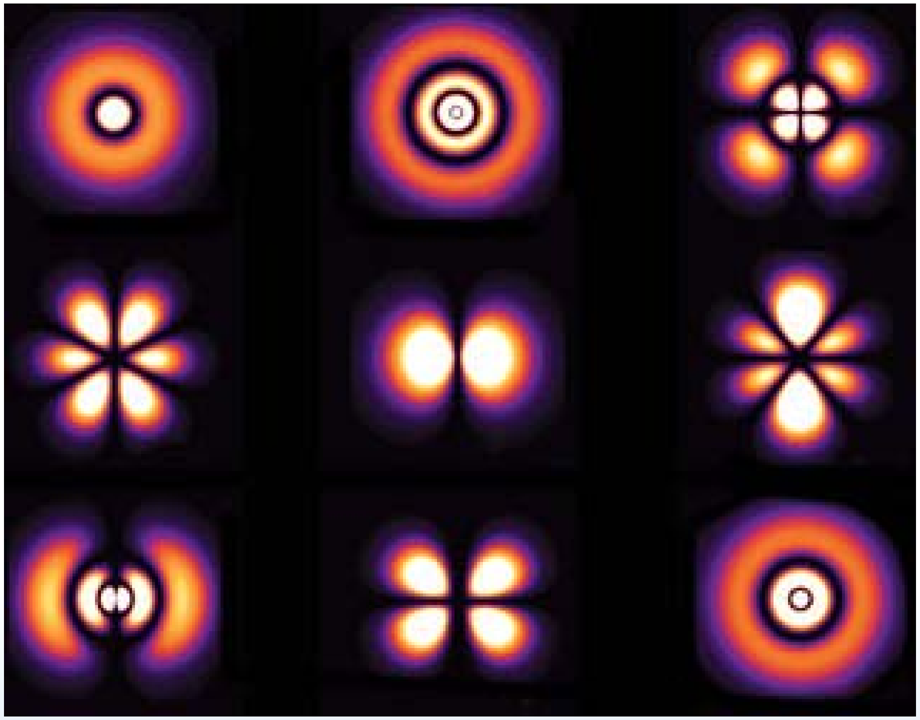
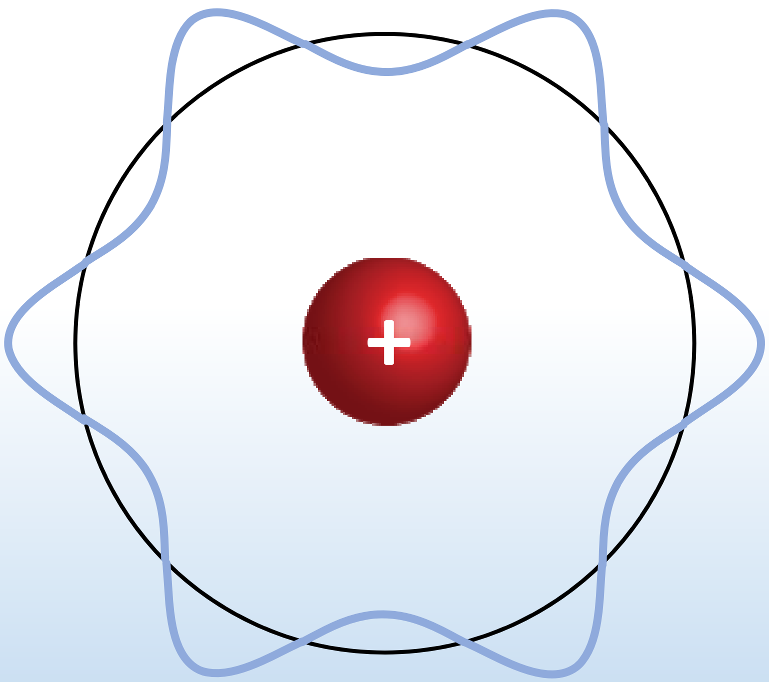


Phys 102 – Lecture 26

The quantum numbers and spin

Recall: the Bohr model

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



SUCCESSES

Correct energy quantization & atomic spectra

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

FAILURES

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*

$$L_n = n\hbar$$

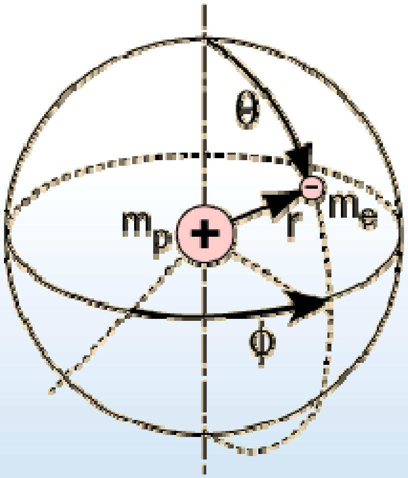
Orbits can hold any number of electrons

Quantum Mechanical Atom

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

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

"Magnetic Quantum Number" $m_\ell = -\ell, \ldots -1, 0, +1 \ldots, \ell$

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

ACT: CheckPoint 3.1 & more

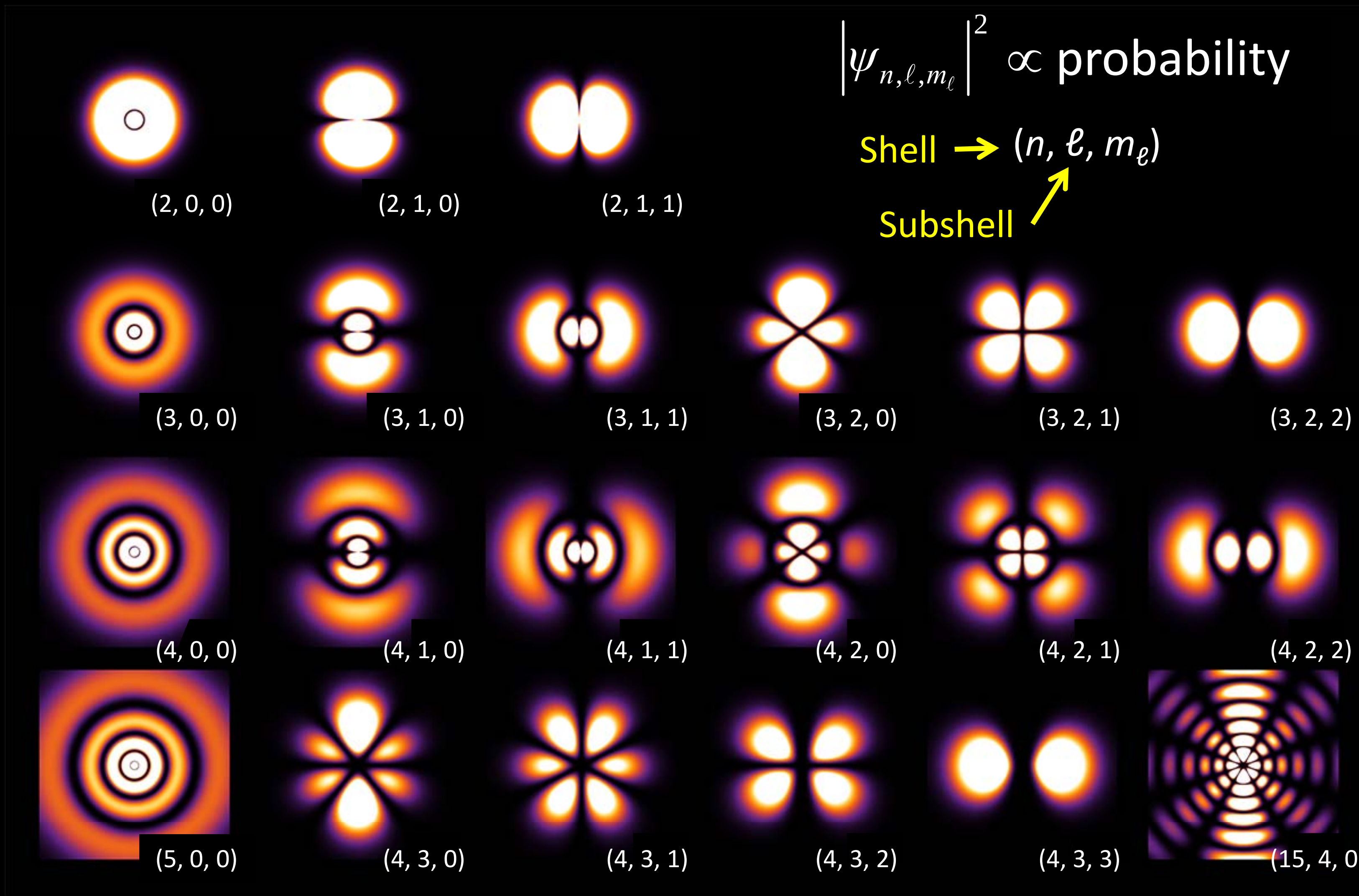
For which state is the angular momentum *required* to be 0?

A. $n = 3$
B. $n = 2$
C. $n = 1$

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

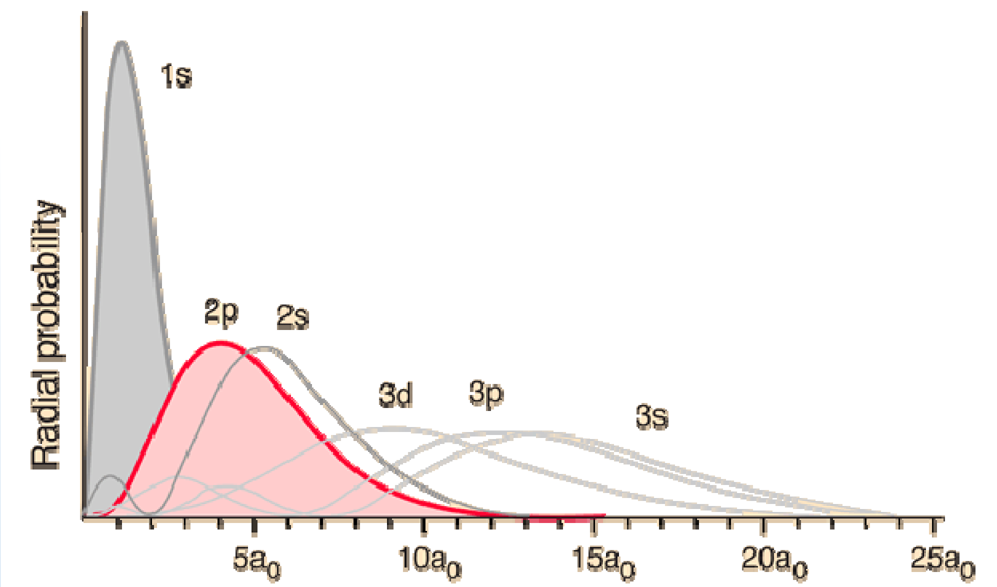
A. 3
B. 5
C. 7

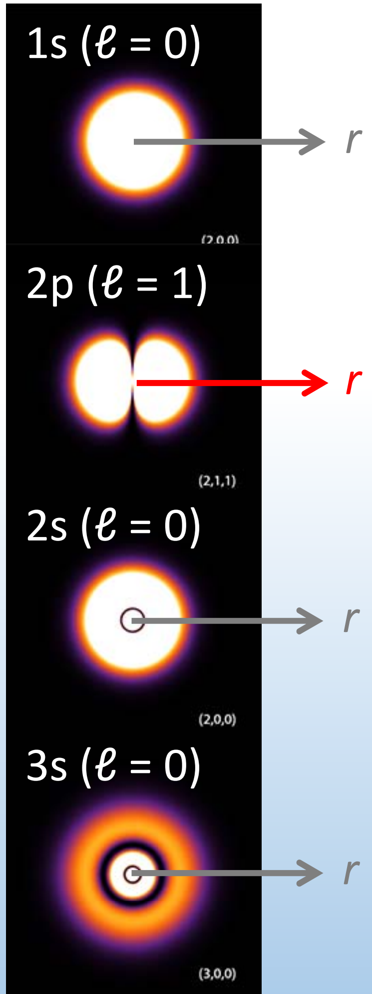
Hydrogen electron orbitals



CheckPoint 2: orbitals

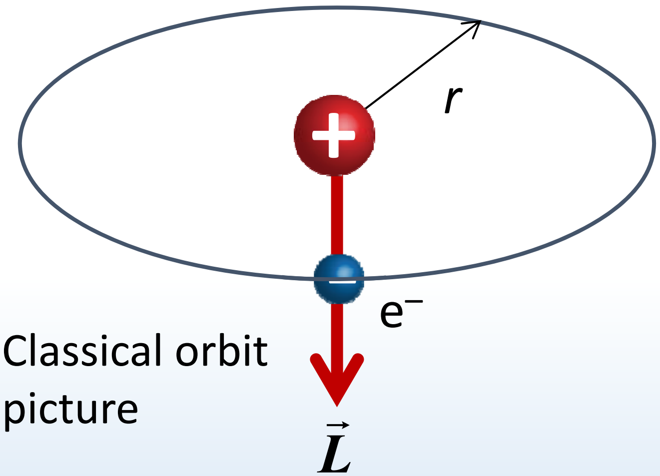
Orbitals represent probability of electron being at particular location





Angular momentum

What do the quantum numbers ℓ and m_ℓ represent?



Classical orbit picture

Magnitude of angular momentum vector quantized

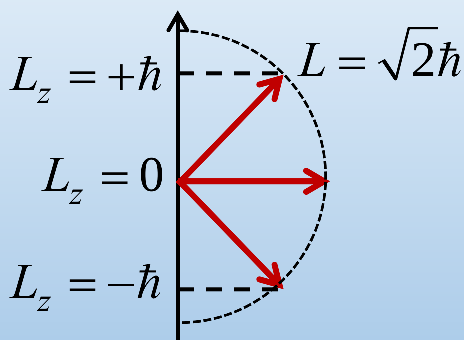
$$\left|\vec{L}\right| = L = \sqrt{\ell(\ell+1)}\hbar \qquad \ell = 0, 1, 2 \cdots n-1$$

Only *one* component of *L* quantized

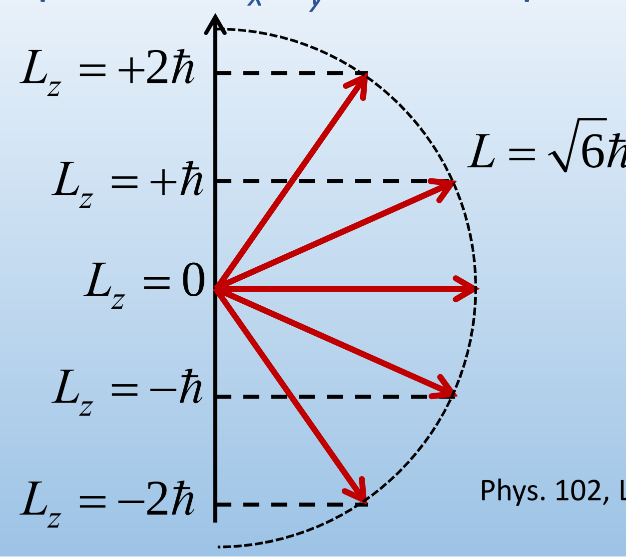
$$L_z = m_\ell \hbar \qquad m_\ell = -\ell, \cdots -1, 0, 1, \cdots \ell$$

Other components L_x, L_y are not quantized

$\ell = 1$

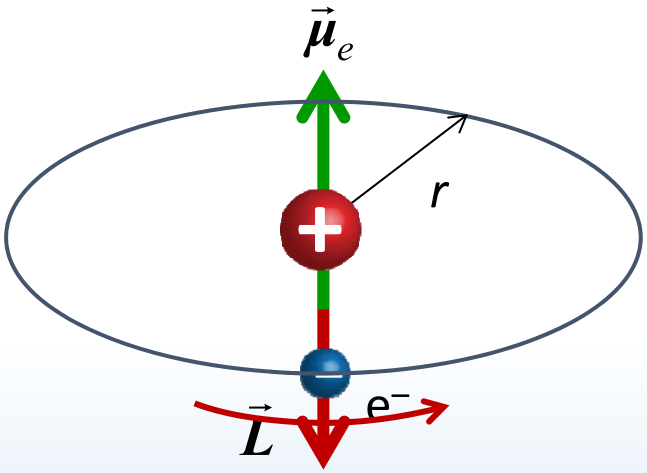


$\ell = 2$



Orbital magnetic dipole

Electron orbit is a current loop and a magnetic dipole



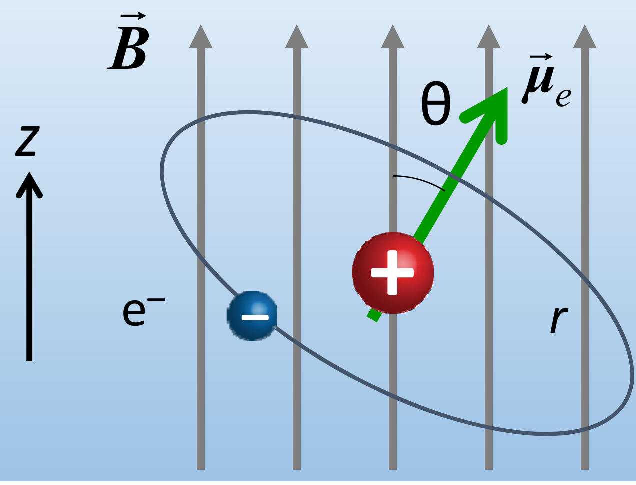
$$\mu_e = IA = -\frac{e}{2m_e} L$$

Recall Lect. 12

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

Dipole moment is quantized

What happens in a *B* field?



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

Recall Lect. 11

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

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

"Bohr magneton"

ACT: Hydrogen atom dipole

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

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

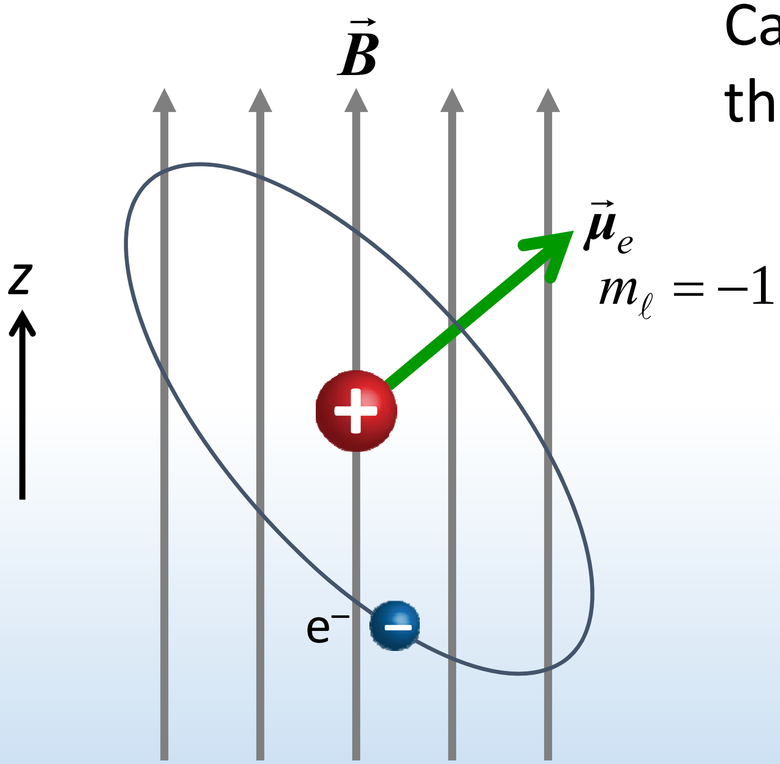
A. $\mu_H = -\frac{e\hbar}{2m_e}$

B. $\mu_H = 0$

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

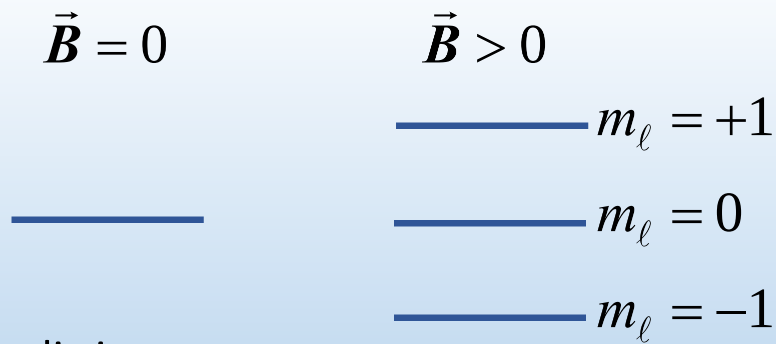
Calculation: Zeeman effect

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



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

For ℓ = 1,
m_ℓ = –1, 0, +1

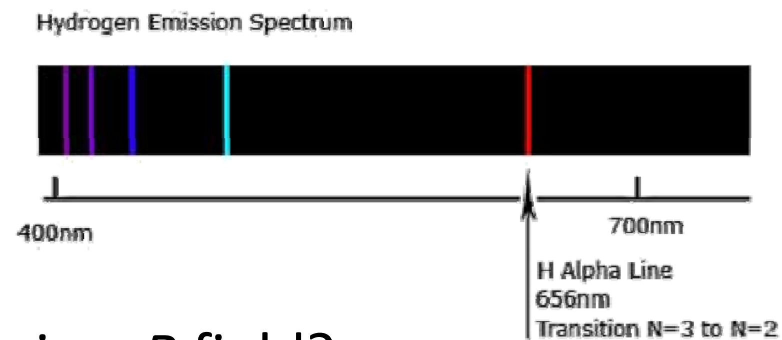


Energy level splits into 3, with energy splitting

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

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 subshells.

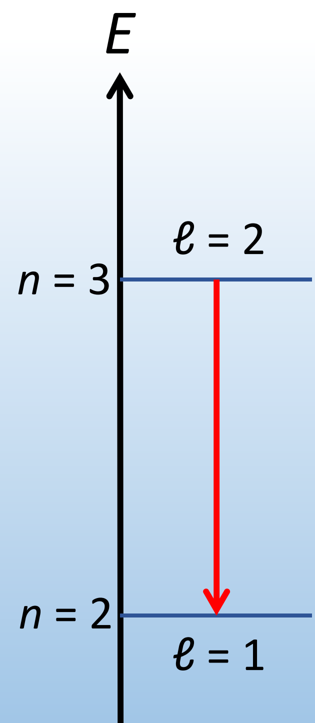


How many spectral lines will appear in a B field?

A. 1

B. 3

C. 5



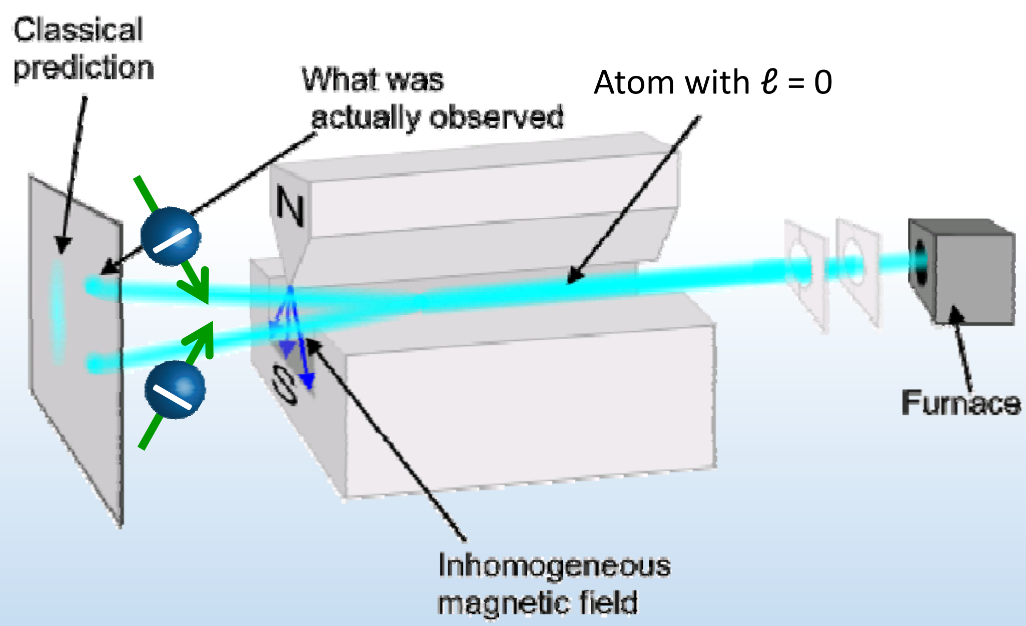
Intrinsic angular momentum

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

n = 1, so ℓ = 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 $\ell = ½$. "Spin"



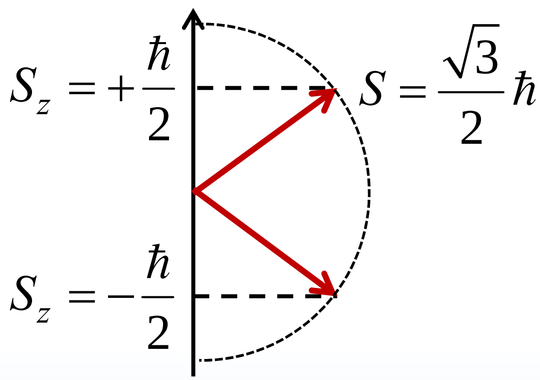
"Stern-Gerlach experiment"

Spin angular momentum

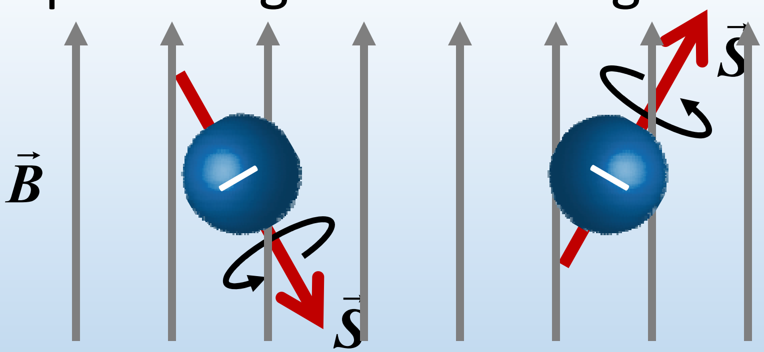
Electrons have an intrinsic angular momentum called "spin"

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

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



Spin also generates magnetic dipole moment



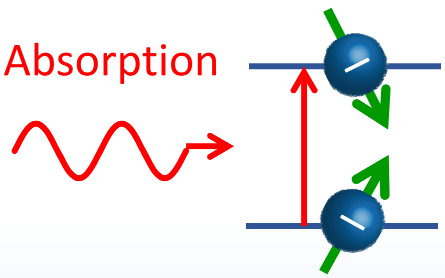
Spin DOWN (– ½) Spin UP (+½)

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

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

Magnetic resonance

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



$m_s = +\tfrac{1}{2}$ $\quad hf = \Delta E$

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

"Electron spin resonance"

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"

Quantum number summary

"Principal Quantum Number", $n = 1, 2, 3, \ldots$

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

"Orbital Quantum Number", $\ell = 0, 1, 2, \ldots, n-1$

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

"Magnetic Quantum Number", $m_l = -\ell, \ldots -1, 0, +1 \ldots, \ell$

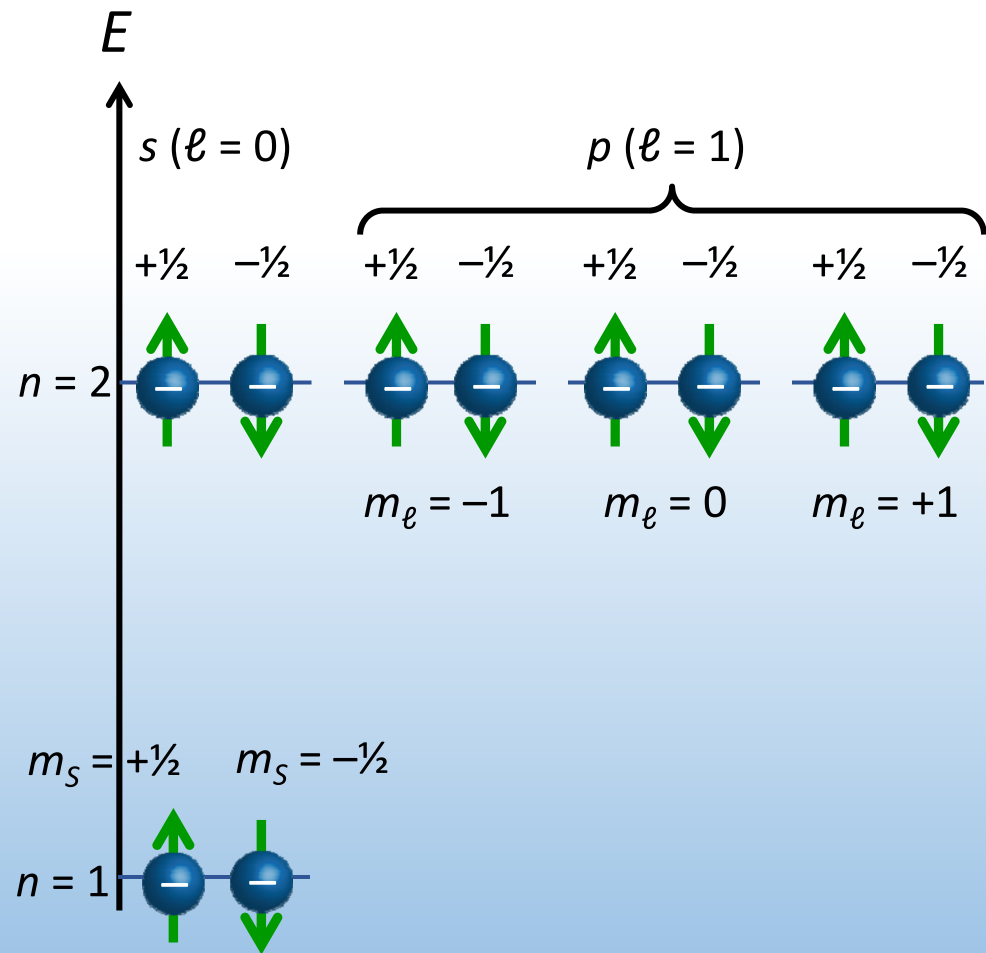
$$L_z = m_\ell \hbar$$ Orientation of angular momentum

"Spin Quantum Number", $m_s = -½, +½$

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

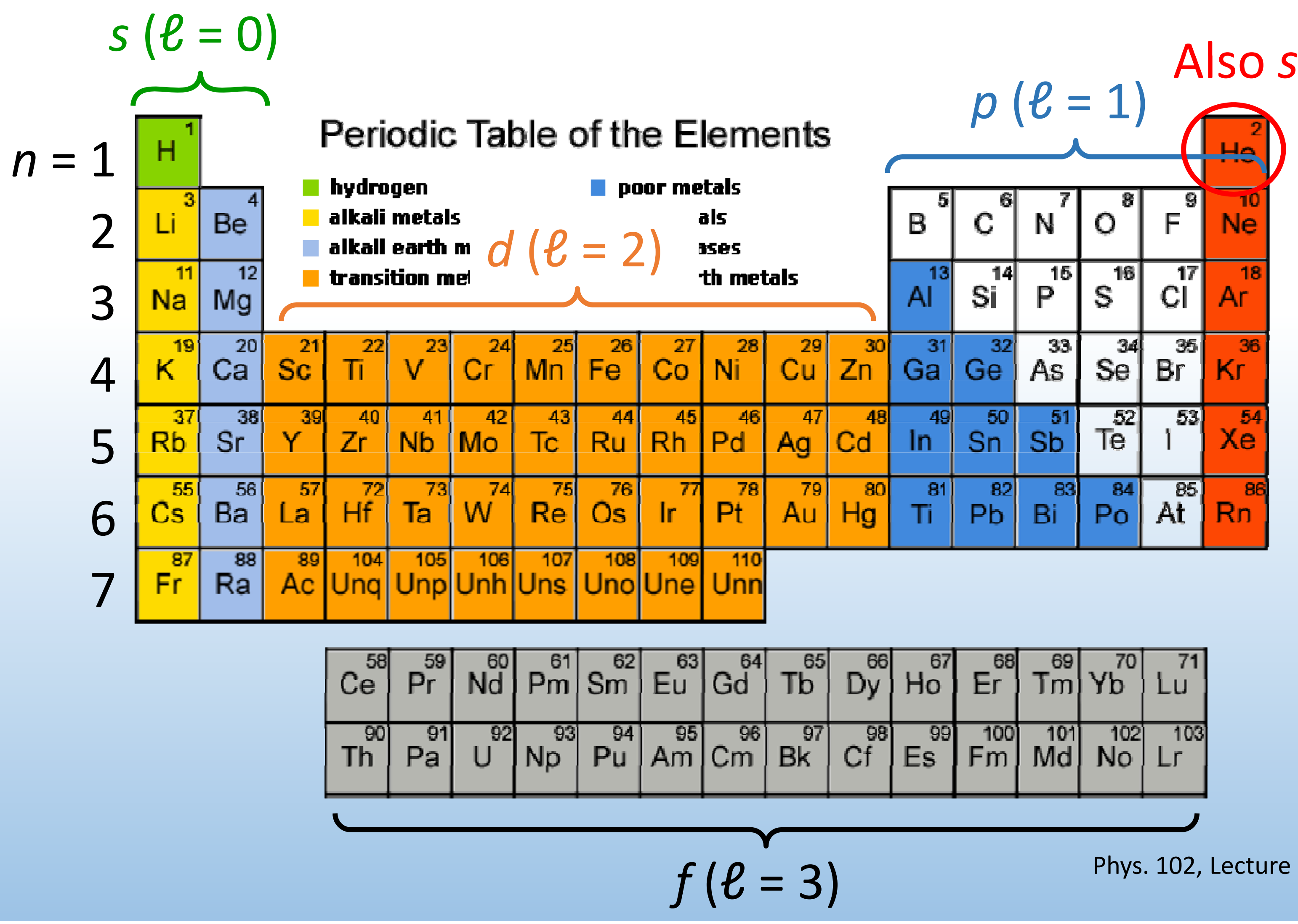
Electronic states

Pauli Exclusion Principle: no two e⁻ can have the same set of quantum numbers



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?

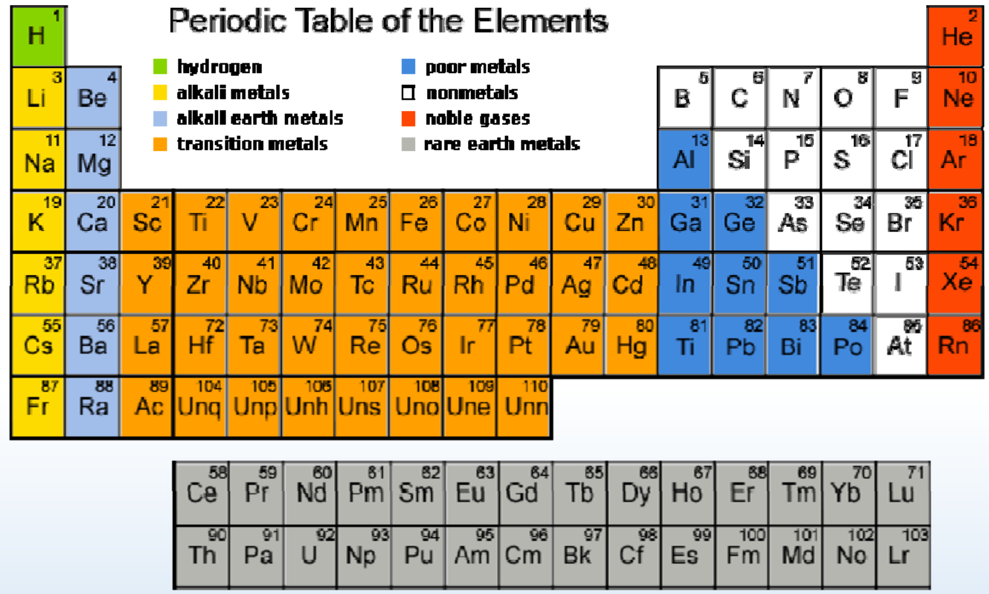
ACT: Quantum numbers

How many total electron states exist with n = 2?

A. 2
B. 4
C. 8

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, $\ell = 4$)

Summary of today's lecture

- Quantum numbers

  Principal quantum number $E = -13.6\,eV / n^2$

  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