Forces, Potentials, and the Shell model

Recall the Infinite Square Well (1D)

Solve Shroedinger's equation: $H\psi = E\psi$

$$\frac{d^2}{dx^2}\psi - V\psi = E\psi$$

Result:
Consideration of boundary conditions (the behavior of the wavefunction at the walls) results in quantization.
Both wavefunctions and eigenstates (energy levels)

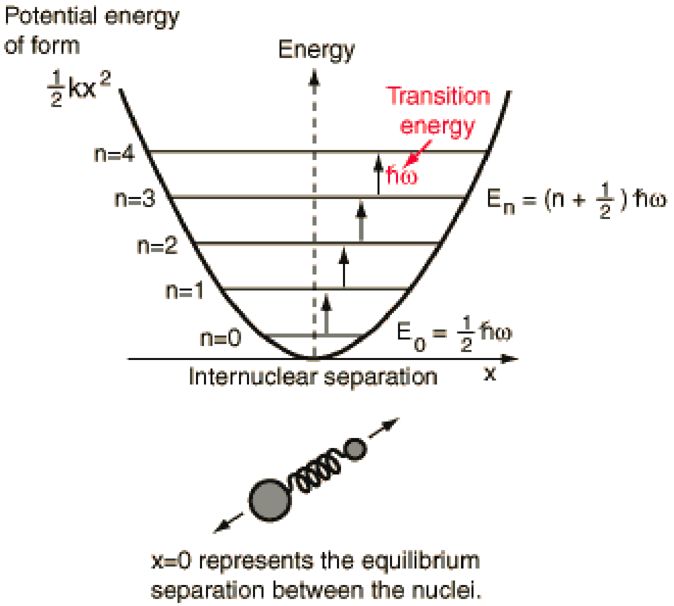
$$E_n = \frac{n^2 h^2}{8mL^2}$$

Notice the dependence of the energy levels on the size of the box, and on the principal quantum number.

Harmonic oscillator (1D)

Hooke's law : $F = -k(x - x_0)$

If , the system is at equilibrium because there is no force. However if is different from there is a force which acts to restore the position to the equilibrium value (Notice the negative sign.)



$$F = -\frac{dV}{dx}$$

Integrating we get,

$$V = \frac{1}{2}k(x - x_0)^2$$

Now solve Schrodinger's equation using this potential.

Eigenvalues: $E_n = (n + \frac{1}{2})\hbar\omega$ where $\omega = \sqrt{\frac{k}{m}}$

Notice the energy spacing for the harmonic oscillator. What is the minimum energy of the harmonic oscillator?

V. Nuclear Shell Model

A. Quantum Properties of Nuclei

1. Discrete Energy Levels
2. Nuclear Spin (I)

a. Summary of experimental facts

e-e : $I = 0$ ALWAYS

e-o, o-e: $I = \frac{n\hbar}{2}$ where n is an odd integer (1, 3,5, ...)

o-o : $I = n\hbar$ where n is an integer (0, 1, 2 ...)

WE'LL USE $\hbar = 1$ for our spins

b. Implication

e-e result implies strong pairing is energetically favorable
therefore, spins must cancel

c. Reason: Nuclear Force is attractive.
in contrast spins are unpaired in a
atomic orbitals due to e-e repulsion
(Pauli exclusion principle)

3. Closed Shells – Unusual Stability

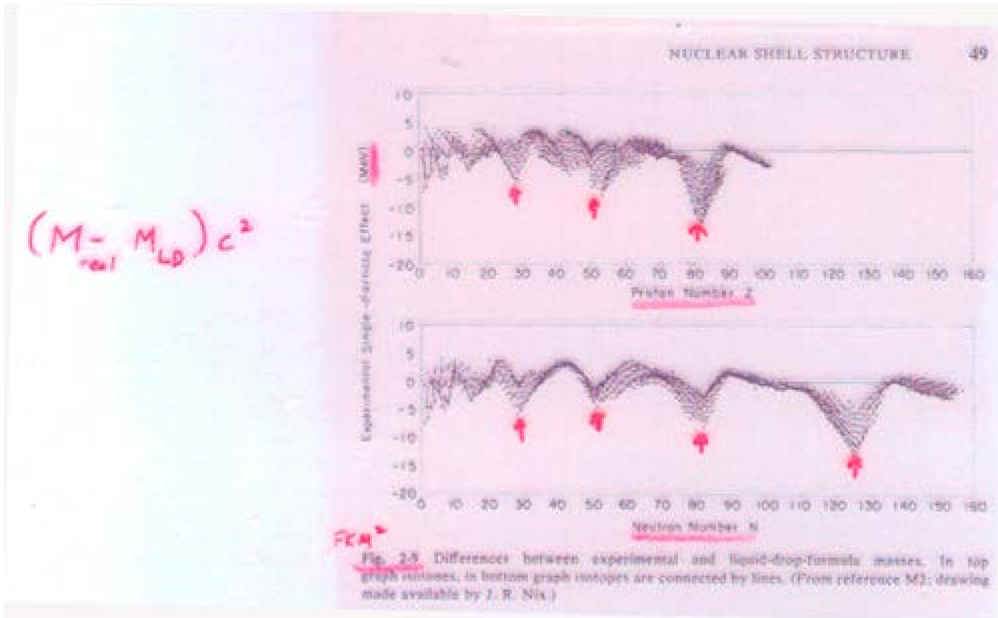


Fig. 2-5 Differences between experimental and liquid-drop-formula masses. In top graph isotones, in bottom graph isotopes are connected by lines. (From reference M2; drawing made available by J. R. Nix.)

a. Magic Numbers

2, 8, 20, 28, 50, 82, 126 (neutrons)

b. Energetics: (MLD – M), Bp, Bn, B_{alpha}

c. Lifetimes:

$^{208}_{82}Pb_{126}$	$^{209}_{82}Pb_{127}$	$^{210}_{84}Po_{126}$	$^{212}_{84}Po_{120}$
STABLE	22y	138d	10^{-7}s

Z=82 & N=126 appear to be stable

4. Magnetic Moments

Moving Charge created a magnetic field with moment μ

$$\mu = \frac{e\hbar}{2Mc} f(I)$$

μ_N = nuclear magneton ($M = M_p$)

a. Expect $\mu_p = \mu_N$ Observe : $\mu_p = 2.793\ \mu_N$

$\mu_n = 0$ $\mu_n = -1.913\ \mu_N$

μ_e agrees with expectations

b. Implication: nucleon has substructure,
since one observes charge on periphery of particle.
e.g., proton +2/3, -1/3, +2/3 ; neutron -1/3, +2/3, -1/3

c. Effect on Chemical Environment

- I = 1/2 for ^{1}H, ^{13}C, ^{57}Fe

- For a nucleus with spin, the magnetic field around the nucleus interacts with the electric field of its electronic environment.

NOTE: $\mu_N << \mu_e$; therefore all e^-s must be paired.

- Interaction is very sensitive to e- orbital distribution and therefore is different for every chemical bond

- Supply rf energy to induce transitions (↑→↓) and get resonance.

d. Result for nuclei:

e-e : $\mu = 0$ ALWAYS
o-e : $\mu \approx \mu_p$
e-o : $\mu \approx \mu_n$
o-o : $\mu \approx \mu_p + \mu_n$

AGAIN, SUPPORTS STRONG PAIRING ARGUMENT

B. Shell Model: Quantum Mechanical Solution (a la hydrogen atom).

1. Schroedinger Equation

a. H = Hamiltonian: Summarizes forces acting on particles
H = T + V(r) = kinetic + potential energy

b. Ψ = Wave function: Describes properties of particles in system;
i.e., Probability distributions in space and time (orbitals)
$\Psi_i = f(x, y, z, t, s, ...)$

(1) Pauli Exclusion Principle
For Fermions (particle with half-integer spins)
Ψi □ Ψj (atoms and molecules also)
i.e., all particles must have different wave functions

(2) Parity (π)
Definition: a mathematical operator that reverses coordinates
$\pi\Psi(x) = \Psi(-x) = \pm\Psi$

Example: EVEN Parity: x^2, x^4, x^6, cos x, s, d, g, …
ODD Parity: x, x^3, x^5, sin x, p, f, h. ...

c. Discrete energy states: Quantum states Produced by action of forces on particles

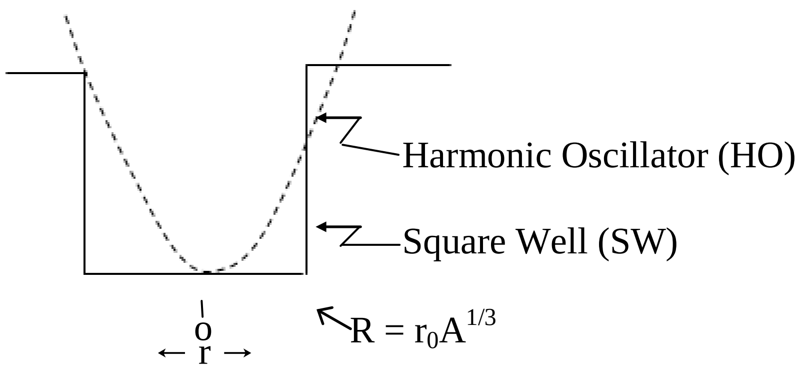
2. Qualitative Expectations for orbitals of the same energy

	Atoms	Nuclei
Pairing	Weak (Hund's rule)	Strong
Shapes	Diffuse (low l preferred)	Compact (high l preferred)
Spin-orbit	Weak ($r_e << r_{atom}$)	Strong ($r_{nucleon} \leq r_{nucleus}$)
Reason	e-e force repulsive	N-N force attractive

Bottom Line: Atomic and Nuclear Shell structure should differ

3. Potential Models: V(r)

This is the "box" that confines the nucleons in the nucleus



Solvable approximations to the nuclear potential; can't solve Fermi function

a. Square Well: $V(r) = -V_0, \ r \le R$ Uniform density sphere

$V(r) = 0, \quad r > R$

b. Harmonic Oscillator:

$V(r) = -V_0 \, [1 - r^2/R^2]$ Parabola

4. HO Solution: Energy Levels

a. $E_{\nu\ell} = [2(\nu - 1) + \ell)]\hbar\omega$

$\nu = 1,2,3,...$ PRINCIPAL Quantum Number

$\ell = 0,1,2,...$ ORBITAL ANGULAR MOMENTUM QN (viz. s,p,d,f,…)

NOTE: ℓ is INDEPENDENT of ν (unlike atoms)

As in atoms there are two other quantum numbers:

$m_\ell = \pm \ell, \pm (\ell - 1) \ ... \ 0$ Magnetic Substate $(2\ell + 1)$

$s = \pm 1/2$ Intrinsic Spin

b. Notation

$\nu\ell$; e.g. $\nu = 2$, $\ell = 4$ is 2 g

Energies for all m_ℓ and s states are same for same ν and ℓ

c. Pauli Exclusion Principle

Each nucleon must have a UNIQUE set of QNs (ν, ℓ, m_ℓ and s)

NOTE: p & n are different particles (i.e., electric charge QN is +1,0)

$\therefore$ they can have the same ν, ℓ, m_ℓ and s)

d. Compare with Magic Numbers: DOESN'T WORK

5. Square-Well Solution -- Doesn't work either

$\therefore$ need ADDITIONAL PHYSICS

6. Empirical Correction

1963 Maria Goeppert Mayer and Hans Jensen – Nobel Prize

ASSUMPTION (1949): Attractive Nuclear Force will lead to a strong interaction between particle spin and its orbit

(e.g., same would be true of moon and earth – if closer/tides)

a. Result: NEW QNs

j = TOTAL ANGULAR MOMENTUM

$$j = \vec{\ell} + \vec{s} = \vec{\ell} \pm \frac{1}{2}$$

b. New QN Notation

$\nu \ell_j$

ν same

ℓ same

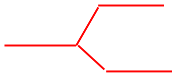
$j = \ell \pm 1/2$

$m_j = +j, (j-1) \ldots -j$ $\quad$ $2j + 1$ values/j

c. Example

$\nu = 1, \ell = 2 \Rightarrow 1d_j$

$j = 2 \pm 1/2 = 3/2, 5/2 \Rightarrow 1\, d_{3/2}$ & $1\, d_{5/2}$



for

$j = 3/2, m_j = 3/2, 1/2, -1/2, -3/2 = 2j + 1 = 4$ possible values

$j = 5/2, m_j = 5/2, 3/2, 1/2, -1/2, -3/2, -5/2 = 2J + 1 = 6$ possible values

Total d states = 10 possible values

d. Effect on Energy States (Levels)

(1) RULE 1:

For same oscillator energy $$E^{HO}_{\nu\ell} = [2(\nu - 1) + \ell)]\hbar\omega$$

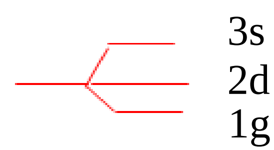
$$\boxed{E_{\ell} < E_{\ell-2} < E_{\ell-4} \ldots}$$

MORE COMPACT ORBITALS (high ℓ) PERMIT STRONGER ATTRACTION (unlike atoms)

Example:

1g, 2d, 3s states all have $E^{HO} = 4\hbar\omega$

Rule says 4 $\hbar\omega$



(2) RULE 2:

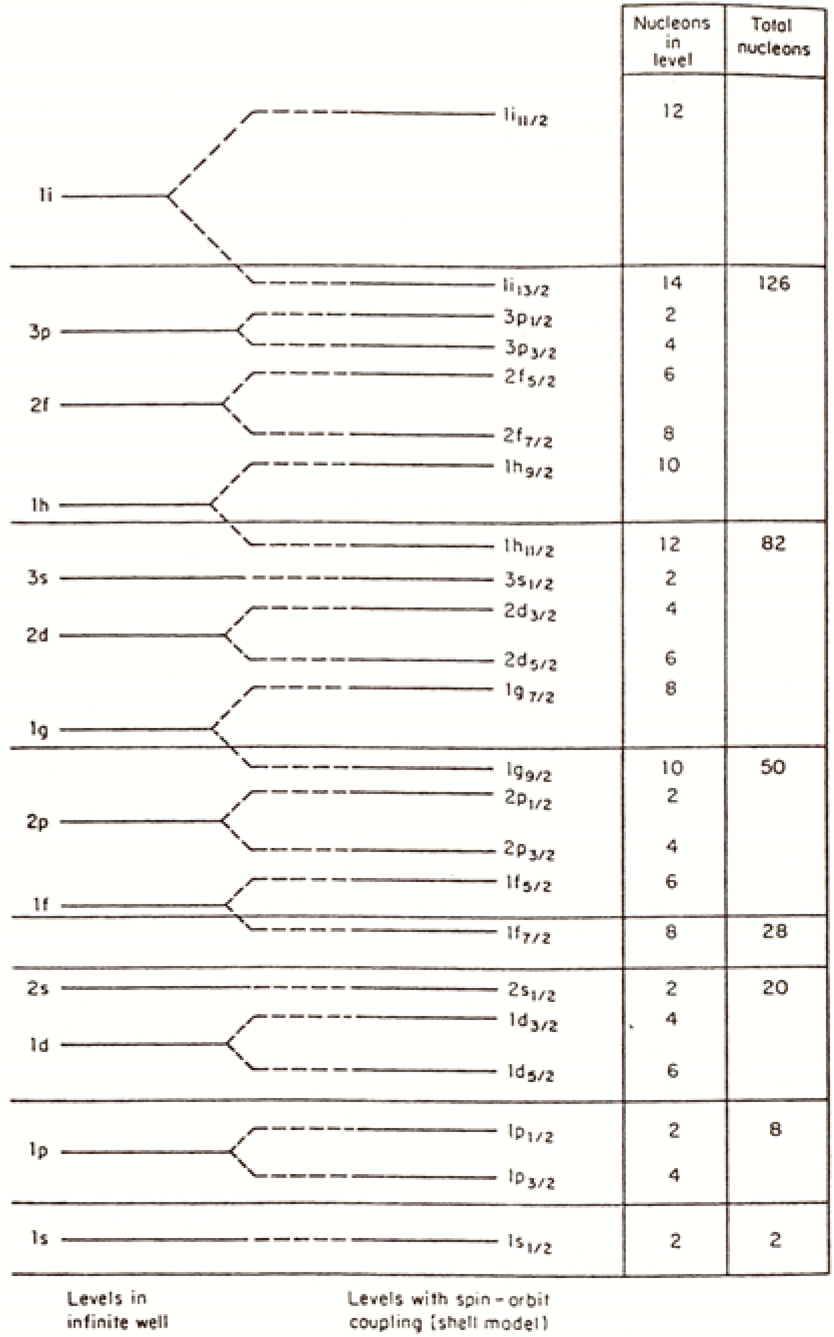
$E_{\ell+1/2} < E_{\ell-1/2}$ for same $\nu\ell$;

(3) RULE 3

$\Delta E_j \propto \ell$

e. Rearranged Level Order

Now matches experimental magic numbers. This is the same trick you play with Bohr model for atoms, except low ℓ preferred to keep electrons as far apart as possible. This is what we will use for predictive purposes.



Comparison of levels in an infinite potential well with spin-orbit coupling level sequence

Table 1 -- Nuclear Shell Structure (from *Elementary Theory of Nuclear Shell Structure*, Maria Goeppert Mayer & J. Hans D. Jensen, John Wiley & Sons, Inc., New York, 1955.)

Angular Momentum ($h\Omega/2\pi$)		Spin-Orbit Coupling (1/2, 3/2, 5/2, 7/2...)	Number of Nucleons: Shell	Number of Nucleons: Total	Magic Number
7	1j				
		1j 15/2	16	[184]	{184}
		3d 3/2	4	[168]	
6	4s	4s 1/2	2	[164]	
6	3d	2g 7/2	8	[162]	
		1i 11/2	12	[154]	
6	2g	3d 5/2	6	[142]	
		2g 9/2	10	[136]	
6	1i				
		1i 13/2	14	[126]	{126}
		3p 1/2	2	[112]	
5	3p	3p 3/2	4	[110]	
		2f 5/2	6	[106]	
5	2f	2f 7/2	8	[100]	
		1h 9/2	10	[92]	
5	1h				
		1h 11/2	12	[82]	{82}
4	3s	3s 1/2	2	[70]	
		2d 3/2	4	[68]	
4	2d	2d 5/2	6	[64]	
		1g 7/2	8	[58]	
4	1g				
		1g 9/2	10	[50]	{50}
		2p 1/2	2	[40]	{40}
3	2p	1f 5/2	6	[38]	
		2p 3/2	4	[32]	
3	1f				
		1f 7/2	8	[28]	{28}
		1d 3/2	4	[20]	{20}
2	2s	2s 1/2	2	[16]	
2	1d	1d 5/2	6	[14]	
		1p 1/2	2	[8]	{8}
1	1p	1p 3/2	4	[6]	
0	1s	1s 1/2	2	[2]	{2}