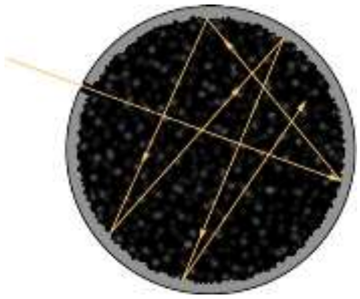
Lecture by: Dr. Ruwaida Saadi Obaid
October 10 2023

Quantum Mechanics

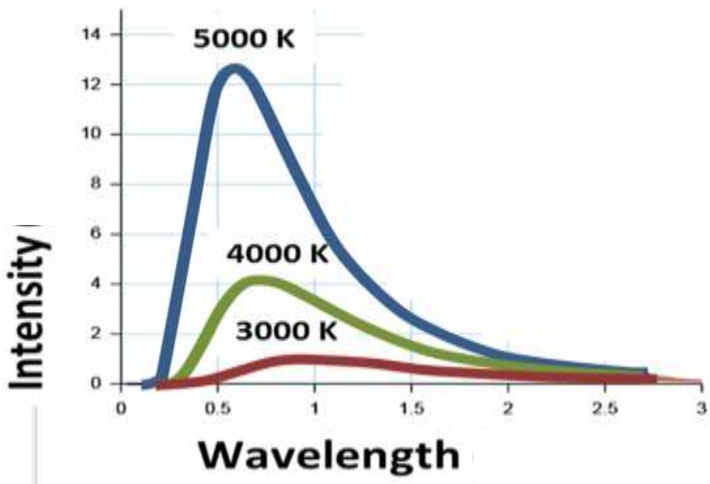
University of Technology
Laser and Optoelectronics Engineering Department
Third Stage

Blackbody Radiation and Plank's Hypothesis

A blackbody is an ideal system that absorbs all radiation incident on it. The electromagnetic radiation emitted by the blackbody is called blackbody radiation. A good approximation of a blackbody is a small opening to the inside of a cavity object as shown in the figure.



Any radiation incident on the opening from outside enters the cavity and is reflected a number times on the interior walls of the cavity; hence the blackbody acts as a perfect absorber. The nature of the radiation leaving the cavity depends only on the temperature of the cavity walls. The peak of the wavelength distribution shifts to shorter wavelength as the temperature increases this behavior described by the following relationship, called **Wien's displacement law**: $\lambda_{max}T = 2.898\times10^{-3}\,\text{m.K}$



Example Find the peak wavelength of the blackbody radiation emitted by the human body when the skin temperature is: (A) 35^0C and (B) 2000K.

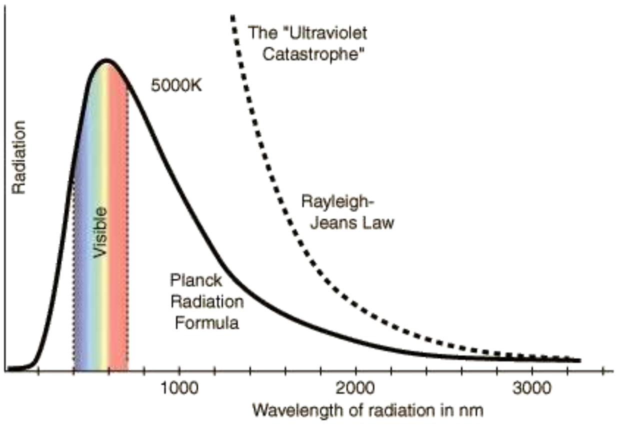
Solution:

$$\lambda_{max} = \frac{2.898\times10^{-3}\,\text{m.K}}{T}$$
$$= \frac{2.898\times10^{-3}\,\text{m.K}}{(35+273)\text{K}} = \frac{2.898\times10^{-3}\,\text{m.K}}{308\text{K}}$$
$$= 9.4\times10^{-6}\,\text{m}$$
$$= 9.4\ \mu\text{m}$$

$$\lambda_{max} = \frac{2.898\times10^{-3}\,\text{m.K}}{T}$$
$$= \frac{2.898\times10^{-3}\,\text{m.K}}{2000\text{K}}$$
$$= 1.4\times10^{-6}\,\text{m}$$
$$= 1.4\ \mu\text{m}$$

Rayleigh-Jeans Law:

The result of a calculation based on a classical theory of blackbody radiation known as the **Rayleigh-Jeans Law,** to describe the distribution of energy from a blackbody, we define $I(\lambda,T)$ to be the intensity $I(\lambda,T) = \frac{2\pi c k_B T}{\lambda^4}$, where k_B is a Boltzmann's constant and c is the speed of light. In this equation, the average energy for each wavelength is assumed to be proportional to $k_B T$. As experimental plot of the blackbody radiation spectrum, together with the theoretical prediction of the **Rayleigh-Jeans Law**, is shown in the below figure.



At long wavelengths, the **Rayleigh-Jeans Law** is reasonable agreement with experimental data, but at short wavelengths, major disagreement is apparent (infinite energy occurs as the wavelength approaches zero). This mismatch of theory and experiments was so disconcerting that scientists called it the **ultraviolet catastrophe**.

Planck-Einstein's visualization of the quantum nature of radiation

Photoelectric Effect

How is the photoelectric effect related to quantum mechanics?

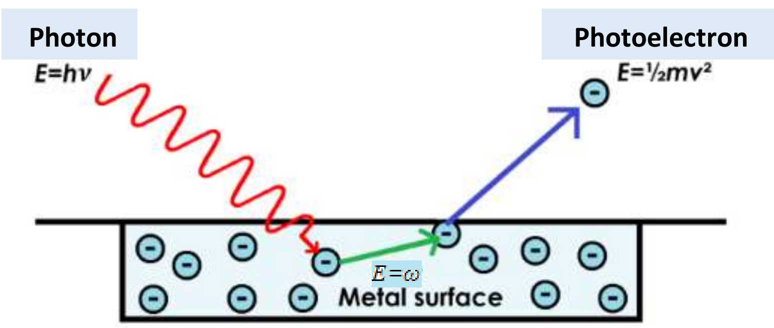
According to **Max Planck**, the radiant energy can have only certain discrete values $E = h\upsilon$ where h is called Planck's constant (h=6.63x10^{-34} J.s) and υ is the frequency of the incident light. In the 19th century, experiments showed that light incident on certain metallic surfaces causes electrons to be emitted from those surfaces, this phenomena is known as the **photoelectric effect** and the emitted electrons are called the **photoelectrons**. In **Einstein's model** of the photoelectric effect, a photon of the incident light gives all its energy $h\upsilon$ to a single electron in the metal. Therefore, the absorption of energy by the electrons is not a continuous absorption process but it is a discontinuous process in which energy is delivered to the electrons in discrete bundles. Let ω be (the work function) i.e. the minimum energy with which an electron is bound in the metal and the photoelectron ejected from the surface with kinetic energy (K_{max}=1/2 mv^2), then $h\upsilon = \omega + \frac{1}{2}mv^2$. If υ_0 is the threshold frequency which just ejects an electron from the metal without any velocity then $\omega = h\upsilon_0$:

$$h\upsilon = \omega + K_{\max}$$

$$h\upsilon = h\upsilon_0 + \frac{1}{2}mv^2$$

$$\frac{1}{2}mv^2 = h\upsilon - h\upsilon_0$$

$$= h(\upsilon - \upsilon_0)$$



Cutoff wavelength

The cutoff frequency is related to the work function through the relationship $\upsilon_c = \omega / h$. The cutoff frequency corresponds to a cutoff wavelength λ_c , where

$$\lambda_c = \frac{c}{\upsilon_c} = \frac{c}{\omega / h} = \frac{hc}{\omega}$$

where c is the speed of light= $3 \text{x} 10^8$ m/s.

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$$1\text{eV} = 1.6 \times 10^{-19}\,\text{J}$$

$$h = 6.63\text{x}10^{-34}\ \text{J.s}$$

$$= 6.63 \times 10^{-34} / 1.6 \times 10^{-19}$$

$$= 4.125 \times 10^{-15}\ \text{eV.s}$$

$$hc = 4.125 \times 10^{-15}\ \text{eV.s} \times 3\text{x}10^{8}\,\text{m/s}$$

$$= 1.2375 \times 10^{-6}\ \text{eV.m}$$

$$1\text{nm} = 10^{-9}\text{m}$$

$$\text{m} = 10^{+9}\text{nm}$$

$$hc = 1.2375 \times 10^{-6}\text{eV}.10^{+9}\text{nm}$$

$$= 1237.5\ \text{eV.nm}$$

$$\simeq 1240\ \text{eV.nm}$$

Example 1 : The photoelectric effect for Sodium:

A Sodium surface is illuminated with light having a wavelength of 300nm. The work function for sodium metal is 2.46 eV.

(A) Find the maximum kinetic energy of ejected photoelectrons.
(B) Find the cutoff wavelength for Sodium.

Solution:

$$E = h\upsilon$$
$$= h\frac{c}{\lambda}$$
$$= \frac{1240 \text{ eV.nm}}{300 \text{ nm}} = 4.13 \text{ eV}$$
$$K_{\max} = h\upsilon - \omega$$
$$= 4.13 \text{ eV} - 2.46 \text{ eV} = 1.67 \text{ eV}$$
$$\lambda_c = \frac{hc}{\omega} = \frac{1240 \text{ eV.nm}}{2.46 \text{ eV}} = 504 \text{ nm}$$

Example 2 : A photoelectric surface has a work function of 4 eV. What is the maximum velocity of the photoelectrons emitted by light of frequency 10^{+15} H_z incident on the surface. Hint: mass of electron is $9x10^{-31}$gm.

Solution:

$$\omega = 4eV \ = 4\times1.6\times10^{-19}\text{ J} = 6.4\times10^{-19}\text{ J}$$
$$K_{\max} = h\upsilon - \omega$$
$$\frac{1}{2}m\nu^2 = 6.63\times10^{-34}\times10^{+15} - (6.4\times10^{-19})$$
$$\frac{1}{2}(9\times10^{-31})\nu^2 = 0.2\times10^{-19}$$
$$\nu^2 = \frac{0.4\times10^{-19}}{9\times10^{-31}}$$
$$\nu = 2\times10^5 \text{ m/s}$$

Example 3 : Calculate the threshold frequency and the corresponding wavelength of radiation incident on a certain metal whose workfunction is 3.31x10^{-19}J.

Solution:

$$\omega = h\upsilon_0$$

$$3.31\times10^{-19}\,\text{J} = 6.63\times10^{-34}\ \text{J.s}\ \upsilon_0$$

$$\upsilon_0 = \frac{3.31\times10^{-19}}{6.63\times10^{-34}}\,\text{s}^{-1} = 5\times10^{14}\,\text{s}^{-1}$$

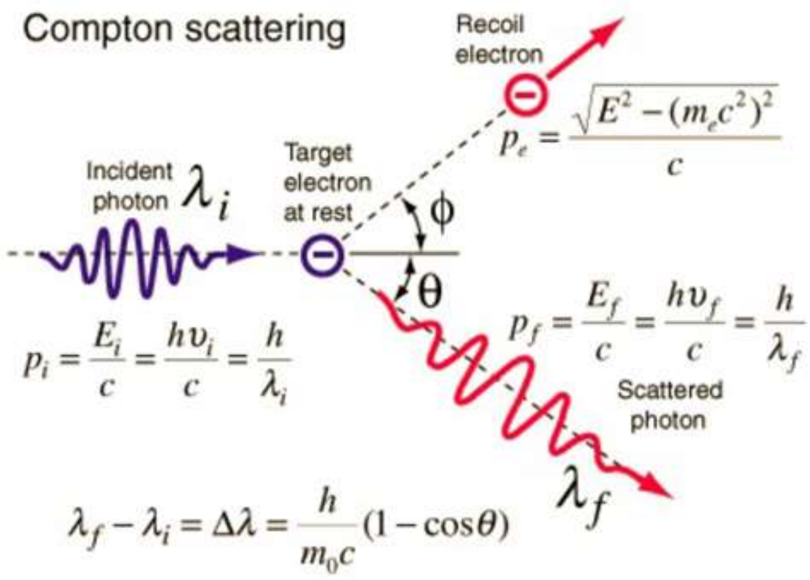
$$\lambda_0 = \frac{c}{\upsilon_0} = \frac{3\times10^{8}\,\text{m/s}}{5\times10^{14}\,\text{s}^{-1}} = 6\times10^{-7}\,\text{m}$$

Home Work: Calculate the longest wavelength of the incident radiation which will eject electrons from a metal work function is 6 eV.

Compton effect

What is the importance of Compton effect in quantum mechanics?

When a photon, usually from the X-Ray spectrum, collides with an electron, or any other charged particle, the wavelength of the scattered X-Ray increases. When the photon comes into contact with the electron, some of its initial energy and momentum are transferred to the charged particle. As such, the scattered photon has less energy than the incident photon and thus, a lower frequency and a higher wavelength, due to their inversely proportional relationship. This phenomenon is known as the **Compton Effect**.



The greatest significance of the Compton effect is that is to provide final and deciding proof for Planck-Einstein's visualization of the quantum nature of radiation. The particle nature of light was established after the discovery of the Compton effect.

Example

X-rays of wavelength λ_0=0.200000 nm are scattered from a block of material. The scattered x-rays are observed at an angle of 45^0 to the incident beam. Calculate their wavelength.

Solution:

$$\lambda - \lambda_0 = \frac{h}{m_0 c}(1-\cos\theta)$$

$$= \lambda_0 + \frac{h}{m_0 c}(1-\cos\theta)$$

$$= 0.200000\times10^{-9}\,\text{m} + \frac{(6.63\times10^{-34}\,\text{J.s})(1-\cos 45^0)}{(9.11\times10^{-31}\,\text{kg})(3\times10^{8}\,\text{m/s})}$$

$$= 0.200710\ \text{nm}$$

Note:

$$1\text{Joule} = \frac{\text{kg.m}^2}{\text{s}^2}$$

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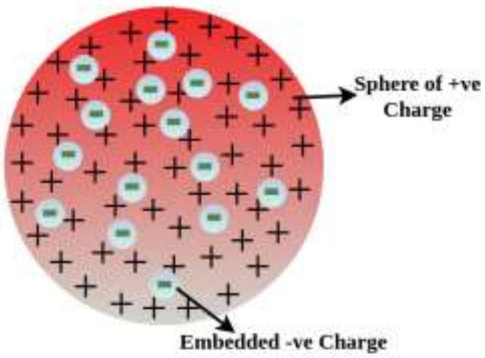
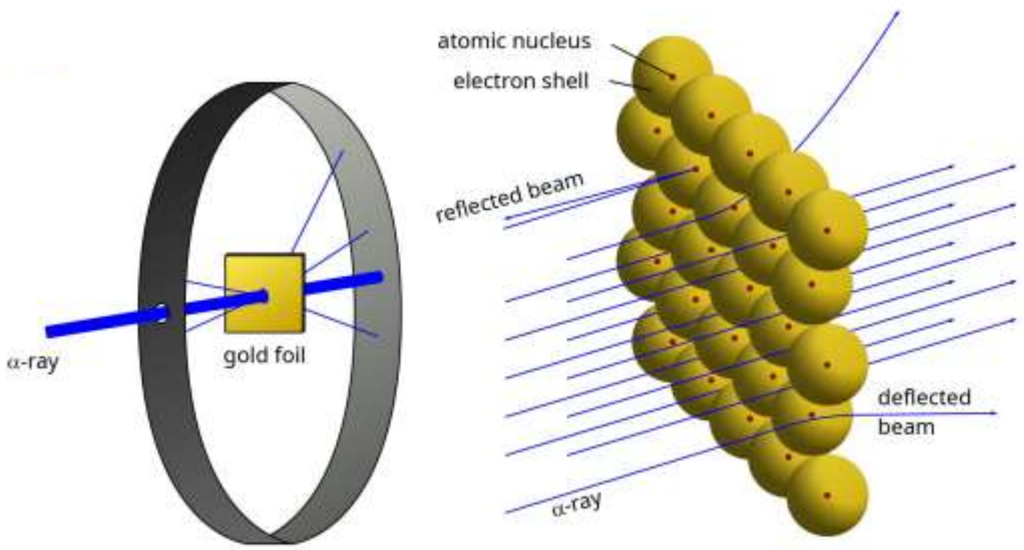
Early Models of the Atom

Thomson (in 1898) suggested a model that describes the atom as a region in which positive charge is spread out in space with electrons embedded throughout the region. The atom as a whole then be electrically neutral.



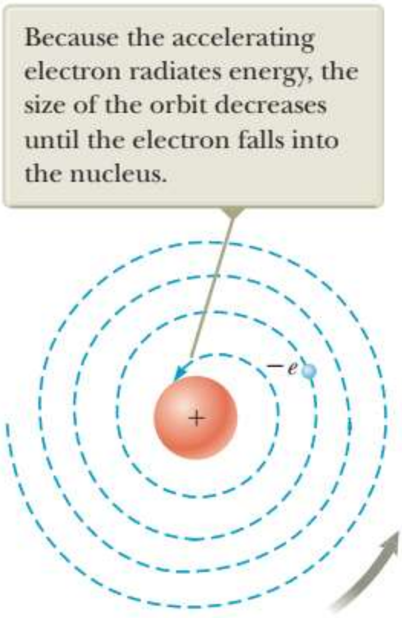
Thomson's Atomic Model

In 1911, Ernest Rutherford performed a critical experiment that showed that Thomson's model could not be correct. In this experiment, a beam of positively charged alpha particles (Helium nuclei) was projected into a thin metallic foil. Most of the particles passed through the foil as if it were empty space, but some of the results of the experiment were astounding. Many of the particles deflected from their original direction of travel were scattered through large angles.



Some particles were even deflected backward completely reversing their direction of travel. When Geiger informed Rutherford that some alpha particles were scattered backward, Rutherford wrote, "It was quite the most incredible event that has ever happened to me in my life". Such large deflections were not expected on the basis of Thomson’s model. According to that model, the positive charge of an atom in the foil is spread out over such a great volume (the entire atom) that there is no concentration of positive charge strong enough to cause any large-angle deflections of the positively charged alpha particles. Furthermore, the electrons are so much less massive than the alpha particles that they would not cause large-angle scattering either. Rutherford explained his astonishing results by developing a new atomic model, one that assumed the positive charge in the atom was concentrated in a region that was small relative to the size of the atom. He called this concentration of positive charge the **nucleus** of the atom. Any electrons belonging to the atom were assumed to be in the relatively large volume outside the nucleus. To explain why these electrons were not pulled into the nucleus by the attractive electric force, Rutherford modeled them as moving in orbits around the nucleus in the same manner as the planets orbit the Sun. For this reason, this model is often referred to as the planetary model of the atom.

Basic difficulties exist with Rutherford's planetary model. Rutherford's electrons are described by the particle in uniform circular motion model; they have a centripetal acceleration.



Bohr's Model of the Hydrogen Atom

Bohr applied Planck's ideas of quantized energy levels (Section 40.1) to Rutherford's orbiting atomic electrons. Bohr's theory was historically important to the development of quantum physics.
Bohr combined ideas from Planck's original quantum theory, Einstein's concept of the photon, Rutherford's planetary model of the atom, and Newtonian mechanics to arrive at a semi-classical structural model based on some revolutionary ideas. The structural model of the Bohr theory as it applies to the hydrogen atom has the following properties:

-The electron moves in circular orbits around the proton under the influence of the electric force of attraction.

-Only certain electron orbits are stable. When in one of these stationary states, as Bohr called them, the electron does not emit energy in the form of radiation, even though it is accelerating.

-The atom emits radiation when the electron makes a transition from a more energetic initial stationary state to a lower-energy stationary state. This transition cannot be visualized or treated classically. In particular, the frequency f of the photon emitted in the transition is related to the

$$E_i - E_f = hf$$

change in the atom's energy and is not equal to the frequency of the electron's orbital motion. The frequency of the emitted radiation is found from the energy-conservation expression

where E_i is the energy of the initial state, E_f is the energy of the final state, and $E_i > E_f$.

We can obtain an expression for *r*, the radius of the allowed orbits,

$$v^2 = \frac{n^2\hbar^2}{m_e^2 r^2} = \frac{k_e e^2}{m_e r}$$

$$r_n = \frac{n^2\hbar^2}{m_e k_e e^2} \qquad n = 1, 2, 3, \ldots$$

v is the electron's speed and *me* is the electron mass.
The orbit with the smallest radius, called the **Bohr radius** a_0, corresponds to $n = 1$ and has the value 0.0529 nm.
These relations give a general expression for the radius of any orbit in the hydrogen atom:

$$r_n = n^2 a_0 = n^2(0.052\,9 \text{ nm}) \qquad n = 1, 2, 3, \ldots$$

To calculate the frequency of the photon emitted when the electron makes a transition from an outer orbit to an inner orbit:

$$f = \frac{E_i - E_f}{h} = \frac{k_e e^2}{2a_0 h}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

Because the quantity measured experimentally is wavelength, Remarkably, this expression, which is purely theoretical, is *identical* to the general form of the empirical relationships discovered by Balmer and Rydberg

$$\frac{1}{\lambda} = \frac{f}{c} = \frac{k_e e^2}{2a_0 hc}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right)$$

Electronic Transitions in Hydrogen

(A) The electron in a hydrogen atom makes a transition from the n=2 energy level to the ground level n=1. Find the wavelength and frequency of the emitted photon.

$$\frac{1}{\lambda} = R_{\mathrm{H}}\left(\frac{1}{1^2} - \frac{1}{2^2}\right) = \frac{3R_{\mathrm{H}}}{4}$$

$$\lambda = \frac{4}{3R_{\mathrm{H}}} = \frac{4}{3(1.097 \times 10^7\ \mathrm{m}^{-1})} = 1.22 \times 10^{-7}\ \mathrm{m} = \boxed{122\ \mathrm{nm}}$$

$$f = \frac{c}{\lambda} = \frac{3.00 \times 10^8\ \mathrm{m/s}}{1.22 \times 10^{-7}\ \mathrm{m}} = \boxed{2.47 \times 10^{15}\ \mathrm{Hz}}$$

(B) In interstellar space, highly excited hydrogen atoms called Redberg atoms have been observed. Find the wavelength to which radio astronomers must turn to detect signals from electrons dropping from the n=273 level to the n=272 level.

$$\frac{1}{\lambda} = R_{\mathrm{H}}\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) = R_{\mathrm{H}}\left(\frac{1}{(272)^2} - \frac{1}{(273)^2}\right) = 9.88 \times 10^{-8}\ R_{\mathrm{H}}$$

$$\lambda = \frac{1}{9.88 \times 10^{-8} R_{\mathrm{H}}} = \frac{1}{(9.88 \times 10^{-8})(1.097 \times 10^7\ \mathrm{m}^{-1})} = \boxed{0.922\ \mathrm{m}}$$

(C) What is the radius of the electron orbit for a Rydberg atom for which n=273?

$$r_{273} = (273)^2\ (0.052\,9\ \mathrm{nm}) = \boxed{3.94\ \mu\mathrm{m}}$$

(D) How fast is the electron moving in a Rydberg atom for which *n*=273?

$$v = \sqrt{\frac{k_e e^2}{m_e r}} = \sqrt{\frac{(8.99 \times 10^9\ \mathrm{N \cdot m^2/C^2})(1.60 \times 10^{-19}\ \mathrm{C})^2}{(9.11 \times 10^{-31}\ \mathrm{kg})(3.94 \times 10^{-6}\ \mathrm{m})}}$$

$$= 8.01 \times 10^3\ \mathrm{m/s}$$

The de Broglie wavelength

In his 1923 doctoral dissertation, Louis de Broglie postulated that because photons have both wave and particle characteristics, perhaps all forms of matter have both properties. This highly revolutionary idea had no experimental confirmation at the time. According to de Broglie, electrons, just like light, have a dual particle–wave nature.

De Broglie suggested that material particles of momentum p have a characteristic wavelength that is given by the *same expression.* Because the magnitude of the momentum of a particle of mass m and speed u is p 5 mu, the **de Broglie wavelength** of that particle is

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

Furthermore, in analogy with photons, de Broglie postulated that particles obey the Einstein relation E 5 hf, where E is the total energy of the particle. The frequency of a particle is then

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

Example

(A) Calculate the de Broglie wavelength for an electron (m_e=9.11x10^{-23} kg) moving at 1.00 x10^{7} m/s.

$$\lambda = \frac{h}{m_e u} = \frac{6.626 \times 10^{-34}\ \text{J}\cdot\text{s}}{(9.11 \times 10^{-31}\ \text{kg})(1.00 \times 10^{7}\ \text{m/s})} = 7.27 \times 10^{-11}\ \text{m}$$

(B) A rock of mass 50 g is thrown with a speed of 40 m/s. What is its de Broglie wavelength?

$$\lambda = \frac{h}{mu} = \frac{6.626 \times 10^{-34}\ \text{J}\cdot\text{s}}{(50 \times 10^{-3}\ \text{kg})(40\ \text{m/s})} = 3.3 \times 10^{-34}\ \text{m}$$

Example

Find the de Broglie wavelength associated with

(1) A 46gm golf ball with velocity 36 m/sec.

$$m = 0.046\ Kg$$

$$\lambda = \frac{h}{mu} = \frac{6.63\times10^{-34}\ J.\text{sec}}{0.046\ Kg \times 36 m/\text{sec}} = 4\times10^{-34} m.$$

(2) An electron with a velocity 10^{7} m/sec.

$$\lambda = \frac{h}{mu} = \frac{6.63\times10^{-34}\ J.\text{sec}}{9.1\times10^{-31}\ Kg \times 10^{7} m/\text{sec}} = 7.3\times10^{-11} m.$$

Home Work: from the results, do you expect there is a wave aspects in the two cases? Why?

Example

Find the kinetic energy of a proton whose de Broglie wavelength is 1fm.

$$pc = \frac{hc}{\lambda} = \frac{6.63\times10^{-34}\ J.\sec\times3\times10^{8} m/\sec}{1\times10^{-15} m}$$
$$=19.89\times10^{-11} J$$
$$= \frac{19.89\times10^{-11}}{1.6\times10^{-19}} eV$$
$$=1243\times10^{6} eV$$
$$=1243\times10^{6}\times10^{-9} GeV$$
$$=1.24 GeV$$

$$E = \sqrt{E_0^2 + p^2c^2}$$
$$= \sqrt{(0.938 GeV)^2 + (1.241 GeV)^2}$$
$$= 1.556 GeV$$
$$KE = E - E_0$$
$$= (1.556 - 0.938) GeV$$
$$= 0.618 GeV .$$

Example:

If the de Broglie wavelength of an electron is 9x10^{-10} m. Calculate its kinetic energy.

$$KE = \frac{1}{2} m \mathrm{v}^2$$

$$\mathrm{v} = \sqrt{\frac{2KE}{m}}$$

$$\lambda = \frac{h}{p} = \frac{h}{m\mathrm{v}}$$

$$\lambda = \frac{h}{m\sqrt{\frac{2KE}{m}}} = \frac{h}{\sqrt{2mKE}}$$

$$KE = \frac{h^2}{2m\lambda^2} = \frac{(6.63\times10^{-34} J.\sec)^2}{2(9.11\times10^{-31} Kg)(9\times10^{-10} m)^2}$$

$$KE = 2.955\times10^{-19} J.$$

Home Work:

Calculate the de Broglie wavelength of a beam of electrons whose energy is 100eV.

Heisenberg Uncertainty Principle

Example:

A microscope, using photons, is employed to locate an electron in an atom to within a distance of $0.2x10^{-10}$ m. what is the uncertainty in the momentum of the electron located in this way?

$$\Delta x \, \Delta p \geq \hbar$$

$$\Delta p \geq \frac{\hbar}{\Delta x}$$

$$\Delta p \geq \frac{1.055\times10^{-34} J.\text{sec}}{0.2\times10^{-10} m}$$

$$\Delta p \geq 5.2\times10^{-24} \frac{J.\text{sec}}{m}$$

Example:

"Locating of electron"

The speed of an electron is measured to be ($5x10^3$ m/sec) to an accuracy of 0.003%. Find the minimum uncertainty in determining the position of this electron.

$$p = m\text{v}$$

$$p = (9.11\times10^{-31} Kg)(5\times10^{3} \frac{m}{\sec})$$

$$p = 4.56\times10^{-27} \frac{Kg.m}{\sec}$$

$$\Delta p = (0.00003)(4.56\times10^{-27} \frac{Kg.m}{\sec})$$

$$\Delta p = 1.37\times10^{-31} \frac{Kg.m}{\sec}$$

$$\Delta x \, \Delta p \geq \hbar$$

$$\Delta x \geq \frac{\hbar}{\Delta p}$$

$$\Delta x \geq \frac{1.055\times10^{-34} J.\sec}{1.37\times10^{-31} \frac{Kg.m}{\sec}}$$

$$\Delta x \geq 3.86\times10^{-4} m.$$

Example:

An electron is confined to a box of length 10^{-10} m. Calculate the minimum uncertainty in its velocity.

$$\Delta x \, \Delta p \geq \hbar$$

$$\Delta p \geq \frac{\hbar}{\Delta x}$$

$$m \, \Delta \text{v} \geq \frac{\hbar}{\Delta x}$$

$$\Delta \text{v} \geq \frac{\hbar}{m \, \Delta x}$$

$$\Delta \text{v} \geq \frac{1.055 \times 10^{-34} \, J.\text{sec}}{(9.11 \times 10^{-31} \, Kg)(10^{-10} \, m)}$$

$$\Delta \text{v} \geq 1.58 \times 10^{6} \, \frac{m}{\text{sec}}$$

Lecture by: Dr. Ruwaida Saadi Obaid
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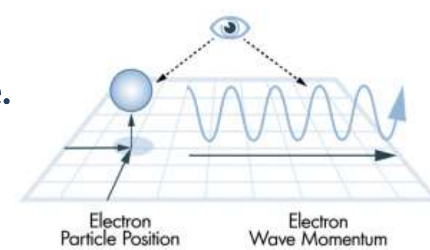
Commutator

Why is the commutator important in quantum mechanics?

Commutators are very important in Quantum Mechanics. As well as being how Heisenberg discovered the Uncertainty Principle. It is known that you cannot know the value of two physical values at the same time if they do not commute.

It is impossible to know both the velocity and position of a particle at the same time.

$$[\hat{X}, \hat{P}] = i\hbar$$



Application:

Show that

$$\left[\frac{\partial}{\partial x}, v\right] = \frac{\partial v}{\partial x}$$

where $v = v(x,t)$ is the potential energy.

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$$\left[\frac{\partial}{\partial x}, v\right]\psi(x,t)$$

$$= \left(\frac{\partial}{\partial x}v - v\frac{\partial}{\partial x}\right)\psi(x,t)$$

$$= \frac{\partial}{\partial x}v\ \psi(x,t) - v\frac{\partial}{\partial x}\psi(x,t)$$

from the question $v = v(x,t)$

$$= \left(\frac{\partial}{\partial x}v(x,t)\right)\psi(x,t) + v(x,t)\frac{\partial}{\partial x}\psi(x,t) - v(x,t)\frac{\partial}{\partial x}\psi(x,t)$$

$$= \left(\frac{\partial}{\partial x}v(x,t)\right)\psi(x,t)$$

$\therefore$

$$\left[\frac{\partial}{\partial x}, v\right]\psi(x,t) = \left(\frac{\partial}{\partial x}v(x,t)\right)\psi(x,t)$$

$$\left[\frac{\partial}{\partial x}, v\right] = \left(\frac{\partial}{\partial x}v(x,t)\right)$$

from the question $v = v(x,t)$

$$\left[\frac{\partial}{\partial x}, v\right] = \frac{\partial v}{\partial x}$$

Application:

Show that

$$\left[\frac{\partial^2}{\partial x^2}, x\right] = 2\frac{\partial}{\partial x}$$

and that this result can be expressed in terms of the momentum operator as

$$\left[p^2, x\right] = -2i\hbar p$$

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$$\left[\frac{\partial^2}{\partial x^2}, x\right]\psi(x,t)$$

$$= \left(\frac{\partial^2}{\partial x^2}x - x\frac{\partial^2}{\partial x^2}\right)\psi(x,t)$$

$$= \frac{\partial^2}{\partial x^2}\left(x\,\psi(x,t)\right) - x\frac{\partial^2}{\partial x^2}\psi(x,t)$$

$$= \frac{\partial}{\partial x}\frac{\partial}{\partial x}\left(x\,\psi(x,t)\right) - x\frac{\partial^2}{\partial x^2}\psi(x,t)$$

$$= \frac{\partial}{\partial x}\left[\left(\frac{\partial x}{\partial x}\psi(x,t)\right) + x\frac{\partial}{\partial x}\psi(x,t)\right] - x\frac{\partial^2}{\partial x^2}\psi(x,t)$$

$$= \frac{\partial}{\partial x}\psi(x,t) + \frac{\partial}{\partial x}\left(x\frac{\partial}{\partial x}\psi(x,t)\right) - x\frac{\partial^2}{\partial x^2}\psi(x,t)$$

$$= \frac{\partial}{\partial x}\psi(x,t) + \frac{\partial x}{\partial x}\frac{\partial}{\partial x}\psi(x,t) + x\frac{\partial^2}{\partial x^2}\psi(x,t) - x\frac{\partial^2}{\partial x^2}\psi(x,t)$$

$$= \frac{\partial}{\partial x}\psi(x,t) + \frac{\partial}{\partial x}\psi(x,t)$$

$$= 2\frac{\partial}{\partial x}\psi(x,t)$$

$$\left[\frac{\partial^2}{\partial x^2}, x\right]\psi(x,t) = 2\frac{\partial}{\partial x}\psi(x,t)$$

$$\left[\frac{\partial^2}{\partial x^2}, x\right] = 2\frac{\partial}{\partial x}$$

we know that $p = -i\hbar \frac{\partial}{\partial x}$

$$\left[\frac{\partial^2}{\partial x^2}, x\right] = 2\frac{\partial}{\partial x}$$

$$\left[(-i\hbar)^2 \frac{\partial^2}{\partial x^2}, x\right] = 2\frac{\partial}{\partial x}(-i\hbar)^2$$

$$\left[p^2, x\right] = -2i\hbar p \quad = 2(-i\hbar)\frac{\partial}{\partial x}(-i\hbar)$$

$$= -2(i\hbar) - i\hbar\frac{\partial}{\partial x}$$

$$= -2i\hbar p$$

Application:

If $\hat{x}$ and $\hat{y}$ are two operators, prove that

$$[\hat{x}, \hat{y}] = -[\hat{y}, \hat{x}]$$

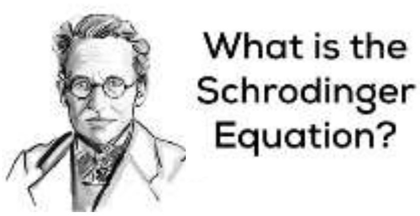
……………………………………………………………………………………….....

$$[\hat{x}, \hat{y}] = [\hat{x}\hat{y} - \hat{y}\hat{x}]$$

$$= -[\hat{y}\hat{x} - \hat{x}\hat{y}]$$

$$= -[\hat{y}, \hat{x}]$$

Schrödinger Equation



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

$$\hat{H}\Psi = E\Psi$$

Hamiltonian Operator (Energy operator) — Energy eigenvalue

The Schrodinger equation gives us a detailed account of the form of the wave functions or probability waves that control the motion of some smaller particles.

Application:

Prove that:

$$k^2 = -\frac{1}{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t)$$

....

$$\psi(x,t) = Ae^{i(kx-\omega t)}$$

$$\frac{\partial}{\partial x}\psi(x,t) = Ae^{i(kx-\omega t)}(ik)$$

$$= Ae^{i(kx-\omega t)}(ik)^2$$

$$= -k^2\psi(x,t)$$

$\therefore$

$$k^2 = -\frac{1}{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t)$$

Application:

Prove that:

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

………………………………………………………………………………………….....

$$E = \frac{p^2}{2m}$$

$$p = \frac{h}{\lambda}.\frac{2\pi}{2\pi}$$

$\therefore$

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

we have:

$$k^2 = -\frac{1}{\psi(x,t)}\frac{\partial}{\partial x}\psi(x,t)$$

Assume that:

$\psi(x,t) = \psi(x)$ ((time independent))

$\therefore$

$$k^2 = -\frac{1}{\psi(x)}\frac{\partial}{\partial x}\psi(x)$$

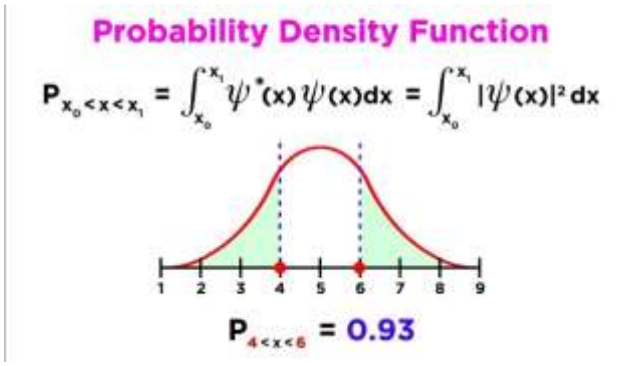
$$E = \frac{\hbar^2\left(-\frac{1}{\psi(x)}\frac{\partial}{\partial x}\psi(x)\right)}{2m}$$

$\therefore$

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

Probability Density in Quantum Mechanics

What is the significance of probability density in quantum mechanics?



The probability density is given by taking the square of the absolute value of the wavefunction. It gives us the likelihood of finding an electron (or some other system) at some given point in space.

Application:

Let two functions ψ and ϕ be defined for $0 \le x < \infty$. Explain why $\psi(x) = x$ cannot be a wavefunction but $\phi(x) = e^{-x^2}$ could be a valid wavefunction.

………………………………………………………………………………………

$$\int_0^\infty |\psi(x)|^2 dx$$

$$= \int_0^\infty |x|^2 dx$$

$$= \left.\frac{x^3}{3}\right|_0^\infty$$

$= \infty$ which gives that the function $\psi(x) = x$ is not square integrable over this range. It cannot be a valid wavefunction

$$\int_0^\infty \left| \phi(x) \right|^2 dx$$

$$= \int_0^\infty \left| e^{-x^2} \right|^2 dx$$

$$= \int_0^\infty e^{-2x^2} dx$$

let

$$2x^2 = z \Rightarrow \therefore x = \sqrt{\frac{z}{2}}$$

$$dz = 4x \ dx$$

$$\therefore dx = \frac{dz}{4x} = \frac{dz}{4\sqrt{\frac{z}{2}}} = \frac{dz}{\sqrt{\frac{16z}{2}}} = \frac{dz}{\sqrt{8z}}$$

then

$$\int_0^\infty e^{-2x^2} dx$$

$$= \frac{1}{\sqrt{8}} \int_0^\infty e^{-z} \frac{dz}{\sqrt{z}}$$

$$= \frac{1}{\sqrt{8}} \int_0^\infty z^{-\frac{1}{2}} e^{-z} dz$$

Hint: using Gamma Function

$$\Gamma(n) = \int_0^\infty z^{n-1} e^{-z} dz$$

$$\Gamma(\frac{1}{2}) = \sqrt{\pi}$$

$\therefore$

$$\frac{1}{\sqrt{8}} \int_0^\infty e^{-z} \frac{dz}{\sqrt{z}}$$

$$= \frac{1}{\sqrt{8}} \Gamma(\frac{1}{2})$$

$$= \sqrt{\frac{\pi}{8}}$$

Lecture by: Dr. Ruwaida Saadi Obaid
November 12 2023

Quantum Mechanics

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Normalization of the wavefuction

The probability of finding the particle between -∞ to ∞ at the time *t* must equal to 1.

$$\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx = 1 \qquad \text{Normalization Condition}$$

Application:

The wavefunction of the particle at a given time is given by

$$\psi(x) = \frac{e^{ikx}}{\sqrt{x^2 + a^2}} \qquad , \; k \text{ and } a \text{ are constant}$$

1. Is $\psi(x)$ normalized?
2. If not, find the normalization constant?
3. Find the probability of finding the particle in the region between $x = \frac{-a}{\sqrt{3}}$ to $\infty = \frac{a}{\sqrt{3}}$.

(1) $\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx$

$= \int_{-\infty}^{\infty} \frac{e^{-ikx}}{\sqrt{x^2+a^2}} \frac{e^{ikx}}{\sqrt{x^2+a^2}}\,dx$

$= \int_{-\infty}^{\infty} \frac{1}{(x^2+a^2)}\,dx$

let: $x = a\tan\theta$

$dx = \frac{a}{\cos^2\theta}d\theta$

$\therefore \int_{-\infty}^{\infty} \frac{1}{(x^2+a^2)}\,dx$

$= \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{1}{(a^2\tan^2\theta+a^2)}\cdot\frac{a}{\cos^2\theta}d\theta$

$= \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{a}{\cos^2\theta(a^2\tan^2\theta+a^2)}d\theta$

$= \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{a}{a^2\cos^2\theta(\tan^2\theta+1)}d\theta$

$= \frac{1}{a^2}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{a}{\cos^2\theta\tan^2\theta+\cos^2\theta}d\theta$

$= \frac{a}{a^2}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{1}{\cos^2\theta\frac{\sin^2\theta}{\cos^2\theta}+\cos^2\theta}d\theta$

$= \frac{1}{a}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{1}{\sin^2\theta+\cos^2\theta}d\theta$

$= \frac{1}{a}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} 1\,d\theta$ ....**

$= \frac{1}{a}\ \theta\Big|_{-\frac{\pi}{2}}^{\frac{\pi}{2}}$

$= \frac{1}{a}\left(\frac{\pi}{2}-\left(-\frac{\pi}{2}\right)\right)=\frac{\pi}{a}$ not normalized

(2) let the normalized wavefunction

$$\psi(x) = N \frac{e^{ikx}}{\sqrt{x^2+a^2}}$$

$$\int_{-\infty}^{\infty} \psi^*(x)\,\psi(x)\,dx = 1 \qquad \text{Normalization Condition}$$

$$= \int_{-\infty}^{\infty} N \frac{e^{-ikx}}{\sqrt{x^2+a^2}} . N \frac{e^{ikx}}{\sqrt{x^2+a^2}}\,dx$$

$$= N^2 \int_{-\infty}^{\infty} \frac{1}{\left(x^2+a^2\right)}\,dx = 1$$

$$= N^2 \left(\frac{\pi}{a}\right) = 1$$

$$\therefore N = \sqrt{\frac{a}{\pi}}$$

$\therefore$ the normalized wavefunction is

$$\psi(x) = \sqrt{\frac{a}{\pi}} \frac{e^{ikx}}{\sqrt{x^2+a^2}}$$

(3) $$\int_{-\frac{a}{\sqrt{3}}}^{\frac{a}{\sqrt{3}}} \sqrt{\frac{a}{\pi}} \frac{e^{-ikx}}{\sqrt{x^2+a^2}} . \sqrt{\frac{a}{\pi}} \frac{e^{ikx}}{\sqrt{x^2+a^2}}\,dx$$

$$= \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{1}{\left(x^2+a^2\right)}\,dx$$

$$= \frac{a}{\pi} \left(\frac{1}{a}\right) \int_{-\theta}^{\theta} d\theta$$ ... return to page 2 to the step with ** to see the details

let: $x = a\tan\theta$

$$x = \frac{a}{\sqrt{3}}$$

$$\frac{a}{\sqrt{3}} = a\tan\theta$$

$$\tan\theta = \frac{1}{\sqrt{3}}$$

$$\therefore \theta = \tan^{-} \frac{1}{\sqrt{3}} = \frac{\pi}{6}$$

$$= \frac{a}{\pi} \left(\frac{1}{a}\right) \int_{-\frac{\pi}{6}}^{\frac{\pi}{6}} d\theta$$

$$= \frac{1}{\pi} \theta \Big|_{-\frac{\pi}{6}}^{\frac{\pi}{6}} \Rightarrow \frac{1}{\pi}\left(\frac{\pi}{6} - \left(-\frac{\pi}{6}\right)\right) \Rightarrow \frac{1}{3}$$

Home Work 1:

Let

$$\psi(x) = Ae^{-\lambda(x-b)^2}$$

Find the normalization constant *A*. λ and b are a real constant.

Hint: let $z^2 = 2\lambda(x-b)^2$ and,

$$\Gamma(n) = \int_0^{\infty} t^{n-1}\, e^{-t} dt$$

$$\Gamma(n) = \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$

Application:

The wavefunction for a particle confines to $0 \le x \le a$ was found to be $\psi(x) = A\sin\left(\frac{\pi x}{a}\right)$ where A is the normalization constant. Find A and determine the probability that the particle is found in the interval $\frac{a}{2} \le x \le \frac{3a}{4}$.

$$(1)\int_0^a |\psi(x)|^2 dx = 1$$

$$= \int_0^a \left| A\sin\left(\frac{\pi x}{a}\right)\right|^2 dx = 1$$

$$= A^2 \int_0^a \sin^2\left(\frac{\pi x}{a}\right) dx = 1$$

$$= A^2 \int_0^a \left(\frac{1-\cos\left(\frac{2\pi x}{a}\right)}{2}\right) dx = 1$$

$$= \frac{1}{2}A^2 \left[\int_0^a dx - \int_0^a \cos\left(\frac{2\pi x}{a}\right)\right] dx = 1$$

$$= \frac{1}{2}A^2 \left[x\Big|_0^a - \frac{a}{2\pi}\sin\left(\frac{2\pi x}{a}\right)\Big|_0^a \right] = 1$$

$$= \frac{1}{2}A^2 [a - 0] = 1$$

$$\therefore A = \sqrt{\frac{2}{a}}$$

$$\therefore \psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right)$$

$$(2)\int_{\frac{a}{2}}^{\frac{3a}{4}} |\psi(x)|^2 dx$$

$$= \int_{\frac{a}{2}}^{\frac{3a}{4}} \left| \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \right|^2 dx$$

$$= \frac{2}{a} \int_{\frac{a}{2}}^{\frac{3a}{4}} \sin^2\left(\frac{\pi x}{a}\right) dx$$

$$= \frac{2}{a} \int_{\frac{a}{2}}^{\frac{3a}{4}} \left(\frac{1-\cos\left(\frac{2\pi x}{a}\right)}{2} \right) dx$$

$$= \frac{2}{a}.\frac{1}{2} \left[\int_{\frac{a}{2}}^{\frac{3a}{4}} dx - \int_{\frac{a}{2}}^{\frac{3a}{4}} \cos\left(\frac{2\pi x}{a}\right) \right] dx$$

$$= \frac{1}{a} \left[x \Big|_{\frac{a}{2}}^{\frac{3a}{4}} - \frac{a}{2\pi} \sin\left(\frac{2\pi x}{a}\right) \Big|_{\frac{a}{2}}^{\frac{3a}{4}} \right]$$

$$= \frac{1}{a}\left(\frac{3a}{4} - \frac{a}{2}\right) - \frac{a}{2\pi} \left(\sin\frac{2\pi\frac{3a}{4}}{a} - \sin\frac{2\pi\frac{a}{2}}{a} \right)$$

$$= \frac{1}{a}\frac{1}{4}a + \frac{1}{a}\frac{a}{2\pi}$$

$$= 0.41$$

Home Work 2:

Normalize the wavefunction:

$$\psi(x) = A\left(ax - x^2\right) \quad \text{for} \quad 0 \le x \le a$$

Lecture by: Dr. Ruwaida Saadi Obaid
November 21 2023, December 5 2023

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Example:

consider a particle whose wavefunction is given by:

$$\psi(x) = Ae^{-\alpha x^2}$$

What is the value of the *A*, if this wavefunction is normalized?

$$\text{Hint}: \Gamma(n) = \int_0^\infty t^{n-1} e^{-t} dt \qquad ; \Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$$

....

$$\int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

$$\int_{-\infty}^{\infty} \left(Ae^{-\alpha x^2}\right)^2 dx = 1$$

$$A^2 \int_{-\infty}^{\infty} e^{-2\alpha x^2} dx = 1$$

$$A^2 \left[\int_0^\infty e^{-2\alpha x^2} dx + \int_{-\infty}^0 e^{-2\alpha x^2} dx\right] = 1$$

$$A^2 \left[\int_0^\infty e^{-2\alpha x^2} dx + \int_{+\infty}^0 e^{-2\alpha x^2} (-dx)\right] = 1$$

$$A^2 \left[\int_0^\infty e^{-2\alpha x^2} dx + (-)\int_0^\infty e^{-2\alpha x^2} (-dx)\right] = 1$$

$$A^2 \left[\int_0^\infty e^{-2\alpha x^2} dx + \int_0^\infty e^{-2\alpha x^2} (dx)\right] = 1$$

$$A^2 \left(2\int_0^\infty e^{-2\alpha x^2} dx\right) = 1$$

let

$$z^2 = 2ax^2$$

$$z = \sqrt{2a}\, x$$

$$dz = \sqrt{2a}\, dx$$

$\therefore$

$$dx = \frac{dz}{\sqrt{2a}}$$

$$2A^2 \int_0^\infty e^{-z^2} \frac{dz}{\sqrt{2a}} = 1$$

$$z^2 = t$$

$$z = \sqrt{t}$$

$$dz = \frac{1}{2} t^{-\frac{1}{2}}\, dt$$

$\therefore$ the equation $2A^2 \int_0^\infty e^{-z^2} \frac{dz}{\sqrt{2a}} = 1$, will be:

$$\frac{2A^2}{\sqrt{2a}} \int_0^\infty e^{-t} \frac{1}{2} t^{-\frac{1}{2}}\, dt = 1$$

$$\frac{A^2}{\sqrt{2a}} \int_0^\infty e^{-t} t^{-\frac{1}{2}}\, dt = 1$$

$$\frac{A^2}{\sqrt{2a}} \sqrt{\pi} = 1$$

$$\therefore A = \left(\frac{2a}{\pi} \right)^{\frac{1}{4}}$$

Dirac Bra-ket Notation

$$\langle \psi_1 | \psi_2 \rangle = \int_{-\infty}^{\infty} \psi_1^* \psi_2 dx$$

Orthonormality of the wavefunction

What is the physical significance of orthonormality?

The physical meaning of their orthogonality is that, when energy is measured while the system is in one such state, it has no chance of instead being found to be in another.

$$\text{Kronecker delta} : \delta_{mn}$$

$$\langle m | n \rangle = \int \Psi_m^* \Psi_n d\tau = \delta_{mn} = \begin{cases} = 0 \text{ if } m \neq n \\ = 1 \text{ if } m = n \end{cases}$$

Example:

$|\psi\rangle = 3i\,|\varphi_1\rangle + 2|\varphi_2\rangle - 4i\,|\varphi_3\rangle$

where $|\varphi\rangle$ are the orthonormal basis. Normalized $|\psi\rangle$.

………………………………………………………………………

$$|\psi\rangle = 3i\,|\varphi_1\rangle + 2|\varphi_2\rangle - 4i\,|\varphi_3\rangle$$

$$\langle\psi| = -3i\,\langle\varphi_1| + 2\langle\varphi_2| + 4i\,\langle\varphi_3|$$

$$\langle\psi|\psi\rangle = \left(-3i\,\langle\varphi_1| + 2\langle\varphi_2| + 4i\,\langle\varphi_3|\right)\left(3i\,|\varphi_1\rangle + 2|\varphi_2\rangle - 4i\,|\varphi_3\rangle\right)$$

$$\begin{aligned}\langle\psi|\psi\rangle &= -3i\,(3i)\langle\varphi_1|\varphi_1\rangle + 2(3i)\langle\varphi_2|\varphi_1\rangle + 3i\,(4i)\langle\varphi_3|\varphi_1\rangle \\ &+ 2(-3i)\langle\varphi_1|\varphi_2\rangle + 2(2)\langle\varphi_2|\varphi_2\rangle + 2(4i)\langle\varphi_3|\varphi_2\rangle \\ &+ (-4i)(-3i)\langle\varphi_1|\varphi_3\rangle + (-4i)(2)\langle\varphi_2|\varphi_3\rangle + (-4i)(4i)\langle\varphi_3|\varphi_3\rangle\end{aligned}$$

where

$$\langle\varphi_m|\varphi_n\rangle = \delta_{mn} = \begin{cases} 0 & \text{if} \quad \mathrm{m} \neq \mathrm{n} \\ 1 & \text{if} \quad \mathrm{m} = \mathrm{n} \end{cases}$$

$\therefore$

$$\begin{aligned}\langle\psi|\psi\rangle &= -3i\,(3i)\langle\varphi_1|\varphi_1\rangle + 2(2)\langle\varphi_2|\varphi_2\rangle + (-4i)(4i)\langle\varphi_3|\varphi_3\rangle \\ &= 9 + 4 + 16 = 29\end{aligned}$$

the normalization constant is the reciprocal of the root of 29

so the normalized wavefunction is

$$|\psi\rangle = \frac{3i}{\sqrt{29}}|\varphi_1\rangle + \frac{2}{\sqrt{29}}|\varphi_2\rangle - \frac{4i}{\sqrt{29}}|\varphi_3\rangle$$

EXPECTATION VALUE OF OPERATOR

Expectation value of Momentum & Energy can thus be written as

$$\langle p \rangle = \int_{-\infty}^{\infty} \hat{p}\,|\Psi|^2 dx = \int_{-\infty}^{\infty} \Psi^* \hat{p}\,\Psi dx = \int_{-\infty}^{\infty} \Psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi dx$$

$$\langle p \rangle = \frac{\hbar}{i}\int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial x} dx$$

$$\langle E \rangle = \int_{-\infty}^{\infty} \hat{E}\,|\Psi|^2 dx = \int_{-\infty}^{\infty} \Psi^* \hat{E}\,\Psi dx = \int_{-\infty}^{\infty} \Psi^* \left(i\hbar\frac{\partial}{\partial t}\right) \Psi dx$$

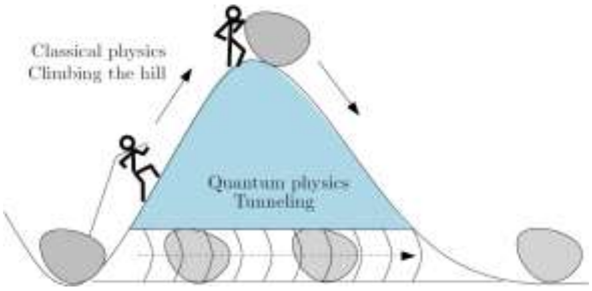
$$\langle E \rangle = i\hbar\int_{-\infty}^{\infty} \Psi^* \frac{\partial \Psi}{\partial t} dx$$

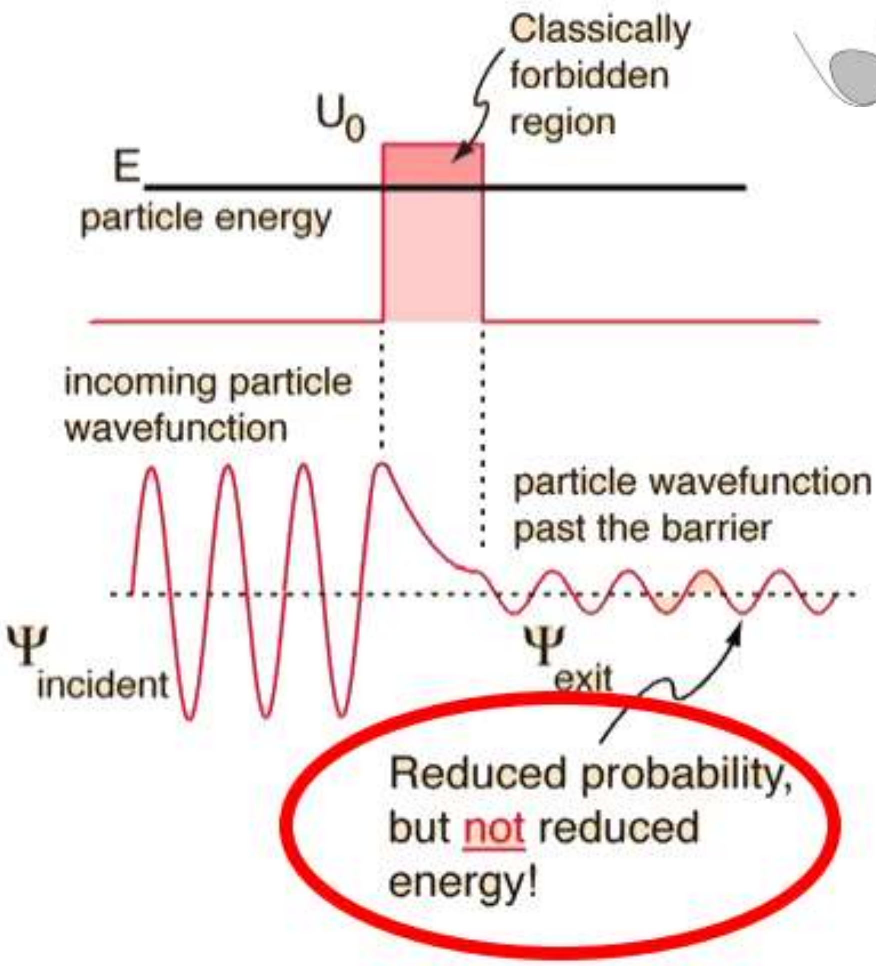
so what is the expectation value in quantum mechanics?

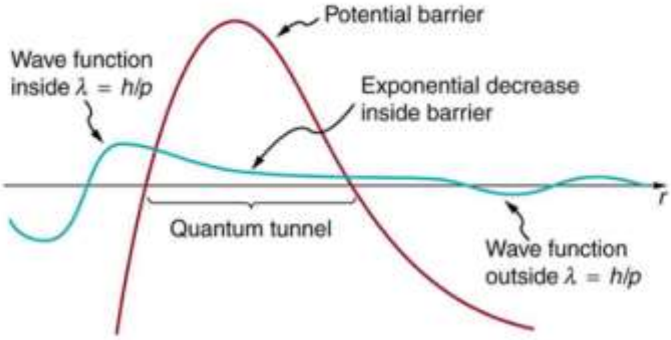
The expectation value of the position operator is the average of the position measurements performed on a large number of identical systems. The expectation value of the Hamiltonian (i.e. energy) operator is the average of the energy measurements performed on a large number of identical systems.

Tunneling effect in quantum mechanics

Tunneling is a quantum mechanical phenomenon when a particle is able to penetrate through a potential energy barrier that is higher in energy than the particle's kinetic energy and this amazing property of microscopic particles.







Application:

A 2eV electroms a barrier 5eV high. What is the probability that it will tunnel through the barrier if the barrier width is (a) 1nm and (b) 0.50nm?

$$T = Ge^{-2\kappa L}$$

$$G = 16\frac{E}{U}\left(1-\frac{E}{U}\right)$$

$$\kappa = \frac{\sqrt{2m(U-E)}}{\hbar}$$

$$G = 16\left(\frac{2.0\text{ eV}}{5.0\text{ eV}}\right)\left(1-\frac{2.0\text{ eV}}{5.0\text{ eV}}\right) = 3.8$$

$$U_0 - E = 5.0\text{ eV} - 2.0\text{ eV} = 3.0\text{ eV} = 4.8\times10^{-19}\text{ J}$$

$$\kappa = \frac{\sqrt{2(9.11\times10^{-31}\text{ kg})(4.8\times10^{-19}\text{ J})}}{1.055\times10^{-34}\text{ J}\cdot\text{s}} = 8.9\times10^{9}\text{ m}^{-1}$$

(a) When $L = 1.00\text{ nm} = 1.00\times10^{-9}\text{ m}$, $2\kappa L = 2(8.9\times10^{9}\text{ m}^{-1})(1.00\times10^{-9}\text{ m}) = 17.8$ and $T = Ge^{-2\kappa L} = 3.8e^{-17.8} = 7.1\times10^{-8}$.

(b) When $L = 0.50$ nm, one-half of 1.00 nm, $2\kappa L$ is one-half of 17.8, or 8.9. Hence $T = 3.8e^{-8.9} = 5.2\times10^{-4}$.

Home Work:

If we take arbitrary an equivalent rectangular barrier of high V_0=15MeV and take the energy of α is E=5MeV then we get for $L=2*10^{-14}$m. Find T.