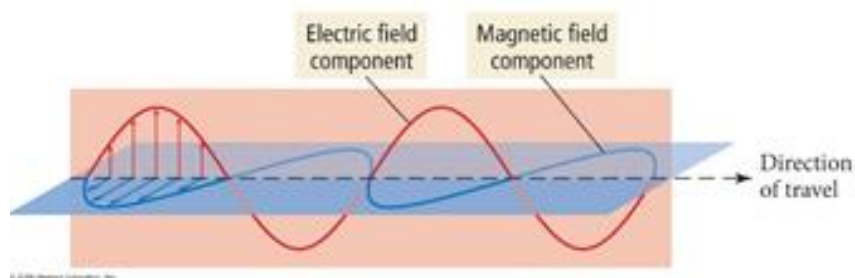
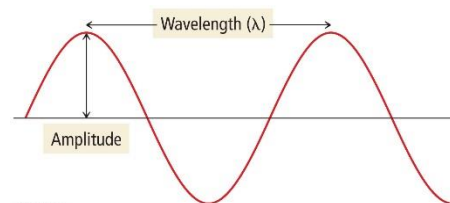


WAVE NATURE OF LIGHT

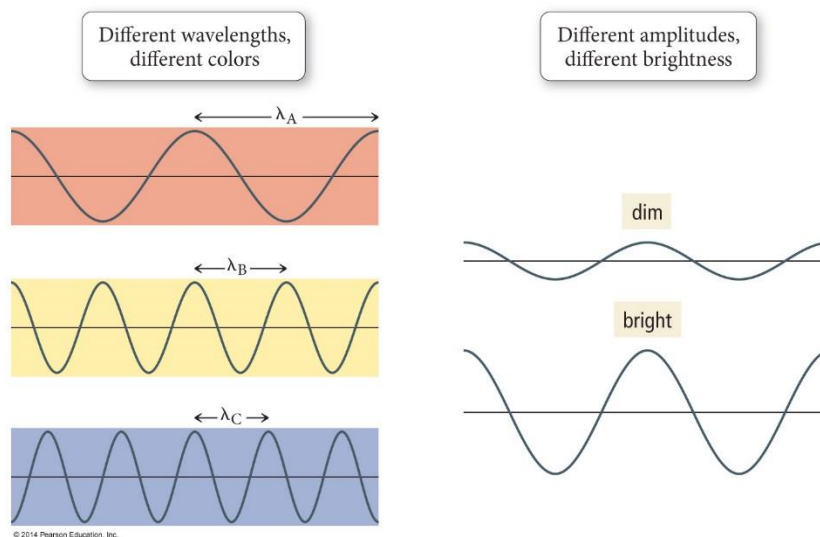
- Light is **electromagnetic radiation**, a type of energy composed of oscillating electric and magnetic fields. The fields oscillate perpendicular to each other. In vacuum, these waves travel at a speed of 3.00×10^8 m/s.



- Waves can be characterized by their **amplitude** or **wavelength** (λ). Wavelength is the distance between adjacent crests. Wavelength is measured in units such as meters, micrometers or nanometers.



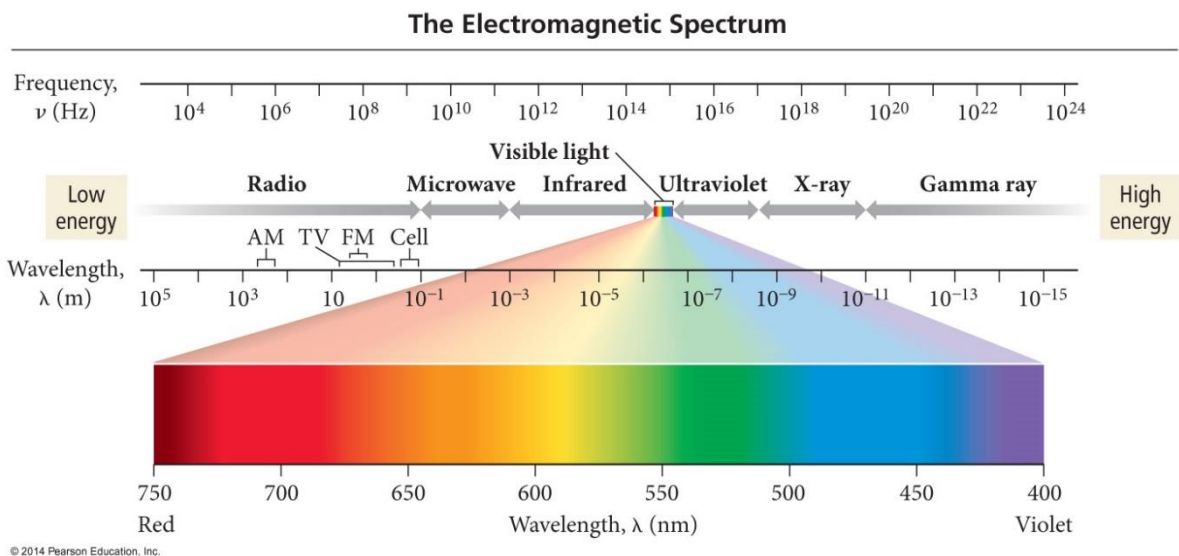
- Wavelength and amplitude are independent properties of light. Amplitude determines light's intensity, while wavelength determines light's color.



- Light is also characterized by its **frequency** (ν), the number of waves crests that pass through a stationary point in a given period of time. The units of frequency are waves/second (s^{-1}) or hertz (Hz).

ELECTROMAGNETIC SPECTRUM

- Visible light is a small portion of the entire *electromagnetic spectrum*, which includes all wavelengths of electromagnetic radiation. These waves include long-wavelength low-frequency waves (radio waves) and short-wavelength, high-frequency waves (gamma rays).

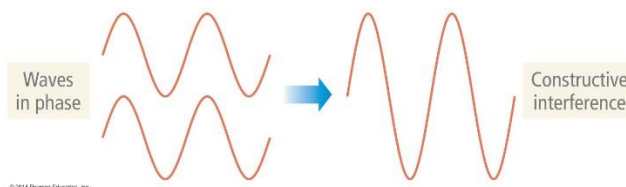


Examples:

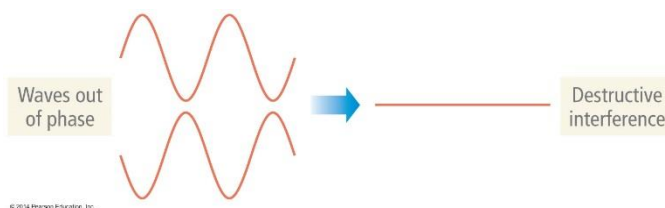
- Arrange the 3 types of radiation—visible light, X-ray and microwave—in order of increasing:
 - wavelength
 - frequency
 - energy
- Arrange the 3 colors of visible light—green, red and blue—in order of increasing:
 - wavelength
 - frequency
 - energy

INTERFERENCE & DIFFRACTION

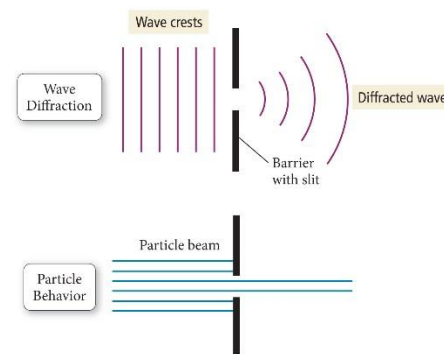
- Waves interact with one another in a characteristic way, called **interference**, by adding or cancelling one another depending on their alignment upon interaction. For example, when two waves of equal amplitude align with each other **in phase**—align with overlapping crests—a wave of twice the amplitude results. This is called **constructive interference**.



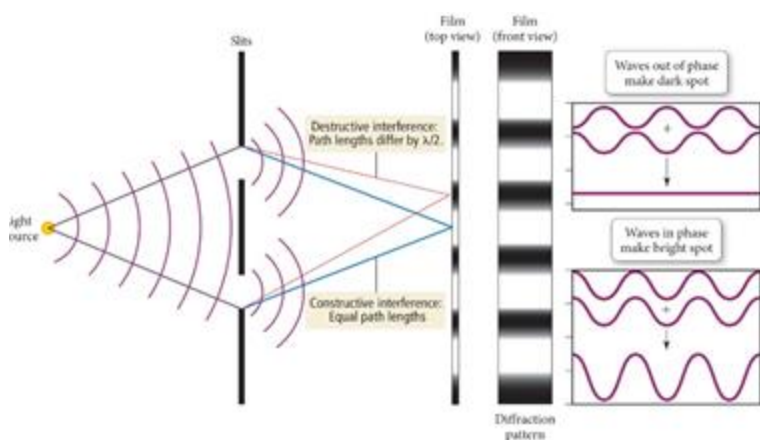
- On the other hand, if the two waves are completely out of phase when they interact—align so that crest of one aligns with trough of the other—the waves cancel by **destructive interference**.



- Another characteristic behavior waves exhibit is called **diffraction**. When waves encounter an obstacle or a slit that is comparable in size to its wavelength, it bend (or diffracts) around it.



- Encountering similar situation, particles, by contrast, do not diffract and pass through the slit.
- The diffraction of light through two slits separated by a small distance, coupled with interference, results in a very characteristic pattern, called **interference pattern**.



PARTICLE NATURE OF LIGHT

- Prior to 1900, light was considered to be purely a wave phenomenon, and its behavior was adequately described by classical electromagnetic theory. However, a number of discoveries in early 1900 brought the classical view of light into question.
- One such discovery was the *photoelectric effect*, the observation that metals emit electrons when light shines upon them. Classic electromagnetic theory attributed this effect to transfer of energy from light to the electron and its dislodgement.
- According to this explanation, only the amplitude (intensity) of the light affected the emission of electrons, not the wavelength. Therefore, it was expected that photoelectric effect would be low with dim light and increase with increased intensity of light.
- Furthermore, dim light would be expected to have a lag time before the initial shining of the light and the dislodgment of the electrons. This lag time would be the minimum time necessary for the dim light to transfer sufficient energy to the electron to dislodge it.
- The experimental results, however, did not support this prediction. Scientists found that a high-frequency, low-intensity light produced electrons without the lag time. Furthermore, the light used to dislodge the electrons exhibits a *threshold frequency*—a frequency below which no photoelectric effect occurs, no matter how high the amplitude or how long the light shines.
- In 1905, Albert Einstein proposed an explanation for the photoelectric effect: light energy must come in fixed amounts (*quantum*). According to Einstein, the energy of light is proportional to its frequency, as shown:

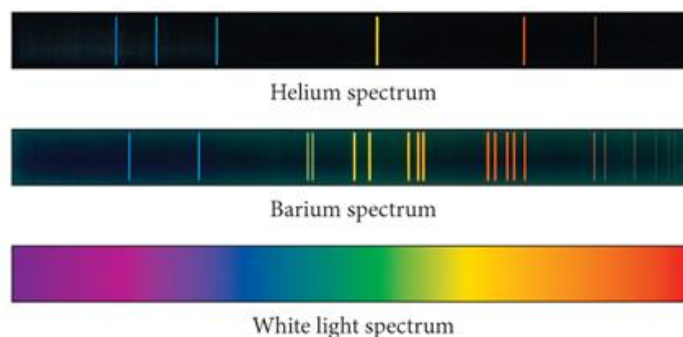
$$E = h \nu \quad \text{where } h, \text{ called Planck's constant} = 6.626 \times 10^{-34} \text{ Js}$$

- A quantum of light is also called a *photon*. The energy of a photon of light can also be expressed in terms of its wavelength:

$$E = \frac{hc}{\lambda}$$

ATOMIC SPECTROSCOPY

- When an atom absorbs energy—in the form of light, heat or electricity—it re-emits the energy as light. A neon light is an example of this effect.
- Close inspection of the light emitted by various atoms reveals that it contains several distinct wavelengths and colors. The components of the light emitted by the atom can be separated by passing the light through a prism. The result is a series of bright lines called an *emission spectrum*. The emission spectrum of a particular element is always the same.



- Note that the white light spectrum is continuous, while the atomic spectra contain only certain wavelengths. Classical physics could not explain why these spectra contained discrete lines.
- Johannes Rydberg, a Swedish mathematician, analyzed many atomic spectra and developed an equation that predicts the wavelengths of the hydrogen emission spectrum. However, this equation (shown below), did not explain why atomic spectra are discrete.

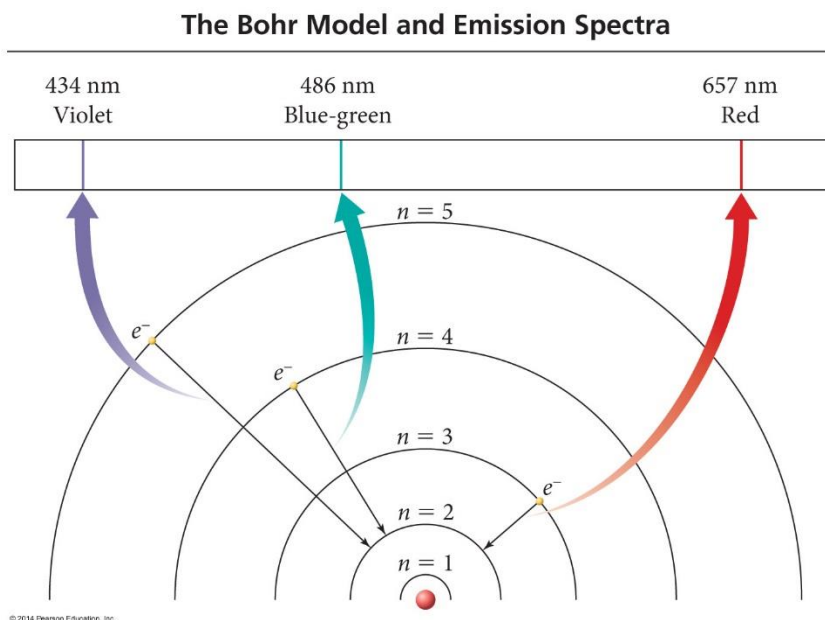
$$\frac{1}{\lambda} = R \left(\frac{1}{m^2} - \frac{1}{n^2} \right) \quad \text{where } R = 1.097 \times 10^7 \text{ m}^{-1}$$

Examples:

1. Calculate the wavelength of light produced when $m=2$ and $n=4$.

BOHR MODEL OF ATOM

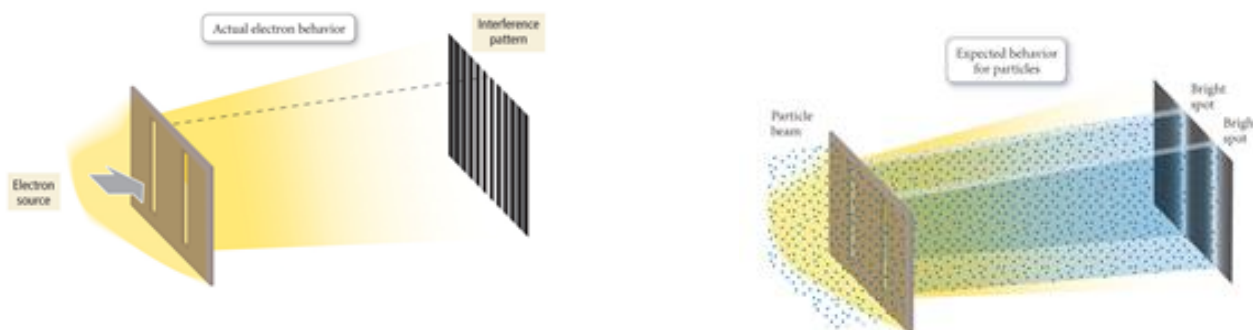
- **Neils Bohr**, a Danish physicist, studied the hydrogen atom extensively, and developed a model for the atom that was able to explain the atomic spectra.
- **Bohr's model** of the atom consisted of electrons orbiting in circular orbits (analogous to planetary orbits around the sun). However, unlike the planetary orbits—which can exist at any distance from the sun—Bohr's orbits exist only at specific, fixed distances from the nucleus. Bohr called these orbits **stationary states**.
- Bohr further proposed that electrons only emit energy when they transition—jump—between orbits. The emission spectrum of an atom consists of discrete lines because the energy of the photon emitted when an electron makes a transition can only be of certain values depending on the difference in the energy of the stationary states. Three of these transitions for the hydrogen atom are shown below:



- In spite of its initial success in explaining the line spectrum of the hydrogen atom, the Bohr model left many unanswered questions. However, it did serve as an intermediate model between the classical view of the electron (particle) and a quantum-mechanical view (particle and wave).
- Bohr model was later replaced with a more thorough quantum-mechanical model that fully incorporates the wave nature of the electron.

WAVE NATURE OF MATTER

- Earlier we described diffraction and interference as characteristic behaviors of waves as they pass through a slit. Similar experiments with electrons passing through two slits resulted in the same interference patterns as observed with light.



- The interference pattern observed with the electrons in these experiments were similar to that expected of waves and not particles. Furthermore, the interference pattern observed with electrons is not caused by pairs of electrons interfering with each other, but rather single electrons interfering with themselves.
- These experimental results led to the proposal by Louis de Broglie in 1924 that electrons—originally thought of as particles—also possesses a wave nature, and its wavelength is related to its kinetic energy by the **de Broglie equation**:

$$\lambda = \frac{h}{mv} \quad \text{where, } h = \text{Planck's constant}$$

$m = \text{mass of electron}$
 $v = \text{velocity of electron}$

- Based on the de Broglie equation, the velocity of a moving electron is related to its wavelength—knowing one is equivalent to knowing the other.
- If de Broglie’s proposal is correct and electrons travel in waves, then they should also exhibit the wave properties of diffraction and interference. A fast moving electron has a wavelength of about 10^{-10} m, so the “perfect” slit would be the natural spacing between crystals in an atom.
- In 1927, C. Davisson and L. Germer guided a beam of electrons at a nickel crystal and obtained an electron diffraction pattern. This experimental observation proved that electrons—particles with mass and charge—create diffraction patterns, just as electromagnetic waves do.
- Although electrons do not have orbits of fixed radius, as de Broglie thought, the energy levels of atoms are related to the wave nature of the electron.

WAVE NATURE OF MATTER

- The table below lists the calculated de Broglie wavelength of several objects.

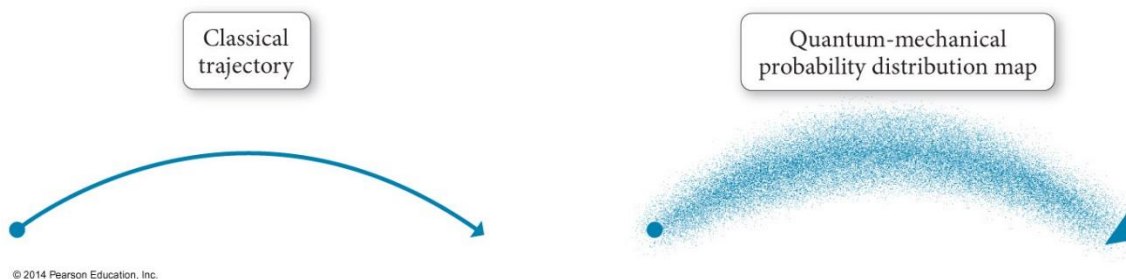
<i>Substance</i>	<i>Mass (g)</i>	<i>Velocity (m/s)</i>	<i>λ (m)</i>
Slow electron	9×10^{-28}	1.0	7×10^{-4}
Fast electron	9×10^{-28}	5.9×10^6	1×10^{-10}
Alpha particle	6.6×10^{-24}	1.5×10^7	7×10^{-15}
Baseball	142	25.0	2×10^{-34}
Earth	6.0×10^{27}	3.0×10^4	4×10^{-63}

Examples:

- If an electron has a velocity of 5.0×10^5 m/s, what is its wavelength in nm?
- What is the velocity of an electron that has a wavelength approximately the length of a chemical bond (1.2×10^{-10} m)?
- Protons can be accelerated to speeds near that of light in particle accelerators. Estimate the de Broglie wavelength (in nm) of such a proton moving at 2.90×10^8 m/s. (mass of a proton = 1.673×10^{-27} kg).

UNCERTAINTY PRINCIPLE

- The wave nature of the electron is difficult to reconcile with its particle nature. How can a single entity behave both as a wave and as a particle?
- To answer this and other related questions, experiments have been done with a single electron aimed at a double slit to observe its properties and determine which slit the electrons passes through. Results of these experiments indicate a very odd occurrence: no matter how hard one tries or whatever method one uses, one cannot both see the interference pattern and simultaneously determine which slit the electron passes through.
- The wave and particle properties of the electron are said to be complimentary properties—they exclude one another. As a result, the more we know about one of them, the less we know about the other, and which property we observe depends on the type of experiment performed. In quantum mechanics, the observation of an event affects its outcome.
- Based on the de Broglie equation, the velocity of an electron is related to its wave nature. The position of an electron, however, is related to its particle nature. Consequently, the inability to observe the wave and particle nature of electron simultaneously means that we cannot simultaneously measure its velocity and position. This is referred to as the *Heisenberg's uncertainty principle*.
- Whereas a classical particle moves in a predicted path and has a defined trajectory, the path of an electron can only be defined by a probability map—a statistical picture of where the electron is most likely to be found. The darker shadings in the probability map indicate greater probability of finding an electron in that region.



<p style="text-align: center;">QUANTUM MECHANICS & THE ATOM</p>
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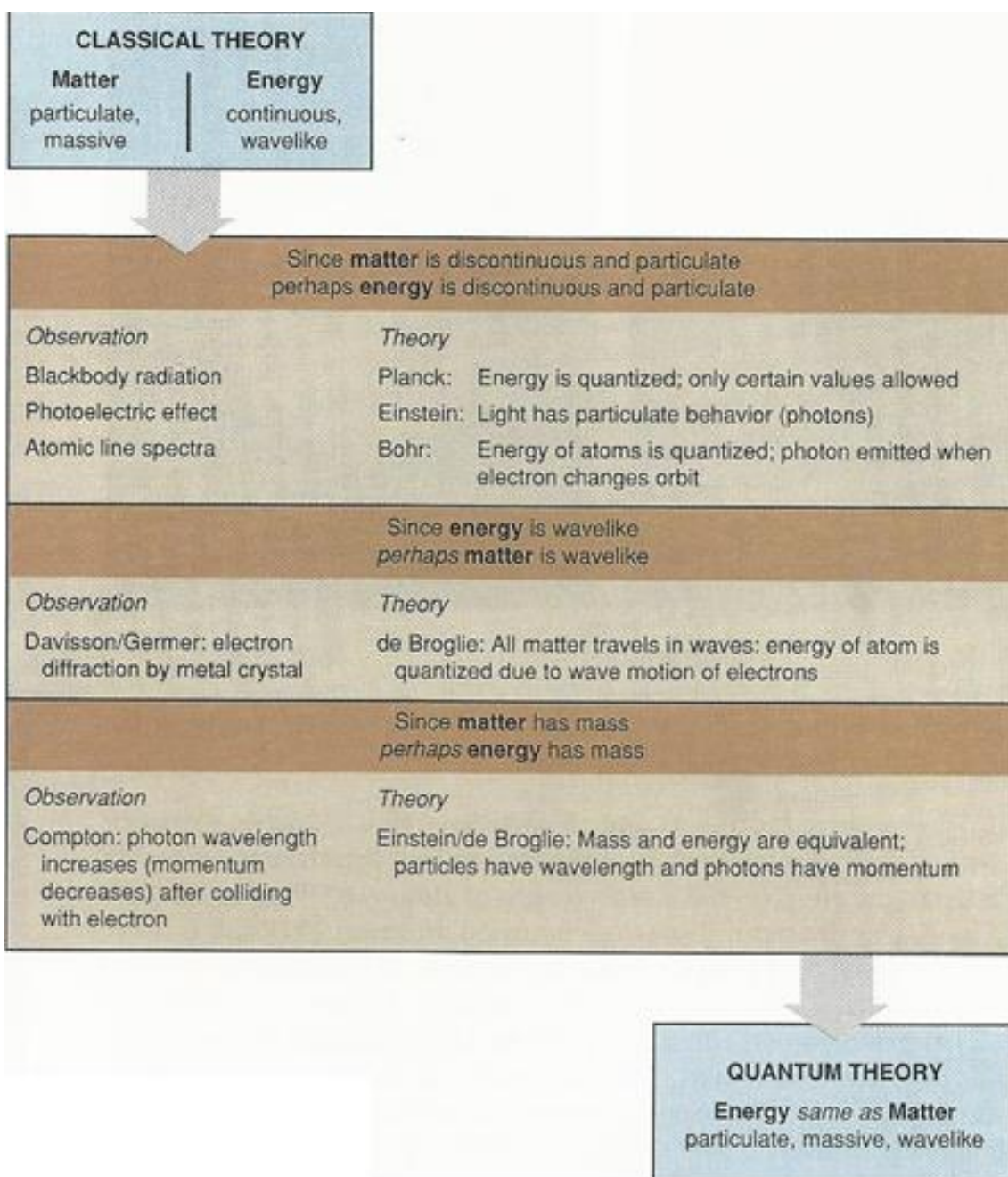
- Recall that the position and velocity of an electron are complementary properties—if we know one accurately, the other becomes indeterminate.
- Since velocity is directly related to energy, position and energy are also complementary properties—the more we know about one, the less we know about the other.
- Many properties of an element depends on the energies of its electrons. For example, whether an electron is transferred from one atom to another to form an ionic bond depends on the relative energies of the electron in the two atoms.
- Because of the complementary nature of position and energy of an electron, we can specify the energy of an electron precisely, but its position can only be described in terms of a probability distribution map, called *orbital*, where the electron is likely to be found.
- The mathematical derivation of energies and orbitals for electrons in atoms comes from solving the Shrodinger equation for the atom of interest. The Shrodinger equation is quite complex because the electron's matter-wave properties occur in 3-dimensional space and is continuously influenced by the nuclear charge. A simplified form of this equation is shown below:

$$\mathcal{H}\psi = E\psi$$

- In this equation, E represents the energy of the atom; the symbol ψ (psi) is called a *wave function* and describes the wavelike nature of the electron; and \mathcal{H} represents a complex set of mathematical operations that, when carried out at a particular ψ , yields an allowed energy state.
- Each solution to the equation is associated with a particular wave function, also called an atomic orbital. Each orbital is specified by three interrelated *quantum numbers*:
 - principal quantum number (n)
 - angular momentum quantum number (l)
 - magnetic quantum number (m_l)
- These quantum numbers all have integer values, and will be discussed in detail individually.

SUMMARY

- The chart below summarizes the major observations and theories leading from classical theory to quantum theory. As happens often in science, an observation (experiment) stimulates the need for an explanation (theory), and/or a theoretical insight provides the impetus for an experimental test.



QUANTUM NUMBERS

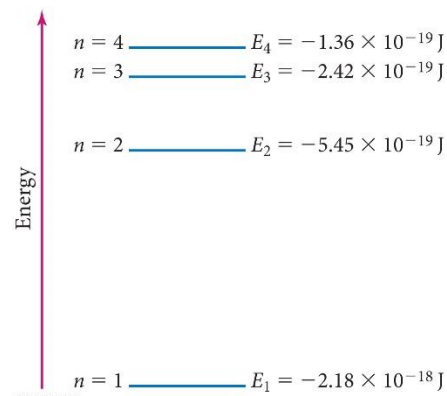
- An atomic orbital is specified by three quantum numbers that are associated, respectively, with orbital's size, shape and orientation in space.
- The quantum numbers have a hierarchical relationship: the size-related number limits the shape-related number, which limits the orientation-related number.

The Principal Quantum Number (n):

- This quantum number is an integer that determines the overall size and energy of an orbital. Its possible values are $n=1, 2, 3, \dots$ and so on.
- For hydrogen, the energy of an electron in an orbital with quantum number n is given by the equation:

$$E_n = -2.18 \times 10^{-18} \text{ J} \left(\frac{1}{n^2} \right) \quad (n=1, 2, 3, \dots)$$

- The energy is negative, because the electron's energy is lowered by its interaction with the nucleus. The constant $2.18 \times 10^{-18} \text{ J}$ is called the Rydberg constant for hydrogen (R_H).
- Orbitals with higher values of n have greater energies (less negative), as shown in the energy level diagram. Note also, that as n increases, the spacing between the energy levels becomes smaller.



The Angular Momentum Quantum Number (l):

- This quantum number (also called azimuthal) is an integer that determines the shape of the orbital. The possible values of l are $0, 1, 2, \dots, (n-1)$. For example, if $n=1$, then the only possible value of l is 0; if $n=2$, the possible values of l are 0 and 1. To avoid confusion between n and l , values of l are assigned letters, shown below:

Value of l	Letter Designation
$l = 0$	s
$l = 1$	p
$l = 2$	d
$l = 3$	f

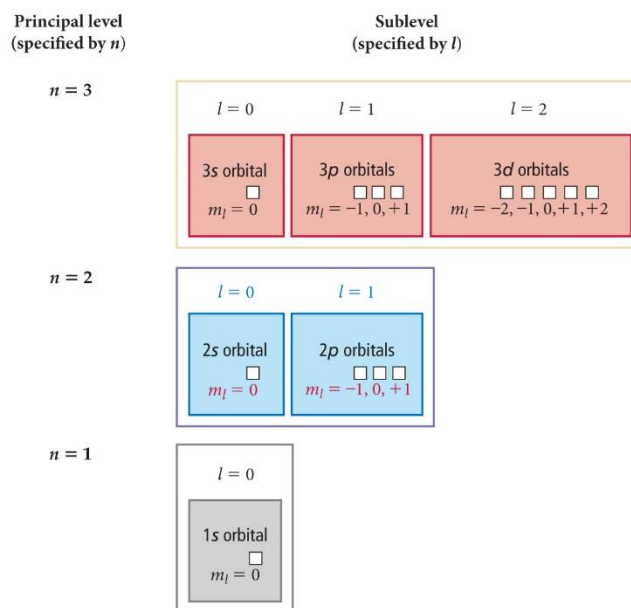
QUANTUM NUMBERS

The Magnetic Quantum Number (m_l):

- This quantum number is an integer that specifies the orientation of the orbital. The possible values of m_l are integer values (including zero) ranging from $-l$ to $+l$. For example, if $l = 1$, then m_l are -1 , 0 and $+1$.
- The chart below shows the hierarchy of quantum numbers for atomic orbitals:

NAME, SYMBOL (PROPERTY)	ALLOWED VALUES	QUANTUM NUMBERS
Principal, n (size, energy)	Positive integer (1, 2, 3, ...)	1, 2, 3
Azimuthal, l (shape)	0 to $n - 1$	For $n=1$: 0 For $n=2$: 0, 1 For $n=3$: 0, 1, 2
Magnetic, m_l (orientation)	$-l, \dots, 0, \dots, +l$	For $n=1, l=0$: 0 For $n=2, l=0$: 0 For $n=2, l=1$: -1, 0, +1 For $n=3, l=0$: 0 For $n=3, l=1$: -1, 0, +1 For $n=3, l=2$: -2, -1, 0, +1, +2

- Each specific combination of the 3 quantum numbers specifies one atomic orbital. For example, the orbital with $n=1$, $l=0$ and $m_l=0$ is known as 1s orbital.
- Orbitals with the same values of n are said to be in the same principal level. Orbitals with the same value of n and l are said to be in the same sublevel.
- The orbitals (and their corresponding quantum numbers) in the first three principal levels are shown on the right.



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QUANTUM NUMBERS

Examples:

1. Write l and m_l values for $n=4$.

2. Supply the missing quantum number(s) or sublevel names below:

<u>n</u>	<u>l</u>	<u>m_l</u>	<u>Name</u>
?	?	0	4p
2	1	0	?
3	2	-2	?
?	?	?	2s

3. Each set of quantum numbers below is supposed to specify an orbital. However, each set contains one quantum number that is not allowed. Replace the quantum number that is not allowed with one that is allowed.

a) $n=3$; $l=3$; $m_l=+2$

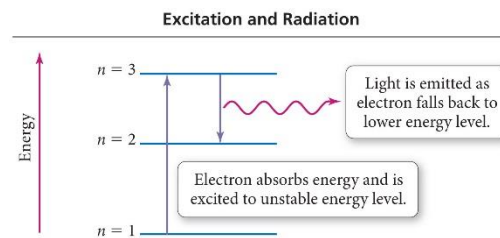
b) $n=2$; $l=1$; $m_l=-2$

c) $n=1$; $l=1$; $m_l=0$

4.

ATOMIC SPECTRA & QUANTUM THEORY

- Quantum theory explains the atomic spectra that was discussed earlier. When an atom absorbs energy, an electron in a lower energy orbital is excited to a higher energy orbital.
- As a result, the atom becomes unstable, and quickly returns to a lower energy orbital, releasing a photon of light containing an amount of energy equal to the energy difference between the two energy levels.
- The difference in the energy between the two levels is given by:

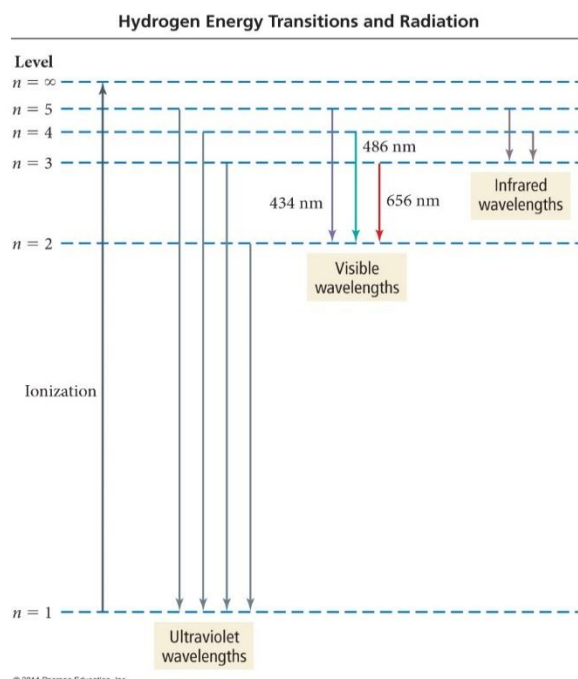


$$\Delta E = E_{\text{final}} - E_{\text{initial}}$$

- Using the equation introduced earlier for calculating the energy of an electron in any orbital, we can arrive at the following relationship:

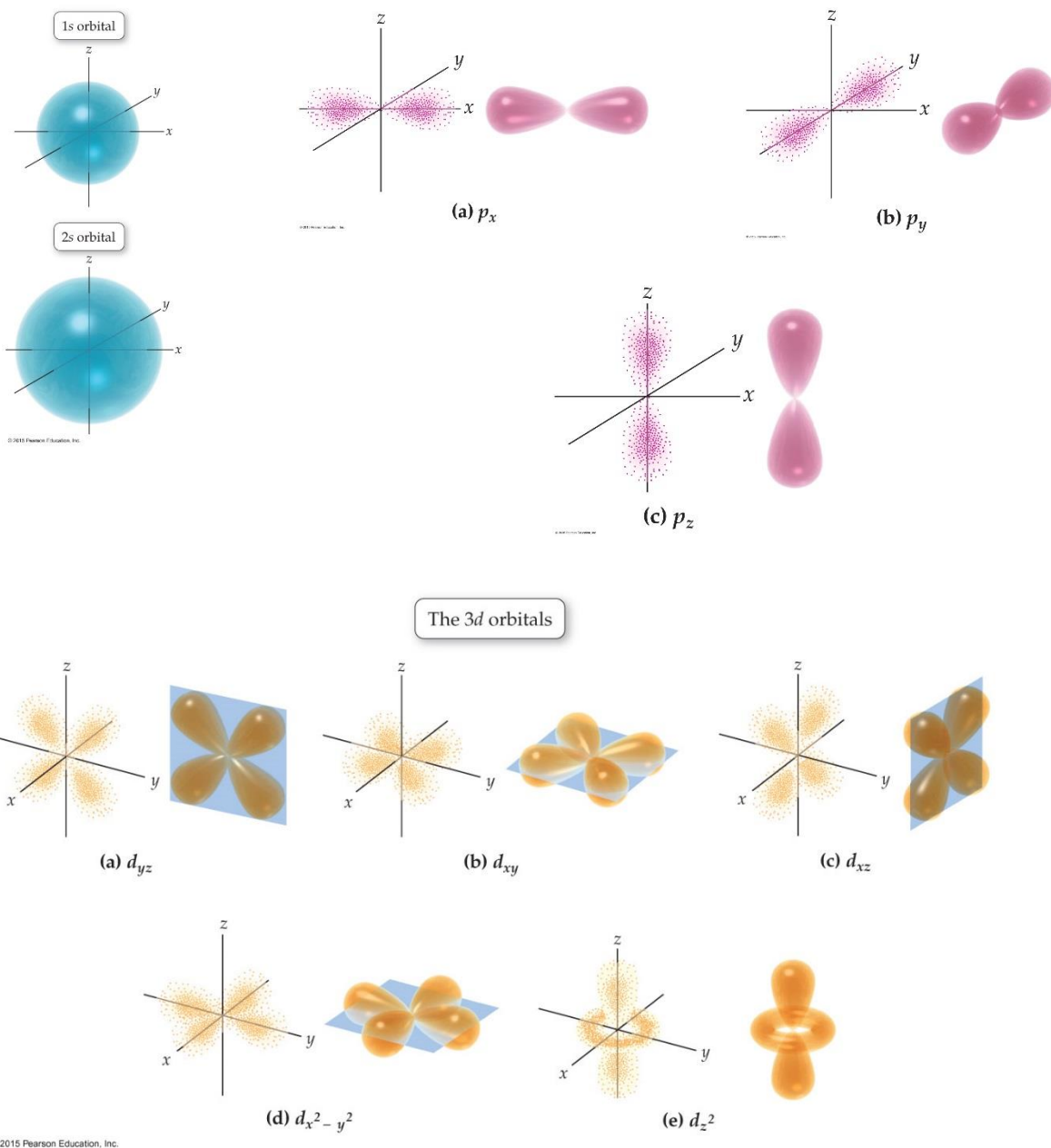
$$\Delta E = -2.18 \times 10^{-18} \text{ J} \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right)$$

- The Rydberg equation can be derived from the relationship above and the relationship discussed earlier between the wavelength and the energy of light.
- Several of the transitions in the hydrogen atom and their corresponding wavelengths are shown below. Note that transitions between orbitals that are further apart in energy produce light that is higher in energy and shorter in wavelength than transitions between orbitals closer together.



ORBITAL SHAPES

- Each orbital type can be represented by a geometric shape that encompasses the volume where the electron is likely to be found.
- These shapes for the s, p and d orbitals are shown below:



ANSWERS TO IN-CHAPTER PROBLEMS:

<i>Page</i>	<i>Example No.</i>	<i>Answer</i>
2	1	649 nm
	2	$5.83 \times 10^{14} \text{ s}^{-1}$
	3	2.5 min
3	1a	x-ray < visible < microwave
	1b	microwave < visible < x-ray
	1c	microwave < visible < x-ray
	2a	blue < green < red
	2b	red < green < blue
	2c	red < green < blue
6	1	435 nm
	2	$3.18 \times 10^{-19} \text{ J}$
	3	541 nm
7	1	486 nm
10	1	1.47 nm
	2	$6.1 \times 10^6 \text{ m/s}$
	3	$1.37 \times 10^{-6} \text{ nm}$
16	1	Discussed in class
	2	Discussed in class
	3	Discussed in class