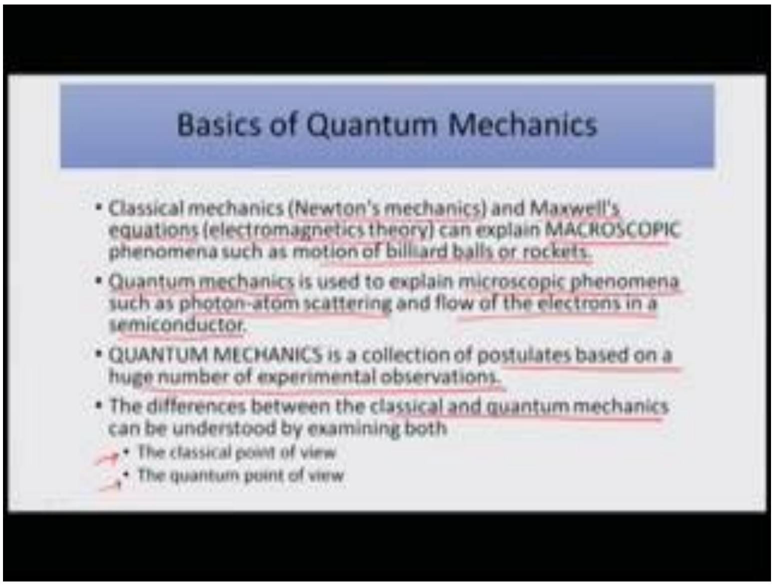
Implementation Aspects of Quantum Computing
Prof. Debabrata Goswami
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture - 11
Basics of Quantum Mechanics

We have been going over the details of quantum computing and the various aspects of bit. And we have also looked at some of the relevant considerations which are required for its implementation. However, one of the basic issues which have come about is that we have not really looked into some of the foundations or the basic aspects of quantum part of this problem.

So, I thought in today's lecture will back a little bit in looking into the Basics of Quantum Mechanics, and take it from there. So, this particular lecture set would be more on the basics of quantum mechanics and looking at some of the aspects related to the quantum phenomena.

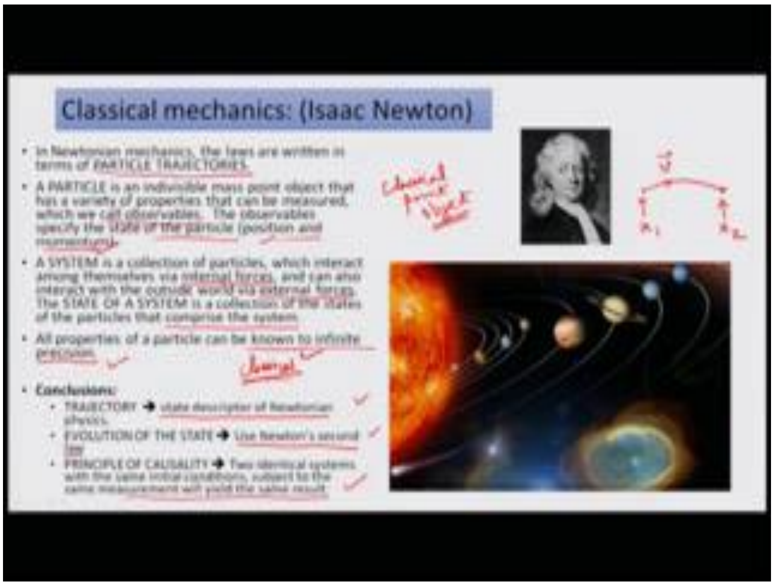
(Refer Slide Time: 01:04)



So, in terms of basics of quantum mechanics we have already realized that it is quite distinct and different from the classical mechanics which we label as the Newton's mechanics or the Newtonian mechanics following the laws of Newton, and Maxwell's equations which are for electromagnetic theory. So, when we consider Newtonian mechanics and Maxwell's equations we can explain macroscopic phenomena such as motion of billiard balls or rockets.

However, when we are looking at microscopic phenomena such as photon-atom is scattering and flow of electrons in a semiconductor or the kinds of discussions where been having until recently which is miniaturization of computing to try to do quantum computing and other things. Quantum mechanics is the main idea. So, quantum mechanics is a collection of postulates based on a huge number of experimental observations. The difference between classical and quantum mechanics can be understood by examining both, the classical point of view as well as the quantum point of view, so let us see.

(Refer Slide Time: 02:30)



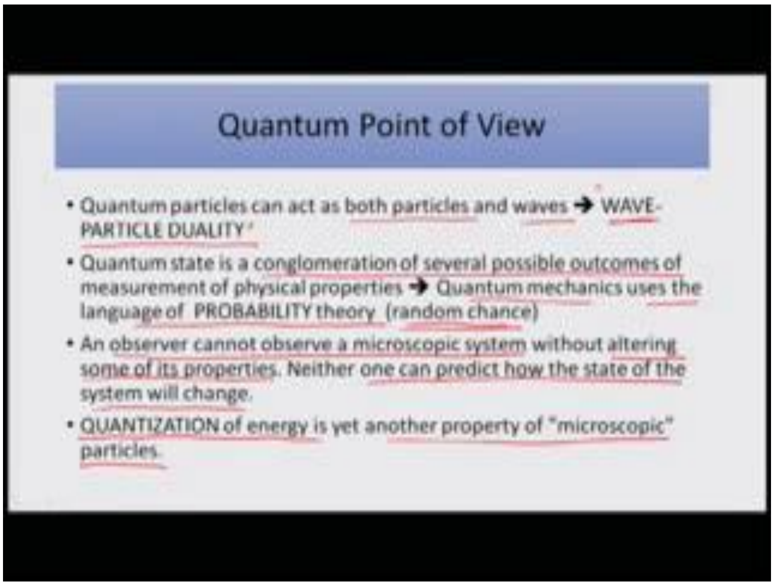
So, the classical point of view the Newtonian one they Isaac Newton's one is the one where the laws are written in terms of particle trajectories. A particle is considered as an in divisible mass point that has a variety of properties that can be measured, all of which we call observables. The observables specify the state of the particle, position and momentum. And here please note that we are mentioning both position and momentum. So, this is what we call the classical particle. And often it is represented in terms of point objects.

Just to make show things simple point objects allow drawing of path between difference points and that is why it is easier to mention in terms of classical point objects, and here both the momentum as well as position. So, these like position x 1, x 2. This is the position as well as this motion associated would be a velocity and so both position and momentum can be specified and this is the classical object point. A system in this concept is a collection of particles which interact among themselves via internal forces and can also interact with the outside world via external forces.

So, the forces are of different kinds; one is the internal force and the other one is the external force. The state of a system is a collection of these states of the particles that comprise the system. All properties of a particle can be known to infinite precision. Now this is the part which is very important in classical mechanics, and we have been used to this principle. So, the conclusions from classical look of how you wanted to state are the trajectory is the state description of Newtonian physics. Evolution of the state is the Newton's second law; the principle of causality is the fact that two identical systems with the same initial conditions subject to the same measurement will yield the same result.

Now, these are the three important aspects of classical concept which give rise to or which we are used to in terms of classical mechanics. So, one of the important applications of classical mechanics we know is always in a astronomical objects, like motion of stars, motion of planets, all of this work quite well, solar system. So, we defined them in terms of systems as well as individual objects. So, this is all what we described in terms of classical.

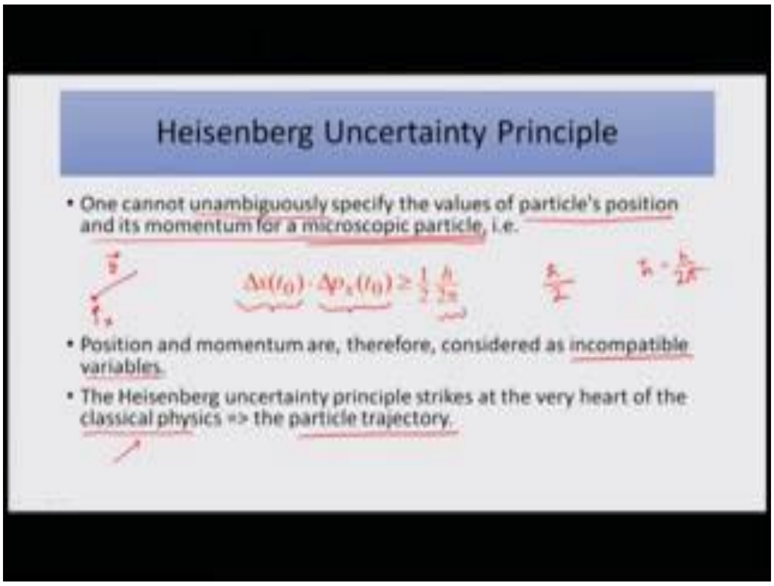
(Refer Slide Time: 05:52)



On the other hand, in terms of quantum point of view quantum particles can act both as particles and waves. So, this is the first very important aspect of quantum mechanics which is it assumes to start with or it has built in wave particle duality. Quantum state is a conglomeration of several possible outcomes of measurement of physical properties, and quantum mechanics uses the language of probability theory. And therefore, a random chance is one of the important aspects that we have to built-in in quantum mechanics.

Another important point here to understand is that the observer in this case cannot observe a microscopic system without altering some of its properties. Neither one can predict how the state of the system will change in terms of absolute precision. And finally, quantization of energy is another property of this microscopic particle which is different from classical system, because in terms of classical mechanics energy can be continuous.

(Refer Slide Time: 07:20)

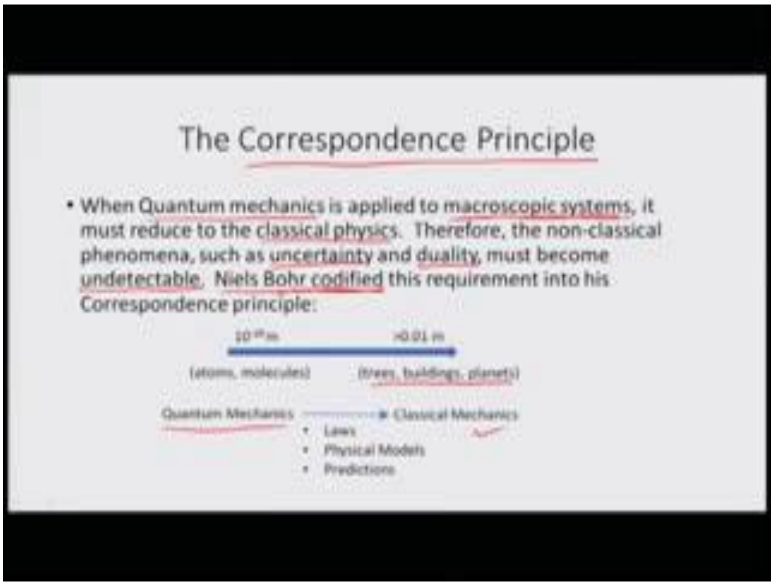


So, one of the most important points mentioned in quantum way of looking at thing is the inability to be certain in measurements and that comes from the famous Heisenberg Uncertainty Principle which says that; one cannot unambiguously specify the values of particle's position and its momentum for a microscopic particle. And this is so different from the classical point of view.

So, this gives rise to the fact that there is always some error in measurement, at any point of time the measurement is being made. So, any measurement which is made will have some error associated with it either in space or in momentum and that product is always going to be act best equal to h cross which we know as h crosses h over 2 pi, which I clarify here. At best it is going to be h cross over 2 or more than that. Position and momentum are therefore considered as incompatible variables or in other words these are the ones which cannot be measured with absolute precision simultaneously.

The Heisenberg uncertainty principle strikes at the very heart of classical physics the particle trajectory, because if we cannot ascertain position and momentum simultaneously the entire picture of trying to draw a particles motion becomes difficult because neither the position nor the momentum can be certain to absolute precision. And that is the reason this becomes one of the biggest problems for classical physics or classical mechanics that is the Heisenberg Uncertainty Principle.

(Refer Slide Time: 09:38)

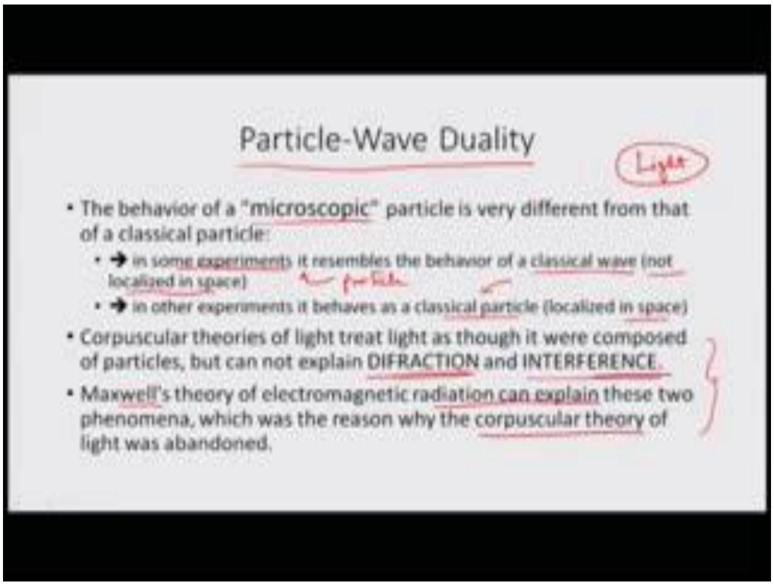


So, how do we apprehend this? In order to make sure that quantum mechanics can still be applied to macroscopic principle where is something which is sort of like known as the Correspondence principle; the idea being that quantum mechanics when applied to macroscopic systems it must reduce to the classical laws or must reduce to the case which the classical physics predicts. And therefore, the non classical phenomena such as uncertainty and duality must become undetectable. Niels Bohr codified this requirement into his Correspondence principle when he postulated his way of looking at quantum mechanics.

Now, Bohr’s theory is something which is still considered as the old quantum mechanics. What we will now look at is how things have evolved. Now for him it was necessary to code this because he wanted the correspondent principle of looking at quantum mechanics or applying quantum mechanics to macroscopic systems. So, that is one wave of looking at it, but there are now the system the ideas have evolved to a wave that it need not be coded it comes automatically the wave the mathematics is done.

So, in principle we have the situation that when we are in the atoms and molecule range in size 10 to the power minus 10 or in that order then we are definitely in this quantum mechanics domain. And when we are in macroscopic domains when we are talking in terms of earth the trees buildings planets for example, then we are all in this classical mechanics principle. And there are laws to connect them, and there are physical models which can lead us to the predictions that we talk about in both these domains.

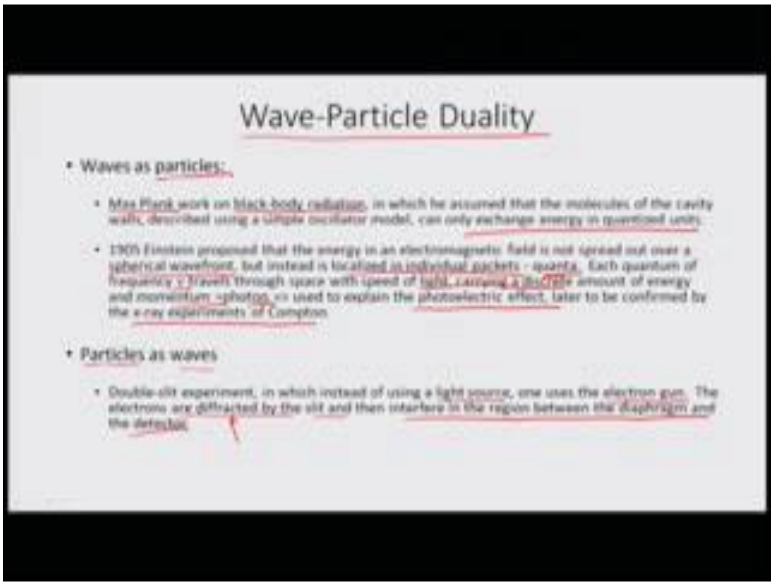
(Refer Slide Time: 11:44)



So, the wave particle duality which is the other main aspect of quantum mechanics gives rise to the very different behavior of microscopic particles from that of classical particles. In a sense in some experiments we have a situation where the behavior of classical wave is shown by particles, so the particle shows resembles the behavior of classical wave that is it is not localized in space. In other experiments the particle behaves like a classical particle localized in space. So, in some sense it is showing a duality between the particle and the wave like picture. Corpuscular theories of light treat light as though it were composed of particles, but cannot explain diffraction and interference.

On the other hand Maxwell's theory of electromagnetic radiation can explain diffraction and interference phenomena, and that was the reason why corpuscular theory was abandoned earlier. So, this is from earlier times. In quantum mechanics we are apprehensive of the fact that both can coexist and that is the reason why the property of light used to have both wave like in terms of Maxwell's phenomena or particle like as for as the corpuscular theory.

(Refer Slide Time: 13:42)



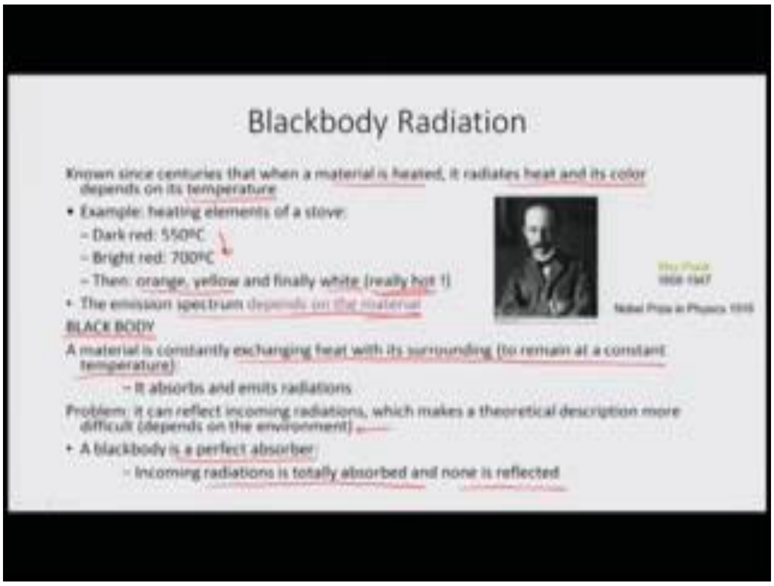
So, in terms of wave particle duality we have specific examples where waves as particles exist Max Planck work on black body radiation in which he assumed that the molecules of the cavity walls described using simple oscillator model can only exchange energy in quantized units. So, that was one place where Max Planck introduced the concept when he used to study the black body radiation.

So, this is the case when particle nature was used. In 1905 Einstein proposed that energy of an electromagnetic field is not spread out over the entire wave front, but localized in individual packets or quanta. Each quantum of frequency new travel through space with speed of light carrying discrete amounts of energy and momentum, which are known as photons which are needs to explain the photoelectric effect. And this was later on confirmed through x-ray experiments of Compton.

So, these are the two cases where for example we have waves to be treated as particles; black body radiation and photo electric effect. Similarly, for particles as wave we have double slit experiments where instead of using a light source if one uses an electro gun; the electrons are diffracted by slit and then interfere in the region between the diaphragm and the detector to give rise to the same kind of pattern which looks like the case of interfering waves.

So, the principle of diffraction and interference are shown by electrons. And therefore, electron particles behave as wave under these conditions.

(Refer Slide Time: 15:56)

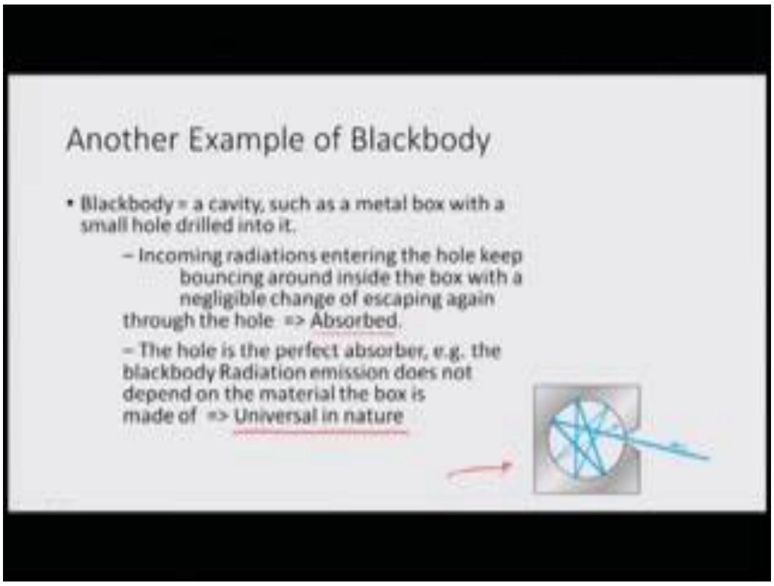


So, little bit more on Blackbody Radiation because this was one of the first important points which gave rise to the idea of quantum mechanics; if this kind of radiation has been known since centuries, since whenever a material is radiated. This kind of radiation has been known for centuries since when a material is heated it radiates heat and its color depends on its temperature. For example, heating elements of a stove turned from dark red to bright red when the temperature goes from 550 degree centigrade to 700 degree centigrade. And it can even further go in to orange and yellow, and finally white when the temperature goes really hot.

So, depending on the temperature the radiation and its color changes, so the emission spectrum as we call it as a result of this change depends on the material heating as well as on the material property. Blackbody is defined as a material that is constantly exchanging heat with its surroundings to remain at a constant temperature. It observes and emits radiation. The problem is it can reflect incoming radiations which makes a theoretical description much more difficult depending on the environment and so on and so forth.

However, a blackbody is a perfect absorber incoming radiations are totally absorbed and none is reflected. So, that is the ideal definition of blackbody.

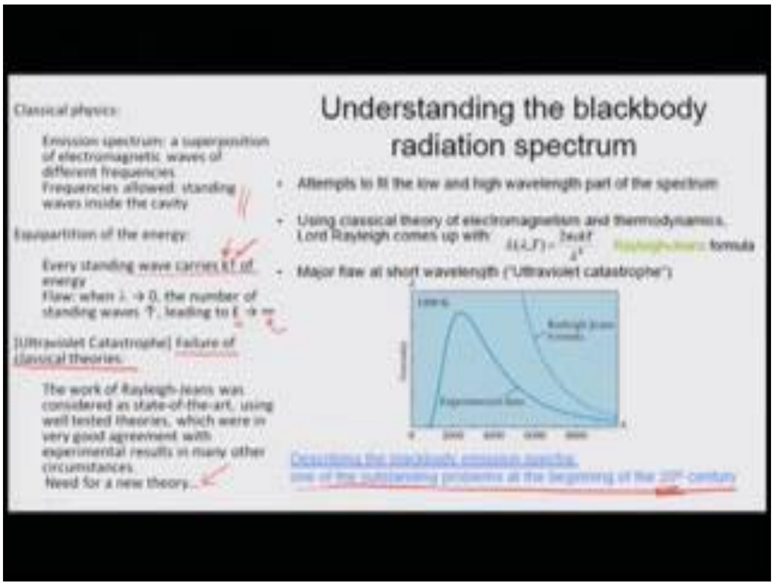
(Refer Slide Time: 17:45)



Another example of blackbody can be something like a cavity which is someone shown here, such that a metal box with a small hold drilled in it the incoming radiation enters the hole keep bouncing around inside the box with negligible change of escaping again through the hole, that means it gets absorbed completely.

The hole is the perfect absorber for example, blackbody radiation emission does not depend on the material the box is made of; this is generally universal in nature. So, there are many ways blackbody and blackbody radiations can be designed and can be checked and it has been there for several. This concept has been around for very long.

(Refer Slide Time: 18:31)

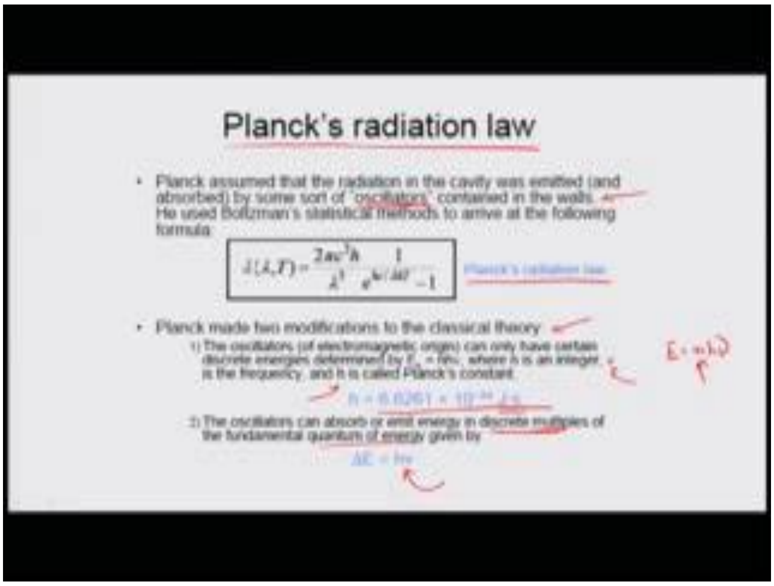


However, the difficulty this principle faced and it was labeled as one of the outstanding problems at beginning of the 20th Century was to describe the blackbody emission spectra. It was difficult because classical physical principles could not quite explain what was going on here. So, when an attempt to fit the low and the high wave length part of this spectrum was tried simultaneously, the theory always failed. The theory worked quite well for the high temperature zone, but it always had a problem when it was trying to fit both low and high wave length part of the spectrum.

That is because as per classical physics emission spectrum is a super position of electromagnetic waves of different frequencies, and the frequencies allowed where the standing waves inside the cavity. Again the equipartition of energy would give rise to the fact that every standing wave carries k t of energy, Boltzmann constant and temperature t of the energy. The flaw is in this approach that when the wave length is approaching 0 the number of standing waves keeps on increasing leading to an energy which goes to infinity. And that is why almost all the laws sort of show the theory in terms of classical physics showed that the energy keeps on increasing as the wave length goes lower.

This came to be known as the ultra of highlight catastrophe, and that led to the failure of the classical theories. One of the most celebrated work in this the work of Rayleigh Jeans was considered as state of the art using well tested theories which have very good agreement with many experimental results in many other circumstances. And even in this case wave length part was well explained only when the wavelengths went to lower numbers it failed. Thus, there was a need of a new theory.

(Refer Slide Time: 20:48)

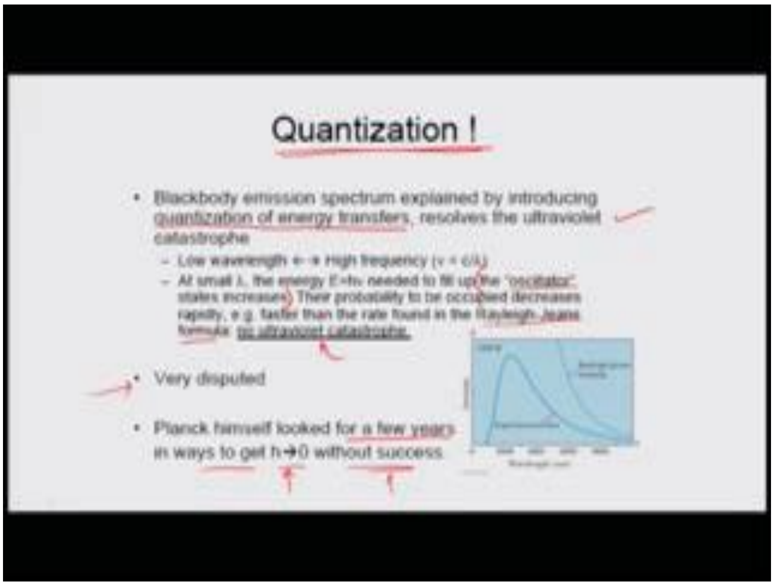


So when Planck looked at this problem, he was also an expert in thermo dynamics, he assumed that the radiation of the cavity was emitted and observed by some sort of oscillators contained in the walls, and this concept is something which he introduce. He uses the Boltzmann statistical methods to arrive at the formula which is the Planck's radiation law.

Now, Planck made two modifications to the classical theory in coming to this form. The oscillators of electromagnetic origin can only have certain discrete energies determined by e equal to h nu n h nu; where n is an integer, nu is the frequency, and h is call the Planck's constant which was given by a number which was very small 6.6 times 10 to power minus 34, however with the units of joule second.

When there the oscillators can absorb or emit energy in discrete multiples of the fundamental quantum of energy given by delta e equals h nu. And that was one of the most important points of the Planck's radiation law which showed that energy was in packets.

(Refer Slide Time: 22:24)

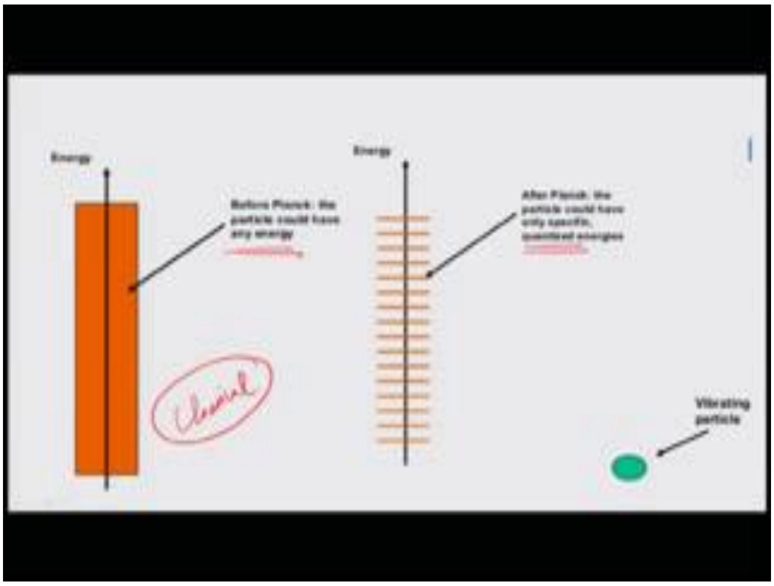


So, this gives rise to the principle of quantization. Blackboard emission spectrum explain by introducing quantization of energy transfers resolved the ultraviolet catastrophe. So, that was one of the most important contributions at that time in this filed by Max Planck. Even at low wave lengths and at high frequencies this particular theory worked. At small wave length the energy h nu needed to fill up the oscillator states the probability of the occupied oscillators decrease rapidly, that is faster than the rate found in the Rayleigh Jeans formula so no ultra violet catastrophe happened.

So, at small lambda the energy h nu needs to fill up, the oscillators straights increase their probability to be occupied then decreases rapidly. For example, faster than the rate in the Rayleigh Jeans formula, so no ultra violet catastrophe happens. However, it became very highly disputed. Planck himself looked for a few years find whether h could be made to go to 0; the Planck constant without any success.

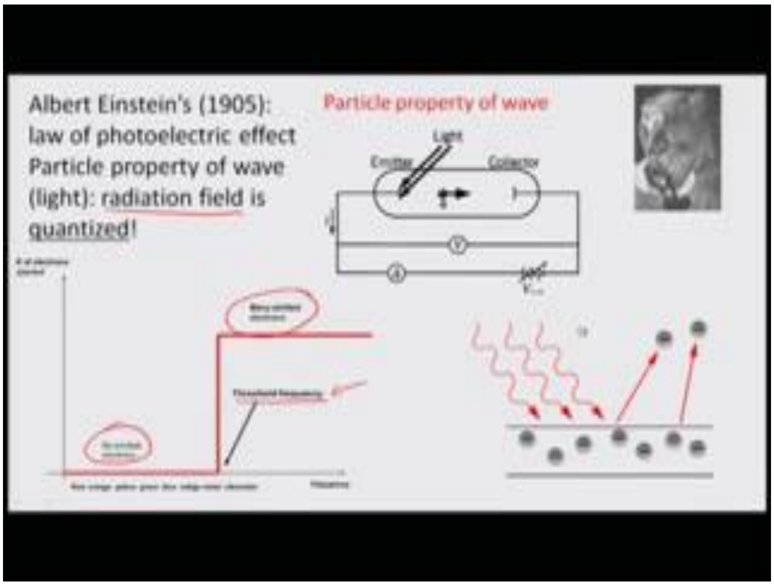
So, that was the basic principle behind quantization where even Planck who discovered it had difficulty in apprehended.

(Refer Slide Time: 23:59)



So, as a result of Planck's law the energy which is the classical one continuous, any energy could be there became discrete. The particle could have only specific quantized energies and this was in conjunction with idea that there was some sort of oscillating vibrating particle inside this entire picture which was being shown to think in terms of blackbody radiation.

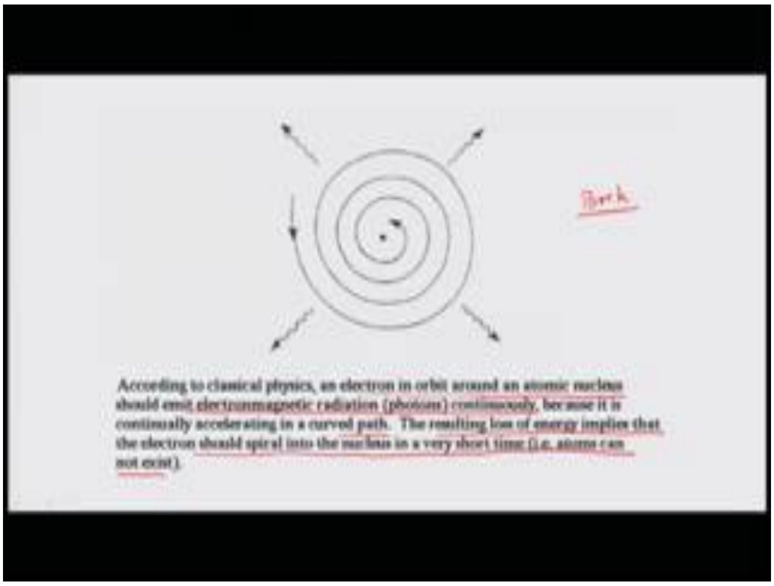
(Refer Slide Time: 24:34)



After this Einstein in 1905 found out that the same principle of quantization was necessary when he was studying the photoelectric effect. What he found that, his law required that the radiation field be quantized; his observations where that, when the light fell on the emitter and photo electrons where being generated which showed as a potential in the circuit there was a threshold frequency until which there were no emitted electrons.

However, once a threshold was reached many emitted electrons came out. So, essentially there was a threshold in terms of the energy which was necessary for the electrons to come out showing that it had a particle property rather than a continuous property. So, this threshold frequency or the threshold energy gave rise to the idea of quantization again.

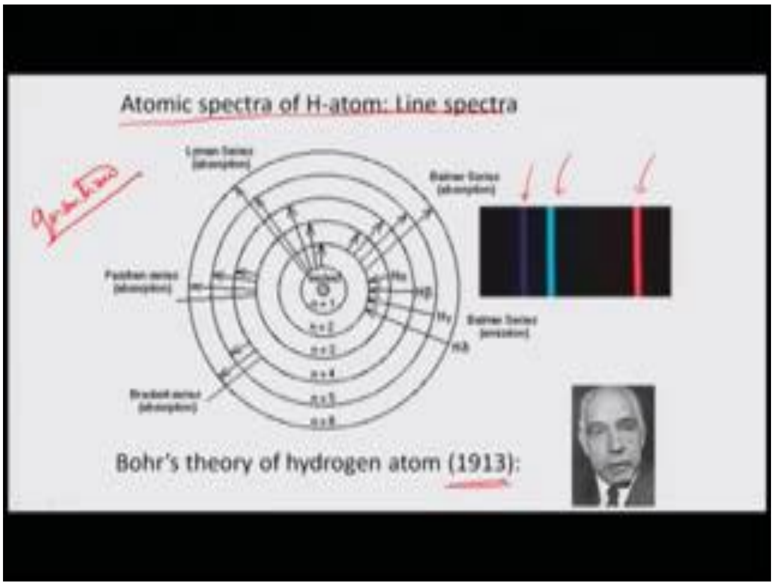
(Refer Slide Time: 25:52)



This led to the other part which was creating a problem in terms of classical mechanics to look at an atom. In terms of classical mechanics an electron in orbit around an atomic nucleolus should emit electromagnetic radiation or photons continuously as per Maxwell equation, because it is continuously accelerating in curved part. The resulting laws in energy imply that the electron should spiral into the nucleolus in a very short time; that is an atom cannot exist.

So, this was one of the issues which the Bohr model was able to handle, because once this concept of classical nature of radiation being emitted at any energy was possible to be looked at differently, he was able to come up with the first quantized atom picture.

(Refer Slide Time: 26:57)



And that immediately explained the atomic spectra of the hydrogen atom the line spectra and all that. So, his theory in 1913 was the one where these energies of these electrons around the nucleolus were considered as quantized so that the transition of an electron could only happen at discrete intervals, and so only discrete line spectra which was always observed was immediately explainable because of this principle. So, the atomic spectra of the hydrogen atom line spectra became understood from this picture introduced by Bohr.

And so that is the first Bohr's theory on the hydrogen atom in terms of quantized aspect which was given. So, will get more into quantum mechanics after this lecture in the next one because we have just come to the point where the first Bohr's model of quantization and the old quantum mechanics as we call it is justified by using the principle of packets or discrete energies which was obvious from the previous experiments and ideas which were necessary to explain this kind of observations that we are observing.

So, both Max Planck and Einstein quantization principle of very small energy packets which were given based on the Planck's constant were being utilized to give rise to this principle of quantum mechanics, more on this in the next lecture.