Introduction to

Modern Physics

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Table of Contents

Preface

Dear students, the purpose of our course this year is to provide an introduction to Modern physics. I hope that I have succeeded in preparing this course and find it easy, understandable and enjoyable as I enjoyed with you during lectures. If there is any comment I would like to hear criticism from my students on my email

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Chapter 1
The Birth of Modern Physics

1.1 What is Physics?

Physics, 'knowledge of nature', from is the natural science that studies matter, its motion and behavior through space and time, and the related entities of energy and force. Physics is one of the most fundamental scientific disciplines, and its main goal is to understand how the universe behaves. Physics is one of the oldest academic disciplines and perhaps the oldest.

Physics intersects with many interdisciplinary areas of research, such as biophysics and quantum chemistry, and the boundaries of physics are not rigidly defined. New ideas in physics often explain the fundamental mechanisms studied by other sciences and suggest new avenues of research in academic disciplines such as mathematics and philosophy.

Advances in physics often enable advances in new technologies. For example, advances in the understanding of electromagnetism, solid-state physics, and nuclear physics led directly to the development of new products that have dramatically transformed modern-day society, such as television, computers, domestic appliances, and nuclear weapons; advances in thermodynamics led to the development of industrialization; and advances in mechanics inspired the development of calculus.

1.2 Classical physics

Classical physics refers to theories of physics that predate modern, more complete, or more widely applicable theories. If a currently accepted theory is considered to be modern, and its introduction represented a major paradigm shift, then the previous theories, or new theories based on the older paradigm, will often be referred to as belonging to the realm of "classical physics".

As such, the definition of a classical theory depends on context. Classical physical concepts are often used when modern theories are unnecessarily complex for a particular situation. Most usually *classical physics* refers to pre-1900 physics, while *modern physics* refers to post-1900 physics which incorporates elements of quantum mechanics and relativity.

The discovery of new laws in thermodynamics, chemistry, and electromagnetics resulted from greater research efforts during the Industrial Revolution as energy needs increased. The laws comprising classical physics remain very widely used for objects on everyday scales travelling at non-relativistic speeds, since they provide a very close approximation in such situations, and theories such as quantum mechanics and the theory of relativity simplify to their classical equivalents at such scales. However, inaccuracies in classical mechanics for very small objects and very high velocities led to the development of modern physics in the 20th century.

1.3 Modern physics

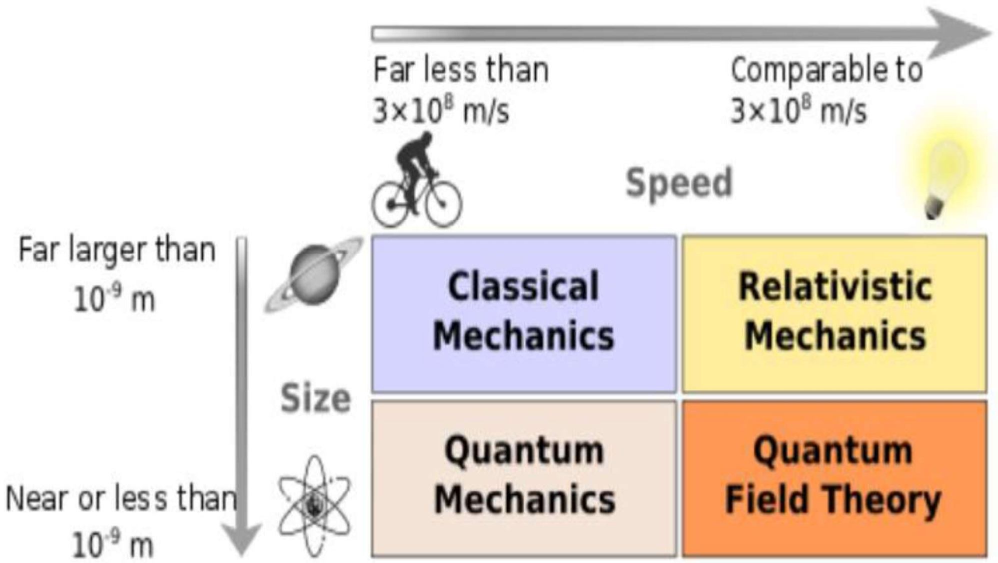
Modern physics began in the early 20th century with the work of Max Planck in quantum theory and Albert Einstein's theory of relativity. Both of these theories came about due to inaccuracies in classical mechanics in certain situations. Classical mechanics predicted a varying speed of light, which could not be resolved with the constant speed predicted by Maxwell's equations of electromagnetism; this discrepancy was corrected by Einstein's theory of special relativity, which replaced classical mechanics for fast-moving bodies and allowed for a constant speed of light.

Black-body radiation provided another problem for classical physics, which was corrected when Planck proposed that the excitation of material oscillators is possible only in discrete steps proportional to their frequency; this, along with the photoelectric effect and a complete theory predicting discrete energy levels of electron orbitals, led to the theory of quantum mechanics taking over from classical physics at very small scales.

Quantum mechanics would come to be pioneered by Werner Heisenberg, Erwin Schrödinger and Paul Dirac. From this early work, and work in related fields, the Standard Model of particle physics was derived. Following the discovery of a particle with properties consistent with the Higgs boson at CERN in 2012, all fundamental particles predicted by the standard model, and no others, appear to exist; however, physics beyond the Standard Model, with theories such as super symmetry, is an active area of research. Areas of mathematics in general are important to this field, such as the study of probabilities and groups.

Modern physics is the post-Newtonian conception of physics. It implies that classical descriptions of phenomena are lacking, and that an accurate, "modern", description of nature requires theories to incorporate elements of quantum mechanics or Einsteinian relativity, or both. In general, the term is used to refer to any branch of physics either developed in the early 20^{th} century and onwards, or branches greatly influenced by early 20^{th} century physics.

Small velocities and large distances is usually the realm of classical physics. Modern physics, however, often involves extreme conditions: quantum effects typically involve distances comparable to atoms (roughly 10^{-9} m), while relativistic effects typically involve velocities comparable to the speed of light (roughly 3×10^{8} m/s). In general, quantum and relativistic effects exist across all scales, although these effects can be very small in everyday life.



Classical physics is usually concerned with everyday conditions: speeds much lower than the speed of light, and sizes much greater than that of atoms.

Modern physics is usually concerned with high velocities and small distances.

1.4 Difference between classical and modern physics

While physics aims to discover universal laws, its theories lie in explicit domains of applicability. Loosely speaking, the laws of classical physics accurately describe systems whose important length scales are greater than the atomic scale and whose motions are much slower than the speed of light. Outside of this domain, observations do not match predictions provided by classical mechanics. Albert Einstein contributed the framework of special relativity, which replaced notions of absolute time and space with spacetime and allowed an accurate description of systems whose components have speeds approaching the speed of light. Max Planck, Erwin Schrödinger, and others introduced quantum mechanics, a probabilistic notion of particles and interactions that allowed an accurate description of atomic and subatomic scales. Later, quantum field theory unified quantum mechanics and special relativity. General relativity allowed for a dynamical, curved spacetime, with which highly massive systems and the large-scale structure of the universe can be well-described. General relativity has not yet been unified with the other fundamental descriptions; several candidate theories of quantum gravity are being developed.

1.5 Summary

In a literal sense, the term *modern physics* means up-to-date physics. In this sense, a significant portion of so-called *classical physics* is modern.

Classical Physics is the name we give to the physical theories generated before the twentieth century. Classical physics is comprised primarily of two areas, mechanics and electro-magnetism. Understanding how physics progressed to the point where modern physics begins is important to understanding modern physics.

Modern Physics is the name we give to the Theoretical advancements in physics since the beginning of the 20th Century, popularly known as Relativity and Quantum Mechanics. In this book, we will examine some of the seminal theoretical and experimental papers that formed the basis of modern physics. Some concepts that will be developed include,

- The electron
- Quantization of energy
- Photo-electric effect
- Compton Scattering
- Schrdinger's Equation
- Quantum Statistics
- Semiconductors
- The Standard Model

Useful Videos

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https://www.youtube.com/watch?v=UbGdcvRMog0

https://www.youtube.com/watch?v=H0m97YJavH4&list=PLybg94GvOJ9FAFBqQGf5-4YbfKpWbJtGn&index=1

Chapter 2
Electromagnetic radiation

2.1 Introduction to Radiant Energy

Electromagnetic radiation, which is the basis of this period, is one form of radiant energy. Visible light is an example of electromagnetic radiation. A change in this magnetic field generates an electric field. We called this electromagnetic induction. Changing electric fields are always accompanied by a changing magnetic field and vice versa. These changing fields allow a changing current in a wire or a moving charge to produce electromagnetic radiation, which is a source of energy. The electromagnetic radiation moves outward from the source as long as the energy that causes the charge to move is present.

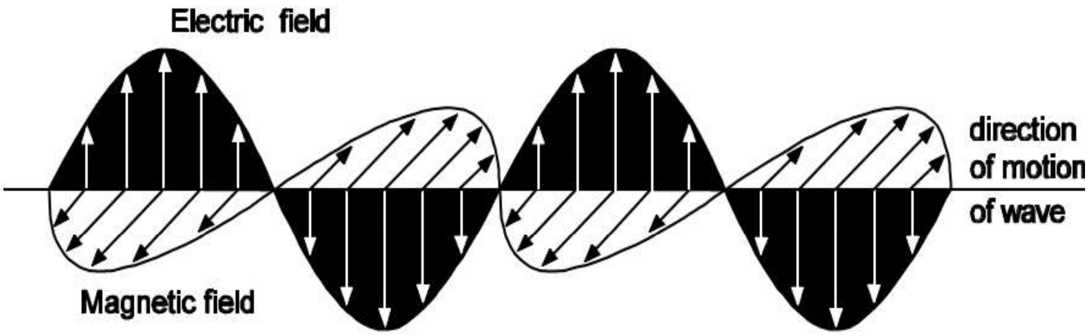


Figure 2.1 illustrates waves of electromagnetic radiation.

You have already seen that the electric field associated with electromagnetic radiation exerts a force on a charge. This fact is used in many devices. Almost every day we experience an example in antennas used for radio, telephone, or television. As we will discuss in

Period 3, electrons in a broadcasting antenna are made to move with some frequency. **Frequency** describes how often something repeats a **cycle**. In this case, the frequency of the electromagnetic radiation being broadcast is the same as the frequency that describes how often the electrons in the broadcasting antenna vibrate per second.

The speed at which radiant energy travels depends on the medium that it is passing through, but in a vacuum it is about 3×10^8 meters per second, or 186,000 miles per second. This speed is true for all frequencies of radiant energy. This constant speed, usually referred to as the speed of light, is given the symbol **c**, that appears in Einstein's famous equation $\mathbf{E = m\,c^2}$, which we will study later this quarter.

2.2 The Wave Model of Radiant Energy

One of the ways to transfer energy without the transfer of mass is to produce a wave. A wave can be a pulse, as in the pulse of sound made by clapping your hands together. Another example of a pulse is a tsunami, a tidal wave of energy that travels many miles over an ocean. But many waves are generated by a cyclic vibration of some given frequency. This type of wave is referred to as a **sine wave**. Sine waves are used to describe many features of radiant energy. We will use the term **electromagnetic wave** to refer to a model that describes radiant energy in terms of sine waves. In Section 2.4 we will discuss the quantum model of radiant energy. Figure 2.2 illustrates sine waves.

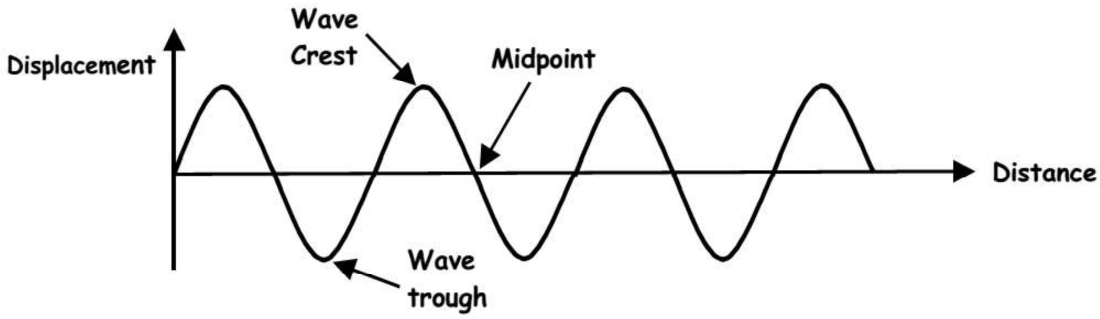


Figure 2.2 Sine Waves

In the case of a sine wave, we associate a **wavelength** with a given frequency. The wavelength is the distance between two adjacent crests of a wave or two adjacent troughs of a wave. All sine waves, regardless of the frequency of the wave, obey the relationship

$$\mathbf{c = f\,L} \qquad \text{(Equation 2.1)}$$

where

c = speed at which radiant energy travels (meters/sec or feet/sec)

f = frequency (cycles/sec, or Hertz)

L = wavelength (in meters or feet)

A wave also has an **amplitude**, which is the maximum height or displacement of the crest of the wave shown in Figure 2.3 above or below its midpoint.

The crest of the longer wavelength of the two waves shown in Figure 2.2 travels past a given point less frequently during a specified period of time than the crest of the shorter wavelength wave. Therefore, the longer wavelength wave has the lower frequency and the shorter wavelength wave has the higher frequency, as shown in

Figure 2.3. The horizontal axis of Figure 2.4 is the time measured at any given point on the horizontal axis of Figure 2.3.

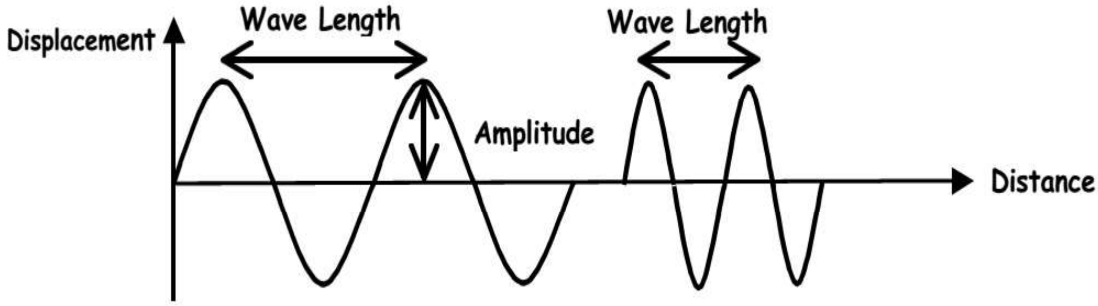


Figure 2.3 Wavelength and Amplitude

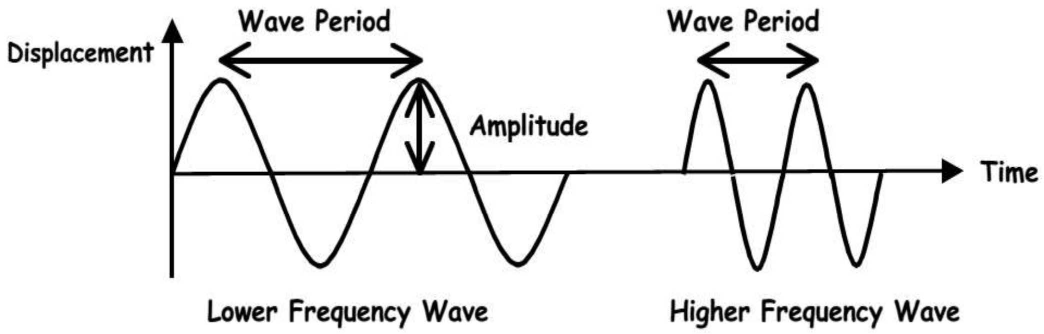


Figure 2.4 Wave Frequency and Period

The time that it takes for a wave to go through one complete cycle is called the **period** of the wave. The shorter the period, the more cycles the wave completes in a given amount of time, and thus the higher its frequency. This can be expressed by the relation given by Equation 2.2.

frequency = 1/ period (Equation 2.2)

Since the period of a wave is expressed in seconds, the frequency of the wave is expressed in 1/seconds, to which we assign the name Hertz (Hz).

2.3 The Electromagnetic Spectrum

All electromagnetic waves are the same, though they may differ in wavelength and frequency. The electromagnetic spectrum can be divided into regions according to wavelength or frequency. These regions are named radio waves, microwaves, infrared radiation, visible light, ultraviolet radiation, X-rays, and gamma rays.

The classifications of some regions of the spectrum are identified by the way that the waves interact with matter. For example, because the typical human eye can see over a certain range of wavelengths, we call that region visible light. Names of other regions of the spectrum are historical. When X-rays were discovered, they were called X-rays because it was not yet known that they were electromagnetic radiation. Next we discuss properties of the various regions of the electromagnetic spectrum, starting with the longest wavelengths and lowest frequencies.

Radio Waves

The longest wavelength region of the spectrum is **radio waves.** They have wavelengths longer than a meter and frequencies lower than about 1×10^8 Hertz. (Radio wave frequencies are often given in megahertz or kilohertz. A megahertz is abbreviated MHz, and is equal to 1×10^6 Hz. A kilohertz is abbreviated kHz, and is equal to 1×10^3 Hz.)

Microwaves

The next region is the **microwave** region of the spectrum. Microwaves have wavelengths of a meter to a few millimeters, and frequencies from about 1×10^8 to 1×10^{11} Hz. You have probably used microwave ovens. Some garage door openers use microwaves. You may also have seen microwave relay stations used by the telephone company for transmission of information over long distances. A small scale microwave generator and receiver will be demonstrated in the classroom.

Infrared Radiation

The region of the spectrum with wavelengths from several milli-meters down to about 7×10^{-7} meters (and frequencies from 1×10^{11} to 4.3×10^{14} Hz) is called the **infrared** region. The fact that radiant energy is present in this region of the spectrum can be illustrated by using a radiometer. We find that the radiometer vanes rotate when exposed to infrared radiation. Another type of device for detecting radiation in the infrared is the photoelectric infrared imaging device. The sniper scope, a particular example of this type of device, will be demonstrated in class. Television remote controls use radiation in this frequency range. The nerves of our skin are sensitive to some of the infrared portion of the spectrum.

Visible Light

Visible light ranges in wavelength from 4×10^{-7} meters (violet light) to 7×10^{-7}meters (red light). Our eyes do not respond to wavelengths outside this small portion of the electromagnetic spectrum. Within this region, our eyes respond to different wavelengths as different colors. In class, we will use prisms and diffraction gratings to separate white light into the colors of the visible spectrum.

Ultraviolet Radiation

Wavelengths of **ultraviolet radiation** extend from the short wavelength end of the visible spectrum (4×10^{-7} meters) to wavelengths as small as 1×10^{-9} meters. The frequencies range from 7×10^{14} Hz to about 3×10^{17} Hz. Ultraviolet radiation can induce fluorescence and can cause tanning in human skin.

X–rays

Even shorter wavelengths (down to about 1×10^{-11} meters) are the **X-ray** region. Frequencies in this region extend from 3×10^{17} Hz to about 3×10^{19} Hz. X-rays have a number of industrial and medical uses, which are associated with the ability of X-rays to penetrate matter. X-rays pass through flesh but are absorbed by bone; thus, Xray photographs can show bone structure and assist the medical profession in diagnosis.

Gamma Rays

Electromagnetic waves with wavelengths shorter than about 1×10^{-11} meters and frequencies above 3×10^{19} Hz are called **gamma rays**. They may be produced by nuclear reactions and will be discussed further in the period on nuclear energy.

2.4 The Quantum Model of Radiant Energy

While many properties of radiant energy are explained by the electromagnetic wave model, some are not. These properties can be explained by a different model, called the **quantum model**. This model treats radiant energy as being composed of small packets of energy called **photons**, or **quanta**. As radiant energy interacts with matter, it absorbs or deposits energy in amounts that are integer multiples of this photon energy. The photon energy can be related to frequency or wavelength by the relation shown in Equation 2.3.

$$\mathbf{E = h\ f = (h\ c)/L} \qquad \text{(Equation 2.3)}$$

Where

E = energy of a photon (joules)

h = is a proportionality constant = 6.63×10^{-34} joule sec

f = frequency (Hertz)

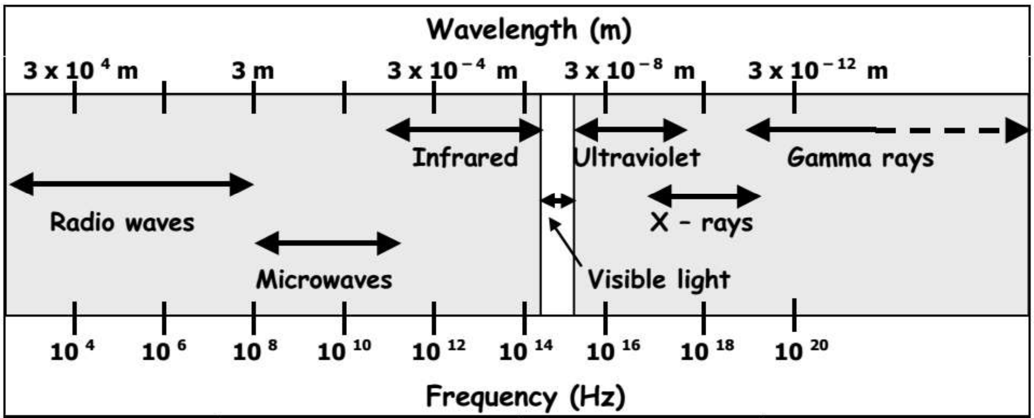
c = speed of the radiant energy = 3×10^{8} meters/sec in a vacuum

L = wavelength (meters).

From these equations, the higher the frequency or the shorter the wavelength, the higher the energy of the photon. The fact that two different models are needed to describe electromagnetic radiation has bothered people for a long time. It is an indication that we still do not have a full understanding of this phenomenon.

Table 2.2 shows the relationship between the wavelength, frequency, and photon energy for radiant energy.

Table 2.2: The Electromagnetic Spectrum



Type of Radiant Energy	Wavelength Range (meters)	Frequency Range (Hertz)	Photon Energy Range (joules)
Radio waves	longer than a meter	below about 1×10^{8} Hz	below about 6.6×10^{-26} J
Microwaves	a meter down to a few millimeters	about 1×10^{8} Hz to 1×10^{11} Hz	about 6.6×10^{-26} J to 6.6×10^{-23} J
Infrared	a few millimeters to 7×10^{-7} meters	about 1×10^{11} Hz to 4.3×10^{14} Hz	about 6.6×10^{-23} J to 2.8×10^{-19} J
Visible light	7×10^{-7} meters to 4×10^{-7} meters	about 4.3×10^{14} Hz to 7.5×10^{14} Hz	about 2.8×10^{-19} J to 5×10^{-19} J
Ultraviolet	4×10^{-7} meters to about 1×10^{-9} meters	about 7×10^{14} Hz to 3×10^{17} Hz	about 4.6×10^{-19} J to 2×10^{-16} J
X-rays	1×10^{-9} meters to about 1×10^{-11} meters	about 3×10^{17} Hz to 3×10^{19} Hz	about 2×10^{-16} J to 2×10^{-14} J
Gamma rays	shorter than about 1×10^{-11} meters	above about 3×10^{19} Hz	above about to 2×10^{-14} J

(Example 2.2)

What is the wavelength of a photon with an energy of 5 x 10^{-20} J?

$$E = \frac{h\,c}{L}$$

$$L = \frac{h\,c}{E}$$

$$L = \frac{(6.63 \times 10^{-34}\,J\,s) \times (3 \times 10^{8}\,m/s)}{5 \times 10^{-20}\,J}$$

$$L = 4.0 \times 10^{-6}\,m$$

Concept Check 2.1

a) What is the wavelength of radiant energy with a frequency of 2 x 10^{9} Hz? __________

b) How much energy does each photon of this radiant energy have? ____

2.5 Summary

2.1: Electrons moving with some frequency produce electromagnetic radiation, or radiant energy. This energy is associated with an electromagnetic field. Radiant energy of any frequency travels in a vacuum at 3×10^8 meters per second, or 186,000 miles per second. This constant is known as the speed of light and is given the symbol **c**.

2.2: Radiant energy can be thought of as a wave with a wavelength and frequency. The speed of a wave = frequency x wavelength: **s = f L** As light passes from one medium to another it is refracted, or bent. Light travels at 3.0×10^8 m/s in a vacuum, but travels at different speeds in materials such as in water or glass. The ratio of these speeds is the index of refraction, n, of the material. n = speed of light in a vacuum speed of light in a material

2.3: The electromagnetic spectrum can be divided into types of radiant energy based on the wavelength or frequency of the radiation: radio waves, microwaves, infrared radiation, visible light, ultraviolet light, X–rays, and gamma rays.

2.4: An explanation of electromagnetic radiation also requires the quantum model, which treats radiant energy as consisting of small packets of energy called photons. Photon energy is related to frequency or wavelength by the relation: **E = h f = (h c)/L**

Exercises

E.1 Each of the following travels, in a vacuum, at the speed of light except

a) radio waves
b) sound waves
c) X-rays
d) infrared rays
e) All of the above travel at the speed of light.

E.2 Which of the following does NOT make use of wave motion?

a) A bowling ball strikes a bowling pin.
b) A radio plays music transmitted from a radio station.
c) A microwave oven heats a slice of pizza.
d) Jane is reading by the light of an incandescent lamp.
e) A tennis ball floating on the river bobs up and down as a boat passes by.

E.3 Estimate the wavelength of a 1500 Hz sound wave. What would be the wavelength of an electromagnetic wave of the same frequency?

a) 0.23 m; 5×10^{-6} m
b) 0.23 m; 2×10^{5} m
c) 4.4 m; 5×10^{-6} m
d) 4.4 m; 2×10^{5} m
e) 8.8 m; 6.2×10^{5} m

E.4 The index of refraction of a piece of glass is 1.5. What is the speed of the photons of light in this glass?

a) 2×10^8 m/s

b) 3×10^8 m/s

c) 4.5×10^8 m/s

d) The speed depends on the period of the electromagnetic wave.

e) The speed depends on the frequency of the wave.

E.5 Which of the following sequences has the various regions of the electromagnetic spectrum arranged in order in increasing wavelength?

a) infrared, visual, ultraviolet, gamma ray

b) radio, infrared, ultraviolet

c) ultraviolet, visual, microwave, radio

d) X-ray, visual, microwave, infrared

e) gamma ray, X-ray, microwave, visual

E.6 In a vacuum, microwaves travel ________ waves of visible light.

a) faster than

b) slower than

c) at the same speed as

E.7 Which of the following statements about the microwaves used in microwave ovens is **not** correct?

a) Microwaves are electromagnetic radiation.

b) Microwaves are the same wavelength as waves used in radio broadcasting.

c) Microwaves have wavelengths longer than those of visible light.

d) Microwaves heat food by the conversion of radiant energy into thermal energy.

e) All of the statements are correct.

E.8 How many photons of wavelength 6×10^{-5} meters are required to produce electromagnetic radiation with 3.32×10^{-15} joules of energy?

a) 1×10^{-6} photons

b) 1×10^{3} photons

c) 1×10^{6} photons

d) 5×10^{6} photons

e) 1×10^{14} photons

Review Questions

R.1 What is the source of radiant energy?

R.2 How are the forms of radiant energy associated with the electromagnetic spectrum similar? How do they differ?

R.3 Give an example of each of the forms of radiant energy.

R.4 How can you find the energy of a photon of radiant energy?

R.5 Compare the speed of sound to the speed of light in air. What is the ratio of the speed of sound to the speed of light?

Useful Videos

https://www.youtube.com/watch?v=6Q1zy0x8q7M

https://www.youtube.com/watch?v=0QZd-rnBV-4

Chapter 3

Interactions of Photons with Matter

Photons are electromagnetic radiation with zero mass, zero charge, and a velocity that is always c, the speed of light.

• Because they are electrically neutral, they do not steadily lose energy via coulombic interactions with atomic electrons, as do charged particles.

• Photons travel some considerable distance before undergoing a more “catastrophic” interaction leading to partial or total transfer of the photon energy to electron energy.

• These electrons will ultimately deposit their energy in the medium.

• Photons are far more penetrating than charged particles of similar energy.

Energy Loss Mechanisms

- photoelectric effect
- Compton scattering
- pair production

3.1 Photoelectric effect

The **photoelectric effect** or *photo ionization* is the emission of electrons or other free carriers when light is shone onto a material. Electrons emitted in this manner can be called *photo electrons*. The phenomenon is commonly studied in electronic physics, as well as in fields of chemistry, such as quantum chemistry or electrochemistry.

According to classical electromagnetic theory, this effect can be attributed to the transfer of energy from the light to an electron. From this perspective, an alteration in the intensity of light would induce changes in the kinetic energy of the electrons emitted from the metal. Furthermore, according to this theory, a sufficiently dim light would be expected to show a time lag between the initial shining of its light and the subsequent emission of an electron. However, the experimental results did not correlate with either of the two predictions made by classical theory.

Instead, electrons are dislodged only by the impingement of photons when those photons reach or exceed a threshold frequency (energy). Below that threshold, no electrons are emitted from the metal regardless of the light intensity or the length of time of exposure to the light (rarely, an electron will escape by absorbing two or more quanta. However, this is extremely rare because by the time it absorbs enough quanta to escape, the electron will probably have emitted the rest of the quanta.). To make sense of the fact that light can eject electrons even if its intensity is low, Albert Einstein proposed that a beam of light is not a wave propagating through space, but rather a collection of discrete wave packets (photons), each with energy hf. This shed light on Max Planck's previous discovery of the Planck

relation ($E = hf$) linking energy (E) and frequency (f) as arising from quantization of energy. The factor h is known as the Planck constant.

The photoelectric effect requires photons with energies approaching zero (in the case of negative electron affinity) to over 1 MeV for core electrons in elements with a high atomic number. Emission of conduction electrons from typical metals usually requires a few electron volts, corresponding to short wavelength visible or ultraviolet light. Study of the photoelectric effect led to important steps in understanding the quantum nature of light and electrons and influenced the formation of the concept of wave–particle duality. Other phenomena where light affects the movement of electric charges include the photoconductive effect (also known as photoconductivity or photo resistivity), the photovoltaic effect, and the photo electrochemical effect.

Photoemission can occur from any material, but it is most easily observable from metals or other conductors because the process produces a charge imbalance, and if this charge imbalance is not neutralized by current flow (enabled by conductivity), the potential barrier to emission increases until the emission current ceases. It is also usual to have the emitting surface in a vacuum, since gases impede the flow of photoelectrons and make them difficult to observe. Additionally, the energy barrier to photoemission is usually increased by thin oxide layers on metal surfaces if the metal has been exposed to oxygen, so most practical experiments and devices based on the photoelectric effect use clean metal surfaces in a vacuum.

When the photoelectron is emitted into a solid rather than into a vacuum, the term *internal photoemission* is often used, and emission into a vacuum distinguished as *external photoemission*.

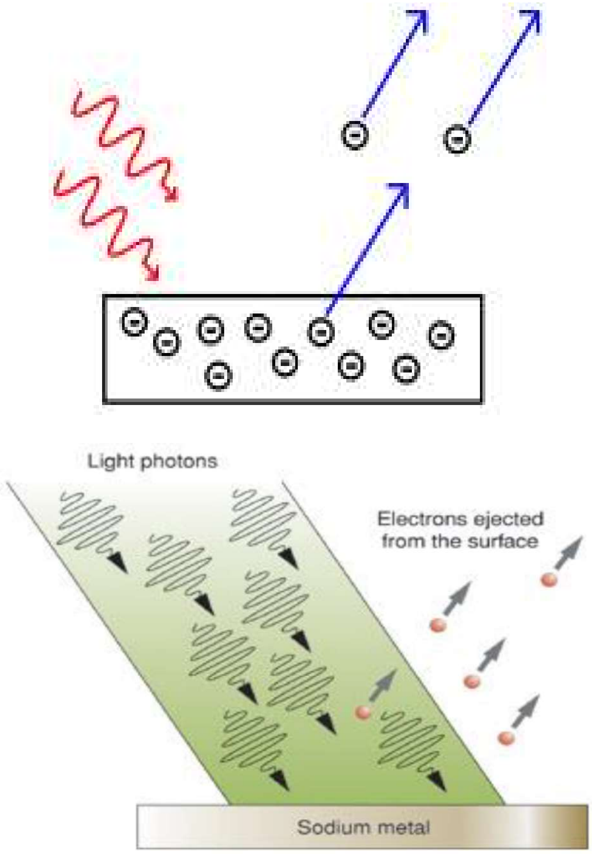


Fig. 1: photoelectric effect

Useful Videos

https://www.youtube.com/watch?v=0b0axfyJ4oo

https://www.youtube.com/watch?v=4EkogMWJJFg

https://www.youtube.com/watch?v=-fKdjBokGVo

3.2 Compton scattering

Compton scattering, discovered by Arthur Holly Compton, is the scattering of a photon by a charged particle, usually an electron. It results in a decrease in energy (increase in wavelength) of the photon (which may be an X-ray or gamma ray photon), called the **Compton effect**. Part of the energy of the photon is transferred to the recoiling electron. **Inverse Compton scattering** occurs when a charged particle transfers part of its energy to a photon

By the early 20th century, research into the interaction of X-rays with matter was well under way. It was observed that when X-rays of a known wavelength interact with atoms, the X-rays are scattered through an angle Θ and emerge at a different wavelength related to Θ. Although classical electromagnetism predicted that the wavelength of scattered rays should be equal to the initial Wavelength, multiple experiments had found that the wavelength of the scattered rays was longer (corresponding to lower energy) than the initial wavelength.

In 1923, Compton published a paper in the Physical Review that explained the X-ray shift by attributing particle-like momentum to light quanta (Einstein had proposed light quanta in 1905 in explaining the photo-electric effect, but Compton did not build on Einstein's work). The energy of light quanta depends only on the frequency of the light. In his paper, Compton derived the mathematical relationship between the shift in wavelength and the scattering angle of the X-rays by assuming that each scattered X-ray photon interacted with only one electron. His paper concludes by reporting on experiments which verified his derived relation:

$$\lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta),$$

where

λ is the initial wavelength,

$\grave{\lambda}$ is the wavelength after scattering,

h is the Planck constant,

m_e is the electron rest mass,

c is the speed of light, and

Θ is the scattering angle.

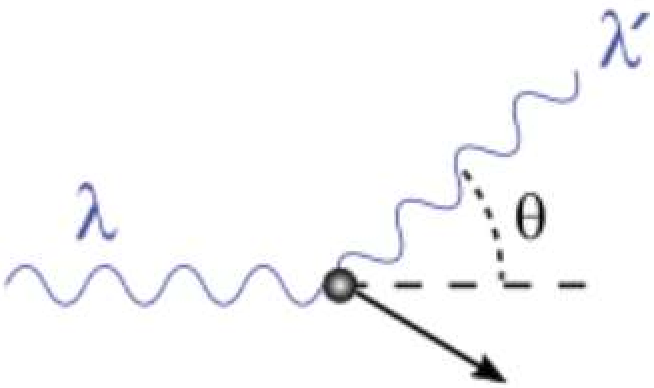


Fig. 2: A photon of wavelength λ comes in from the left, collides with a target at rest, and a new photon of wavelength $\grave{\lambda}$ emerges at an angle θ. The target recoils, carrying away an angle-dependent amount of the incident energy.

Useful Videos

https://www.youtube.com/watch?v=QsCmslcSlEs

https://www.youtube.com/watch?v=rGy7nsC8O_Y

https://www.youtube.com/watch?v=lzuiPoJffV4

3.3 Pair production

Pair production is the creation of an elementary particle and its antiparticle. Examples include creating an electron and a positron, a muon and an antimuon, or a proton and an antiproton. Pair production often refers specifically to a photon creating an electronpositron pair near a nucleus but can more generally refer to any neutral boson creating a particleantiparticle pair. In order for pair production to occur, the incoming energy of the interaction must be above a threshold in order to create the pair – at least the total rest mass energy of the two particles – and that the situation allows both energy and momentum to be conserved. However, all other conserved quantum numbers (angular momentum, electric charge, lepton number) of the produced particles must sum to zero – thus the created particles shall have opposite values of each other. For instance, if one particle has electric charge of +1 the other must have electric charge of -1, or if one particle has strangeness of +1 then another one must have strangeness of -1. The probability of pair production in photon-matter interactions increases with photon energy and also increases approximately as the square of atomic number of the nearby atom.

For photons with high photon energy (MeV scale and higher), pair production is the dominant mode of photon interaction with matter. These interactions were first observed in Patrick Blackett's counter controlled cloud chamber, leading to the 1948 Nobel Prize in Physics. If the photon is near an atomic nucleus, the energy of a photon can be converted into an electron positron pair:

$$\gamma \rightarrow e^{-} + e^{+}$$

The photon's energy is converted to particle's mass through Einstein's equation, $E=mc^2$; where E is energy, m is mass and c is the speed of light. The photon must have higher energy than the sum of the rest mass energies of an electron and positron (2 × 0.511 MeV = 1.022 MeV) for the production to occur. The photon must be near a nucleus in order to satisfy conservation of momentum, as an electron positron pair producing in free space cannot both satisfy conservation of energy and momentum. Because of this, when pair production occurs, the atomic nucleus receives some recoil. The reverse of this process is electron positron annihilation.

Useful Videos

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Chapter 3

Interactions of Photons with Matter

Photons are electromagnetic radiation with zero mass, zero charge, and a velocity that is always c, the speed of light.

• Because they are electrically neutral, they do not steadily lose energy via coulombic interactions with atomic electrons, as do charged particles.

• Photons travel some considerable distance before undergoing a more "catastrophic" interaction leading to partial or total transfer of the photon energy to electron energy.

• These electrons will ultimately deposit their energy in the medium.

• Photons are far more penetrating than charged particles of similar energy.

Energy Loss Mechanisms

- photoelectric effect
- Compton scattering
- pair production

3.4 Photoelectric effect

The **photoelectric effect** or *photo ionization* is the emission of electrons or other free carriers when light is shone onto a material. Electrons emitted in this manner can be called *photo electrons*. The phenomenon is commonly studied in electronic physics, as well as in fields of chemistry, such as quantum chemistry or electrochemistry.

According to classical electromagnetic theory, this effect can be attributed to the transfer of energy from the light to an electron. From this perspective, an alteration in the intensity of light would induce changes in the kinetic energy of the electrons emitted from the metal. Furthermore, according to this theory, a sufficiently dim light would be expected to show a time lag between the initial shining of its light and the subsequent emission of an electron. However, the experimental results did not correlate with either of the two predictions made by classical theory.

Instead, electrons are dislodged only by the impingement of photons when those photons reach or exceed a threshold frequency (energy). Below that threshold, no electrons are emitted from the metal regardless of the light intensity or the length of time of exposure to the light (rarely, an electron will escape by absorbing two or more quanta. However, this is extremely rare because by the time it absorbs enough quanta to escape, the electron will probably have emitted the rest of the quanta.). To make sense of the fact that light can eject electrons even if its intensity is low, Albert Einstein proposed that a beam of light is not a wave propagating through space, but rather a collection of discrete wave packets (photons), each with energy hf. This shed light on Max Planck's previous discovery of the Planck

relation ($E = hf$) linking energy (E) and frequency (f) as arising from quantization of energy. The factor h is known as the Planck constant.

The photoelectric effect requires photons with energies approaching zero (in the case of negative electron affinity) to over 1 MeV for core electrons in elements with a high atomic number. Emission of conduction electrons from typical metals usually requires a few electron volts, corresponding to short wavelength visible or ultraviolet light. Study of the photoelectric effect led to important steps in understanding the quantum nature of light and electrons and influenced the formation of the concept of wave–particle duality. Other phenomena where light affects the movement of electric charges include the photoconductive effect (also known as photoconductivity or photo resistivity), the photovoltaic effect, and the photo electrochemical effect.

Photoemission can occur from any material, but it is most easily observable from metals or other conductors because the process produces a charge imbalance, and if this charge imbalance is not neutralized by current flow (enabled by conductivity), the potential barrier to emission increases until the emission current ceases. It is also usual to have the emitting surface in a vacuum, since gases impede the flow of photoelectrons and make them difficult to observe. Additionally, the energy barrier to photoemission is usually increased by thin oxide layers on metal surfaces if the metal has been exposed to oxygen, so most practical experiments and devices based on the photoelectric effect use clean metal surfaces in a vacuum.

When the photoelectron is emitted into a solid rather than into a vacuum, the term *internal photoemission* is often used, and emission into a vacuum distinguished as *external photoemission*.

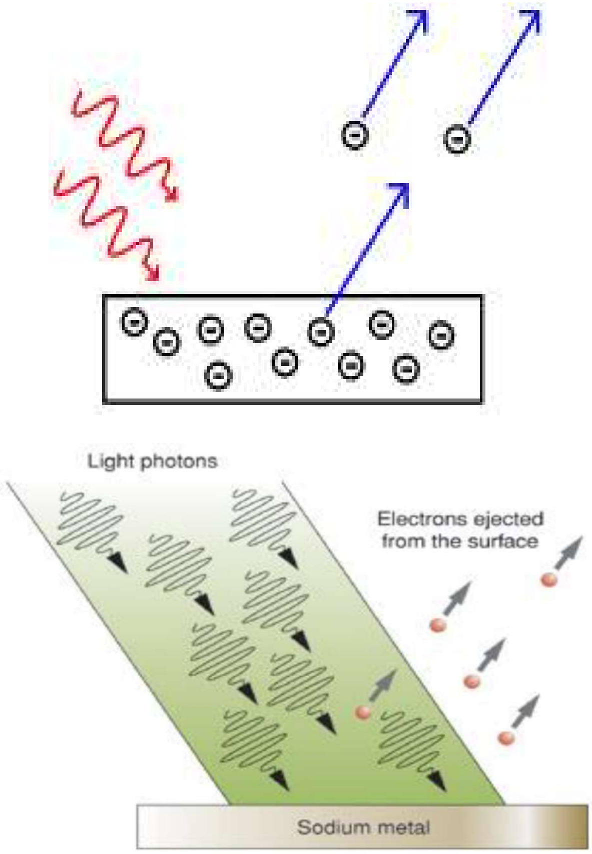

Fig. 1: photoelectric effect

Useful Videos

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By the early 20th century, research into the interaction of X-rays with matter was well under way. It was observed that when X-rays of a known wavelength interact with atoms, the X-rays are scattered through an angle Θ and emerge at a different wavelength related to Θ. Although classical electromagnetism predicted that the wavelength of scattered rays should be equal to the initial Wavelength, multiple experiments had found that the wavelength of the scattered rays was longer (corresponding to lower energy) than the initial wavelength.

In 1923, Compton published a paper in the Physical Review that explained the X-ray shift by attributing particle-like momentum to light quanta (Einstein had proposed light quanta in 1905 in explaining the photo-electric effect, but Compton did not build on Einstein's work). The energy of light quanta depends only on the frequency of the light. In his paper, Compton derived the mathematical relationship between the shift in wavelength and the scattering angle of the X-rays by assuming that each scattered X-ray photon interacted with only one electron. His paper concludes by reporting on experiments which verified his derived relation:

$$\lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta),$$

where

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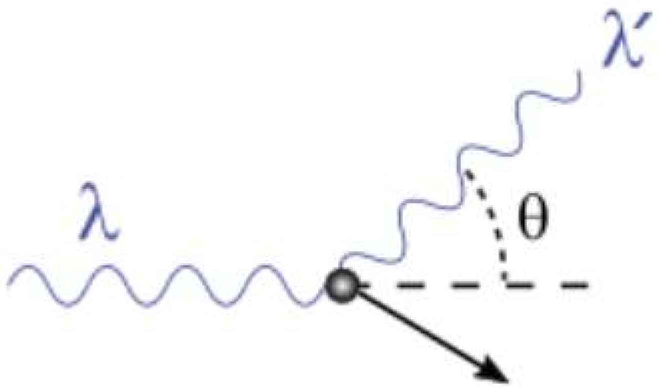

Fig. 2: A photon of wavelength λ comes in from the left, collides with a target at rest, and a new photon of wavelength $\grave{\lambda}$ emerges at an angle θ . The target recoils, carrying away an angle-dependent amount of the incident energy.

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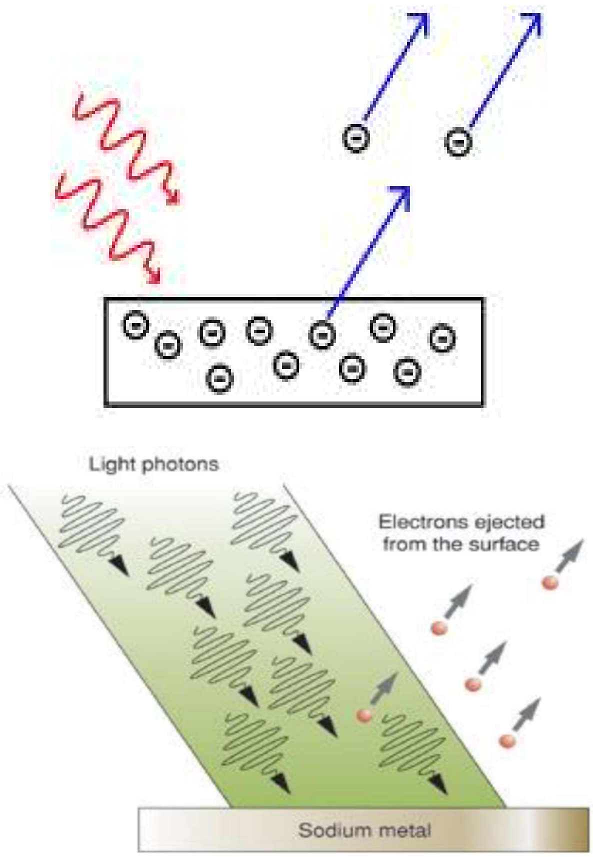

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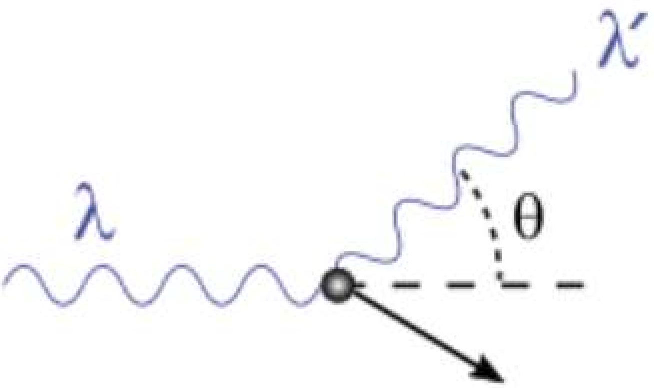

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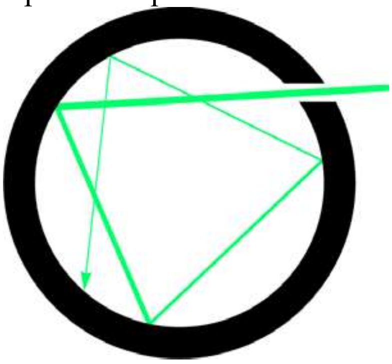
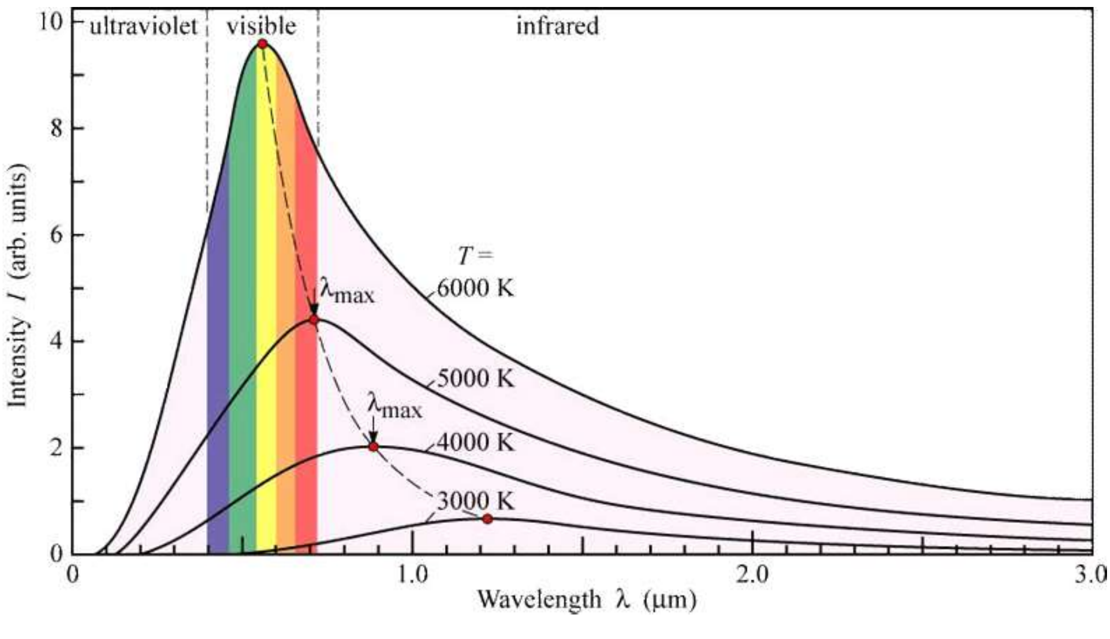
Modern Physics

Blackbody radiation

Experience show that the temperature of a hot and a cold object placed close to each other equalize in vacuum as well. All macroscopic objects in all temperature emit (and absorb) thermal radiation spontaneously. This radiation consists of electromagnetic waves.
The energy of the electromagnetic waves emitted by a surface, in unit time and in unit area, depends on the nature of the surface and on its temperature.
The thermal radiation emitted by many ordinary objects can be approximated as blackbody radiation. A perfectly insulated cavity that is in thermal equilibrium internally contains black-body radiation and will emit it through a hole made in its wall, provided the hole is small enough to have negligible effect upon the equilibrium.



The (absolute) blackbody absorbs all energy, and reflects nothing, which is of course an idealization. A black-body at room temperature appears black, as most of the energy it radiates is infra-red and cannot be perceived by the human eye. Black-body radiation has a characteristic, continuous frequency spectrum that depends only on the body's temperature. The spectrum is peaked at a characteristic frequency that shifts to higher frequencies (shorter wavelengths) with increasing temperature, and at room temperature most of the emission is in the infrared region of the electromagnetic spectrum.



Wien's displacement **law** indicates that the maximum of the energy distribution is displaced within the radiation spectrum of a blackbody in case of a change in temperature.

$$\lambda_{\max} T = b$$

where b is called Wien's displacement constant, is equal to 2.89×10^{-3} Km.

The **Stefan–Boltzmann law** states that the power emitted by the surface of a black body is directly proportional to the fourth power of its absolute temperature and, of course, its surface area A:

$$P = \sigma T^4 A$$

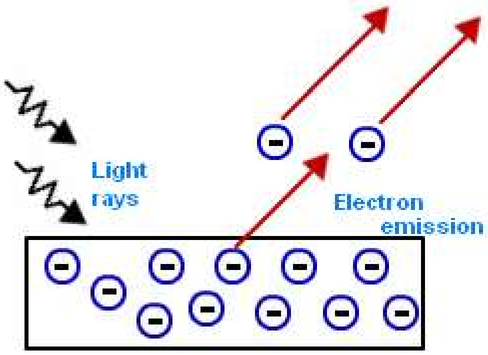
where $\sigma \approx 5{,}67 \cdot 10\text{-}8 W/(m^2K^4)$ is the Stefan–Boltzmann constant.
It was impossible to explain the measured spectral emissivity distribution by the concepts and laws of classical physics. In 1900 Max Planck theoretically derived a formula, which accurately described the radiation. In order to do that, he had to suppose that **energy** of the **electromagnetic field** inside the cavity **does not exist in a continuous, but only in quantized form**, in other words, the energy could only be a multiple of an elementary unit

$$\boxed{E = h f}$$

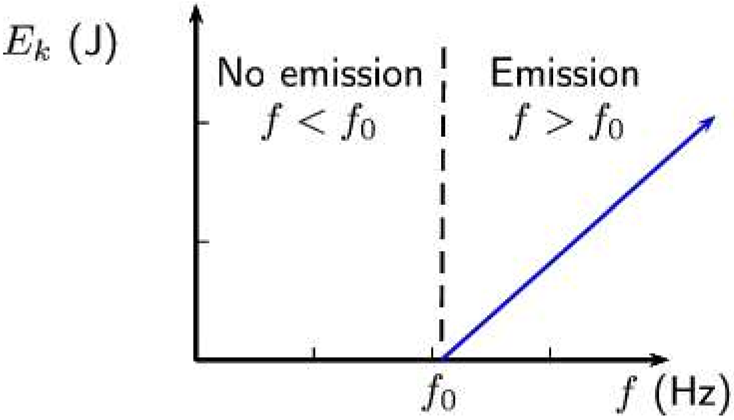
where h is Planck's constant, $h = 6{,}626 \cdot 10^{-34}$ Js. Planck's quantum hypothesis is a pioneering work, heralding advent of a new era of modern physics and quantum theory.

Photoelectric effect

Scientists observed that many metals emit electrons when illuminated by ultraviolet light. In case of alkali metals this effect can be generated by visible light as well. The emitted electrons are called photoelectrons.



Experimental observations of photoelectric emission:
1. For a particular metal, there exists a certain minimum frequency (so called threshold frequency f_0) of incident radiation below which no photoelectrons are emitted, regardless of the intensity of light.
2. Above the threshold frequency, the maximum kinetic energy of the emitted photoelectron depends on the frequency of the incident light and on the material, but is independent of the intensity of the incident light.
3. The rate at which photoelectrons are ejected is directly proportional to the intensity of the incident light.
4. The time lag between the incidence of radiation and the emission of a photoelectron is very small, less than 10^{-8} second.



The theory of the photoelectric effect must explain the experimental observations of the emission of electrons from an illuminated metal surface. But these experimental observations can't be explained by the wave properties of light. In order to solve this problem 1905, Albert Einstein developed Planck's theory. He described light as composed of discrete quanta, now called **photons**, rather than continuous waves.

The energy of the photon is directly proportional to its frequency: $E=hf$, where h is the Planck constant. Now we can apply the conservation of energy to the ideal process when all of the incoming energy is transferred to an electron:

$$hf = W_{out} + \frac{1}{2} m_e \mathrm{v}_{\max}^2$$

W_{out} is the so called **work function**, usually denoted by φ. This is the minimum work (i.e. energy) needed to remove an electron from a solid to a point in the vacuum immediately outside the solid surface. Its value is characteristic for the metal and can be determined by the threshold frequency f_0 :

$$hf_0 = W_{out} = \varphi$$

If the light can be considered not only as waves but as **particles**, one have to determine the mass and momentum of these particles. If we use the famous Einstein-relation

$$\mathrm{E} = \mathrm{m} \cdot \mathrm{c}^2 ,$$

we obtain for the mass of the photon:

$$\mathrm{m} = \frac{\mathrm{E}}{\mathrm{c}^2} = \frac{\mathrm{hf}}{\mathrm{c}^2} = \frac{\mathrm{h}}{\mathrm{c}} \cdot \frac{\mathrm{f}}{\mathrm{c}} = \frac{\mathrm{h}}{\mathrm{c} \cdot \lambda}$$

Now the momentum of the photon:

$$p = \mathrm{m} \cdot \mathrm{c} = \frac{\mathrm{h}}{\lambda}$$

Expressed by the wave-number:

$$\vec{p} = \hbar \vec{k}$$

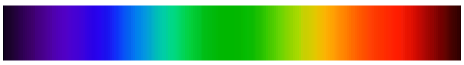
where $\hbar = \frac{h}{2\pi}$ is the so called reduced Planck's constant

We emphasize that Einstein did not negate that the electromagnetic radiation propagates as waves. Instead, he proposed that light has a dual nature: it can behave as a wave and as a collection of particles as well.

Line spectra of atoms

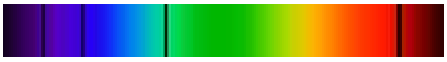
The quantum hypothesis also plays an important role in the understanding of atomic spectra which were started to be explored more than two centuries ago.

The spectrum emitted by a hot solid (such as the filament of a light bulb) is continuous, all wavelengths are present.

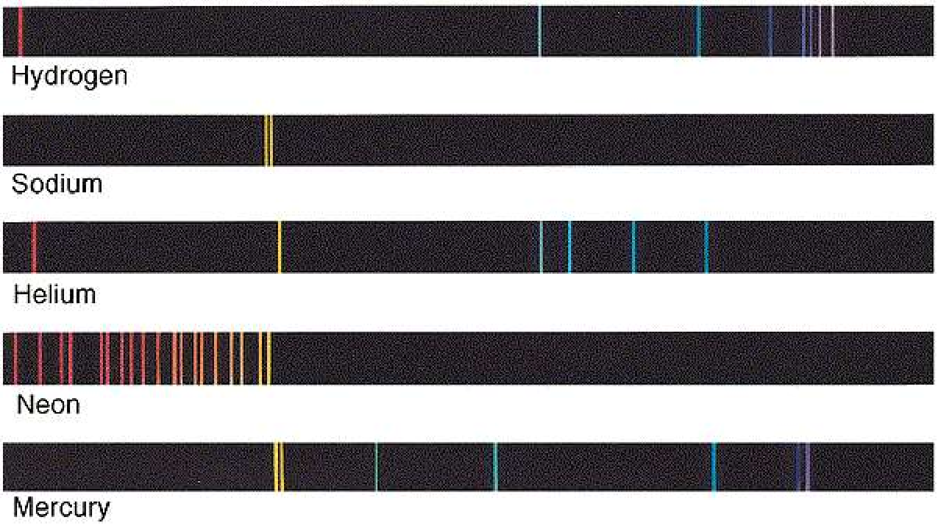


But if the source is a heated gas or vapour, the spectrum includes only a few colours in the form of isolated lines. This is called emission line spectrum, and the lines are called spectral lines. The wavelengths or frequencies of the lines are characteristic of the element emitting the light.

An absorption line is produced when photons from a hot, broad (continuous) spectrum source pass through a cold material. The intensity of light, over a very narrow frequency range, is reduced due to absorption by the material



Spectral lines are highly atom-specific, and can be used to identify the chemical composition of any medium capable of letting light pass through it (typically gas is used). Several elements were discovered by spectroscopic means, e.g. helium,



Suggested basic level video:
https://www.youtube.com/watch?v=ssFHlRKMRGs

Bohr model of atoms

It was proposed before Bohr that the electron in a hydrogen atom travels around the nucleus in a circular orbit. However, this violates the principles of classical electrodynamics. The energy of the electron in an orbit is increasing with its distance from the nucleus. As the electron is accelerating, it should generate electromagnetic radiation, thereby lose energy, continuously spiralling into the nucleus. In the reality this does not happen and it was Bohr who explained it first.

Bohr's postulates

A) Only a limited number of orbits with certain energies are allowed as stationary orbits of the electron. In other words, the orbits are quantized.

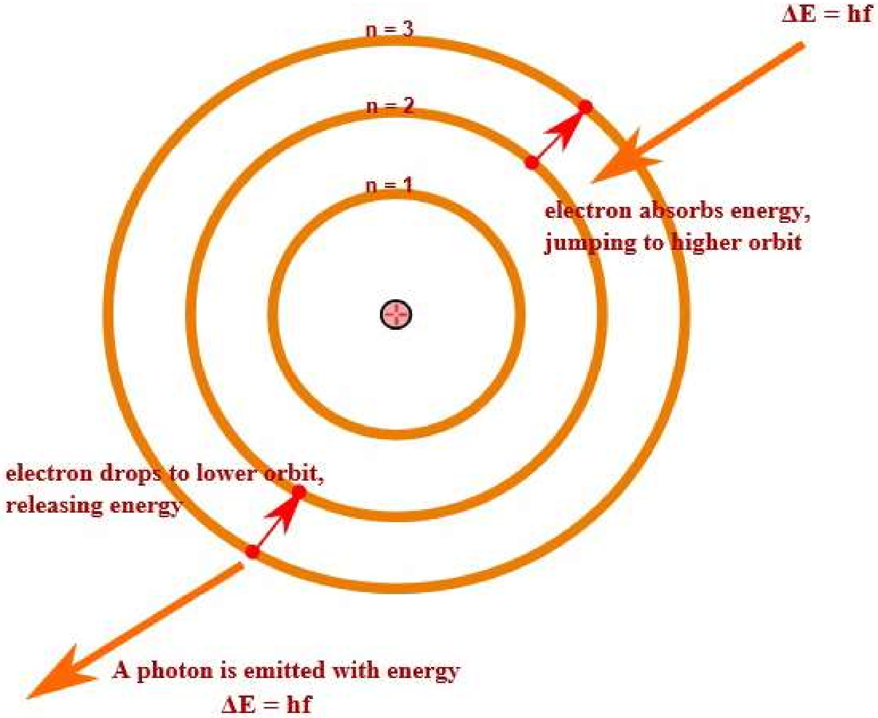
B) For hydrogen, the only orbits that are allowed are those for which the angular momentum of the electron is an integral multiple of the reduced Planck's constant.

$$L_{e^-} = n\hbar, \quad n = 1,2,3...., \quad \hbar = \frac{h}{2\pi}$$

The integer number n here is a quantum number describing the stationary state of the electron.

C) Light is absorbed when an electron jumps to a higher energy orbit and emitted when an electron falls into a lower energy orbit. The energy of the light emitted or absorbed is exactly equal to the difference between the energies of the orbits.

$$E_i - E_k = hf_{ik}$$



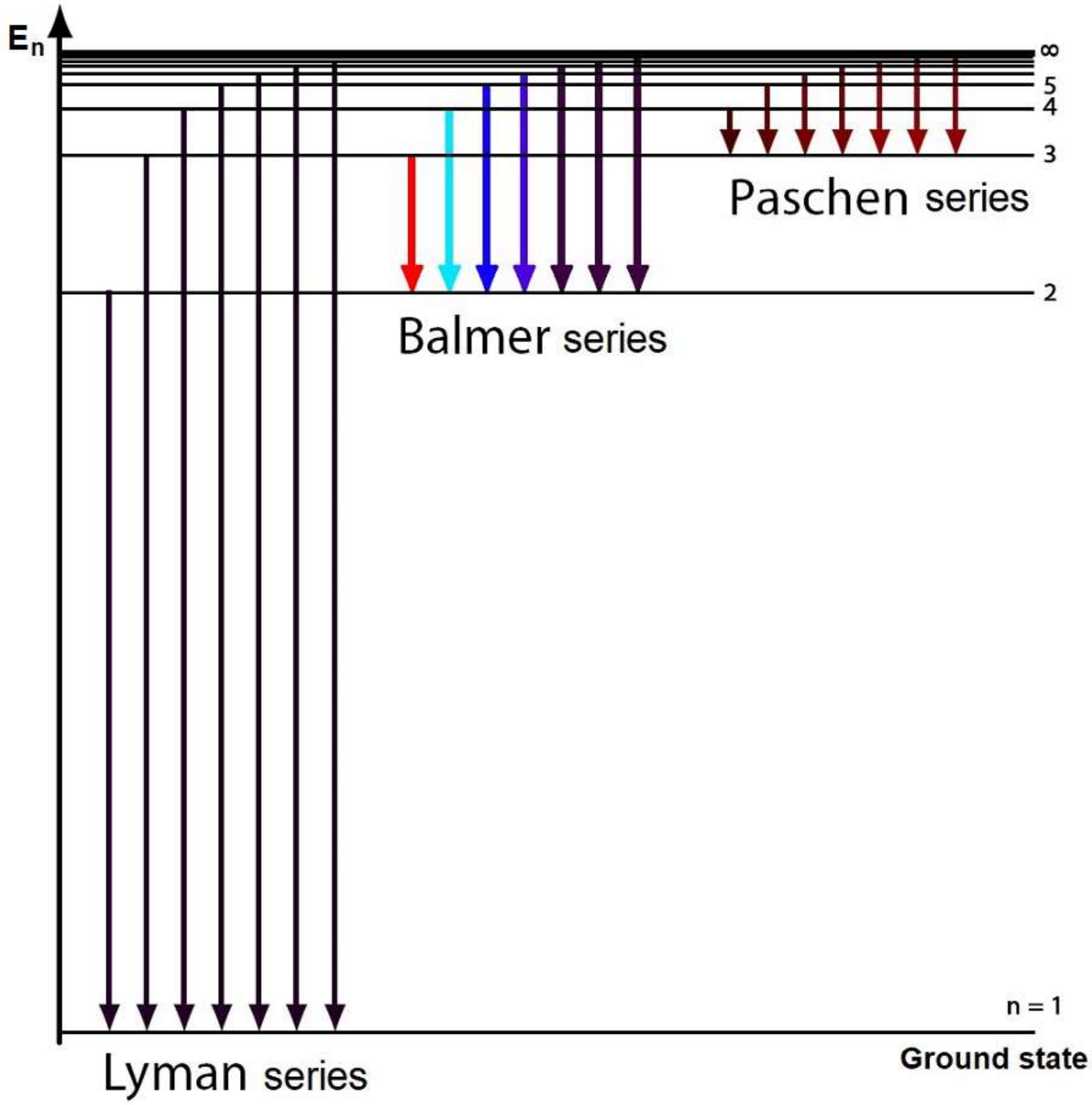
Apart from his postulates, Bohr applied classical physics, (Newton and Coulomb laws) during his work. He derived the energy levels in the Hydrogen atom,

$$E_n = -E^* z^2 \cdot \frac{1}{n^2}$$

Therefore he managed to deduce the already known frequencies of the emitted light:

$$f_{nm} = \frac{E_n - E_m}{h} = \frac{E^*}{h}\left(\frac{1}{m^2} - \frac{1}{n^2}\right) = R\left(\frac{1}{m^2} - \frac{1}{n^2}\right)$$

where R is the Rydberg-constant.



The predicted and measured Rydberg constant R was in good agreement.
The Bohr model was successful in case of one-electron atoms or ions, such as

- hydrogen
- singly ionized helium He^{+}
- doubly ionized lithium Li^{++} and so on.

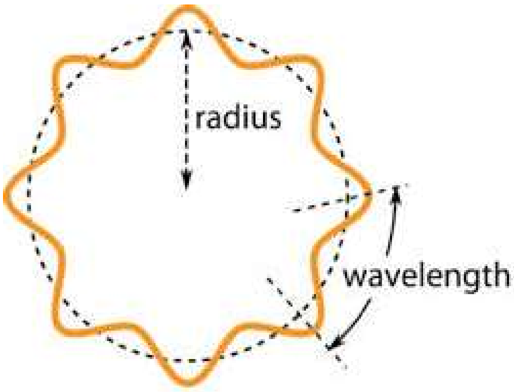
Such atoms are called hydrogen-like atoms.
The most serious **problem** with the Bohr model is that it does not properly work for multi-electron atoms, and in the model the atom seems to be a disk, but in the reality it is a sphere.

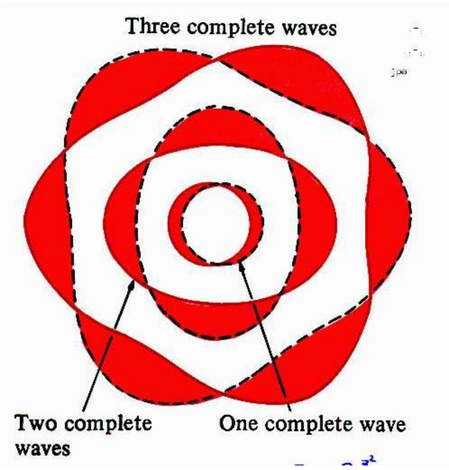
Wave particle duality of particles, de-Broglie hypothesis

We have already seen the double nature of electromagnetic radiation or light. We concluded that light can behave like a wave or particle. This was called wave particle duality.
In 1924 de-Broglie suggested the same duality in case of particles like protons or **electrons**.
He asked the question: If the momentum of a photon can be calculated from its wavelength: $p = \frac{h}{\lambda}$
then why can't we reverse this relation to calculate the wavelength of an electron from its momentum: $\boxed{\lambda = \frac{h}{p}}$

An electron possessing wave properties is subject to constructive and destructive interference. As will be shown this leads naturally to quantization of electron momentum and kinetic energy. In order to avoid destructive interference, the wave must be a standing wave, i.e. the electron's wavefunction must be single-valued, which in this application requires a circular boundary condition: the wavefunction must match at points separated by one circumference

$$n\lambda = 2\pi r$$





Using the assumption

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

we obtain

$$\frac{nh}{mv} = 2\pi r$$

and therefore the angular momentum is

$$L = mvr = n\hbar .$$

It means that de-Broglie derived one of the postulates of Bohr. A few years later, in 1927 Davisson and Germer verified experimentally the existence of matter waves showing interference of electrons. The obtained wavelength was in good agreement with the de-Broglie hypothesis.

However, later it turned out that the Bohr model gives an **incorrect** value $L = \hbar$ for the ground state (n=1) orbital angular momentum. Instead, L=0 in this case, which cannot be explained by classical physics.

Although the Bohr model and its underpinning by de-Broglie is not really perfect, the wave–particle duality, which proposes that every elementary particle exhibits the properties of not only particles, but also waves, was a key step in the development of quantum mechanics. The next important steps in this new branch of science was made by Schrödinger and Heisenberg in 1925 and 1926.

Wave Function

The so called **wave function** describes the state of the electron (or any physical system). Usually the Greek letter psi (or sometimes φ) is used, and in general

$$\Psi(x, y, z, t) ,$$

or in one dimension $\Psi(x,t)$.

The values of Ψ are usually complex numbers.

Only continuous, bounded functions can describe a real physical system, and usually there is a requirement that the square-integral of Ψ should be bounded: $\int_{\substack{full\\space}} |\Psi|^2 dV < C$

What is the physical meaning of the wave function Ψ for a particle?
The wave function describes the distribution of the particle in space. It is related to the probability of finding the particle in various regions. If we imagine a volume element dV around a point, the probability that the particle can be found in that volume element is measured by $|\Psi|^2 dV$. The so called probability density is

$$\rho = |\Psi|^2 \equiv \Psi^*\Psi \,.$$

The probability of finding a particle in an arbitrary volume is the integral of the probability density:

$$p(\mathrm{V}) = \int_V \rho dV = \int_V |\Psi|^2 dV < 1$$

One can have the information only about where the particle is likely to be, not where it is for sure.

Principle of superposition: If ψ_1 and ψ_2 are possible wave-functions of the system, then the

$$\psi = c_1\psi_1 + c_2\psi_2$$

linear combination is also a possible wave-function.

We note that in quantum computing, a qubit or quantum bit is a unit of quantum information—the quantum analogue of the classical binary bit. A qubit is a two-state quantum-mechanical system. In a classical system, a bit would have to be in one state or the other. However, quantum mechanics allows the qubit to be in a superposition of both states at the same time, a property that is fundamental to quantum computing.

Operators

The observables, i.e. those physical quantities which are dynamical variables (i.e. not constants like m or q) are represented by linear operators, denoted by “hat” on the top of the letter: $\hat{O}$.

To obtain specific values for physical quantities, for example energy or momentum, you operate on the wavefunction with the quantum mechanical operator associated with that quantity.

In linear algebra, an eigenvector of a square matrix is a vector that points in a direction which is invariant under the associated linear transformation (*eigen* here is the German word meaning self or own). In other words, if $\vec{v}$ is a nonzero vector, then it is an eigenvector of a square matrix A if $A\vec{v}$ is a scalar multiple of $\vec{v}$. Similarly in case of functions, f is an eigenfunction of an operator $\hat{A}$ if the action of that operator is only a multiplication of that function by a number:

$$\hat{A}f = af$$

where a is a real or complex number. For example, $\frac{d}{dx}$ is a linear operator and if

$\mathrm{f}(x) = e^{ax}$ then

$$\frac{d}{dx}e^{ax} = ae^{ax} = a \cdot f \,,$$

therefore this f is an eigenfunction and the eigenvalue is a.

A number *a* can be the value of an observable only if *a* is an eigenvalue of the operator $\hat{A}$ which represents the observable. We have 2 cases:

- The wave function of the system is an eigenfunction of $\hat{A}$, i.e. the system is an eigenstate of the operator. In this case the value of any (precise) measurement of the physical quantity will be *a*.
- The wave function of the system is not an eigenfunction of different numbers. For example the system has the wave function

$$\psi = c_1\psi_1 + c_2\psi_2$$

which is a combination of eigenstates, i.e.

$$\hat{A}\psi_1 = a_1\psi_1$$

$$\hat{A}\psi_2 = a_2\psi_2 \,.$$

Now the result of the measurement can be different numbers. We will measure a_1 with probability $|c_1|^2$ and a_2 with probability $|c_2|^2$.

The eigenvalues a_n may be discrete, and in such cases we can say that the physical variable is "quantized" and that the index n plays the role of a "quantum number" which characterizes that state.

Concrete form of the operators

As the first example, there is an x-position operator, which is a simple multiplication:

$$\hat{x} = x \cdot .$$

It turns the wave function Ψ into xΨ.
Instead of a linear momentum $p_x = mv_x$ there is an x-momentum operator

$$\boxed{\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}}$$

similarly

$$\hat{p}_y = \frac{\hbar}{i}\frac{\partial}{\partial y}, \quad \hat{p}_z = \frac{\hbar}{i}\frac{\partial}{\partial z} \quad \text{and} \quad \hat{y} = y \cdot \,, \quad \hat{z} = z \cdot \,,$$

The kinetic energy in classical physics:

$$T = \tfrac{1}{2}mv^2 = \tfrac{p^2}{2m} = \tfrac{1}{2m}(p_x^2 + p_y^2 + p_z^2)$$

In quantum physics:

$$\hat{T} = \tfrac{1}{2m}(\hat{p}_x\hat{p}_x + \hat{p}_y\hat{p}_y + \hat{p}_z\hat{p}_z) =$$

$$= \frac{1}{2m}\left[\frac{\hbar}{i}\frac{\partial}{\partial x}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) + \frac{\hbar}{i}\frac{\partial}{\partial y}\left(\frac{\hbar}{i}\frac{\partial}{\partial y}\right) + \frac{\hbar}{i}\frac{\partial}{\partial z}\left(\frac{\hbar}{i}\frac{\partial}{\partial z}\right)\right] =$$

$$\frac{1}{2m}\left[\left(\frac{\hbar}{i}\right)^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\right] = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) = -\frac{\hbar^2}{2m}\Delta$$

$$\hat{T} = -\frac{\hbar^2}{2m}\Delta$$

The potential energy of a particle depends on the position of the particle, thus the operator is the multiplication by the potential function:

$$\hat{V}\psi(x, y, z, t) = V(x, y, z, t) \cdot \psi(x, y, z, t)$$

Following the Newtonian analogy, the total energy operator, indicated by **H**, is the sum of the kinetic energy operator and the potential energy operator $\hat{V}$:

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + \hat{V} \cdot$$

H is called the **Hamiltonian**.
Sample video about this topic: https://www.youtube.com/watch?v=cUUFIk0ISuY

Schrödinger equation

Schrödinger wrote his famous equation to describe the motion of the electron. This is the fundamental equation of quantum mechanics. In this course we examine only the simplest case, e.g. only time-independent potentials. Thus we study only the **time-independent** version of the Schrödinger equation. This is the **energy-eigenvalue equation**:

$$\boxed{\hat{H}\psi(\vec{r}) = E\psi(\vec{r})}$$

or in an other form:

$$-\frac{\hbar^2}{2m}\Delta\varphi(\vec{r}) + V(\vec{r})\varphi(\vec{r}) = E\varphi(\vec{r})$$

This is a second order partial differential equation for the energy-eigenvalues and eigenfunctions of the system. Any wave-function can be the stationary wave-function of the system only if it is a solution of this energy-eigenvalue equation, thus the energy has a certain, well defined value.
Thus if we want to examine the stationary behaviour of an electron, we must incorporate all relevant interactions into the potential energy term and then solve the Schrödinger equation. After that we can calculate the values of physical quantities represented by operators.

Heisenberg's uncertainty principle

There is a fundamental limit to the precision with which certain pairs of physical properties of a particle (or any system) can be known simultaneously. These pairs are known as complementary variables, for example position x and momentum p.

$$\left.\begin{aligned} \Delta x \Delta p_x &\geq \frac{\hbar}{2} \\ \Delta y \Delta p_y &\geq \frac{\hbar}{2} \\ \Delta z \Delta p_z &\geq \frac{\hbar}{2} \\ \Delta E \Delta t &\geq \frac{\hbar}{2} \end{aligned}\right\} \text{Heisenberg uncertainty relations}$$

Here the Greek letter Δ means the uncertainty, mathematically the (standard) deviation.
The uncertainty appears when the system is not in the eigenstate of the particular operator. Heisenberg uncertainty relations state that there is no function which is an eigenfunction of e.g. both the momentum and the position operator.
Historically, the uncertainty principle has been confused with a similar effect in physics, called the observer effect, which notes that measurements of certain systems cannot be made

without affecting the systems. Heisenberg offered such an observer effect at the quantum level as a physical "explanation" of quantum uncertainty. However, it has since become clear that the uncertainty principle is inherent in the properties of all wave-like systems. Thus, the uncertainty principle actually states a fundamental property of quantum systems, and is **not** a statement about the observational success of current or future technology.

The last inequality can be interpreted in case of stationary states as the following: if ψ is an eigenfunction of the Hamiltonian, then the uncertainty of the energy is zero, thus the uncertainty of the time must be infinity, therefore this state can persist forever, which means that the state is stationary.

Free particle in 1D

The simplest case is when the potential V is zero everywhere. Then the potential term is missing from the Schrödinger equation, thus we get:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2} = E\varphi(x)$$

we can rearrange it:

$$\frac{d^2\varphi}{dx^2} = -\frac{2mE}{\hbar^2}\varphi$$

and introduce new notation: $k = \frac{\sqrt{2mE}}{\hbar}$. Now the equation it is very simple:

$$\frac{d^2\varphi}{dx^2} = -k^2\varphi$$

The solution:

$$\boxed{\varphi(x) = Ae^{\mathrm{ikx}}},$$

where k is an arbitrary real number. Let us calculate the momentum:

$$\hat{p}_x\varphi = \frac{\hbar}{i}\frac{\partial}{\partial x}\left(Ae^{\mathrm{ikx}}\right) = \frac{\hbar}{i}\cdot ik\cdot Ae^{\mathrm{ikx}} = \hbar k\varphi$$

thus momentum of the particle is

$$p = \hbar k = \frac{h}{\lambda}$$

and we get back the assumption of de Broglie. Now we can write the wave-function into an other form:

$$\varphi\left(x\right) = Ae^{\frac{i}{\hbar}p_x x}$$

We obtain the energy of the particle similarly:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\varphi(x)}{\partial x^2} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\left(Ae^{\mathrm{ikx}}\right) = \frac{\hbar^2 k^2}{2m}\varphi(x) = E\varphi(x)$$

Thus the energy is:

$$E = \frac{\hbar^2 k^2}{2m}$$

As k was an arbitrary real number, the energy of the free particle can be any positive number, so the energy-spectrum is continuous. If k>0, the momentum and therefore the velocity of the particle is positive, which means that the particle is travelling to the right. The particle can be in a superposition of a left-moving and a right moving wave:

$$\varphi(x) = Ae^{\text{ikx}} + Be^{\text{-ikx}}$$

This is also a solution of the Schrödinger equation above, because only k^2 is present in the expression of energy.

If A=B, then the above solution can be given in a new form using the Euler identity $e^{ix} = \cos x + i \sin x$:

$$\varphi(x) = A(e^{ikx} + e^{-ikx}) = 2A\cos kx .$$

Similarly, if $A = -B$:

$$\varphi(x) = A(e^{ikx} - e^{-ikx}) = 2A\sin kx .$$

Thus the sin and cos functions are also good solutions of the energy-eigenvalue equation, and they represent standing waves.

Infinite 1D potential well (particle in a box)

We solve this problem only in 1D, where the potential limits the motion of the particle into the $(0, a)$ interval:

$$V(x) = \begin{cases} \infty, & \text{if } x < 0 \\ 0, & \text{if } 0 \le x \le a \\ \infty, & \text{if } x > a \end{cases}$$

Thus outside the $(0, a)$ interval, $\varphi \equiv 0$.

Now we have a nontrivial continuity requirement:

$$\varphi(0) = \varphi(a) = 0$$

Inside the well, (in the $0 \le x \le a$ section) the Schrödinger-equation has the form:

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} = E\varphi$$

It is very similar to the case of the free particle. However, the absolute value of the $e^{\pm\text{ikx}}$ function is 1, thus these functions never reach zero, which contradicts the continuity requirement. We can write the general solution of this equation:

$$\varphi = A \cdot \sin(kx) + B \cdot \cos(kx) .$$

The continuity requirement φ(0)=0 yields B=0, thus the wave function is purely a sine wave.

φ(a)=0 yields:

$$Asin(ka) = 0 \Leftrightarrow ka = n\pi,$$

where n is an integer number, which will be our first quantum number.

So we have the wave function: $\varphi_n = A\sin\frac{n\pi}{a}x$

Physically this means a standing wave for each n>0. In order to obtain the possible energy values we substitute back the expression $k = \frac{\sqrt{2mE}}{\hbar}$, and obtain:

$$\frac{\sqrt{2mE}}{\hbar} a = n\pi \,.$$

After rearrangement

$$2mEa^2 = n^2\pi^2\hbar^2 = n^2\pi^2 \frac{h^2}{4\pi^2}$$

One can see that the energy is quantized and proportional to the square of the n quantum number:

$$E = \frac{h^2}{8ma^2} n^2$$

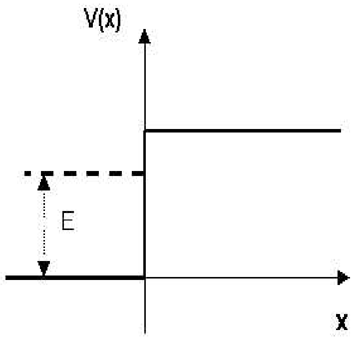
See for example: https://www.youtube.com/watch?v=nFHhLJGDNHA

Solution of Schrödinger equation for a step potential

Suppose that at x=0 there is a discontinuity in the potential:

$$V(x) = \begin{cases} 0, & \text{if } x < 0 \\ \text{V}, & \text{if } 0 \le x \end{cases}$$

We examine the case when a particle is coming from the left side with kinetic energy less than V.



As a particle approaches the barrier, it is described by a free particle wavefunction. The solution of the Schrödinger equation on the left side is usual:

$$\varphi_1(x) = Ae^{\frac{i}{\hbar}p_x x} + Be^{-\frac{i}{\hbar}p_x x}, \quad p_x > 0$$

The second term represents the reflected wave, thus $B \le A$.
When it reaches the barrier, it must satisfy the Schrödinger equation in the form

$$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} + V\varphi = E\varphi \,.$$

If we introduce $q = \sqrt{2m(V-E)} > 0$ and rearrange the equation:

$$\frac{d^2\varphi}{dx^2} = \frac{q^2}{\hbar^2}\varphi$$

Now the mathematical solution is a combination of exponential functions with real exponent:

$$\varphi(\mathrm{x}) = Ce^{-\frac{q}{\hbar}x} + De^{\frac{q}{\hbar}x}$$

The second term is problematic:

$e^{\frac{q}{\hbar}x} \to \infty$, if $x \to \infty$, which is nonphysical. Thus D=0 and the solution is an **exponentially decreasing real function**:

$$\varphi_2(x) = Ce^{-\frac{q}{\hbar}x}$$

The probability density

$$\rho(x) = \phi^*(x)\cdot\phi(x) = C^*\cdot C\cdot e^{\frac{-2q}{\hbar}x} = |C|^2\cdot e^{\frac{-\sqrt{8m(V-E)}}{\hbar}x}$$

According to classical physics, a particle of energy E less than the height V of a barrier could not penetrate - the region inside the barrier is classically forbidden. But the wavefunction associated with a free particle must be continuous at the barrier and will show an exponential decay inside the barrier.
The **penetration depth** is the distance inside the potential-step where the probability decreases by a factor e:

$$\rho(\mathrm{x_p}) = e^{-1}\rho(\mathrm{x_0})$$

Now the penetration depth is inversely proportional to the square root of the mass and the missing energy:

$$\mathrm{x}_p = \frac{\hbar}{\sqrt{8m(V-E)}},$$

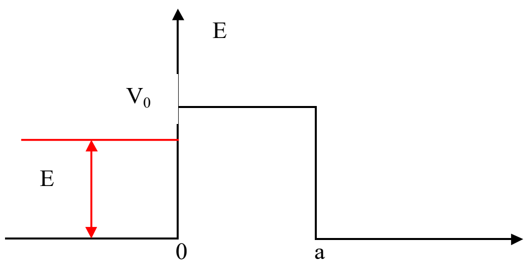
and with this notation:

$$\rho(x) = |C|^2\cdot e^{-\frac{x}{x_p}}$$

Quantum Tunnelling

Consider now a potential barrier:

$$V(x) = \begin{cases} 0, & \text{if } x<0 \\ \mathrm{V}, & \text{if } 0\le x\le a \\ 0, & \text{if } x>a \end{cases}$$

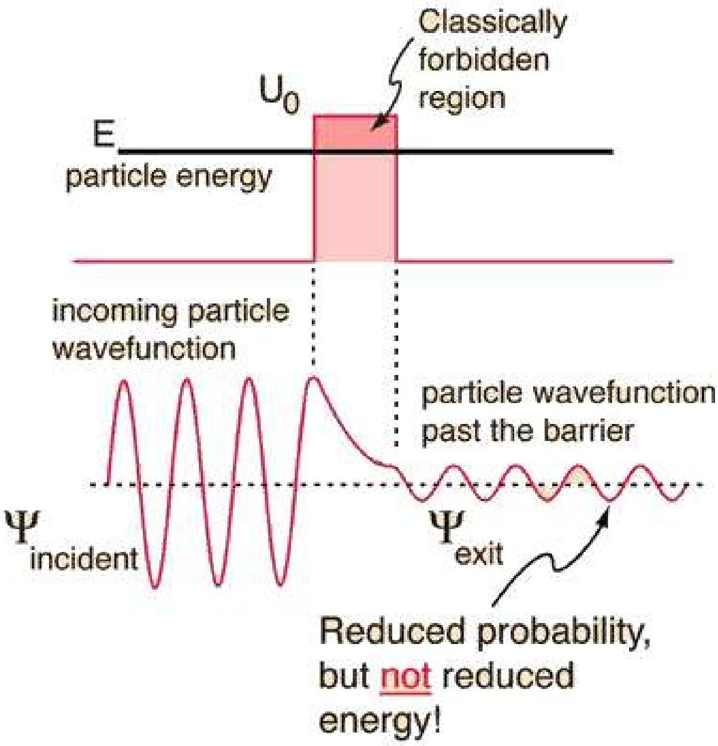


Let examine a particle coming from the left with kinetic energy less than V.
As the left part of the potential is the same as in the previous case, we use the information obtained for the step potential. Most importantly the wave function inside the barrier is an exponentially decreasing function. The wavefunction must be continuous at both side of the barrier, so there is a finite probability that the particle will tunnel through the barrier. If this happens, the energy of the particle will be the same as before meeting the potential barrier.

The transmission coefficient T and reflection coefficient R are used to describe the behaviour of waves incident on a barrier. The transmission coefficient represents the probability of the particle to cross the barrier.

$$T = \frac{\rho(\mathrm{a})}{\rho(0)} = \frac{|C|^2\cdot e^{-\frac{\mathrm{a}}{\mathrm{x_p}}}}{|C|^2} = e^{-\frac{\mathrm{a}}{\mathrm{x_p}}} = e^{-\frac{\sqrt{8m(V-E)}}{\hbar}\mathrm{a}}$$

while $R = 1 - T$.

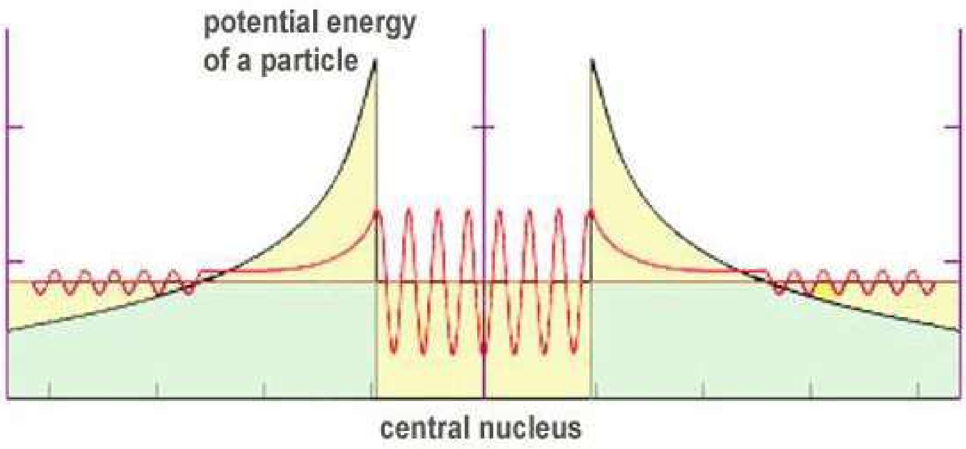


Thus in quantum mechanics, the particle can go across energy barriers which – according to classical physics – too high and therefore impenetrable for them. This is a manifestation of Heisenberg's uncertainty principle. However, as the size of the particle or the width of the potential barrier is increasing, the probability of violating classical physics is rapidly decreasing.

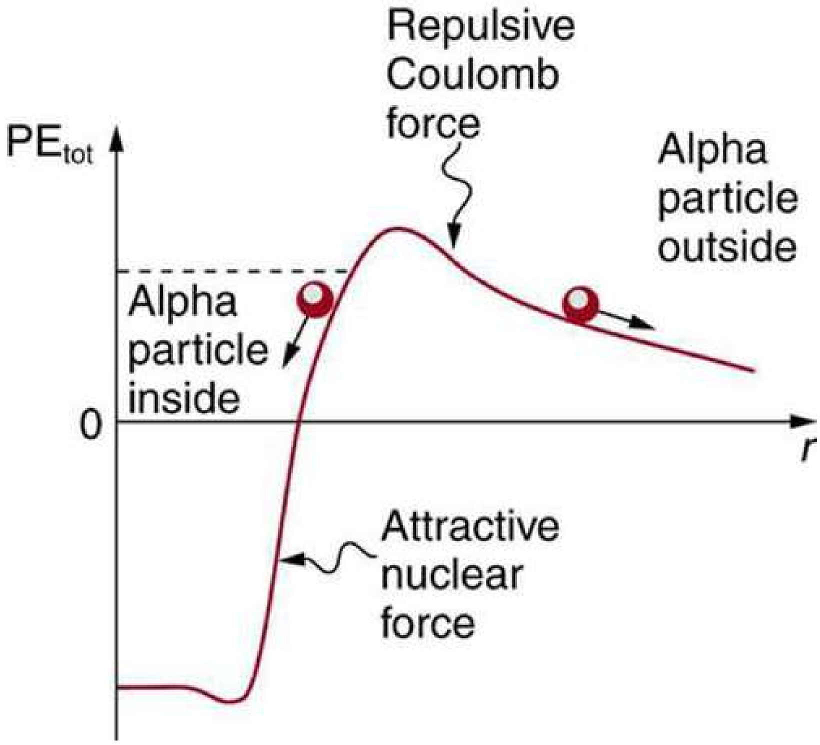
Examples:

Tunnelling occurs with barriers of thickness around 1-3 nm and smaller, but it is the cause of some important macroscopic physical phenomena. For instance, tunnelling is a source of current leakage in very-large-scale integration (VLSI) electronics and results in the substantial power drain and heating effects that plague high-speed and mobile technology; it is considered the lower limit on how small computer chips can be made.

Nuclear fusion
Fusion occurs in most stars like the Sun. The temperatures in the Sun are actually many times cooler than the extreme high temperatures which are theoretically needed to provide the incoming protons with enough energy and speed to overcome the strong repulsive electromagnetic force of the receiving hydrogen atoms. By virtue of quantum tunnelling and Heisenberg's uncertainty principle, the protons can tunnel through the barrier even given the apparently insufficient temperature and energy. The probability of this tunnelling is quite low, that is why the sun shines approximately constantly over several millions of years.



Radioactive decay
Radioactive decay is the process of emission of particles and energy from the unstable nucleus of an atom to form a stable product. This is done via the tunnelling of a particle out of the nucleus. This was the first application of quantum tunnelling.



Cold emission
Cold emission of electrons is relevant to semiconductors and superconductor physics. It is similar to thermionic emission, where electrons randomly jump from the surface of a metal to follow a voltage bias because they statistically end up with more energy than the barrier, through random collisions with other particles. When the electric field is very large, the barrier becomes thin enough for electrons to tunnel out of the atomic state, leading to a current that varies approximately exponentially with the electric field. These materials are important for flash memory, vacuum tubes, as well as some electron microscopes.

Tunnel junction

A simple barrier can be created by separating two conductors with a very thin insulator. These are tunnel junctions, the study of which requires quantum tunnelling. For example when you twist two copper wires together or close the contacts of a switch, current passes from one conductor to the other despite a thin insulator oxide layer between them. The electrons go through this thin insulating layer by the tunnel effect. If there are only a few atomic layers between the two conductors, the tunnelling probability is enough for conducting.
In case of superconductors, Josephson junctions take advantage of quantum tunnelling.

Tunnel diode
A tunnel diode is a type of semiconductor device that is capable of very fast operation, well into the microwave frequency region, made possible by the use of the quantum tunneling. There is a voltage-region where the differential resistance is negative because the current decreases with increasing voltage.

Angular momentum in quantum physics

The angular momentum operator plays an important role in the theory of atomic physics and other quantum problems involving rotational symmetry.
In classical physics:

$$\vec{L} = \vec{r} \times \vec{p}$$

This can be carried over to quantum mechanics, by reinterpreting r as the quantum position operator and p as the quantum momentum operator. L is then an operator, specifically called the orbital angular momentum operator. Specifically, L is a vector operator, meaning $\mathbf{L} = (L_x, L_y, L_z)$, where L_x, L_y, L_z are three different operators.

However, there is another type of angular momentum, called **spin** angular momentum (more often shortened to spin), represented by the spin operator $\hat{S}$.
Because of the Heisenberg's uncertainty principle, the x, y and z component of the angular momentum cannot be measured simultaneously, they have no definite values at the same time. If L_z and L^2 is determined (these two are the usual choice), than L_x and L_y are completely undetermined. So it is possible to solve only the L_z and L^2 eigenvalue-equation simultaneously to obtain the possible values for the angular momentum.
The orbital angular momentum is quantized according to the relationship:

$L^2 = \hbar^2 l(l+1)$ where $l = 0,1,2,\dots$ is the angular or azimuthal quantum number.

The z-component of the angular momentum takes the form

$L_z = \hbar m$, where $m = -\ell, -\ell+1, \dots, 0, 1, 2, \dots, \ell-1, \ell$ is the magnetic quantum number

As these formulas can be derived from a very general way, these applies to orbital angular momentum, spin angular momentum, and the total angular momentum for an atomic system.
We recall that angular momentum quantization was put into the semi-classical Bohr model as an ad hoc assumption with no fundamental justification and the concrete $L_{e^-} = n\hbar$ formula was not correct. However, by the real quantum mechanics, the quantization and the correct values come out automatically.

Quantum numbers in an atom contains 1 electron

From the Heisenberg's uncertainty relation $\Delta x \Delta p_x \geq \frac{\hbar}{2}$ we obtain $\Delta x \cdot m \cdot \Delta v_x \geq \frac{\hbar}{2} \approx 10^{-34}$

For the electron in the atom, the uncertainty of the position is roughly the size of the atom: $\Delta \mathrm{x} \cong 10^{-10}\,\mathrm{m}$ and the mass is $m \cong 10^{-30}\,kg$, thus

$$\Delta v_x \cong \frac{10^{-34}}{10^{-10} \cdot 10^{-30}} = 10^{6}\,\frac{m}{s}.$$

This is so high that we can state that the electron has no trajectory in the atom. If we would localize the electron even more, the uncertainty is even higher.
We need to find a more relevant and usable description and it is possible with quantum numbers.
We have to solve the Schrödinger-equation with the Coulomb-potential:

$$-\frac{\hbar^2}{2m}\Delta\psi - k\frac{Ze^2}{r}\psi = E\psi;$$

The solution consists of complicated functions, where the quantum numbers are the parameters of these functions.

1. The principal quantum number (n) describes the electron shell, or energy level, of an atom. The value of n ranges from 1 to the shell containing the outermost electron of that atom, i.e.

   $$E_n = -Z^2 \cdot E^* \cdot \frac{1}{n^2}\ ,\ \text{where n = 1, 2, ...}$$

2. The angular or azimuthal quantum number (ℓ) (also known as the orbital quantum number) describes the subshell, and gives the magnitude of the orbital angular momentum through the relation

   $$L^2 = \hbar^2 \ell(\ell+1)\ ,\ \text{where } \ell = 0, 1, 2,..., n-1.$$

   "ℓ = 0" is often called an s orbital, "ℓ = 1" a p orbital, "ℓ = 2" a d orbital, and "ℓ = 3" an f orbital.

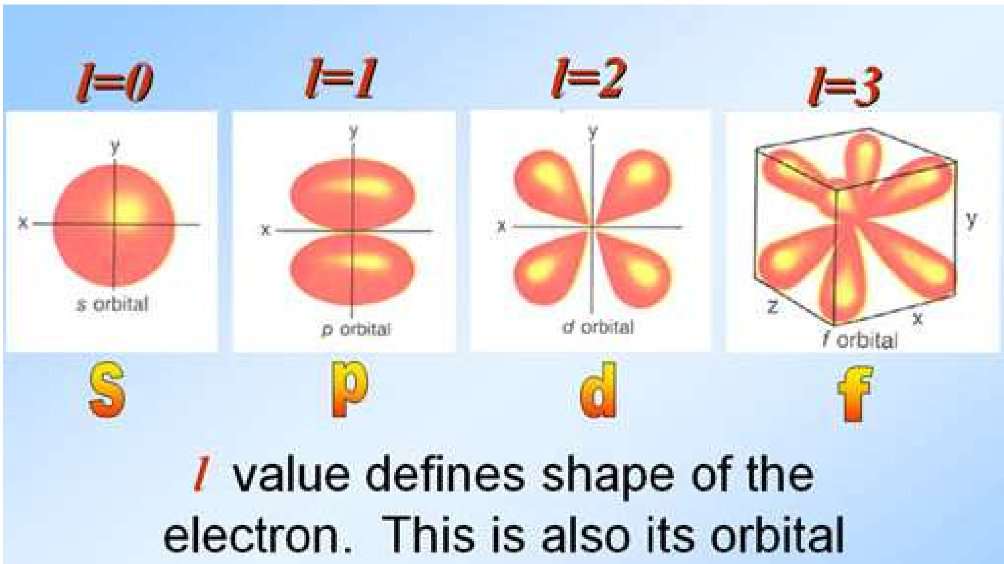
3. The magnetic quantum number (m) describes the specific orbital (or "cloud") within that subshell, and yields the projection of the orbital angular momentum along a specified axis:

   $$L_Z = \hbar m\ ,\ \text{where}\quad m = -\ell, -\ell+1, ..., 0, 1, 2, ..., \ell-1, \ell$$

   As the magnetic moments have a potential energy in magnetic field (this is the Zeeman-energy), if $\vec{H} \neq 0$ then the energy of the electron depends on H as well.

4. The spin quantum number or more precisely the spin projection quantum number (m_s or sometimes s) describes the spin (intrinsic angular momentum) of the electron within that orbital, and gives the projection of the spin angular momentum S along the specified axis:

   $$S_z = \hbar m_s \text{ where } m_s = -\frac{1}{2}, +\frac{1}{2}$$



https://www.youtube.com/watch?v=GordTWgyQnA

Quantum Statistics

In statistical mechanics, the **classical** or **Maxwell–Boltzmann statistics** describes the average distribution of distinguishable particles over various energy states in thermal equilibrium if quantum effects are negligible. The expected number of particles in a state with energy E_i

$$f_{MB}(E_i) = \frac{1}{Ae^{\frac{E_i}{kT}}} = \frac{1}{A}e^{-\frac{E_i}{kT}},$$

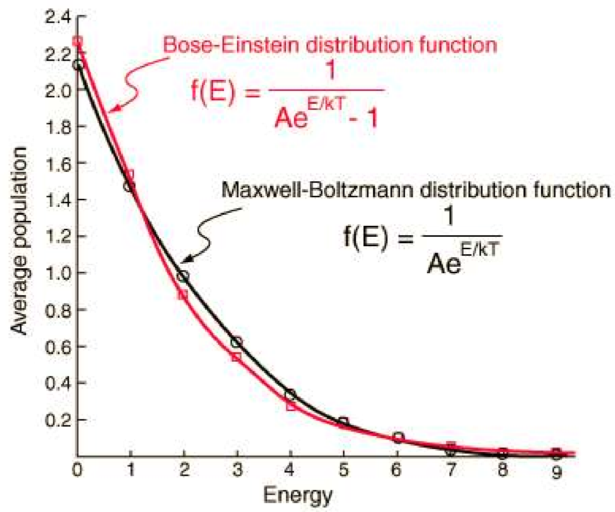
where k is Boltzmann's constant, T is the absolute temperature, A is a normalization constant (which keeps the number of particles constant).

In **quantum** statistics, there are **two** possible ways in which a collection of non-interacting indistinguishable particles may occupy a set of available discrete energy states, at thermodynamic equilibrium. One of them is the Bose–Einstein statistics (B–E statistics) and the other is the Fermi–Dirac statistics.

The **Bose–Einstein statistics** apply only to those particles not limited to single occupancy of the same state — that is, particles that do not obey the Pauli exclusion principle restrictions. Such particles have integer values of spin and are named **bosons**, after the statistics that correctly describe their behaviour. If we have a state i with energy E_i , then the average number of particles in that state is

$$f_{BE}(E_i) = \frac{1}{Ae^{\frac{E_i}{kT}} - 1}$$

Examples for bosons are the photons, the He nucleus and the Higgs boson.



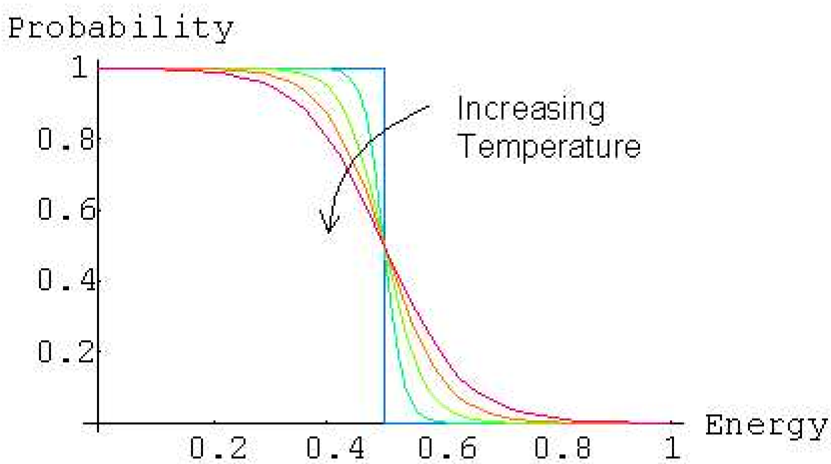
The other statistics is **Fermi–Dirac statistics**, which describes a distribution of particles over energy states in systems consisting of particles that **obey the Pauli exclusion principle**. It is most commonly applied to electrons, protons and neutrons, which are **fermions** with spin 1/2. If we have a state i with energy E_i , then the average number of Fermi particles in that state is

$$f_{FD}(E_i) = \frac{1}{Ae^{\frac{E_i}{kT}} + 1}$$

It can be calculated that the normalization constant A is $A = e^{-\frac{E_F}{kT}}$, where E_F is the **Fermi energy**. Now we have:

$$\boxed{f_{FD}(E_i) = \frac{1}{e^{\frac{E_i - E_F}{kT}} + 1}}$$

The denominator cannot be less than one, $f\left(E_i\right) < 1$, thus one can see that it reflects the Pauli principle. Therefore we can say $f\left(E_i\right)$ is the probability of occupying the particular state.



Even if the temperature is absolute zero, the fermions cannot occupy the state with the minimal energy, because they are already occupied by other fermions.

At low temperatures, bosons can behave very differently than fermions because an unlimited number of them can collect into the same energy state, a phenomenon called "condensation".

If the energy E is much larger than kT, the $e^{\frac{E}{kT}}$ term is much greater than 1, thus the quantum statistics tend to the classical one.

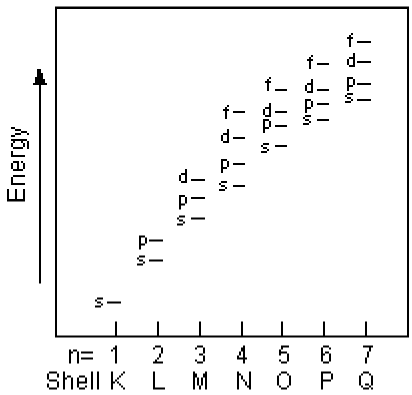
Quantum numbers for atoms with more electrons and the periodic table

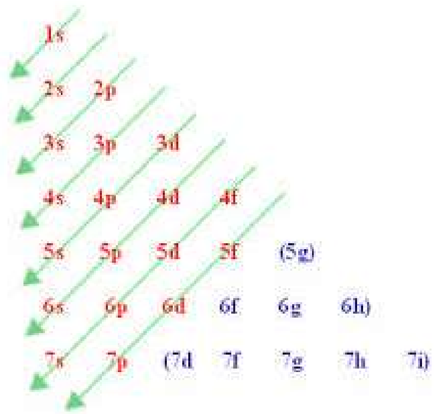
It is very hard to solve the Schrödinger equation if the number of electrons is greater than one. The results will be similar to the case of one electron, but now the quantum numbers have no exact meaning, they describe the behaviour of the electrons only approximately. The most important difference from the one-electron case is that now the energy depends on the angular quantum number:

$$E_{n,\ell} < E_{n,\ell+1}$$

The order of the energy levels:

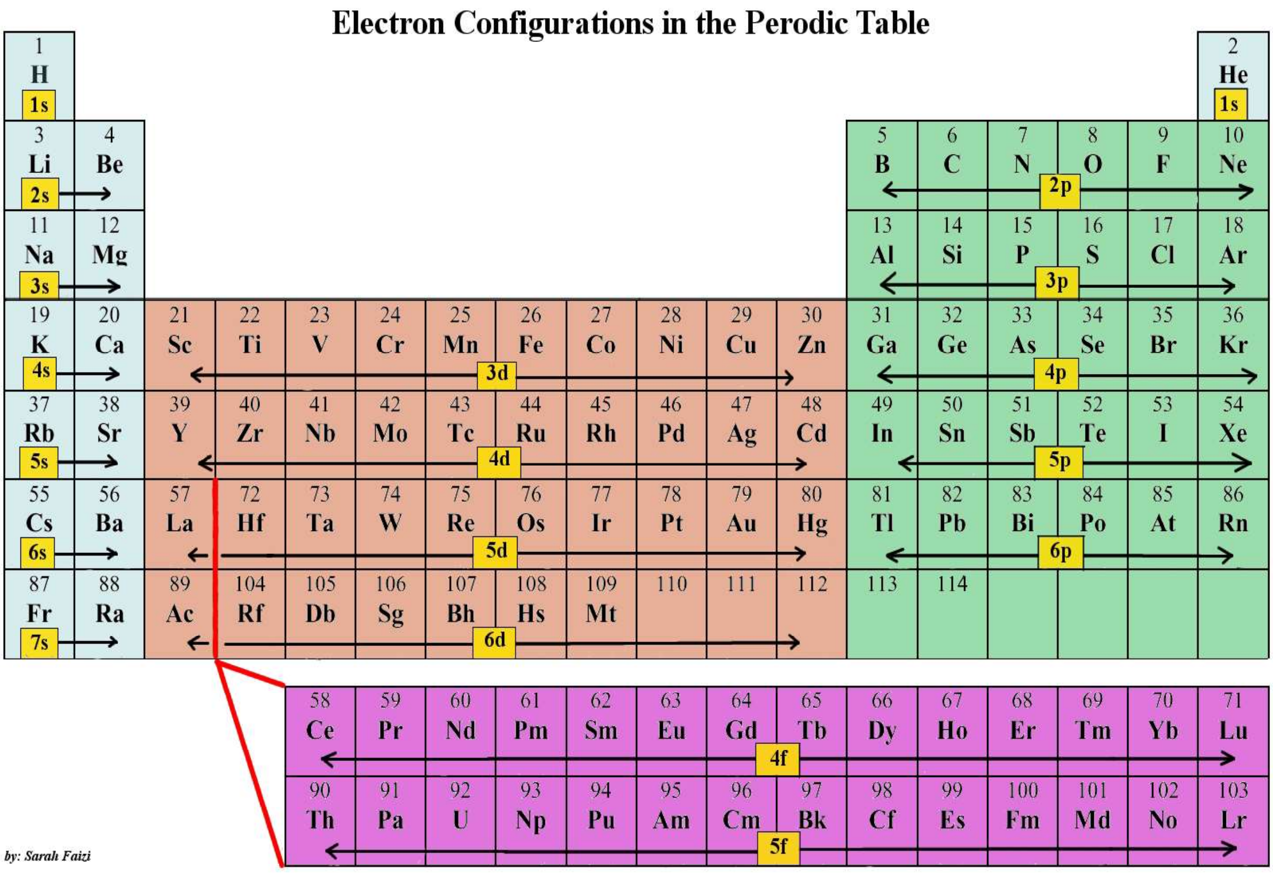
1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p





To understand the periodic table, we need the Pauli principle and the energy-minimum principle applied to these concrete energy-levels.
An element's location on the periodic table reflects the quantum numbers of the last orbital filled. The period indicates the value of principal quantum number for the valence shell. The lanthanides and actinides, indicated by pink-purple, are in periods 6 and 7, respectively. Each of them contains 14 elements, because if $\ell = 3$, m has 7 possible values (from -3 to 3), and 2*7=14.

The block indicates the value of the angular quantum number ℓ for the last subshell that received electrons in building up the electron configuration. The blocks are named for subshells (s, p, d, f)



Each block contains a number of columns equal to the number of electrons that can occupy that subshell

The s-block (in light blue) has 2 columns, because a maximum of 2 electrons can occupy the single orbital in an s-subshell.

The p-block (in green) has 6 columns, because a maximum of 6 electrons can occupy the three orbitals in a p-subshell.

The d-block (in orange) has 10 columns, because a maximum of 10 electrons can occupy the five orbitals in a d-subshell.

The f-block (in pink/purple) has 14 columns, because a maximum of 14 electrons can occupy the seven orbitals in a f-subshell.

Possible elaborative questions:

1) Blackbody radiation
2) Photoelectric effect and the momentum of the photon
3) Line spectra of atoms and the Bohr model
4) Wave particle duality of particles, de-Broglie hypothesis
5) Wave Function and the principle of superposition
6) Operators and eigenvalues
7) The concrete form of the operators and the Schrödinger equation
8) Heisenberg's uncertainty principle
9) Free particle in 1D
10) Infinite 1D potential well (particle in a box)
11) Solution of Schrödinger equation for a step potential and quantum tunnelling
12) The essence of quantum tunnelling and some examples
13) Angular momentum and atoms with 1 electron
14) Quantum Statistics
15) Atoms with more electrons and the periodic table

Sample questions:

Which is true for the photoelectric effect?

A) If the incoming intensity is large, the effect always immediately occurs.

B) The effect occurs only if the frequency is large enough.

C) We can always see the effect independently of the frequency of the light.

D) The energy of the incoming photon is always smaller than the energy of the emitted electron.

E) The effect occurs only in the case of some discrete frequencies.

F) If the incoming intensity is small, we have to wait for the effect for hours or days.

Which one in <u>not</u> true for the wave function of a given electron in a given infinite potential well?

A) **It is continuous.**
B) **It is zero at the edge of the wall.**
C) **It can be zero in some points inside the well far from the edges.**
D) **The energy can be arbitrary.**
E) **The kinetic energy is positive.**
F) **The energy can be determined without deviance.**