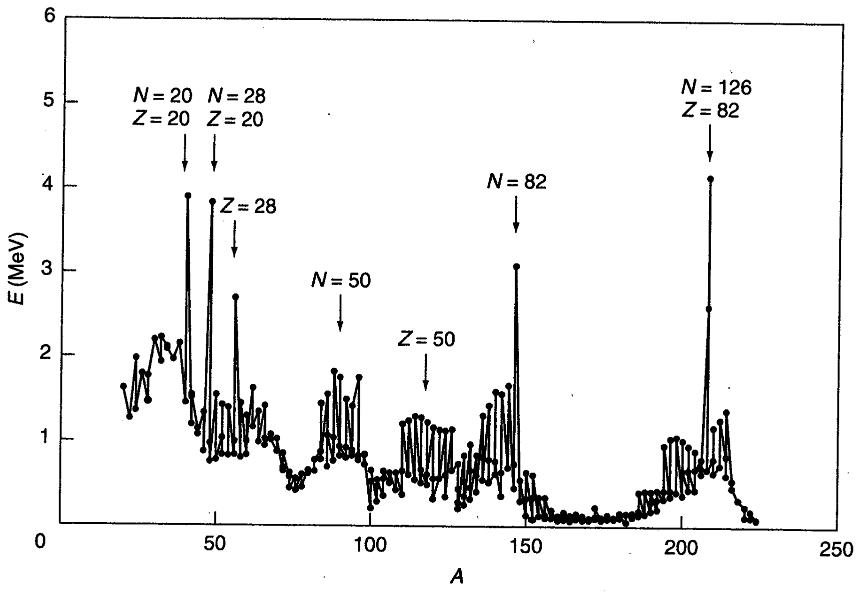


Data from D. J. Hughes and D. Sherman, *Phys. Rev.* *78* (1950), 632. Copyright 1950 by the American Physical Society.

Further Evidence for a Nuclear Shell Model

Figure 5.8 | Energies of the First Excited 2^+ States of Even–Even Nuclei as a Function of *A* and *Z*

The relevance of the first excited 2^+ state is discussed in Chapter 6.

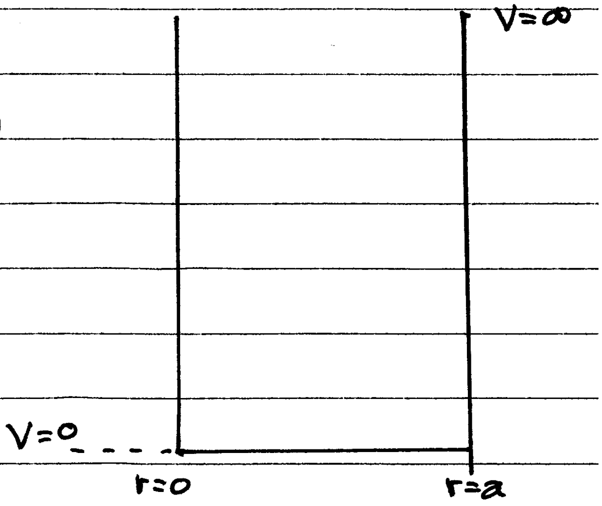


First Approach to a Nuclear Shell Model

1. The Infinite Square Well Potential

$$V(r)=\begin{cases}0 & r<a\\ \infty & r>a\end{cases}$$

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(\psi = E\psi$$



$$\psi(r,\theta,\varphi) = R_{n\ell}(r)\, Y_{\ell m}(\theta,\varphi)$$

The radial part of the Schrödinger Equation:

① $$-\frac{\hbar^2}{2m}\left[\frac{d^2R}{dr^2}+\frac{2}{r}\frac{dR}{dr}\right]+\left[V(r)+\frac{\hbar^2\ell(\ell+1)}{2mr^2}\right]R=ER$$

Section 4.1.3 of Griffiths

Convert the radial equation using a change of variables:

Let $u(r)\equiv r\,R(r)$

Then the radial part of the Schrödinger Equation can be written as:

② $$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\underbrace{\left[V(r)+\underbrace{\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}}_{\text{Centrifugal term}}\right]}_{\text{Effective Potential}}u=E\,u$$

In the radial part of the Schrödinger Equation:

Normalization $\Longrightarrow$ $\int_0^\infty |R|^2 r^2\, dr = 1$ & $\int_0^{2\pi}\int_0^{\pi} |Y|^2 \sin\theta\, d\theta\, d\varphi=1$

In our case (Eq.2) we have $\int_0^\infty |u|^2\, dr = 1$

Approach to a Nuclear Shell Model

Consider Eq. 2 for the infinite square well potential and $\ell = 0$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} = Eu \quad \Rightarrow \quad \frac{d^2u}{dr^2} + k^2u = 0$$

where: $k_n = \frac{\sqrt{2mE_n}}{\hbar} = \frac{n\pi}{a}$ $\qquad u(r) = A\sin k_n r + B\cos k_n r$

$R(r) = \frac{u(r)}{r}$ and $\frac{\cos kr}{r} \to \infty$ as $r \to 0$. So, $B = 0$

So, $R(r) = \frac{\sqrt{\frac{2}{a}}\,\sin k_n r}{r}$ $\qquad Y_{00} = \frac{1}{\sqrt{4\pi}}$

$$\boxed{\psi_{n00} = \frac{1}{\sqrt{2\pi a}}\,\frac{\sin\left(\frac{n\pi}{a}r\right)}{r}}$$

Solution for $\ell = 0$

$n = 1, 2, 3, \ldots$

$$\boxed{E_{n\underset{\uparrow \ell=0}{0}} = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

What are the solutions for an arbitrary integer ℓ ?

Now we must solve: $\frac{d^2u}{dr^2} + \left[k^2 - \frac{\ell(\ell+1)}{r^2}\right]u = 0$

The solution to this equation is:

$$u(r) = A\,r\,\underset{\uparrow \text{sph. Bessel}}{j_\ell(kr)} + B\,r\,\underset{\uparrow \text{sph. Neumann}}{\eta_\ell(kr)}$$

$B = 0$ because $\eta_\ell(kr) \to \infty$ as $r \to 0$

So, $u(r) = A\,r\,j_\ell(k_n r) = r\,R(r)$

Table 5.3 Example of Spherical Harmonics for Small Values of *l*

l	m_l	$Y_{lm_l}(\theta, \phi)$
0	0	$(1/4\pi)^{1/2}$
1	0	$(3/4\pi)^{1/2} \cos\theta$
1	±1	$\mp(3/8\pi)^{1/2} \sin\theta\, e^{\pm i\phi}$
2	0	$(5/16\pi)^{1/2} (3\cos^2\theta - 1)$
2	±1	$\mp(15/8\pi)^{1/2} \sin\theta \cos\theta\, e^{\pm i\phi}$
2	±2	$(15/32\pi)^{1/2} \sin^2\theta\, e^{\pm 2i\phi}$

Table 5.4 Some Examples of Spherical Bessel Functions

l	$j_l(kr)$
0	$\sin kr/(kr)$
1	$[\sin kr/(kr)^2] - [\cos kr/(kr)]$
2	$[3\sin kr/(kr)^3] - [3\cos kr/(kr)^2] - [\sin kr/(kr)]$

Figure 5.10 Spherical Bessel Functions for *l* = 0, 1, and 2

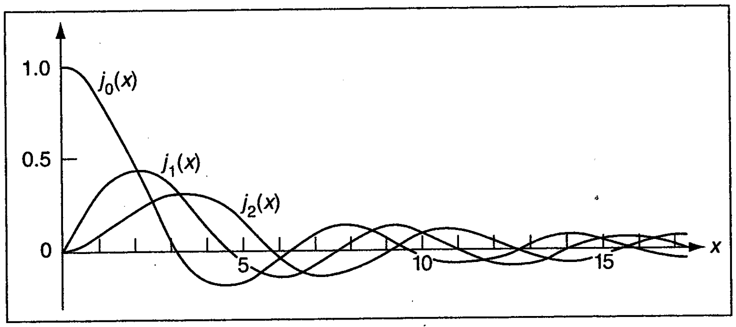


Table 5.5 The First Four Zeros of the Spherical Bessel Functions as a Function of *l*

l	$z_n(l)$
0	3.1416, 6.2832, 9.4248, 12.5664, ...
1	4.4934, 7.7253, 10.9041, 14.0662, ...
2	5.7635, 9.0950, 12.3229, 15.5146, ...
3	6.9879, 10.4171, 13.6980, 16.9236, ...
4	8.1826, 11.7049, 15.0397, 18.3013, ...
5	9.3558, 12.9665, 16.3547, 19.6532, ...
6	10.5128, 14.2074, 17.6480, 20.9835, ...
7	11.6570, 15.4313, 18.9230, 22.2953, ...

What are the energy levels for these wavefunctions?

$R(0) = \text{finite}$ $\qquad$ $R(a) = 0$ $\qquad$ $\boxed{R(r) = A_{n\ell}\, j_\ell(k_n r)}$

$\boxed{k_n a = \beta_{n\ell}}$ $\qquad$ $\beta_{n\ell} = n^{th}$ zero of the ℓ^{th} spherical Bessel function

$$E_{n\ell} = \frac{\hbar^2 k_{n\ell}^2}{2m} \qquad \boxed{E_{n\ell} = \frac{\hbar^2 \beta_{n\ell}^2}{2ma^2}}$$

⇐ Energy levels depend on $\underline{\underline{n \text{ and } \ell}}$

$$\psi_{n\ell m} = R_{n\ell}(r)\, Y_{\ell m}(\theta, \varphi)$$

$$\boxed{\psi_{n\ell m} = A_{n\ell}\, j_\ell\left(\frac{\beta_{n\ell}}{a} r\right) Y_{\ell m}(\theta, \varphi)}$$

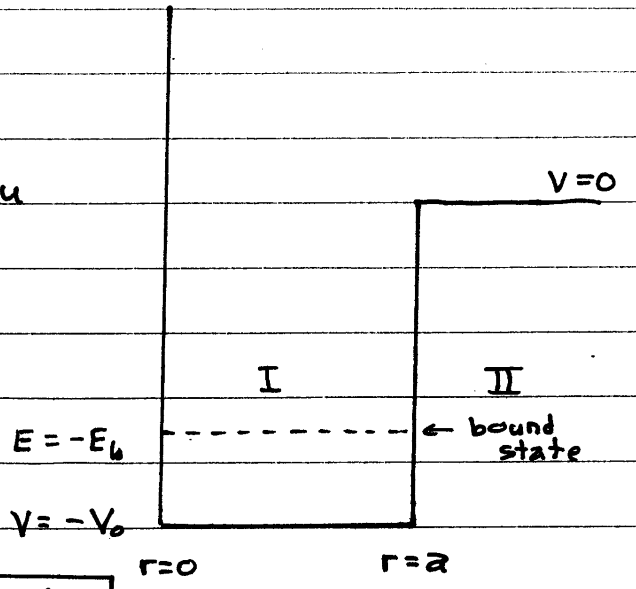
Table 5.6 | Energies and Occupancy of Nucleon States for the Infinite Square Well Potential

n	l	Notation	E/E_0	Occupancy	Accumulated Occupancy
1	0	1s	1.00	2	2
1	1	1p	2.05	6	8
1	2	1d	3.37	10	18
2	0	2s	4.00	2	20
1	3	1f	4.96	14	34
2	1	2p	6.04	6	40
1	4	1g	6.78	18	58
2	2	2d	8.38	10	68
1	5	1h	8.88	22	90
3	0	3s	9.00	2	92
2	3	2f	10.99	14	106
1	6	1i	11.20	26	132
3	1	3p	12.05	6	138
1	7	1j	13.76	30	168

Infinite Square Well → Finite Square Well

The radial equation:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\hbar^2\ell(\ell+1)}{2mr^2}\right]u = Eu$$



Region I : Use $u(r) = A_{n\ell}\, r\, j_\ell(kr)$

Region II : Use $u(r) = C e^{-\kappa(r-a)}$

$$k = \sqrt{\frac{2mc^2(V_0 - E_b)}{(\hbar c)^2}}$$

$$\kappa = \sqrt{\frac{2mc^2 E_b}{(\hbar c)^2}}$$

$\boxed{\text{This for } \ell = 0}$

$$u(r) = \begin{cases} \frac{c_1}{k}\sin(kr) & 0 \le r \le a \\ \frac{c_1}{k}\sin(ka)\, e^{-\kappa(r-a)} & a \le r < \infty \end{cases}$$

Using the B.C.'s at r=a, you can determine the normalization constant (c_1) and the binding energy (E_b).

Note: there can be multiple binding energies dependending on the width and depth of the well.

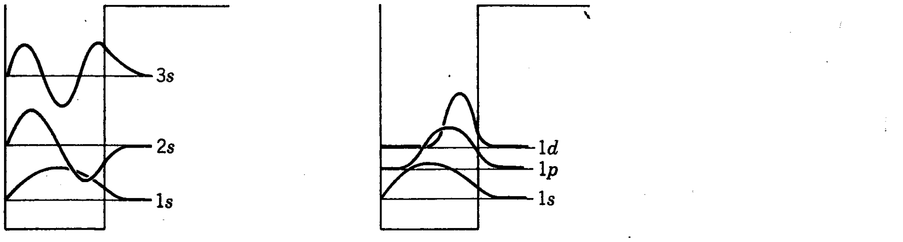
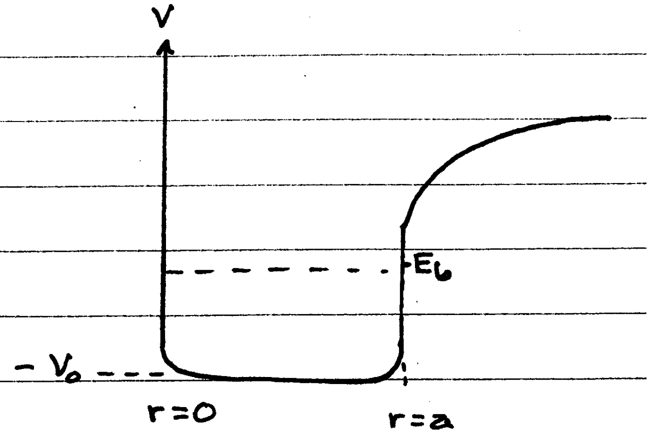


Figure 15-17 *Left:* Illustrating qualitatively the product rR of the radial coordinate r and the radial dependence R of the eigenfunction ψ for states, of the indicated three-dimensional square well, with $l = 0$ and $n = 1, 2, 3$. Each is shown by using its energy level as an r axis. Since the radial probability density is $P = 4\pi r^2 R^* R = 4\pi(rR)^2$, if the student visualizes the squares of the functions depicted he can make comparisons with the radial probability densities for states of a one-electron atom Coulomb potential, or a multielectron atom Hartree net potential, by looking also at Figures 7-5 or 9-10. In so doing, he should keep in mind that the quantum number n is used differently in atomic physics. The fact that the radial node quantum number n of nuclear physics just specifies the number of nodes of rR within the well is made apparent by this figure. *Right:* The same for states with $n = 1$ and $l = 0, 1, 2$. The way that what might be called a centrifugal effect tends to prevent a nucleon from approaching $r = 0$ as the orbital angular momentum quantum number l becomes larger than 0 is seen in this figure.

Other forms of the nuclear potential

① Rounded Edges $V(r) = \dfrac{-V_0}{1 + e^{+(r-a)/z}}$



② Rounded Edges + Spin Orbit Coupling

a = nuclear radius

z ~~τ~~ surface thickness t

$$z = \frac{t}{4\ln 3}$$

How do we introduce spin-orbit coupling in the nucleus?

$$V(r) \longrightarrow V(r) + f(r)\,\vec{S}\cdot\vec{L}$$

where f(r) is a function of position and $\vec{S}$ & $\vec{L}$ are the nucleon spin and orbital angular momenta

- The spin-orbit interaction cancels out in the interior of the nucleus.
- The spin-orbit interaction is most important at the edge of the nucleus.

$$f(r) \propto \frac{1}{r}\frac{dV}{dr}$$

Recall that for complex atoms where we studied the spin-orbit interactions, we have a term for the perturbation potential energy:

$$V_{\vec{S}\cdot\vec{L}} = \vec{S}\cdot\vec{L}\, f_c(r) \quad \text{where } f_c(r) = \frac{1}{2mc^2}\frac{dV_c}{dr}$$

where V_c was the PE of the electron with a "screened" nuclear charge.

⟹ For a hydrogen-like atom $V_c(r) = \dfrac{e^2}{4\pi\varepsilon_0}\dfrac{1}{r}$ & the perturbation hamiltonian became $H'_{so} = \left(\dfrac{e^2}{8\pi\varepsilon_0}\right)\dfrac{1}{m^2c^2r^3}\,\vec{S}\cdot\vec{L}$ (including $\frac{1}{2}$ for Thomas Precession)

Spin-Orbit Coupling (Atomic & Nuclear)

In the case of complex atoms we found the following splittings in the energy levels:

for complex atoms

$$\langle V_{\vec{S}\cdot\vec{L}} \rangle = \frac{\hbar^2}{2} \underset{\underset{\text{Coulomb}}{\uparrow}}{\langle f_c(r) \rangle} \times \begin{cases} l & \text{for } j = l + 1/2 \\ -l-1 & \text{for } j = l - 1/2 \end{cases}$$

In other words, doublet splitting for every non-zero l.

Spin-Orbit Splitting in the Nucleus

1. Spin-Orbit interactions are very strong in the nucleus. Especially when it is compared to the $\vec{S}\cdot\vec{L}$ interaction in complex atoms.
2. Spin-Orbit interactions in the nucleus gives rise to the "magic numbers" observed for N and Z.

need the minus sign in nuclear $\vec{S}\cdot\vec{L}$ interactions.

$$\boxed{V_{\vec{S}\cdot\vec{L}}\ (\text{nucleus}) = -\frac{a_{SL}^2}{r}\,\frac{dV}{dr}\,\vec{S}\cdot\vec{L}}$$

In the case where there is strong $\vec{S}\cdot\vec{L}$ coupling the energy levels are determined by the total angular momentum $\vec{J} = \vec{L} + \vec{S}$

The spin of nucleons is $\frac{1}{2}\hbar$ $(s = 1/2)$, so,

$$j = l + \tfrac{1}{2} \quad \text{or} \quad j = l - 1/2$$

As in atomic physics $\vec{J}\cdot\vec{J} = (\vec{L}+\vec{S})\cdot(\vec{L}+\vec{S})$ and $\vec{S}\cdot\vec{L} = \frac{1}{2}(J^2 - L^2 - S^2)$

and $\langle \vec{S}\cdot\vec{L} \rangle = \frac{\hbar^2}{2}\left[j(j+1) - l(l+1) - s(s+1) \right]$

The change in PE for $j = l + 1/2 \leftrightarrow j = l - 1/2$ is $\boxed{\Delta V \propto 2l + 1}$

Spin-Orbit Coupling in the Nucleus

This ΔV due to $j = \ell + 1/2$ and $j = \ell - 1/2$, coupled with the measured "minus sign" in $V_{\vec{S}\cdot\vec{L}}$ (nucleus) leads to

$j = \ell - 1/2$ "higher" energy state

$j = \ell + 1/2$ "lower" energy state

... the opposite of the $\vec{S}\cdot\vec{L}$ splitting into doublet states found in complex atoms.

The spectroscopic notation for nuclear states reflects the fact that n, ℓ, and j are good quantum numbers.

$n\ell_J$ ⇐ Spectroscopic notation for nuclear states.

See how the spin-orbit interaction in the nucleus significantly changes the energy levels.

① The j-state has $2j+1$ degenerate states

② The occupancy is $2(2j+1)$ because of the Pauli Exclusion Principle

Example: Consider a $1g$ state. $\ell = 4$

"lower" energy → $j = \ell + \frac{1}{2} = 9/2$ 10 degenerate states (m_J's)

"higher" energy → $j = \ell - \frac{1}{2} = 7/2$ 8 degenerate states (m_J's)

Figure 5.11 | Nuclear Energy Levels for an Infinite Square Well, a Finite Square Well, a Square Well with Rounded Edges, and a Square Well with Rounded Edges Including Spin Orbit Coupling

The numbers on the right hand side of the figure show the cumulative occupancy for the final case. The harmonic oscillator energy levels are shown for comparison.

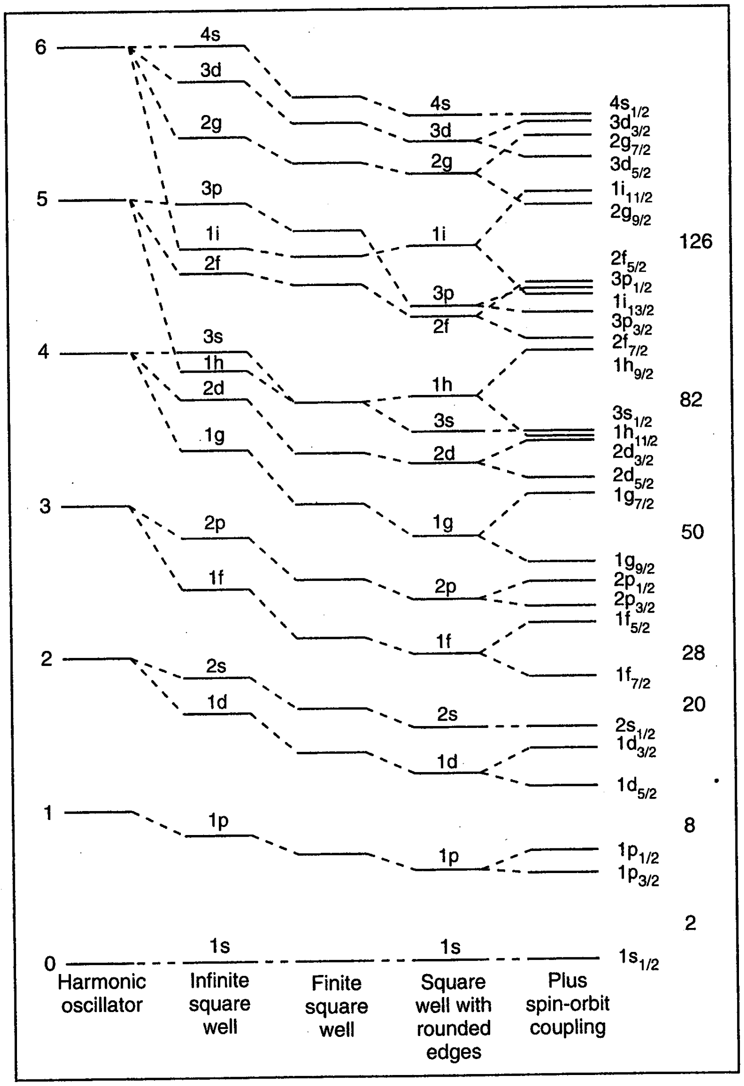


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Figure 5.14 Comparison of Nuclear Energy Levels for (a) Neutrons and (b) Protons