UNIT II

Quantum Mechanics

Dr. Swati Gahlot
Physics Department
SVNIT, Surat

Introduction

Classical Mechanics is based mainly on three Newton's laws

- Law of Inertia
- Law of Force
- Law of action and reaction

Concepts involved are

- Absolute time, mass and space
- Explains correct motion of macroscopic and microscopic bodies moving with non-relativistic speeds ($v<<<<c$)

Principles involved in classical mechanics

In **classical mechanics**

- Time and space are two independent entities
- No limit in particle velocity
- Since everything is deterministic, we can measure all quantities simultaneously
- The outcome of all measurements are repeatable and depends only on the accuracy of measuring device

Principles involved in classical mechanics

Light: Waves or particles

1678 : Huygens principle

Every point on primary wave front serves as a source of secondary wavelets such that the primary wave front at some time later time is the envelope of these wavelets

1704 : Newton's principle

Corpuscular theory: Due to the fact that light travels in straight line according to classical physics

Principles involved in classical mechanics

Light: Waves or particles

1801 : Thomas Young

Uses wave theory of light to produce constructive and destructive interference and explained Newton's rings

Thomas Young
1773-1829

Principles involved in classical mechanics

1816 : Polarization

Arago and Fresnel investigated the interference of polarized rays of light and found that two rays of polarized light at right angles to each other will never interfere.

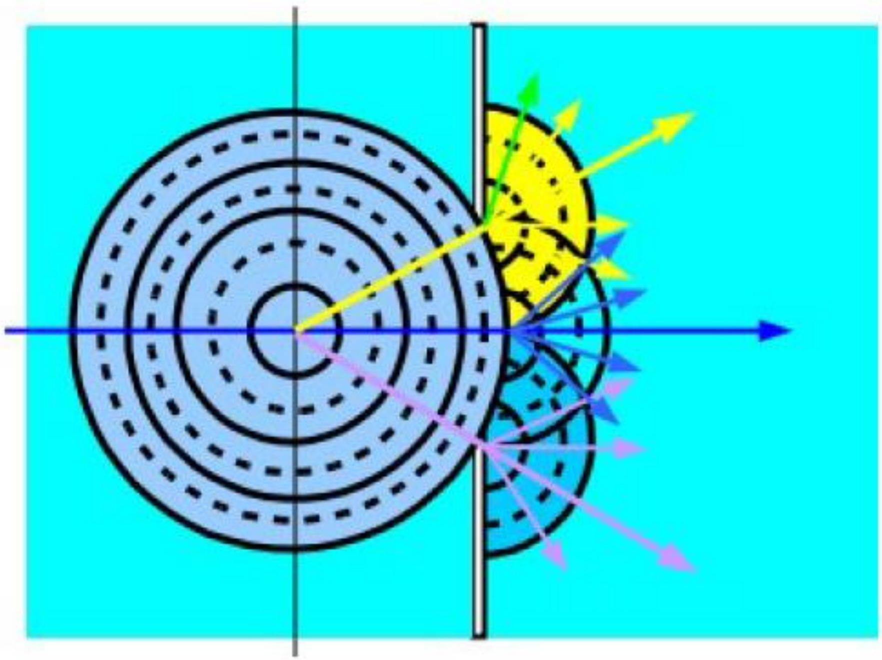
Dominique François Jean Arago 1786-1853

Augustin Jean Fresnel 1788-1827

Principles involved in classical mechanics

1818 : Diffraction

Fresnel by using Huygen's concept of secondary wavelets and explanation of interference, developed the theory of diffraction.



Augustin Jean Fresnel 1788-1827

Principles involved in classical mechanics

1865 : Electromagnetism

Maxwell's equations

James Clerk Maxwell
(1831-1879)

$\vec{H}$	***Magnetic Field Intensity***	$\left[A \cdot m^{-1}\right]$
$\vec{D}$	***Electric Displacement***	$\left[A \cdot s \cdot m^{-2}\right]$
$\vec{E}$	***Electric Field Intensity***	$\left[V \cdot m^{-1}\right]$
$\vec{B}$	***Magnetic Induction***	$\left[V \cdot s \cdot m^{-2}\right]$

Inadequacies of Classical Mechanics

Classical mechanics

- At the end of 19th century, Physics has evolved to the point at which Classical Mechanics was well established.

  - ✓ Thermodynamics and kinetic theory was well established
  - ✓ Geometrical and physical optics was well established
  - ✓ Conservation laws for energy and momentum

"There is nothing new to be discovered in Physics now. All that remains is more and more precise measurement" – *Lord Kelvin*

Inadequacies of Classical Mechanics

This is just before Relativity and Quantum mechanics appeared on the scene and opened up the ways for new exploration

Inadequacies of Classical Mechanics

- It does not holds good for atomic dimensions (non-relativistic speeds) i.e., electrons, protons, neutrons, etc.,
- Could not explain the stability of atoms
- Could not explain the observed spectrum of black body radiation
- Could not explain the variation of specific heat
- Could not explain the origin of discrete spectra
- Splitting of spectral lines

Origin of Quantum mechanics

- Classical mechanics does not give any pointers to understand the quantum world.

- So, it became challenge for the young minds to understand exactly how the quantum world works…

- The features relating to quantum world were really obvious only through the atomic and sub microscopic phenomena.

Origin of Quantum mechanics

- That is not to say that quantum mechanics does not hold good for macroscopic objects.

- In fact several macroscopic phenomena, I can think of ferromagnetism, paramagnetism in liquids right away…which can only be explained on the basis of quantum mechanics.

- Old quantum theory was proposed and developed by Neils Bohr, J.J.Thomson, etc.,

Origin of Quantum mechanics

- But Einstein found that no definitions, procedures and laws will work out when we deal with microscopic and sub-atomic particles.

- Thus, a new theory for dealing sub microscopic particles was developed and we call it now as Quantum Mechanics.

- Two master minds led this theory successful. They were the primary architects of quantum mechanics.

  - ✓ W.Heisenberg - matrix mechanics - Observables
  - ✓ E.Schroedinger - wave mechanics - Wavefunction & probability

Outcomes of Quantum mechanics

Dual nature of light and matter:

Wave nature of light……

- ✓ Interference
- ✓ Diffraction
- ✓ Polarization….

Particle / Corpuscular nature of light……

- ✓ Photoelectric effect
- ✓ Compton effect
- ✓ Discrete emission and absorption of radiation…
- ✓ Light is propagated in small packets or bundles of energy $h\nu$ or $\hbar\omega$
- ✓ These packets are called photons (or) quanta and behave like corpuscles (particles)

Outcomes of Quantum mechanics

De Broglie waves (or) Matter waves…………

- ✓ In 1923-24, he proposed that idea of dual nature can be extended to all sub-atomic particles
- ✓ According to de Broglie a moving particle whatever its nature has a wave properties associated with it.
- ✓ The waves associated with material particles are called de Broglie waves (or) matter waves.

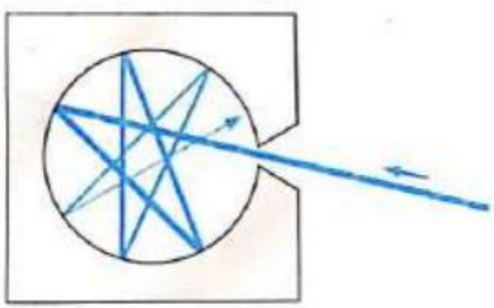
$$\lambda = h / p$$

$$\lambda = h / mv$$

L. de BROGLIE

BLACK BODY RADIATION

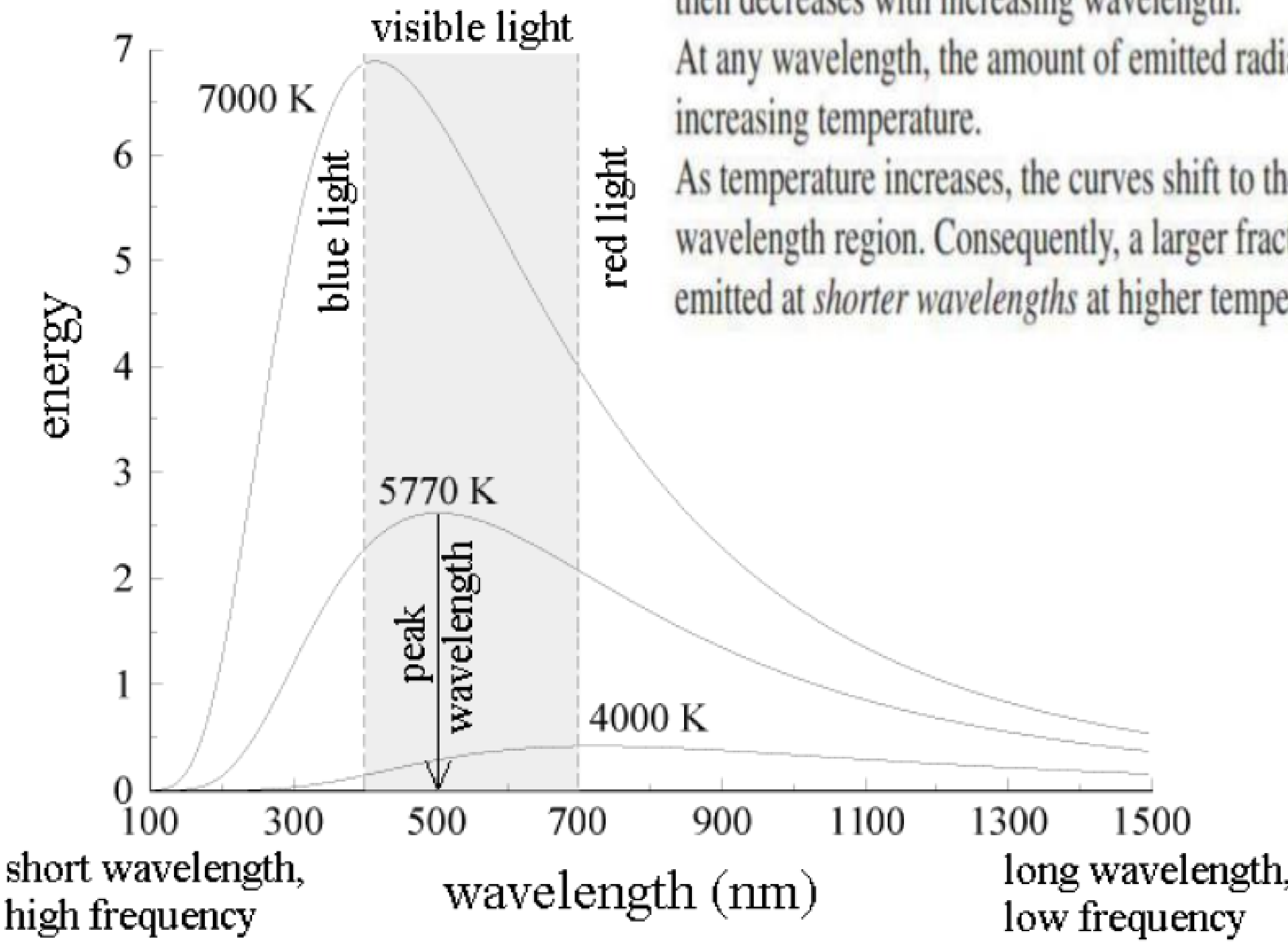
A body at temp. above absolute zero emits radiation in all directions over a wide range of wavelength.



blackbody

A blackbody is a surface that

- completely absorbs all incident radiation
- emits radiation at the maximum possible monochromatic intensity in all directions and at all wavelengths.



The emitted radiation is a continuous function of *wavelength*. At any specified temperature, it increases with wavelength, reaches a peak, and then decreases with increasing wavelength.

At any wavelength, the amount of emitted radiation *increases* with increasing temperature.

As temperature increases, the curves shift to the left to the shorter-wavelength region. Consequently, a larger fraction of the radiation is emitted at *shorter wavelengths* at higher temperatures.

The Explanation of Classical physics

1. Light is an electromagnetic wave that is produced when an electric charge vibrates. Now recall that heat is just the kinetic energy of random motion. In a hot object, electrons vibrate in random directions and produce light as a result. A hotter object means more energetic vibrations and so more light is emitted by a hotter object --- it glows brighter. So far, so good. But classical physics could not explain the shape of the blackbody spectrum.

2. The electrons in a hot object can vibrate with a range of frequencies, ranging from very few vibrations per second to a huge . Classical physics said that each frequency of vibration should have the same energy. This means that, there should be no limit to the energy of the light produced by the electrons vibrating at high frequencies. WRONG!!

Experimentally, the blackbody spectrum always becomes smaller. (short wavelength, high frequency).

At about 1900, Max Planck came up with the solution:

He proposed that

The classical idea that each frequency of vibration should have the same energy must be wrong.

Instead, he said that energy is not shared equally by electrons that vibrate with different frequencies. Planck said that energy comes in clumps. He called a clump of energy a quantum. The size of a clump of energy --- a quantum --- depends on the frequency of vibration. Here is Planck's rule for the a quantum of energy for a vibrating electron:

$$E = h f$$

where h, the calibration constant, is today called Planck's constant. Its value is about 6 x 10-34, very tiny

So how does this explain the spectrum of blackbody radiation?

Planck said that an electron vibrating with a frequency f could only have an energy of 1 hf, 2 hf, 3 hf, 4 hf, ... ; that is,

energy of vibrating electron = (any integer) x hf

But the electron has to have at least one quantum of energy if it is going to vibrate. If it doesn't have at least an energy of 1hf, it will not vibrate at all and can't produce any light . Planck said: at high frequencies the amount of energy in a quantum, hf, is so large that the high-frequency vibrations can never get going! This is why the blackbody spectrum always becomes small (high frequency) .

DEFINITIONS

Total energy density (u) at any point denotes the total radiant energy for all wavelengths from 0 to ∞ per unit volume around that point. Its unit is Jm^{-3}.

Spectral energy density (u_λ) for the wavelength λ is a measure of the energy per unit volume per unit wavelength. Therefore, $u_\lambda d\lambda$ denotes the energy per unit volume in the wavelength range between λ and $\lambda + d\lambda$. It is related to total energy density through the relation

$$u = \int_0^\infty u_\lambda \, d\lambda$$

Total emissive power E of the surface of the body at a given temperature is defined as the amount of total energy radiated by unit area of its surface in unit time. Unit- $J\,m^{-2}s^{-1}$

Spectral emissive power E_λ of a body for the wavelength λ signifies the radiant energy per second per unit surface area per unit range of wavelength. Therefore, $E_\lambda d\lambda$ denotes the energy per unit area per second in the wavelength range between λ and $\lambda + d\lambda$. It is related to emissivity through the relation

cal

$$\mathbf{E} = \int_0^\infty E_\lambda \, d\lambda$$

Emissivity of a surface → Ratio of the radiation emitted by the surface at a given temperature to the radiation emitted by a blackbody at the same temperature.

$$\boxed{e = \frac{E(T)}{E_b(T)}} \qquad 0 \le e \le 1$$

Emissivity of real surfaces = f(T, λ, direction of radiation)

Spectral absorptivity (a_λ) is defined as the fraction of incident energy absorbed per unit surface area per second at wavelength λ. Suppose that δQ_λ radiation of wavelength between λ and λ + dλ is incident on a unit area of the surface of the body per second from all possible directions. If $a_\lambda \delta Q_\lambda$ is the amount of radiation absorbed, then a_λ signifies the absorptivity of the body for wavelength λ. a_λ has no dimensions;

KIRCHHOFF'S LAW: RELATION BETWEEN e_λ AND a_λ

The Kirchhoff's law states that *the ratio of the spectral emissive power* e_λ *to the spectral absorptivity* a_λ *for a particular wavelength* λ *is the same for all bodies at the same temperature and is equal to the emissive power of a perfectly black body at that temperature*. Mathematically, we write

$$\frac{e_\lambda}{a_\lambda} = E_\lambda$$

where E_λ is emissive power of a perfectly blackbody. Note that the ratio e_λ/a_λ is a universal function of λ and T.

Wien Displacement Law Formula The Wien's Displacement Law provides the wavelength where the spectral radiance has maximum value. This law states that the black body radiation curve for different temperatures peaks at a wavelength invers proportional to the temperature.

Maximum wavelength = Wien's displacement constant / Temperature

The equation is:

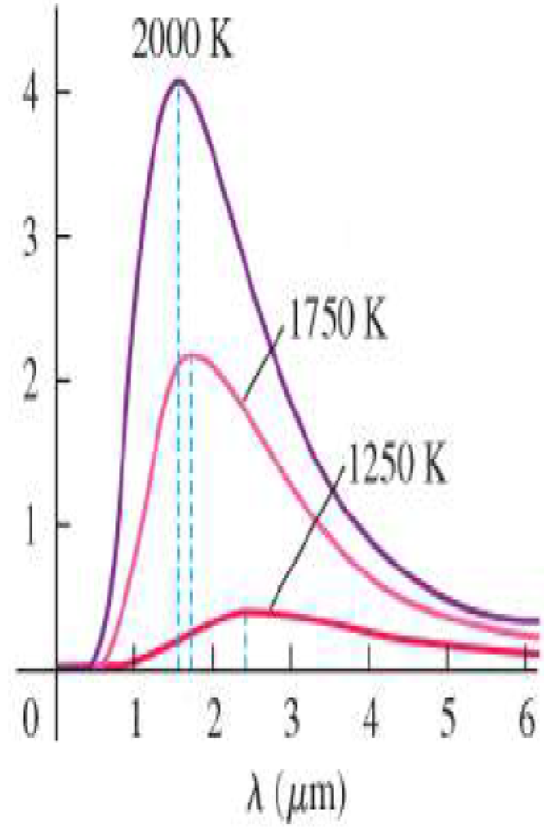
$\lambda_{max} = b/T$

Where:

λ_{max}: The peak of the wavelength

b: Wien's displacement constant. ($2.9*10^{(-3)}$ m K)

T: Absolute Temperature in Kelvin.



Plank's Radiation Law (1900)-

* Blackbody chamber is filled up not only with radiation but also with simple harmonic oscillators of molecular dimensions.
* The oscillator in cavity walls could not have a continuous distribution of possible energies ϵ, but must have only energies. $E_n = nh\nu$

  $(n = 0, 1, 2, 3 \ldots)$
* An oscillator emits radiation of freq. 'ν' when it drops from one energy state (E_2) to the lower one (E_1) & it absorbes radiation of freq. 'ν' while going to the higher energy state (i.e. $E_1 \rightarrow E_2$)
* Each discrete bundle of energy is called a 'quantum'.
* With oscillator energy limited to $nh\nu$, the average energy per oscillator in cavity walls and so per standing waves (as in R. Jeans) turns out not

equal to kT but different from it.
In order to derive Plank's radiation law, we shall first derive the no. of resonators per unit volume lying in the freq. range ν & $\nu + d\nu$ & the av. energy of Plank's resonator.

Thus, the no of modes of vibrations per unit volume with freq. range ν & $\nu + d\nu$.

$$= \frac{4\pi \nu^2 \, d\nu}{c^3}$$

Blackbody radiation travel with velocity of light 'c' & are transverse in character.

As there are 2 possible polarisation state for each transverse wave, so the no. of modes of vibration per unit volume within freq. range ν & $\nu + d\nu$.

$$= 2 \times \frac{4\pi \nu^2 \, d\nu}{c^3} = \frac{8\pi \nu^2 \, d\nu}{c^3} \quad \text{—(1)}$$

Average Energy of Plank's Oscillator -

If 'N' is the total no. of Planck's resonators & E their total energy, then av. energy per Planck oscillator is given by,

$$\bar{\epsilon} = \frac{E}{N} \quad -(2)$$

According to Maxwell's law of molecular motion if ϵ is a certain amount of energy, the probabilities that a system will have energies $0, \epsilon, 2\epsilon, \dots r\epsilon, \dots$ are in the ratio

$$1 : e^{-\epsilon/kT} : e^{-r\epsilon/kT} : \dots \text{ etc}$$

If N_0 is the no. of resonators having energy zero, then the no. of resonators N_1 having energy ϵ will be $N_0 e^{-\epsilon/kT}$, the no of resonators N_2 having energy 2ϵ will be $N_0 e^{-2\epsilon/kT}$, no of resonators N_r having energy $r\epsilon$ is $N_0 e^{-r\epsilon/kT}$

$\therefore \quad N = N_0 + N_1 + N_2 \cdots + N_r + \cdots$

$$= N_0 + N_0 e^{-\epsilon/kT} + N_0 e^{-2\epsilon/kT} + \cdots N_0 e^{-r\epsilon/kT}$$

$$= N_0 \left[1 + e^{-\epsilon/kT} + e^{-2\epsilon/kT} + \cdots e^{-r\epsilon/kT} + \cdots\right]$$

putting $\quad e^{-\epsilon/kT} = y \quad$ — (3)

$$N = N_0 \left[1 + y + y^2 + \cdots y^r \cdots\right]$$

or

$$N = \frac{N_0}{1-y} \quad \text{— (4)}$$

Total energy of Plank's resonator

$$E = 0 \times N_0 + \epsilon \times N_1 + 2\epsilon \times N_2 + \cdots r\epsilon \times N_r + \cdots$$

$$= 0 + \epsilon N_0 e^{-\epsilon/kT} + 2\epsilon N_0 e^{-2\epsilon/kT} + \cdots + r\epsilon N_0 e^{-r\epsilon/kT} + \cdots$$

$$= N_0 \epsilon \left[e^{-\epsilon/kT} + e^{-2\epsilon/kT} + \cdots e^{-r\epsilon/kT} + \cdots\right]$$

$$= N_0 \epsilon \left[y + 2y^2 + \cdots ry^r + \cdots\right]$$

Let $\quad S = y + 2y^2 + \cdots ry^r + \cdots$

$\therefore \quad Sy = y^2 + 2y^3 + \cdots ry^{r+1}$

Substract $\Rightarrow$ $\quad S - Sy = y + y^2 + \cdots + y^r + \cdots$

$$S(1-y) = \frac{y}{1-y}$$

$$S = \frac{y}{(1-y)^2}$$

$$E = N_0 \epsilon S$$

$$= N_0 \epsilon \frac{y}{(1-y)^2} \quad - (5)$$

therefore the average energy of a resonator will be

$$\bar{\epsilon} = \frac{E}{N} = \frac{N_0 \epsilon \frac{y}{(1-y)^2}}{\frac{N_0}{(1-y)}}$$

$$= \frac{\epsilon y}{1-y} = \frac{\epsilon e^{-\epsilon/kT}}{1-e^{-\epsilon/kT}}$$

$$\bar{\epsilon} = \frac{\epsilon}{e^{\epsilon/kT}-1} \quad - (6)$$

According to Planck's hypothesis of quantum theory $\epsilon = h\nu$

$$\bar{\epsilon} = \frac{h\nu}{e^{h\nu/kT}-1} \quad - (7)$$

per unit volume, in the freq. range ν & $\nu + d\nu$ i.e.,

$$E_\nu d\nu = \left(\frac{8\pi\nu^2 d\nu}{c^3}\right)\left(\frac{h\nu}{e^{h\nu/kT}-1}\right)$$

or

$$E_\nu d\nu = \frac{8\pi\nu^2}{c^3}\frac{h\nu}{e^{h\nu/kT}-1} d\nu \quad -(8)$$

where $E_\nu d\nu$ is energy density (i.e. total energy per unit volume) belonging to the range $d\nu$.

Eqⁿ (8) is called Planck's radiation law in terms of freq.

$$E_\lambda d\lambda = \frac{8\pi hc}{\lambda^5}\frac{d\lambda}{e^{hc/\lambda kT}-1} \quad -(9)$$

This is Planck's radiation law in terms of wavelength.

for shorter wavelength $e^{\hbar c/\lambda k T}$ becomes large as compared to unity & hence Planck's law reduces to

$$E_\lambda d\lambda = \frac{8\pi \hbar c}{\lambda^5} \cdot \frac{1}{e^{\hbar c/\lambda k T}} d\lambda$$

$$= \frac{8\pi \hbar c}{\lambda^5} e^{-\hbar c/\lambda k T} d\lambda \quad - (10)$$

which is wien's law

for longer wavelengths $e^{\hbar c/\lambda k T}$ may be approximated to $\left(1 + \frac{\hbar c}{\lambda k T}\right)$ &

hence Planck's law reduces to

$$E_\lambda d\lambda = \frac{8\pi \hbar c}{\lambda^5} \left(\frac{1}{1 + \frac{\hbar c}{\lambda k T} - 1} \right) d\lambda$$

$$= \frac{8\pi \hbar c}{\lambda^5} \cdot \frac{\lambda k T}{\hbar c} d\lambda$$

$$E_\lambda d\lambda = \frac{8\pi k T}{\lambda^4} d\lambda \quad - (11)$$

which is Rayligh - Jean's law.