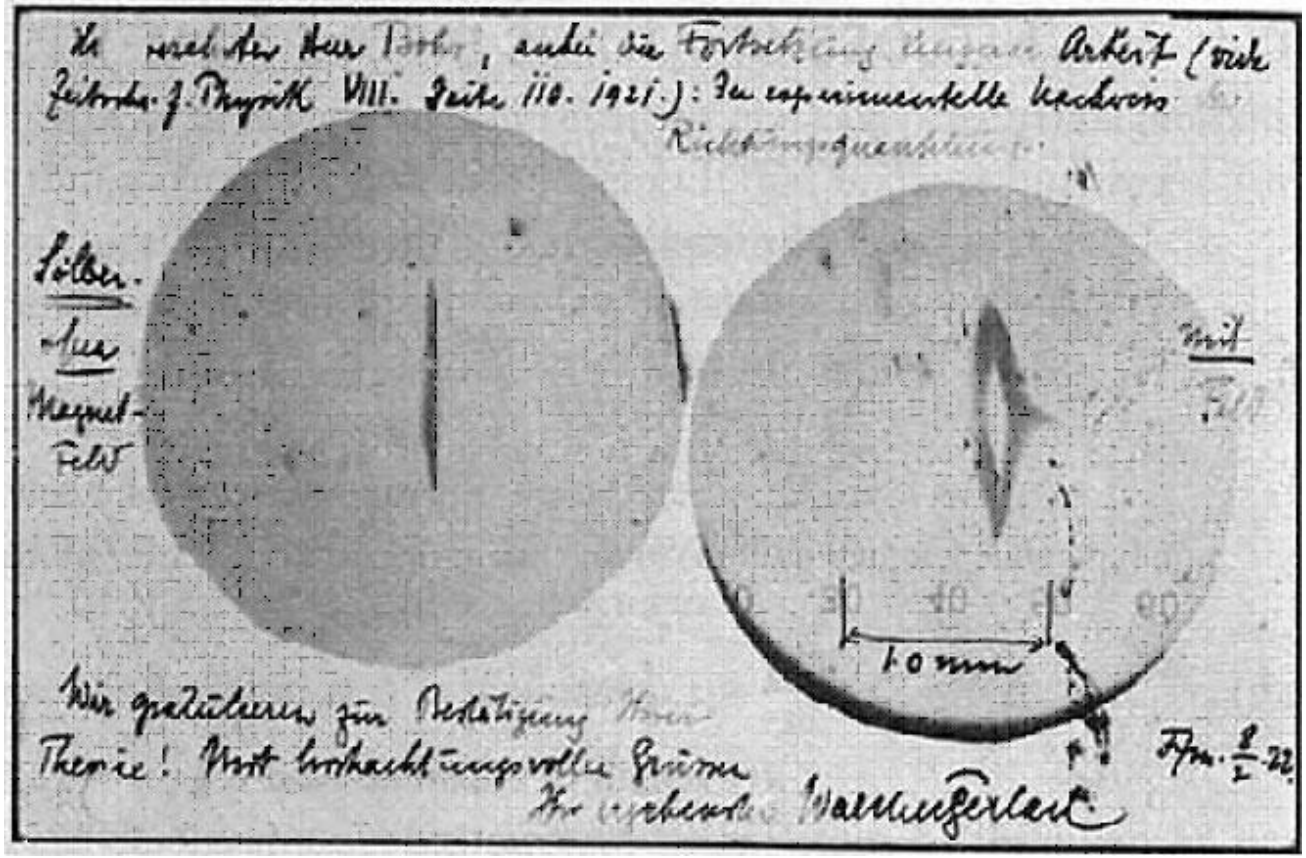
Pre-AP Chemistry

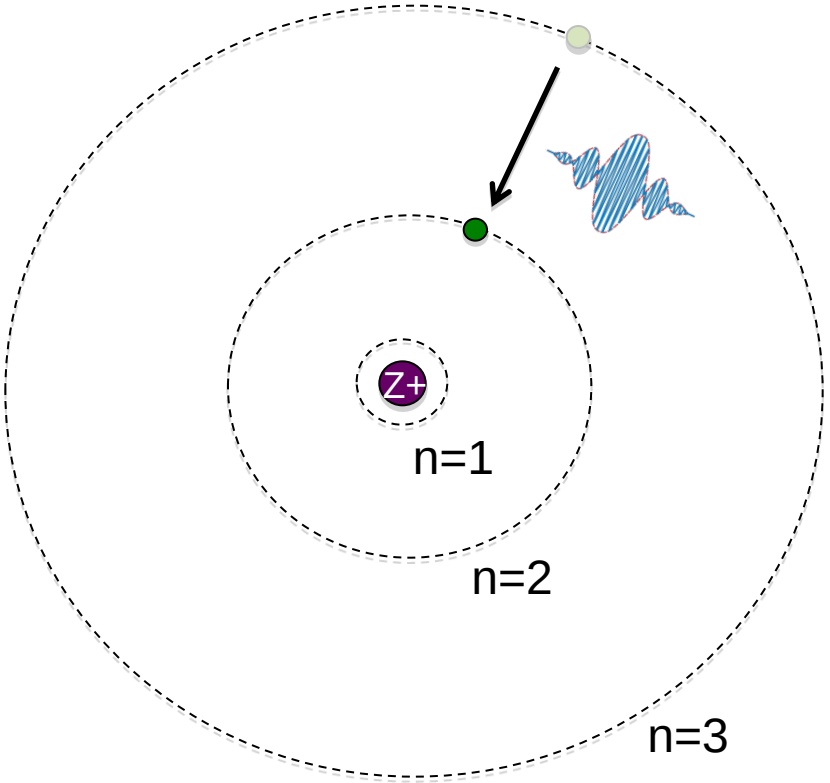
September 4, 2011

8. Electrons in Atoms II



Review

- Electrons in atoms can only occupy specific orbitals
- Light with energy equal to the difference in orbital energies is absorbed or emitted when electrons jump between these orbitals



$$\Delta E = h\nu$$

- Is light absorbed or emitted when an electron jumps from
  - 1) n = 1 to n = 2 ?
  - 2) n = 3 to n = 1 ?
- Is more energy released when an electron jumps from n = 3 to n = 1 or from n = 3 to n = 2?

Outline

- Wave-Particle Duality
- Quantum Numbers

- Wave-Particle Duality
  - Light Particles vs Electron Waves
  - Uncertainty Principle
  - Orbitals as Probabilities
- Quantum Numbers
  - Principal, n
  - Angular Momentum, l
  - Magnetic, m_l
  - Spin, m_s

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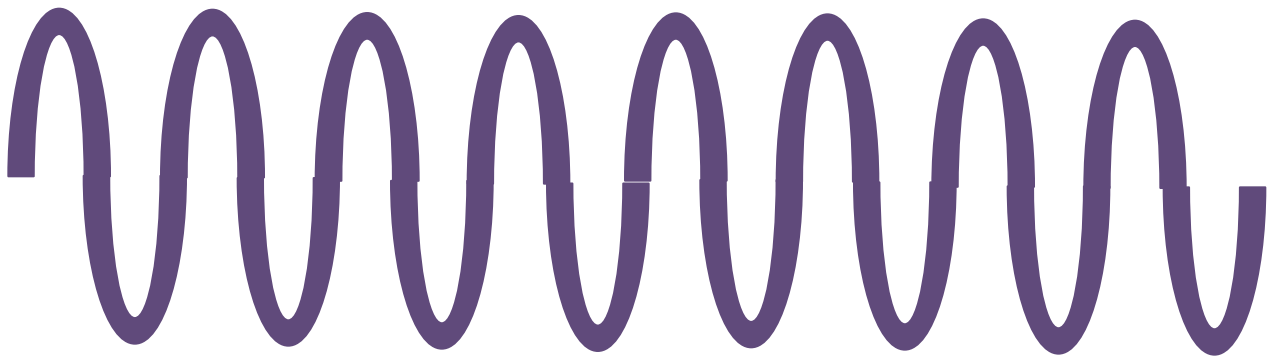
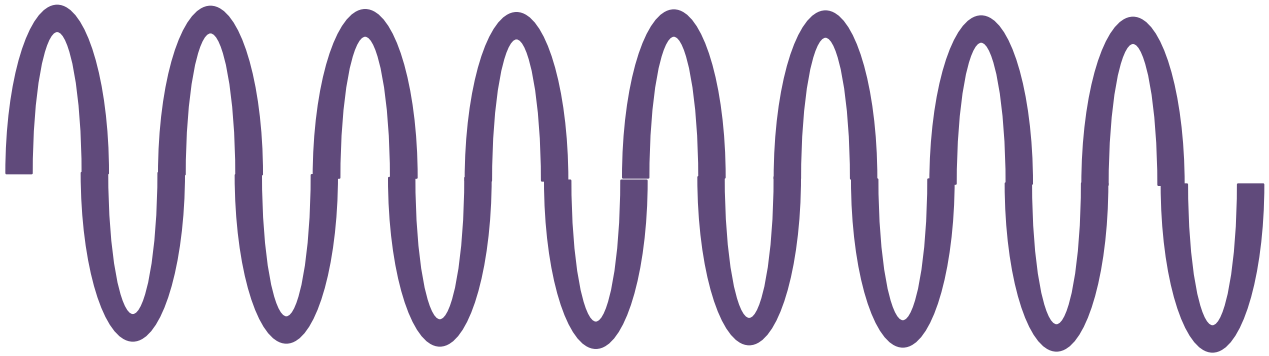
Light: Waves and Particles

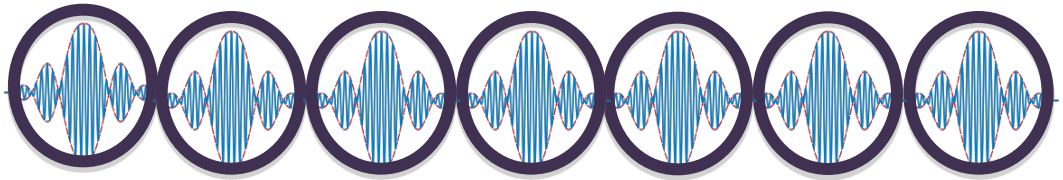
- We think of light in two ways
  1. As **Waves** (**radiation**): frequency, wavelength, etc.

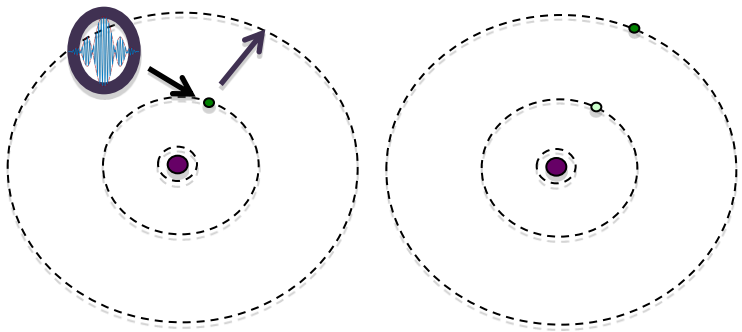


Light: Waves and Particles

- We think of light in two ways
  1. As **Waves** (**radiation**): frequency, wavelength, etc.
  2. As **Particles** (**photons**): kicking electrons between orbits

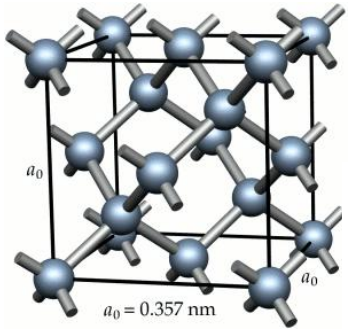


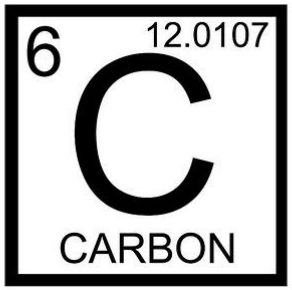


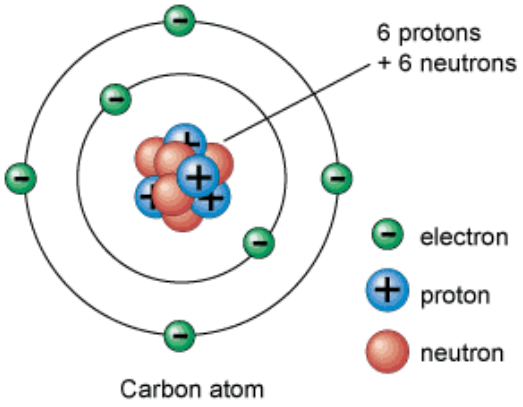


Matter Particles

- So far, we have thought of matter as composed of particles
  - Solids, liquids, gases
  - Molecules
  - Atoms
  - Protons, Neutrons, Electrons







Matter Waves

- Matter (particles) can also be described in terms of waves
- The **wavelength of a particle** is **inversely proportional** to its **mass** and velocity

People have mass, but I don't feel very wavy …

Matter Waves

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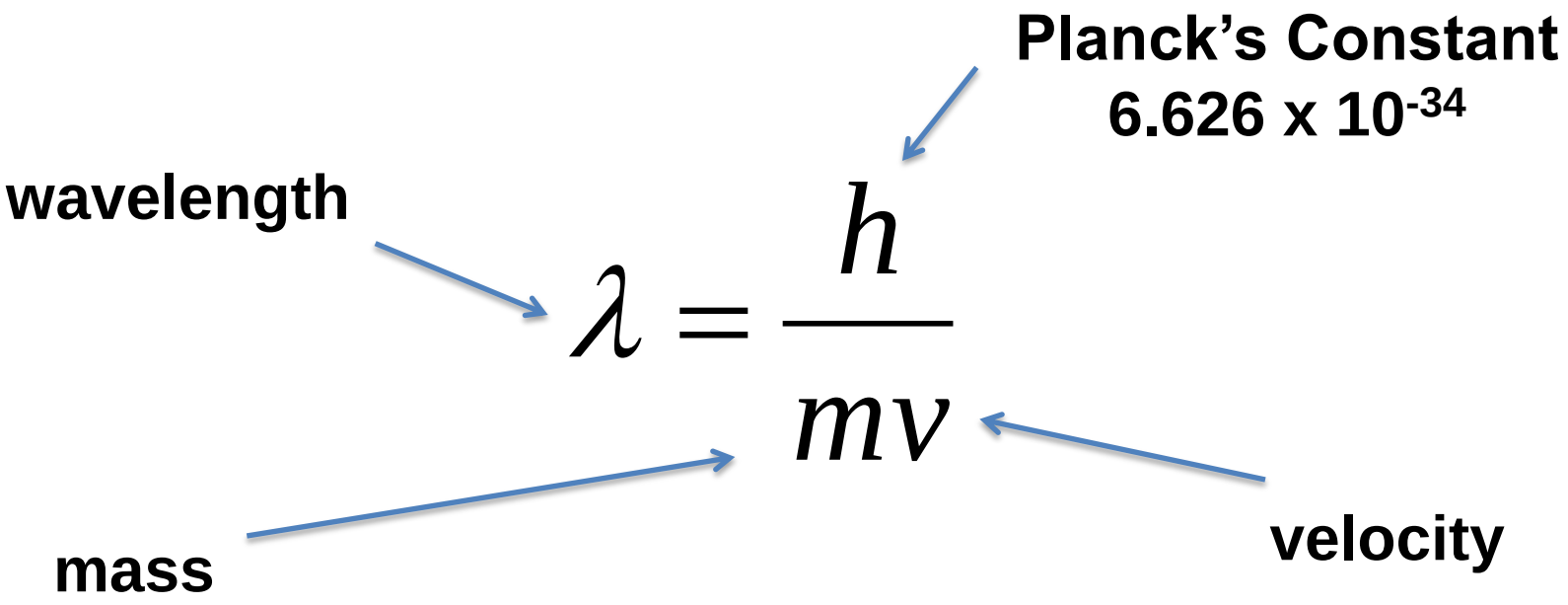


De Broglie Equation

Mini Quiz

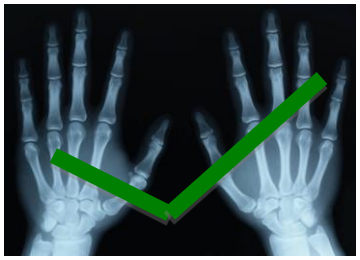
$$\lambda = \frac{h}{mv}$$

Object	Mass	Velocity	Wavelength	Wave-like?
	73 kg	3.8 m/s	?	
-	9.1E-31 kg	1E+6 m/s	?	

Only very small particles – like electrons – are wave-like

Matter Waves

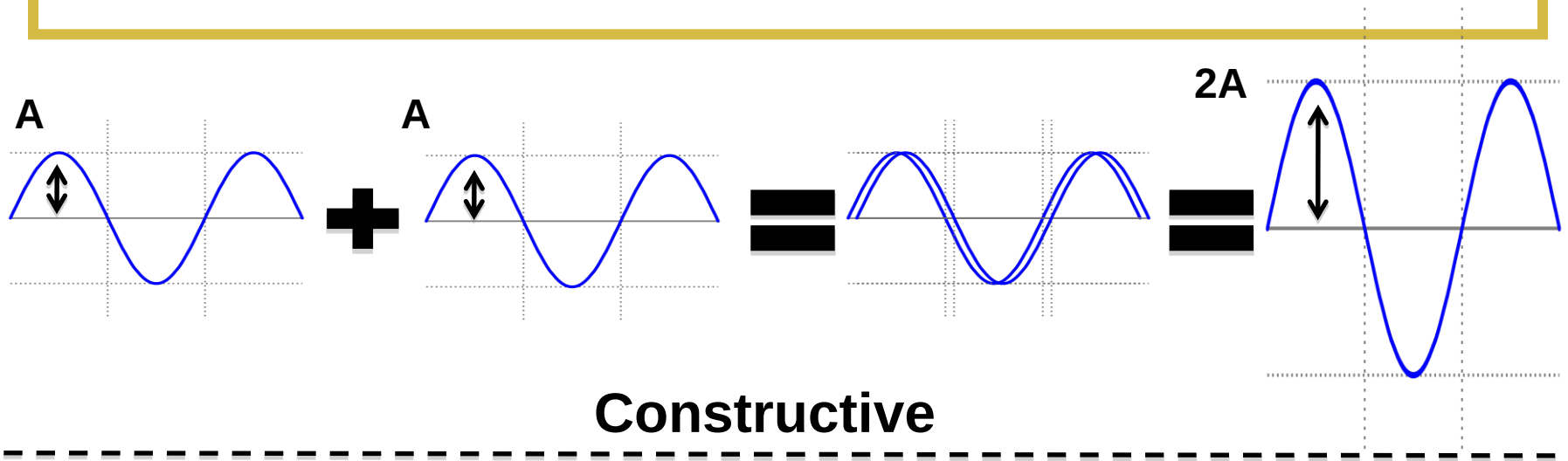
$$\lambda = \frac{h}{mv}$$

Object	Mass	Velocity	Wavelength	Wave-like?
	73 kg	3.8 m/s	2.7E-36 m	
	9.1E-31 kg	1E+6 m/s	7.3E-10 m	

Only very small particles – like electrons – are wave-like

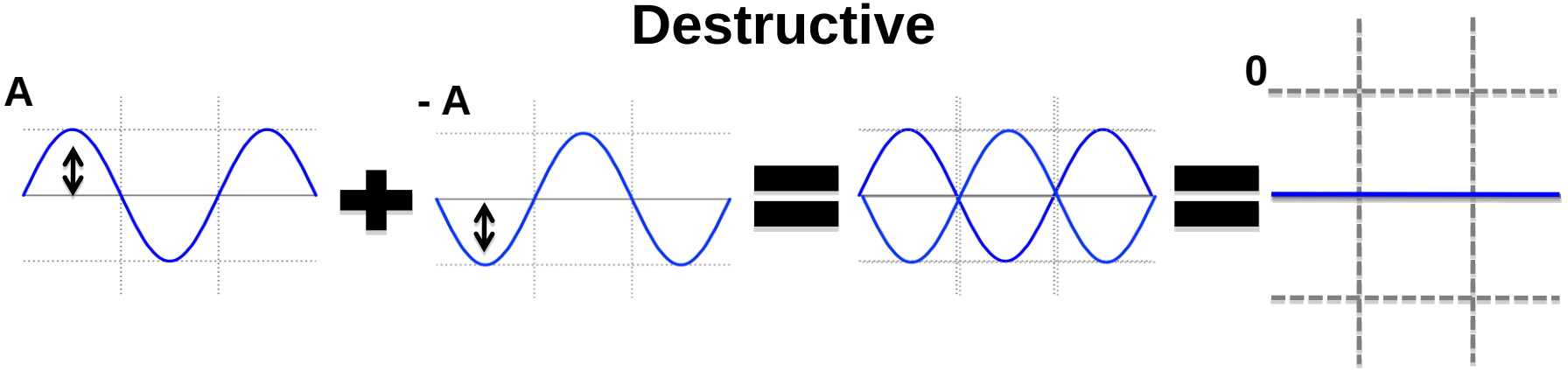
Interference

- Waves can add to each other **constructively** and **destructively**



Constructive

Destructive



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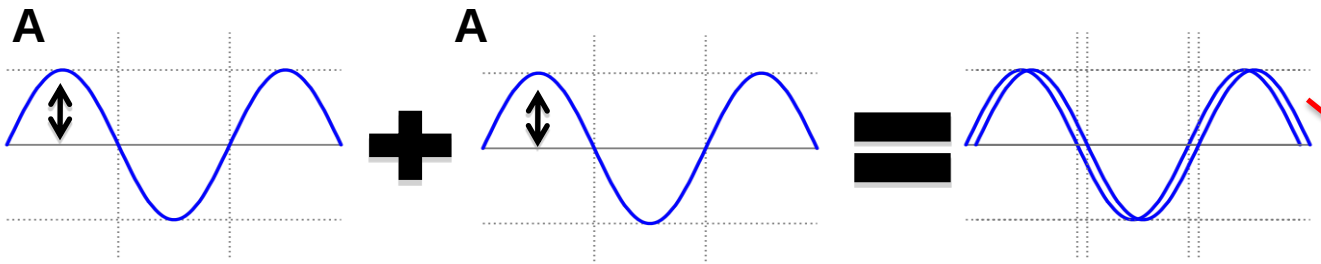

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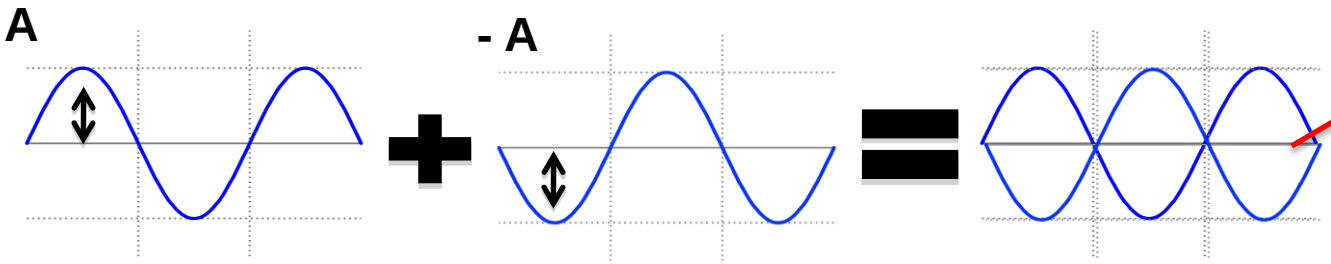
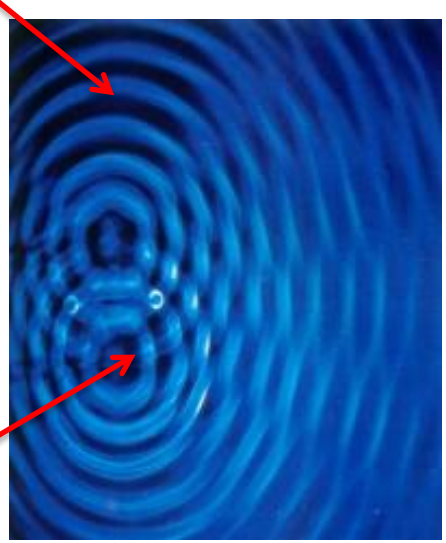
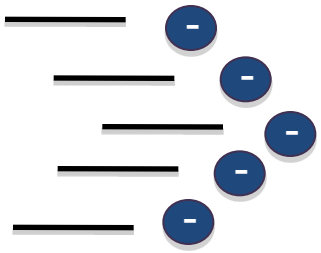
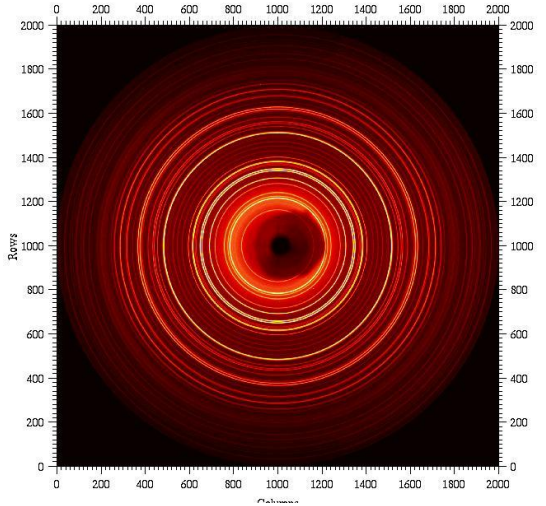




Interference

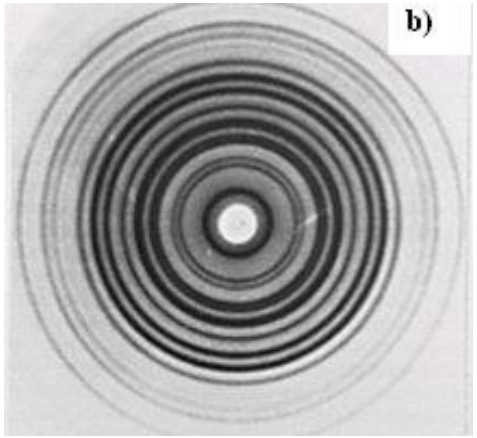
- Electrons also show interference when shot through matter





ELECTRONS

WATER



X-RAYS

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Uncertainty Principle

- If an electron can be a wave, how do we find it's position?

Uncertainty Principle

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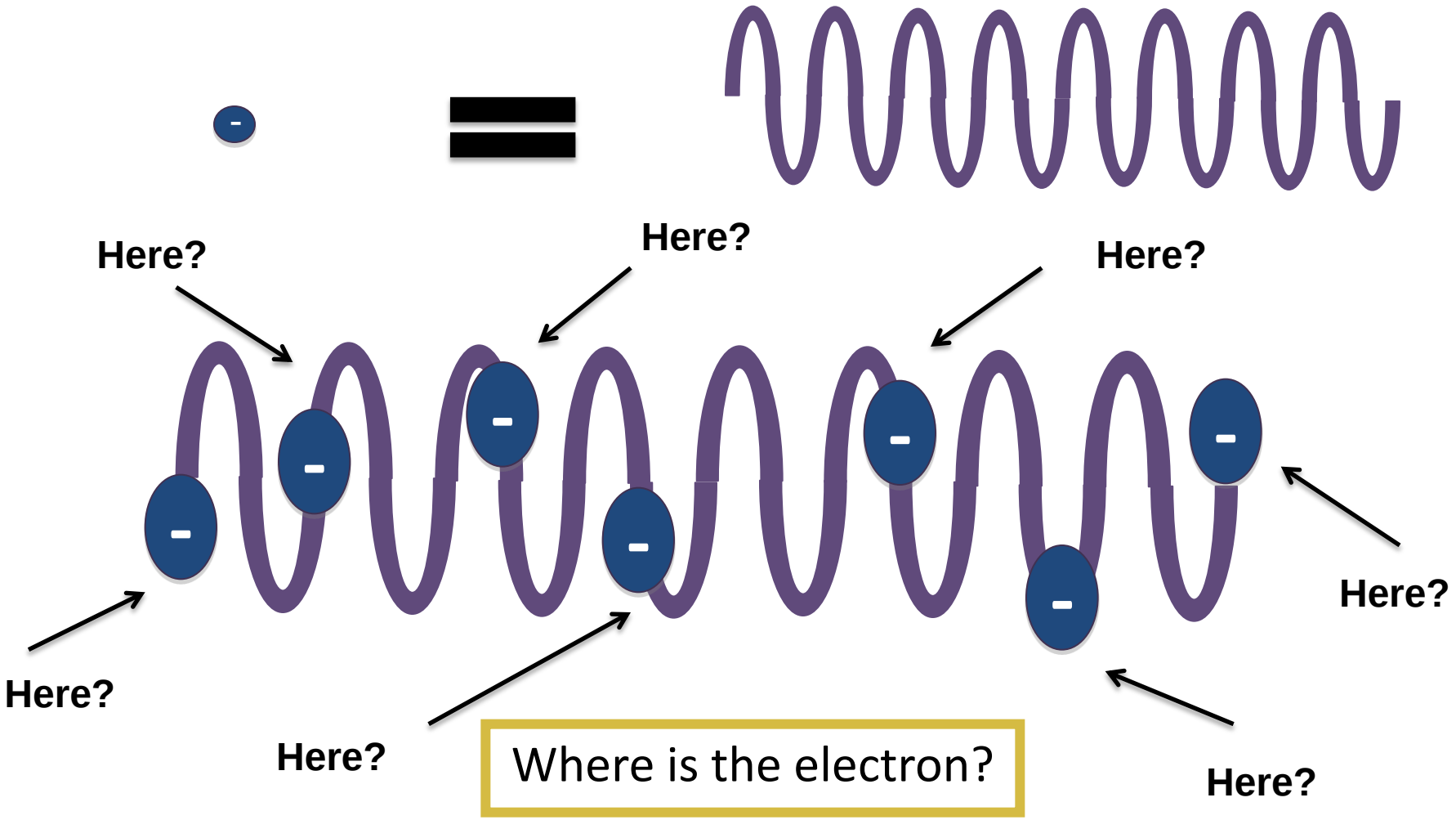


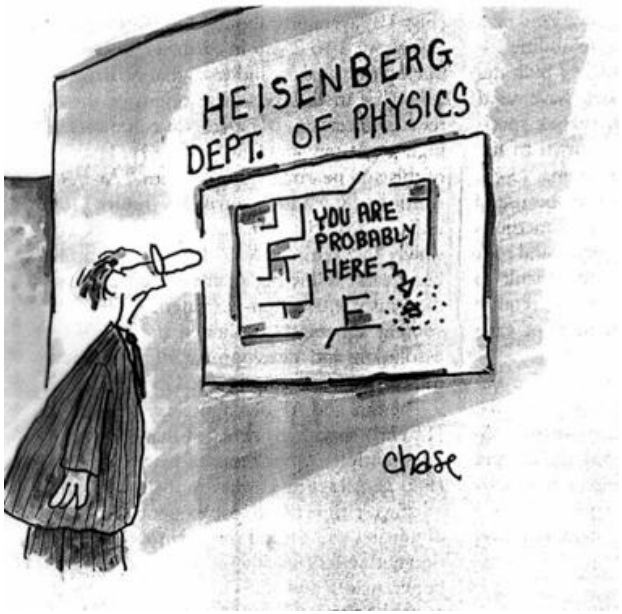
Uncertainty Principle

- There is a limit to how precisely we can know the position and momentum of a particle.

Uncertainty in Position

Uncertainty in Momentum

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$

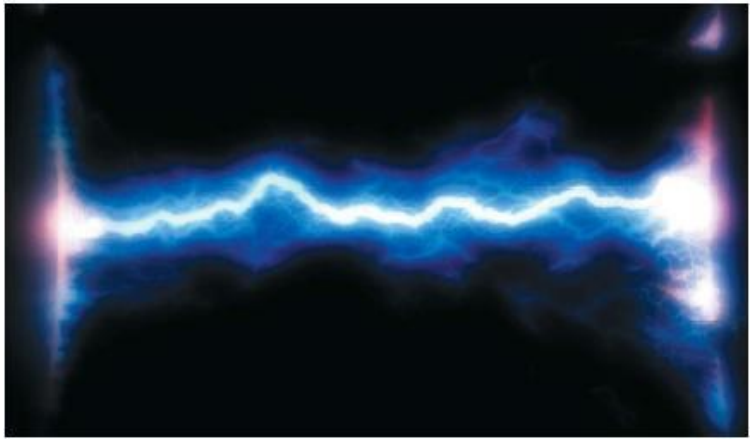


What does this mean for accuracy and precision in scientific measurements?

Uncertainty Principle

- There is almost **no uncertainty** in the position and velocity of **things we can see**
- For very small objects – like an electron – we can never know its exact location or speed

$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi} \approx 10^{-34} \frac{kg \cdot m^2}{s^2}$$



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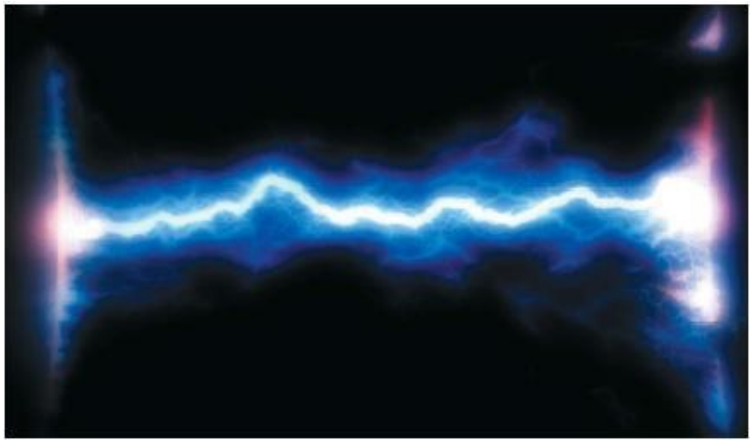


$$\Delta p = 10^{2} \ \frac{kg \cdot m}{s}$$

$$\Delta p = 10^{-24} \ \frac{kg \cdot m}{s}$$

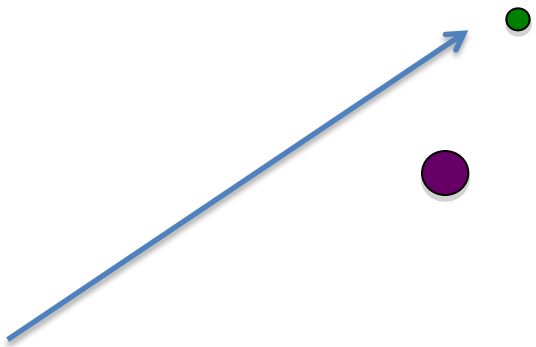
$$\Delta x \approx 10^{-36} m$$

$$\Delta x \approx 10^{-10} m$$

Uncertainty Principle

- The uncertainty in the position of an electron in an atom is as big at the atom itself!

- Uncertainty in electron position: 10^{-10} m
- Electron radius: 10^{-15} m
- Atomic radius: 10^{-10} m



- An electron could be here …

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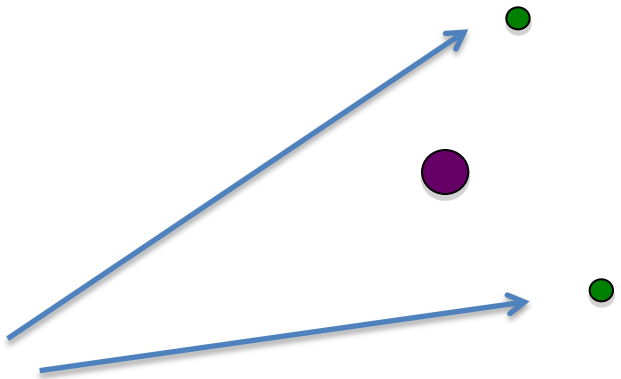
- Atomic radius: 10^{-10} m

- … or here …



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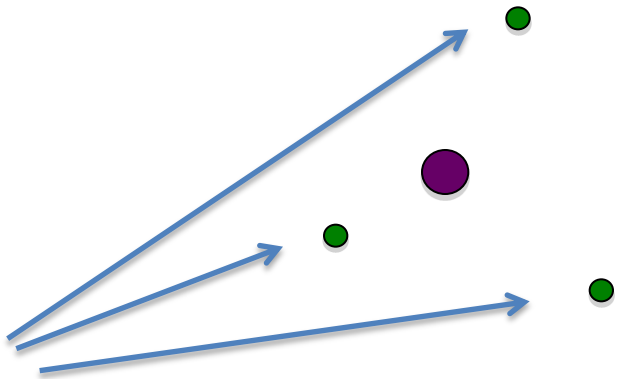

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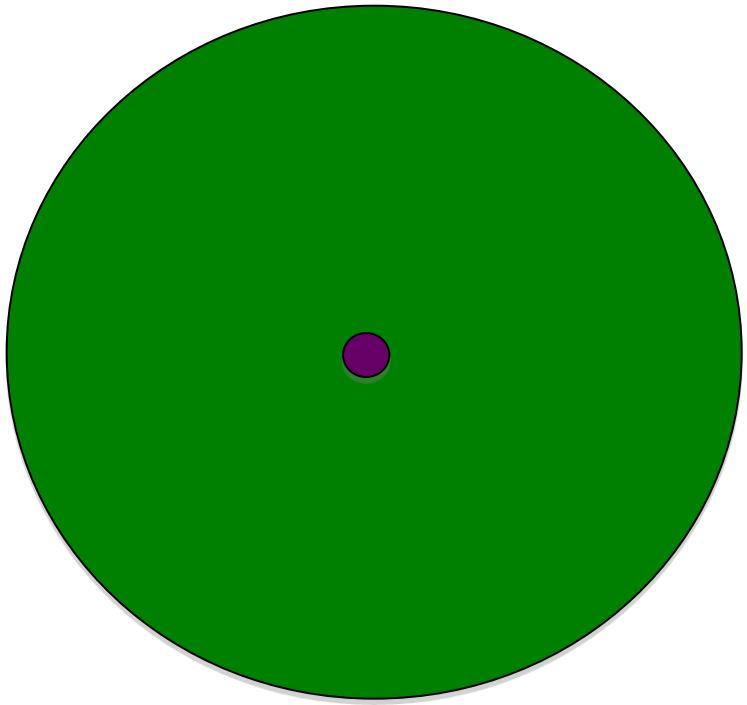

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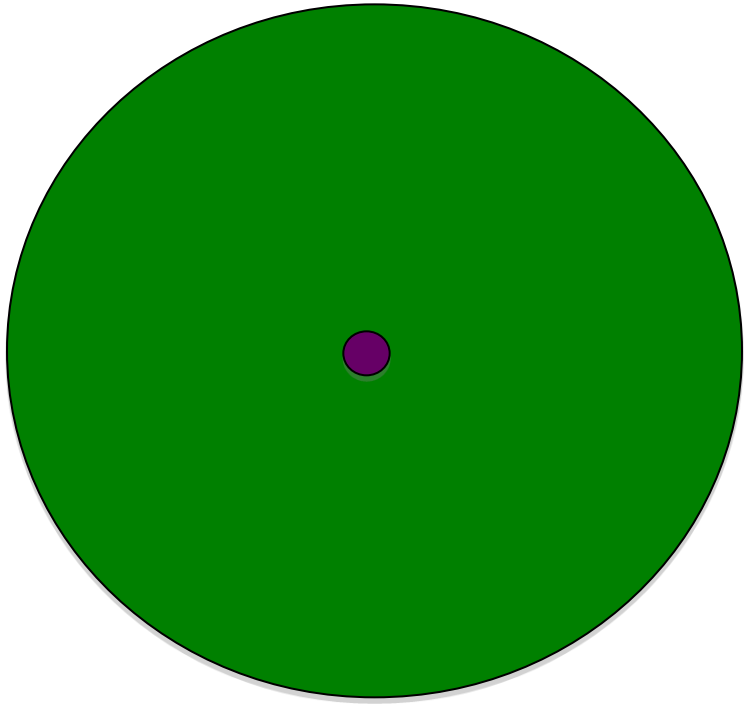

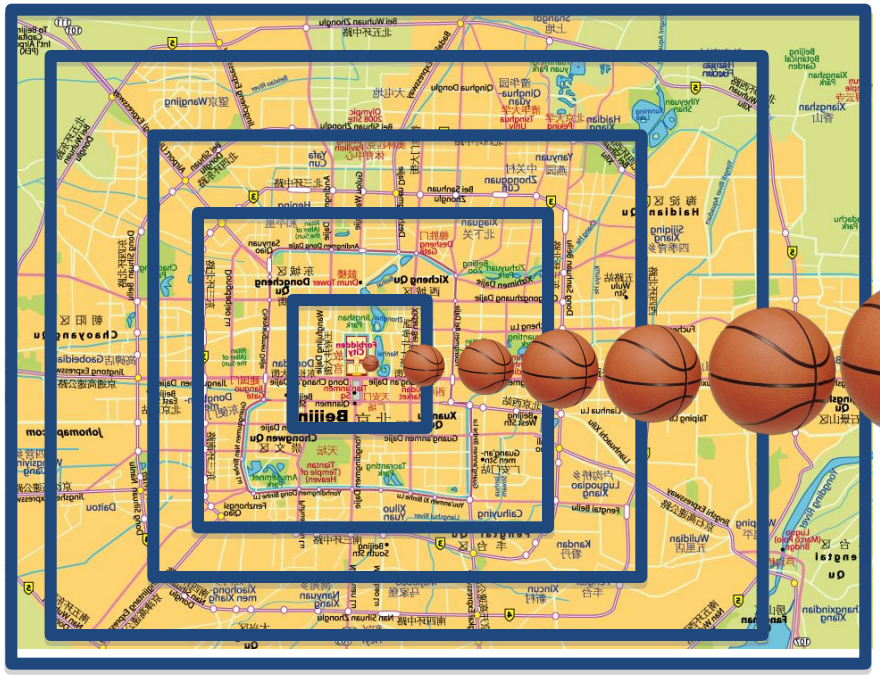

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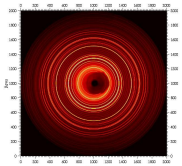
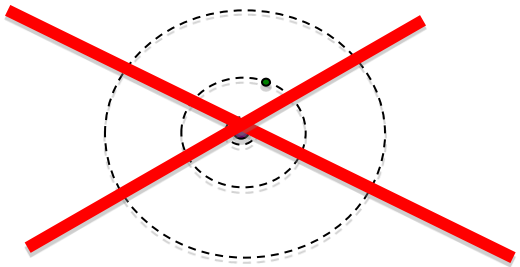
Orbitals as Probabilities

- Because there is uncertainty in the position of very small particles …

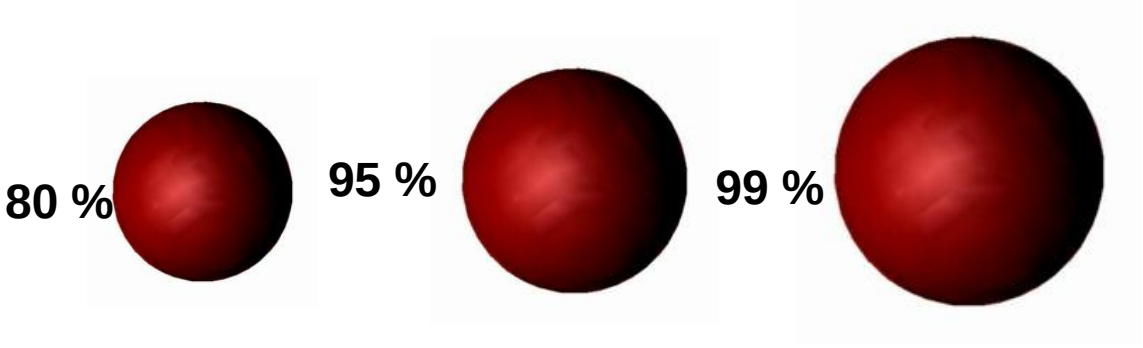
$$\Delta x \cdot \Delta p \geq \frac{h}{4\pi}$$





… electron orbits are not well-defined circles (sorry, Bohr) …

… but only give the probability of finding an electron in a given space around the nucleus.



Orbitals as Probabilities

- So how do we calculate the probability of finding an electron at a given position in an atom?

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$$H\psi = E\psi$$

The Schrodinger Equation (aka the King of all Equations)

Orbitals as Probabilities

- So how do we calculate the probability of finding an electron at a given position in an atom?

$$H\psi = E\psi$$

$$\sum_i \left(-\frac{h^2}{8\pi^2 m_e}\nabla_i^2 - \sum_j \frac{kq_e^2}{r_{ij}} + \sum_n \frac{kq_e^2}{r_{in}} \right)\psi(r) = E\psi(r)$$

The Schrodinger Equation

Mini Quiz

- Solve for ψ(r).

$$\sum_i \left(-\frac{h^2}{8\pi^2 m_e} \nabla_i^2 - \sum_j \frac{k q_e^2}{r_{ij}} + \sum_n \frac{k q_e^2}{r_{in}} \right) \psi(r) = E \psi(r)$$

Mini Quiz

- A little help …

$$\sum_i \left(-\frac{h^2}{8\pi^2 m_e} \nabla_i^2 - \sum_j \frac{kq_e^2}{r_{ij}} + \sum_n \frac{kq_e^2}{r_{in}} \right) \psi(r) = E\psi(r)$$

$$\sum_i \left(-\frac{h^2}{8\pi^2 m_e} \left(\frac{\partial}{\partial x_i}^2 + \frac{\partial}{\partial y_i}^2 + \frac{\partial}{\partial z_i}^2 \right) - \sum_j \frac{kq_e^2}{r_{ij}} + \sum_n \frac{kq_e^2}{r_{in}} \right) \psi(r) = E\psi(r)$$

Mini Quiz

- The hydrogen atom should be easy …

$$-\left(\frac{h^2}{8\pi^2 m_e}\nabla^2 + \frac{kq_e^2}{r}\right)\psi(r) = E\psi(r)$$

Mini Quiz

- The hydrogen atom should be easy …

$$-\left(\frac{h^2}{8\pi^2 m_e}\nabla^2 + \frac{kq_e^2}{r}\right)\psi(r) = E\psi(r)$$

$$\psi_{nlm}(r,\phi,\varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}} e^{-\frac{r}{na_0}} \left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right) \cdot Y_l^m(\phi,\varphi)$$

Laguerre Polynomial

Spherical Harmonic

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Quantum Numbers

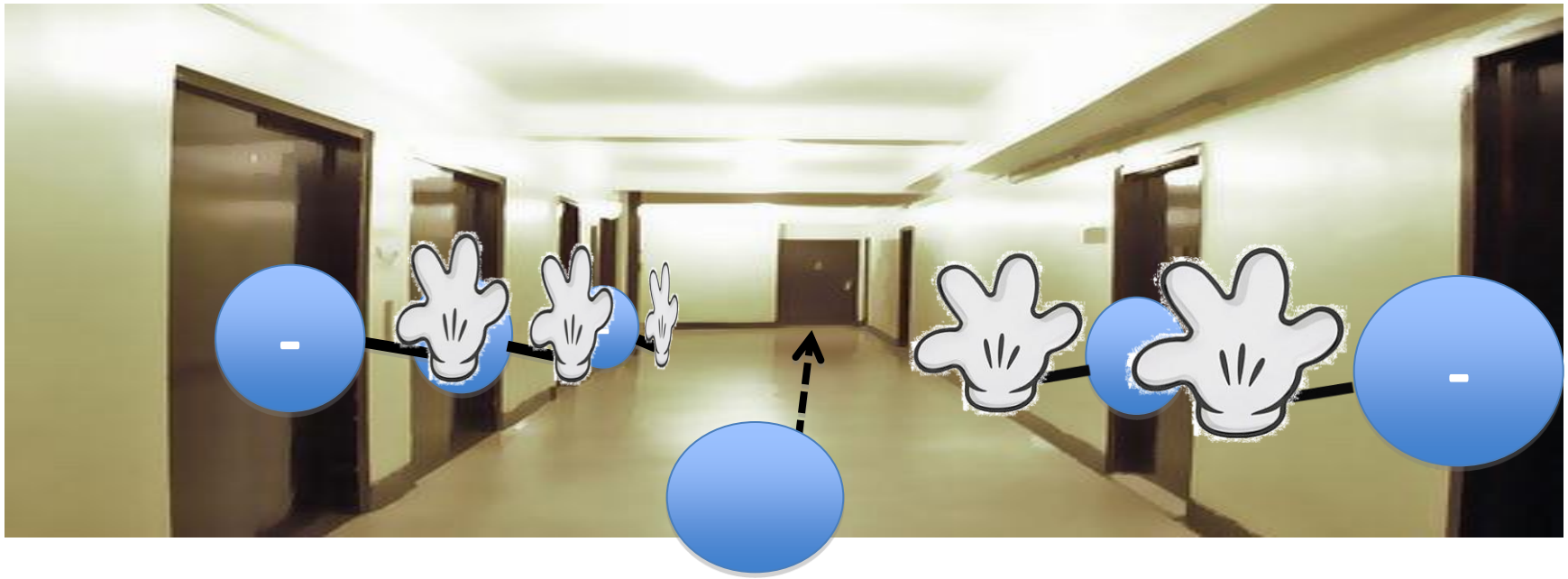
- We call the orbits – ψ(r) – that electrons may occupy around the nucleus **orbitals**
- Electrons can occupy orbitals of **different energies, shapes, and orientations**

$$\psi_{nlm}(r,\phi,\varphi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}} e^{-\frac{r}{na_0}} \left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{2l+1}\left(\frac{2r}{na_0}\right) \cdot Y_l^m(\phi,\varphi)$$

- In most of chemistry (and for this class !), we don't need any crazy math
- A few **quantum numbers** tell us everything we need to know about the orbitals

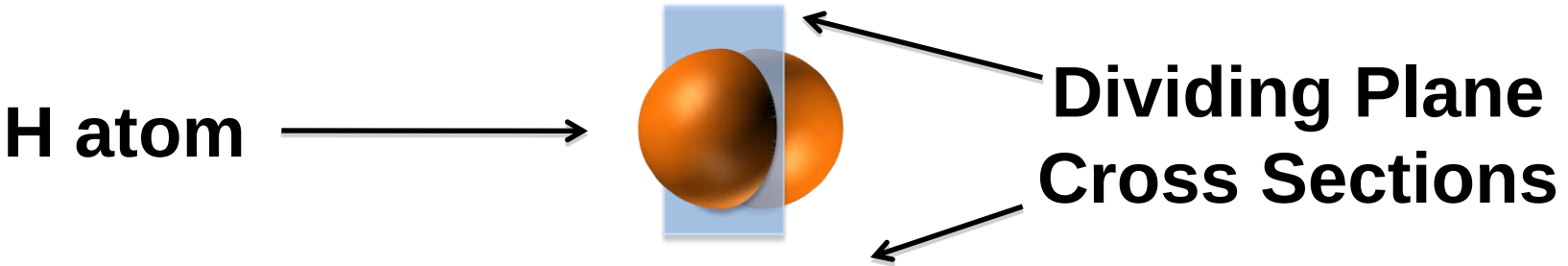
Quantum Numbers

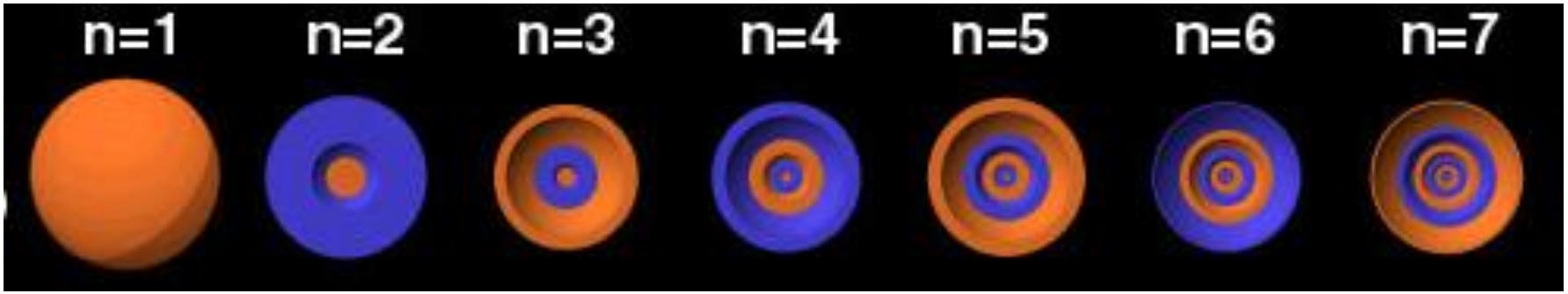
- The **quantum numbers** of an electron are its **address**, telling you exactly which orbital it occupies
- **Pauli Exclusion Principle**: No two electrons in an atom have exactly the same set of quantum numbers



Principle Quantum Number (n)

- Related to the closeness of an electron to the nucleus
- Lower n = higher probability of being closer to the nucleus
- n = 1, 2, 3, 4, …





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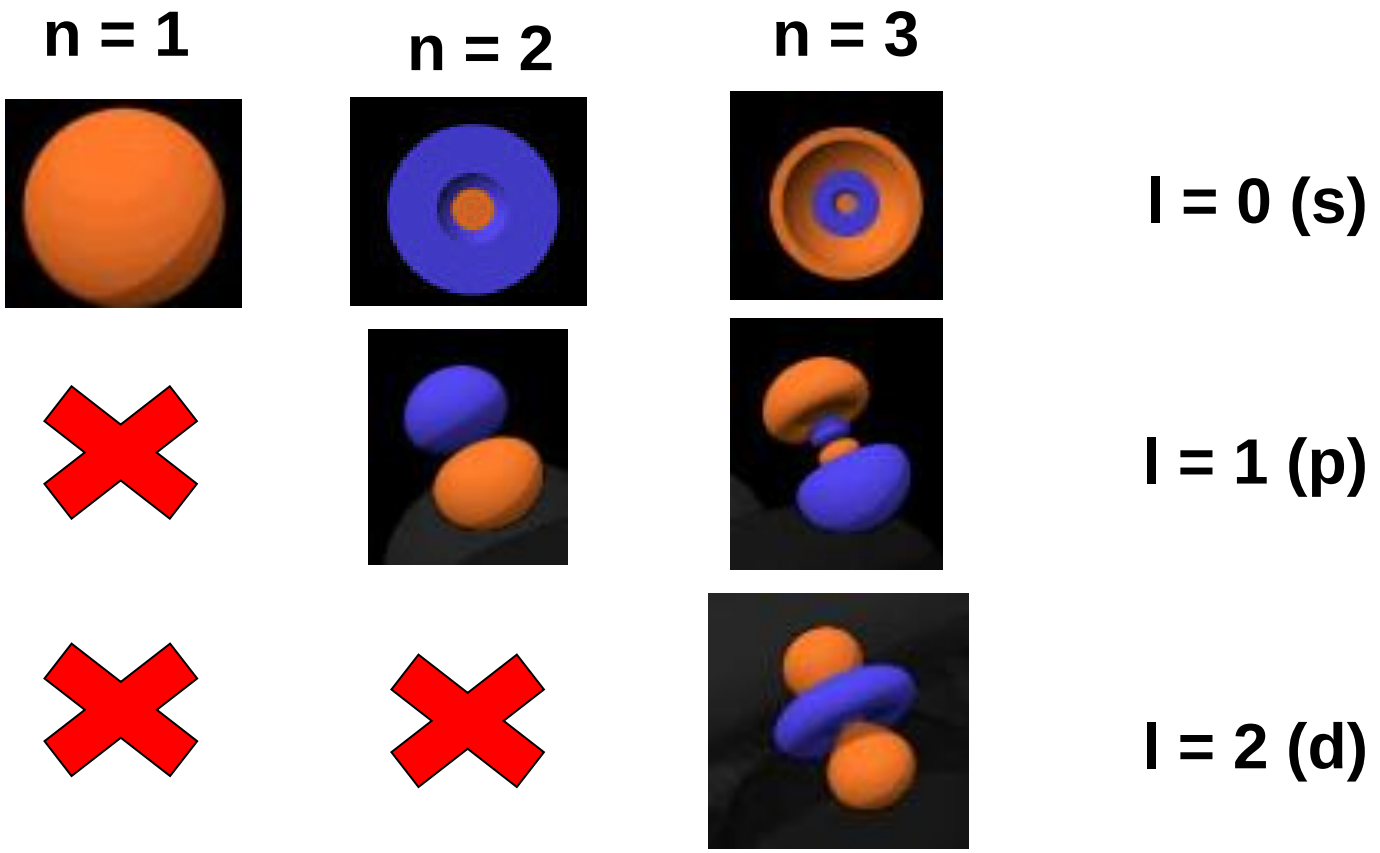
Angular Momentum (l)

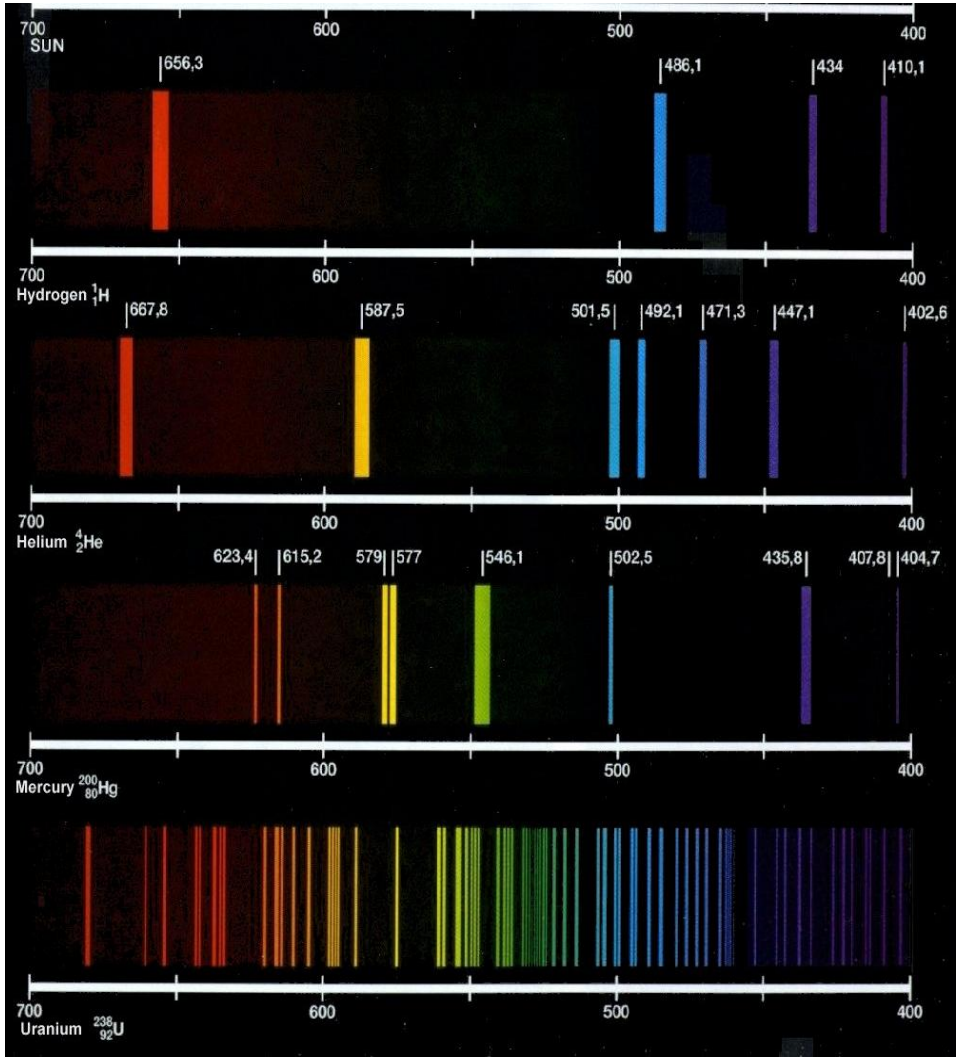
- Related to the shape of an orbital
- For a given n, l = 0, 1, 2, 3, …, (n-1)
- Each l value has a corresponding letter
  - 0 = s, 1 = p, 2 = d, 3 = f, … (don't worry about the others)



Angular Momentum (l)

- Where did the letters – s, p, d, f – come from?

- Described how similar atomic spectra were to hydrogen line spectrum
  - s = ‘sharp’
  - p = ‘principal’
  - d = ‘diffuse’
  - f = ‘fundamental’



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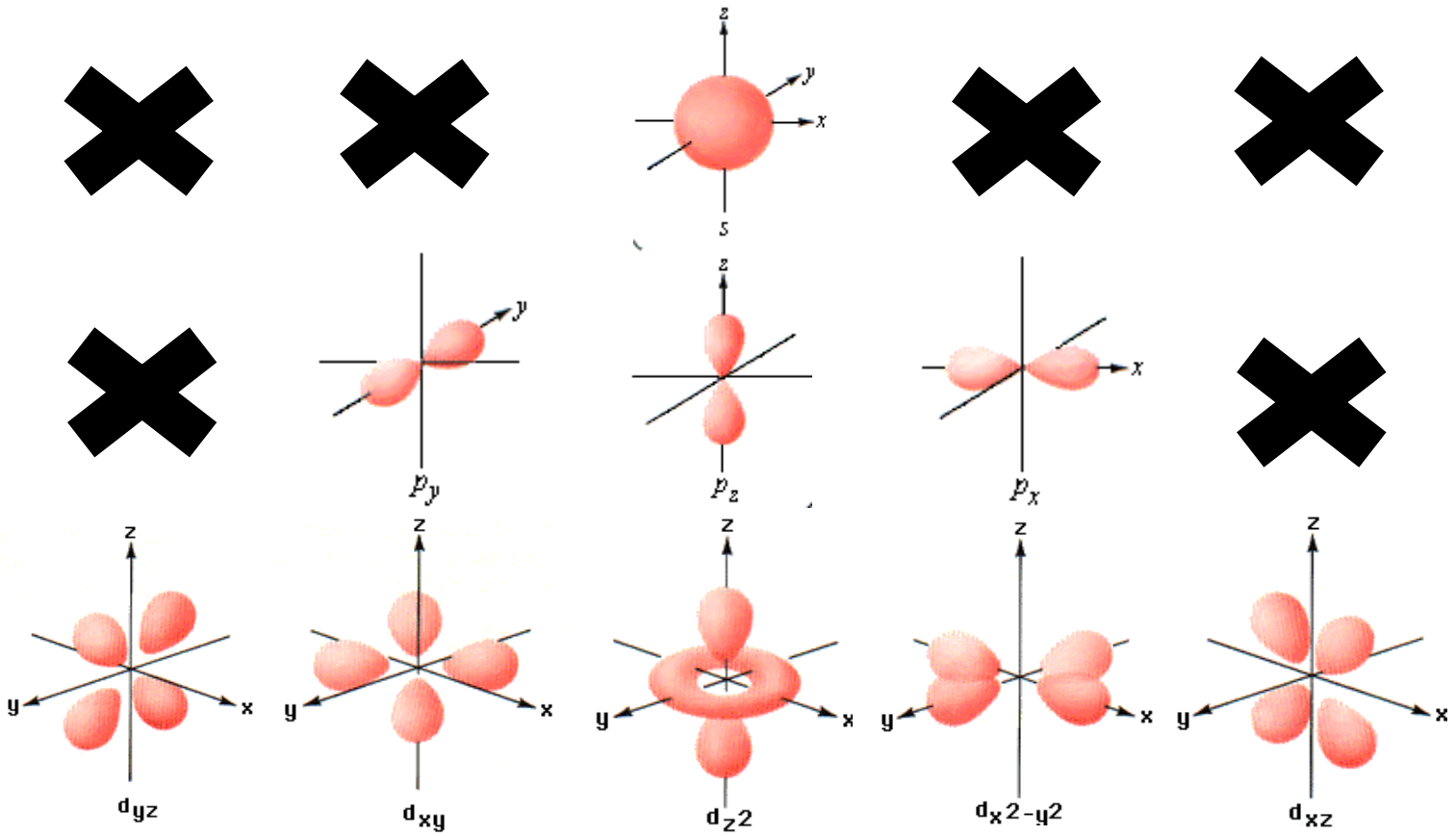
Magnetic (m_l)

- Related to the orientation of an orbital
- For a given l, m_l = -l, 1 – l, 2 – l, … , 0, 1, 2, …, l

l = 0 (s)

l = 1 (p)

l = 2 (d)



m_l = - 2 m_l = - 1 m_l = 0 m_l = 1 m_l = 2

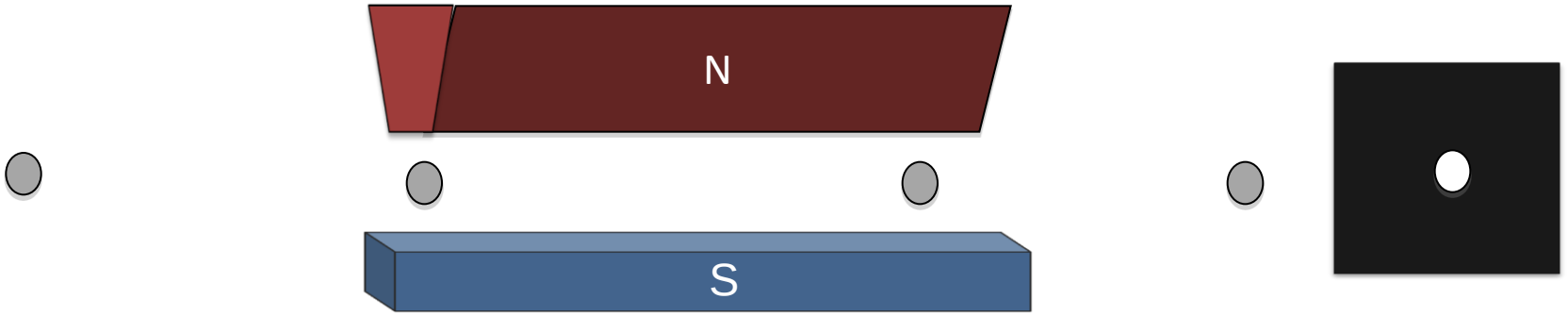
Outline

- Wave-Particle Duality
- Quantum Numbers

- Wave-Particle Duality
  - Light Particles vs Electron Waves
  - Uncertainty Principle
  - Orbitals as Probabilities
- Quantum Numbers
  - Principal, n
  - Angular Momentum, l
  - Magnetic, m_l
  - Spin, m_s

Stern-Gerlach Experiment

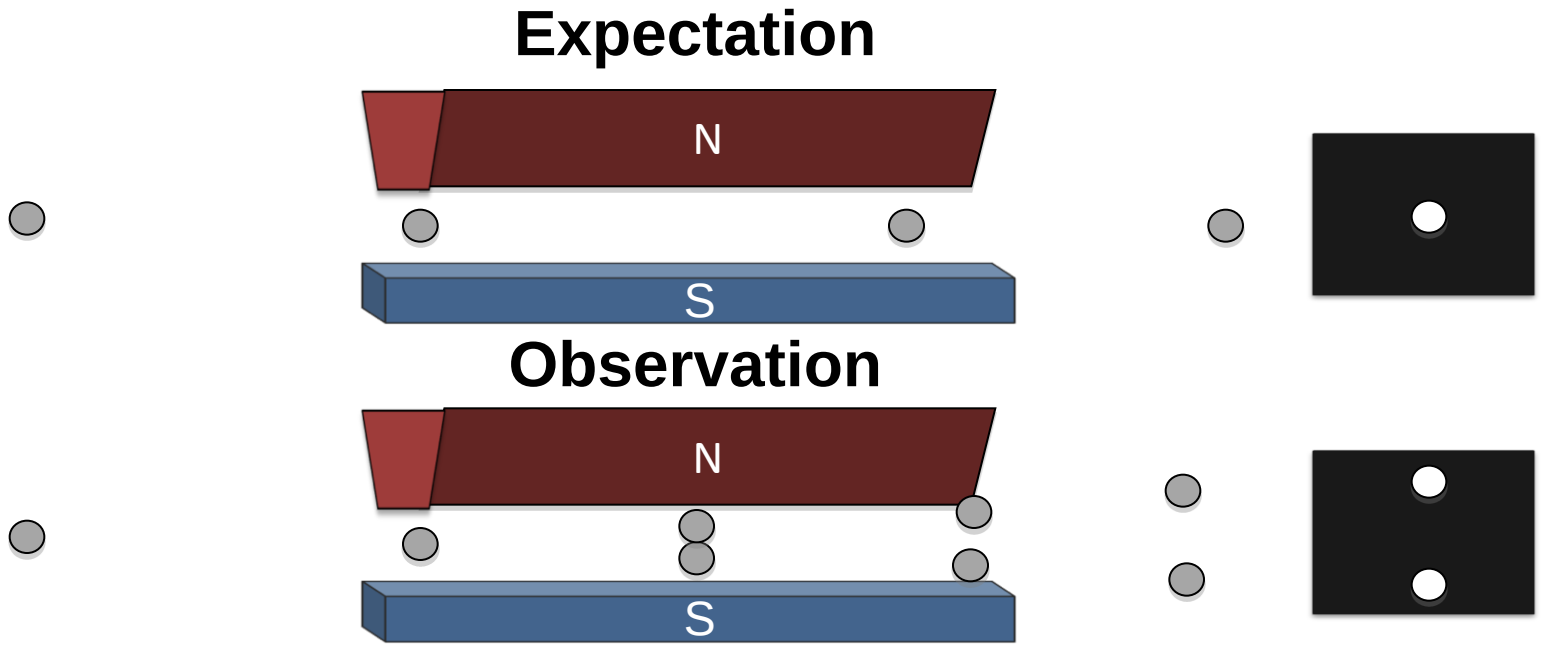
- Shot a beam of silver atoms through a magnetic field
- Watched the pattern formed when the silver atoms hit a photographic plate



- **Important**: Silver atoms can be thought of as single electrons **with spin** but **without charge** – we'll find out why next class

Stern-Gerlach Experiment

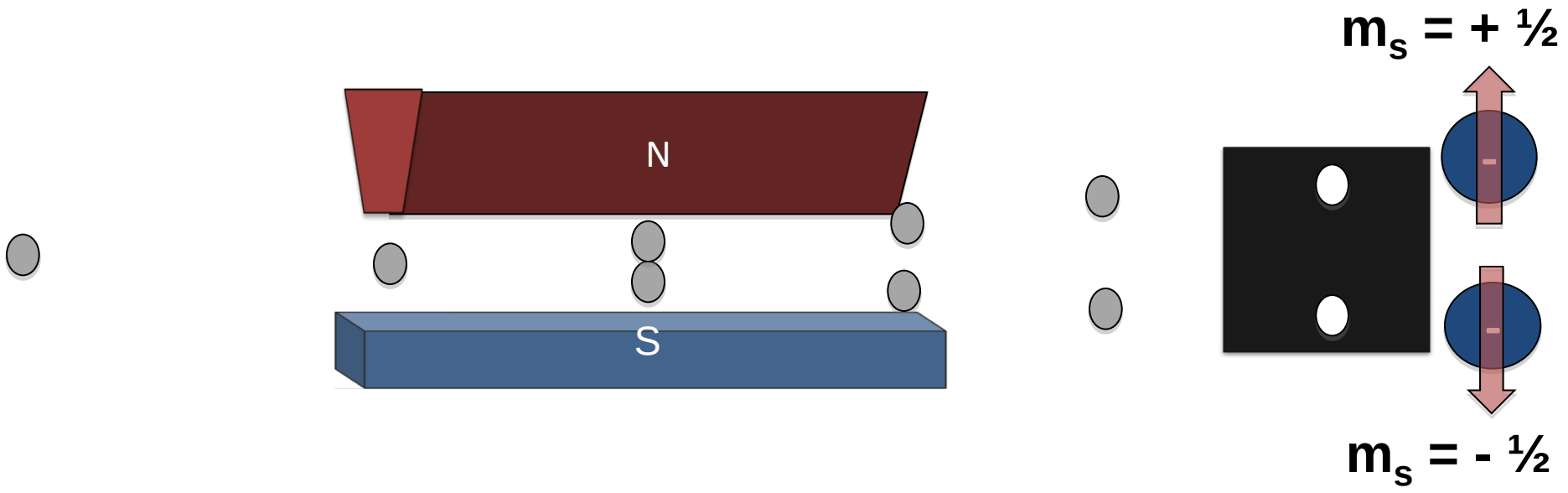
- Classically, we would expect silver particles to travel straight through magnets (one photographic spot)
- Instead, we observe two spots, indicating electrons take one of two paths



- Electrons must have a property **not observed** in macroscopic objects!

Spin (m_s)

- Related to the behavior of an electron in a magnetic field
- m_s= + ½ or -½
- Value does not depend on other quantum numbers



- Electron is **NOT** spinning!
- **Spin** is purely **quantum mechanical** – macroscopic objects do NOT possess it

Mini-Quiz

- Consider two electrons, one in an orbital with n = 3 and one in an orbital with n = 5.

- Which electron has a higher probability of being found close to the nucleus?

- What are the possible values of l for each electron?

- What are the possible values of m_l?

- What are the possible values of m_s?

- If one electron is in a p orbital, what is its l value? What does this tell you about the orbital that electron is in?

Summary

- Light and matter have both wave and particle characteristics
- Electron orbitals show the probability of finding an electron near the nucleus

Quantum Number	Principal	Angular Momentum	Magnetic	Spin
Symbol	n	l	m_l	m_s
Values	1,2,3, …	0,1,2, … (n-1)	-l, 1-l, …, l-1, l	+½, -½
Related To	Distance from Nucleus	Orbital Shape	Orbital Orientation	Magnetic Behavior

Homework

- Handout on Electrons in Atoms (Due Friday)