AKTU Energy Science & Engineering

For B.Tech Second Year

Strictly acording to the latest Syllabus Prescribed by

Dr.A.P.J.Abdul Kalam Technical University, Lucknow

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786

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Preface

The book "*AKTU Energy Science & Engineering* "is intended to serve as a text book for B.Tech Second year students of Abdul Kalam Technical University - Lucknow.Each chapter of the book covers the revised and latest syllabii of AKTU university. The book is written to provide a simple, clear and logical presentation of subject with a large number of diagrams and illustrations . The basic concepts and derivations are included in a simple and easy manner so that the students do not find any difficulty in going through the different chapters of the book. In all chapters of the book emphasis has been laid on the physical concepts. No elementary books are required to supplement the study material as each and every derivation numerical explanation carries a step by step solution.

Previous year papers are included for students to get an idea of exam pattern. Each chapter contains question with answers.

E-book of same is avaliable on kdpkindle.

In spite of best efforts of the author, it is possible that few unintentional errors and misprints might have come. Any suggestion for the improvement of the book would be accepted. One can mail their doubts or suggestions on *divyaghildyal@gmail.com.*

Authors will be all the more happy to serve in future.

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About the Author

Dr. Divya Ghildyal (MSc, MPhil, Phd) has done her doctorate in Physics from Lucknow University. She is presently working in a reputed Engineering college in Noida, India.She has over 15 years of teaching experience in Physics to engineering students.

She has previously worked as Content Cordinator for various entrance exams with Physics as her subject. An expert in solving Multiple Choice Questions asked in various competitive exams, along with alternative and short cut methods for approaching the exam paper in stipulated time frame.

She has done her PhD in Physics from Lucknow University in the area of magnetic resonance. She has authored 4 books out of which 2 are for undergraduate level students in engineering college and 2 for students aspiring to compete the entrance tests in various medical and engineering fields. She has published more 15 research papers and has participated and presented research papers in several national and international conferences.

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Contents

AKTU - Energy Science and Engineering

Engineering Science Courses for B.Tech.(AICTE Model Curriculum) 2nd Year (effective from the session 2019-20)

Subject Code: KOE033/043

Unit-I Energy and its Usage: Units and scales of energy use, Mechanical energy and transport, Heat energy: Conversion between heat and mechanical energy, Electromagnetic energy: Storage, conversion, transmission and radiation, Introduction to the quantum, energy quantization, Energy in chemical systems and processes, flow of CO2, Entropy and temperature, carnot and Stirling heat engines, Phase change energy conversion, refrigeration and heat pumps, Internal combustion engines, Steam and gas power cycles, the physics of power plants. Solid-state phenomena including photo, thermal and electrical aspects.

Unit-II Nuclear Energy: Fundamental forces in the universe, Quantum mechanics relevant for nuclear physics, Nuclear forces, energy scales and structure, Nuclear binding energy systematics, reactions and decays, Nuclear fusion, Nuclear fission and fission reactor physics, Nuclear fission reactor design, safety, operation and fuel cycles.

Unit-III Solar Energy: Introduction to solar energy, fundamentals of solar radiation and its measurement aspects, Basic physics of semiconductors, Carrier transport, generation and recombination in semiconductors, Semiconductor junctions: metal-semiconductor junction & p-n junction, Essential characteristics of solar photovoltaic devices, First Generation Solar Cells, Second Generation Solar Cells, Third Generation Solar Cells.

Unit-IV Conventional & non-conventional energy source: Biological energy sources and fossil fuels, Fluid dynamics and power in the wind, available resources, fluids, viscosity, types of fluid flow, lift, Wind turbine dynamics and design, wind farms, Geothermal power and ocean thermal energy conversion, Tidal/wave/hydro power.

Unit-V Systems and Synthesis: Overview of World Energy Scenario, Nuclear radiation, fuel cycles, waste and proliferation, Climate change, Energy storage, Energy conservation. Engineering for Energy conservation: Concept of Green Building and Green Architecture; Green building concepts, LEED ratings; Identification of energy related enterprises that represent the breath of the industry and prioritizing these as candidates; Embodied energy analysis and use as capacity consumption

1. Energy and Its Usage

Unit-I Energy and its Usage: Units and scales of energy use, Mechanical energy and transport, Heat energy: Conversion between heat and mechanical energy, Electromagnetic energy: Storage, conversion, transmission and radiation, Introduction to the quantum, energy quantization, Energy in chemical systems and processes, flow of CO2, Entropy and temperature, carnot and Stirling heat engines, Phase change energy conversion, refrigeration and heat pumps, Internal combustion engines, Steam and gas power cycles, the physics of power plants. Solid-state phenomena including photo, thermal and electrical aspects.

➢ ENERGY AND IT'S USAGE

Energy is the potential to exert force from a distance, it is defined as that capacity a body or substance possesses which can result in the performance of work. Two broad categories of energy are stored (potential) energy and working (kinetic) energy. For example, the food we eat contains chemical energy, and our body stores this energy until we release it when we work.

Few more examples of energy are:

S.No.	Energy	Properties
1.	Potential Energy	Stored energy, energy of position (=mgh) ,where m is mass, g is acceleration due to gravity, h is height.
2.	Kinetic Energy	Energy in motion, (=$mv^2/2$) where m is mass, v is velocity, eg. Motion of waves, molecules, electrons, atoms etc.
3.	Chemical Energy	Energy stored in the bonds of atoms and molecules. eg.petroleum, natural gas, propane, coal etc.
4	Nuclear Energy	Energy stored in the nucleus of an atom, eg nucleus of uranium atom stores energy
5	Radiant energy	Energy in electromagnetic waves, travels in transverse waves,eg, solar energy
6	Thermal Energy	Internal energy in substance ie the vibration and movement of atoms and molecules within substances eg. Geothermal energy
7.	Electrical energy	Movement of electrons,eg lightning and electricity.

➢ Grades of Energy

High Grade Energy:

Electrical and chemical energy are high-grade energy, because the energy is concentrated in a small space. Even a small amount of electrical and chemical energy can do a great amount of work. The molecules or particles that store these forms of energy are highly ordered and com- pact and thus considered as high grade energy. High-grade energy like electricity is better used for high grade applications like melting of metals rather than simply heating of water.

Low-Grade Energy:

Heat is low-grade energy. Heat can still be used to do work(example of a heater boiling water), but it rapidly dissipates. The molecules, in which this kind of energy is stored (air and water molecules), are more randomly distributed than the molecules of carbon in a coal.

- **Units and Scales of energy use**:

The energy units are wide and varied. The usage of units varies with country, industry sector, systems such as FPS, CGS, MKS and SI, and also with generations of earlier period using FPS and recent generations using MKS. Even technology/equipment suppliers adopt units that are different from the one being used by the user of that technology/equipment.

What are three examples of units used for energy. (AKTU-2021)

EnergyUnits and Conversions

1 Joule (J) is the MKS unit of energy, equal to the force of one Newton acting through one meter.
1 Watt is the power of a Joule of energy per second
Power = Current x Voltage (P = I V)
1 Watt is the power from a current of 1 Ampere flowing through 1 Volt.
1 kilowatt is a thousand Watts.
1 kilowatt-hour is the energy of one kilowatt power flowing for one hour. (E = P t).
1 kilowatt-hour (kWh) = 3.6 x 10^6 J = 3.6 million Joules.
1 calorie of heat is the amount needed to raise 1 gram of water 1 degree Centigrade.
1 calorie (cal) = 4.184 J
(The Calories in food ratings are actually kilocalories.)
A BTU (British Thermal Unit) is the amount of heat necessary to raise one pound of water by 1 degree Farenheit (F).
1 British Thermal Unit (BTU) = 1055 J (The Mechanical Equivalent of Heat Relation)
1 BTU = 252 cal = 1.055 kJ
1 Quad = 10^{15} BTU (World energy usage is about 300 Quads/year, US is about 100 Quads/year in 1996.)
1 therm = 100,000 BTU
1,000 kWh = 3.41 million BTU

Power Conversion:

1 horsepower (hp) = 745.7 watts

Gas Volume to Energy Conversion

One thousand cubic feet of gas (Mcf) -> 1.027 million BTU = 1.083 billion J = 301 kWh
One therm = 100,000 BTU = 105.5 MJ = 29.3 kWh
1 Mcf -> 10.27 therms

Energy Content of Fuels

Coal	25 million BTU/ton
Crude Oil	5.6 million BTU/barrel
Oil	5.78 million BTU/barrel = 1700 kWh / barrel
Gasoline	5.6 million BTU/barrel (a barrel is 42 gallons) = 1.33 therms / gallon
Natural gas liquids	4.2 million BTU/barrel
Natural gas	1030 BTU/cubic foot

Wood 20 million BTU/cord

CO_2 Pollution of Fossil Fuels

Pounds of CO_2 per billion BTU of energy

Coal 208,000 pounds

Oil 164,000 pounds

Natural Gas 117,000 pounds

Ratios of CO_2 pollution:

Oil / Natural Gas = 1.40

Coal / Natural Gas = 1.78

Pounds of CO_2 per 1,000 kWh, at 100% efficiency:

Coal 709 pounds

Oil 559 pounds

Natural Gas 399 pounds.

Electricity

The energy unit used for everyday electricity, particularly for utility bills, is the kilowatt-hour (kWh); one kWh is equivalent to 3.6×10^6 J (3600 kJ or 3.6 MJ). Electricity usage is often given in units of kilowatt-hours per year (kWh/yr). This is actually a measurement of average power consumption, i.e., the average rate at which energy is transferred. One kWh/yr is about 0.11 watts.

Natural gas

Natural gas in the US is sold in Therms or 100 cubic feet (100 ft^3 = 1 Ccf). One Therm is equal to about 105.5 megajoules. In Australia, natural gas is sold in Cubic Meters (1m^3 = 38 megajoules). In the most of the world, natural gas is sold in gigajoules.

Food industry

Calorie is defined as the amount of thermal energy necessary to raise the temperature of one gram of water by 1 Celsius degree, from a temperature of 14.5 °C, at a pressure of 1 atm. For thermochemistry a calorie of 4.184 J is used, but other calories have also been defined, such as the International Steam Table calorie of 4.1868 J. Food energy is measured in large calories or kilocalories.

Atomic physics and chemistry

In physics and chemistry, it is still common to measure energy on the atomic scale in the non-SI, but convenient, units electronvolts (eV). The Hartree (the atomic unit of energy) is commonly used in calculations.

Explosions

A gram of TNT releases 980–1100 calories upon explosion. To define the tonne of TNT, this was arbitrarily standardized by letting 1000 thermochemical calories = 1 gram TNT = 4184 J (exactly).

Spectroscopy

In spectroscopy and related fields it is common to measure energy levels in units of reciprocal centimetres. These units (cm^{-1}) are strictly speaking not energy units but units proportional to energies,

- **Mechanical energy and transport**

Mechanical energy can be **converted** into **heat**, and **heat** can be **converted** into some **mechanical energy**. This idea of work and heat equivalence is stated in the First law of thermodynamics, which says that the change in internal energy of a system is the sum of the work done and the heat added to any system

Mechanical energy is the sum of potential energy and kinetic energy. It is the macroscopic energy associated with a system. The principle of conservation of mechanical energy states that if an isolated system is subject only to conservative forces, then the mechanical energy is constant. If an object moves in the opposite direction of a conservative net force, the potential energy will increase; and if the speed (not the velocity) of the object changes, the kinetic energy of the object also changes.

Many devices are used to convert mechanical energy to or from other forms of energy, e.g. an electric motor converts electrical energy to mechanical energy, an electric generator converts mechanical energy into electrical energy and a heat engine converts heat energy to mechanical energy.

Energy is a scalar quantity and the mechanical energy of a system is the sum of the potential energy (which is measured by the position of the parts of the system) and the kinetic energy (which is also called the energy of motion).

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$$\mathbf{E_{mechanical} = U + K}$$

The potential energy, *U*, depends on the position of an object subjected to a conservative force. It is defined as the object's ability to do work and is increased as the object is moved in the opposite direction of the direction of the force. If *F* represents the conservative force and *x* the position, the potential energy of the force between the two positions x_1 and x_2 is defined as the negative integral of *F* from x_1 to x_2:

$$\boxed{\boldsymbol{U = -\int_{x1}^{x2} F.dx}}$$

The kinetic energy, *K*, depends on the speed of an object and is the ability of a moving object to do work on other objects when it collides with them. It is defined as one half the product of the object's mass with the square of its speed, and the total kinetic energy of a system of objects is the sum of the kinetic energies of the respective objects

$$\boxed{K = \frac{mv^2}{2}}$$

Question:A force of 250N is used for pushing a 70kg box through a distance of 3m along a horizontal floor. Calculate the work done and energy transformed.

Solution: Work = Force x Distance

W = 250 x 3 = 750 Joules

Examples:

Swinging pendulum

A swinging pendulum with the velocity vector (green) and acceleration vector (blue). The magnitude of the velocity vector, the speed, of the pendulum is greatest in the vertical position and the pendulum is farthest from Earth in its extreme positions.The pendulum reaches greatest kinetic energy and least potential energy when in the vertical position, because it will have the greatest speed and be nearest the Earth at this point. On the other hand, it will have its least kinetic energy and greatest potential energy at the extreme positions of its swing, because it has zero speed and is farthest from Earth at these points. However, when taking the frictional forces into account, the system loses mechanical energy with each swing because of the negative work done on the pendulum by these non-conservative forces.

- A **satellite** of mass at a distance from the centre of Earth possesses both kinetic energy, (by virtue of its motion) and gravitational potential energy, , (by virtue of its position within the Earth's gravitational field; Earth's mass is). Hence, mechanical energy of the satellite-Earth system is given by

$$\boxed{E = U + K}$$

$$E = \frac{GM_e m}{r} + \frac{mv^2}{2}$$

In case the satellite is in circular orbit, the energy conservation takes the form

$$E = \frac{GM_e m}{2r}$$

Many devices are used to convert mechanical energy to or from other forms of energy, e.g. an electric motor converts electrical energy to mechanical energy, an electric generator converts mechanical energy into electrical energy and a heat engine converts heat energy to mechanical energy.

Transport phenomena is the subject which deals with the movement of different physical quantities in any chemical or mechanical process and describes the basic principles and law of transport.It also describes the relations and similarities among different types of transport that may occur in any system. Transport in a chemical or mechanical process can be classified into three types:

(i)Momentum Transport: Momentum transport deals with the transport of momentum in fluids and is also known as fluid dynamics
(ii)**Energy Transport** : Energy transport deals with the transport of different forms of energy in a system and is also known as heat transfer.
(iii)**Mass Transport**: Mass transport deals with the transport of various chemical species themselves.
NOTE: Mechanical energy is a useful concept for flows that do not involve significant heat transfer or energy conversion, such as flow of gasoline from an underground tank into a car.
Electromagnetic energy is a form of **energy** that is reflected or emitted from objects in the form of electrical and magnetic waves that can travel through space.e**xample**: Radio Waves,Radarwaves,Heat (infrared radiation), Ultraviolet Light (This is what causes Sunburns),X-rays Short waves,Microwaves, Gamma Rays.

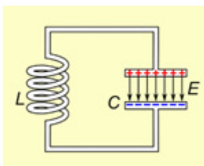
Sunlight is also a form of electromagnetic energy. Electromagnetic radiation is created when an atomic particle, such as an electron is accelerated by an electric field, causing it to move.The movement produces oscillating electric and magnetic fields. The movement produces oscillating electric and magnetic fields, which travels at right angles to each other in a bundle of light energy called a photon. Photons travel in harmonic waves at the fastest speed possible in the universe.The transfer of energy by an electromagnetic wave is at right angles to both electric and magnetic components of the wave vibration and its rate is proportional to the vector product of their amplitudes as per **Poynting Theorem.(S = E x H)**

$$\boldsymbol{U} = \frac{\boldsymbol{\varepsilon_0 E^2}}{\mathbf{2}} + \frac{\boldsymbol{\mu_0 H^2}}{\mathbf{2}}$$

Electromagnetic Energy Storage in L.C. circuit

LC circuits are **circuits** that contain inductors and capacitors. Therefore, we see that the **energy stored** within an LC circuit oscillates back and forth between the electric fields of the capacitor and the magnetic field of the inductor. This oscillation is known as electromagnetic oscillation.

The energy stored on a capacitor can be calculated from the equivalent expressions:



L is Inductor
C is Capacitor
E the Electric Field

$$\boxed{U = \frac{1}{2}\frac{Q^2}{C} = \frac{1}{2}QV = \frac{1}{2}CV^2}$$

This energy is stored in the electric field.
The energy stored on a capacitor is in the form of energy density in an electric field is given by

$$\boxed{\eta_E = \frac{energy}{volume} = \frac{1}{2}\varepsilon E^2}$$

This can be shown to be consistent with the energy stored in a charged parallel plate capacitor

$$\begin{aligned} Energy = \eta V &= \frac{1}{2}\varepsilon E^2 Ad \\ &= \frac{1}{2}\varepsilon \frac{V^2}{d^2} Ad \\ &= \frac{1}{2}\frac{\varepsilon A}{d} V^2 = \frac{1}{2}CV^2 \end{aligned}$$

Energy in an Inductor

When a electric current is flowing in an inductor, there is energy stored in the magnetic field. Considering a pure inductor L, the instantaneous power which must be supplied to initiate the current in the inductor is

$$\boxed{P = iv = Li\frac{di}{dt}}$$

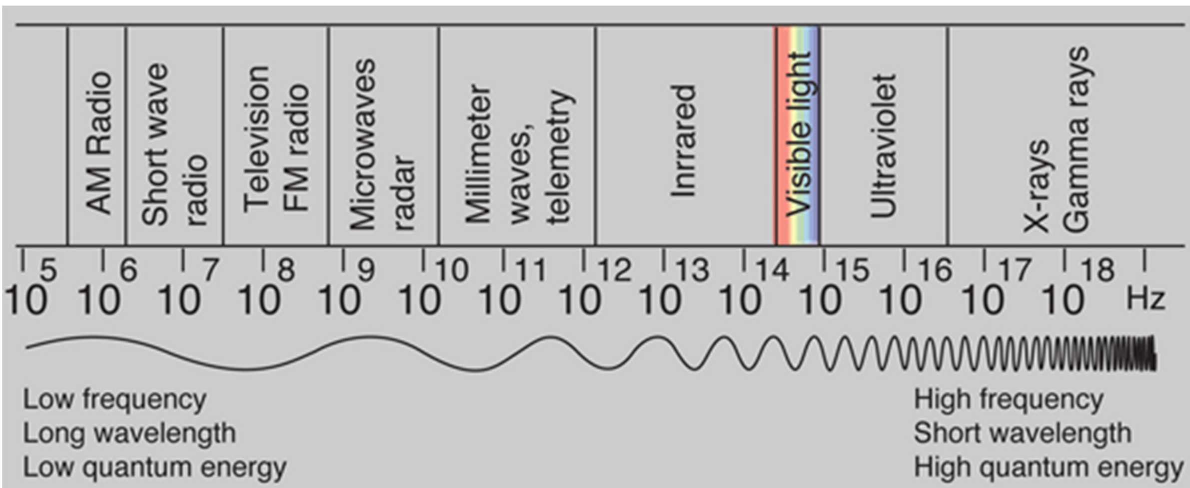
so the energy input to build to a final current i is given by the integral

$$\text{Energy stored} = \int_0^t P dt = \int_0^I L i' di' = \frac{1}{2} L I^2$$

Storage, conversion, transmission and radiation

Electromagnetic energy can be **stored** in the form of an electric field or a magnetic field, the latter typically generated by a current-carrying coil. Practical electrical **energy storage** technologies include electrical double-layer capacitors (EDLCs or ultracapacitors) and superconducting magnetic **energy storage** (SMES)

Magnetic reconnection is a fundamental process of **electromagnetic energy conversion** into kinetic **energy** and heat that operates in the solar corona, astrophysical accretion disks, active galactic nuclei, and planetary magnetospheres



$c = \nu\lambda$ **, where c is velocity of light , ν is frequency, λ is wavelength**

The different parts of the electromagnetic spectrum have very different effects upon interaction with matter. Starting with low frequency radio waves, the human body is quite transparent. In the lower ultraviolet range, all the Ultra Violet radiations from the sun are absorbed in a thin outer layer of humanskin.Each portion of the electromagnetic spectrum has quantum energies appropriate for the excitation of certain types of physical processes. The energy levels for all physical processes at the atomic and molecular levels are quantized, and if there are no available quantized energy levels with spacings which match the quantum energy of the incident radiation, then the material will be transparent to that radiation, and it will pass through. If electromagnetic energy is absorbed, butcannot eject electrons from the atoms of the material, then it is classified as non-ionizing radiation, and will typically just heat the material.

Question: Define energy with it forms.

ANS. Energy is defined as the ability to do work. Energy comes in various forms. Here are 10 common types of energy and examples of them

1. **Mechanical Energy**-Mechanical energy is energy that results from movementor the location of an object. Mechanical energy is the sum ofkineticenergy and potential energy.**examples:** An object possessing mechanical energy has both kinetic and potential energy, although the energy of one of the forms may be equal to zero. A moving car has kinetic energy. If you move the car up a mountain, it has kinetic and potential energy. A book sitting on a table has potential energy.

2. **Thermal Energy-**Thermal energy or heat energy reflects the temperature difference between two systems. **example:** A cup of hot coffee has thermal energy. You generate heat and have thermal energy with respect to your environment.

3. **Nuclear Energy-**Nuclear energy is energy resulting from changes in the atomic nuclei or from nuclear reactions. **example:** Nuclear fission, nuclearfusion, and nuclear decay are examples of nuclear energy. An atomic detonation or powers from a nuclear plant are specific examples of this type of energy.

4. **Chemical Energy-**Chemical energy results from chemical reactions between atoms or molecules. There are different types of chemical energy, such as electrochemical energy and chemiluminescence. **example:** A good example of chemical energy is an electrochemical cell or battery.

5. **Electromagnetic Energy-**Electromagnetic energy (or radiant energy) isenergy from light or electromagnetic waves. **example:** Any form oflight has electromagnetic energy, including parts of the spectrum we can't see. Radio, gamma rays, x-rays, microwaves, and ultraviolet light are some examples of electromagnetic energy.

6.**Sonic Energy-**Sonic energy is the energy of sound waves. Sound waves travel through the air or another medium. **example**: A sonic boom, a song played on a stereo, yourvoice.

7-**Gravitational Energy-**Energy associated with gravity involves the attraction between two objects based on their mass. It can serve as a basis for mechanical energy, such as the potential energy of an object placed on a shelf or the kinetic energy of the Moon in orbit around the Earth. **example**: Gravitational energy holds the atmosphere to the Earth.

8. **Kinetic Energy**-Kinetic energy is the energy of motion of a body. It rangesfrom 0 to a positive value. Example: An example is a child swinging on a swing. No matter whether the swing is moving forward or backward, the value of the kinetic energy is nevernegative.

9. **Potential Energy**-Potential energy is the energy of an object's position. Example: When a child swinging on a swing reaches the top of the arc, she has maximum potential energy. When she is closest to the ground, her potential energy is at its minimum (0). Another example is throwing a ball into the air. At the highest point, the potential energy is greatest. As the ball rises or falls it has a combination of potential and kineticenergy.

10. **Ionization Energy**-Ionization energy is the form of energy that bindselectrons to the nucleus of its atom, ion, or molecule. Example: The first ionization energy of an atom is the energy needed to remove one electron completely. The second ionization energy is energy to remove a second electron and is greater than that required to remove the firstelectron.

What is the importance of Quantum mechanics .(AKTU 2021)

- **Introduction to the quantum energy**

The electrons in free atoms can only be found in certain discrete **energy** states. One of the implications of these **quantized energy** states is that only certain photon **energies** are allowed when electrons jump down from higher levels to lower levels, producing the hydrogen spectrum. **Quantum mechanics** is an **important** tool to understand at the theoretical level the electronic structure of chemical compounds and the mechanism, thermodynamics, and kinetics of chemical reactions.

The **quantization of energy** refers to the fact that at subatomic levels, **energy** is best thought of as occuring in discreet "packets" called photons, photons come in different denominations. Each photon contains a unique amount of discreet energy **(E = hν)**

Wave Particle Duality: As stated by Einstein, the energyof light is concentrated in small bundles called photon. Hence, light behaves as a wave and as a particle, this nature of light is known as dual nature, while this property of light is known as wave particle duality.

Wave function and its significance: The quantity whose variation builds up matter waves is called **wave function (ψ).**The probability of finding the particle at a given point is proportional to $|\psi|^2$ at that point and the probability of finding the particle within an element of volume **dτ = dxdydz** is$|\psi|^2 d\tau$. Since the particle is necessarily somewhere in space the integral over the whole space must be unity, that is

$$\boxed{\int_{-\infty}^{\infty} |\psi|^2 d\tau = 1}$$

A wave function ψ satisfying the above relation is called **normalized wave function**. Every acceptable wave function must be normalized.

Conditions for wave function to be acceptable:

(i) Normalised wave function must be single valued
(ii) It must be finite everywhere
(iii) Ψ must be continuous throughout the entire space of the system and have a continuous first derivative.

Schrodinger's Wave Equation: This wave equation is a fundamental equation in quantum mechanics and describes the variation of wave function **ψ**in space and time.

The three dimensional time dependent Schrodinger wave equation is expressed as

$$\left(\frac{-h^2}{2m}\nabla^2 + V\right)\psi = i\hbar\frac{\partial\psi}{\partial t} \text{-----------------------} \quad (1)$$

Wave function ψ can be expressed as the product of two functions , one position dependent f(x,y,z) and the other time dependent Φ(t) as

$$\Psi = f(x,y,z)\,\Phi(t) \qquad \text{-----------------------} \ (2)$$

Putting the value of ψ in equation(1) , we get

$$\left(\frac{-h^2}{2m}\nabla^2 + V\right) f(x,y,z)\Phi(t) = i\hbar\frac{\partial}{\partial t}\lfloor f(x,y,z)\Phi(t)\rfloor$$

Dividing both sides by f(x, y, z)Φ(t), we get

$$\frac{1}{f(x,y,z)}\left(\frac{-h^2}{2m}\nabla^2 + V(x,y,z)\right)f(x,y,z) = i\hbar\frac{1}{\Phi(t)}\frac{\partial\Phi(t)}{\partial t} \text{ ---------------------- (3)}$$

The left hand side of equation (3) is independent of time t and right side is independent of x.This is possible only when they are separately equal to a constant. Let the constant be E

Then $\frac{1}{f(x,y,z)}\left(\frac{-h^2}{2m}\nabla^2 + V(x,y,z)\right)f(x,y,z) = E$ -------------------------- (4)

$i\hbar\frac{1}{\Phi(t)}\frac{\partial\Phi(t)}{\partial t} = E$ ----------------------- (5)

Since f(x,y,z) = ψ(x,y,z) , hence equation(4) can be rewritten as

$$\boxed{\nabla^2\psi + \frac{2m}{h^2}(E-V)\psi = 0}$$

This is **Schrodinger Time Independent Wave Equation** having solution ψ(x,y,z).

Solving equation(5)

$i\hbar\frac{\partial\Phi(t)}{\partial t} = E\Phi(t)$ ---------------------------- (6)

$\frac{\partial\Phi(t)}{\partial t} = \frac{E}{i\hbar}\partial t$ ------------------------------ (7)

On integrating we get

$$log\Phi(t) = \frac{Et}{i\hbar}$$

$\Phi(t) = e^{\frac{-iEt}{h}}$

The solution represented by equation(2) of time dependent Schrodinger equation is

$$\boxed{\Psi = f(x,y,z)e^{\frac{-iEt}{h}}}$$

The values of energy for which steady state equation (time independent) can be solved are called **eigen values** and the corresponding wave functions are called **eigen functions**.

de Broglie waves or matter waves:

1. When a material particle moves in a medium , a group of waves is associated with it due to which it shows the wave particle duality. These waves are known as matter waves or de Broglie waves.
2. According to de Broglie's, each ,material particle in motion behaves as waves, having wavelength λ associated with moving particle of momentum p.

$$\boxed{\boldsymbol{\lambda = \frac{h}{p}}}$$

where h is planks constant and p is momentum

Let the potential U(x) in the time-independent Schrodinger equation to be zero inside a one-dimensional box of length L and infinite outside the box. For a particle inside the box a free particle wavefunction is appropriate, but since the probability of finding the particle outside the box is zero, the wavefunction must go to zero at the walls. This constrains the form of the solution to

V = 0 for 0 < x < L

V = ∞ for 0 < x and x > L.

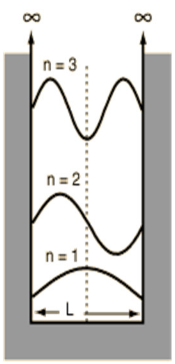
The Schrodinger equation for the particle within the box (V = 0) is

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0$$

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

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0$$

Particle in a Box



x = 0 at left wall of box.

Assume the potential U(x) in the time-independent Schrodinger equation to be zero inside a one-dimensional box of length L and infinite outside the box. For a particle inside the box a free particle wavefunction is appropriate, but since the probability of finding the particle outside the box is zero, the wavefunction must go to zero at the walls. This constrains the form of the solution to

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The Schrodinger equation for the particle within the box (V = 0) is

$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0$ -------------------------------- (1)

Let $\frac{2m}{\hbar^2} E = k^2$ -------------------------------- (2)

$\frac{d^2\psi}{dx^2} + k^2\psi = 0$ ------------------------------ (3)

The general solution of equation(3) is of the form

Ψ (x) = A sin kx + B cos kx ----------------------------- (4)

Where A and B are unknown constants found by applying boundary conditions, ψ = 0 at x = 0 and x = L

For boundary condition ψ = 0 at x = 0 to equation(4) , we get

0 = Asin0 + Bcos0 or B = 0 ------------------------------ (5)

When ψ = 0 at x = L we get

AsinkL = 0 orkL =nπ

$k = \frac{n\pi}{L}$ -------------------------- (6)

Where n = 1, 2, 3 …………….

Putting the value of k from equation(6) in equation (2) we get

$$\boxed{E_n = \frac{n^2h^2}{8mL^2}}$$

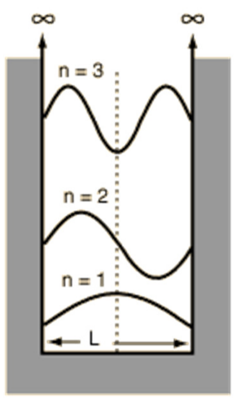
From the above equation it is clear that particle can have only **certain** discrete energy corresponding to n = 1, 2, 3 ……………

Normalization, Particle in Box

For the particle in a box with infinite walls, the probability must be equal to one for finding it within the box. The condition for normalization is then

$$\int \Psi^*\Psi\, dx = \int_0^L A_n^2 \sin^2\left(\frac{n\pi}{L}x\right) dx = 1$$

$$= A_n^2 \left[\frac{x}{2} - \frac{\sin\left(\frac{2n\pi}{L}x\right)}{4n\pi / L} \right]_0^L$$



x = 0 at left wall of box.

The sin terms drop out, leaving $A_n^2 \frac{L}{2} = 1$

so the normalized wavefunctions are:

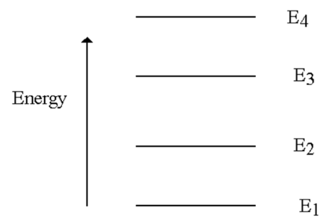
$$\Psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x \qquad n = 1,2,3,\ldots$$

Particle in the Box

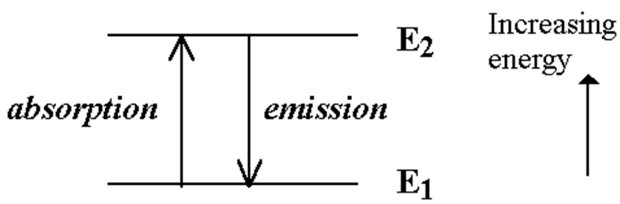
- The energy of a particle is quantized. This means it can only take on discreet energy values.
- The lowest possible energy for a particle is **NOT** zero (even at 0 K). This means the particle always has some kinetic energy.
- The square of the wavefunction is related to the probability of finding the particle in a specific position for a given energy level.
- The probability changes with increasing energy of the particle and depends on the position in the box you are attempting to define the energy for

Energy Quantisation:

Any atom or molecule can **ONLY HAVE CERTAIN FIXED ENERGIES**, energy is **QUANTISED** and an atom or molecule can exist only in certain discrete levels.



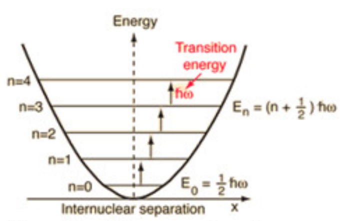
Since, the minimum energy is ½*h*□ the molecule is always vibrating. It is *never* at rest. It has ZERO-POINT energy, which must be allowed for many applications.



The ***Bohr-Einstein*** condition is:

$$\boxed{\Delta E = E_2 - E_1 = h\nu}$$

where ν is the frequency of the light absorbed/emitted and *h* is Planck's constant. ***h*ν is a quantum ("packet") of energy - called a photon.**



Quantised Energy Levels

Example: Find the energy of an electron moving in one dimension in an infinitely high potential box of width 1A^0 (mass of the electron is 9.11 x 10^{-31} kg and h = 6.63 x 10^{-34} J-s).

Solution: From equation

$$E_n = \frac{n^2 h^2}{8mL^2}$$

For n = 1 we get

$$E_n = \frac{h^2}{8mL^2}$$

Putting the numerical values we get
m = 9.11 x 10^{-31}kg, h = 6.63 x 10^{-34} joule-sec and L = 1A^0 = 10^{-10}m
we get
E = 6.03 x 10^{-18} joule or 37.69eV