Your questions/comments

ANNOUNCEMENTS: Prof. Oono will hold my Mon. 3-4pm office hour today.
End of semester coming soon! ICES evaluation & check your gradebook!
Final exam May 13 & 15: cumulative, will cover material evenly
James Scholar Credit projects due Sat., May 2

Exam 1-3
3/4 of material

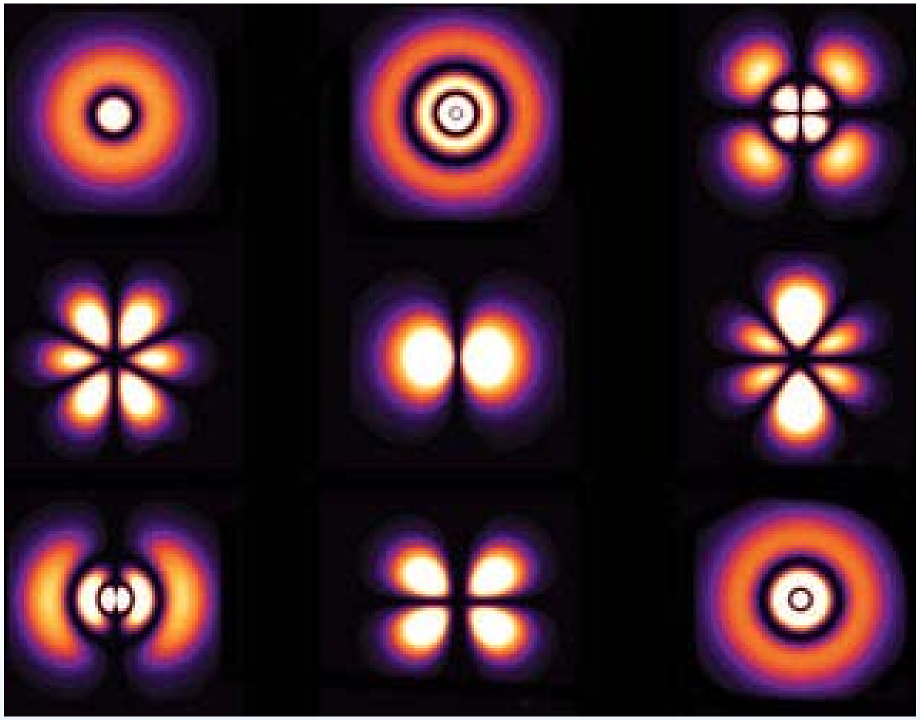
"If you can't find your keys, you probably know too much about their momentum."

"If atoms act like magnets, is that how Magnetic Resonance Imaging is able to work?"

"What. Is. Happening. Why have Chemistry and Physics have combined to create this monstrous entity called "Quantum Physics"."

"Quick review on shortcuts for determining the number of electrons, shell configurations, etc. when given a set of quantum numbers?"

"That's a lot of chemistry…and did we learn the bohr model to then learn that it is wrong? Interesting"



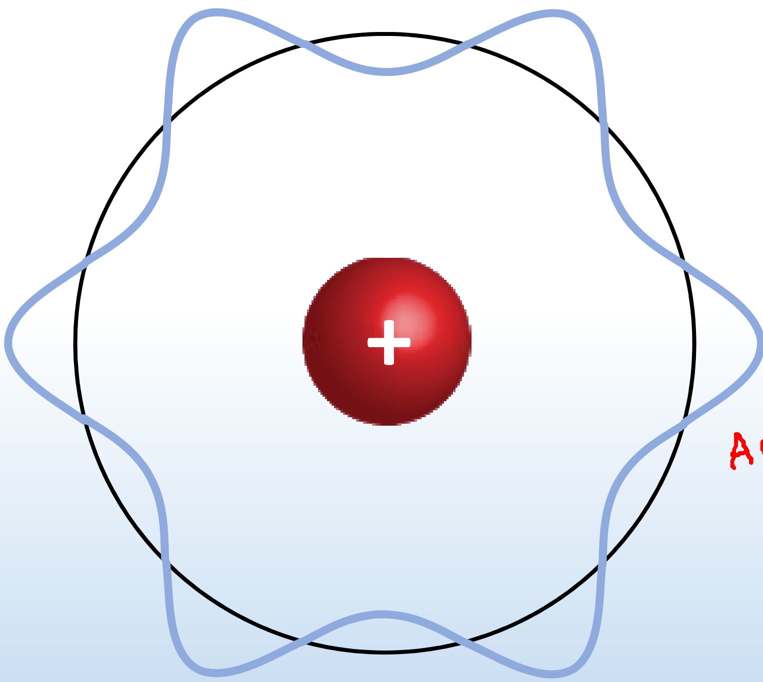
Phys 102 – Lecture 26

The quantum numbers and spin

Recall: the Bohr model

+ de Broglie

Only orbits that fit *n* e⁻ wavelengths are allowed



e⁻ wave

SUCCESSES H, single e⁻

Correct energy quantization & atomic spectra

$$E_n = -\frac{m_e k^2 e^4}{2\hbar^2} \cdot \frac{Z^2}{n^2} \qquad n = 1, 2, 3, \ldots$$

FAILURES

ACT Radius & momentum quantization violates Heisenberg Uncertainty Principle

$$r_n = \frac{n^2\hbar^2}{m_e k e^2} \equiv n^2 a_0 \qquad \Delta r \cdot \Delta p_r \geq \frac{\hbar}{2}$$

Electron orbits cannot have zero *L*

$$L_n = n\hbar$$

Orbits can hold any number of electrons

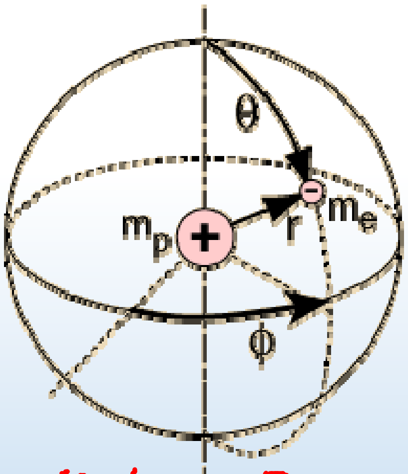
Quantum Mechanical Atom

1925

Schrödinger's equation determines e^- "wavefunction"

$$\left(-\frac{\hbar^2}{2m_e}\nabla^2 - \frac{ke^2}{r}\right)\psi(r,\theta,\varphi) = E\psi(r,\theta,\varphi) \quad \Rightarrow \quad \psi_{n,\ell,m_\ell}$$

3 quantum numbers determine e^- state



"SHELL"

"Principal Quantum Number" n = 1, 2, 3, …

$$E_n = -\frac{m_e k^2 e^4}{2\hbar^2}\frac{1}{n^2}$$ Energy

13.6eV

Same as Bohr

s, p, d, f "SUBSHELL"

"Orbital Quantum Number" ℓ = 0, 1, 2, 3 …, n–1

$$L = \sqrt{\ell(\ell+1)}\hbar$$ Magnitude of angular momentum

Diff. than Bohr

"Magnetic Quantum Number" $m_\ell = -\ell$, …–1, 0, +1…, ℓ

$$L_z = m_\ell \hbar$$ Orientation of angular momentum

ACT: CheckPoint 3.1 & more

For which state is the angular momentum *required* to be 0?

A. $n = 3$

B. $n = 2$

C. $n = 1$

$\ell = 0, 1, 2, 3 \ldots, n-1$
so for $n = 1$, $\ell = 0$

How many values for m_ℓ are possible for the *f* subshell ($\ell = 3$)?

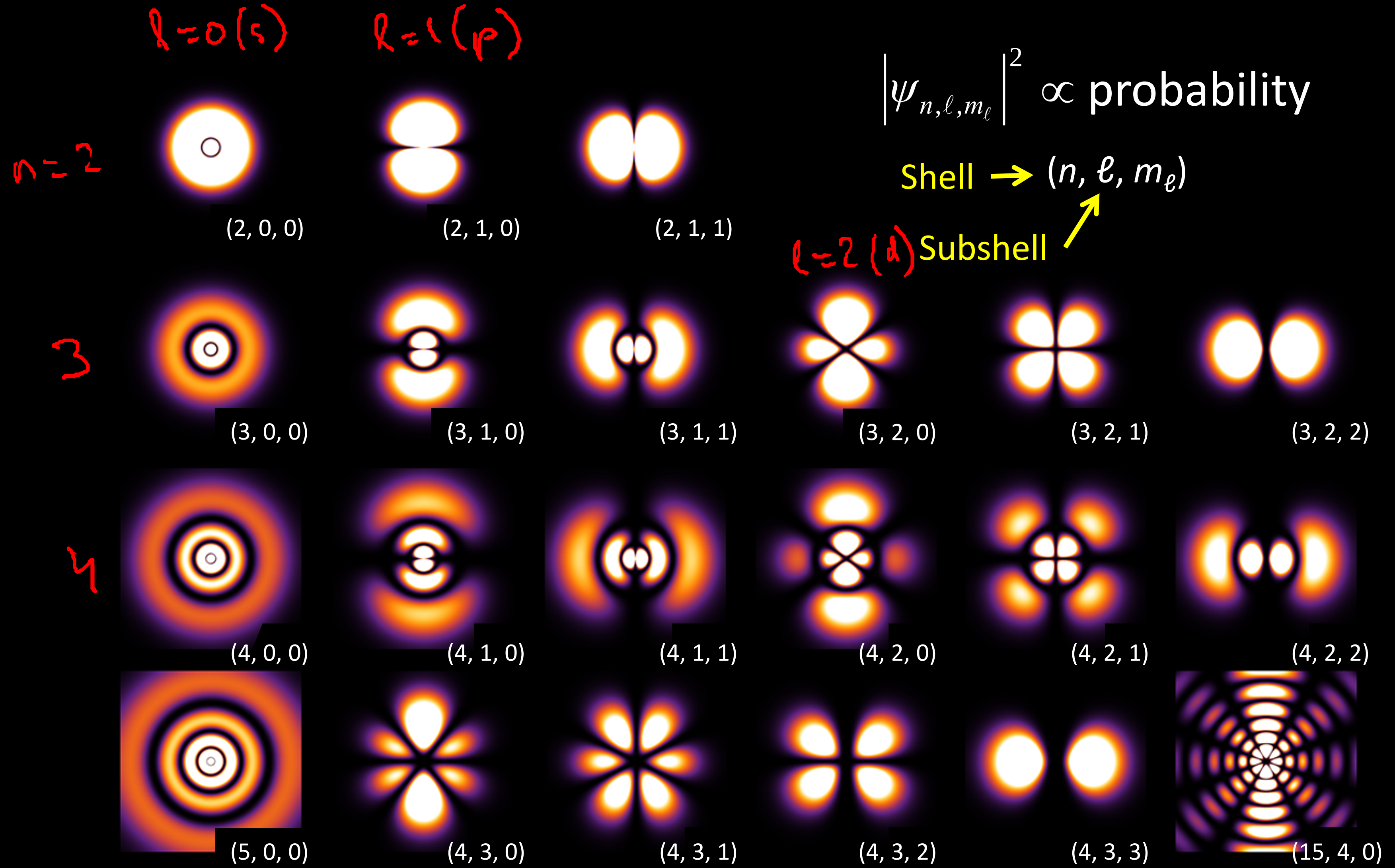
A. 3

B. 5

C. 7

$m_\ell = -\ell, \ldots -1, 0, +1 \ldots, \ell$
so for $\ell = 3$, $m_\ell = \underbrace{-3, -2, -1, 0, +1, +2, +3}_{2\ell + 1 \text{ terms}}$

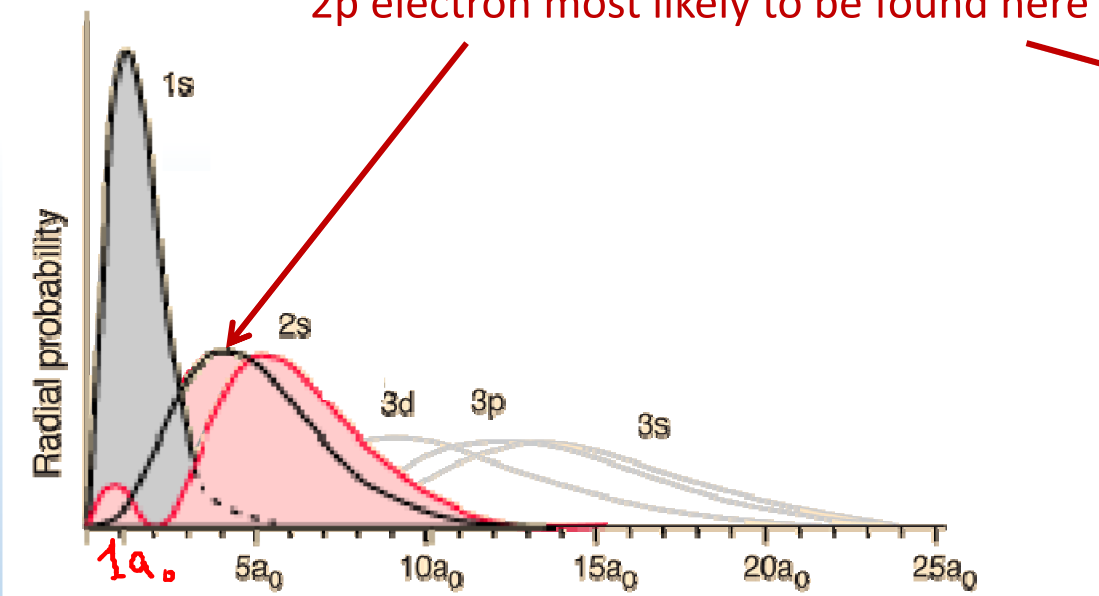
Hydrogen electron orbitals

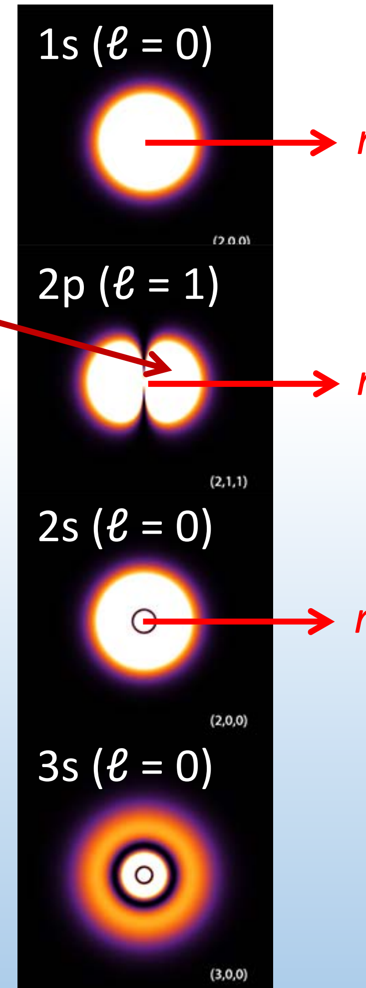


CheckPoint 2: orbitals

Orbitals represent *probability* of electron being at particular location

2p electron most likely to be found here

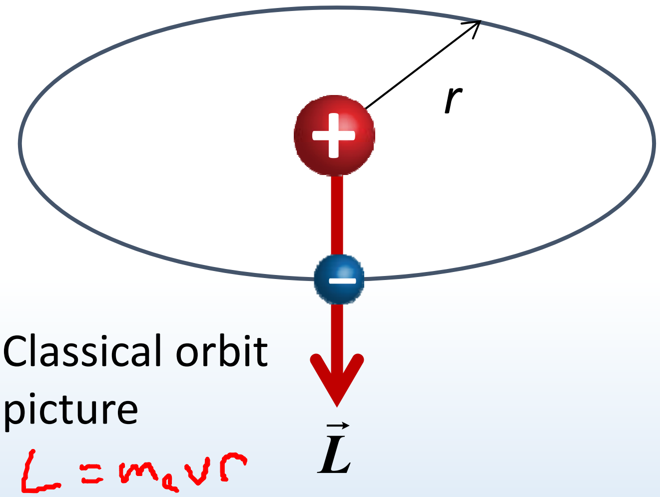




Bohr radius $a_0 \equiv \dfrac{\hbar^2}{m_e k e^2}$

Angular momentum

What do the quantum numbers ℓ and m_ℓ represent?



Classical orbit picture

$L = m_e v r$

Magnitude of angular momentum vector quantized

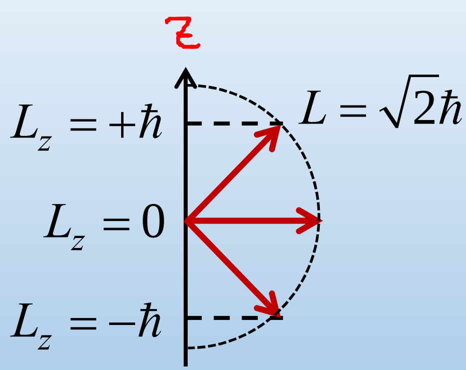
$$|\vec{L}| = L = \sqrt{\ell(\ell+1)}\hbar \qquad \ell = 0, 1, 2 \cdots n-1$$

Only *one* component of *L* quantized

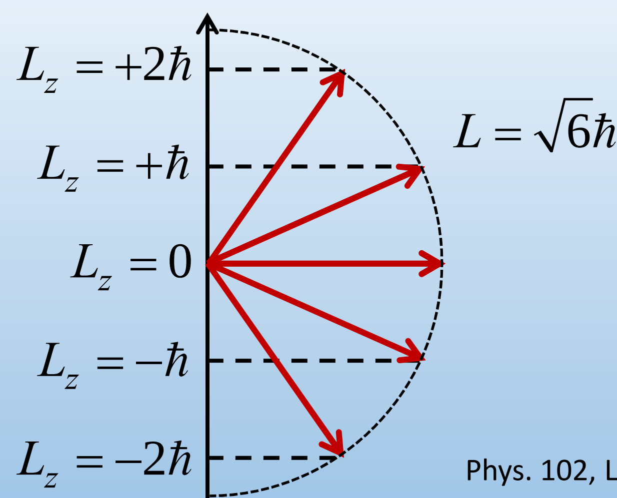
$$L_z = m_\ell \hbar \qquad m_\ell = -\ell, \cdots -1, 0, 1, \cdots \ell$$

Other components L_x, L_y are not quantized

$\ell = 1$

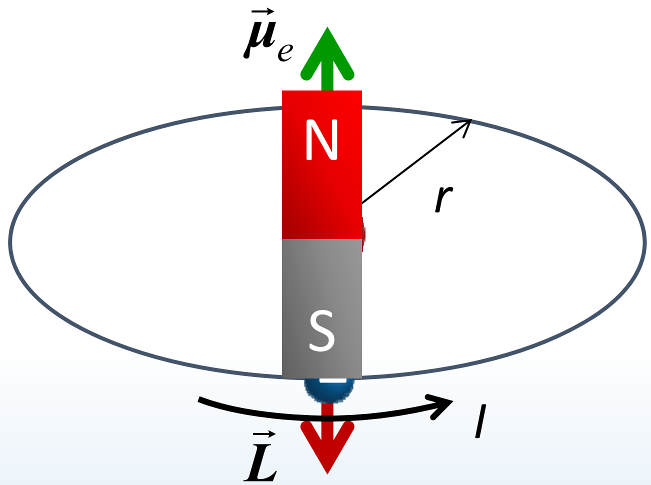


$\ell = 2$



Orbital magnetic dipole

Electron orbit is a current loop and a magnetic dipole



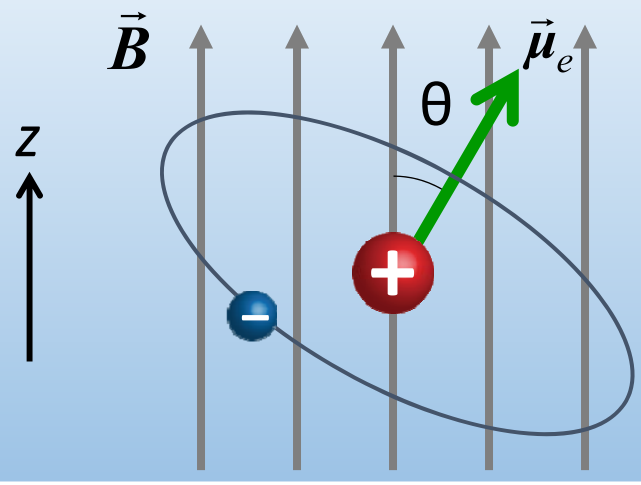
$$\mu_e = IA = \frac{\Delta q}{\Delta t}\pi r^2 = \frac{ev}{2\pi r}\pi r^2 = -\frac{e}{2m_e} m_e v r$$

Recall Lect. 12

$$\boxed{\vec{\mu}_e = -\frac{e}{2m_e}\vec{L}}$$

Dipole moment is quantized

What happens in a *B* field?



Recall Lect. 11

$$U = -\mu_e B\cos\theta = \frac{eB}{2m_e}L_z = \frac{e\hbar}{2m_e}Bm_\ell$$

Orbitals with different *L* have different quantized energies in a *B* field

ACT: Hydrogen atom dipole

What is the magnetic dipole moment of hydrogen in its ground state due to the orbital motion of electrons?

$n = 1$

$$\boxed{\vec{\boldsymbol{\mu}}_e = -\frac{e}{2m_e}\vec{\boldsymbol{L}}}$$

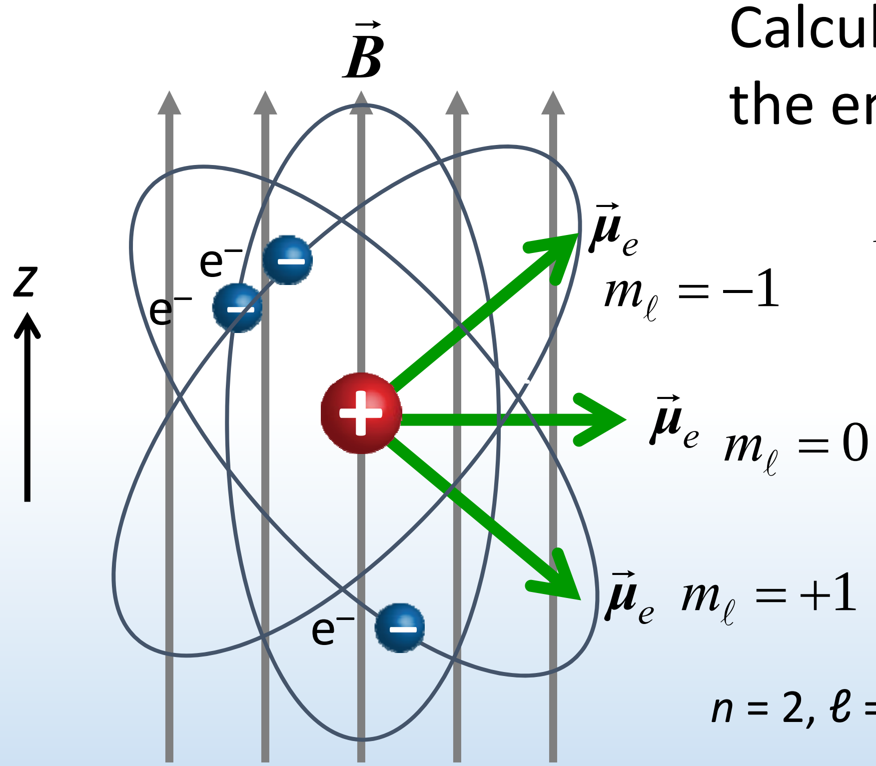
A. $\mu_H = -\dfrac{e\hbar}{2m_e}$

B. $\mu_H = 0$

C. $\mu_H = +\dfrac{e\hbar}{2m_e}$

CheckPoint 3.1. In ground state, $n = 1$ and $\ell = 0$, so $\mu_e = 0$

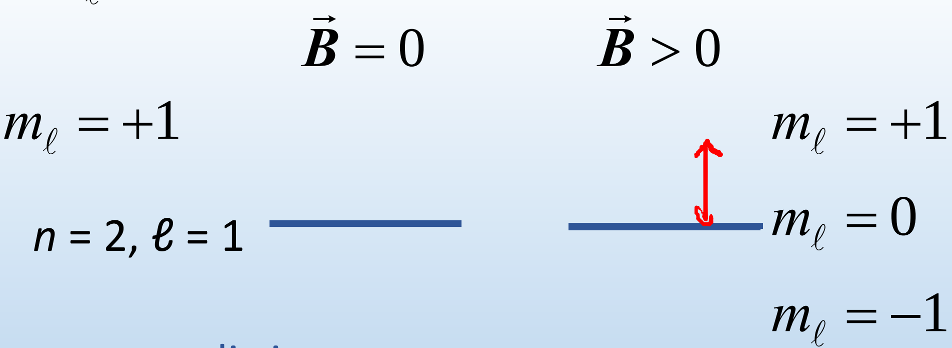
Calculation: Zeeman effect



Calculate the effect of a 1 T *B* field on the energy of the 2p (*n* = 2, *ℓ* = 1) level

$$E_{tot} = E_{n=2} - \mu_e B\cos\theta$$
$$= -\frac{13.6\,\text{eV}}{4} + \frac{e\hbar}{2m_e} B m_\ell$$

For $\ell = 1$, $m_\ell = -1, 0, +1$



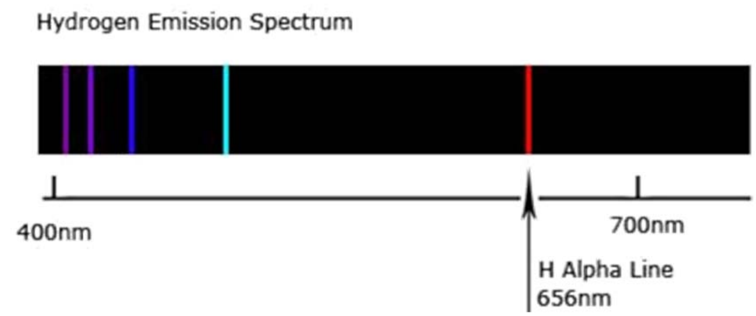
Energy level splits into 3, with energy splitting

$$\Delta E \equiv \frac{e\hbar B}{2m_e} = 5.8\times10^{-5}\,\text{eV} \qquad \mu_B \equiv \frac{e\hbar}{2m_e} = 5.8\times10^{-5}\,\frac{\text{eV}}{\text{T}}$$

"Bohr magneton"

ACT: Atomic dipole

The H α spectral line is due to e⁻ transition between the *n* = 3, ℓ = 2 and the *n* = 2, ℓ = 1 sub-shells.

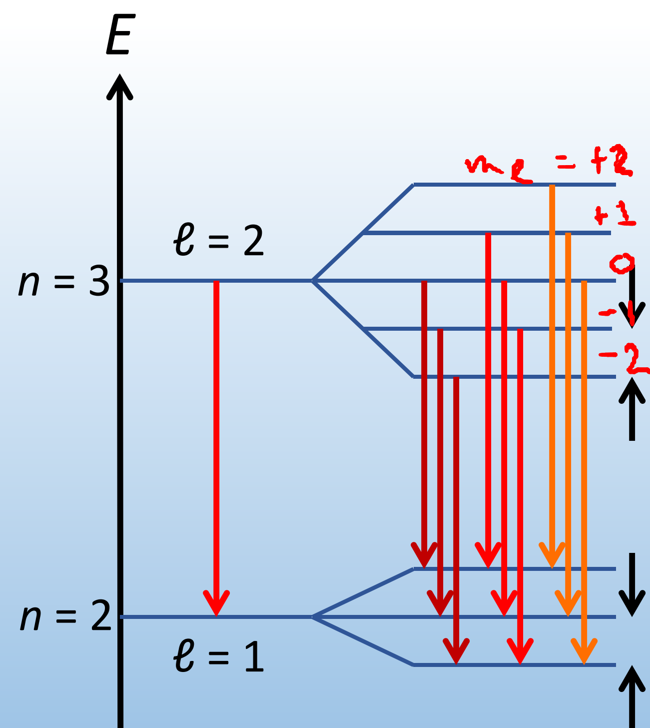


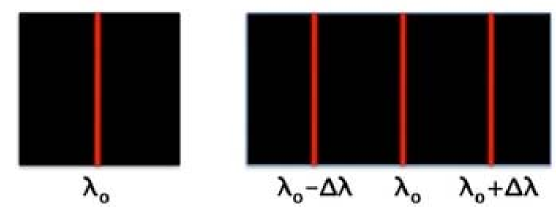
How many levels should the *n* = 3, ℓ = 2 state split into in a *B* field?

A. 1

B. 3

C. 5





$$\Delta E = \frac{e\hbar}{2m_e}B$$

Intrinsic angular momentum

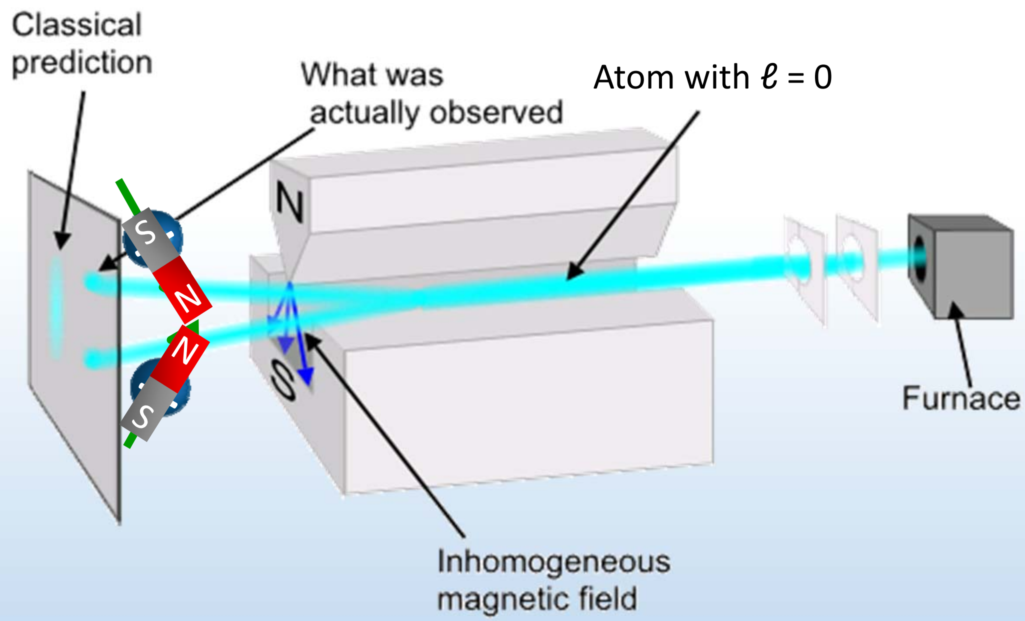
A beam of H atoms in ground state passes through a *B* field

$n = 1$, so $\ell = 0$ and expect NO effect from *B* field

Instead, observe beam split in two!

Since we expect $2\ell + 1$ values for magnetic dipole moment, e^- must have *intrinsic* angular momentum with $\ell = ½$.

"Spin" *s*



"Stern-Gerlach experiment" 1922

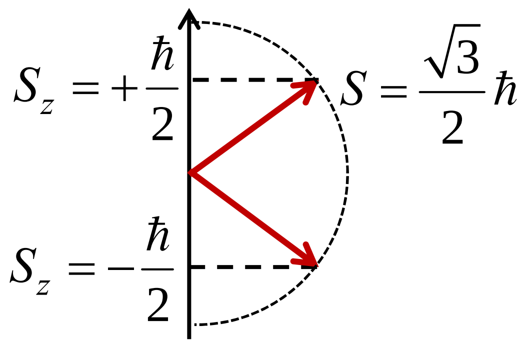
Spin angular momentum

spin-½ particle

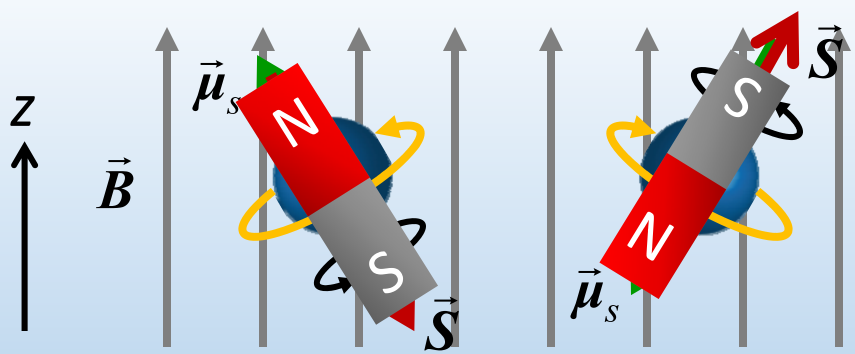
Electrons have an intrinsic angular momentum called “spin”

$$\left|\vec{S}\right| = S = \sqrt{s(s+1)}\hbar \qquad \text{with } s = ½$$

$$S_z = m_s\hbar \qquad m_s = -\tfrac{1}{2}, +\tfrac{1}{2}$$



Spin also generates *magnetic* dipole moment



Spin DOWN (–½)   Spin UP (+½)

$$\boxed{\vec{\mu}_s = -\frac{e}{2m_e} g\vec{S}} \qquad \text{with g} \approx 2$$

$$U = -\mu_s B\cos\theta = \frac{ge\hbar}{2m_e} B m_s \cos\theta$$

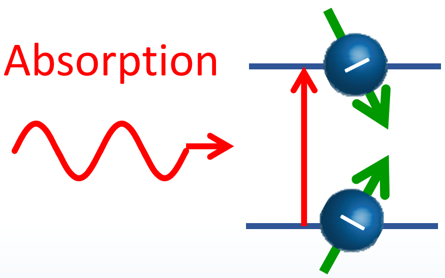
$m_s = +\frac{1}{2}$

$\vec{B} > 0$

$m_s = -\frac{1}{2}$

Spin resonance

e^- in B field absorbs photon with energy equal to splitting of energy levels



$$m_s = +\tfrac{1}{2}$$

$$m_s = -\tfrac{1}{2}$$

$$\begin{aligned} hf &= \Delta E \\ &= \frac{ge\hbar}{2m_e}B \\ &= g\mu_B B \approx 2\cdot 5.8\times10^{-5}\,\frac{\text{eV}}{\text{T}}\cdot 1\text{T} \approx \underbrace{11.6\times10^{-5}\,\text{eV}}_{\text{28 GHz}} \end{aligned}$$

"Electron spin resonance (ESR)"

Typically microwave EM wave

Protons & neutrons also have spin ½

$$\vec{\boldsymbol{\mu}}_{prot} = +\frac{e}{2m_p} g_p \vec{\boldsymbol{S}} << \vec{\boldsymbol{\mu}}_s \qquad \text{since } m_p >> m_e$$

"Nuclear magnetic resonance (NMR)"

Typically radio EM wave

For B = 1 T, *f* = 43 MHz

Sensitive probe for local chemical environment: Local B fields (ex: from e^- orbitals) change energy splitting slightly "Chemical shift"

Quantum number summary

"Principal Quantum Number", n = 1, 2, 3, …

$$E_n = -\frac{m_e k^2 e^4}{2\hbar^2}\frac{1}{n^2}$$ Energy

"Orbital Quantum Number", ℓ = 0, 1, 2, …, n–1

$$L = \sqrt{\ell(\ell+1)}\hbar$$ Magnitude of angular momentum

"Magnetic Quantum Number", m_ℓ = –ℓ, … –1, 0, +1 …, ℓ

$$L_z = m_\ell \hbar$$ Orientation of angular momentum

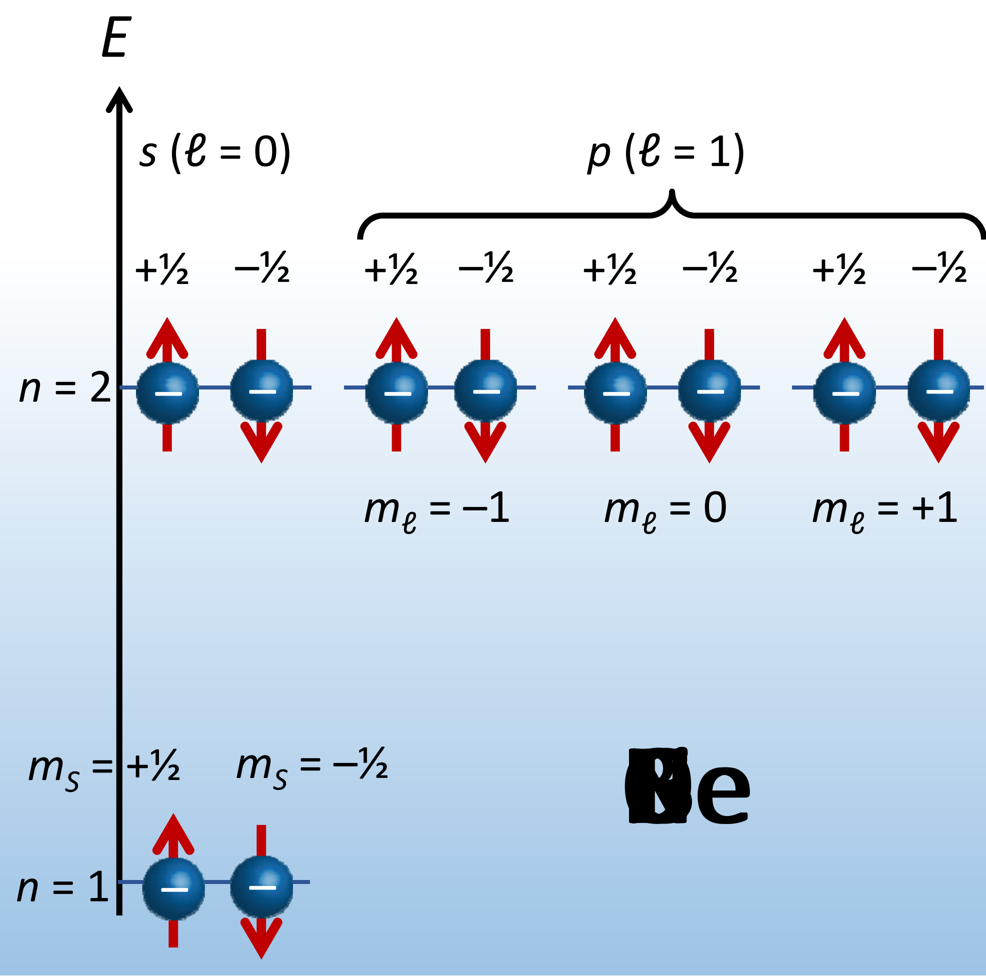
"Spin Quantum Number", m_s = –½, +½

$$S_z = m_s \hbar$$ Orientation of spin

Electronic states

spin ½ particle

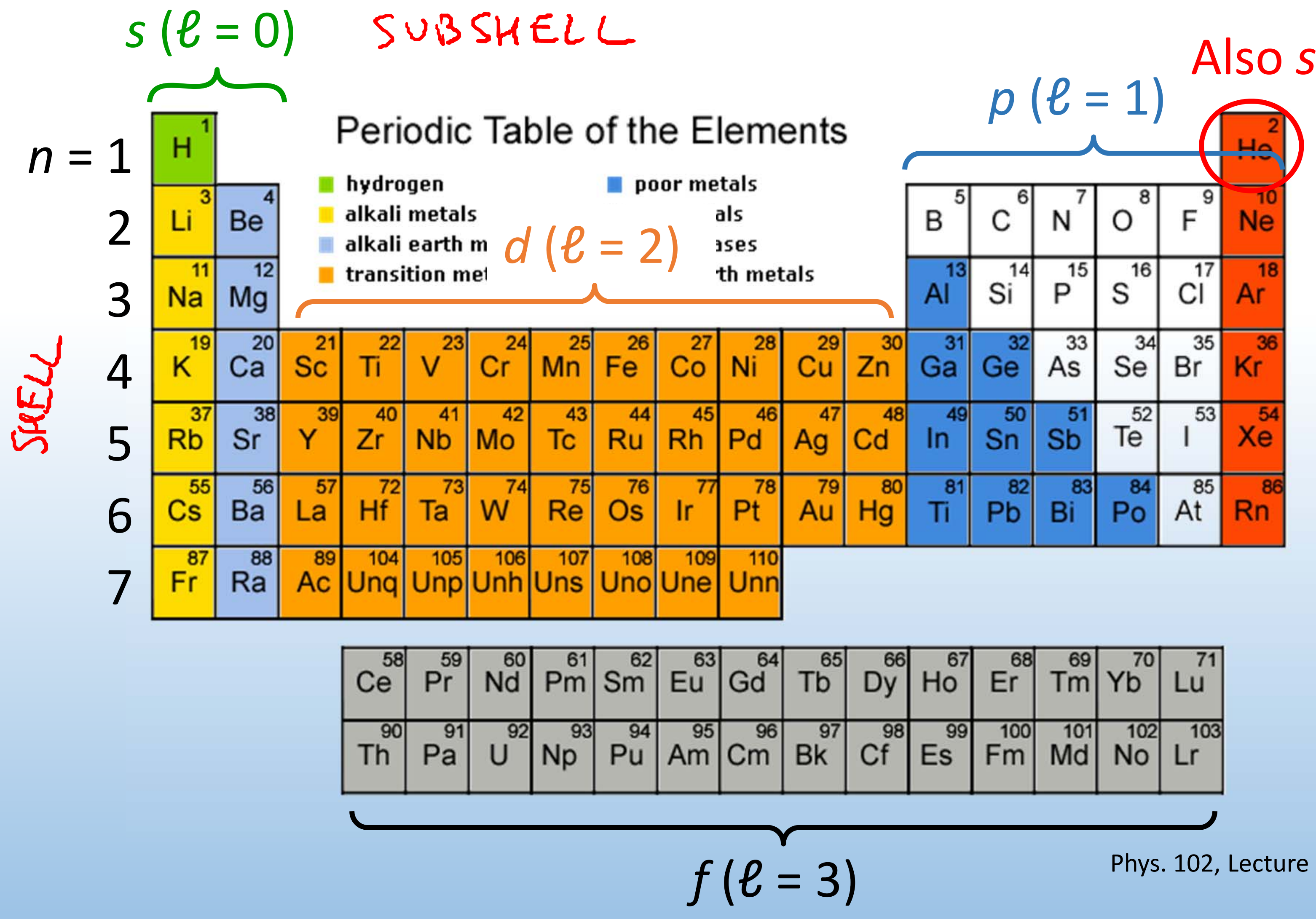
Pauli Exclusion Principle: no two e^- can have the same set of quantum numbers n, ℓ, m_ℓ, m_s



As e^- are added, they must occupy higher energy levels

The Periodic Table

Pauli exclusion & energies determine sequence



CheckPoint 3.2

How many electrons can there be in a 5g (n = 5, ℓ = 4) sub-shell of an atom?

$$2\ell+1 \begin{cases} m_\ell = +4 & m_s = +\tfrac{1}{2}, -\tfrac{1}{2} & \text{2 states} \\ m_\ell = +3 & m_s = +\tfrac{1}{2}, -\tfrac{1}{2} & \text{2 states} \\ m_\ell = +2 & m_s = +\tfrac{1}{2}, -\tfrac{1}{2} & \text{2 states} \\ m_\ell = +1 & m_s = +\tfrac{1}{2}, -\tfrac{1}{2} & \text{2 states} \\ m_\ell = 0 & m_s = +\tfrac{1}{2}, -\tfrac{1}{2} & \text{2 states} \\ m_\ell = -1 & m_s = +\tfrac{1}{2}, -\tfrac{1}{2} & \text{2 states} \\ m_\ell = -2 & m_s = +\tfrac{1}{2}, -\tfrac{1}{2} & \text{2 states} \\ m_\ell = -3 & m_s = +\tfrac{1}{2}, -\tfrac{1}{2} & \text{2 states} \\ m_\ell = -4 & m_s = +\tfrac{1}{2}, -\tfrac{1}{2} & \text{2 states} \end{cases}$$

There are a total of

$$2(2\ell+1) = 18$$

states within one subshell

ACT: Quantum numbers

How many total electron states exist with $n = 2$?

A. 2

B. 4

C. 8

$\ell = 0$ (s sub-shell)

$1 \left\{ m_\ell = 0 \right.$ $m_s = +\frac{1}{2}, -\frac{1}{2}$ 2 states

$\ell = 1$ (p sub-shell)

$$3 \left\{ \begin{array}{lll} m_\ell = +1 & m_s = +\frac{1}{2}, -\frac{1}{2} & \text{2 states} \\ m_\ell = 0 & m_s = +\frac{1}{2}, -\frac{1}{2} & \text{2 states} \\ m_\ell = -1 & m_s = +\frac{1}{2}, -\frac{1}{2} & \text{2 states} \end{array} \right.$$

There are a total of

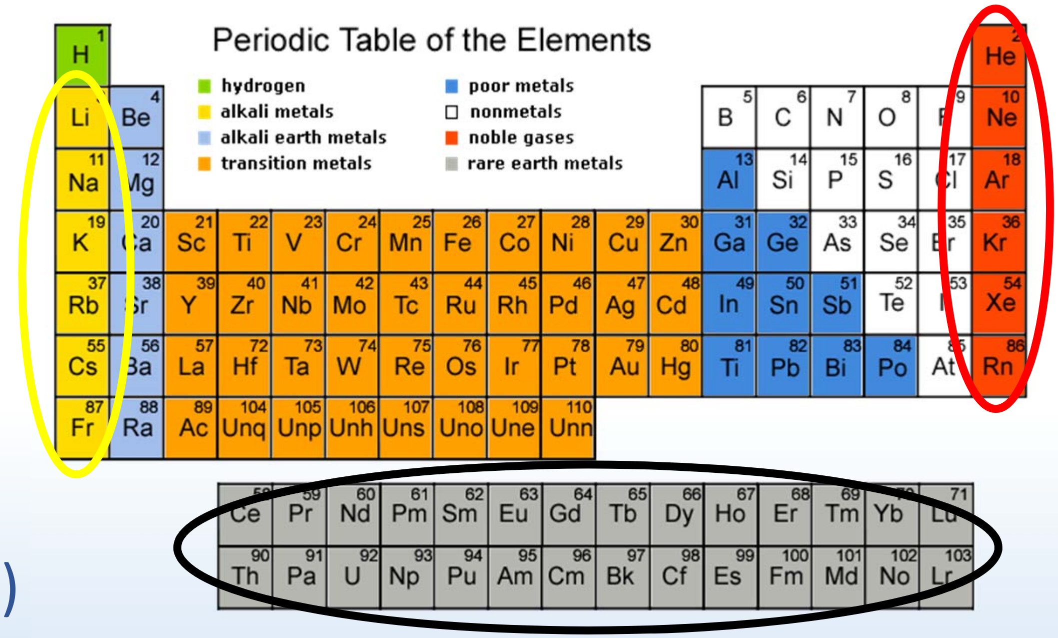
$2n^2 = 8$

states in one shell

For general n, there are a total of: $2\times(1 + 3 + 5 + ...(2n-1)) = 2n^2$ states

ACT: Magnetic elements

Where would you expect the most *magnetic* elements to be in the periodic table?



A. Alkali metals (s, $\ell = 1$)
B. Noble gases (p, $\ell = 2$)
C. Rare earth metals (f, $\ell = 4$)

Magnets are made from elements in the *d* and *f* subshells.
High ℓ means high dipole moment Ex: Fe, Co, Nd, Sm

$$\boxed{\vec{\mu}_e = -\frac{e}{2m_e}\vec{L}}$$

Summary of today's lecture

- Quantum numbers

  Principal quantum number $E_n = -Z^2/n^2 \times 13.6\,\mathrm{eV}$

  Orbital quantum number $L = \sqrt{\ell(\ell+1)}\hbar, \quad \ell = 0, 1, n-1$

  Magnetic quantum number $L_z = m_z\hbar, \quad m_\ell = -\ell, \ldots, 0, \ldots \ell$

- Spin angular momentum

  e⁻ has intrinsic angular momentum $S_z = m_s\hbar \quad m_s = -\frac{1}{2}, \frac{1}{2}$

- Magnetic properties

  Orbital & spin angular momentum generate magnetic dipole moment

- Pauli Exclusion Principle

  No two e⁻ can have the same quantum numbers