FOUNDATION OF QUANTUM MECHANICS

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“മാതാ പിതാ ച മേ ശത്രുര്യേന ബാല്യേനപാഠ്യതേ
സഭാമദ്ധ്യേ ന ശോഭതേ ഹംസമദ്ധ്യേ ബകോയഥാ”

“ചെറുപ്പത്തിൽ വിദ്യാഭ്യാസം ചെയ്യിപ്പിക്കാത്ത
മാതാപിതാക്കൾ ശത്രുക്കൾക്ക് സമാനമാകുന്നു.
അത് എന്തെന്നാൽ വിദ്യ അഭ്യസിച്ചിട്ടില്ലാത്തവൻ ഒരു
സഭാമദ്ധ്യത്തിൽ ചെന്നാൽ അരയന്നങ്ങളുടെ
ഇടയിൽ അകപ്പെട്ട കൊക്കിനു സമം തന്നെ.”

- Quantum Mechanics explains operation of Lasers, microchips, stability of DNA, **α** particle tunneling etc.

- Quantum Physics, developed during the first quarter of the century (1900 -1926), which provides a conceptual frame work to understand the physical processes taking place at the atomic scale

- Classically, we may describe the state of a system by specifying, at some time t the generalized coordinates and momenta

- In quantum mechanics, it is not possible to give such a complete specification to arbitrary precision

- non-intuitive
- defies commonsense
- essentially mathematical
- cannot be simplified
- Never tasted failure
- Revolutionized our view of physical world
- Quantum physics constitutes the "foundation stone "for many fields of modern science

Solid state physics and material science
Band theory – semiconductor electronics
Superconductors, Lasers, Nanotechnology
Quantum chemistry, Catalysis and surface science
Biochemistry, Nuclear Physics, Nuclear weapons
Nuclear fission and fusion, Particle Physics, Quarks
Microprocessors …

- Testing theories by experiment is a hall mark of Physics (Science)
- The interplay between theory and experiment is still the best way to proceed in the world of acceptable science
- Galileo devised experiments
- Isaac Newton
- James Clarke Maxwell
- Lord Kelvin spoke of relativity & quantum theory
- Albert Michelson – What remains to be filled is sixth decimal place !!

Classical aesthetics

- Universe is like a machine set in a frame work of absolute time and space
- Newtonian synthesis implied that all motion had a cause
- If state of motion is known at one point-say present- it could be determined at any other point in future or past.Nothing was uncertain (principle of determinism)
- Properties of light are described by electromagnetic theory
- Energy in motion is either particle or a wave and these pictures are mutually exclusive.

The International Solvay Institutes for Physics and Chemistry, located in Brussels, were founded by the Belgian industrialist Ernest Solvay in 1912

famous conference - Fifth Solvay International Conference on Electrons and Photons, October 1927

Eminent physicists met to discuss the newly formulated quantum theory

The leading figures were Albert Einstein and Niels Bohr

Einstein, disenchanted with Heisenberg's "Uncertainty Principle" remarked "God does not play dice." Bohr replied, "Einstein, stop telling God what to do."

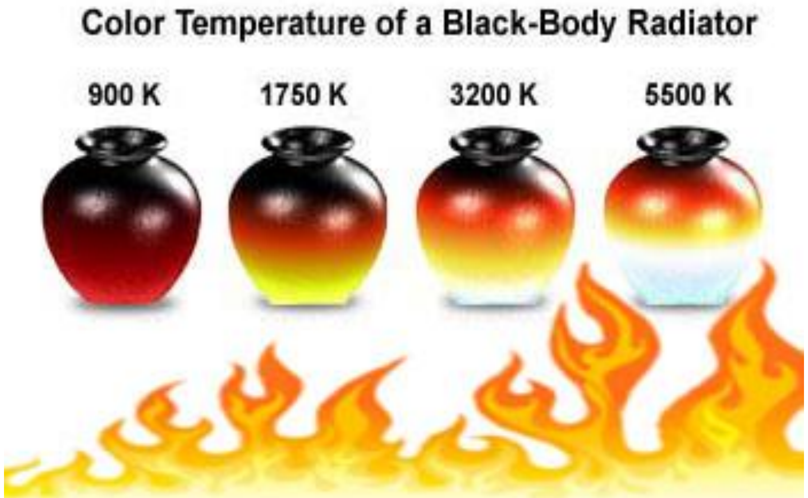
Seventeen of the twenty-nine attendees were or became Nobel Prize winners, including Marie Curie, who alone among them, had won Nobel Prizes in two separate scientific disciplines.

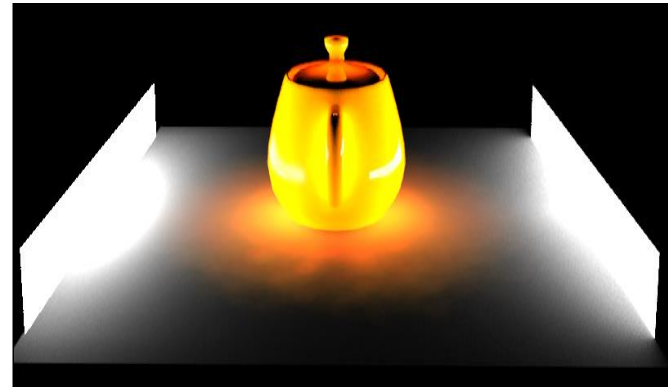
Back row L-R: A Piccard, E Henriot, P Ehrenfest, Ed Herzen, Th. De Donder, E Schroedinger, E Verschaffelt, W Pauli, W Heisenberg, R. H Fowler, L Brillouin
Middle row L-R: P Debye, M Knudsen, W. L Bragg, H. A Kramers. P. A. M Dirac, A. H Compton, L. V. De Broglie, M Born, N Bohr
Front row: L-R: Angmeir, M Planck, M Curie, H. A Lorentz, A Einstein, P Langevin, Ch. E Guye, C. T. R Wilson, O. W Richardson

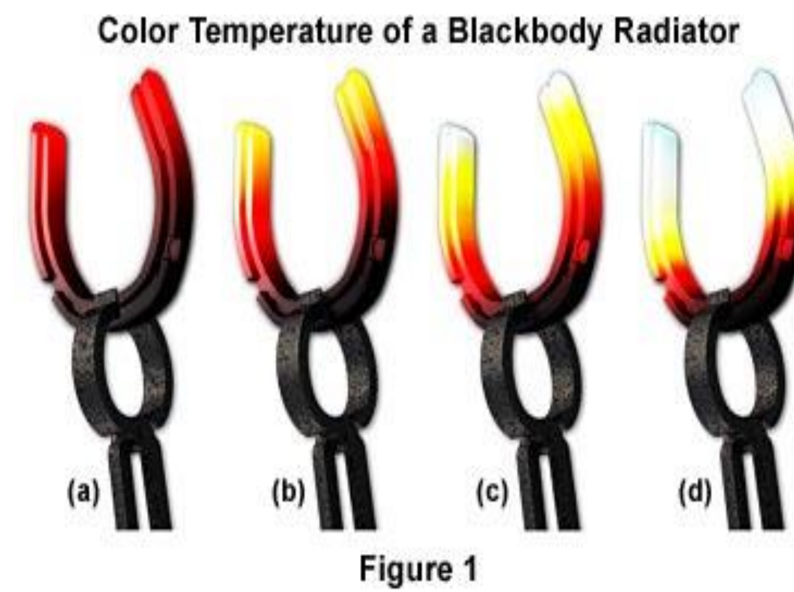
POTTERS GUIDE
(Josiah wedgewood-1792)

- 550ºc - DARK RED
- 750ºc - CHERRY RED
- 900ºc - ORANGE
- 1000ºc - YELLOW
- 1200ºc - WHITE

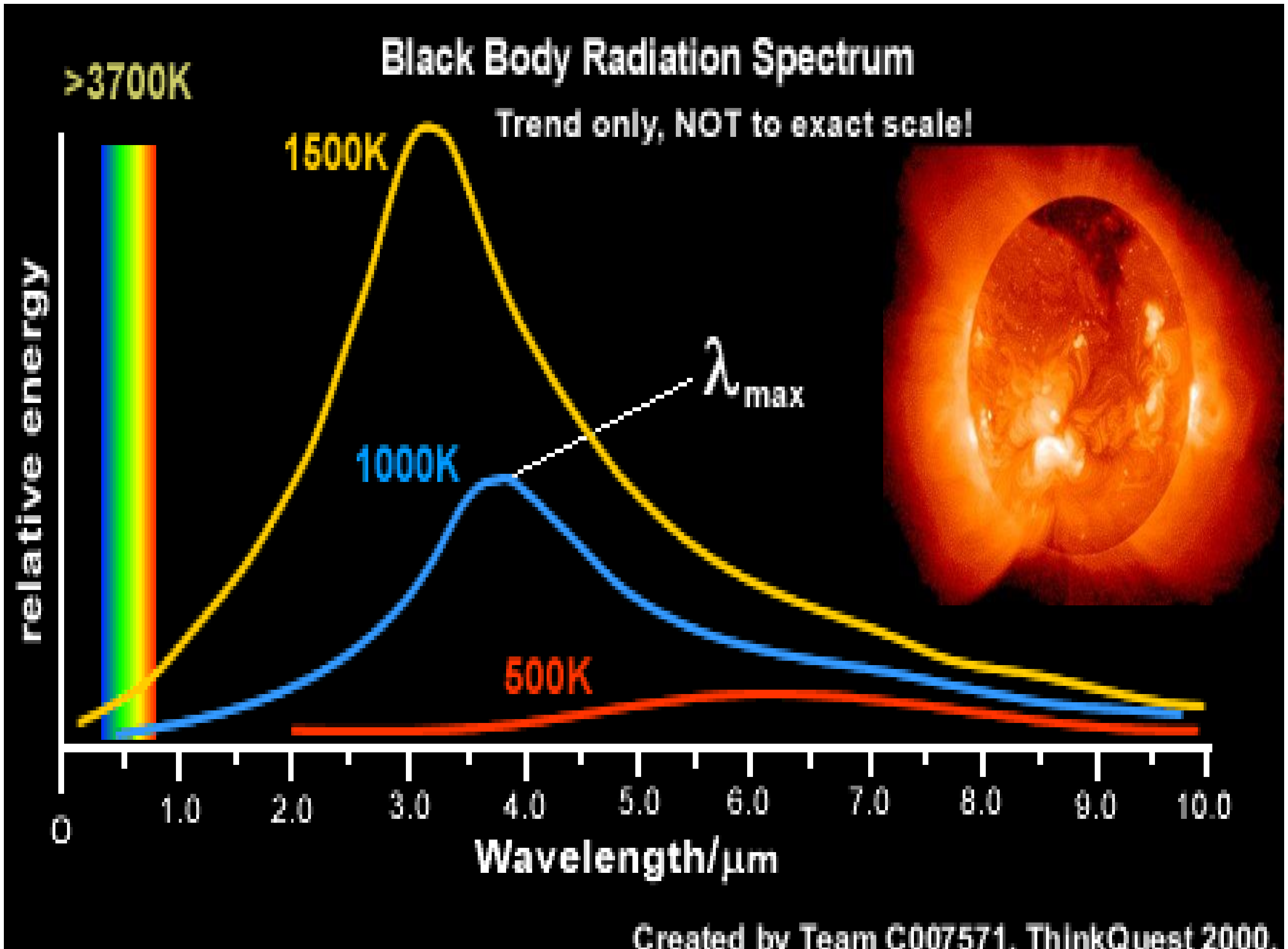
Temperatupa, °C	Color
550	
630	
680	
740	
770	
800	
850	
900	
950	
1000	
1100	
1200	
1300	


Color Temperature of a Black-Body Radiator
900 K
1750 K
3200 K
5500 K




Color Temperature of a Blackbody Radiator
(a)
(b)
(c)
(d)
Figure 1

BLACK BODY RADIATION SPECTRUM



CLASSICAL APPROACH TO BLACK BODY

- The Stefan-Boltzman law (1879) relates the total amount of radiation emitted by an object to its temperature

$$\mathbf{E = \sigma T^4}$$

- The Wien's Displacement Law (1893) state that the wavelength carrying the maximum energy is inversely proportional to the absolute temperature of a black body.

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

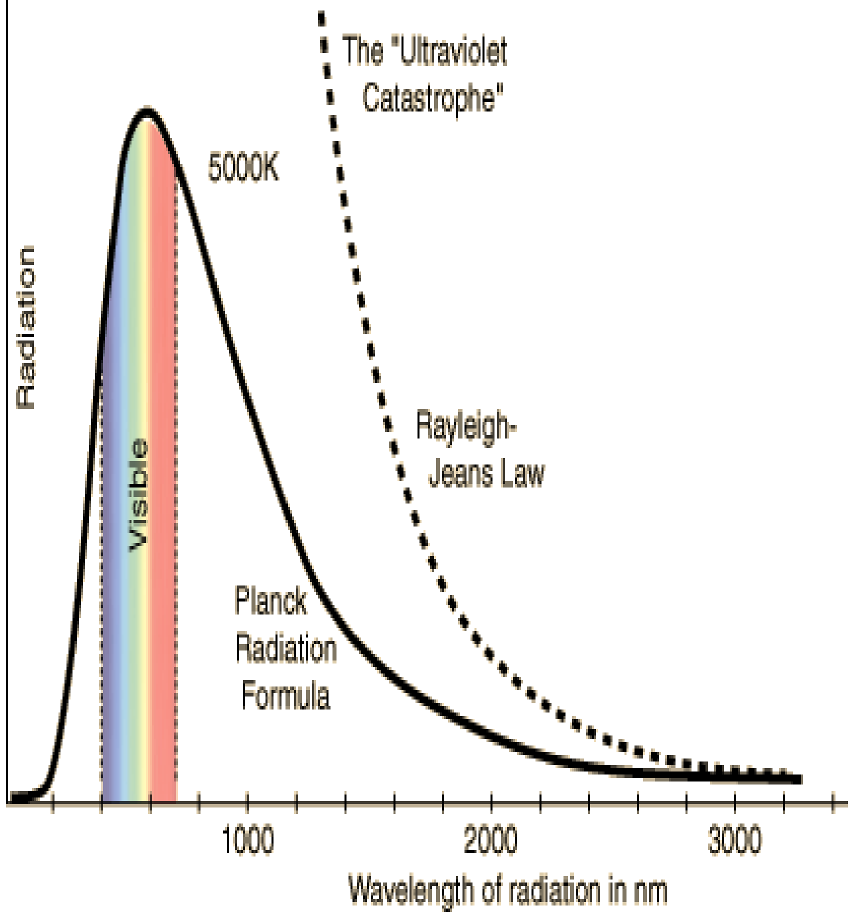
- A classical law approximately describing the intensity of radiation emitted by a blackbody, derived by Rayleigh and Jeans by counting the number of standing wave modes in an enclosure

$$u(v)dv = \frac{8\pi kT}{C^3} v^2 \, dv$$

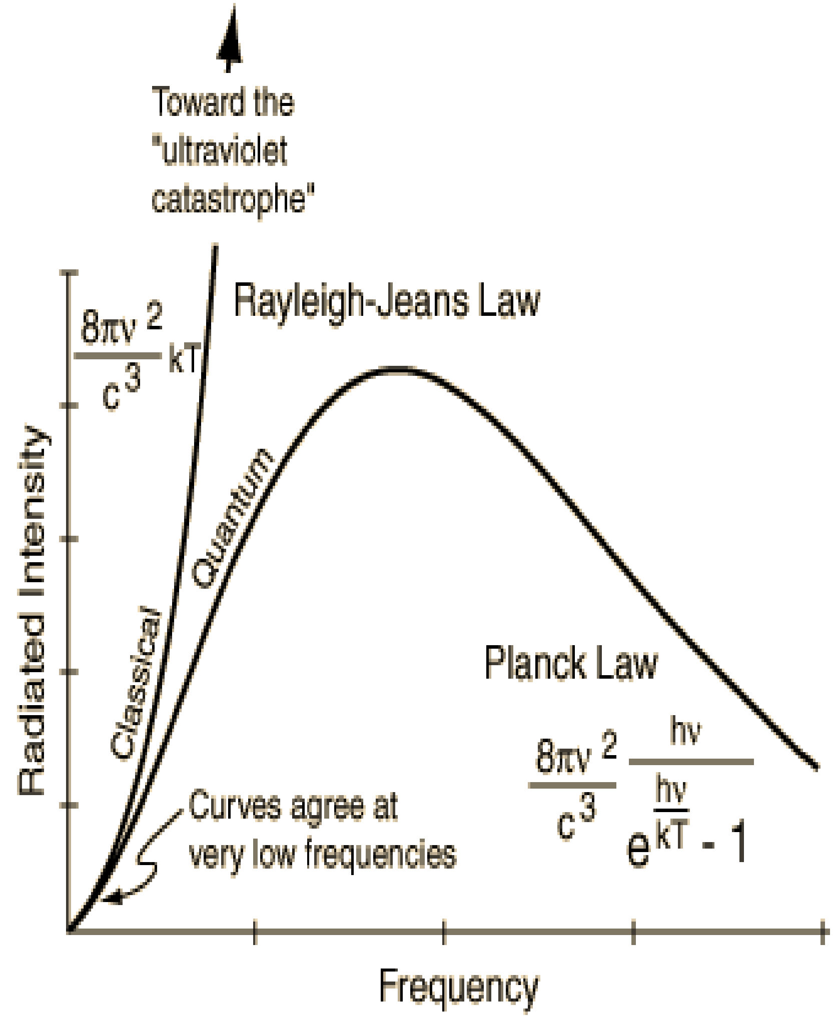
‘CLASSIC’AL CONCLUSIONS

- There is an infinite total energy in the cavity. This cannot be immediately disproved because total energy is not an observable quantity directly,but it is an unpleasant result
- The radiation in cavity has infinite specific heat. This cannot be true because temperature can be increased by providing finite amount of energy
- The specific heat is independent of temperature and total energy is proportional to temperature. Thermodynamically and also experimentally, the total energy in the cavity is proportional to fourth power of temperature.

- The energy is concentrated at high frequencies and energy per unit frequency range is proportional to square of the frequency. This is not true since experiments show that the energy is a function of frequency and has a definite maximum at frequency which is a function of temperature.
- From Rayleigh – Jeans formula as frequency υ increases towards the ultraviolet end of the spectrum the energy density should increase as υ^2. In the limit of infinitely high frequencies, total energy density $u(\upsilon)\,d\upsilon$ per unit volume therefore should also go to infinity. In reality, the energy density falls to 0 as υ tends to infinity.This discrepancy became known as the ultraviolet catastrophe.



The "Ultraviolet Catastrophe"
5000K
Radiation
Visible
Rayleigh-Jeans Law
Planck Radiation Formula
1000
2000
3000
Wavelength of radiation in nm



Toward the "ultraviolet catastrophe"
$\frac{8\pi\nu^2}{c^3}kT$
Rayleigh-Jeans Law
Radiated Intensity
Quantum
Classical
Planck Law
$\frac{8\pi\nu^2}{c^3}\frac{h\nu}{e^{\frac{h\nu}{kT}}-1}$
Curves agree at very low frequencies
Frequency

PLANCK RADIATION FORMULA

In 1900, the German Physicist Max Planck solved the problem by introducing a constant *h* called Planck's constant.

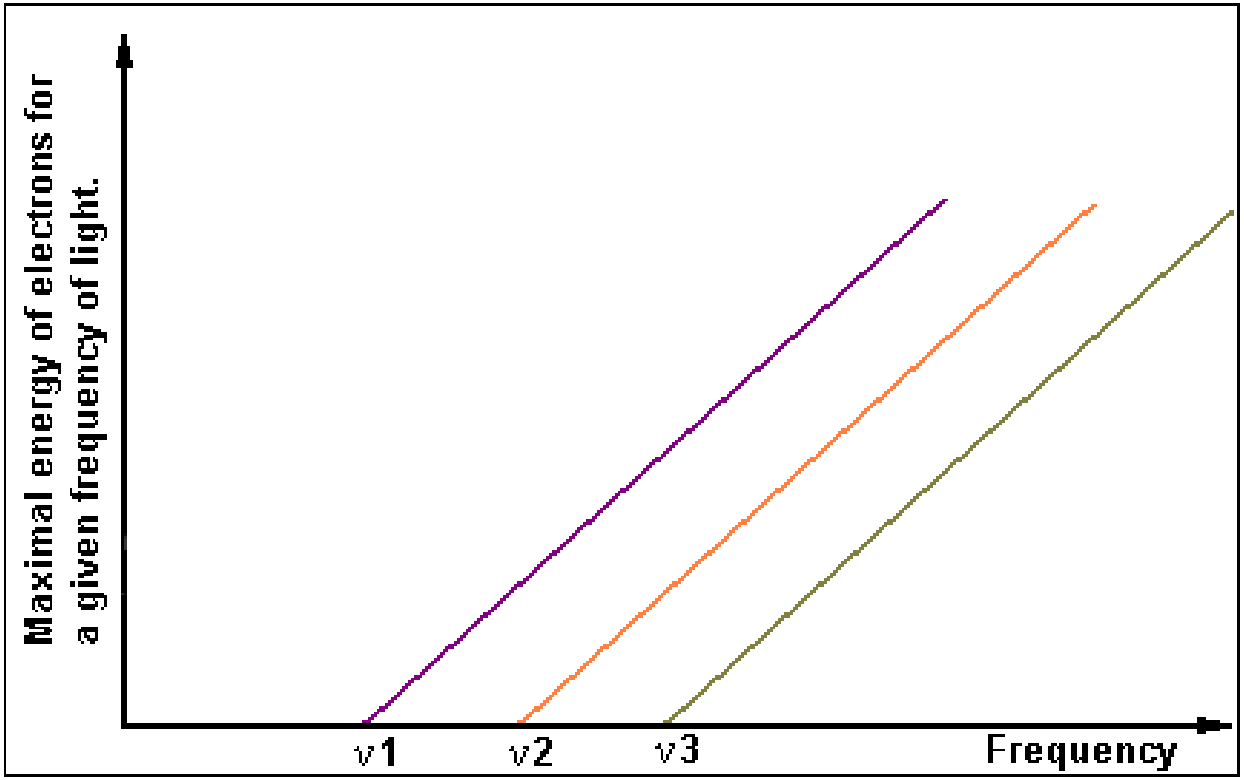
His "lucky guesswork" (as he later called it) resulted in a formula for the spectral energy density of blackbody radiation.

$$u(v)dv = \frac{8\pi h}{c^3} \frac{v^3}{e^{\frac{hv}{kT}} - 1} dv$$

PHOTOELECTRIC EFFECT

Albert Einstein (1879 - 1955) published his theory of photoelectric effect in 1905, the same year in which he published the Special Theory of Relativity and the paper on molecular dimensions which earned him his Ph.D from the University of Zurich. Then, in 1921 Einstein won the Nobel Prize for the theory of photoelectric effect.

$$h\nu = KE_{max} + \varphi$$



The diagram shows the interdependence between light frequency and the maximal energy of electrons emitted from metal. It show the interdependence for three different metals. See that it clearly shows the limiting frequencies - different for different metals

Millikan verified Einstein's explanation during 1912-1917.He obtained linear results so accurate that Einstein's predictions are proved.

"Contrary to all my expectations I am compelled to assert its unambiquous experimental verification inspite of its unreasonableness. The hypothesis was made solely because it furnished a ready explanation of the fact that the energy of an ejected electron is independent of the intensity of light but depend on the frequency.I understand even Einstein him self no longer accepts it".

- Niels Bohr (1885-1955) :

  Privileged Orbits
- Quantum number : To represent the state of a system
- Pauli - idea of 'hidden rotation'
- To account for both fine structure in spectral lines and anomalous Zeeman effect, two Dutch graduate students, Samuel Goudsmit and George Uhlenbeck proposed in 1925 that every electron has intrinsic angular momentum, called spin

Basics of quantum mechanics - particle-wave duality

- The behavior of a "microscopic" particle is very different from that of a classical particle:
  - ➔ in some experiments it resembles the behavior of a classical wave (not localized in space)
  - ➔ in other experiments it behaves as a classical particle (localized in space)
- Corpuscular theory of light treat light as though it were composed of particles, but can not explain DIFFRACTION and INTERFERENCE.
- Maxwell's theory of electromagnetic radiation can explain these two phenomena, which was the reason why the corpuscular theory of light was abandoned.

Dual nature of radiation and matter

radiation- dual nature (postulate of Einstein)

Louis de Broglie – duality is general (1924)

$$\lambda = \frac{h}{P}$$

- Quantum particles can act as both particles and waves ➔ WAVE-PARTICLE DUALITY
- Quantum state is a conglomeration of several possible outcomes of measurement of physical properties ➔ Quantum mechanics uses the language of PROBABILITY theory (random chance)
- An observer cannot observe a microscopic system without altering some of its properties. Neither one can predict how the state of the system will change.
- QUANTIZATION of energy is yet another property of "microscopic" particles.
- Watch Quantum Mechanics Explained

- Triple Birth of Quantum Mechanics
- Werner Heisenberg (1901-1976) with Max Born and Pascual Jordan - matrix mechanics

Heisenberg picture of atom
Not to treat atom as a solar system
Consider as a virtual oscillator
$[x,p] = ih/2\pi$

- Erwin Schrodinger – Wave Mechanics
- Paul Dirac – Quantum Algebra
- Electrons were shown to obey a new type of statistical law, Fermi-Dirac statistics. It was recognized that all particles obey either Fermi-Dirac statistics or Bose-Einstein statistics, and that the two classes have fundamentally different properties.

- Paul A. M. Dirac developed a relativistic wave equation for the electron that explained electron spin and predicted antimatter. He also laid the foundations of quantum field theory by providing a quantum description of the electromagnetic field.
- Dual nature of light is free of paradox for those who can follow the mathematics
- His work was carried forward by Richard Feynmann, Freeman Vyson, Julian Schwinger & Tomaonaaga – QED
- QED describes interaction of light and matter with remarkable accuracy

Principle of Complimentarity

Classical Physicist : If two descriptions are mutually exclusive then atleast one of them must be wrong

Quantum Physicist : Whether an object behaves as a particle or a wave depends on our choice of apparatus for looking at it

Suppose one set of experimental evidence can only be interpreted on the basis of wave properties and other by particle properties, these sets are not contradictory. They are obtained under different experimental conditions, cannot be combined in a single picture and is regarded as complimentary.

COPENHAGEN INTERPRETATION

The description of a state of an atomic system before measurement is undefined having only potentiality of certain values with certain probabilities

Niels Bohr together with Heisenberg, Pauli and Born

Postulates Of Quantum Mechanics

- State of a quantum mechanical system is described by a vector in an abstract Hilbert space
- If $|\psi_1\rangle$ and $|\psi_2\rangle$ represent state vectors of two states of given system then $c_1|\psi_1\rangle + c_2|\psi_2\rangle$ also represents the state of the system

  (Closure property of vector space-superposition principle)

- Dynamical variables are represented by linear operators. Corresponding to every observable there exists a Hermitian operator. The measurable values of an observable are eigen values
- For Energy $H|\psi\rangle = E|\psi\rangle$

Postulates of QM Contd.

The expectation value of an operator corresponding to a state vector is the possible result of a large number of measurements of the dynamical variable represented by the operator

$$<A> = \frac{<X/A/X>}{<X/X>}$$

Postulates of QM Contd.

Any pair of canonically conjugate operators will satisfy the Heisenberg commutation relations

$$[\widehat{q_l}, \widehat{q_k}] = 0 \qquad [\widehat{q_l}, \widehat{p_k}] = \frac{ih\hat{I}}{2\pi}\delta_{lk}$$

$$[\widehat{p_l}, \widehat{p_k}] = 0$$

Postulates of QM Contd.

The time development of state function is given by

$$\widehat{H}|\psi> = \frac{ih}{2\pi}\frac{d|\psi>}{dt}$$

Time development of operator is given by

$$\frac{d\hat{F}}{dt} = \frac{\partial\hat{F}}{\partial t} + \frac{2\pi i}{h}\,[\hat{H},\hat{F}]$$

Time- Dependent Schrodinger Wave equation

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t)$$

Total E term | K.E. term | P.E.term

$$\Psi(x,t) = e^{-iEt/\hbar}\psi(x)$$

Time-Independent Schrodinger Wave Equation

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

Quantum theory is based on two constructs: wave .functions and operators

The state of the system is represented by its waves function, observables are represented by operators. Mathematically, wave functions satisfy the defining conditions for abstract vectors, and operators act .on them as linear transformation

So the natural language of quantum mechanics is . linear algebra

Vectors in an n-dimension space

we want to generalize precedent ◘ concepts to n-dimension real space

: Orthonormal basis •

A vector a can be expressed in this Orthonormal basis as

$$\vec{a} = \sum_{i=1}^{n} \vec{a}_i \vec{e}_i$$

:Inner Product •

$$(\vec{a},\vec{b}) = \sum_{i=1}^{n} a_i b_i$$

If the vectors are complex, then

$$(\vec{a},\vec{b}) = \sum_{i=1}^{n} a_i^* b_i$$

We observe that for any vector

$$(\vec{a},\vec{a}) = \sum_{i=1}^{n} a_i^* a_i = \sum_{i=1}^{n} |a_i|^2$$

Inner Product

If we have two vectors•

, $\vec{a} = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$ $\vec{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$

Then, the scalar product or inner product is defined by

$$(\vec{a},\vec{b}) = \sum_{i=1}^{3} a_i b_i$$

Orthogonal and orthonormal basis

A basis $\{u_i\}$ is said to be orthogonal if •

$$(\vec{a},\vec{b}) = 0$$

.Where a, b any two vectors in a basis

A basis $\{u_i\}$ is said to be orthonormal if•

$$(a_i, a_j) = \delta_{ij} \qquad i, j = 1, 2, \ldots$$

$$\delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

- The set of vectors $\{\vec{a}_1, \ldots \vec{a}_n\}$ is **linearly independent** if

$$c_1\vec{a}_1 + \ldots + c_n\vec{a}_n = 0$$

can only be satisfied when

$$c_1 = c_2 = \ldots = c_n = 0$$

:Inner Product •

$$(\vec{a},\vec{b}) = \sum_{i=1}^{n} a_i b_i$$

If the vectors are complex, then

$$(\vec{a},\vec{b}) = \sum_{i=1}^{n} a_i^* b_i$$

We observe that for any vector

$$(\vec{a},\vec{a}) = \sum_{i=1}^{n} a_i^* a_i = \sum_{i=1}^{n} |a_i|^2$$

The norm or length of a vector a define as ◘

$$N = (a,a)^{1/2}$$

Then a vector whose norm is unity is said ◘

. to be **normalized**

$$(\vec{a},\vec{a}) = \sum_{i=1}^{n} a_i^* a_i = \sum_{i=1}^{n} |a_i|^2 = 1$$

Linear Dependence and Independence

The set of vectors $\{\vec{a}_1, \ldots \vec{a}_n\}$ in a vector space V is said to be **linearly dependent** if there exist scalars $c_1, c_2, \ldots, c_n$, not all zero, such that

$$c_1\vec{a}_1 + \ldots + c_n\vec{a}_n = 0$$

- The set of vectors $\{\vec{a}_1, \ldots \vec{a}_n\}$ is **linearly independent** if

$$c_1\vec{a}_1 + \ldots + c_n\vec{a}_n = 0$$

can only be satisfied when

$$c_1 = c_2 = \ldots = c_n = 0$$

Hilbert Space

- In quantum mechanics , very often we deal with complex function and the corresponding function space is called .the Hilbert Space
- the Hilbert Space is a complete linear .vector space with an inner product

an example of Hilbert Space is $L^2(R)$, the space of square-integrable functions $f(x)$ on the real line. Here the inner product :is define by

$$(f,g)=\int_{-\infty}^{\infty} dx f^*(x)g(x),$$

Orthogonal functions

The important definitions regarding .Orthogonal functions

The Inner Product of two functions ◘ F(X) and G(X) define in the interval $a \leq x \leq b$ denoted as (F,G) OR (F |G), is

$$(F,G) = \int_a^b F^*(x)G(x)dx$$

These functions are **Orthogonal** if:

$$(F,G) = \int_a^b F^*(x)G(x)dx$$

A function is **normalized** if its norm is: unity

$$(F,F)^{1/2} = \left[\int_a^b |F(x)|^2 dx\right]^{1/2} = 1$$

These functions are **Orthogonal** if

$$(F,G) = \int_a^b F^*(x)G(x)dx$$

A function is **normalized** if its norm is unity:

$$(F,F)^{1/2} = \left[\int_a^b |F(x)|^2 dx\right]^{1/2} = 1$$

Functions that are Orthogonal and normalized are called orthonormal .Functions

$$(F_i, F_j) = \delta_{ij}, i = j = 1, 2, \ldots$$

A set of functions $F_1(X), F_2(X)$ is linearly dependent if

$$\sum c_i F_i(x) = 0$$

Where ci are not all zero. Otherwise they are linearly independent

The expansion theorem

Any function $\phi(x)$ defined in the same interval can be expanded in terms of the set of linearly-independent functions as

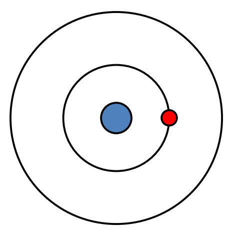
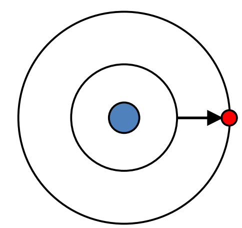
$$\phi(x) = \sum_i c_i F_i(x)$$

Then, the coefficients are given by

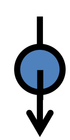
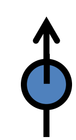
$$c_i = (F_i, \phi)$$

Qubits

- Qubit is the unit of quantum information.
- A qubit is any quantum system with exactly **two** degrees of freedom; we use them to represent binary ‘0’ and ‘1’
- Hydrogen atom:

Ground state:  **Excited state:** 

- Spin-1/2 electron:

Spin-down (-ħ/2) state:  **Spin-up (+ħ/2) state:** 

- The state of a quantum system is described by a **state vector**, written $|\psi\rangle$
- If the basis states for a qubit are written $|0\rangle$ and $|1\rangle$, then the state vector for the qubit is

$$|\psi\rangle = \alpha\,|0\rangle + \beta\,|1\rangle$$

where α and β are complex numbers with

$$\alpha^2 + \beta^2 = 1$$

- A Quantum computer is a computation device that makes direct use of quntum mechanical phenomena, such as: superposition and entanglement, to perform operation on data.

Watch Landmark in quantum computing