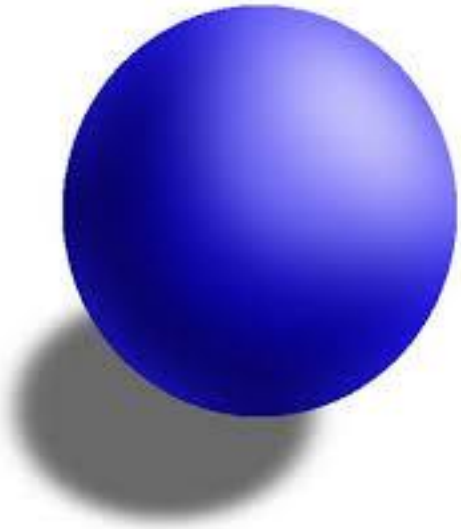
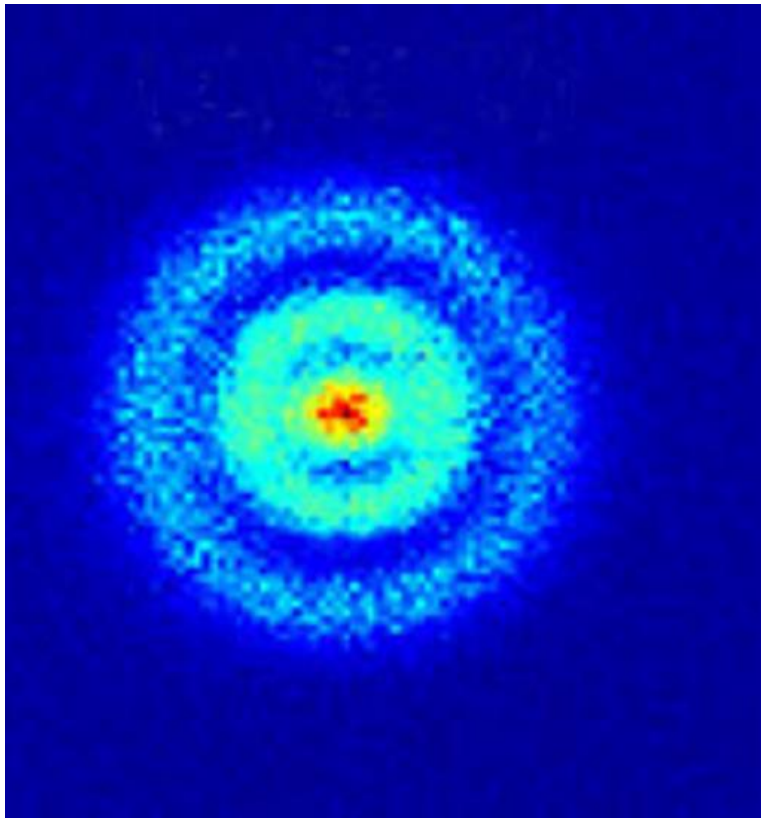
Chapter 6
Electronic Structure of Atoms

How do We get From Here….. To here





Dalton, indivisible

Schroedinger/Heisenberg
Quantum mechanical object

The shortest history of science ever

Experiments.

Atomic spectra

- Bunsen, Kirchhoff, 1860
  - 1st spectroscope
  - 1st line spectrum
- Lockyer, 1868
  - He in solar system
- Balmer,1885
  - H line spectrum

Theory

Quantum/em theory

- Maxwell, 1861
  - Relate Electricity and magnetism
- Plank,1900
  - Black body radiation
- Einstein, 1905
  - Photoelectric effect
- Bohr, 1913
  - Applied to atom structure

More experiments

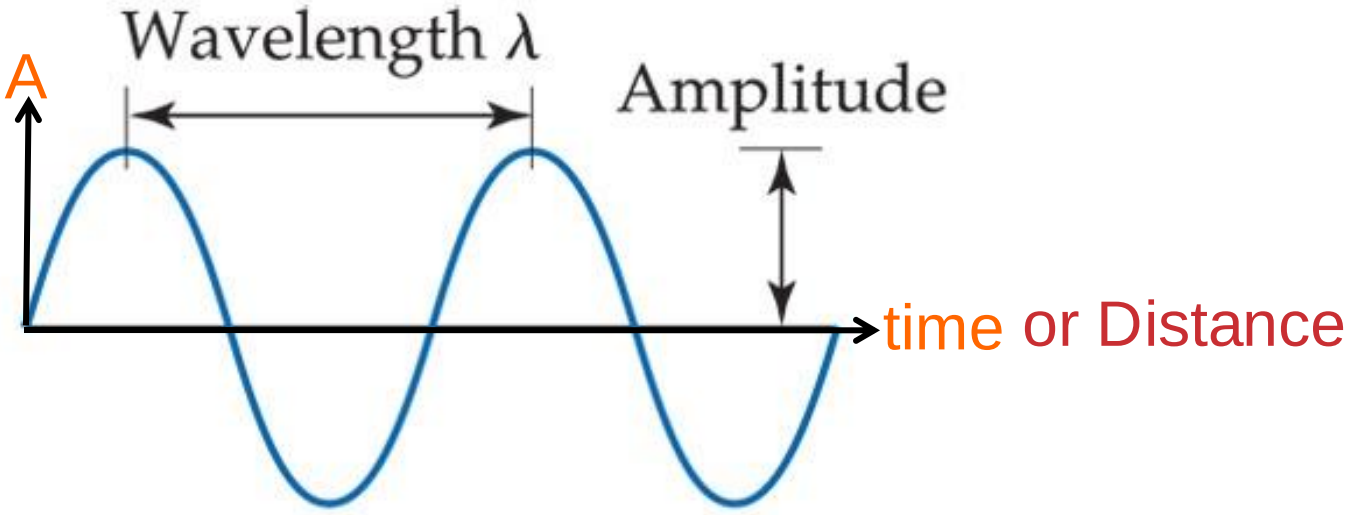
Atomic structure

- Dalton, 1803
  - atomic nature
- Faraday, 1834
  - Electricity & Mag.
- Thompson, 1897
  - electrons e/m
- Millikan, 1911
  - oil drop
- Rutherford, 1911
  - gold foil/nucleus

Electro-magnetic radiation (light)

- Light is a wave
  - The nature of waves
    - What is a wave?
    - What is waving?

Waves

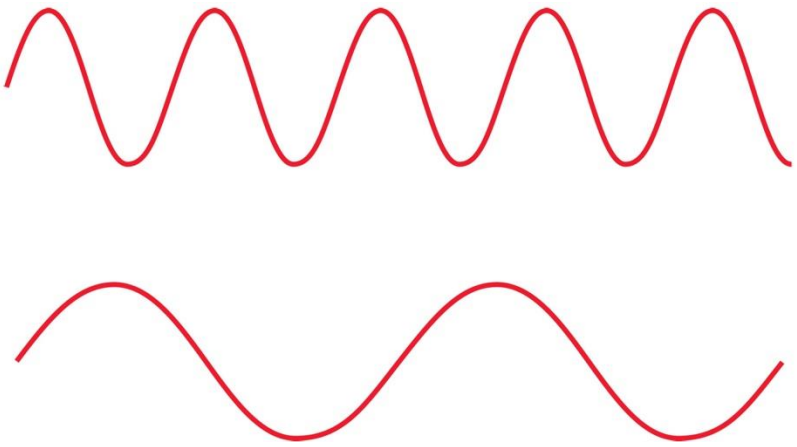


- Wave: some sort of periodic function
  - ➢ something that periodically changes vs. time.
- wavelength (λ): distance between equivalent points
- **Amplitude:** "height" of wave, maximum displacement of periodic function.

Waves

Higher frequency

shorter wavelength

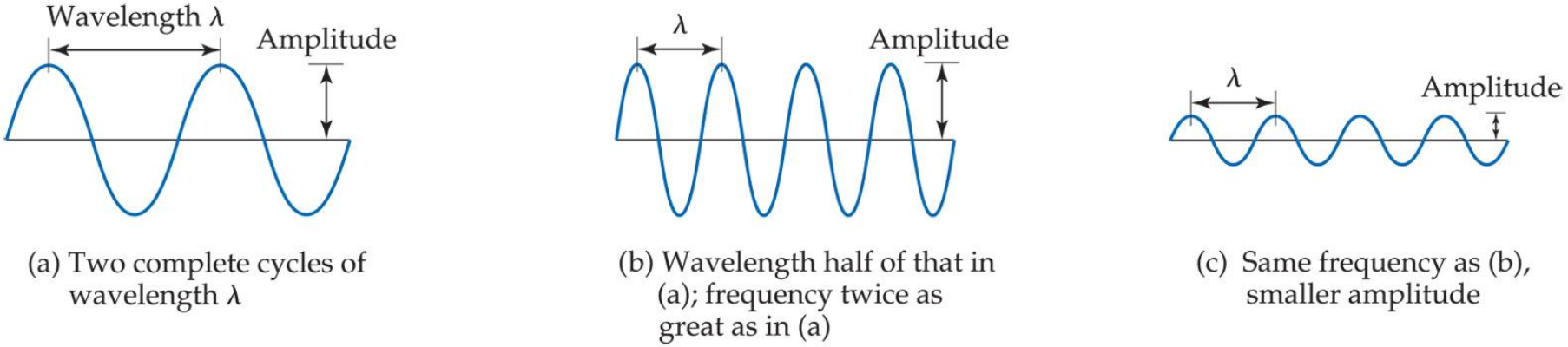


lower frequency

longer wavelength

- The number of waves passing a given point per unit of time is the frequency (ν).
- For waves traveling at the same velocity, the longer the wavelength, the smaller the frequency.

Waves



(a) Two complete cycles of wavelength λ

(b) Wavelength half of that in (a); frequency twice as great as in (a)

(c) Same frequency as (b), smaller amplitude

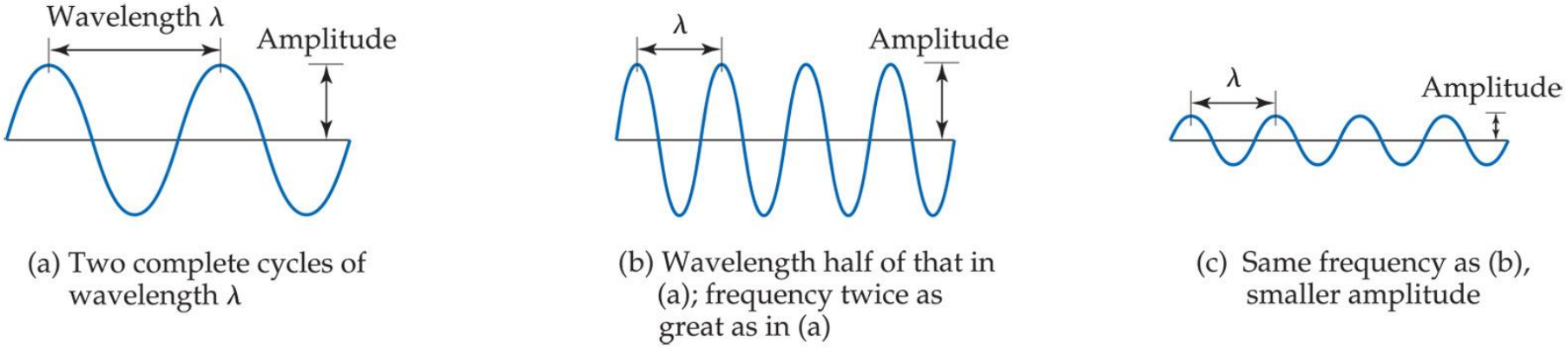
For any wave:

v = wavelength x frequency

meters x (1/sec) = m/sec

$$\mathbf{v = \lambda\nu}$$

Waves



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For any wave:

v = wavelength x frequency

meters x (1/sec) = m/sec

$$v = \lambda\nu$$

What is the velocity if the wavelength is 2 m and the frequency is 20 sec^{-1} (m/sec)?

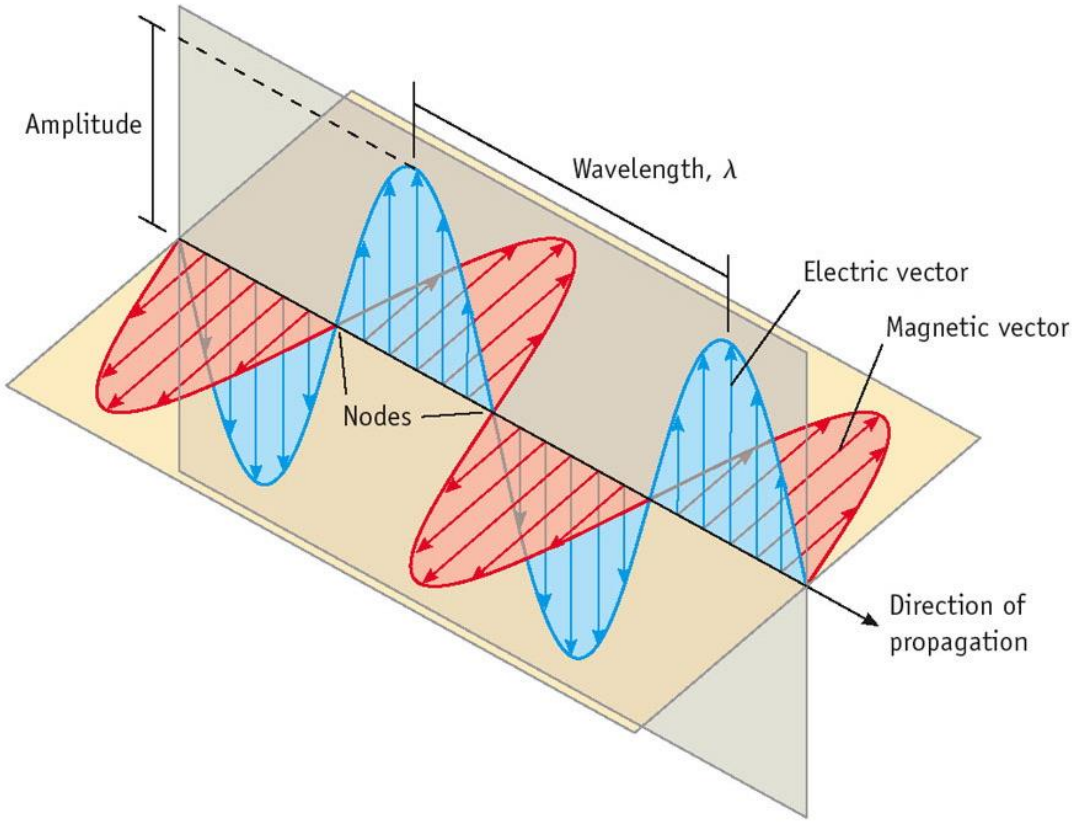
A. 2
B. 10
C. 20
D. 40

Waves

Major question:

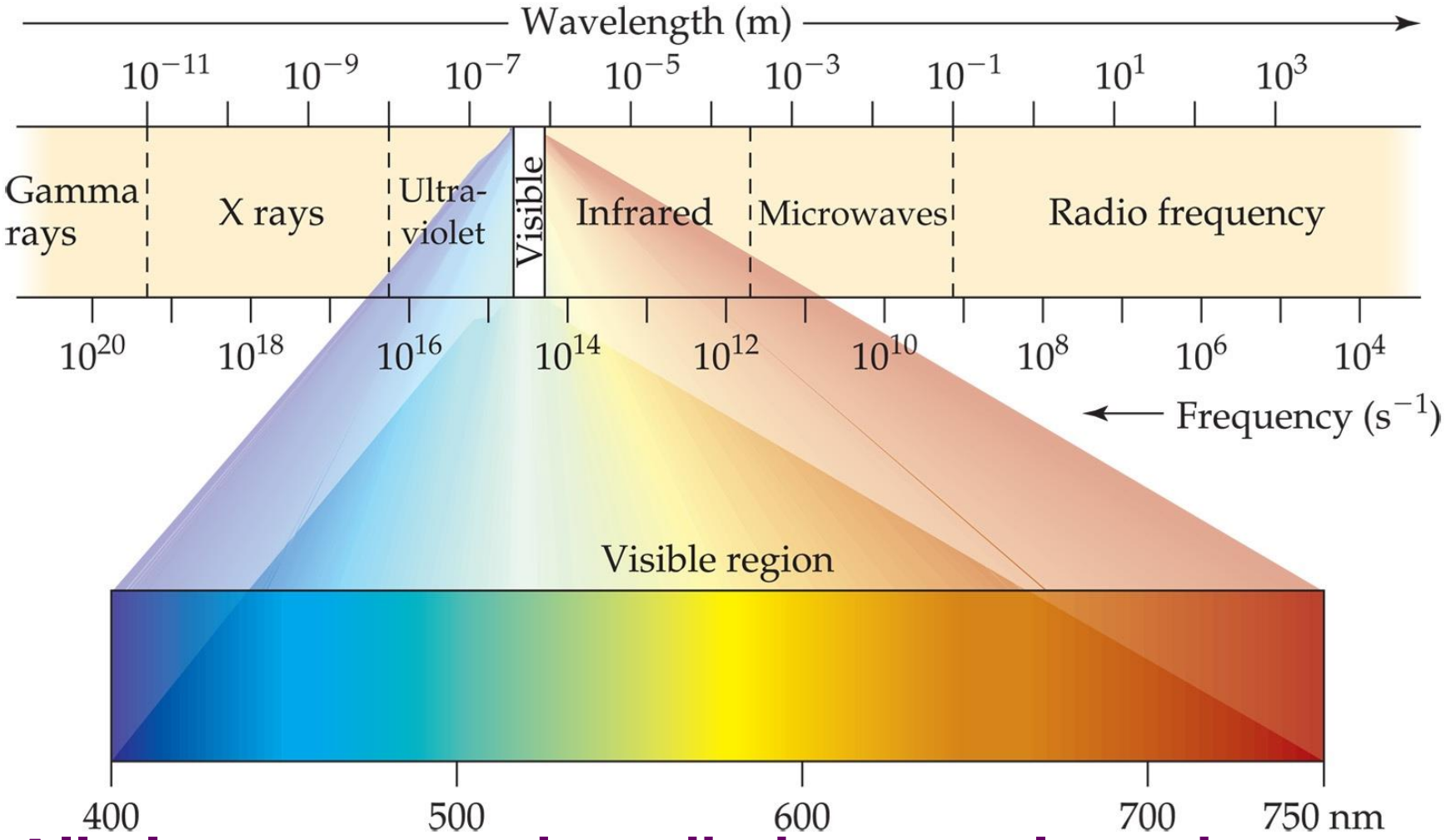
- What is waving?
- water wave:
  - water height(pressure)
- Sound wave:
  - air pressure
- Light?

Light waves.



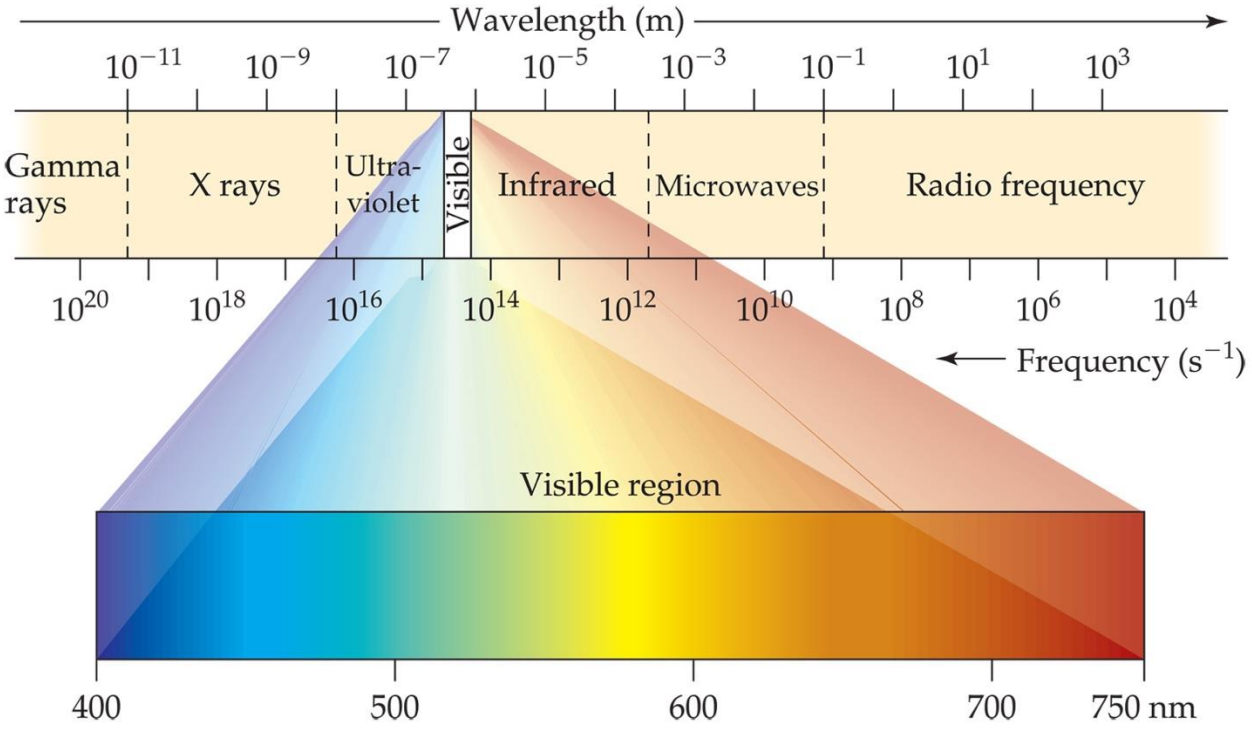
- What is waving? Electric field, and perpendicular magnetic field.
- Faraday thought this, Maxwell proved it (1865).

Electromagnetic Radiation



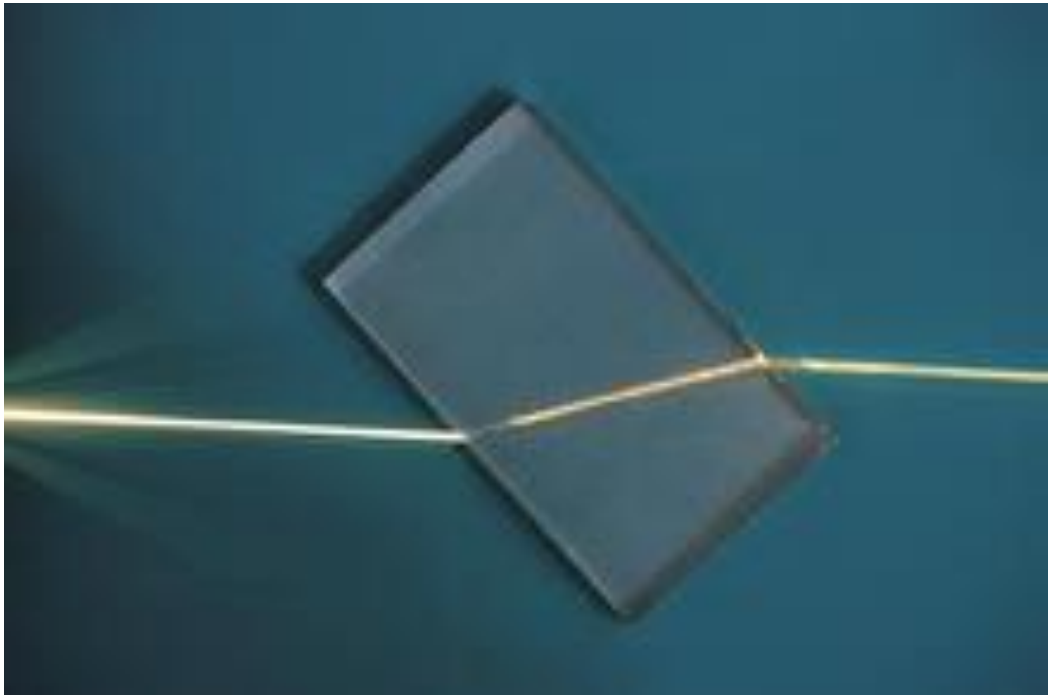
- **All electromagnetic radiation travels at the speed of light (*c*), 3.00 × 10⁸ m/s (in a vacuum).**
- **Therefore:** $c = \lambda\nu$

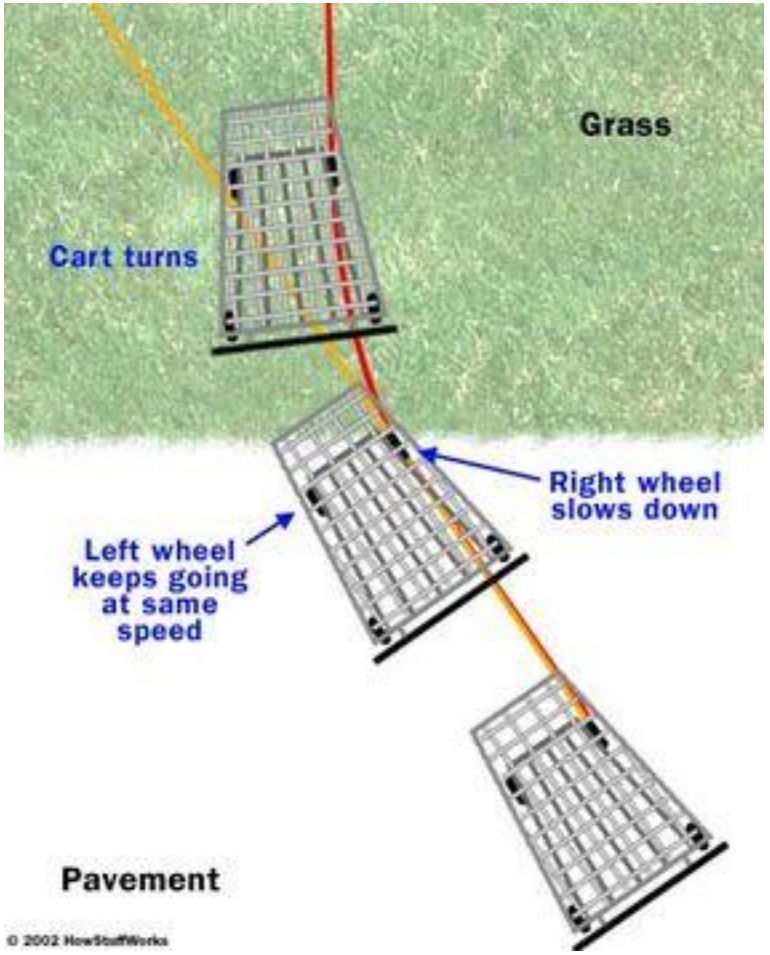
Electromagnetic Radiation



- **Which radiation moves the fastest?**
  - **A. Infrared**
  - **B. Radio**
  - **C. Ultraviolet**
  - **D. None (all equal)**

Electromagnetic Radiation





- **All electromagnetic radiation travels the speed of light (*c*), 3.00 × 10⁸ m/s (in a vacuum).**
- **Therefore:** $c = \lambda\nu$
- ***But not in other media.***

This causes the light to ***bend*** when it travels from one medium to another

Speed of light in other materials

Index of refraction is: **n = c/v**

The speed of light is only a constant in a vacuum.

The index of refraction of some common materials are given below.

material	n	material	n
Vacuum	1	Grown Glass	1.52
Air	1.0003	Salt	1.54
Water	1.33	Asphalt	1.635
Ethyl Alcohol	1.36	Heavy Flint Glass	1.65
Fused Quartz	1.4585	Diamond	2.42
Whale Oil	1.460	Lead	2.6

Values of n come from the CRC Handbook of Chemistry and Physics

The major issue of late 19th century physics

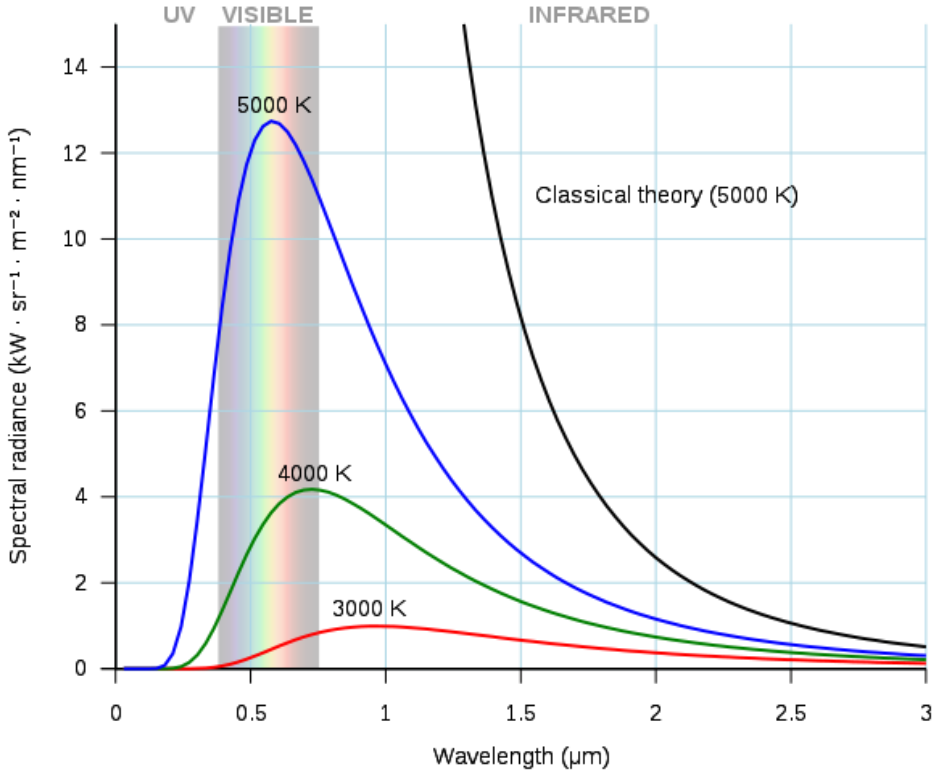
- What is light?
- What is the relationship between light and energy?
- How does light interact with **matter**?

The three mysteries of 19th century physics

Mystery #1: Blackbody radiation

- **Why does metal glow when heated?**
- ***Heating*, so K.E.**
- **What light is given off?**

Black Body Radiation



Spectral output of a black body.

Black shows that predicted from classical electricity & magnetism

Colored curves are what you actually get.

Light is **emitted** when **atoms vibrate** (or oscillate). But the K.E. at higher :

Expect atoms moving at **higher frequency, shorter wavelength**

The ultraviolet catastrophe!

Something is wrong.

Mystery 1: Black body radiation

- Higher T leads to shorter wavelength of light
- More K.E., more E
- **But not short enough!**
- Doesn't fit K.E. prediction.
- Plank concluded that light energy is ***quantized.*** *It comes in packets (like fruit snacks) and is* proportional to frequency:

$$E = h\nu$$

where *h* is Planck's constant, 6.63×10^{-34} J-s. The *minimum packet* of E.

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Which light has higher Energy?

A. Light with higher frequency
B. Light with lower frequency
C. Light with longer wavelength?
D. They all have the same energy

What did Einstein get the Nobel Prize for?

What did Einstein get the Nobel Prize for?

The photoelectric effect.

What is the photoelectric effect?

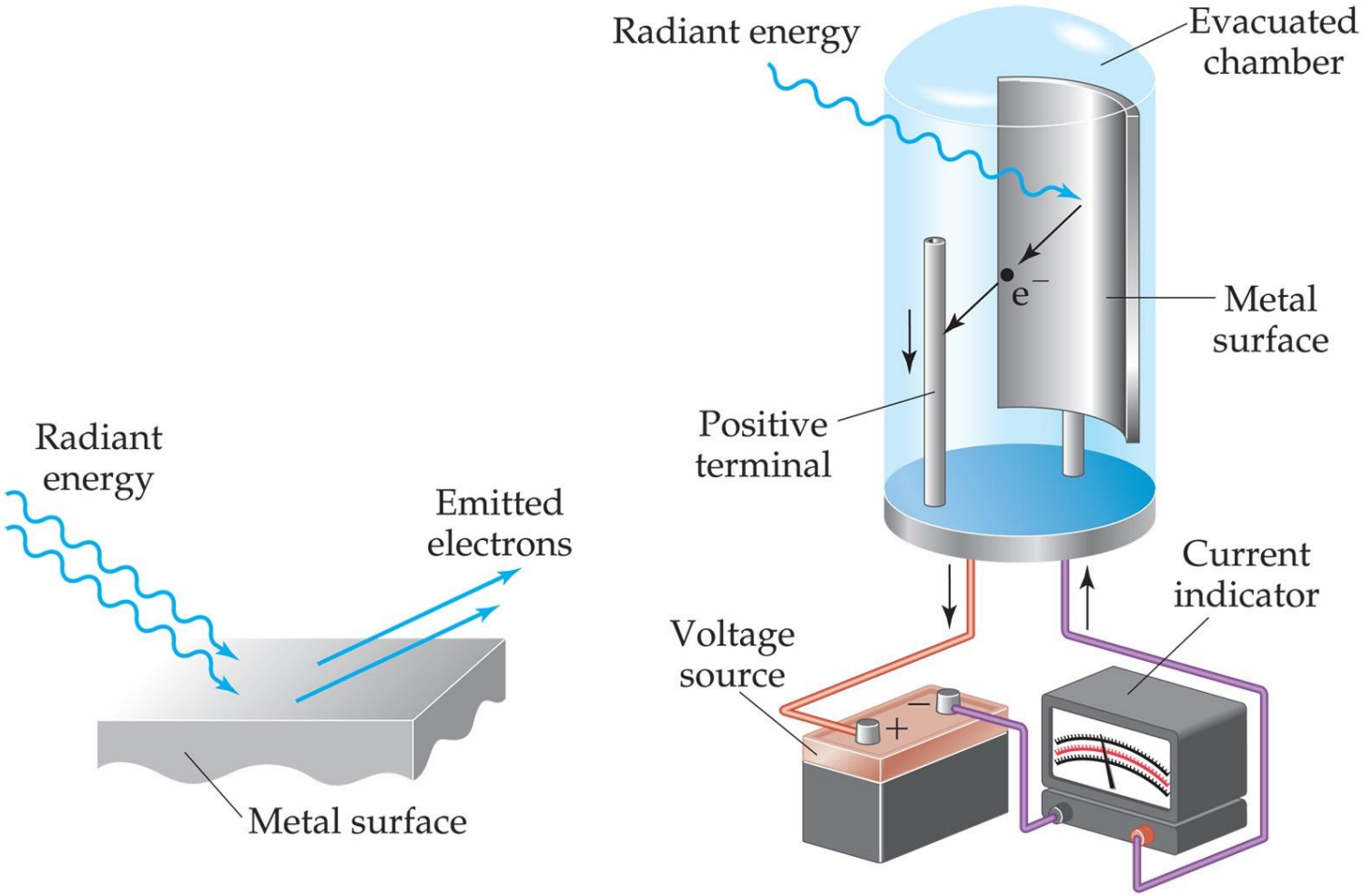
A. Electricity used in photography

B. Absorption of electrons upon light irradiation

C. Emission of electrons upon light irradiation.

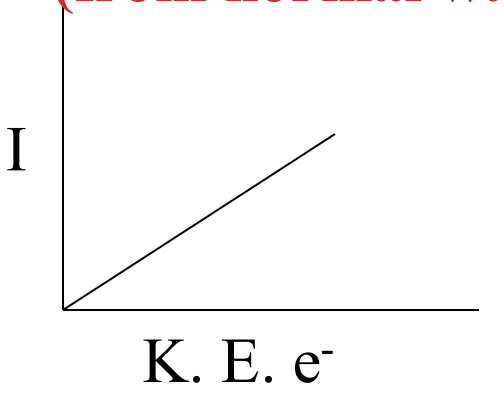
D. Emission of light upon electron irradiation.

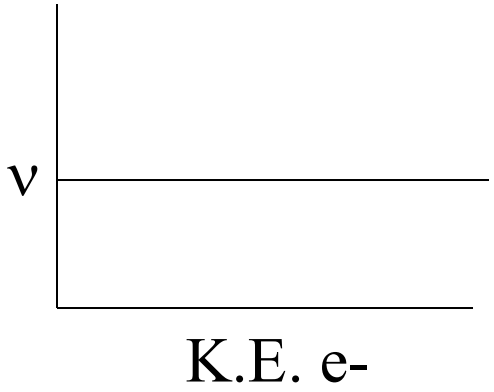
Mystery #2: The Photo-electric effect



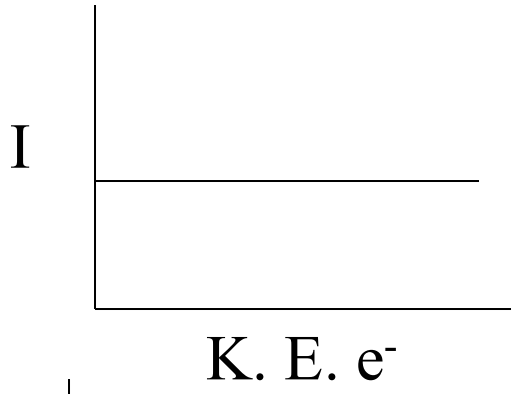
Note, this is what a photocell does
Turn light into work (current)

What you might expect (from normal waves)

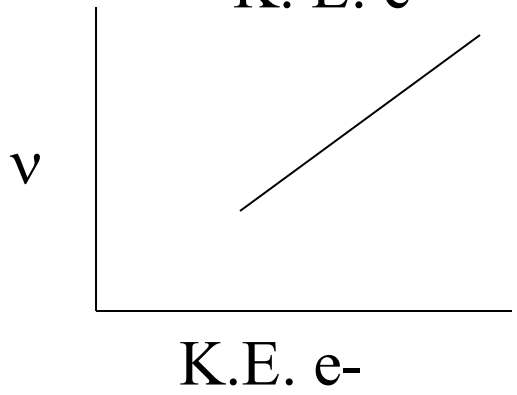


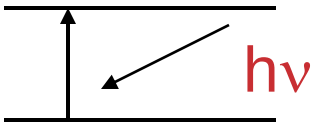


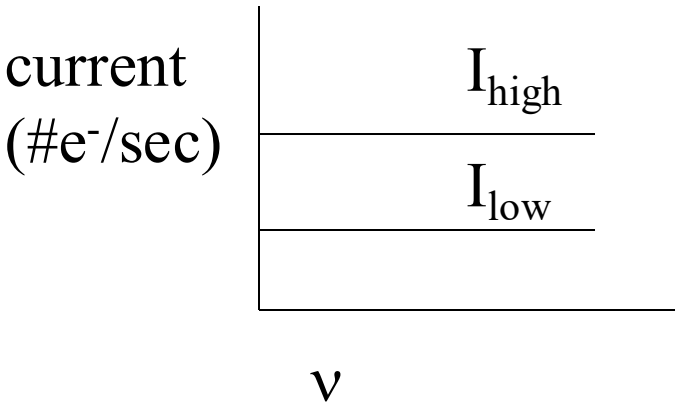
what do you see?

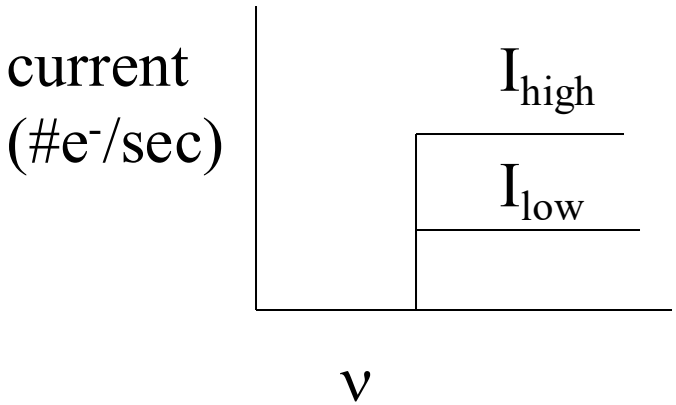


Constant ν









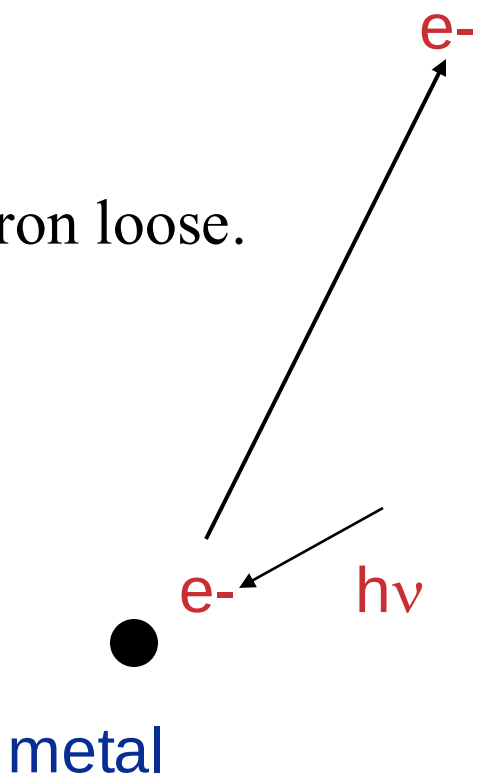
Einstein: Light is both a particle and a wave.

e- K.E. "escape energy"

$$E_{photon} = 1/2 m_e v_e^2 + h\nu_o = E_{electron}$$

Light comes in **packets of energy**.
Each **packet** runs into **one electron**.
Each packet must have enough E to break electron loose.
The rest of the energy goes into kinetic energy.

Frequency tells us the E of each packet.
I tells us how many **packets/second** we get.
More packets, more current (more electrons knocked off).



The Nature of light Energy

- Energy, λ, ν, related:

$$c = \lambda\nu$$

$$E = h\nu$$

c= speed of light in vacuum, constant

The Three great mysteries:

1. Black body radiation

1. $E=h\nu$

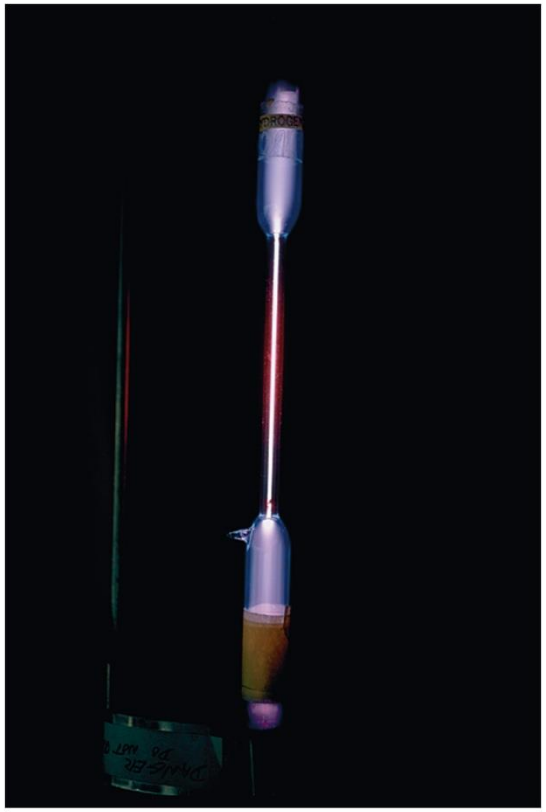
2. The photoelectric effect.

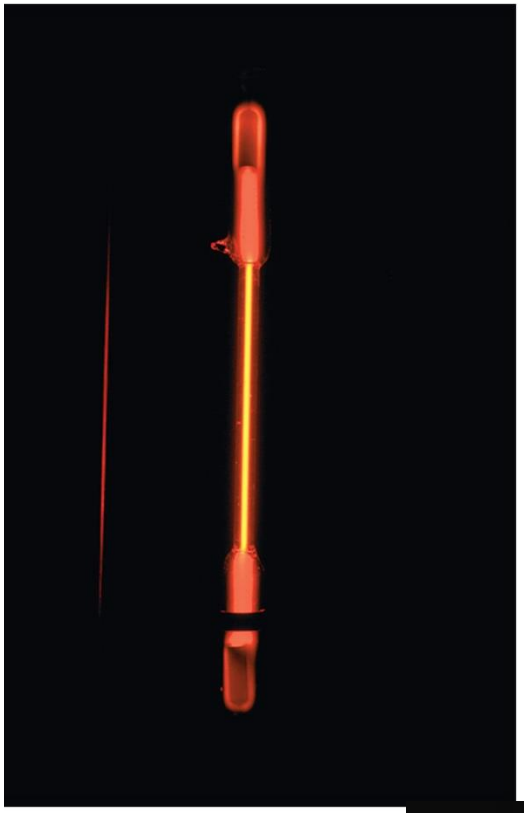
e- K.E. "escape energy"

$$E_{photon} = 1/2mv^2 + h\nu_o = E_{electron}$$

Light acts like a particle AND a wave.

Mystery number 3: element line spectrum Known since 1853-54.

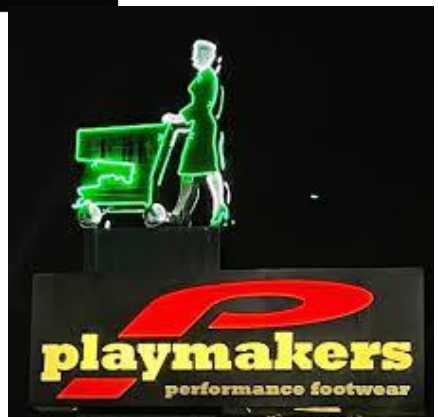




Hydrogen Neon

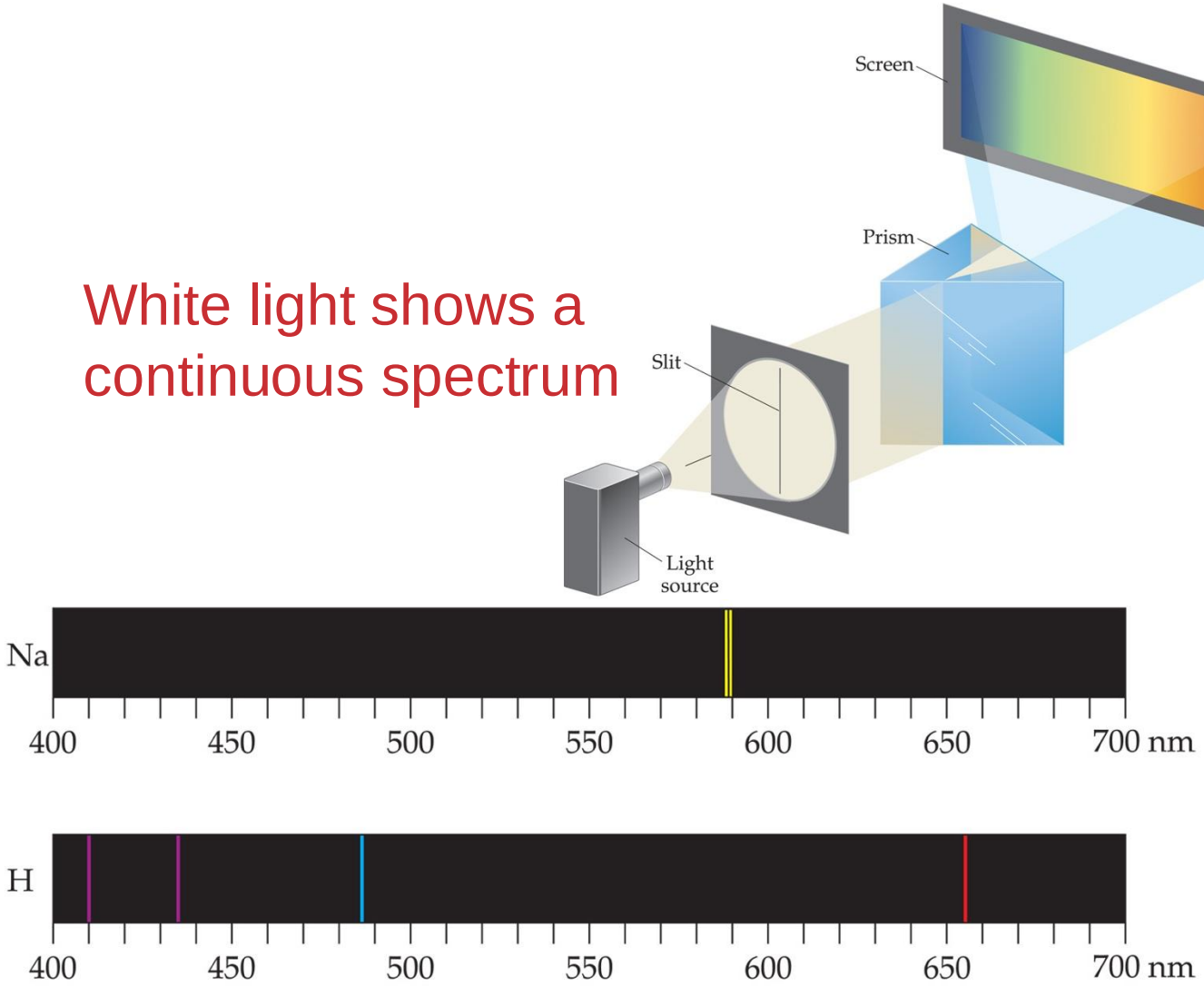
- Gas discharge tube (full of some elemental gas)
- Gives off specific frequencies of light only.
- Different elements give off different colors.
- i.e. *different energies.*

This is all a neon light is.



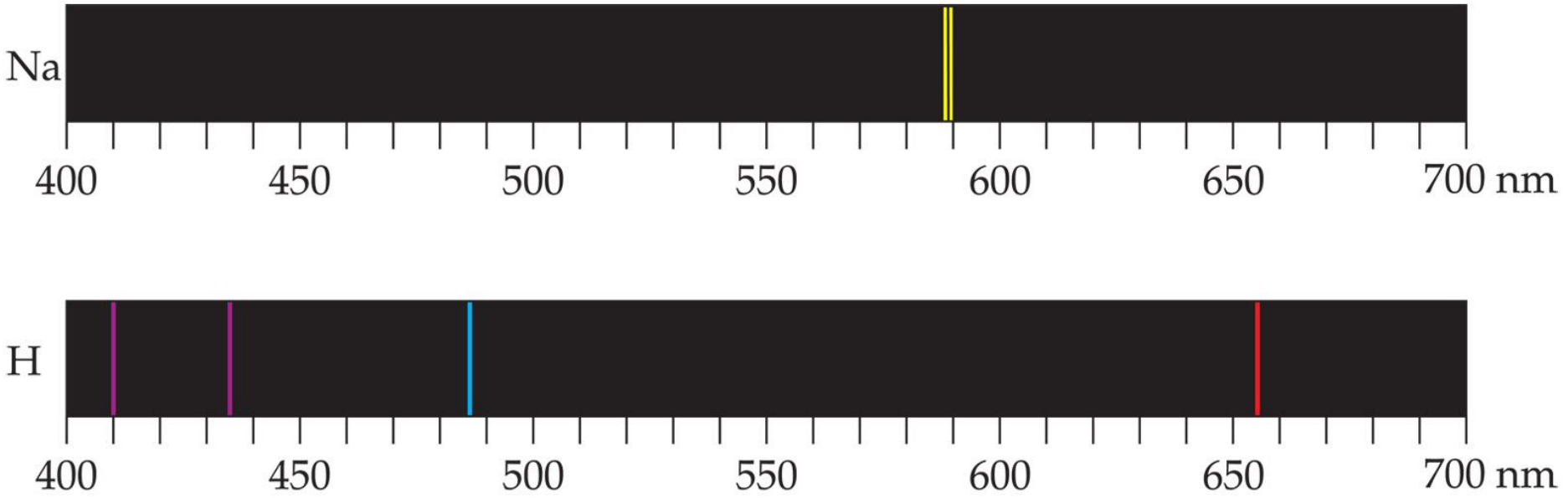
Elemental Line spectra

White light shows a continuous spectrum



- A **line spectrum** of discrete wavelengths is observed from element discharge.

Hydrogen Line spectra



Johann Balmer, School teacher

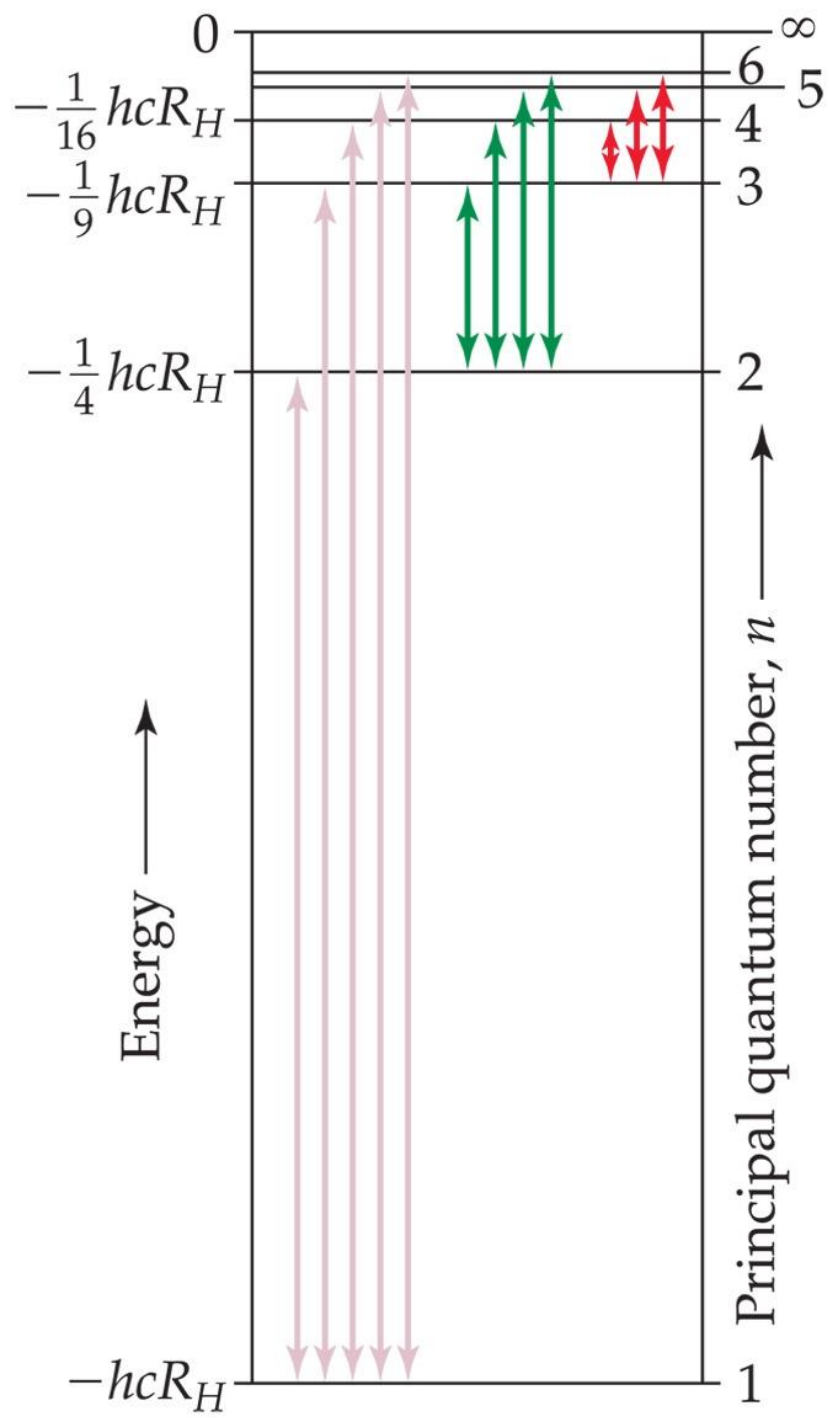
In 1885 figured out that the H lines fit a simple equation:

R_H=constant

n_1 and n_2 are integers

$$\frac{1}{l} = (R_H)\left(\frac{1}{n_1^2} - \frac{1}{n_2^2}\right)$$

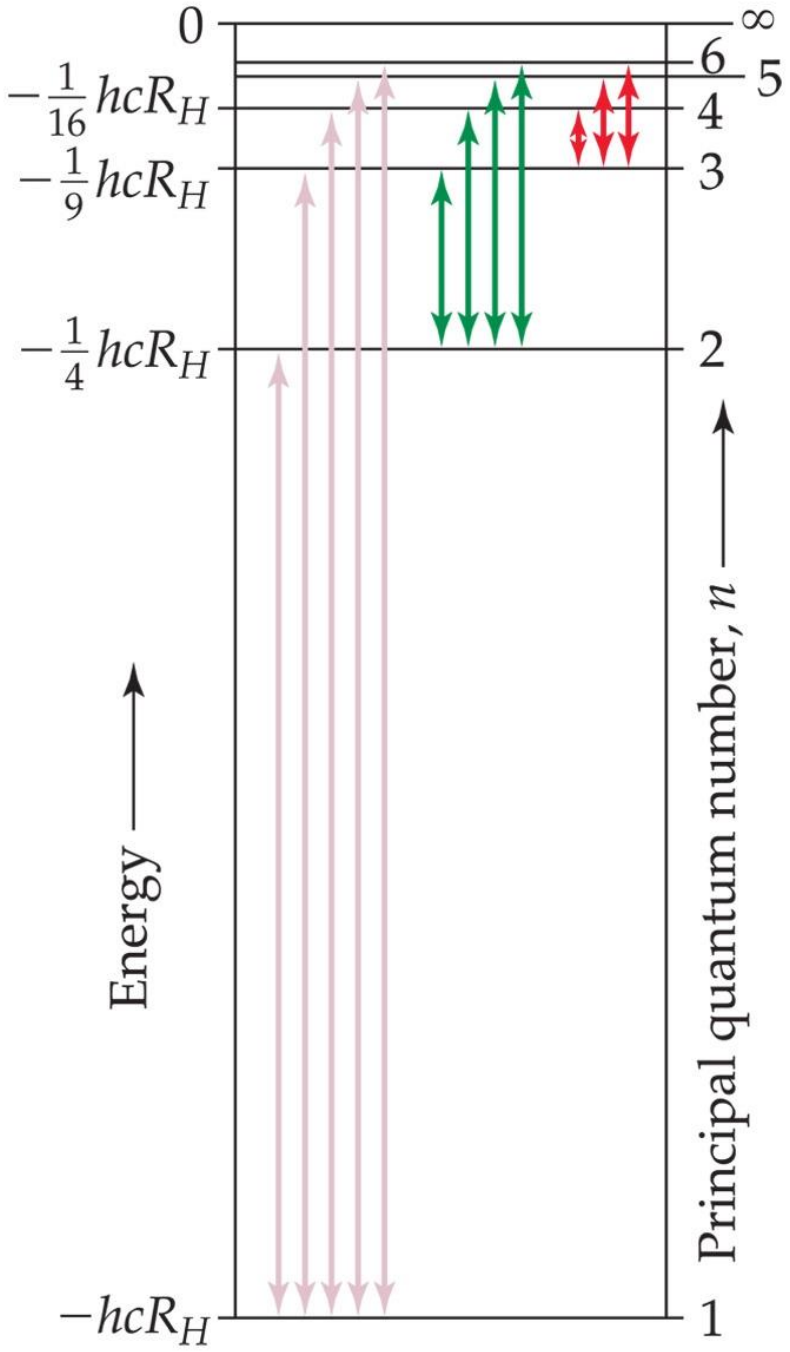
But why?



Light and matter

Niels Bohr adopted Planck's assumption and explained these phenomena in this way:

1. **Electrons in an atom can only occupy certain orbits (corresponding to certain energies).**
    1. **What do we mean by "energy" in this case? *How stuck the e^- is to the atom.***

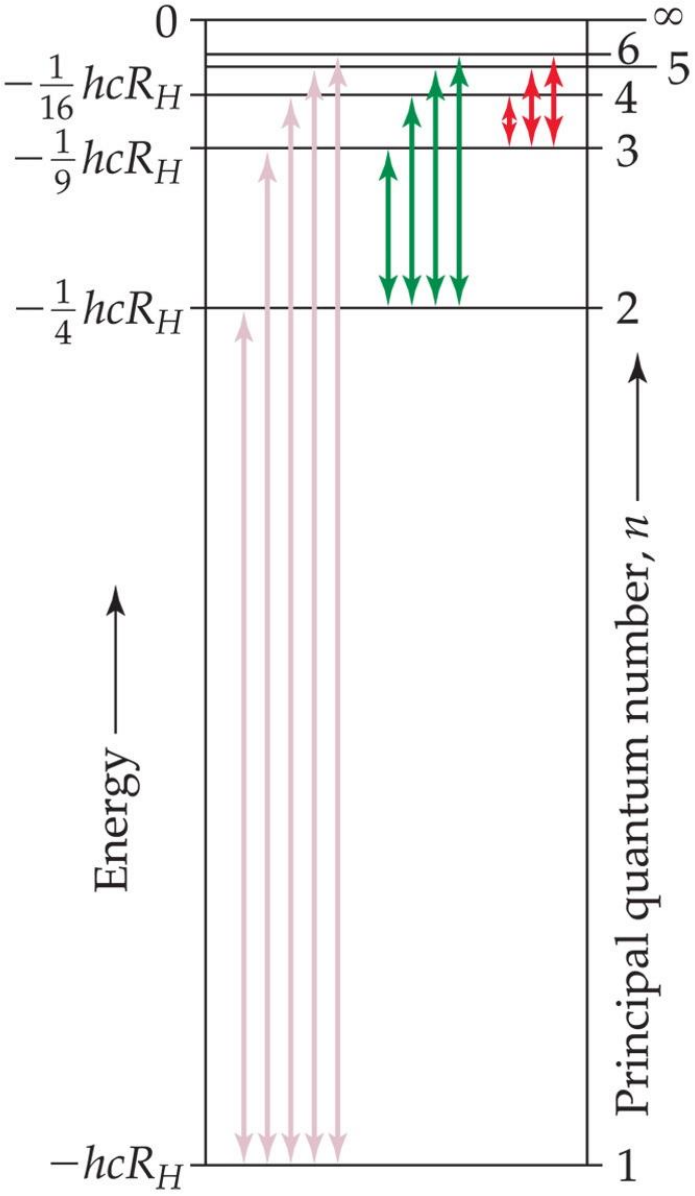


Light and matter

- Niels Bohr adopted Planck's assumption and explained these phenomena in this way:

2. **Electrons in permitted orbits have specific, "allowed" energies;**

Light and matter

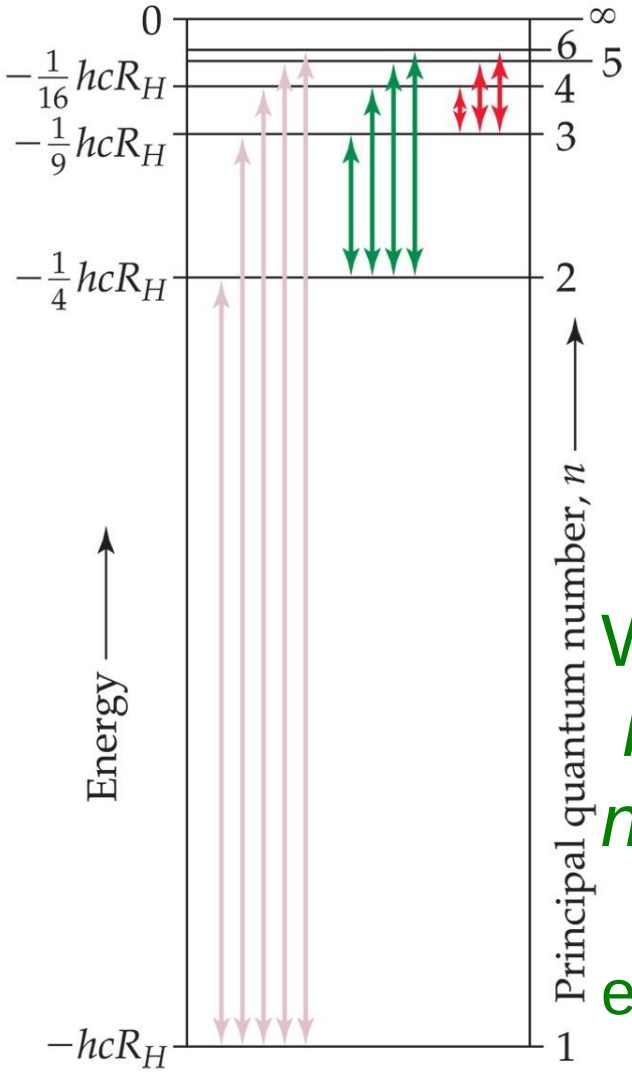


- Niels Bohr adopted Planck's assumption and explained these phenomena in this way:

3. **Energy can only be absorbed or emitted to move an electron from one "allowed" energy state to another; the energy is defined by**

$$E = h\nu$$

Light and matter



The energy absorbed or emitted from electron promotion or demotion can be calculated by the equation:

$$\Delta E = -R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

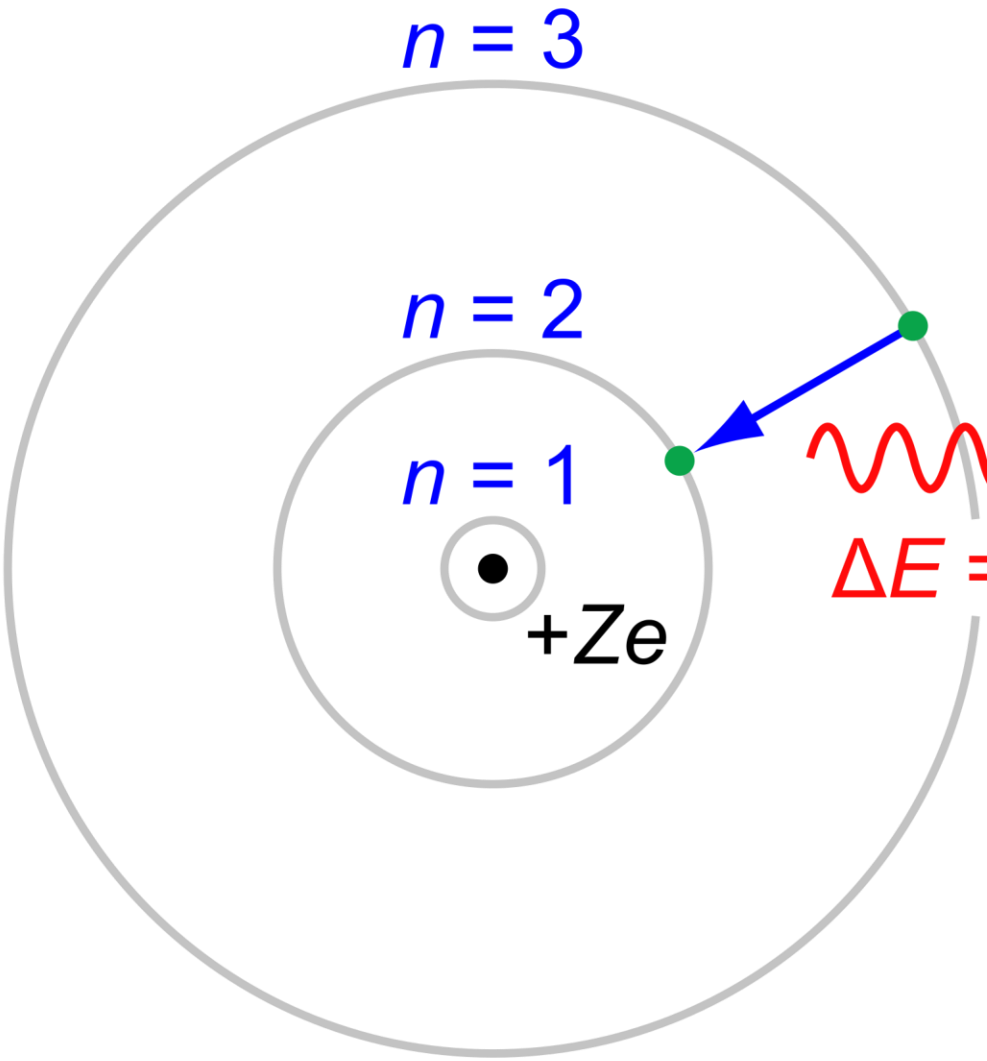
Where:

R_H: Rydberg constant, 2.18×10^{-18} J

n_i and n_f are integers:

initial and final energy level of the electron.

Bohr.



- Using a model that had electrons orbiting the nucleus like planets, Bohr could explain H, but no other elements.

$$\Delta E = -R_H \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

$$R_E = 1/2 mec^2 (k_e e^2/\cancel{h}c)^2$$

The Wave Nature of Matter

- Louis de Broglie, 1924 Ph. D. thesis: if light can be a particle, maybe **matter** can be **wave-like**.

$$Velocity = l\, n$$

$$n = \frac{velocity}{l}$$

like $E=mc^2$

$$E = m(velocity)^2 = hn = h\frac{velocity}{l}$$

$$l = \frac{h}{m(velocity)}$$

Wave-like nature of matter

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

However, the higher the mass, the smaller the wavelength & h=6.63 $\times$ 10^{-34} J-s, is a ***really small*** number.

Example; What is λ for a 1 g ball going 1 meter per second?

$$\lambda = \frac{6.63 \times 10^{-34} \text{kgm}^2/\text{s}}{.001\text{kg}(1\text{m/s})} = 6.63 \times 10^{-31} \text{ m}$$

wavelengths of everyday objects too small to measure.

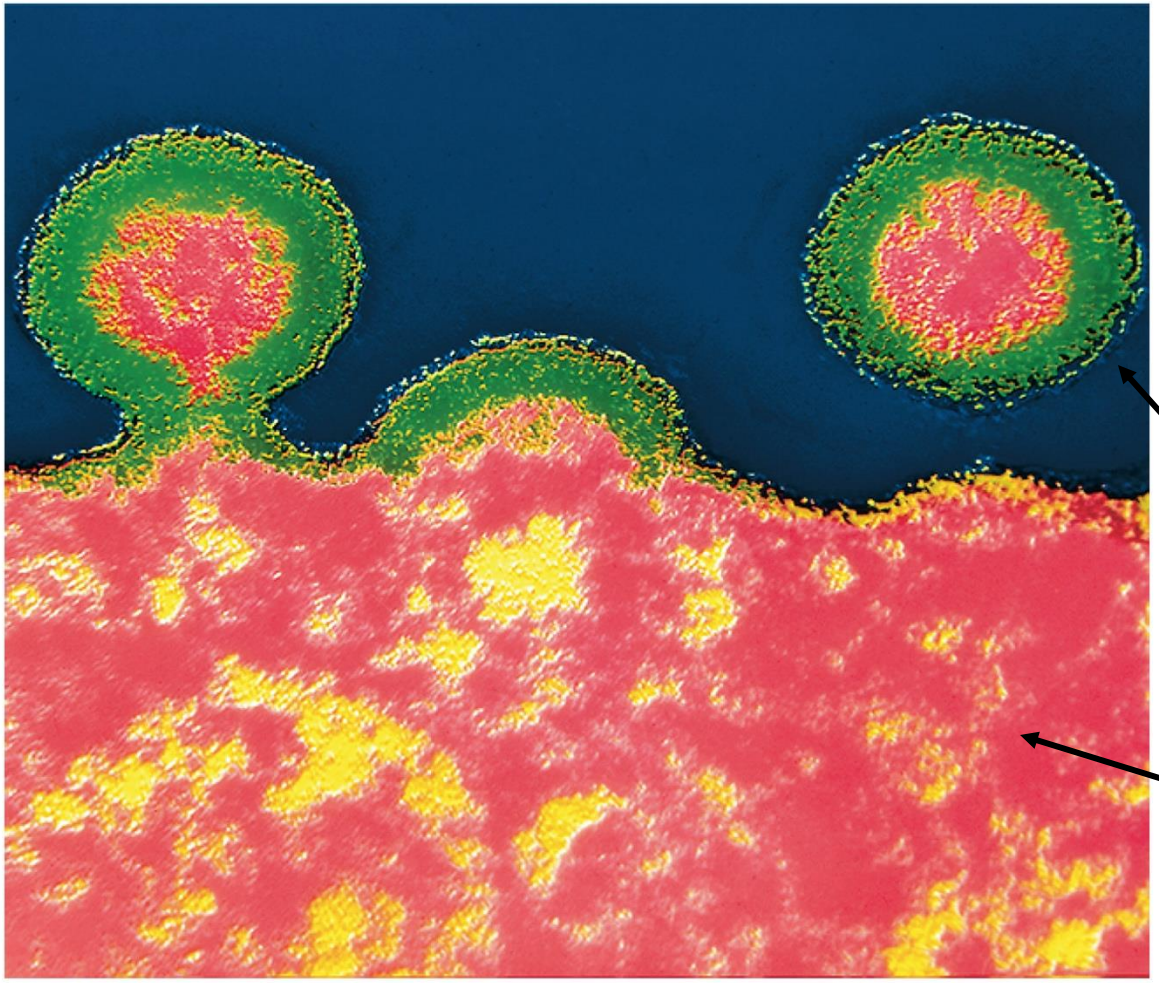
Wave-like nature of matter

- What about an electron? v = 6 x 10^{6} m/s:
- m = 9.1 x 10^{-28} g.

$$\lambda = \frac{6.63 \times 10^{-34} \text{kgm}^2/\text{s}}{9.1 \times 10^{-28} \text{ g } (6 \times 10^{6} \text{ m/s})} = 1.22 \times 10^{-10} \text{ m} = .122 \text{ nm}$$

Wavelength of X-rays

Electron microscopy

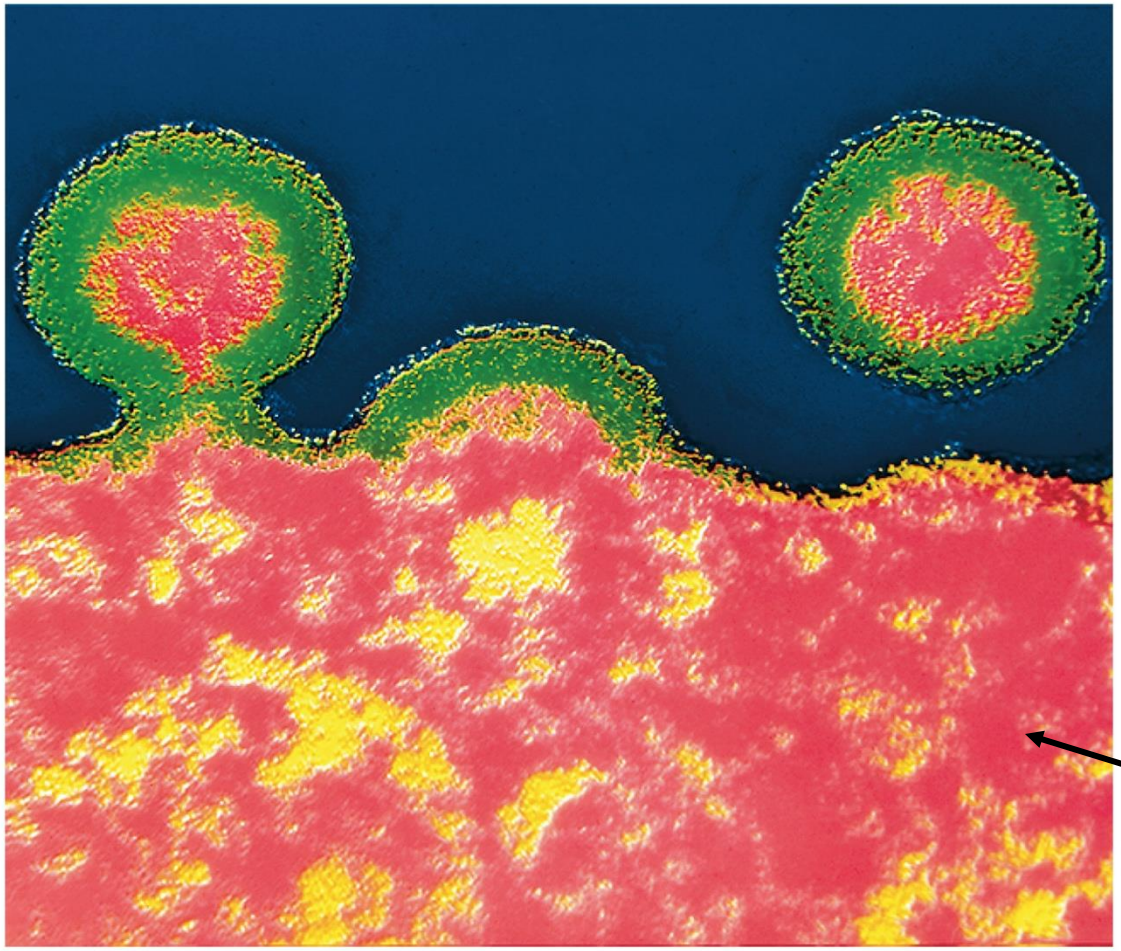


Because electron wavelengths are very small, you can use them to look at very small things.

HIV virus
100 nm, (light microscope limit 400 nm)

T-lymphocyte

Electron microscopy



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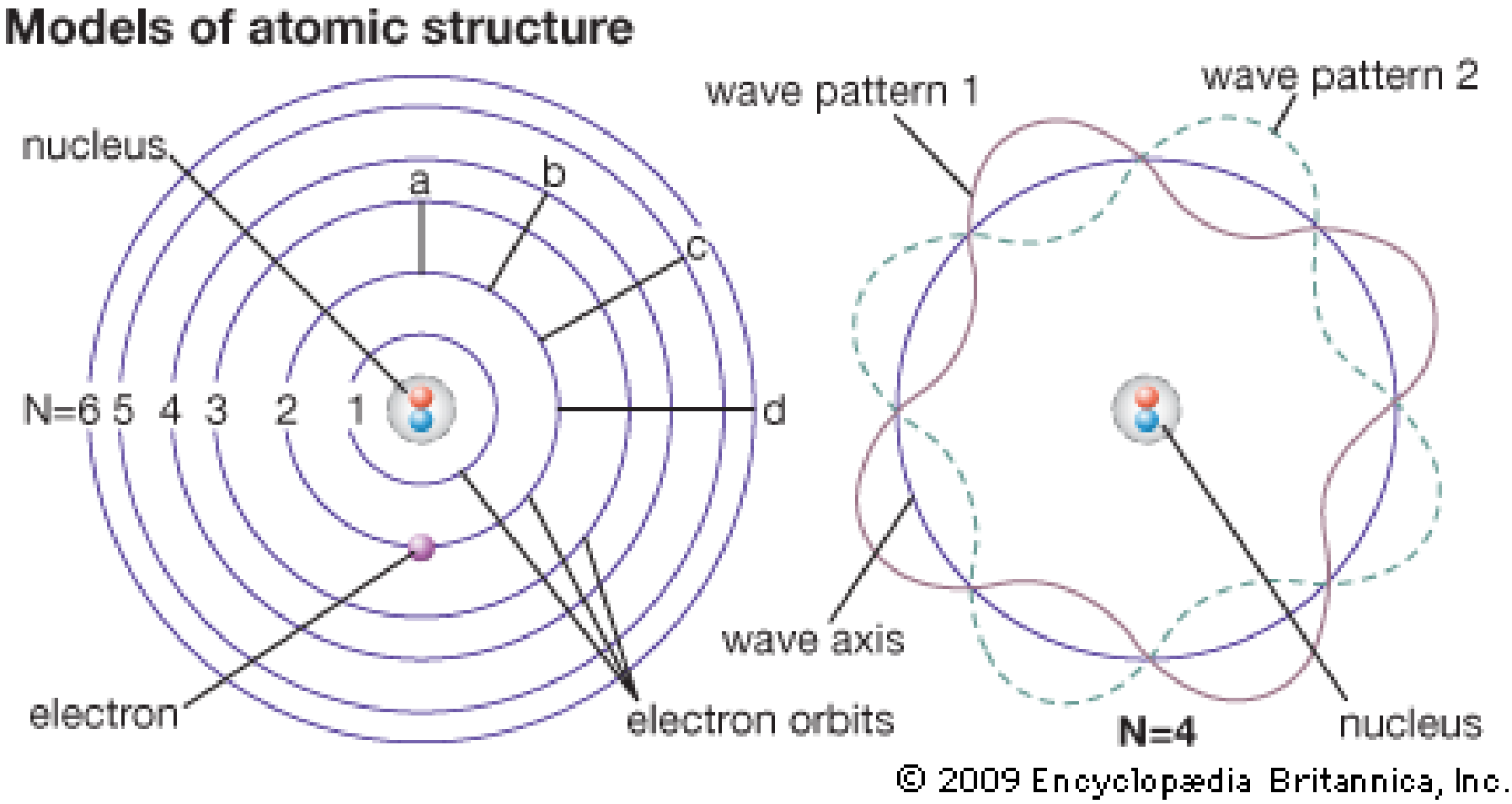
Nobel Prize in Chemistry 2017:
Jacques Dubochet, Joachim Frank, Richard Henderson
Electron Microscopy

Modified pictures of the atom



Both are wrong!

The Uncertainty Principle

- Heisenberg showed that the more precisely the momentum of a particle is known, the less precisely is its position known:

$$(\Delta x)\,(\Delta mv) \geq \frac{h}{4\pi}$$

- our uncertainty of the whereabouts of an electron can be greater than the size of the atom!

This is a result of the wave/particle duality of matter

The Uncertainty Principle

- Heisenberg showed that the more precisely the momentum of a particle is known, the less precisely is its position known:

$$(\Delta x)\,(\Delta mv) \geq \frac{h}{4\pi}$$

- h = 6.626 x 10^{-34} J-Hz
- What's the range of positional error (**estimate**) for a bullet weighing 0.025 Kg travelling at 200 m/sec?
- A 1 m
- B 1 x 10^{-34} m
- C 1 x 10^{34} m
- D 1 x 10^{-3} m

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$$(\Delta x)\,(\Delta mv) \geq \frac{h}{4\pi}$$

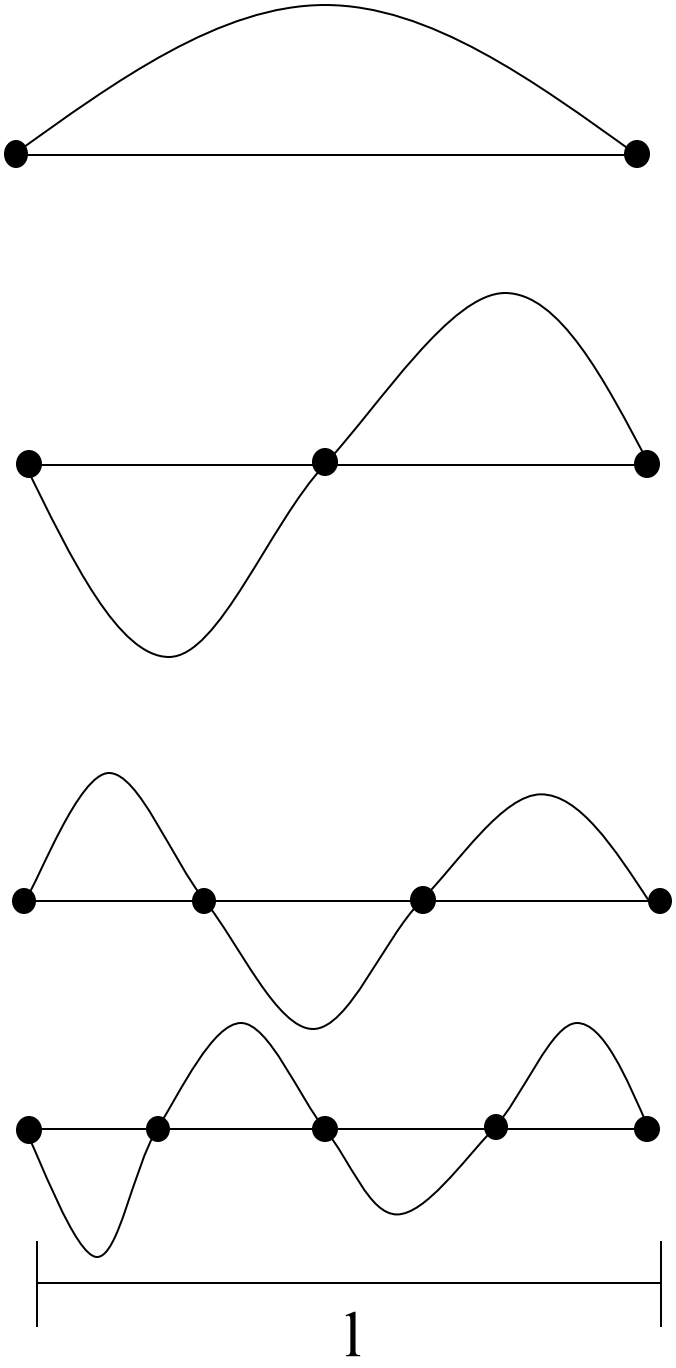
- h = 6.626 x 10^{-34} J-Hz
- What about an electron in an atom?
- Atom size: 1 x 10^{-10} m.
- Electron mass: 9.91 x 10^{-31} kg
- Can easily be **larger** than the size of an **atom**!
- So Heisenberg says we have no idea where an electron is in an atom at any given moment.

“The clues”

- 1. Plank: **E of light is quantized** & depends on **frequency**
- 2. Einstein/photo-electric effect: Light behaves like a particle when it interacts with matter.
- 3. Emission spectra/Bohr: Potential E. of electrons are quantized in an atom.
- 4. Debroglie: wave/particle duality of electrons (matter).
- 5. The Heisenberg Uncertainty Principle
- 6. Standing waves: ***are quantized inherently***

Born/Schroedinger/Jordan: use standing wave analogy to explain electron P.E. in atoms. *Quantum Mechanics*

Standing waves



l=(**1**/2)λ
1ν_O=frequency
nodes = 2 (gotta have 2)

l = (**2**/2)λ = λ
2ν_O=frequency
nodes = 3

l=(**3**/2)λ
3ν_O=frequency
nodes = 4

l=(**4**/2)λ=2λ
4ν_O=frequency
nodes = 5

1 dimensional standing waves.

Allowed n and l *quantized.*

l = (**n**/2)λ,

n is integer/quantum #

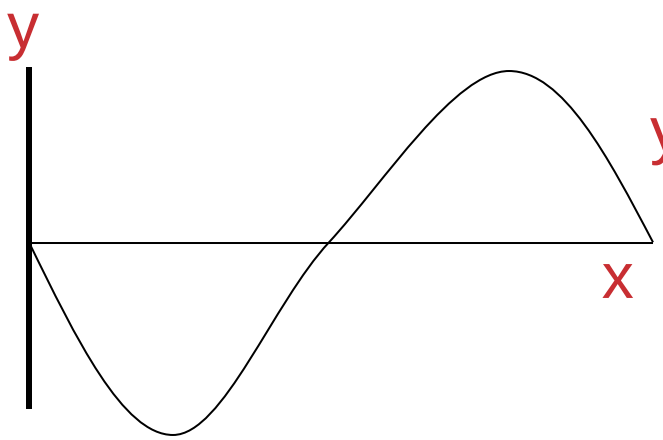
frequency = **n**ν_O

Quantum mechanics

- Each electron can be described using a standing wave equation (***wavefunction***)
- Quantized **frequency** corresponds to quantized **Energy** (Debroglie, Plank, etc.)
- Integer values are critical to this description: ***quantum numbers.***

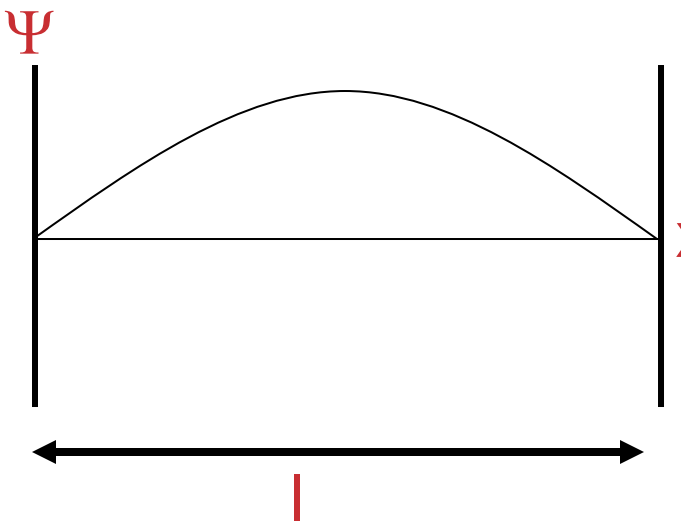
Quantum mechanics

Examples of wave equations



y = sinx

Propagating wave



$$Y = \sqrt{\frac{2}{l}} \sin \frac{px}{l}$$

Standing wave

l=1/2λ

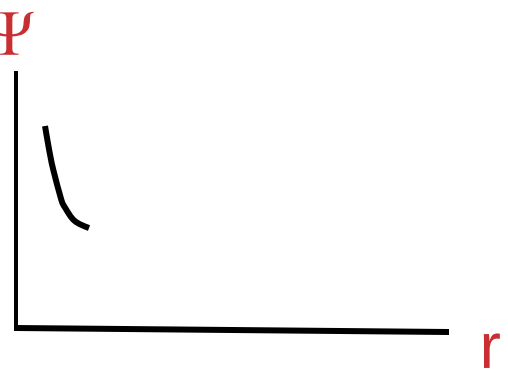
ν_O=frequency

nodes = 2

Quantum mechanics

- Using math we do NOT want to deal with, you can do the same thing for an electron in hydrogen:

$$\Psi = \frac{1}{\sqrt{\pi}} e^{-r}$$



But what, physically is Ψ? **What is waving?**

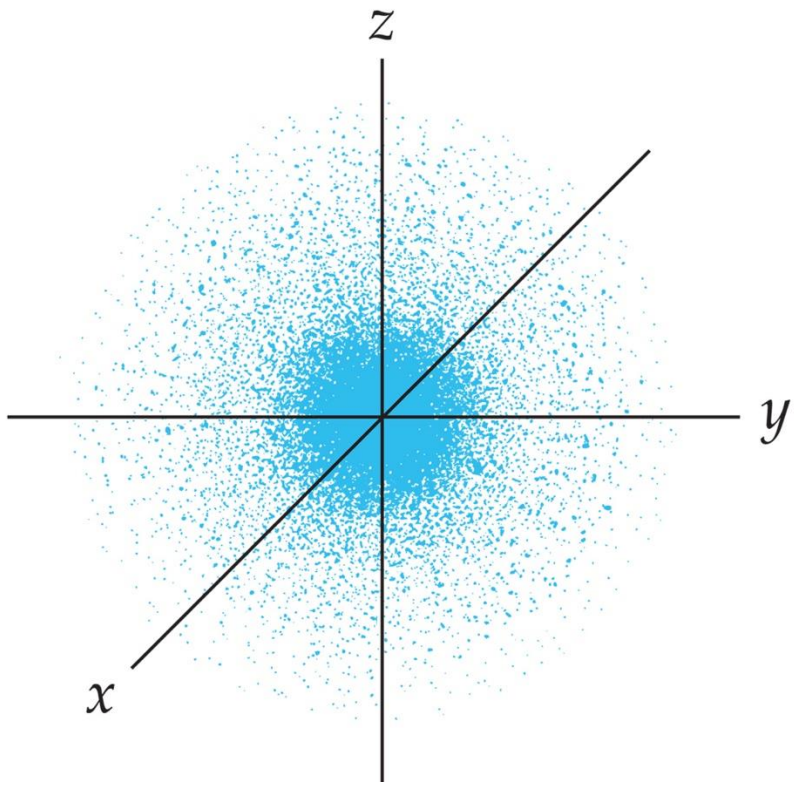
Born (1926):

Ψ^2= probability/volume of finding the electron.

Quantum Mechanics

Plot of Ψ^2 for hydrogen atom.

The closest thing we now have to a physical picture of an electron trapped in an atom.

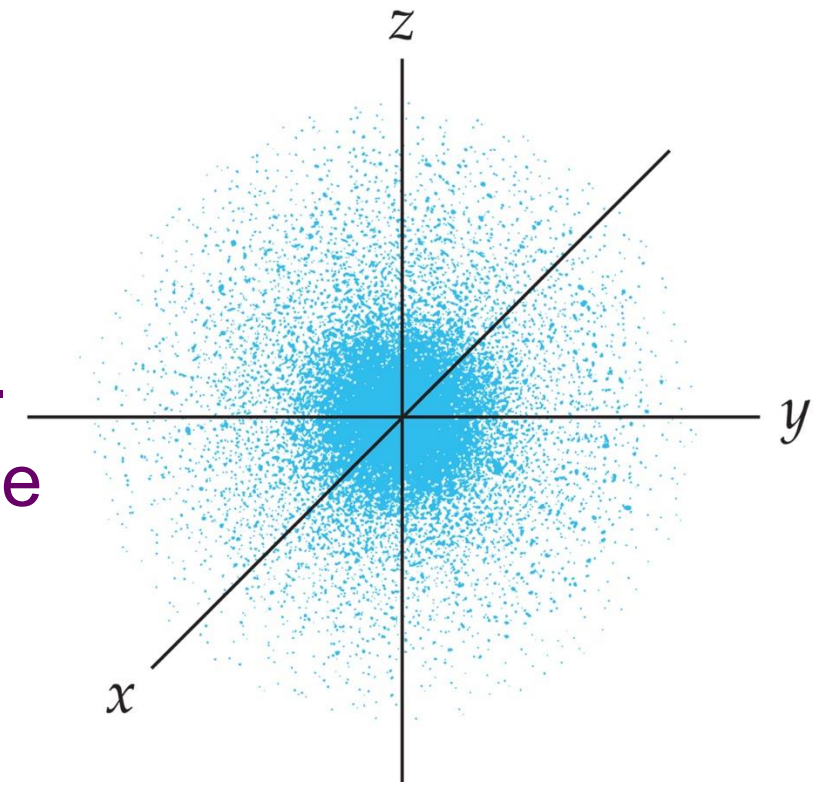


90% contour:

will **find** electron in **blue stuff 90%** of the time.

Quantum Mechanics

- The wave equation designated with a lower case Greek *psi* (ψ).
- ψ^2, gives the probability density of electron location.
- Where it's "most likely" to be



Quantum Numbers

- Solving the wave equation gives a set of wave functions, or ***orbitals***, and their ***energies***.
- Each ***orbital*** describes:
  - a spatial distribution of electron density (location)
  - A very precise ***Potential Energy*** for the electron.
- An orbital is described by a set of three quantum numbers (integers)
- Why three?
  - A One for protons, neutrons and electrons
  - B. One for E, one for charge, one for mass.
  - C. Describes three dimensions
  - D. None of the above.

Quantum numbers

- **3 dimensions.**

- Need three quantum numbers to define a given wavefunction.
- Another name for **wavefunction**: **Orbital** (because of Bohr).
- **Orbital = Wavefunction**

Principal Quantum Number, *n*

- The principal quantum number, *n*, describes the **energy level** on which the orbital resides.
- Largest E difference is between E levels
- The values of *n* are integers > 0.
- 1, 2, 3,...n.

Azimuthal Quantum Number, *l*

- Defines **shape** of the orbital.
- Allowed values of ***l*** depend on **n**:
  - integers ranging from **0 to *n* − 1**.
- We use letter designations for the different values of *l* and, therefore, the shapes and types of orbitals.
- *Note, allowed quantum number possibilities depend on each other.*

Azimuthal Quantum Number, *l*

l = 0, 1…,n-1

Value of *l*	0	1	2	3
Type of orbital	*s*	*p*	*d*	*f*

So each of these letters corresponds to a shape of orbital.

If n=2, can there be and l=3 (f orbital?)

A. yes

B. no

Magnetic Quantum Number, m_l

- Describes, primarily, the **three-dimensional orientation** of the orbital.
- Values are integers ranging from -*l* to *l*:

$$-l \leq m_l \leq l.$$

- Therefore, *on a given energy level*, there *can* be:
- 1 *s orbital (l=0),* (m_l=0),
- 3 *p* orbitals *(l=1),* (m_l=-1,0,1)
- 5 *d* orbitals *(l=2),* (m_l=-2,-1,0,1,2)
- 7 *f* orbitals *(l=3),* (m_l=-3,-2,-1,0,1,2,3)

Magnetic Quantum Number, m_l

- Orbitals with the same value of *n* form a shell.
- Different orbital types within a shell are subshells (s, p, d, f).

n	Possible Values of *l*	Subshell Designation	Possible Values of m_l	Number of Orbitals in Subshell	Total Number of Orbitals in Shell
1	0	1*s*	0	1	1
2	0	2*s*	0	1	
	1	2*p*	1, 0, −1	3	4
3	0	3*s*	0	1	
	1	3*p*	1, 0, −1	3	
	2	3*d*	2, 1, 0, −1, −2	5	9
4	0	4*s*	0	1	
	1	4*p*	1, 0, −1	3	
	2	4*d*	2, 1, 0, −1, −2	5	
	3	4*f*	3, 2, 1, 0, −1, −2, −3	7	16

Magnetic Quantum Number, m_l

n	Possible Values of l	Subshell Designation	Possible Values of m_l	Number of Orbitals in Subshell	Total Number of Orbitals in Shell
1	0	1*s*	0	1	1
2	0	2*s*	0	1	
	1	2*p*	1, 0, −1	3	4
3	0	3*s*	0	1	
	1	3*p*	1, 0, −1	3	
	2	3*d*	2, 1, 0, −1, −2	5	9
4	0	4*s*	0	1	
	1	4*p*	1, 0, −1	3	
	2	4*d*	2, 1, 0, −1, −2	5	
	3	4*f*	3, 2, 1, 0, −1, −2, −3	7	16

- If n=4 and l=0 which values can m_l have?

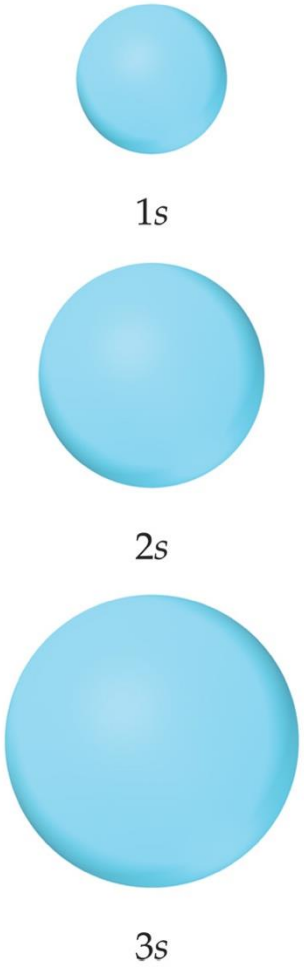
  A. 0

  B. 1

  C. -1

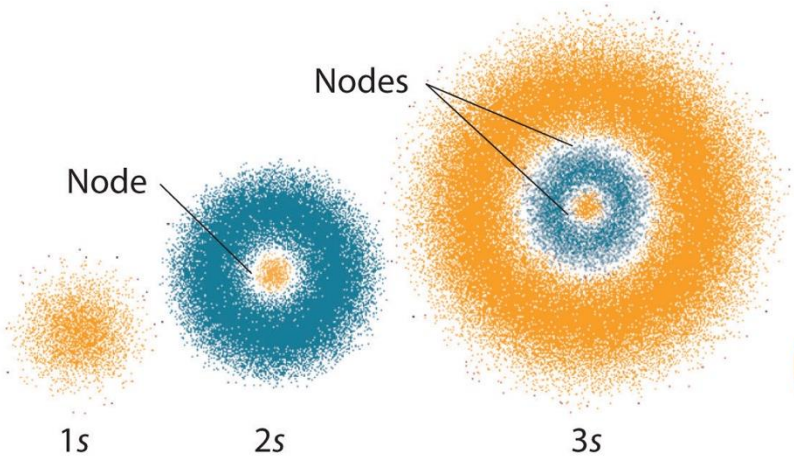
  D. All of the above

s Orbitals

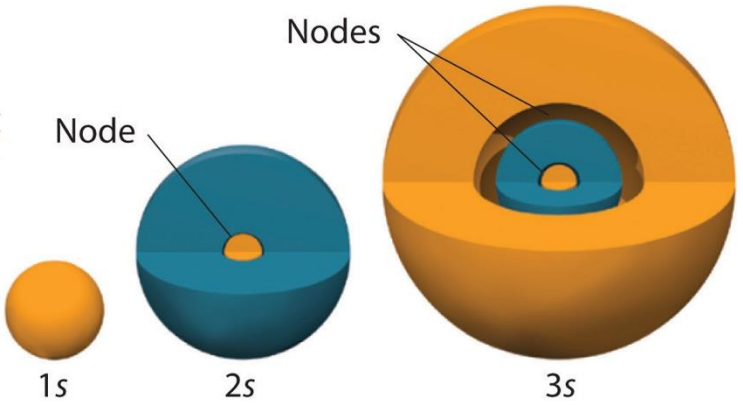


- $l = 0$.
- Spherical in shape.
- Radius of sphere increases with increasing value of *n*.

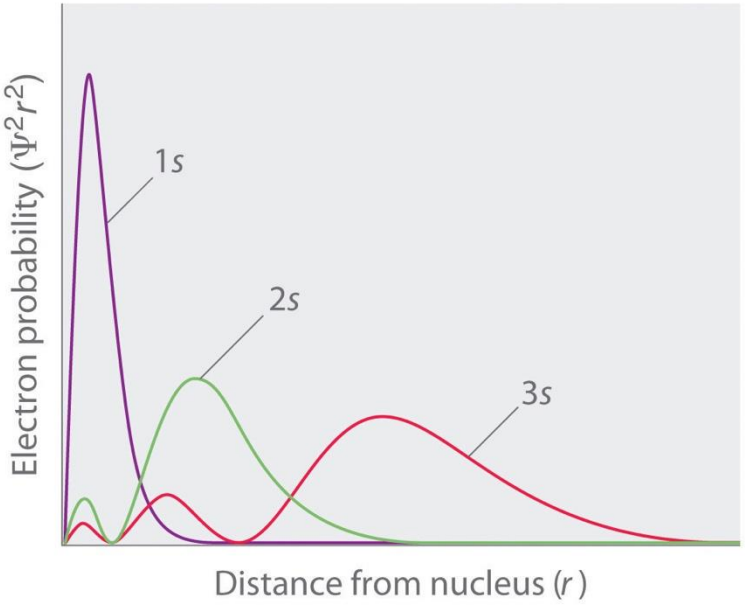
s Orbitals



(a) Electron probability



(b) Contour probability



(c) Radial probability

s orbitals: $n-1$

Nodes:

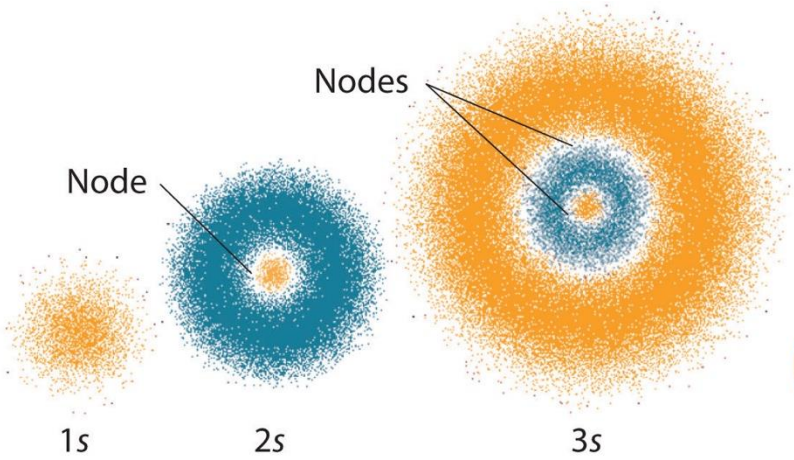
Node: 0 amplitude

0 probability

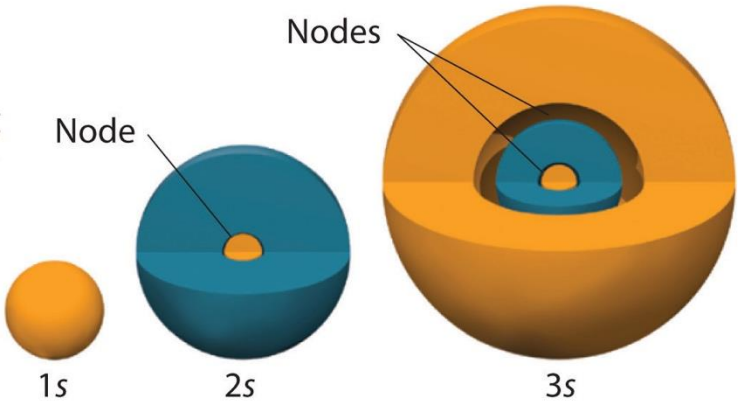
Note; 1s orbitals have 0 nodes!

The nucleus is not a node

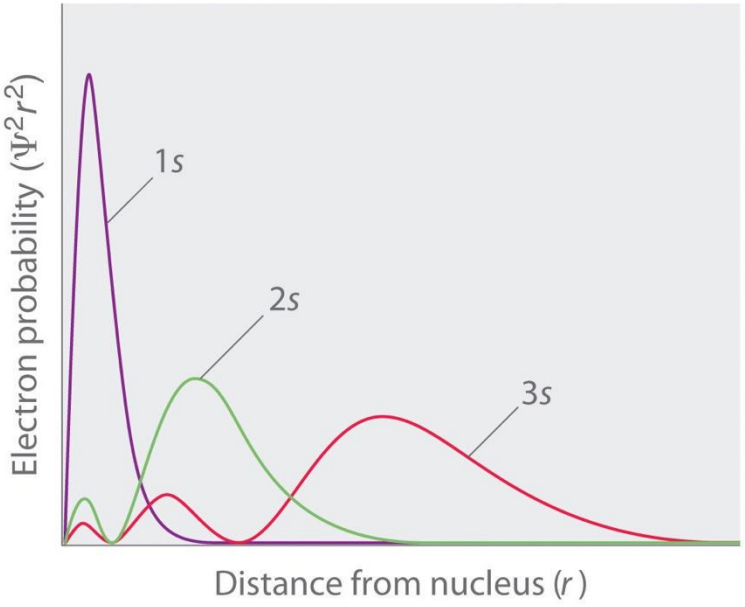
s Orbitals



(a) Electron probability



(b) Contour probability



(c) Radial probability

How many nodes does a 4s orbital have?

A. 0

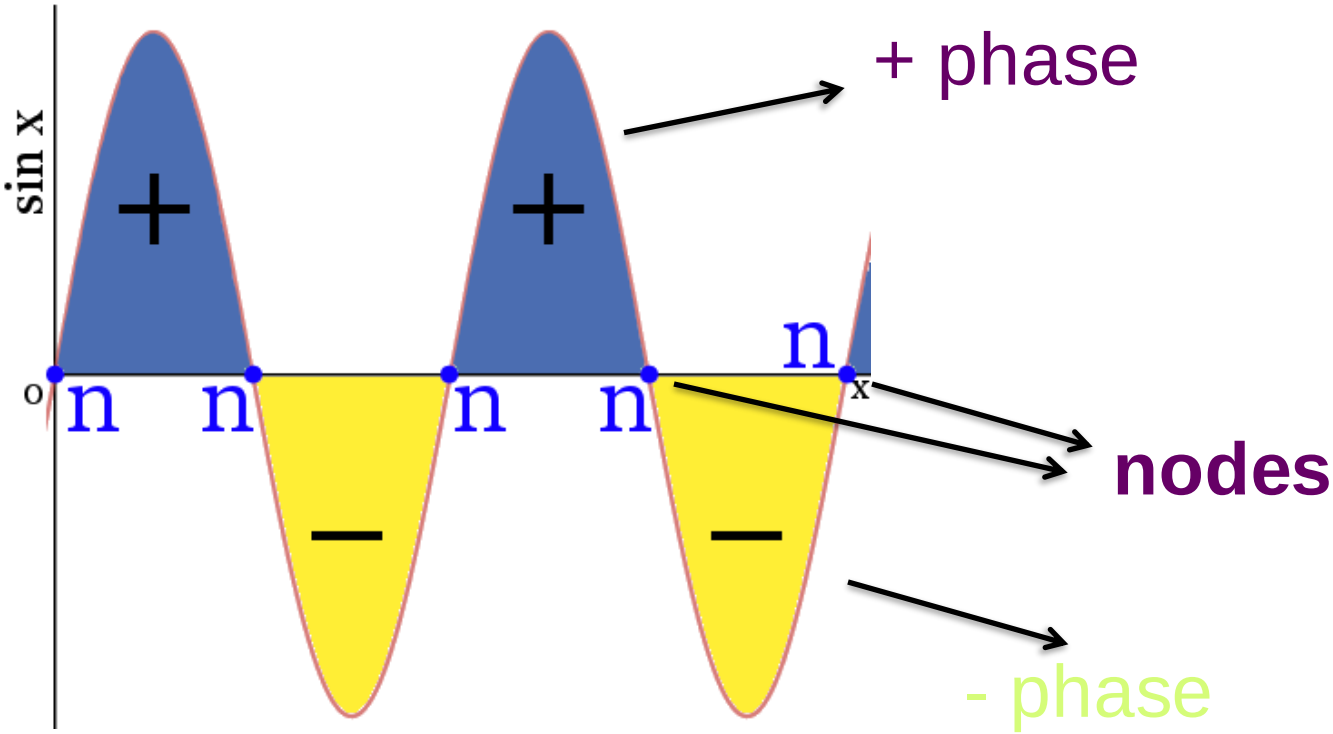
B. 1

C. 2

D. 3

E. 4

Nodes and Waves.

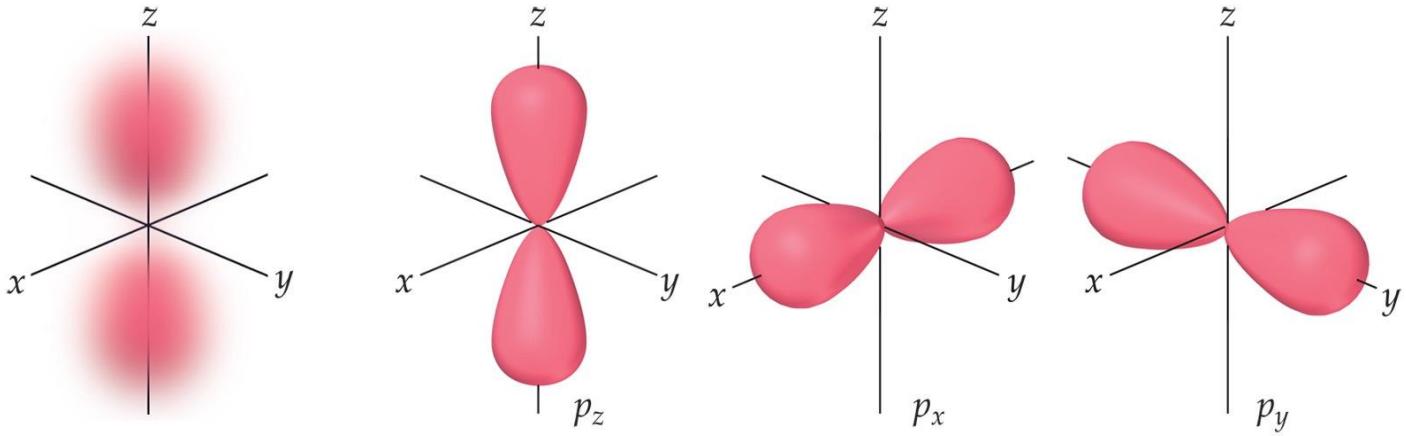


Note: when you square the wave, the phase change goes away.

$(-x)^2 = x^2$

p Orbitals

- Value of *l* = 1.
- Have two lobes with one angular node (nodal plane) between them.



Note: always 3 p orbitals for a given n

What values of m_l can a p orbital have?

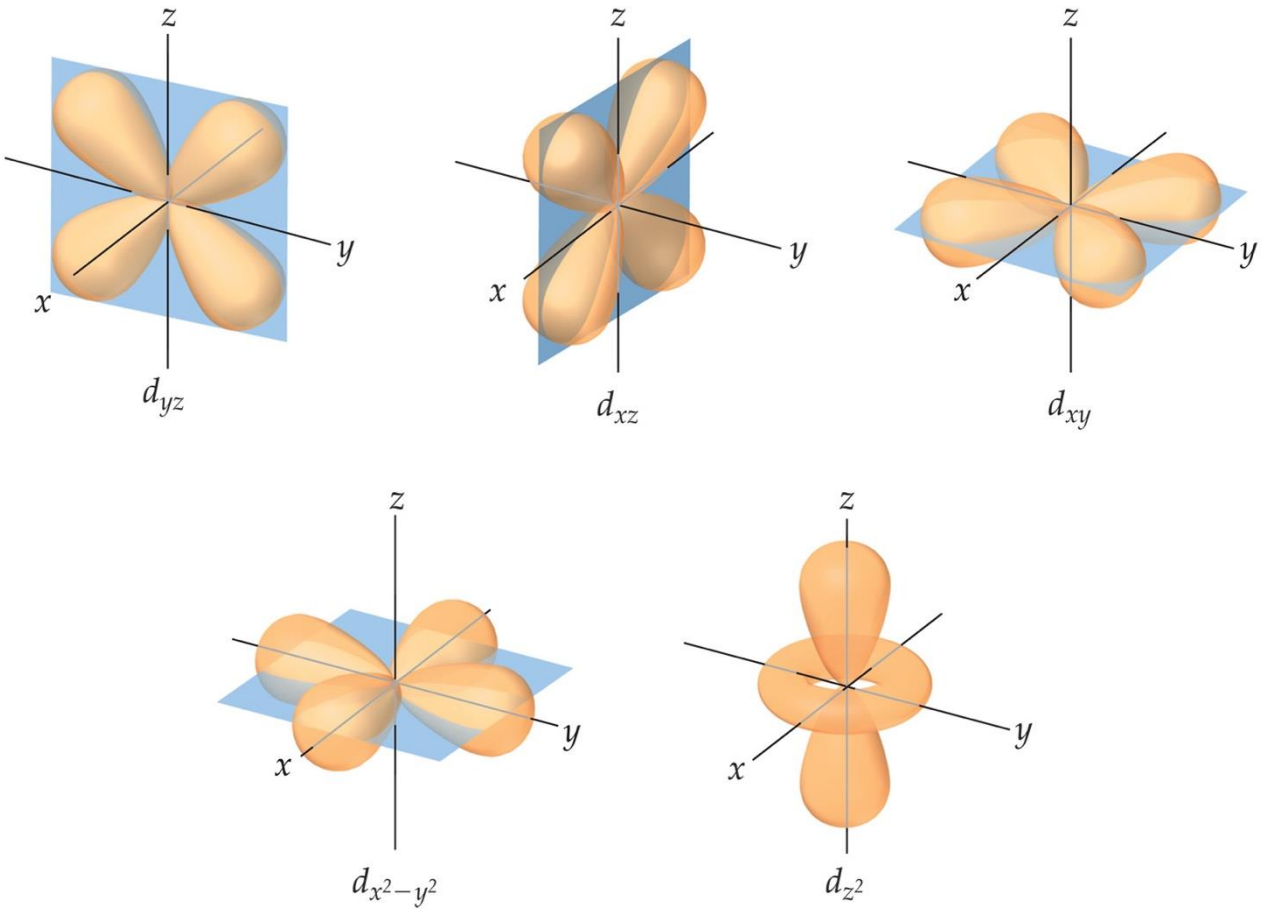
A. 0

B. -1

C. 1

D. All of the above

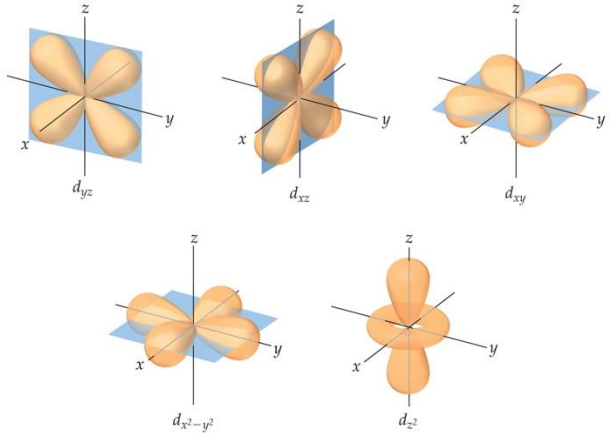
d Orbitals

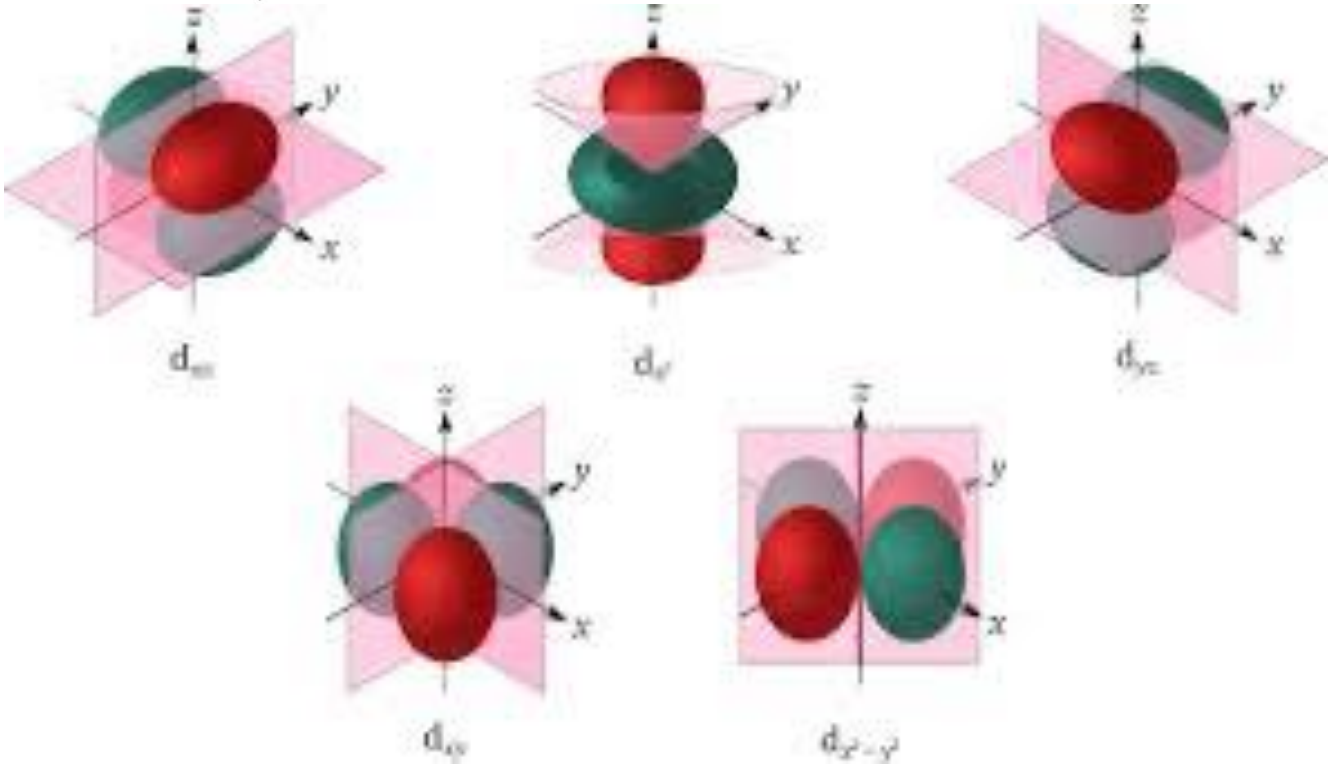


- Value of ***l* is 2.**
- Four of the five orbitals have 4 lobes; the other resembles a *p* orbital with a doughnut around the center.

Note: always 5 d orbitals for a given n.

d Orbitals

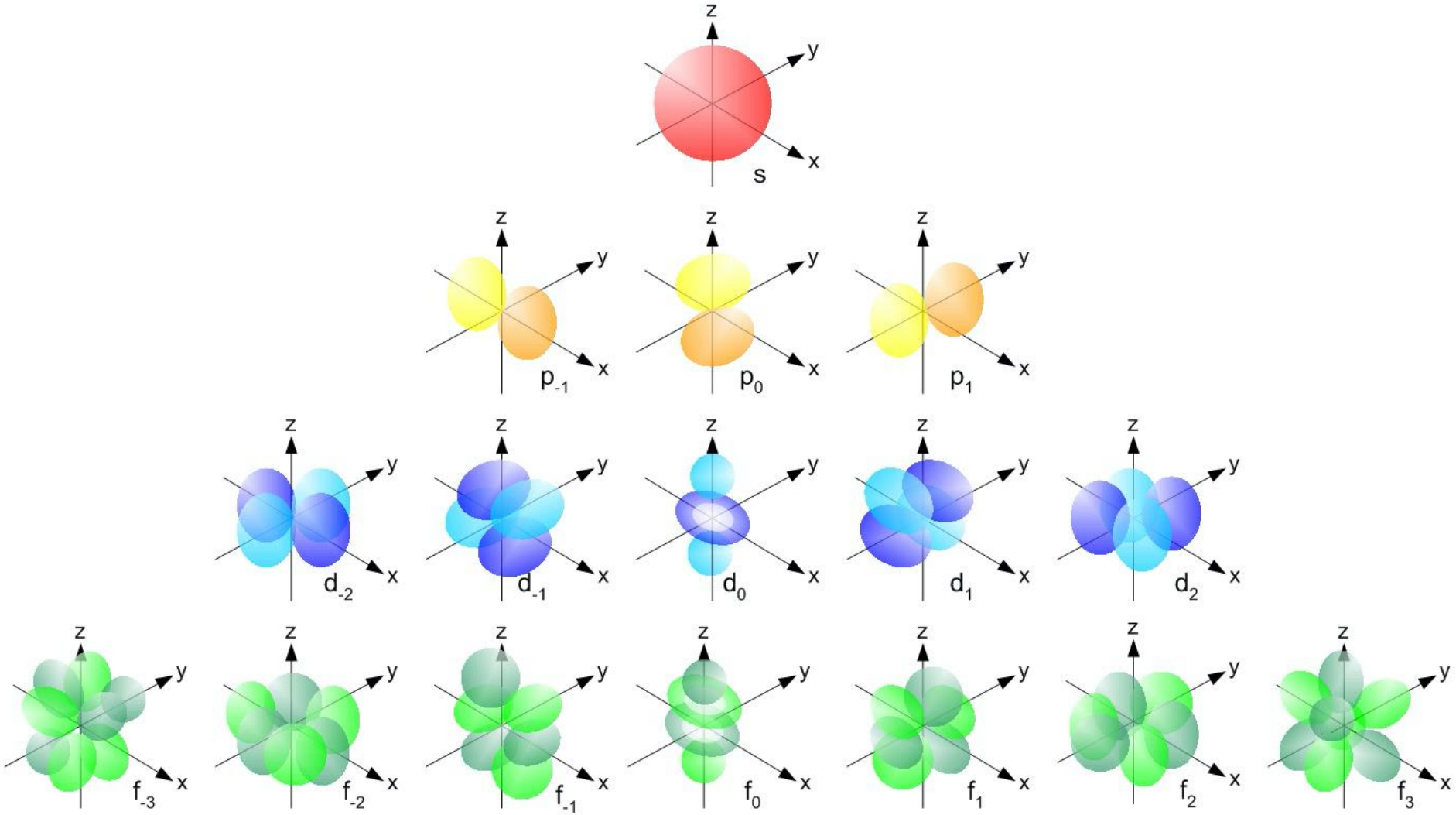




- Value of *l* is 2.
- Four of the five orbitals have 4 lobes; the other resembles a *p* orbital with a conical collar around the center.
- **2 angular nodes**

Note: always 5 d orbitals for a given n.

Shapes of all the orbitals



Orbitals and nodes

Orbital	Symmetry	Node geometry	radial nodes/shell*	Orbitals /E level
s	spherical	radial (spherical)	n-1	1
p	cylindrical around x, y, or z axis	**1 angular (planar)** remainder spherical	n – 2	3
d	complex	**2 angular nodes** diagonal to Cartesian axis; remainder spherical	n - 3	5
f	complex	complex	n - 4	7

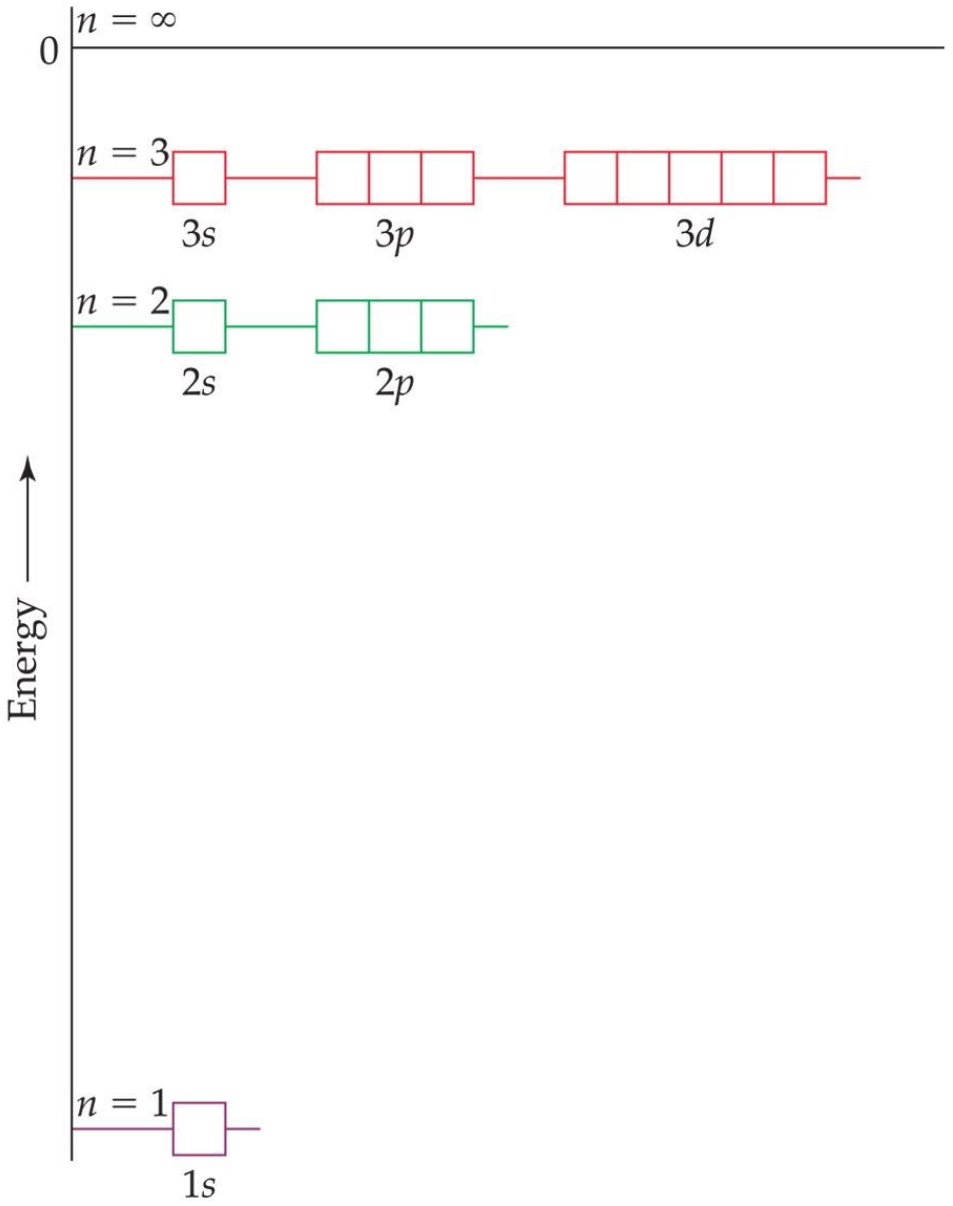
•n = the shell, with n = 1 the ground state or lowest possible energy shell. Thus n may have integral values from 1 - infinity.

•Nodes:

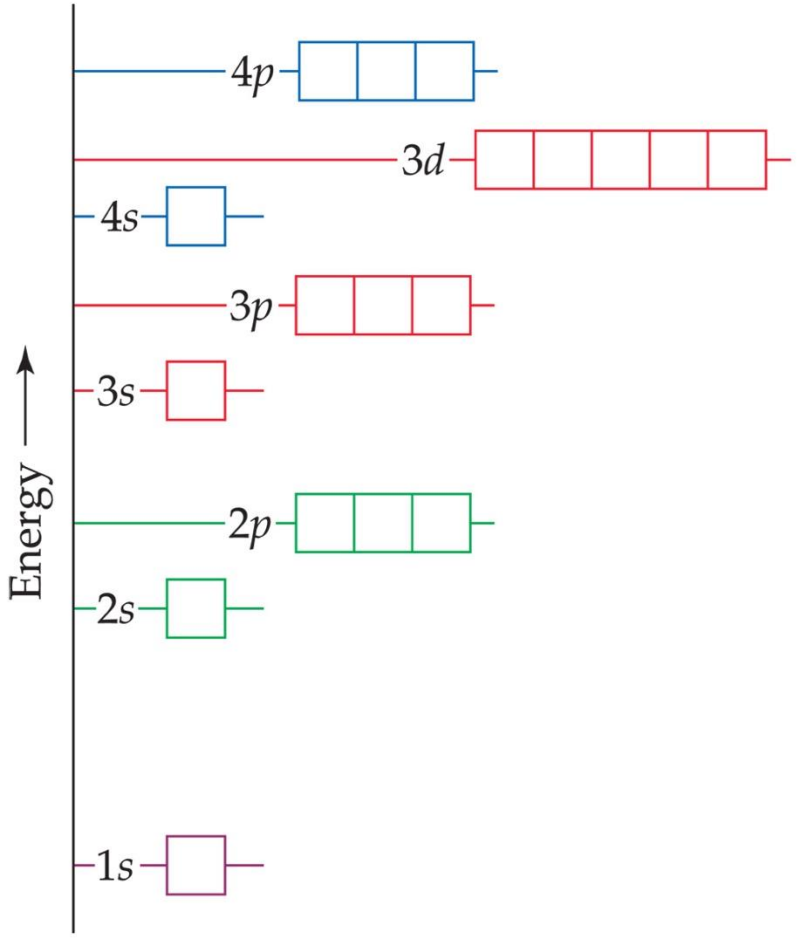
- Total # of nodes = n -1
- # of angular (planar) nodes = l
- # radial (spherical) nodes = n – 1 - l

Energies of Orbitals

- For a one-electron atom (hydrogen), orbitals on the same energy level have the same energy.
- That is, they are **degenerate.**
- **Note. H atom has all these orbitals, even though it only has *1 electron.***
- ***The rest are empty.***

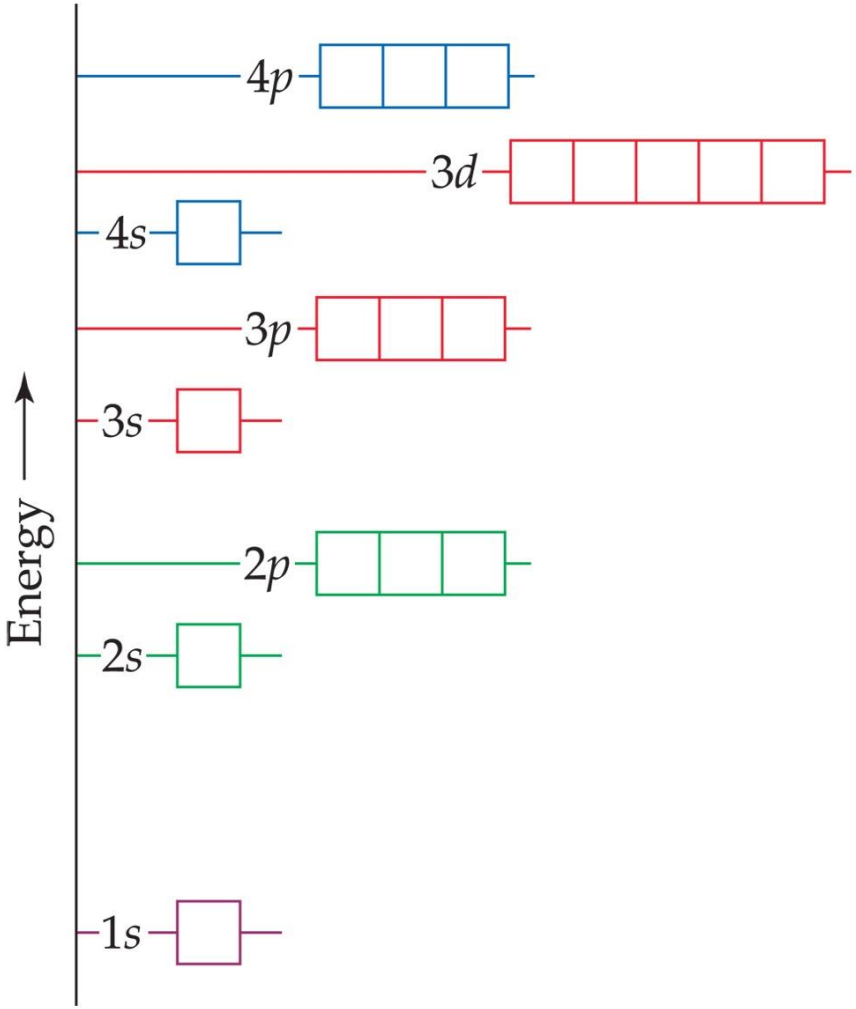


Energies of Orbitals
Many electron atom



- Electrons in the same atom repel each other.
- Therefore, in many-electron atoms, ***orbitals on the same energy level are no longer degenerate***.

Energies of Orbitals



- For a given energy level (n):
- Energy:
- s<p<d<f (**Always)**
- s lowest energy, where electrons go first
- Next p
- Then d

Why?

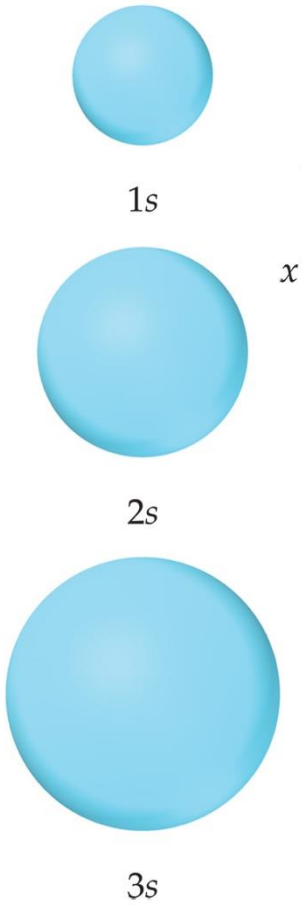
A. Because of the way electrons move in spheres versus dumbells

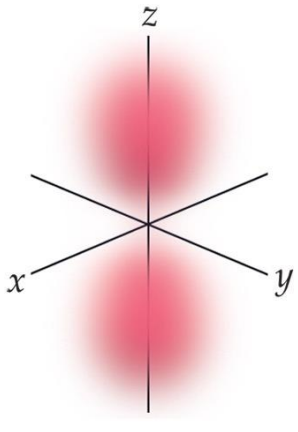
B. It's harder for the electron to "jump" a planar node

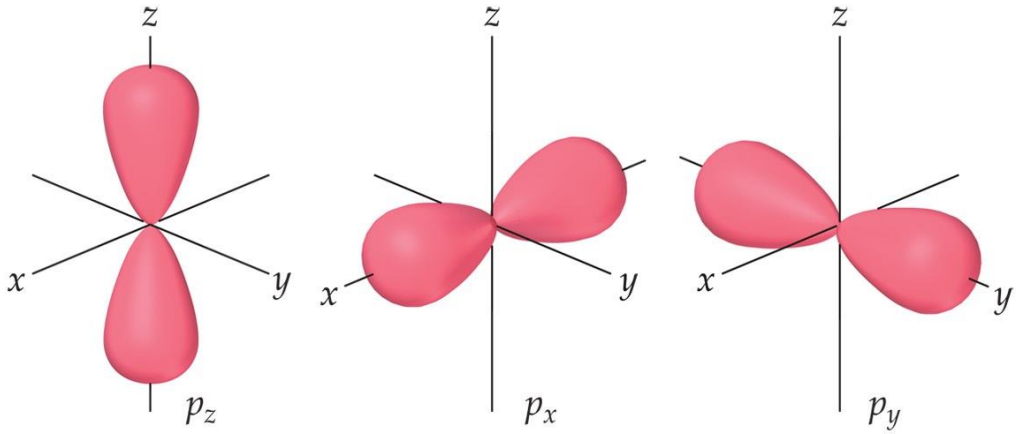
C. E is dependent on distance of the electron from the nucleus.

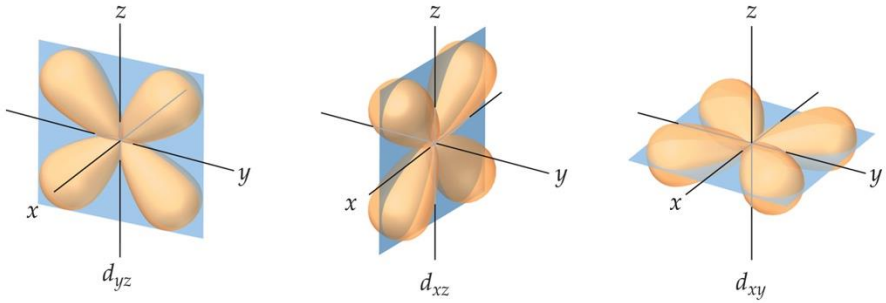
closest

Less close

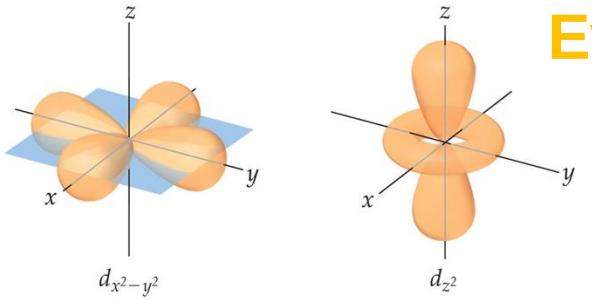








Even Less close

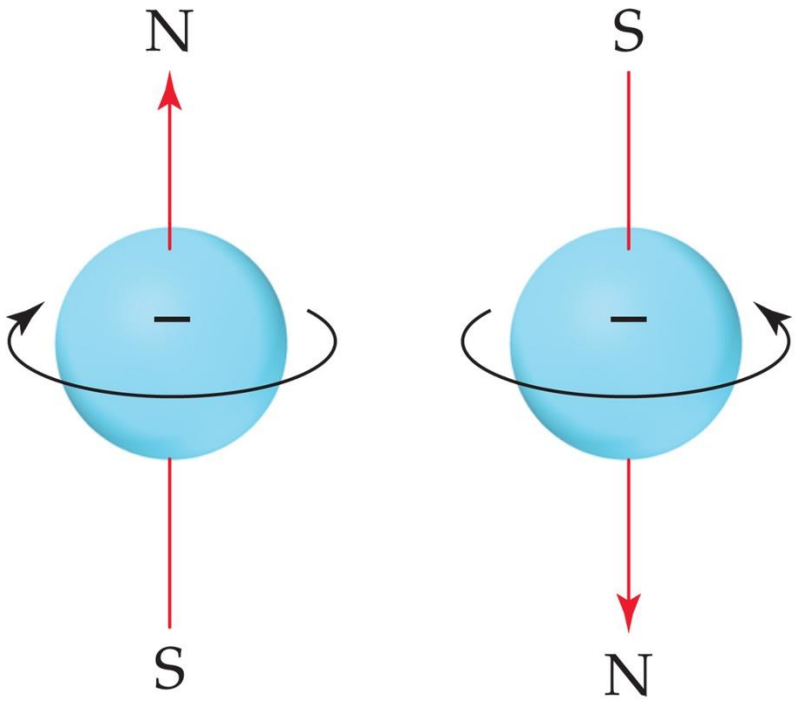


The closer to the nucleus, the lower the potential energy

Lower PE, more tightly stuck to the atom.

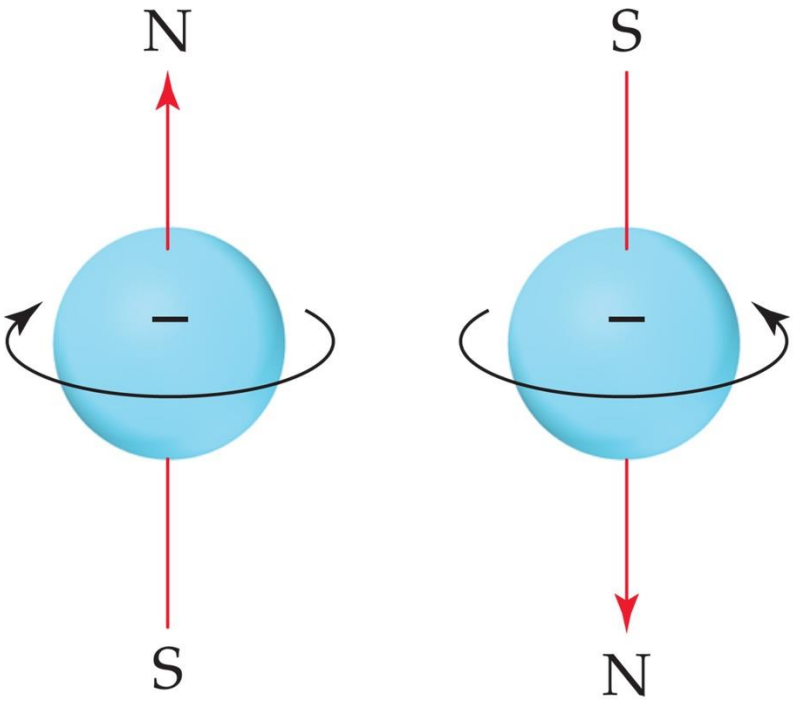
Spin Quantum Number, m_s

- A fourth QM required. Why?
  - A electrons move in a mysterious fourth spatial dimension
  - B Need a dimension for charge.
  - C Need a dimension for mass
  - D Need a dimension for time.



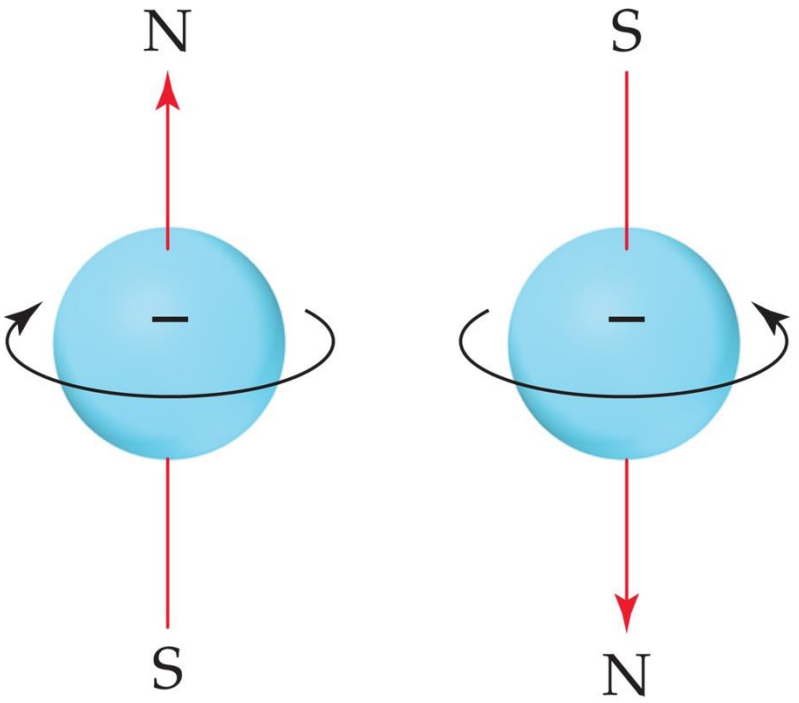
Spin Quantum Number, m_s

- A fourth dimension required. Why?
- **Time. Adding time changes E**
- Another quantum number needed.
- Time *dependent Schroedinger equation.*

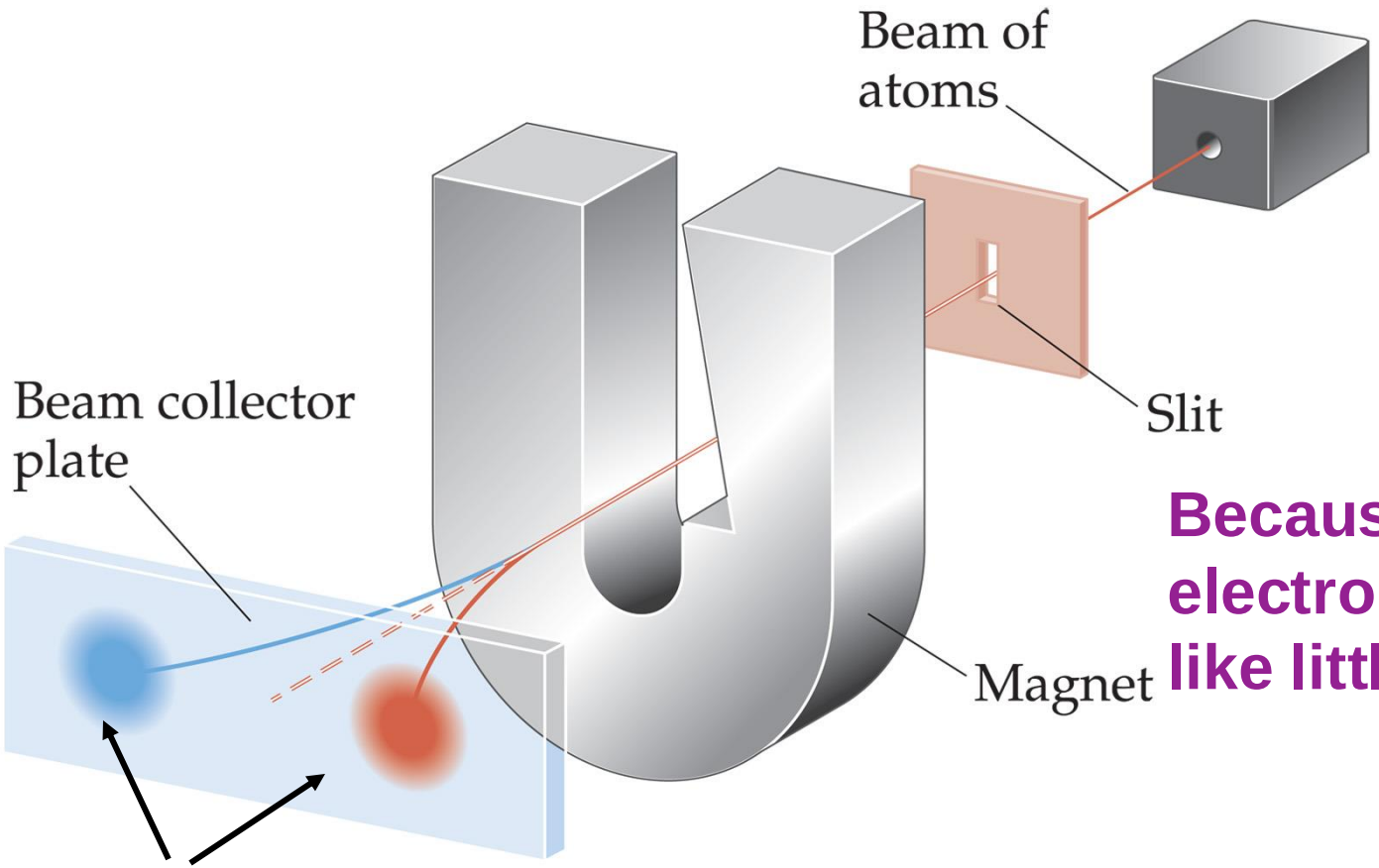


Spin Quantum Number, m_s

- This leads to a fourth quantum number, the spin quantum number m_s.
- The spin quantum number has only 2 values **+1/2 and -1/2**
- **Describes magnetic field vector of electron**



Why do we call it "spin"

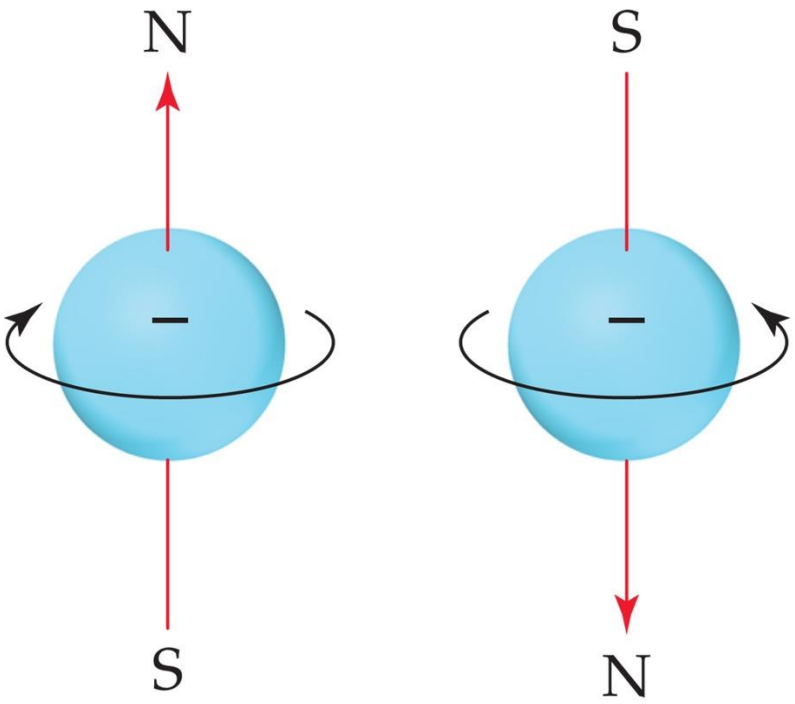


Because electrons behave like little magnets

Note: apparently only two values for the magnetic field

Spin Quantum Number, m_s

- And charges that spin produce magnetic fields

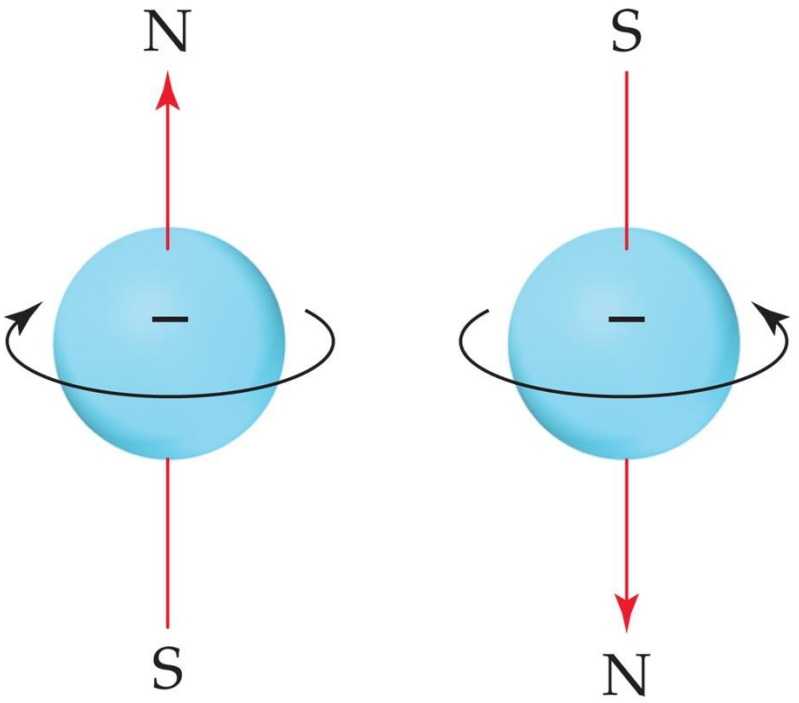


The problem with quantum mechanics

- It's not too hard to solve equations for the various wavefunctions if there is only 1 electron (like H)
- The problem: what happens in the presence of other electrons
- **The electron interaction problem**
- Electron interaction so complex, exact solutions are only possible for H!
- Why?
  - Electron probabilities overlap a lot, must interact a lot, repulsion keeps them from ever "touching"

Pauli Exclusion Principle

- No two electrons in the same atom can have exactly the same energy.
- No two electrons in the same atom can have **identical sets of quantum numbers**.

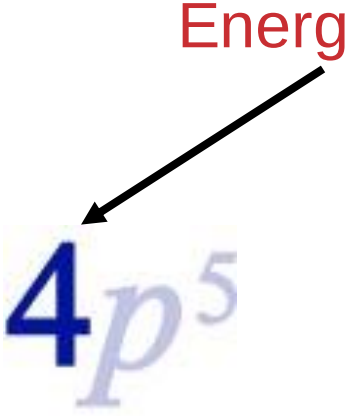


Electron Configurations Every electron has a home

- Address of each electron **unique**
- Address consists of four numbers:
- n,l,m_l,m_s
- Example:
- 578 S Shaw Ln. East Lansing MI
- Note, in an address each part depends on others
- Rome Ga, not the same as Rome Italy.
- Quantum numbers are similar.

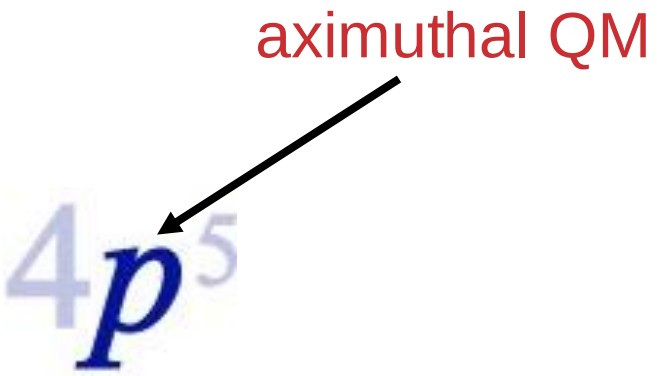
Electron Configurations

Energy level



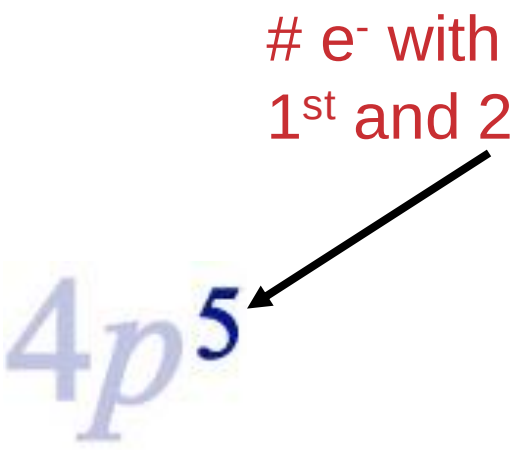
- Distribution of all electrons in an atom
- Consist of
  - Number denoting the energy level

Electron Configurations



- Distribution of all electrons in an atom
- Consist of
  - Number denoting the energy level
  - Letter denoting the l quantum number, “orbital type”

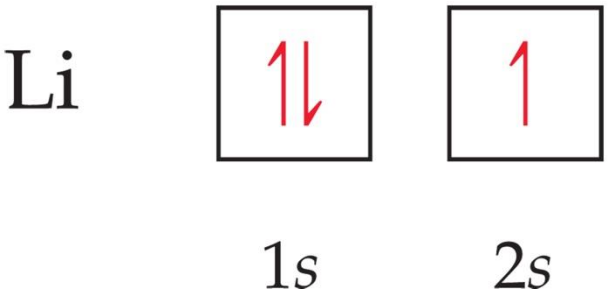
Electron Configurations



- Distribution of all electrons in an atom.
- Consist of
  - Number denoting the energy level.
  - Letter denoting the type of orbital.
  - Superscript denoting the total number of electrons in those orbitals.

Orbital Diagrams

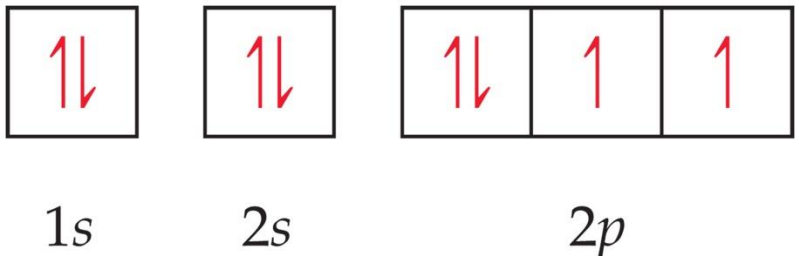
- Each box represents one orbital.
- Half-arrows represent the electrons.
- The direction of the arrow represents the spin of the electron.



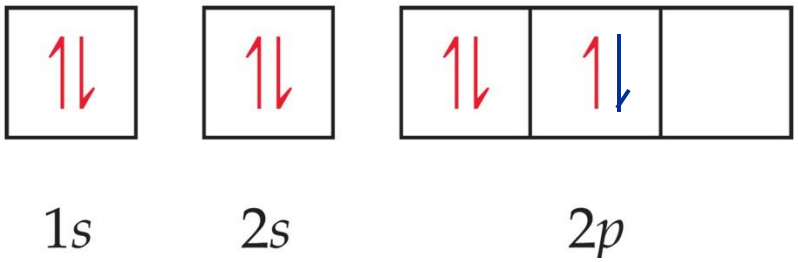
$1s^2 2s^1$

Hund's Rule

(of maximum multiplicity)



NOT:



"For degenerate orbitals, the lowest energy is attained when the number of electrons with the same spin is maximized."

Electrons prefer to be in their own orbital.

Electron configurations

TABLE 6.3 Electron Configurations of Several Lighter Elements

Element	Total Electrons	Orbital Diagram (1s, 2s, 2p, 3s)	Electron Configuration
Li	3	↿⇂ | 1 | | | | |	$1s^2 2s^1$
Be	4	↿⇂ | ↿⇂ | | | | |	$1s^2 2s^2$
B	5	↿⇂ | ↿⇂ | 1 | | | |	$1s^2 2s^2 2p^1$
C	6	↿⇂ | ↿⇂ | 1 | 1 | | |	$1s^2 2s^2 2p^2$
N	7	↿⇂ | ↿⇂ | 1 | 1 | 1 | |	$1s^2 2s^2 2p^3$
Ne	10	↿⇂ | ↿⇂ | ↿⇂ | ↿⇂ | ↿⇂ | |	$1s^2 2s^2 2p^6$
Na	11	↿⇂ | ↿⇂ | ↿⇂ | ↿⇂ | ↿⇂ | 1	$1s^2 2s^2 2p^6 3s^1$

- What's the electron configuration for Mg?
- A $1s^2 2s^2$
- A. $1s^2 2s^2 2p^8$

C. $1s^2 2s^2 2p^6 3s^1$

D. $1s^2 2s^2 2p^6 3s^2$

Why do we accept this wacko stuff?

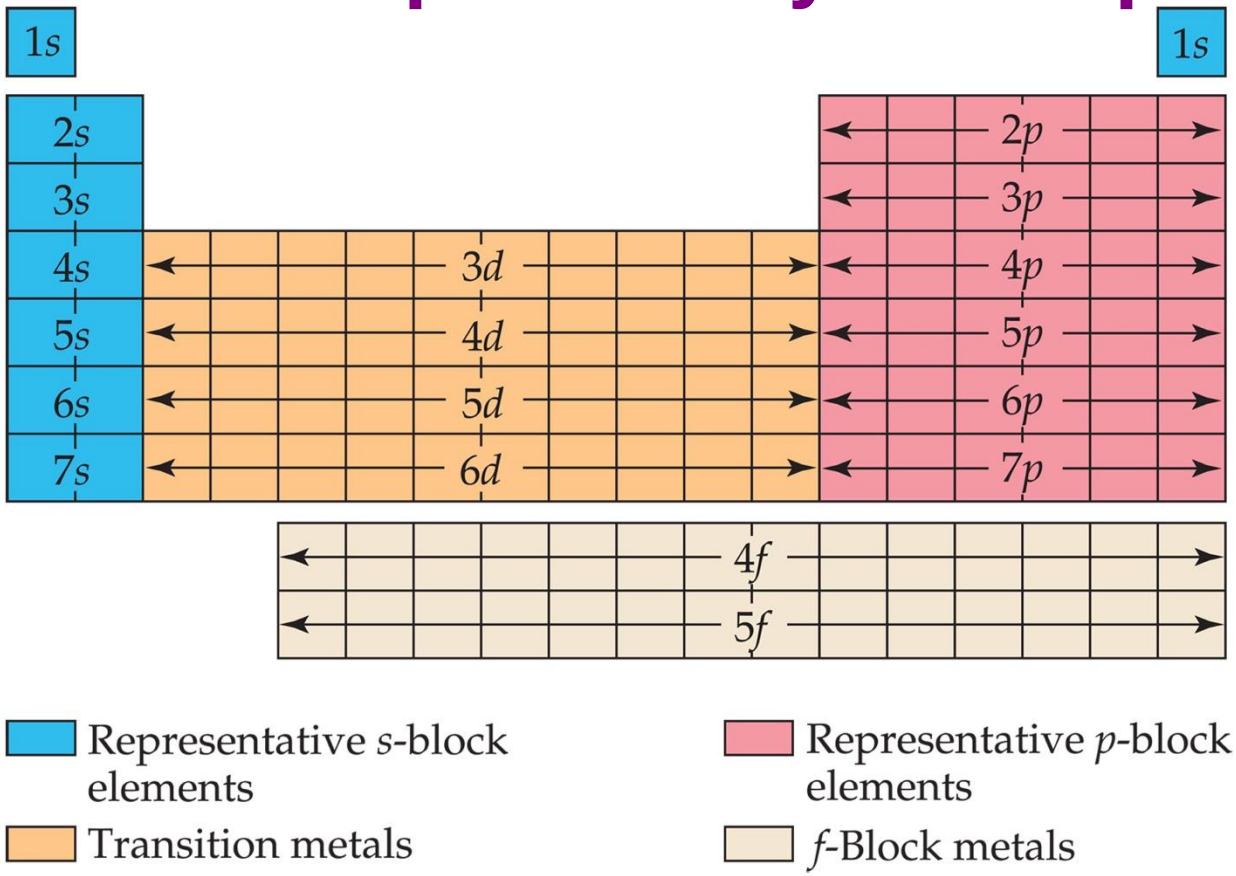
- It must explain all the data
- It should predict things

- Q.M. is consistent with all our data
  - Black body radiation
  - photoelectric effect,
  - emission spectra of elements,
  - dual wave/particle weirdness, etc.

- **One prediction:**
  - elements with similar electron configuration should have similar chemical properties

Why do we accept this wacko stuff?

It predicts the periodicity of the periodic table!!



1868: mystery discovered

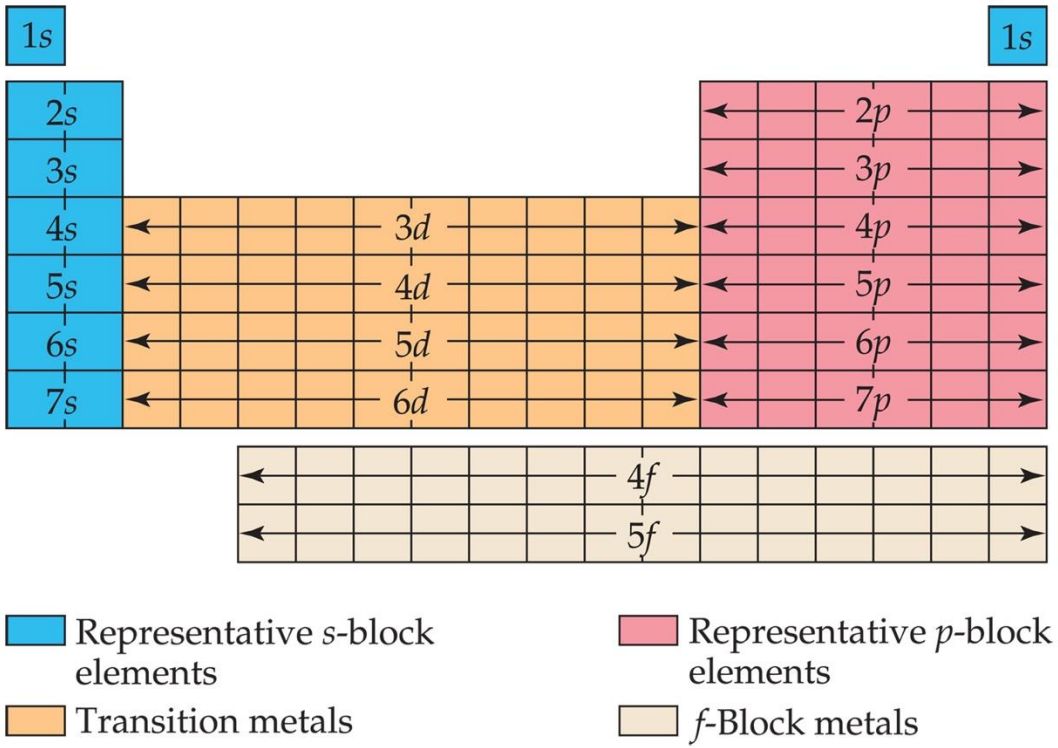
1920's: QM Mystery solved.

- **We fill orbitals in increasing order of energy.**
- **Different blocks on the periodic table, then correspond to different types of orbitals.**

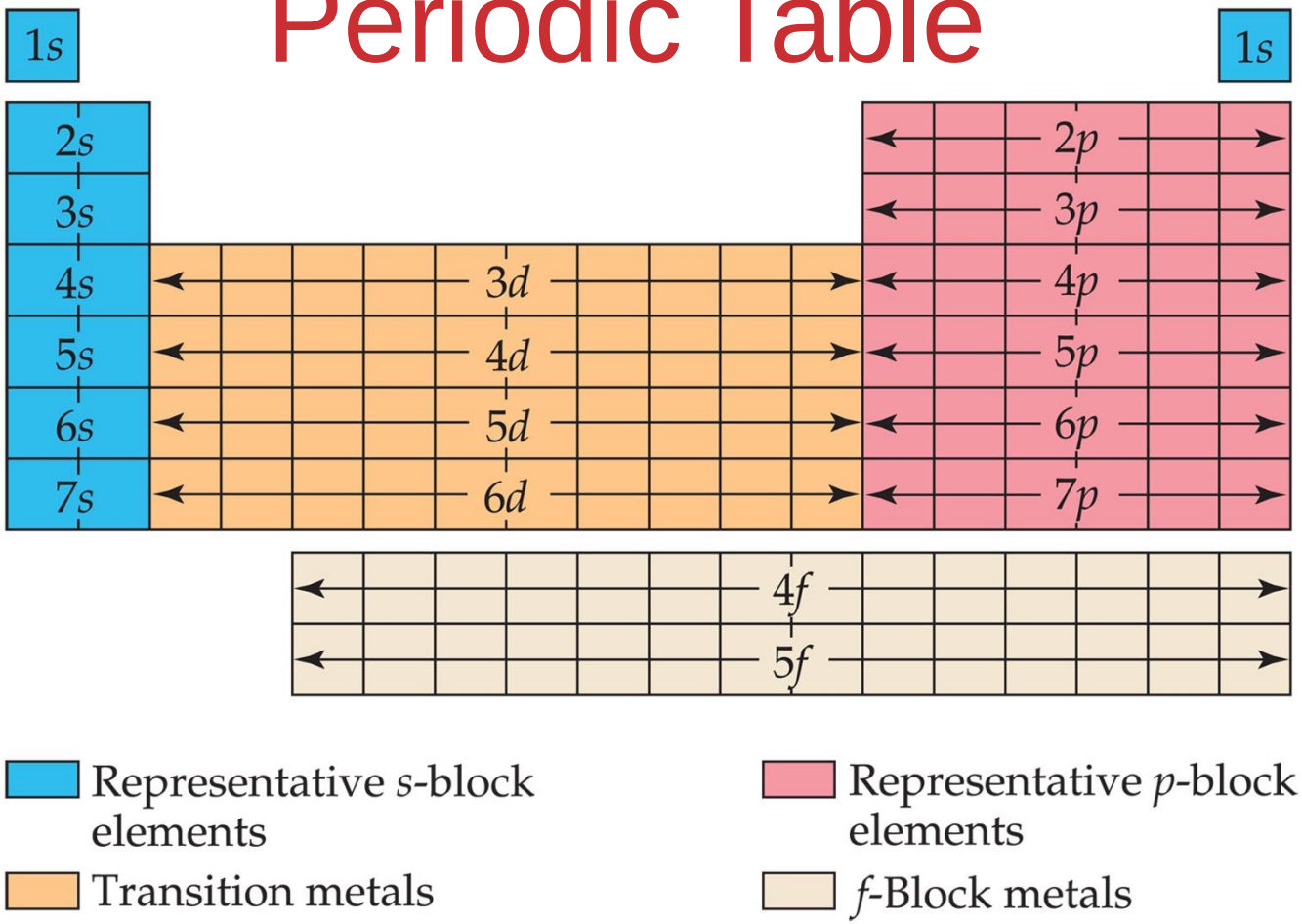
Why do we accept this wacko stuff?

It predicts the periodicity of the periodic table!!

- **Remember: The periodic table was arranged the way it was based on chemical properties.**
- **Totally empirical,**
  - **until now. Based only on observation.**



Periodic Table



- **Periodic table tells you about the last electron that went in!!!**
  - **Which will be the highest energy electron, most reactive**
- **Periodic table also makes it easy to do electron configurations.**

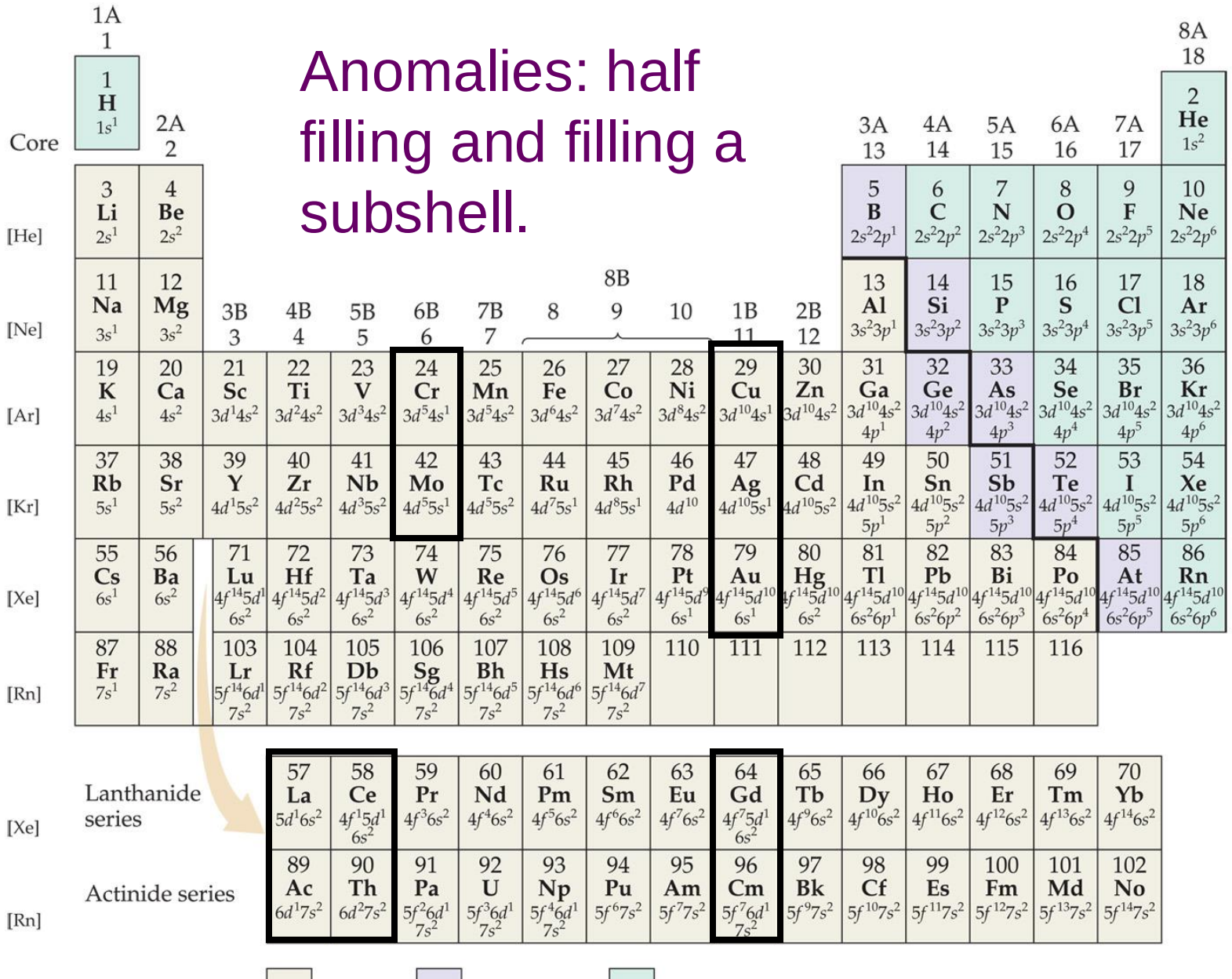
Short cut for writing electron configurations

TABLE 6.4 Electron Configurations of the Group 2A and 3A Elements

Group 2A	
Be	$[He]2s^2$
Mg	$[Ne]3s^2$
Ca	$[Ar]4s^2$
Sr	$[Kr]5s^2$
Ba	$[Xe]6s^2$
Ra	$[Rn]7s^2$
Group 3A	
B	$[He]2s^2 2p^1$
Al	$[Ne]3s^2 3p^1$
Ga	$[Ar]3d^{10} 4s^2 4p^1$
In	$[Kr]4d^{10} 5s^2 5p^1$
Tl	$[Xe]4f^{14} 5d^{10} 6s^2 6p^1$

Some Anomalies

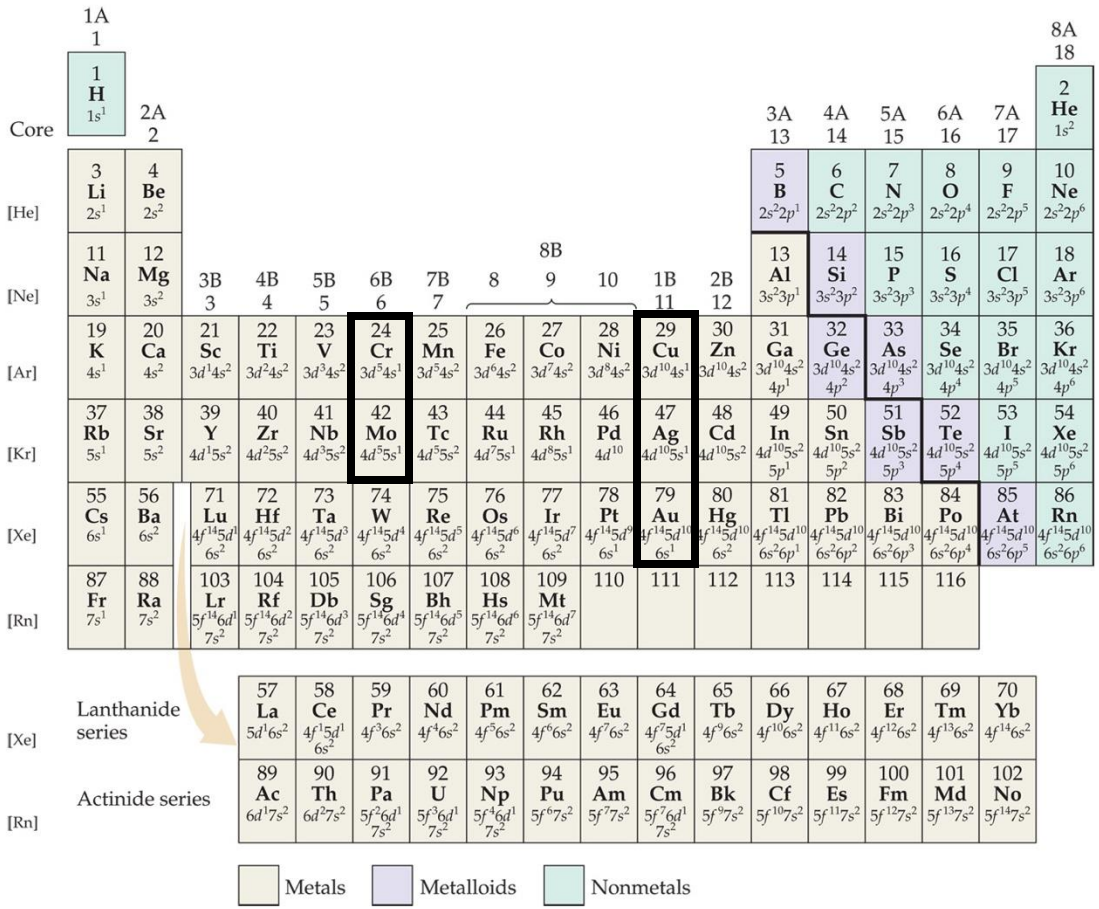
Anomalies: half filling and filling a subshell.



Cu: [Ar] $4s^1 3d^{10}$

Ag: [Kr] $5s^1 4d^{10}$

Some Anomalies



For instance, the electron configuration for Copper, is

[Ar] $4s^1$ $3d^{10}$

rather than the expected

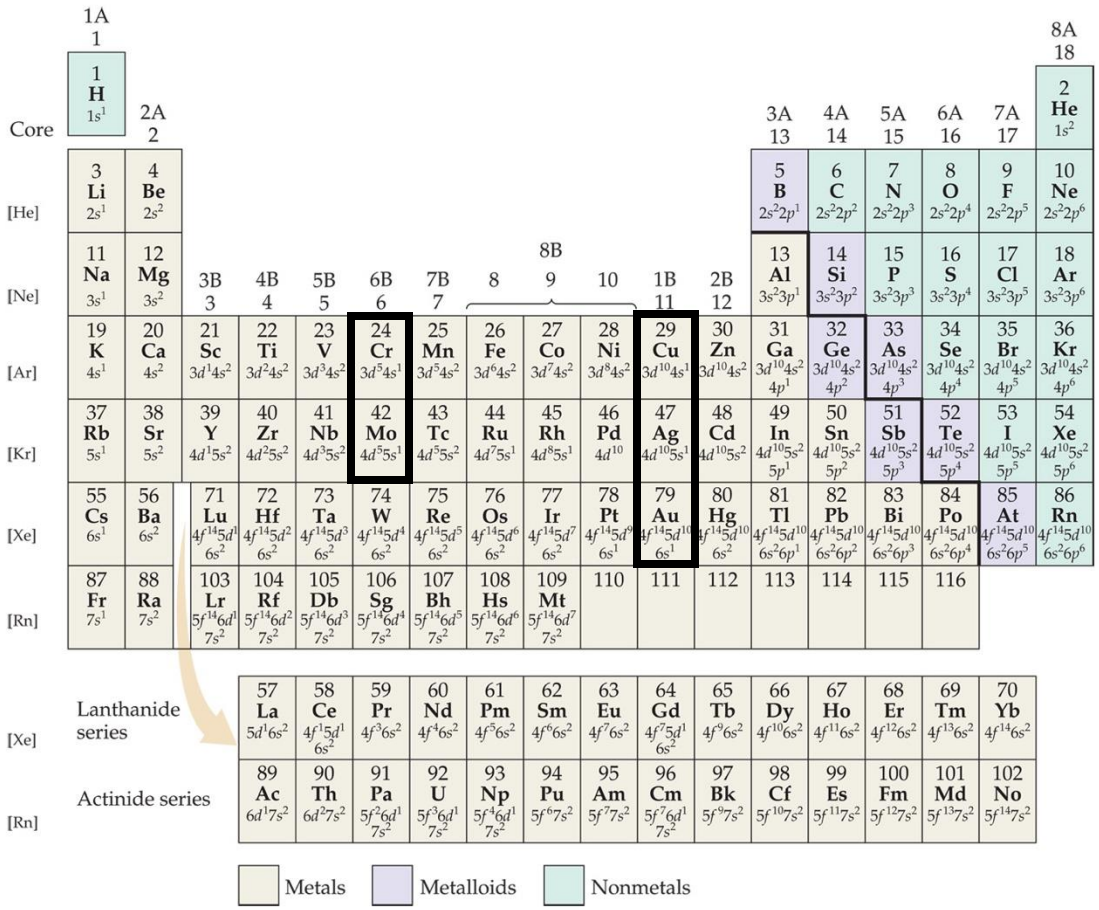
[Ar] $4s^2$ $3d^9$.

Filling d shell preferred.

Explains why:

Cu^{1+}, Ag^{1+}, Au^{1+} common ions.

Some Anomalies



And: the electron configuration for Chromium, is

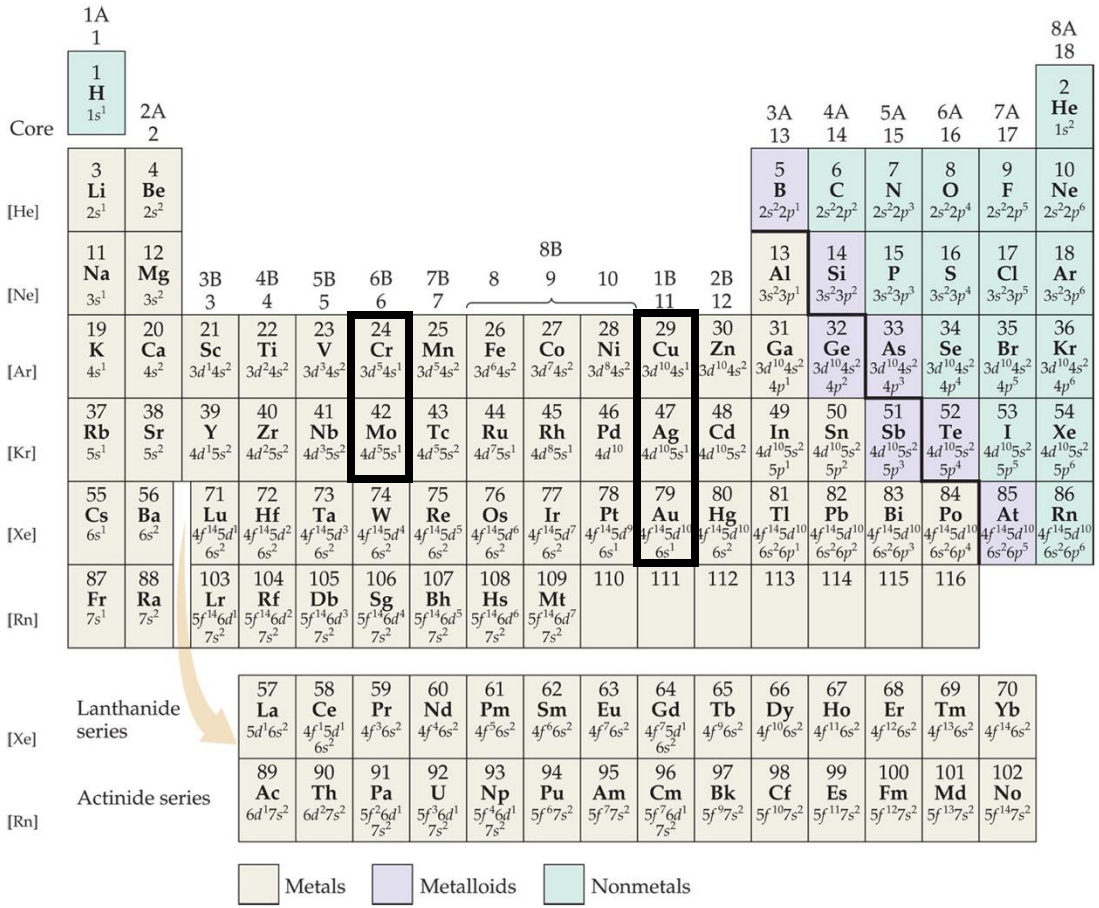
[Ar] $4s^1\ 3d^5$

rather than the expected

[Ar] $4s^2\ 3d^4$.

For exam: I don't care about these ones.

Some Anomalies



What's the electon configuration of Au^{1+} ion?

A. $[Xe]6s^2\ 4f^{14}\ 5d9$

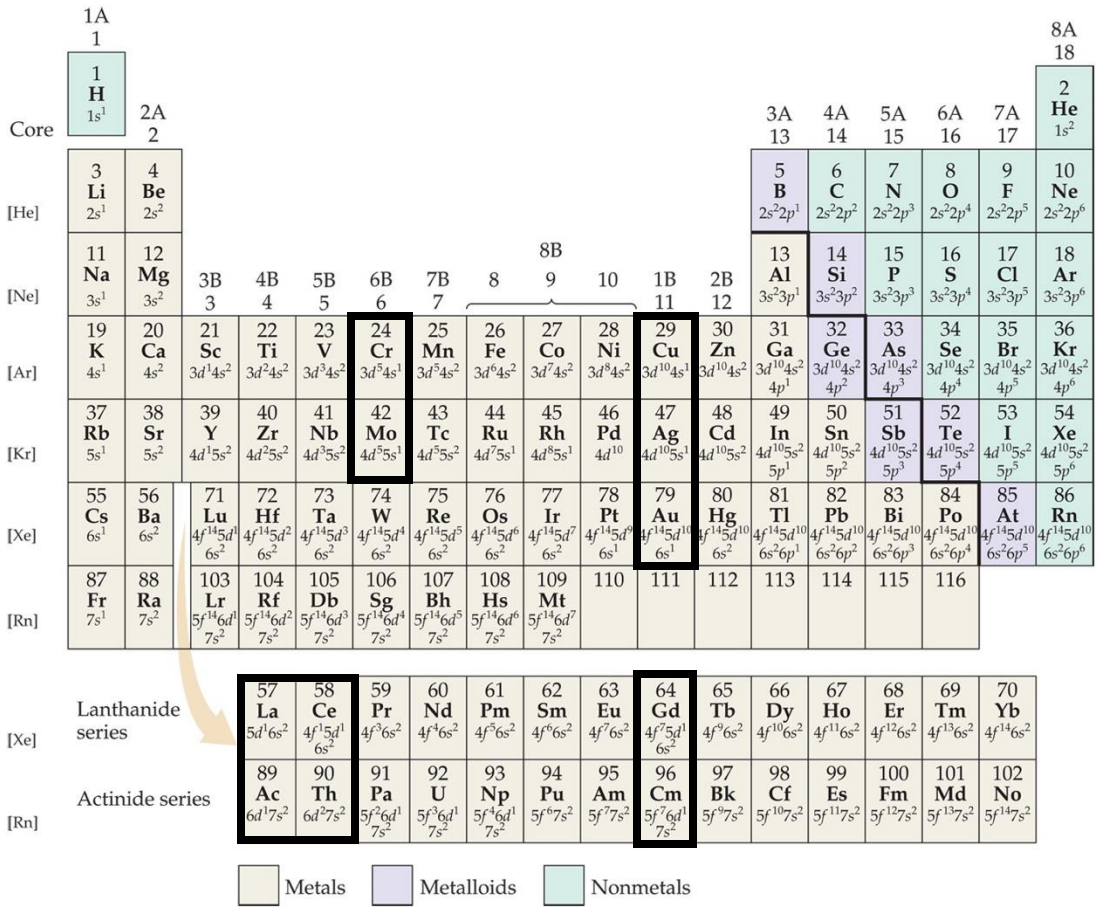
B. $[Xe]6s^2 5d^8$

C. $[Xe]6s^1 5d^9$

D. $[Xe]5d^{10}$

E. $[Xe]5d^9$

Some Anomalies



- This occurs because the 4*s* and 3*d* orbitals are very close in energy.
- These anomalies occur in *f*-block atoms, as well.
- Exam: NO F block anomalies!

The Nobel Prize 2024

- David Baker Demis Hassabis John M. Jumper
- Protein Design Protein structure prediction
  - » Using A.I./ machine learning
  - » Computer scientist
  - » Not chemists.

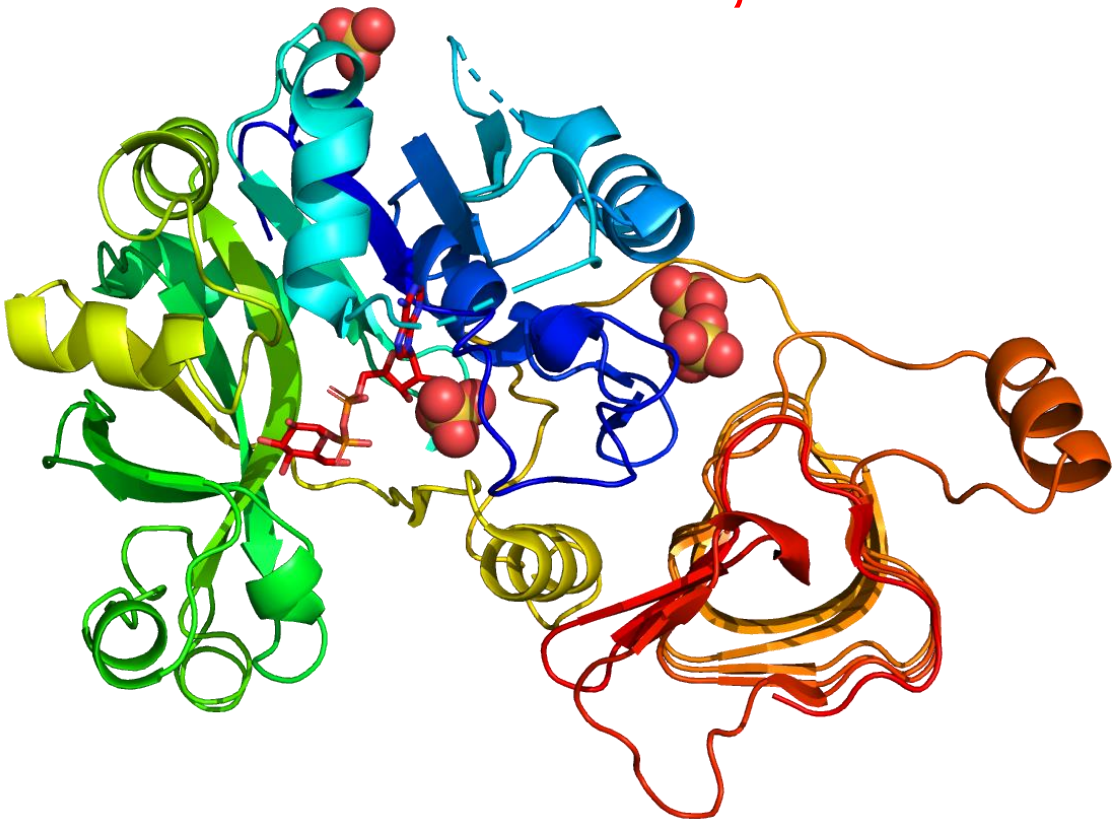
Predict 3D protein structure from amino acid sequence.

Turn this

Millions of sequences

MAVSDSQNSQTCLDPDASRSVLGI
ILGGGAGTRLYPLTKKRAKPAVPL
GANYRLIDIPVSNCLNSNISKIYV
LTQFNSASLNRHLSRAYASNMGGY
KNEGFVEVLAAQQSPENPDWFQGT
ADAVRQYLWLFEEHTVLEYLILAG
DHLYRMDYEKFIQAHRETDADITV
AALPMDEKRATAFGLMKIDEEGRI
IEFAEKPQGEQLQAMKVDTTILGL
DDKRAKEMPFIASMGIYVISKDVM
LNLLRDKFPGANDFGSEVIPGATS
LGMRVQAYLYDGYWEDIGTIEAFY
NANLGITKKPVPDFSFYDRSAPIY
TQPRYLPPSKMLDADVTDSVIGEG
CVIKNCKIHHSVVGLRSCISEGAI
IEDSLLMGADYYETDADRKLLAAK
GSVPIGIGKNCHIKRAIIDKNARI
GDNVKIINKDNVQEAARETDGYFI
KSGIVTVIKDALIPSGIII

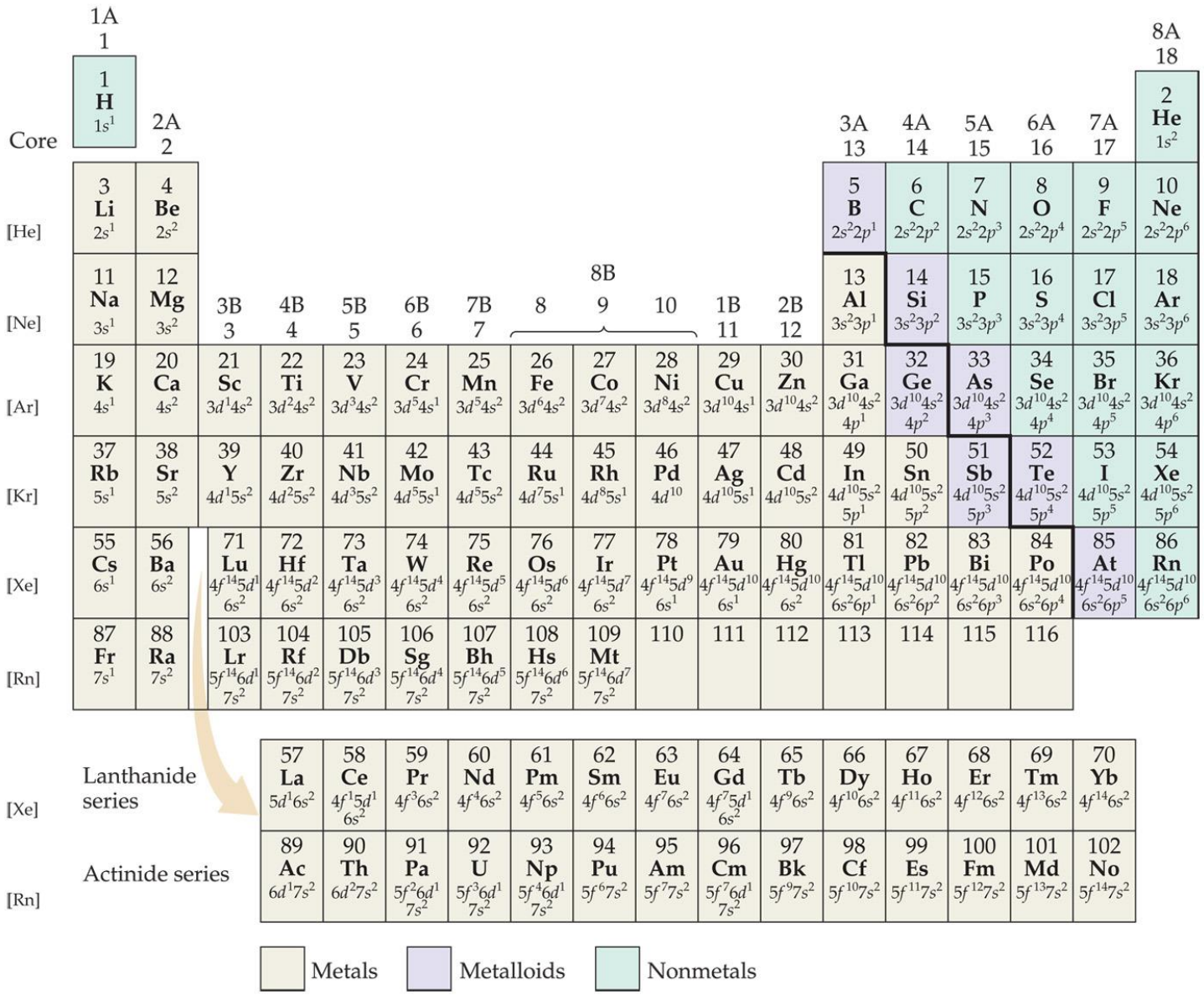
about 5,000 folds



how was this done?

Artificial Intelligence/
"Machine Learning"

Electron configurations of the elements



What's on the exam?

- Chapter 4, (essentially everything)
- Chapter 5 (everything)
- Chapter 6 everything

Chapter 4.

Solution stoichiometery

Strong vs. weak electrolytes

Know strong electrolytes

strong acids

soluble salts

precipitation reactions

Ionic equation

net ionic equation

Neutralization reactions

gas forming reactions

H_2CO_3 ---- CO_2 H2O

Chapter 4.

- Solution stoichiometery
  - Molarity
  - Dilution
  - Titration
  - Oxidation reduction
    - assigning oxidation numbers
    - who is oxidizing and reducing?
  - Activity series

Chapter 5

- Heat and work
- $E = q + w$
- H = q at constant P (q_P)
- Use ΔH_f to find ΔH_{rxn}.
- Calorimetry problems.
- Changes of state and heat.

Chapter 6

- History of Light
- $v=\lambda\nu$
- Electromagnetic radiation order
- Blackbody radiation
- Photo electric effect
- $E = h\nu$
- The uncertainty principle.
- Standing waves are quantized.

Chapter 6

- Standing waves are quantized.
- Quantum mechanics
  - Quantum numbers
    - n,l,m_l,s
    - $n=1,2,3,\ldots$
    - $l=0,1,2,3\ldots n-1$
    - $m_l=-l,\ldots 0,\ldots l$
    - $s=+1/2$ or $-1/2$
    - What's a shell? (all the orbitals/electrons in an E level
    - What's a subshell? (all the orbitals/electrons with same n and l (the 2s orbital, the three 4p orbitals etc.)
    - Shapes of orbitals and their nodes.
    - Energies of orbitals
    - How electrons are filled in any element.
    - How you can use the periodic table to know electron configuration

Test breakdown:

Ch. 4:

- Strong/weak electrolytes (1)
- Neutralization/titration (1)
- Assign/change in Ox Numbers (1)
- Activity series (1)

Ch. 5

Work calculation (1)

ΔH/ ΔE work/heat calculation (1)

Enthalpy of rxn via enthalpy of formation calc (1)

Enthalpy of phase change (1)

Calorimetry/specific heat (1)

CH 6.

$v=\lambda\nu$ (1)

$E=hv$ (1)

Photo electric effect (1)

EM radiation (1)

Quantum numbers (1)

Shells subshells (2)

Electron configurations (3)

Shape of orbitals (1)

- Which of the following types of electromagnetic radiation has the highest energy?
  - a. microwaves
  - b. infrared
  - c. ultraviolet
  - d. X-rays

  Which species is neither reduced nor oxidized in the following reaction
  $AgCl(s) + Na \rightarrow Ag(s) + NaCl$
  a. Ag
  b. Ag^+
  c. Na
  d. Na^+
  e. Cl^-

- How many electrons are there in the 3p sub shell of Argon (Ar)?
- a. 2 c. 6
- b. 4 d. 8

- How many unpaired electrons does an oxygen atom (0) have?
- a. 0
- b. 1
- c. 2
- d. 3
- e. 4

- Which of the following types of electromagnetic radiation has the highest energy?
  - a. microwaves
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  $AgCl(s) + Na \rightarrow Ag(s) + NaCl$
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  c. Na
  d. Na^{+s}
  e. Cl^{-}

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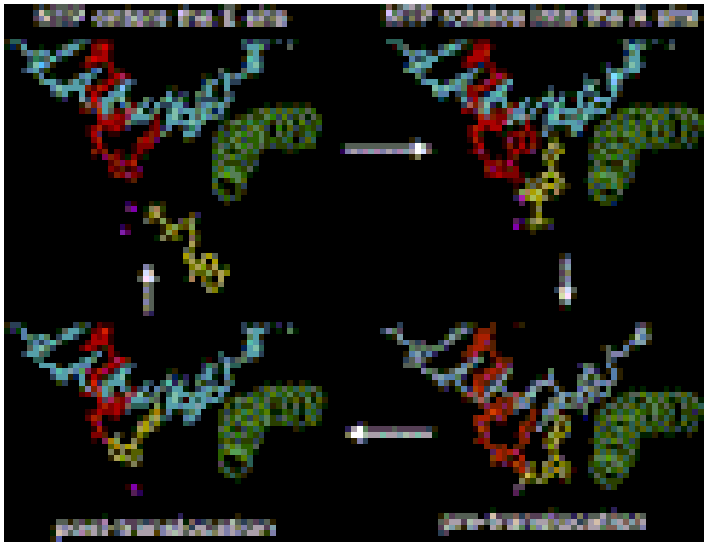
- How many unpaired electrons does an oxygen atom (0) have?
- a. 0
- b. 1
- c. 2
- d. 3
- e. 4

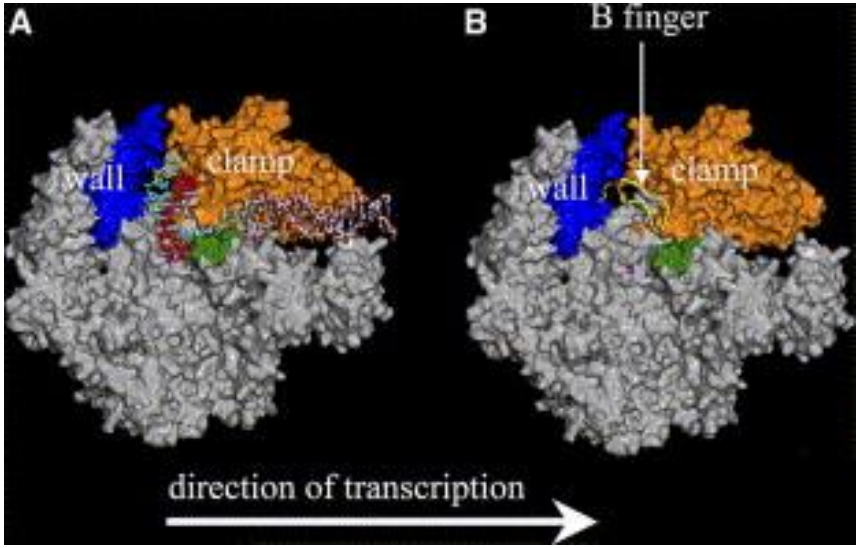
The Nobel Prize in Chemistry 2008

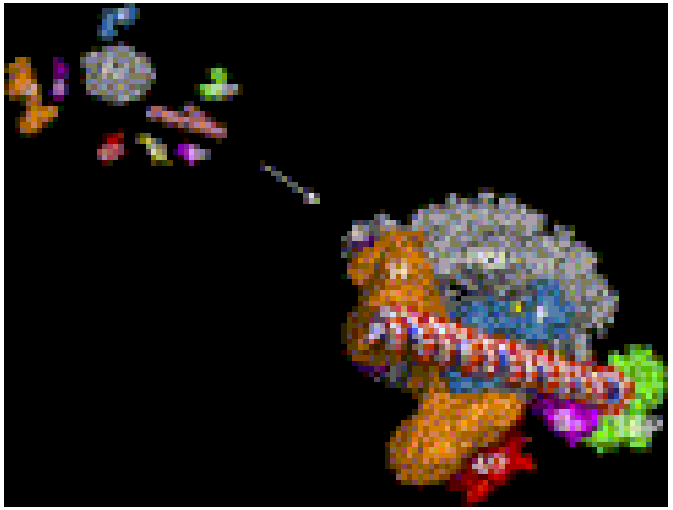
Roger Kornberg

X-ray crystallography

How does RNA Pol II decode DNA into RNA?

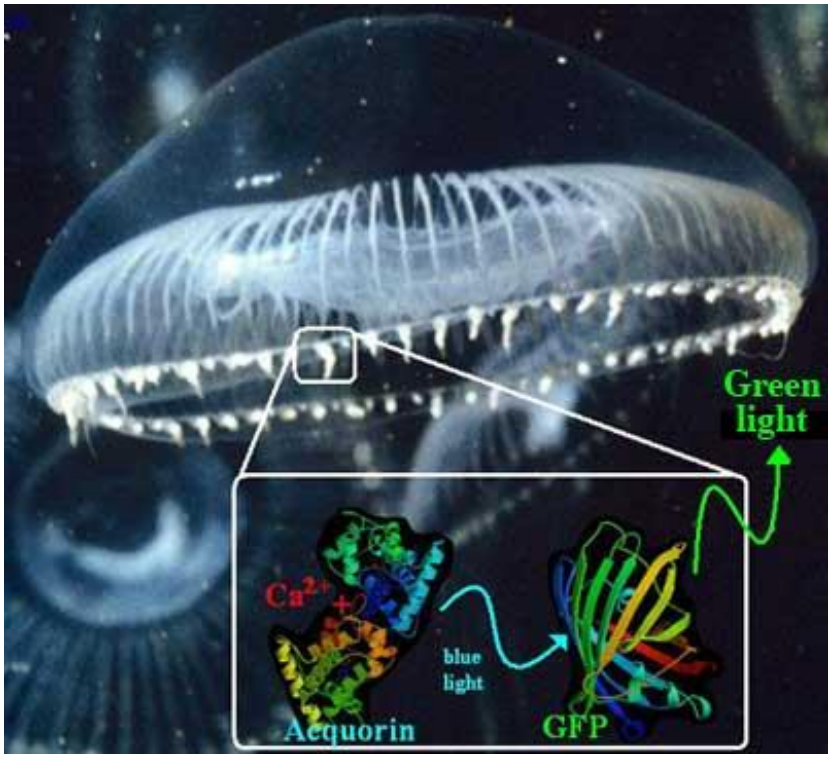




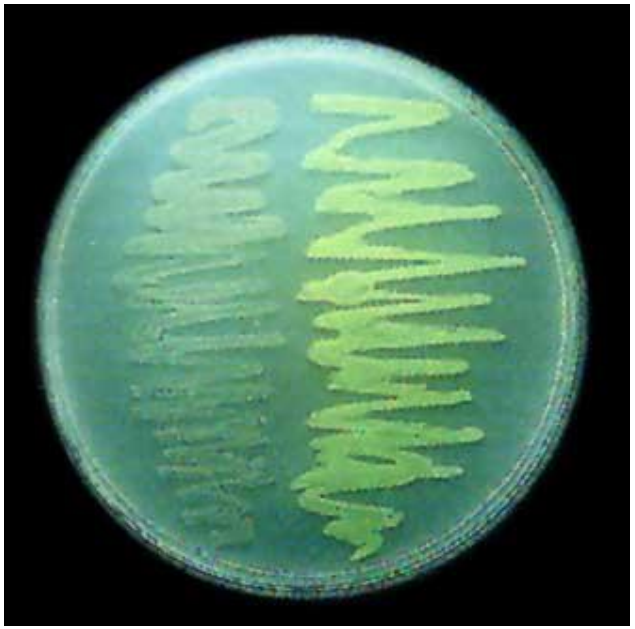


Nobel Prize in Chemistry

- Green Fluorescent protein



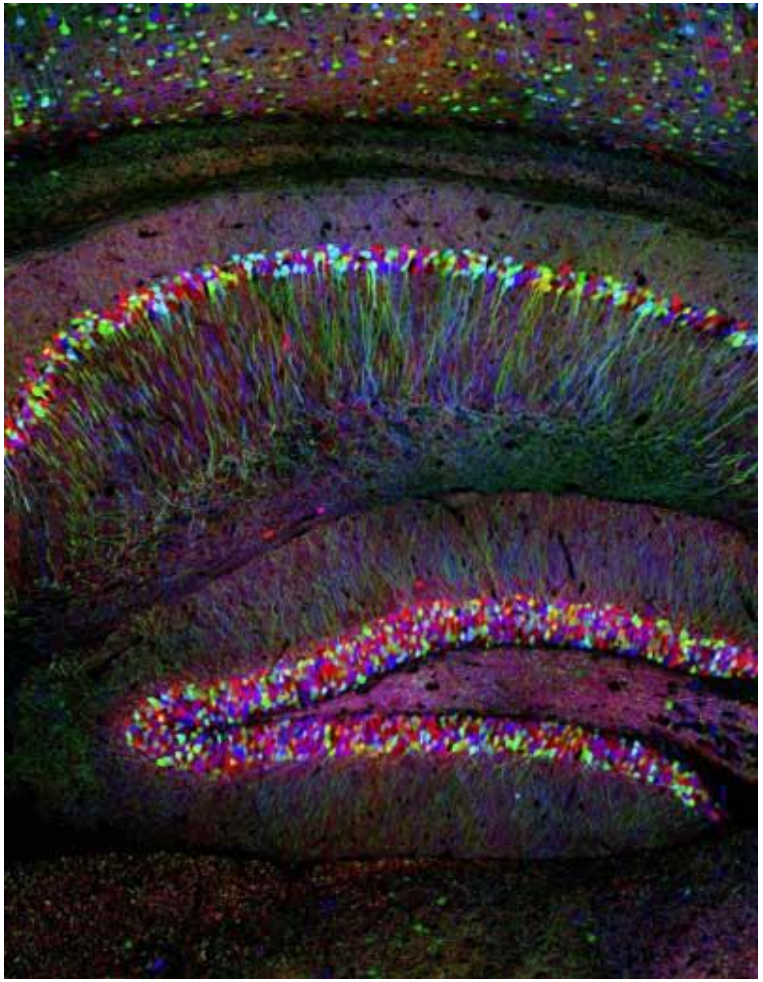
Osamu Shimonura



Marty Chalfie

GFP

Roger Tsien



Cerebral cortex
Tsien/Chalfie
Lictman/Sanes

Gunpowder

$$10\ KNO_3 + 3\ S + 8\ C \rightarrow 2\ K_2CO_3 + 3\ K_2SO_4 + 6\ CO_2 + 5\ N_2.$$