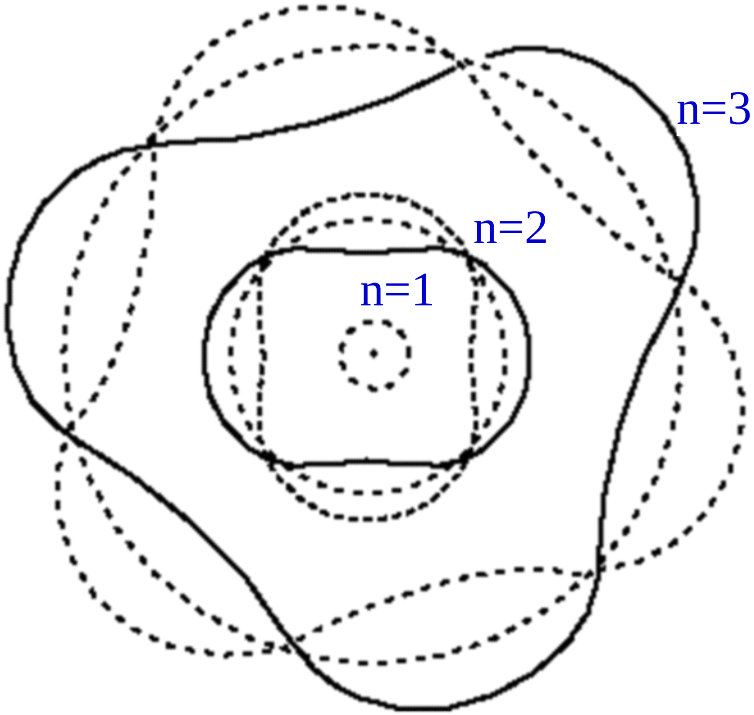
electron orbitals

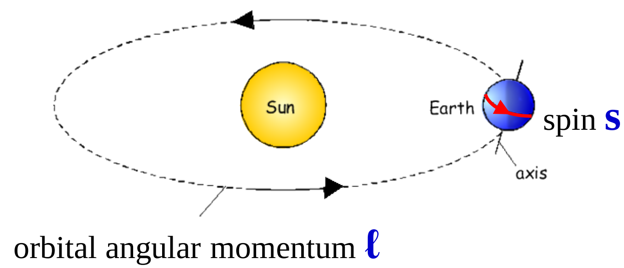


electrons in an atom

quantum numbers:

n	(principal)	**1,2,3,…**
ℓ	(orbital angular momentum)	**0 → n-1**
m	(magnetic)	**-ℓ ≤ m ≤ +ℓ**
s	(spin)	↑↓ or **+½ħ -½ħ**

classical analogy



sun ≡ nucleus
earth ≡ electron

protons and neutrons** have **ℓ** and **s

total angular momentum: $\vec{j} = \vec{\ell} + \vec{s}$

total nuclear spin: $I = \sum j$

electron is structure less and hence can not rotate
***spin s** is a quantum mechanical concept*

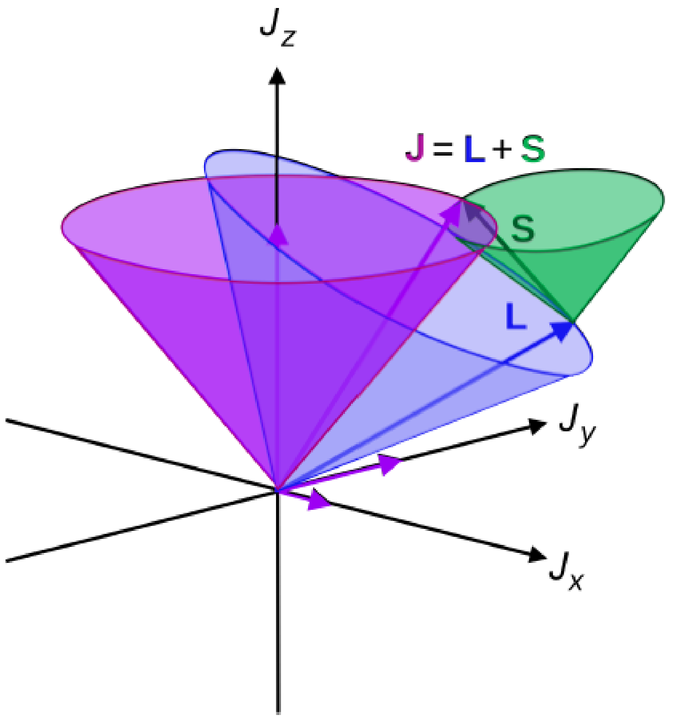
Nuclear spin quantum number

***protons and neutrons** have orbital angular momentum* $\boldsymbol{\ell}$ *and spin* $\mathbf{s}$

total angular momentum: $\vec{j} = \vec{\ell} + \vec{s}$

total nuclear spin: $I = \sum j$

$$I = |j_1 + j_2 + \cdots j_n|, |j_1 + j_2 + \cdots j_n| - 1, \cdots, |j_1 - j_2 - \cdots - j_n|$$ quantum mechanics



Nuclear spin quantum number

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- ^{1}H = 1 proton, so I = ½
- ^{2}H = 1 proton and 1 neutron, so I = 1 or 0

- For larger nuclei, it is not immediately evident what the spin should be as there are a multitude of possible values.

mass number	number of protons	number of neutrons	spin (I)	example
even	even	even	0	^{16}O
	odd	odd	integer (1,2,…)	^{2}H
odd	even	odd	half-integer ($^1/_2, ^3/_2, \cdots$)	^{13}C
	odd	even	half-integer ($^1/_2, ^3/_2, \cdots$)	^{15}N

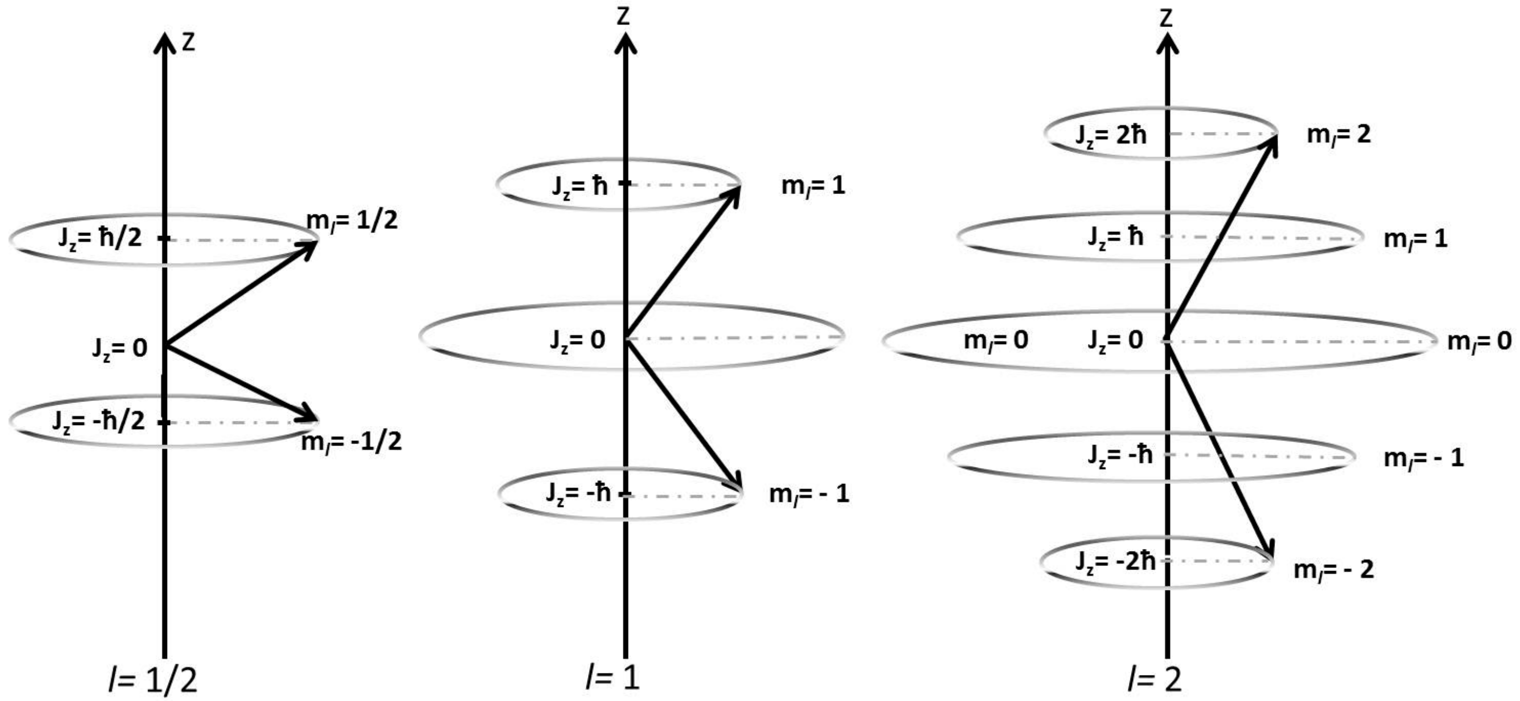
Nuclear spin quantum number

The magnitude is given by

$$L = \hbar\sqrt{I(I+1)}$$

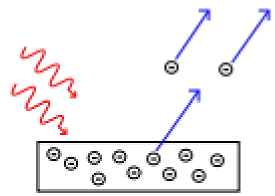
The projection on the z-axis (arbitrarily chosen), takes on discretized values according to m, where

$$m = -I, -I+1, -I+2, \cdots, +I$$



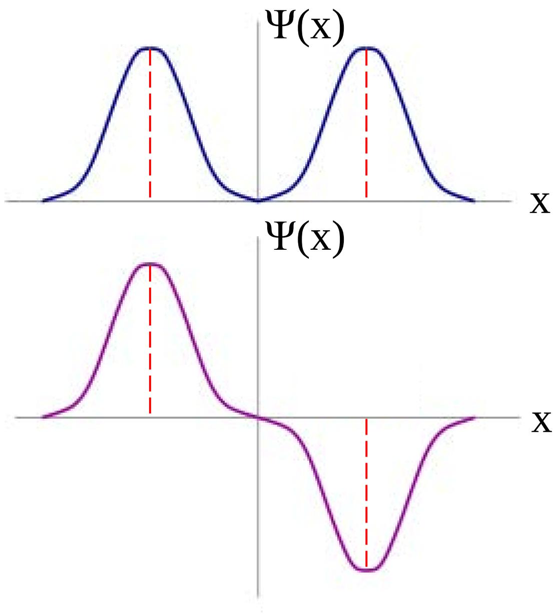
Parity

wave – particle duality:



photoelectric effect

wave function



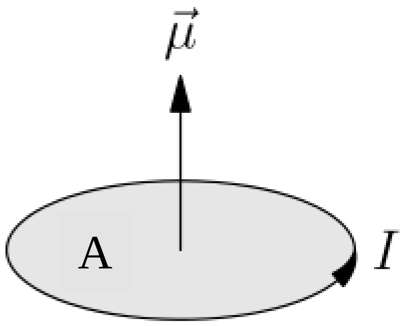
$\Psi(x) = \Psi(-x) \;\rightarrow\;$ parity = even (+)

$\ell = 0, 2, 4, \ldots$ even

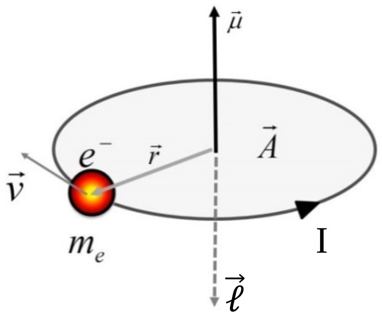
$\Psi(x) = -\Psi(-x) \;\rightarrow\;$ parity = odd (-)

$\ell = 1, 3, 5, \ldots$ odd

Magnetic moment



$$\vec{\mu} = I \cdot A$$



$$\ell = m_e v \cdot r \qquad v = \frac{2\pi r}{t} \quad \rightarrow \quad t = \frac{2\pi r}{v}$$

$$I = \frac{e}{t} = \frac{e \cdot v}{2\pi r}$$

$$\mu = \frac{e \cdot v}{2\pi r} \cdot \pi r^2 = \frac{e \cdot v \cdot r}{2}$$

$$\mu = \frac{e \cdot v \cdot r}{2} \cdot \frac{m_e v \cdot r}{m_e v \cdot r} = \frac{e \cdot \ell}{2m_e} \qquad \mu_{Bohr} = \frac{e \cdot \hbar}{2m_e}$$

$$\mu_\ell = \mu_B \cdot \frac{\ell}{\hbar}$$ electron orbital magnetic moment

$$\mu_\ell = \mu_N \cdot \frac{\ell}{\hbar}$$ proton orbital magnetic moment $\mu_N = \frac{e \cdot \hbar}{2m_p}$

Magnetic moment

$$\mu_\ell = \mu_B \cdot \frac{\ell}{\hbar}$$

electron orbital magnetic moment

$$\mu_s = -2.0023 \cdot \mu_B \cdot \frac{s}{\hbar}$$

electron spin magnetic moment (Dirac equation)

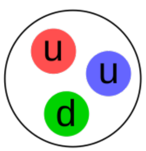
$$\mu_s = +5.585691 \cdot \mu_N \cdot \frac{s}{\hbar}$$

proton spin magnetic moment

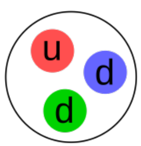
$$\mu_s = -3.826084 \cdot \mu_N \cdot \frac{s}{\hbar}$$

neutron spin magnetic moment

Why has a neutron a magnetic moment when it is uncharged?



proton
+1e



neutron
0e

u-quark: $+\,^2/_3\, e$
d-quark: $-\,^1/_3\, e$

neutrons and protons are not elementary particles
internal structure: they have charges.

$$\mu_s({}^2_1H) = (5.59 - 3.83) \cdot \mu_N \cdot \frac{1}{2} = 0.87980\mu_N$$

$$= 0.8574 \cdot \mu_N \quad \text{(experiment)}$$

Magnetic resonance imaging (MRI)

$$\mu_s = +5.585691 \cdot \mu_N \cdot \frac{s}{\hbar}$$

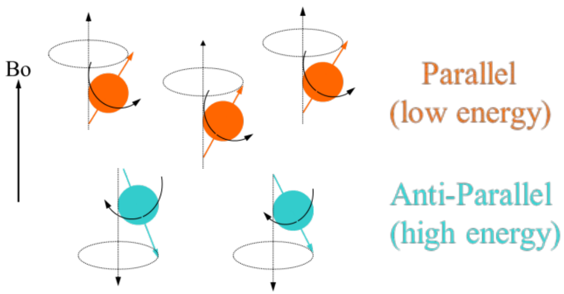
proton spin magnetic moment

$$\boxed{\mu_I = \gamma \cdot I}$$

gyromagnetic ratio $\gamma = g \cdot \frac{\mu_N}{\hbar} = g \cdot 47.89 \cdot 10^6 \quad [T^{-1}s^{-1}]$

proton g-factor: +5.585691, spin I: ½ ħ

proton in magnetic field



energy difference between states

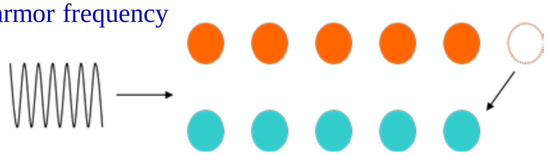
$$\Delta E = h \cdot \nu$$

$$\Delta E = 2 \cdot \mu_I \cdot B_0$$

$\nu = {}^{\gamma}/_{2\pi} \cdot B_0$ Larmor frequency

${}^{\gamma}/_{2\pi} = 42.57 \quad [{}^{MHz}/_{T}]$ for proton

Larmor frequency



low energy

high energy

low energy

high energy