Introductory Quantum Mechanics and Spectroscopy
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Lecture - 1
Chemistry I – CY1001

Welcome to this course. The first part of this course in Chemistry, which is introductory, is on Atomic Structure and Spectroscopy. What we would do in the limited period, of this six to eight weeks, is to introduce the Basic Theory and Methods which are used to understand atomic and molecular structure, and also to explain what we see in the experiments, namely in a spectroscopy. Spectroscopy is the interaction of radiation with matter; and also provides the experimental tool and verification for all the things that we have understood so far in molecular and atomic quantum mechanics.

Being an introductory course meant for the first or second year students entering the college, I would keep the mathematics to a reasonably low level. However, I do not want to make any approximate statements, as far as possible; I want to make the statements as quantitatively as I can. There are, obviously, exercises and assignments for you to practice that. Then you can have this also discussed with your teachers in class, in some sort of a reversed class mode to have the teachers interact with you and solve problems for you. The only way to learn this subject is by solving as many problems; that is, by learning by doing. I would very strongly recommend that you solve every problem that is proposed in this lecture series, every assignment that is given, and also every in-class exercise, which is provided along with the lectures.

The first introduction to quantum mechanics is something that needs a little bit of elaboration as to why it is important. Almost at the turn of the last century - to be precise, 1900 - Max Planck came up with the hypothesis that energy emitted or absorbed by the material bodies does not happen in a continuous fashion, but that it is emitted in packets - quantas.

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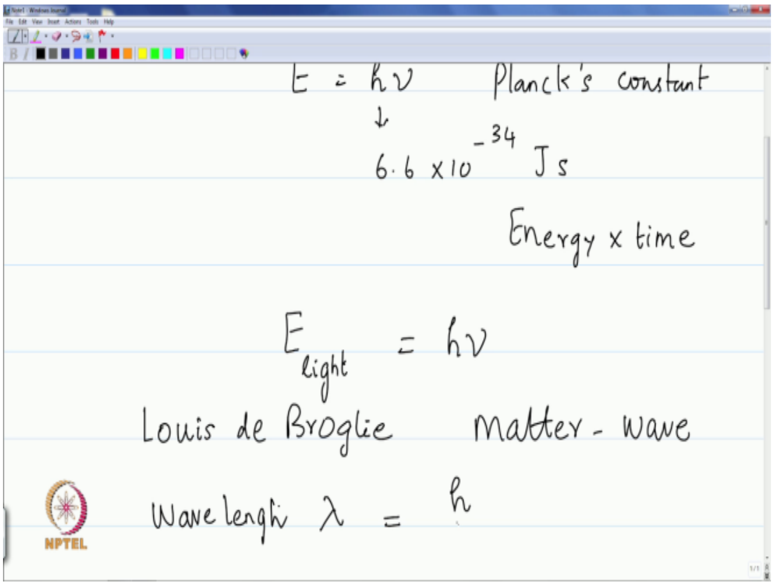

He came up with this famous formula for energy in terms of quantas and in terms of the frequency of light that gets emitted, by the formula, E is equal to h nu; where, nu is the frequency of the radiation that gets emitted or that radiation that gets absorbed by the material bodies. He introduced a constant, which was not known until then, and called this as the Planck's constant - he did not call it, all the others did, since it was his fundamental contribution.

He proposed the values somewhere around 6 point 6 into 10 raised to minus 34 Joule second. Since this is energy, and the frequency is per second, the dimension of the constant - the Planck's constant - is energy into time. There are other ways of decomposing these dimensions, but after Planck introduced this, it was not something that everybody accepted it as is - they thought that with his prescription of the discretization of the transaction of energy by the material bodies, he could explain, at that point of time, very satisfactorily what was known as the Black Body Radiation Phenomenon, which could not be explained by any classical mechanical methods.

Just about five years later, it was Albert Einstein who threw in the next tantrum, if I may say so, to the whole field of physics with his hypothesis or his proposition that light itself consisted of packets of energy. If you recall elementary physics, Newton many, many years ago - I mean hundreds of years ago - proposed that light consists of corpuscles or particles - particulate; that was disputed later by Huygens and many others through the experiments of diffraction, interference, and many well established physical experiments. They proposed that light had to be a wave. Later, the fact that light was a wave was further generalized by Maxwell through his theory of electromagnetic radiation, in which he considered light to be part of the general field called the electromagnetic radiation, in which electric and magnetic fields oscillate in time.

So, the property that light is a wave was well established for more than 200 years; but then, Einstein, in explaining the photoelectric effect of the emission of electrons by metals - when light falls on the metals - he came up with this proposal that light itself consists of packets of energy, and he used exactly the same formula that Planck had; except that now I will put the as subscript light. The packet of energy also is given by this formula that h nu, where h was the Planck's constant, which was introduced by Max Planck five years before that; and nu is the frequency of light.

So, there was this difficulty: how can light be both wave and particle? This discussion continued for some time. It was Louis de Broglie, who added some more light into this whole process of description; namely, that all material particles, which are in motion, can be ascribed with a wavelength in addition to a momentum which involves the mass, and the mass is, of course, localized; therefore, all material particles which are localized while they are travelling, while they are moving, can be associated with a wavelength. He called it as the matter wave; in this process, he introduced the wavelength lambda to be again involving the Planck's constant.

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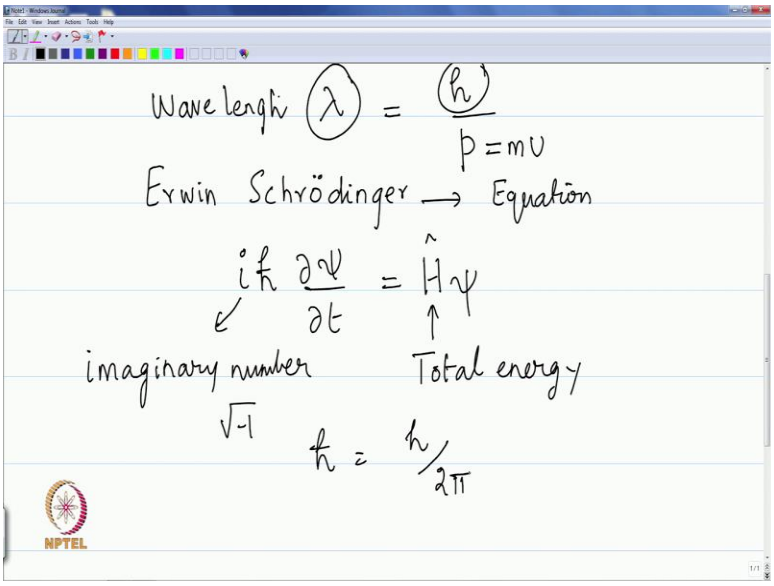

The momentum of the particle, this is for particle which travels not with the speed of light, but much less than the speed of light, which you can write as the mass times the velocity; so, here is again the Planck's constant. This idea that particles in motion can actually be associated with a wavelength, now brought into question by someone who would contribute to the most fundamental equation of matter for the next 100 years - by Erwin Schrödinger. Schrödinger asked himself the question: what the dynamical equations, governing such matter waves would be? Why this question? Because Newton and many others had described the planetary motion, and the motion of macroscopic particles through their equations of motion, the dynamics in time - that is how things change in time; that dynamics was well known through Newton's equation of motion.

Then, the dynamics of electromagnetic radiation; I mean the properties of electromagnetic radiation were, obviously, described by Maxwell known as the Theory of Classical Electromagnetism. So, there were theories for the time evolution of waves, and the time evolution of particles, but things which behave particle and wave like, is there a separate dynamical equation that will govern their evolution in time. Schrödinger came up with a proposal and an answer, which became the most famous equation of the last century called the Schrödinger equation and I will write that out.

The Schrödinger equation comes up with a function psi, which is a function of time, and a quantity called the Hamiltonian or the total energy of the system, and it involves the imaginary number - square root of minus one - and h bar is again Planck's constant, h, divided by 2 pi. Schrödinger proposed this equation as the equation that the matter waves would satisfy and he proposed the function psi as a property of the system. Since it is the property which describes how the system evolves in time, psi itself is a function of time.

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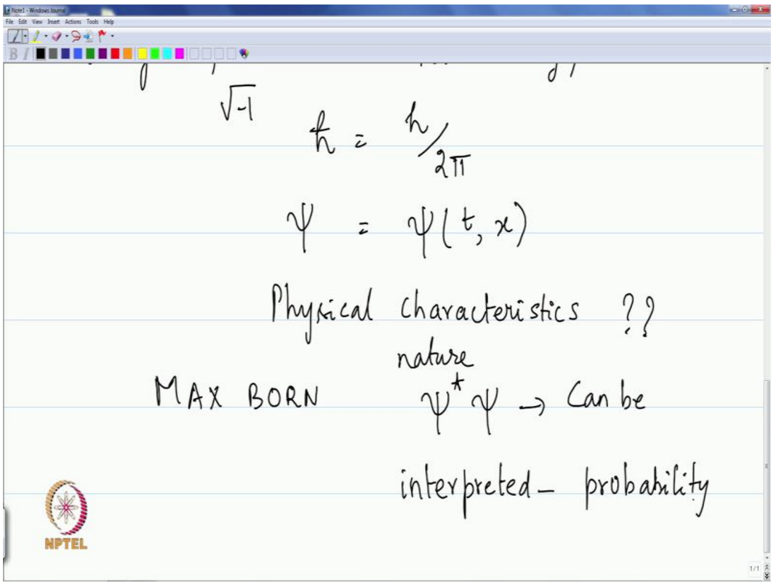

But in addition to time, it is also a function of the position or the momentum, but not both. The x here represents position in one dimension or one-dimensional motion, but if the motion happens in three dimensions it is a function of all the three positional coordinates of that system or the particle, but it is also a function of time. Schrödinger proposes wave function, and then, when the question was asked - what does this wave function mean - even he had difficulty explaining the physical property or the physical characteristics of the wave function or nature - what is it? In fact, Schrödinger made a mistake; his interpretation was proved to be wrong.

Later, it was Professor Max Born who came up with the correct interpretation that most of us accept today - that it is not the wave function which is important, given that this equation is an equation containing - you see this particular one that you have here; let me highlight it. This particular equation, which has the total energy on one side and it has a wave function on the other side, but it also contains the imaginary number; therefore, it is possible that wave function psi itself is imaginary or complex. And if it is complex, then we do not have a physical interpretation for the wave function itself, but it was Max Born who said it is not the wave function psi, but it is the complex conjugate times the wave function itself - the product - that can be interpreted through probability statements. It is associated with the probability of something. We will see all of this in this whole course, the entire course. In the entire course, it would be nice for me to actually solve the time dependent equation, but I am not going to.

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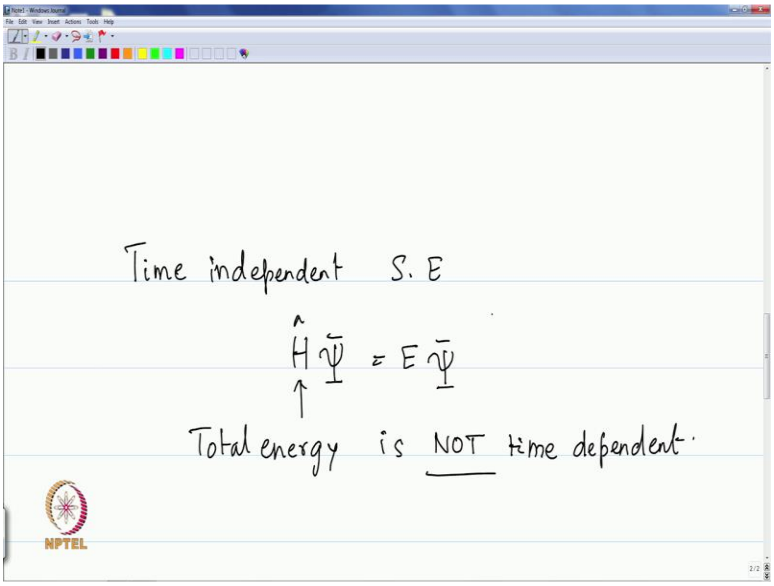

I would limit myself to a much smaller subset of the Schrödinger equation, known as the Time independent Schrödinger equation, which is given by the symbol H. Let me write it with a different wave function psi capital, as a constant times psi, and this is time independent, in the sense that the Hamiltonian or the total energy associated with that system is not time dependent or it is time independent.

If radiation interacts with matter for a brief time, as we do in spectroscopy, during the interaction period, the system, total energy is dependent on time, because the radiation itself is an oscillating electric and magnetic field in some approximation, in the wave approximation. Therefore, the Hamiltonian, can in principle be dependent on time or we may introduce a force for a short period, a changing force; therefore, the Hamiltonian which represents the total energy of the system may actually depend on time, but we will not consider those cases, we will consider those problems in this particular course, in the short eight weeks or ten weeks period, we would study only the time independent Schrödinger equation.

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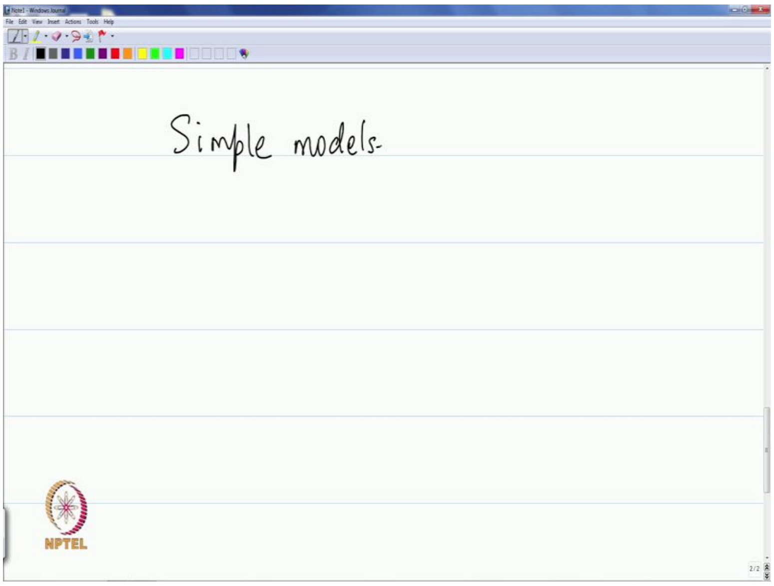

This would be done with simple model problems in the entire course; and these models will later be associated with the chemical systems in order to give you the feel for why chemists are interested in it.

I welcome you all to this course, and I hope that you will enjoy the learning process in the next eight weeks or so, but please do answer all the assignments; please do attempt all the assignments; please do answer all the questions which are discussed either in your class related to the subject or given to you for your own attempt. Without solving those problems, you will not even be able to appreciate what all of this is about and I wish you all the best. We will continue that in the next lecture.

Thank you.