Symmetry and Group Theory

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Lecture -57
Introduction to Spectroscopy Part - I

So, in this week of lectures we will be discussing the last of the applications which is application of group theory to spectroscopy.

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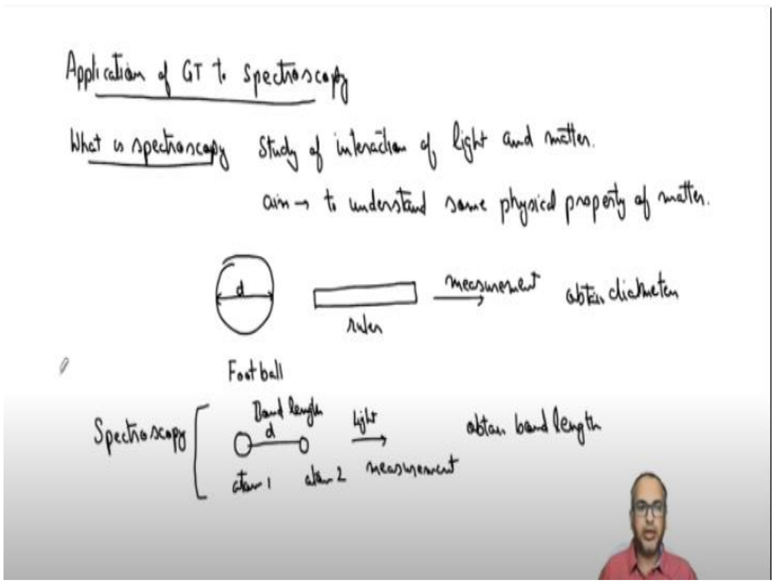

So, before we discuss these applications, let us give a brief overview on what is spectroscopy? Because some of you might not have actually gone through this course of spectroscopy by now. So, let us first discuss. So, what is spectroscopy? Spectroscopy is the study of interaction of light and matter. Now what is the aim here? Why do we study this? Our aim is to determine or to understand some physical property of matter.

Now what is that matter? What is the physical property? What kind of light we are going to use? All of this dictates what kind of spectroscopy we are going to be using. So, let us see, for example let us say if you have a classical object let us say a football, a football is there. But let us say you have a football and you want to determine the diameter of this. So, this is diameter.

So, what you do is you will take a typical ruler and do the measurement, and obtain diameter. This is a typical setup when you want to do any kind of measurement in a classical system. Now in case of quantum systems, you cannot really let us say again you have an atom and you have another atom. Atom 1, atom 2 and now you want to let us say you want to measure the distance between the two atoms, or you can also call it if they are connected you can call it as a bond.

So, bond length, you want to determine the bond length. Now you cannot really have a ruler to measure these distances. So, what instead you would do is you would shine some sort of a light and you will do a measurement and, in the process, you will obtain bond length. This is just one example of one physical property. There can be other examples. Now this particular process is study of interaction of light with matter to obtain some physical property is called as spectroscopy.

So, what is spectroscopy is clear. So, now there can be different types of spectroscopy. What do you mean by different types of spectroscopy? So, before we actually go to different types of spectroscopies, let us look at what is light.

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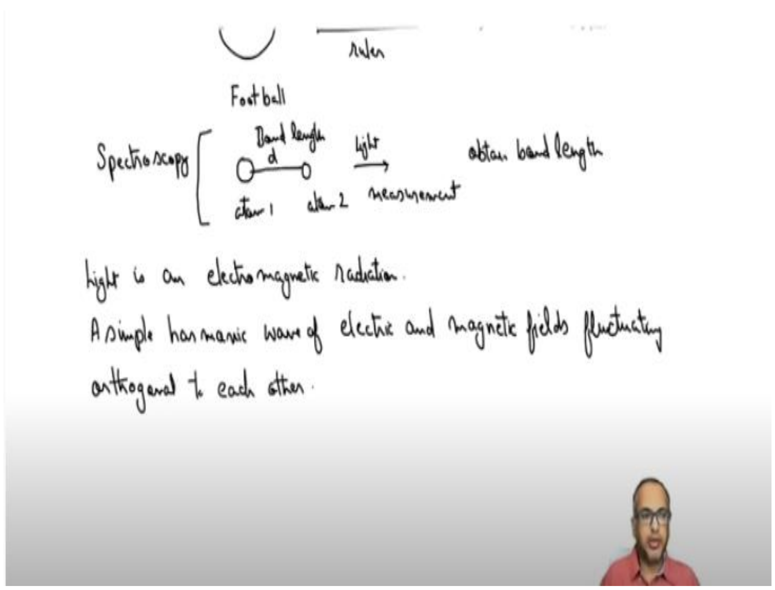

So, light is an electromagnetic radiation. Some of you might know this. So, this will be a little revision for those, but if you do not know just also go through some basic spectroscopy book, it will be beneficial. So, light is an electromagnetic radiation. What do you mean by electromagnetic radiation? So, electromagnetic radiation is a simple harmonic wave of electric and magnetic fields fluctuating orthogonal to each other.

So, there can be different types of lights. But any kind of light, for example, you can have gamma rays, you can have x-rays, you can have IR infrared radiation, radio waves. All of these can be described as a simple harmonic wave of electric and magnetic fields which are fluctuating orthogonal to each other. What do you mean by that?

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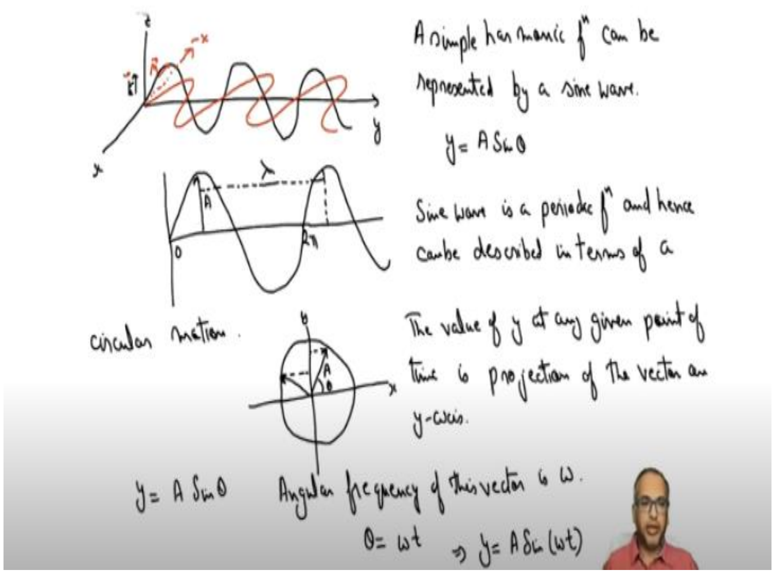

So, let us try to draw a typical wave. So, if my electric component is oscillating in y, z plane, this is my electric field. So, my electric field is oscillating in y, z and then I will draw using another colour which is now vibrating in x, y plane something like this. So, now this is in x, y plane. This is my magnitude along the x axis will be the magnetic field. This is electric field, this is magnetic field. Now these two are orthogonal to each other and these two are drawn in phase.

So, you have electric and magnetic fields fluctuating orthogonal to each other. Now this overall is called as light. So, this is a simple harmonic wave. So, how else you can mathematically what you can say is, you can say a simple harmonic, see because it is a function so you can always describe it mathematically. So, a simple harmonic function can be represented by a sine wave. So, let us say if you have y is equal to you can describe as A sine theta.

Now you can also describe this function as a circular motion. So, let us first draw this as a wave and look at what is A, what is theta, what are different characteristics of a wave? So, if you have a simple harmonic sine wave, the maximum amplitude here is A and this will be the wavelength which is described by lambda and this is 0, this is 2 pi. So, this is how a typical wave can be described. Now sine wave is a periodic function that means which repeats itself.

So, if you see that this function actually is repeating itself after a finite interval of time. So, that is why it is called a periodic function. So, periodic function and hence can be described in terms of a circular motion. So, how do you describe it in circular motion? So, you can also draw this as let us say if you have only x and y coordinate systems. So, you draw a circle around here. Again it is not a very good drawing and if I draw a vector like this with the length A and this angle as theta.

So, I can say that the value of y at any given point let us say that this vector is actually rotating along this circle. So, this is the angle theta and the radius of the circle is A. So, now the vector is doing circular motion. So, the value of y at any given point of time is the projection of the vector on y axis. So, if you draw a projection of this vector onto y axis this length will be the value of y at any given point.

So, let us say the vector at some point is let us say here then the projection will be this length. If the vector is here the projection will be this length. So, this projection will keep on changing. So, how this will keep on changing? So, this will be changing with this relation. So, y is equal to A times sine theta which we had written here, which is nothing but projection of this vector A onto y axis.

So, this comes from a simple trigonometry that this particular side of the triangle will be A sine theta. If this is my base this is my hypotenuse then and whatever is the angle then you will get is sine theta. So, this comes from basic trigonometry. Now let us say the angular frequency of this vector that means the speed with which this vector is rotating is omega. So, then you can say that theta is equal to omega t, omega times t.

So, the velocity into time during time t how much this vector has rotated in terms of angle. So, you will get this angle by omega t. So, that is easy to understand. Now you can then describe the wave as y is equal to A sine omega t because theta is your omega t. So, that should be very, very clear.

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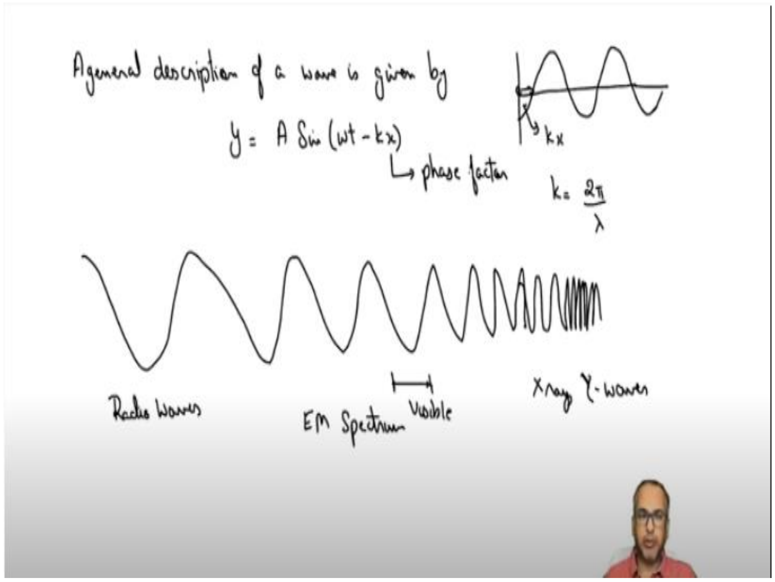

Now in general any wave function or any wave, sorry, a general description, let us say, of a wave is given by y is equal to A sine omega t minus kx, where kx is the phase factor. How do you show it in a diagram? So, if I instead of starting from origin let us say my wave is starting like this. So, it is not perfect the phase is not 0 here. So, then this particular length is given by kx where k is equal to 2 pi by lambda.

So, lambda is the wavelength which is the distance between two crests or two troughs. So, now that should be clear. Now any given wave can be described in terms of wavelength. So, from radio waves, let us say if you draw the electromagnetic spectrum, it looks something like this. So, the far end far left-hand side so this is an electromagnetic spectrum which comprises of all the radiations present in the universe.

So, you have radio waves here and at the far end you have gamma waves or gamma rays, gamma radiation. So, you have x-rays and in between you have visible light and so on. So, you have UV, infrared, microwave, all sorts of things coming in between. Now depending on what kind of information you want from spectroscopy, you shine different types of wavelength onto the material or the matter, and corresponding change in matter is observed and you measure that change. So, you can never measure any absolute property in spectroscopy.

What you have to do is you have to always measure a change in some particular property and from there you draw correlations to understand what is the physical property we are trying to understand. So, what you do here is let us say you are shining radio waves.

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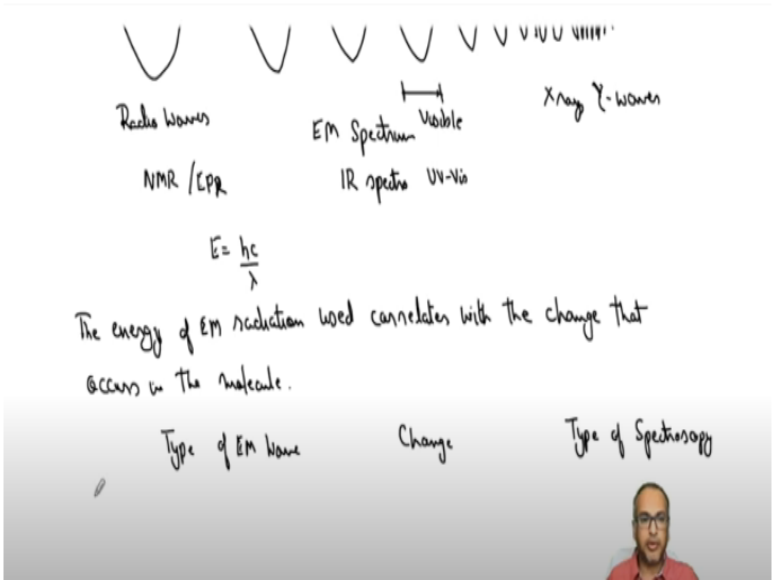

So, you are doing NMR spectroscopy or EPR spectroscopy. So, in some sense here you are doing let us say IR spectroscopy then UV, visible is in this range and so on so forth. So, different types of radiation are associated with different types of energy. Why is that? Because the energy of a wave is equal to hc by lambda so, if the wavelength changes this is Planck's constant, speed of light, the energy of the radiation changes.

If the energy of the radiation will change, it will bring out a different level of change in the subject matter. For example, if you have more energy, you can jump let us say up to the first floor like from ground floor to first floor you require a lot of energy to jump. But if you have only a small amount of energy with you then you will be able to jump only a feet or so. So, it depends on what is the energy available with the radiation which you are shining.

And correspondingly the change will happen in the matter which is under study. So, let us see what do I mean by that. So, let us try to write down a few changes and few types of spectroscopy. So, the energy of electromagnetic radiation used correlates with the change that occurs in the molecule. So, for example let us write down a few types of radiations. So; the type of EM wave, then change, and type of spectroscopy.

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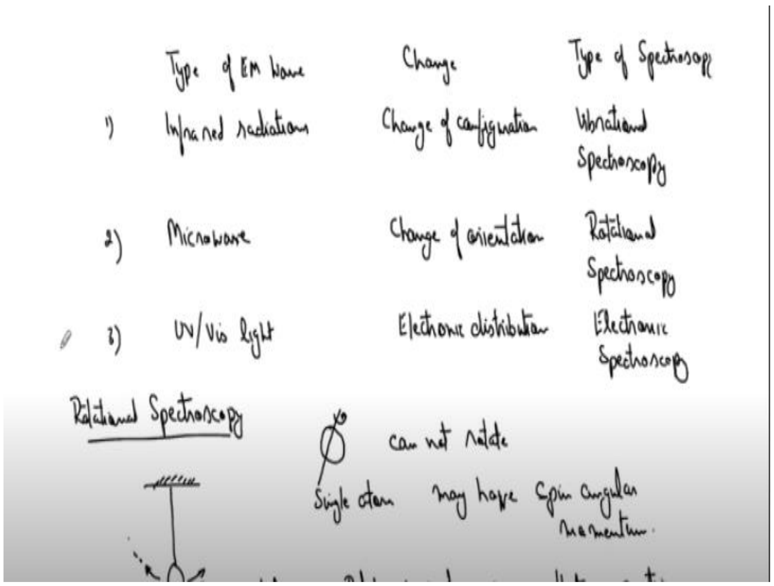

So, first is let us say if we are dealing with infrared radiations. So, infrared radiations are the same radiations that you use on a day-to-day basis in remote controls like with where you control operate TVs and other electronic devices using a remote. So, those are typically infrared. Some of them are also based on wi-fi that is radio waves. But typically, these are infrared radiations. What kind of change they bring out in the molecule?

They change the configuration of the molecule. So, we will come to that in a later class. So, basically it will create a different, it will excite different vibrational levels and the bond vibrations will be affected and hence the configurations will be different. So, this is called vibrational spectroscopy. Now the second is the microwave. Again, you must have all used to microwave in day-to-day life.

So, it is a part of almost everybody's kitchen now, where you excite water molecules and you let the water molecules heat up the food which is kept in here. So, what happens there, there is a change of orientation of the molecule. Because with a microwave what you are doing is you are actually rotating the molecules. So, change of orientation and this is called rotational spectroscopy. So, let us also see UV visible light.

So, again you are also aware of UV visible light. So, you must have I mean visible light everybody is aware of and UV light is also everybody is aware of. What you do here is you change electronic distribution. So, if you change electronic distribution, this is called electronic spectroscopy. So, these are a few examples. So, let us discuss one by one. So, let us start with rotational spectroscopy.

We will discuss a little bit of rotational and then we will go to vibrational spectroscopy and we will see how group theory can be used in all of this. So, application of group theory will not start by today or in the next class, maybe a class after. So, let us start with rotational spectroscopy. What is rotational spectroscopy? So, if you take a single atom let us say you have a single atom. This cannot rotate.

So, you cannot associate rotation with a single point with a single atom. So, let us say if there is an axis and it is spinning about its own axis then the atom may possess, may have spin angular momentum. But there is no rotation as such. This is called spinning motion. So, it has spin angular momentum but no rotation. So, for rotation you would need to tie this up with let us say if you tie this atom up with a thread.

So, this looks like a simple (wrongly written and spoken as bar) pendulum now where you have what you have done is you have suspended a mass a ball of mass m with a thread onto a rigid support. Now this can do oscillatory motions. These kinds of motions this can undergo. Now these oscillatory motions are nothing but if you complete the full circle this will be a rotational motion. So, this is a rotational motion. So, a single atom can undergo rotational motion only if it is tied to a particular rigid end, rotational motion or oscillatory motion.