



Introductory Quantum Chemistry
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Lecture - 2
Standing Waves


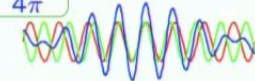
So, in the last lecture, we saw that electrons, neutrons, protons over these microscopic things have a dual nature; they have a particle nature as well as a wave nature. And as you would know, the most important characteristic of a wave is its wave lengths. And for a particle you would obviously say one of the most important things is the momentum. And in fact, a relationship between the wave length, that is associated with the particle and its momentum was adjusted by de Broglie. We will discuss the De Broglie relationship later hopefully.

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De Broglie - Heisenberg

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

de Broglie

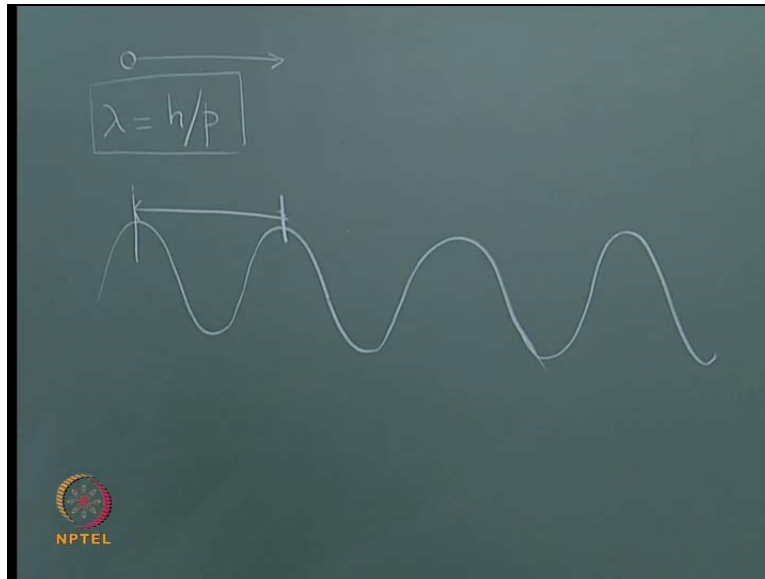
 $\Delta x \Delta p \geq \frac{h}{4\pi}$ 

Heisenberg



But let me just remind you, because you would already be familiar at least a little bit with this. It may remind you what the De Broglie relationship is. According to him, imagine that you have a particle that is moving with a momentum, which we denote as p.

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So, here is the particle; it is moving with a momentum, which I shall denote by the symbol p . Then according to him, you say this particle because of its dual nature, it has a wave nature and wave... There should be a wave length that is associated with the particle. And so if I draw the wave, the wave would be something like this. And when I say the wave length, what is the wave length? The wave length is this distance, is the wave length of the particle. And De Broglie suggested that, the two are related. Wave length – we will denote by the symbol λ . And he suggested that, λ is given by the relationship – it is equal to h by p .

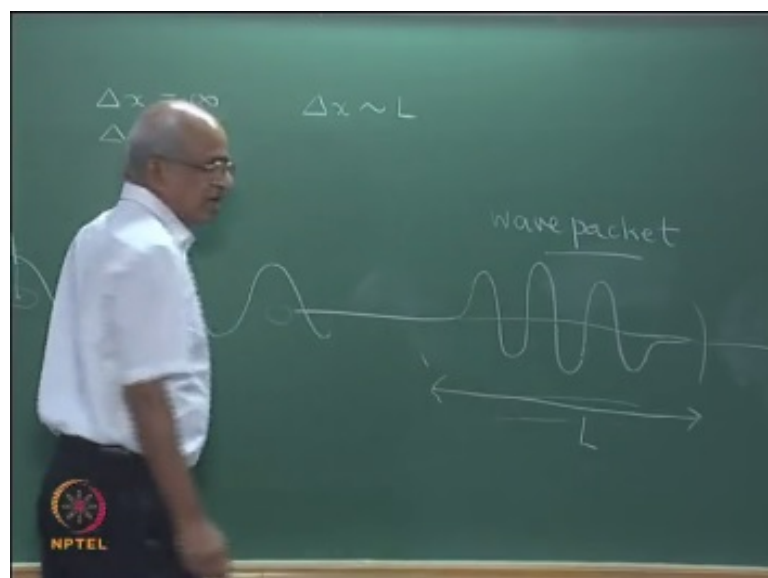
Now, it is very interesting that, De Broglie actually belong to the royal family. He was a prince. And originally, he had wanted to study history. He was a student of history, but then he found history not very interesting; and he switched over to physics. And this was his PhD thesis. The suggestion was his PhD thesis. And the people did not believe in the suggestions; and the thesis was likely to be rejected. And if it was note for Einstein, it would might have been rejected. And Einstein that, maybe there is some truth in the suggestion, and therefore, the thesis was eventually accepted. But, then at the time of the viva voce of the thesis, viva voce examination, the examiners actually asked him, when this is only theoretically, can you suggest some experiment, which will verify this relationship that you are suggesting. And then he said, you know that in the case of x-rays, x-rays have a wavelength, which is comparable to the spacing between atoms in a

crystal lattice. And therefore, we can see x-ray diffraction, because the wave length is comparable to the spacing between the different items in a crystal lattice.

So, maybe what you can do is you can have electrons; we can make them in such a fashion that their wave length will match the spacing between atoms in a crystal lattice and then maybe it will be possible to see the phenomenon of electron diffraction. This was suggested by him. And it was experimentally observed within 2-3 years. And therefore, their relation was experimentally verified. So, what I want to tell is an important consequence of this. One important consequence of this is actually the Heisenberg's – so-called Heisenberg's uncertainty principle.

So, to demonstrate you how the uncertainty principle comes around or comes about, you imagine that, you have a particle; this is the particle that is moving with a momentum. I will say I have indicated p ; and the momentum... I know precisely what the momentum of the particle is. If I know the momentum precisely, then of course, I will know the wave length. If this relationship is valid, I will also know the wave length precisely. And the wave length will be given by this relationship. So, I note precisely what the wave length is. And so what will happen is that, I will have a wave, which looks like this; and its wave length is very well-defined. So, it will be repeating again and again with periodicity when that is equal to λ ; it will go on repeating again and again and again and again. In principle, it will extend from minus infinity to plus infinity.

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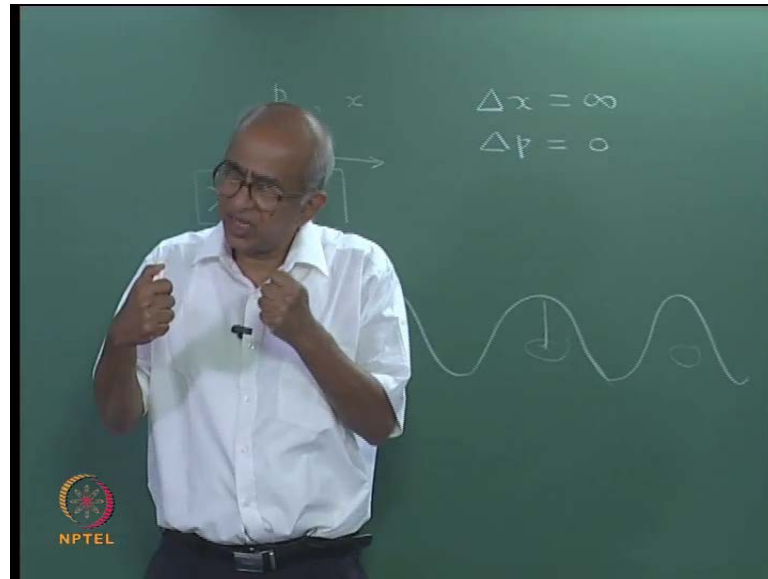


On the other hand, if I had a wave, which is probably something like this; suppose I had a wave, which is of this form; then, it is not possible to say precisely what the wave length is, because you see this distance would you say is the wave length or would you say that distance is the wave length. So, wave length is ill-defined for such a wave. So, in order to have a very well-defined wave length, I should have a very long wave with it repeating periodically in these shapes – sinusoidal in shape so to say. It has to go on repeating. Therefore, if you say this is the kind of associated with this particle, which has a well-defined momentum and then if you ask me where we... Suppose I do an experiment where I am going to find where the particle is; suppose this is the wave associated with the particle, I mean, this is eventually going to be associated with the wave function – this wave that I have.

So, we know that... Maybe what I can say is, wherever the value of the wave is large, I will probably find the particle there if I do an experiment. Therefore, if you look at this, you can say, with the way it is drawn, at this location, it has a value; and at that location also it has a same value. Even here it has a same value. My drawing is not perfect, but you can imagine it is perfectly periodic. And so you see that, there are different points, where it has exactly the same value. And therefore, you would say if I did an experiment, maybe the particle may be found somewhere; in this locality, you may be somewhere there or may be somewhere there or may be somewhere there and so on.

Therefore, you realize that, if I did an experiment, the particle can be found in principle anywhere between minus infinity and plus infinity, because the wave extends over such a region. And therefore, what has happen is that, experimentally if I try to determine the position of the particle, I would find that, my answer is each time it is going to very very very different. Sometimes I may find it here, some other times I may find it there, some other times I may find it there. So, where I will have a huge uncertainty in the experimentally observed values of position; that means, if I denote the position by the symbol x , it is a large uncertainty in the huge uncertainty.

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Therefore, I will say that, this is a situation where the uncertainty in the measured position of x is large. In fact, it would be infinity in principle if I had such a wave. Now, look at the situation why no momentum precisely. Therefore, I have no uncertainty in momentum; momentum is precisely known for this particle. So, if I had Δp uncertainty in momentum equal to 0, then if I measure the position; if the answers are going to be so different that I would have a huge uncertainty in the value of position.


On the other hand, if suppose you say, no, I do not want this; I do not want the position to have such a large uncertainty, then what should I have? I should have maybe a wave, which is of this shape. And this wave has the characteristic that it is 0; say it is nonzero only in this region; and outside, the wave is 0. So, if we wanted to have such a wave; why do I want to have such a wave? That if I have such a wave, when I measure the position of the particles, sometimes I will find it here, sometimes I will find it there, maybe sometimes here and so on. But, the uncertainty will not be very large. It will be... It will not definitely be not infinity. So, here Δx will be finite. Correct? But, then you ask what is the wave length of this; that means the answer is ill-defined, and then because I mean you have to think of a wave length for this; we will see how it may be done in the next few pictures.

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De Broglie - Heisenberg

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

de Broglie

 $\Delta x \Delta p \geq \frac{h}{4\pi}$

Heisenberg



So, this is the first wave that I talked about the wave actually. ((Refer Time: 09:26)) has a definite wave length; it extends from minus infinity to plus infinity. Now, suppose I want to construct a wave of this shape, how will I go about doing that? That is made clear in the next few pictures. So, you think of this red wave and you also think of this green wave. If you look at it carefully, you would realize that, the wave lengths are slightly different; the wave lengths of the two waves are slightly different; they are not the same. And now, suppose you added these two waves, what will be the result? If I am adding these two waves, the answer you can see; what is going to happen? If you think of a point here – right at that location, the green wave has a displacement, which is downwards; the red also has a displacement, which is downwards. So, if you added the two of these, you will have a larger displacement at the downward direction.

But, if you thought of a point somewhere here, what will happen? The green wave has an upward displacement while the red one has a downward displacement; the two will nullify each other. So, if we added these two, what will be the result? That is shown in the blue curve; that is shown here; I have drawn all the three waves. You see this blue wave is actually the result of adding the red and the green. And you can see that, by adding these two together, I have managed to have something, which looks like this. If you actually added the two waves, what will happen is that, you will have this being repeated again and again and again. That is what happens. But, the point is that, by

adding two waves of slightly different wave length, I can actually make the wave function, have a large value in some region and smaller values elsewhere.

But, now, suppose I am not going to add just two waves; I am going to add a large number of waves having slightly different wave lengths; then, what I can do is I can have a situation; this is actually mathematically possible to demonstrate. But, we would not do that; we will have to believe me when I say I can have a wave, which probably is of this form; its value outside is 0; its value in that region also is 0; and the wave is localized only in this region. All the other regions you see I can cancel everything and have an answer 0 everywhere else, but only in a small region. But, for that to happen, what I should have is I will have to add together several waves of slightly varying wave lengths. And this is something that we can refer to as a wave packet. The mathematics of this I hope to discuss maybe after something like 10-20 lectures. So, that will come later. But, this is the idea. So, then, this is actually such a wave, is a super position of waves of different wave lengths.

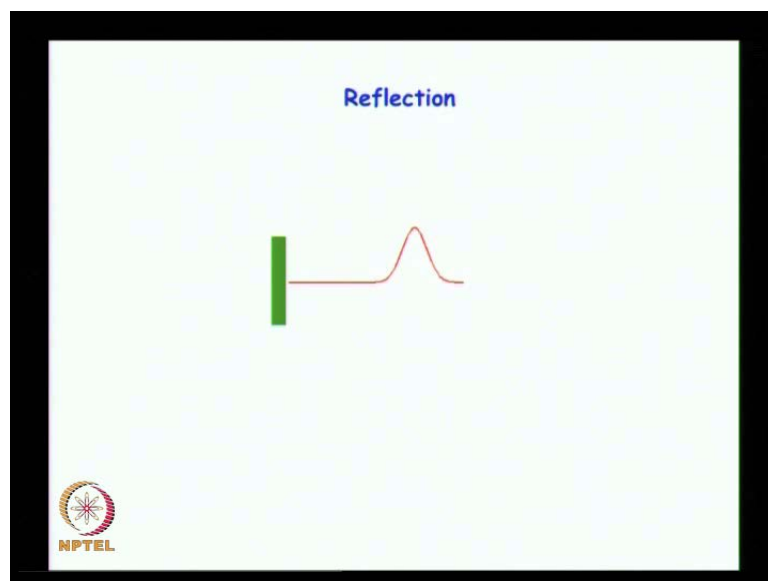
Now, why did I do it? Because I wanted to have uncertain in position small; uncertain in position is now of the order of this distance; it is of the order of this distance. And this I shall denote as L . So, this is a situation, where Δx is of the order of L . And for such a situation, what has happened, the momentum... Earlier in this case, the momentum was well-defined; there was no uncertainty in momentum. But, to have this, I have to superpose the waves of varying wave length. And so momentum has become uncertain; or, the wave length; instead of saying momentum, I should say the wave length has become uncertain. If the wave length has become uncertain, naturally, if λ is uncertain, then momentum is uncertain. Now, if you want to make this wave packet narrower, you can do that; but then you will have to superpose waves of even widely varying wave lengths. And therefore, the moment you try to reduce the uncertainty in position, what happens, uncertainty in momentum starts increasing. So, there is an inverse relationship between uncertainty in position and uncertainty in momentum.

This was mathematically analyzed by Heisenberg. And he came up with this relationship. He said that... He could show... I mean this is something that I hope to do later in the course, but here I am just giving an overview. He could show that, $\Delta x \Delta p$ must be greater than or equal to $\frac{h}{4\pi}$. This is one of the consequences of this wave particle duality. And I wanted to talk about another one, which is of great interest

to us particularly when we are thinking of atomic orbitals, molecular orbitals and so on. See suppose I now imagine that, I have a very long string lets me say. One end of the string is attached to that wall and I am going to take hold of the other end here. And very quickly, what I will do is I will stretch it tight and then I will just move my hand up and down.

And then, what will happen, I would have produced a disturbance, which will travel. Or, you say you stretch it tight and then maybe I will just lift up a part of the string and very quickly and then release it. Then, what will happen, I would have produced a disturbance in that string. And that disturbance naturally, it will travel on the string and it will reach the wall; from the wall, it will be reflected, because it cannot go further. So, it is going to get reflected. And what you are going to see is an animation, which shows this reflection.

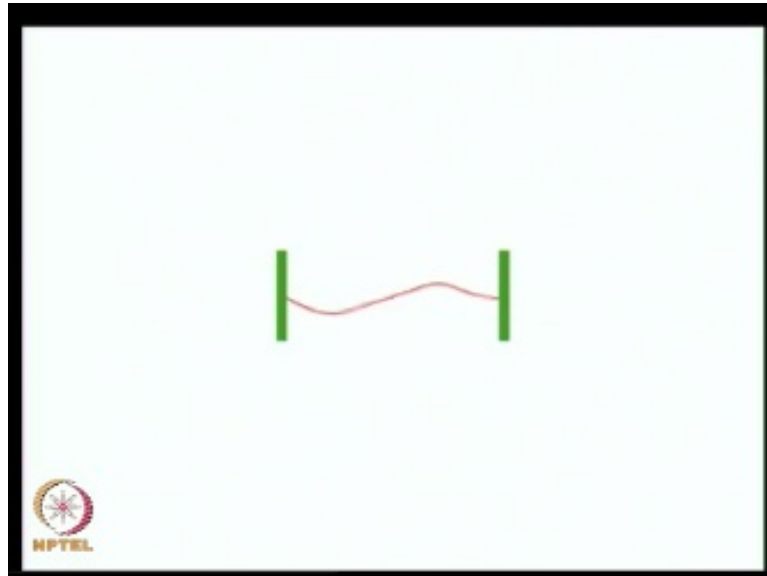
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So, you imagine this is the... I mean this kind of displacement is difficult to produce, but imagine I can... I am able to produce such a displacement initially and imagine that it goes towards the wall. Then, it is going to get reflected. And how will it get reflected? You can see that as an animation. But, the way the animation is made, you see the reflection process is shown again and again and again several times. That is how the reflection process actually takes place. It goes, hits the wall and gets reflected. So, if you had a wave in a medium... What is it? I have a string; that is the medium. And I have produced a wave; the wave is moving in the medium; but then if I put an obstruction,

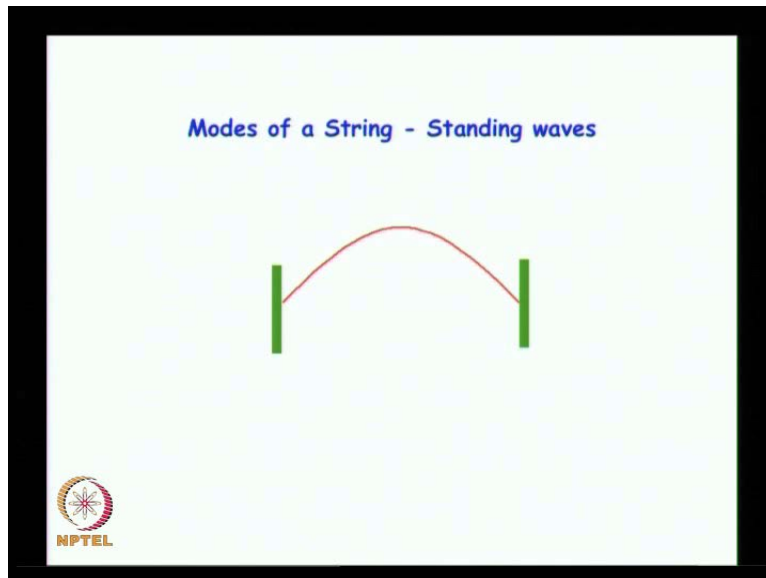
what will happen, I would have reflections. I would have a reflection from the obstruction.

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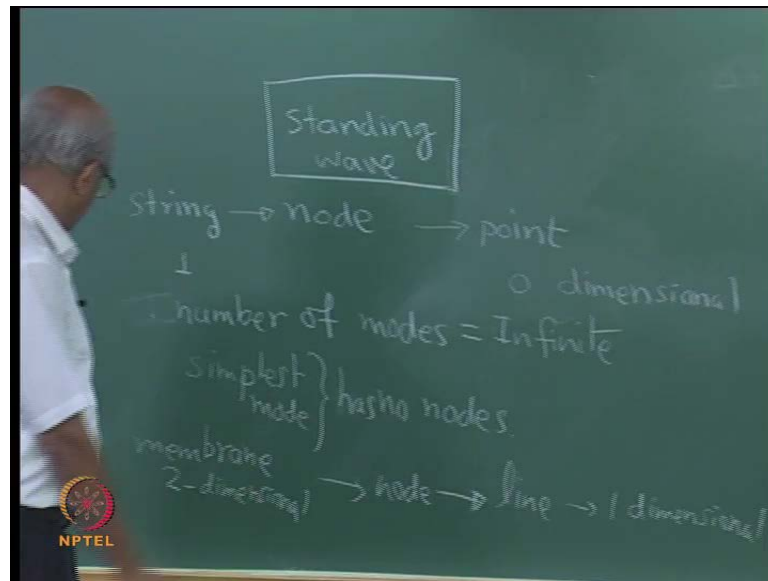
Now, suppose I put two walls. Therefore, I am going to now imagine that I have two walls here let us say; and I have a string, which is stretched tight between the two. So, then, imagine that. And then what I will do is I will take my hand and hit the string. And then, what will happen? The string will start vibrating. You can see the kind of things that can do in the next animation. So, here what is happening is that, you see the initial displacement that I have produced; it is this one. This is the initial displacement; and then, it goes on changing its shape and so on. So, what is happening is that, the wave is reflected not from one side alone, but it is reflected from the other wall also. Therefore, you have reflection from this side; you have reflection from the other side; and also, you should notice that, the shape of this disturbance that I have produced is going on changing; it is going on changing all the time. That is what you see. But, then in the case of a string, we now experimental it that, it is possible for one to produce certain special kinds of displacements. They are special and they are very nice.

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Let me show you one of them and tell you how this actually comes about. So, this is a special kind of displacement. You can see that, the whole of the string goes up and then goes down; and it is going up and down with a certain number of times in a second. So, that we refer to as the frequency of vibration of the string; it goes up and down with a certain definite frequency. Here what is happening is that, the disturbance that you have produced; it is definitely getting reflected from this side and from the other side. But, what has happened is that, the original disturbance and the reflections actually combine to retain the shape of the disturbance. See in the earlier disturbance that I have shown, that was not the way it was; the ((Refer Time: 19:07)) reflection and the reflections were actually causing the change in the shape of the wave. But, that does not happen in this case. Here what is happening is that, there are reflections, but the reflections and the original disturbance are such that they manage to retain the shape. And this is referred to as a standing wave pattern.

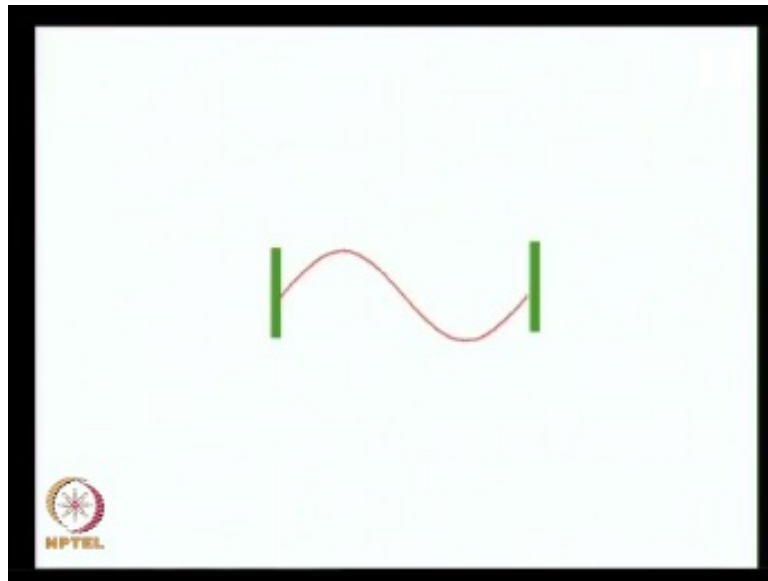
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And, further you see earlier you would have seen that, the disturbance is actually moving back and forth. So, you would have referred to it as a traveling on the string. But, in this case, see it is not moving back and forth on the string. All that is happening is that, the whole string goes up and down; it goes up and down in the perpendicular direction, not on the string itself. So, this is something where it is referred to as the standing wave pattern and it is special. Why is it special? Because first of all, it has a definite frequency. The second thing is that, its shape is not really changing. When I say shape, you see it is the shape like this. And the magnitude of the displacement actually changes; but other than that, the actual shape is not changing. But, this is not the only standing wave pattern that I can imagine. These are also referred to as normal modes of motion of the string. And in fact, this is the simplest possible normal mode of motion of the string.

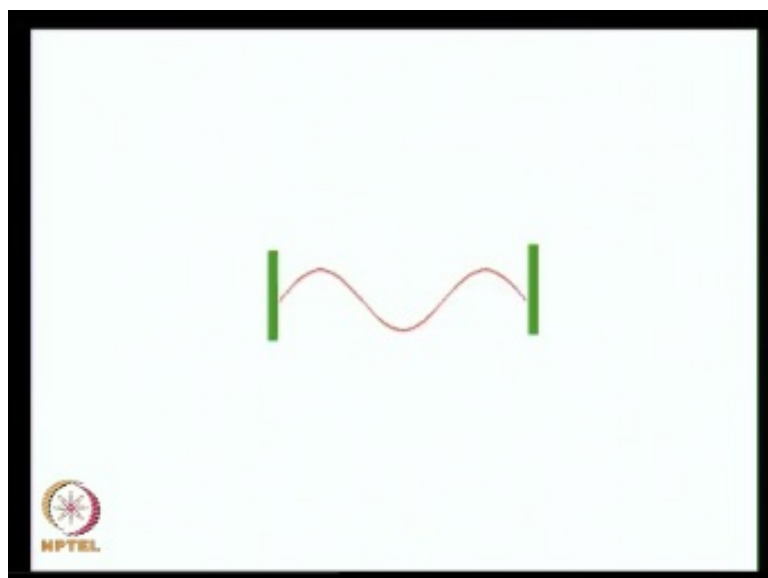
But, suppose you had lot of other possible normal modes of motion; this is another possible normal mode of motion, where what is happening is that, the half of the string – imagine it is going up; then, the other half is actually going down. So, it vibrates like this. And further right in the middle of the string, at this point, what is happening, there is no displacement of the string. The action is happening, not at the middle, but elsewhere. So, that particular point... Actually at that particular point, what is happening is that, there is no displacement of the string. And therefore, I will refer to that; that is a special point; and I will say that, it is a node.

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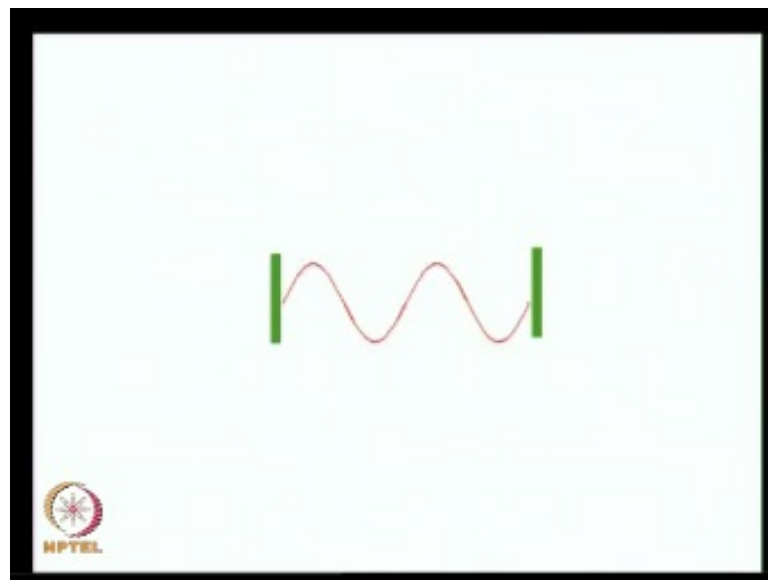
So, in this case – in the case of a string, you would say agree when I say that, the string is a 1 dimensional object. What has happened, I have a particular point, where there is no displacement. And that is referred to as a node. So, here the node is actually a point. That is the case of the string actually. And string of course, you will agree when I say that it is 1 dimensional; it is a one dimensional object and it is a point. Mathematically speaking, its dimension is what it is 0 dimensional.

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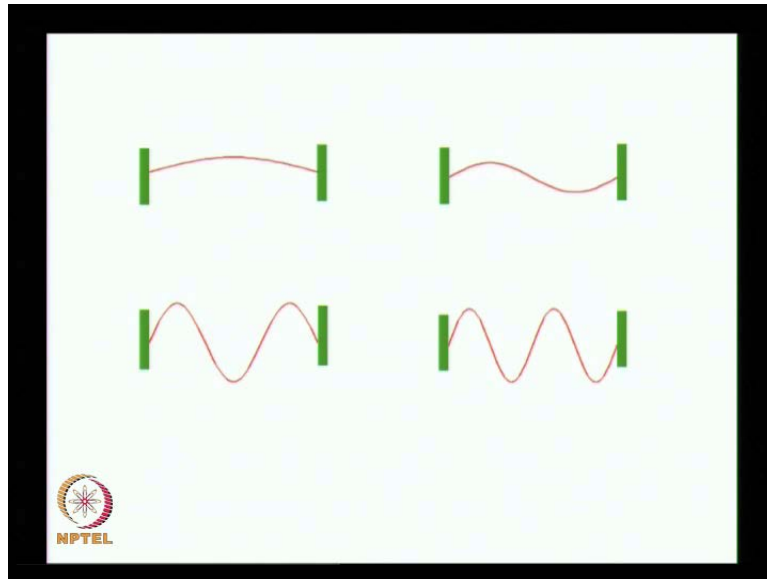
Now, this is another normal mode of motion. You can think of other normal modes of motion. This is yet another one. And the major difference between this and the previous one is that, this has two nodes. And what about the simplest one that we had? The first one; the first one you can see again. This is the first one. And this obviously, has no nodes. As you saw, the first one has 0 nodes; second one has 1 node; the third one has 2 nodes. And then, obviously, you can imagine other normal modes of motion. They will have 3, 4, 5, 6, etcetera nodes. And so in principle, if you do not worry too much about the atomic structure and if you are asked the question, how many normal nodes are possible; then, the answer is infinite. They are all characterized by the number of nodes – 0, 1, 2, 3, 4, etcetera. So, infinite... And one more point maybe I should rather simply write simplest mode; it has no nodes.

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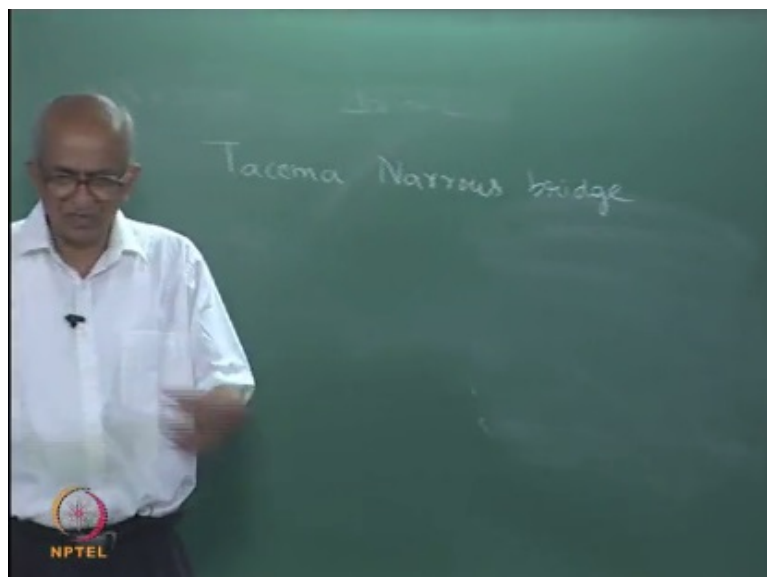
So, this is the next one. And all of them are... I mean the four that I have shown you are all shown here. But, of course, it is easy think of other higher modes.

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This is an interesting thing. This again has nothing to do with the quantum mechanics actually. This shows you, standing waves can be set up in a bridge for example. And something very unfortunate happened long ago around 1942. This shows you are the... This is everyday which I will play for a few minutes. There was a very very famous bridge.

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It is referred to as Tacoma narrows bridge. This is a... In the US, it was a very long narrow bridge and it was built around 1940-41. And this was in a region where there

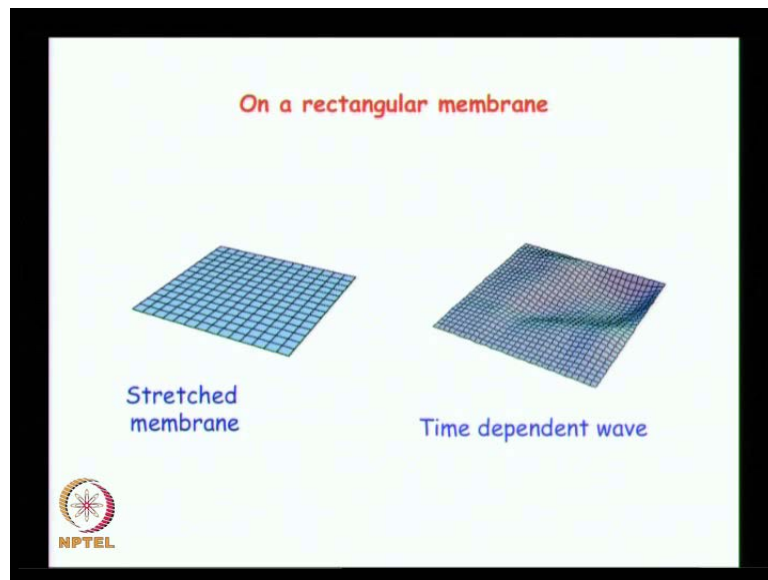
were strong winds. And after the bridge was built, it was found that, because of the winds, there were standing waves wave kind of things set up in the bridge. And these standing waves... I mean there was some kind resonance; the waves that were set up were very large, their amplitude was very large. And so now, you can see what the result was.

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So, this is view of the bridge on a particular day. And these were the oscillations caused by the wind. We can see them very clearly the modes; the mode that was set up – it is quite interesting if you have not seen it. There is a car sitting on top of the bridge. The story is that, there was a dog inside; the man was sitting and sitting; he came out and crawled to safety. But, the dog perished, because of the collapse of the bridge. And later on, they constructed. I mean they realized that, the engineering was not correct. So, they constructed another proper bridge. This is from you tube.

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We have thought of a something that is 1 dimensional. But, imagine I have a drum; and the membrane of the drum is obviously 2 dimensional. And normally, as you know drums are actually having nice circular shape. But, let us imagine for a few minutes that, I have a rectangular drum; I am crazy I have made a rectangular drum let us say. And how would the membrane look like. This will be the membrane and you should realize that, along the periphraes, the membrane is fixed. Along the periphraes, the membrane is fixed.

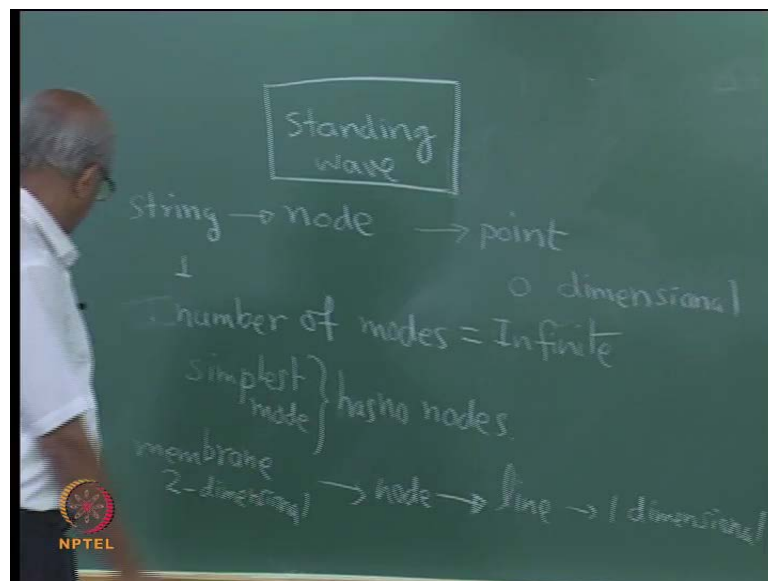
Therefore, if I take my hand and hit it, what would happen? I would have produced a displacement of the membrane; and that displacement will move, because the membrane is stretched tight. It will move on to the membrane, but it will hit the periphraes. And from there, what will happen? It will get reflected. And what is going to happen is that, as you watch the shape... I mean if you can watch it of course, the shape of the membrane will go on changing. I mean you will have to do speed photography to actually see it, but this is how it will go. I mean if I have taken this and then hit the membrane, then I will have some kind of disturbance, which goes around something like this.

But, just as in the previous case, here again the move in the video is not the video. But, the animation is repeated again and again and again. But, just as in the previous case, it is possible for it to produce what are afraid to us – standing waves. These are waves that

their shapes go on changing, but it is possible for me to produce waves, which are standing. In what sense? They are not actually moving around.

Here if the wave is ((Refer Time: 29:45)) the disturbance is moving around. So, this is a very special kind of disturbance over the displacement that we can produce. What is happening is that, the whole of the membrane goes up or it goes down. And that happens with a particular frequency. And I am sure you will agree when I say that, here this is the simplest possible pattern and that does not have any nodes; there is no point inside the membrane, where the displacement is 0. So, that immediately tells me that it should be possible to think of other modes; which is the next one that I can think of a mode like this. And if you look at this, you will agree that, there is 1 node. Where is the node? Actually, if you look at it carefully, you will see that, it is this line – this particular line. Along that line, there is no displacement. And so it is a node. So, this in the case of the membrane... I hope this is visible.

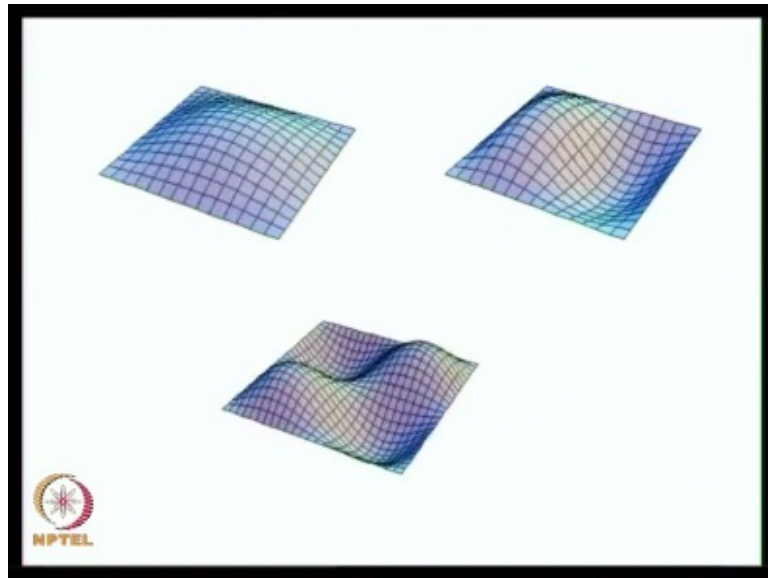
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Membrane is 2 dimensional. What has happened is that, the node is actually... It is not a point anymore. The node is actually a line; it is a line. And the line you will say, what it mathematically speaking, what is the dimension of a line; it is 1 dimensional. So, when you have membrane, which is 2 dimensional, you have line, which is node, which is a line, which is 1 dimensional. And how many such modes can we imagine? You can have 0 nodes, then you can have 1 node, then maybe 2, 3, 4, etcetera and so up to infinity at

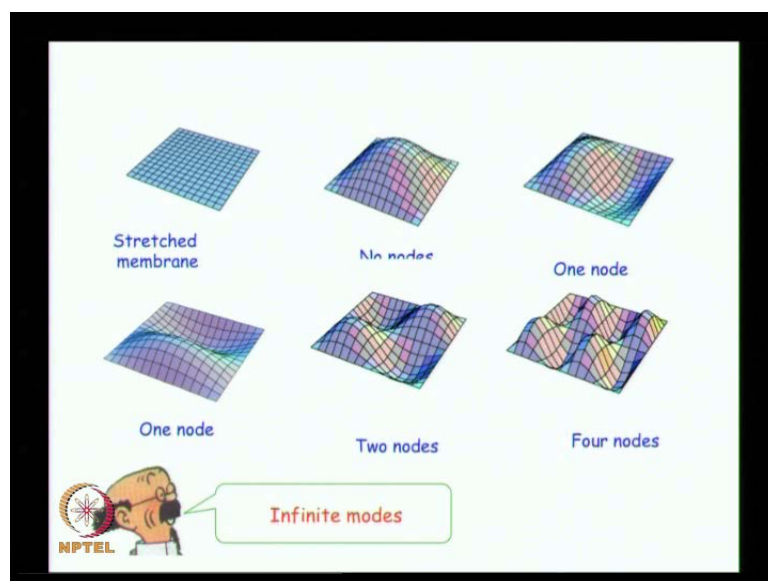
least in principles. So, you can see that... You see this one is another disturbance. So, what is the characteristic? It has two lines along which the displacement is 0 and these two lines are perpendicular to each other. Correct?

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So, I have shown you 3 of the normal modes. All of them together are as shown in this animation. But, then I have one more picture; it is not an animation, but it shows you the different modes.

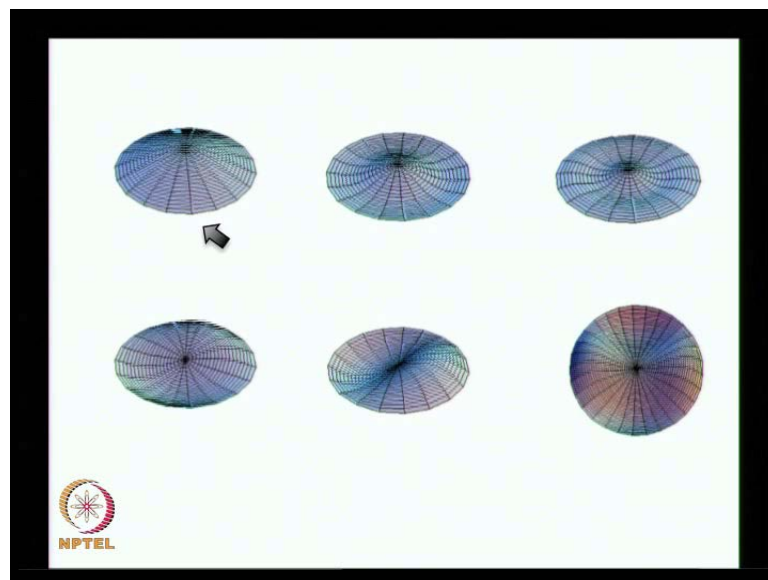
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This is the membrane. The membrane is now displaced, but then this is a displacement, which has no nodes; a normal mode of motion in which there is not displacement. This has one node; this also... This is a... This is not the same as that displacement. That also you should notice. What is the difference between two? You will see that, the nodes are actually different. This one has a node along that particular line; while this one actually you cannot see the line; the line is perpendicular to the line in the previous case. So, now, this mode is different from that mode. And then, you have may be a situation with two nodes. We have already seen the animation. And then, maybe you can have a situation like this one. This one is drawn in such a fashion that there are four nodes.

So, you can have 0 or you can have 1, then 2, 3, 4, etcetera in principle up to infinity. So, in the case of the membrane also, what happens, you would have infinite number of modes of motion – normal modes of motion. And the simplest possible one has of course, 0 node. Not only that, if you have wave in 2 dimensions, what happens, the nodes are actually 1 dimensional. And if we have waves in a string which is 1 dimensional, what happens, the nodes are actually 0 dimensional. So, there are infinite such modes.

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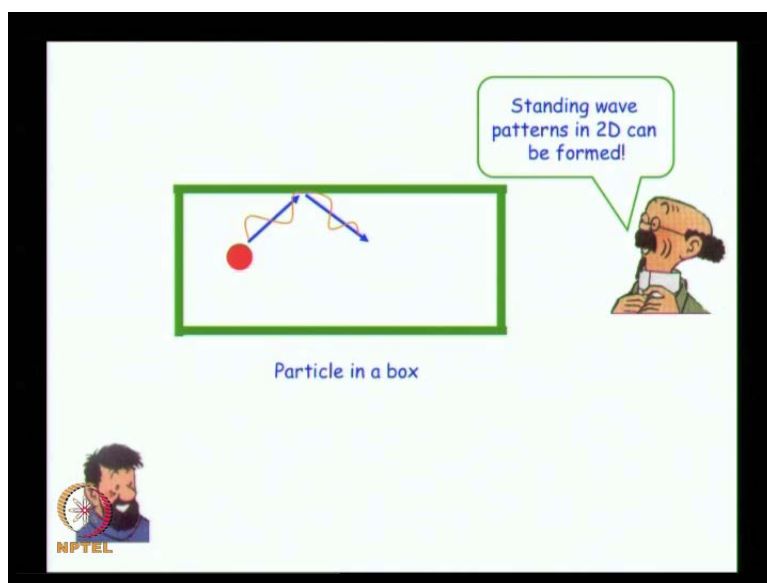


Now, as I said, a drum is circular usually. So, you may ask what happens if we have a circular membrane? That is shown here in this picture. You will see that, there are nodes; but if you look at this one, this is the simplest possible standing wave pattern that we can have; it has no nodes; the whole of the membrane goes up and down. If you look at this

one, what would you say? Here if you look at it carefully, you would realize that it has just 1 node – 1 node where the displacement of the membrane is 0. And that one node is actually having the shape of a circle. This one if you look at it and think about it carefully, you would realize that, it has two nodes; the two nodes are both circular – circles; I mean along the circles, there is no displacement of the membrane. While this one has 1 node and that node is actually roughly along this particular line – this line – a line which runs like that.

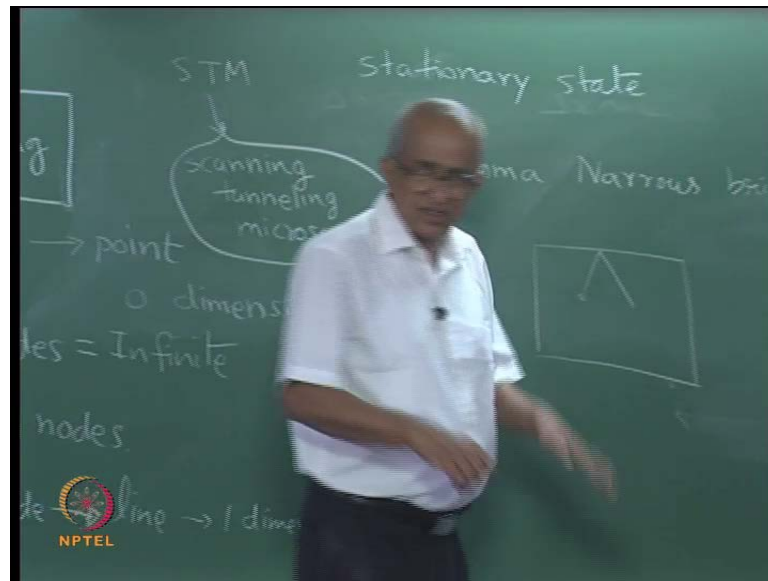
And, this one has nodes which is perpendicular to that line. There are 2 nodes: this one was 1 node; this one has another node and the two lines are actually perpendicular to one another. While the last one; it has two nodes; that the mode itself has 2 nodes; both are lines perpendicular to each other. And then if you are asked, how many such modes can you think of; again, the answer is in principle infinite number of such modes are there. Of course, here also the simplest one, it does not have any nodes. And as you go up, what is happening is that, the number of nodes go on increasing.

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You may ask what is the relevance of all these to chemistry, because you see this is a course on a quantum chemistry. And so I should make connection with chemistry. So, let me do that. Imagine that, I have a particle. We will see examples later. And this is confined to a box. So, let us say...

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To make things simple, imagine that, everything is 2 dimensional. So, therefore, this region is a box – two-dimensional box; such a thing you know it does not really exist. But, let us... We can have close approximations to this as we will see in a few seconds. Imagine I have a box like this and electron is confined to this box. What does it mean? You see if it hits the boundaries of the box, it is going to get reflected; which is what is shown in the picture. So, you see. So, the electron has a wave associated with it. So, if I am confining the electron to this box, what will happen is that, the wave associated with it also is confined; it cannot go out. And if it does not go out, what does it mean? The wave is going to get reflected from the boundaries.

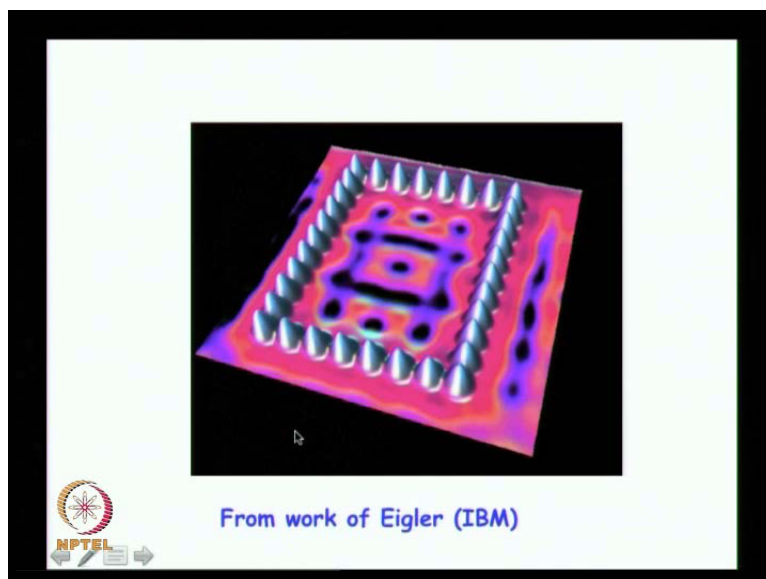
So, like the figure that is shown in the in the picture here, you see that, the wave is getting reflected. So, in such a situation, what is possible? You see you have waves in a 2 dimensional medium. That is essentially what you have. You have waves in 2 dimensions and you have confined. So, naturally, there will be reflections from the boundaries. And then, you can immediately say this is like the waves in a membrane. And those waves if you have remember, they could have had a time dependent behavior, where the shape is changing. But, it is also possible for us to have ((Refer Time: 38:13)) to a standing wave patterns.

And, what can you say about the standing wave patterns? Basically, I can say that, I can have any... I can imagine an infinite number of such standing wave patterns. The

simplest one would not have any nodes; the next one would have one node; the next would have 2, 3, 4, etcetera. This is definitely possible. The wave associated with the electron can have a state. Notice the wave – a new wave that I have introduced can have a state, where the wave associated with it forms a standing wave pattern. The simplest state would be that one in which the wave associated with it has no nodes.

The next one would have 1 node; it would have 2 nodes; the next would have 3, 4, 5, etcetera. So, different standing wave patterns can be formed. And these are the things that you refer to as stationary state in quantum mechanics. So, what is actually a stationary state in quantum mechanics? This is a state in which the wave forms a standing wave pattern. That is what it is. A stationary state is nothing but a state, where the wave associated with a particle forms a standing wave like what has happened in the case of the membrane. So, standing wave patterns in 2 dimensions can be formed.

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As I said, this is somewhat of an idealization, but these can be realized experimentally. And these are experiments taken from Eigler, who works at IBM. I will not go into the details of this, but I will tell you what the ideas were. See what Eigler has done is, he built an STM microscope. STM stands for standing tunneling microscope. And the beauty of this is that, you see this is possible for you to image even single atoms sitting on a surface; you can image even single atom sitting on a surface. Not only that, one that he built he could operate at very low temperatures. In fact, it was one of the first to

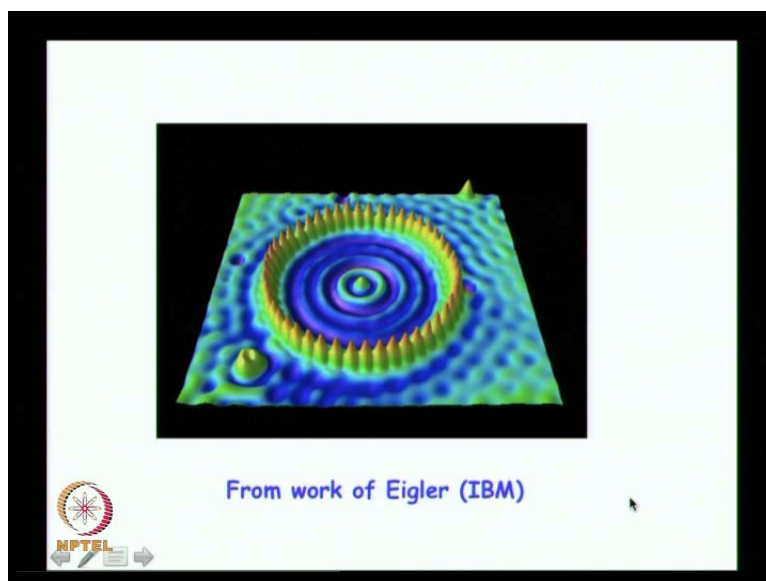
operate at 4 kelvin or below. And not only that, he can actually pick up a zener atom, which is sitting on to the surface. Imagine you have a zener atom, which is sitting on a surface. He could pick it up using the tip of this microscope. There is a sharp tip using which we can pick up an atom and put it elsewhere. Therefore, it is possible to move the atoms on a surface. And what he did was, he had ion atoms sitting on a copper surface – ion atoms sitting on a cooper surface. Using the tip of this scanning tunneling microscope, he could move these ion atoms and arrange them, so that they formed a rectangle, which is shown in this picture.

You look at this picture. This rectangle is formed of ion atoms. And in fact, these peaks that you see here actually, is representing the electron densities of these ion atoms; which could be imaged using this scanning tunneling microscope. So, he arranged ion atoms in the form of a rectangle on the surface of copper. And then, you think of electrons; you see electrons in copper. Suppose you have an electron inside this region; that electron – actually it is confined within something like a two dimensional box, because this is the error; these ion atoms, which are acting as obstructions.

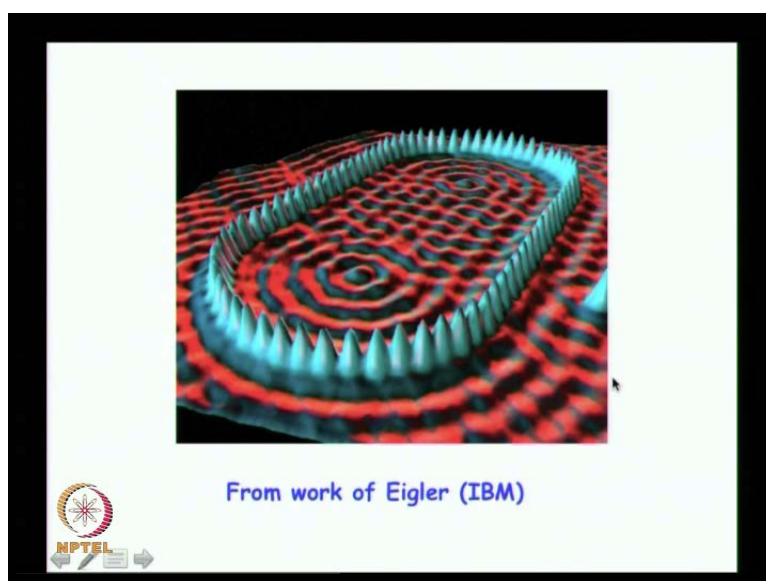
So, what is going to happen is that, the wave associated with these electrons; they will form a standing wave pattern within the box, within this rectangular box. And if they form a standing wave pattern, what will happen to their electron density? They will have a wave-like pattern formed inside the box. And that can be imaged using the same microscope. And he did that. And you can see that, there is an evidence for wave nature of electrons, because you see the electron density within this has undulations; it varies from point to point with wave nature. And so you can see that. So, this was one of the very clear experimental demonstrations of wave nature of the electrons.

Now, here he has a rectangular box; but why should you have a rectangular box? We can have a circular one. And this is what he did; he put a circular barrier made up of ion atoms and then observed that, the electron density within this; actually he has this wave-like behavior again showing, proving the wave nature of electrons. This is actually experimental data. This image has become so famous that, it is available in many many many books; you might have seen this already. Instead of having a circular stadium, this may be referred to as a circular stadium.

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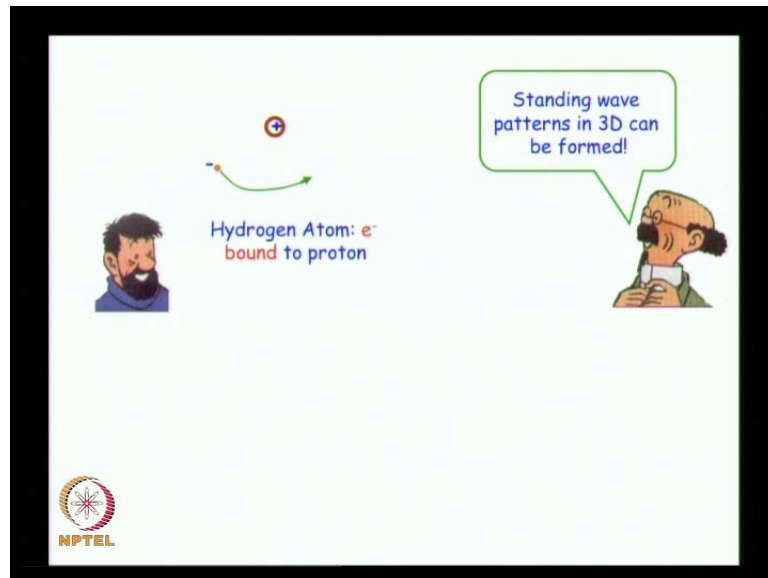


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We can also have an elliptical one. And even there we can see these interference patterns right the way the evidence of wave nature in the electron density that excess inside this. So, that is from the work of Eigler. But, then again you may say. that is all very much difficult; very much difficult in the sense, these are very difficult experiments. What is the relevance of all these things to ask chemists in our everyday life. And that is uncertainty next 2-3 slides. You imagine you have a hydrogen atom. What is the hydrogen atom? You have a proton and you have an electron. And imagine that, I have a situation, where the electron has been put close to the proton.

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And, I know that, the proton is positively charged, the electron is negatively charged. So, that will be attractive interaction between the coulombic attractions that will actually lower the energy of the system. So, if I started with the electron close to the proton, the energy of the system I expect will be low. And unless I supply energy, I cannot take it far away; I cannot take the electron far away. If I wanted it to take the electron far away, I will have to supply energy from outside.

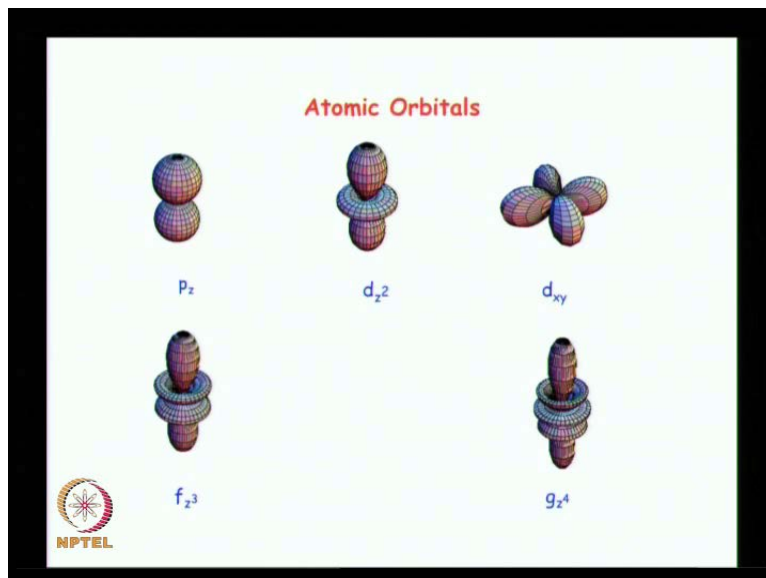
If I do not give that energy, then what is going to happen; the electron is going to be in the vicinity of the proton. So, if it goes in this direction; suppose it goes in that direction, then it will not be able to go to infinity; it will have to eventually turn back. So, what will happen to the wave associated with the electron? The wave associated with the electron also will turn back.

So, effectively, even though I do not have actually a boundary, what is happening is that, the proton is there and the attractive interaction with the proton actually puts something like a boundary, not exactly a boundary, because the electron cannot go far away; it is going to get turned around; that means essentially it is going to get reflected. So, what will happen; the wave associated with this electron – it will get reflected; it is confined; it cannot go to infinity. And if you have confined waves, how is the confinement done here? It is simply because of the interaction between the proton and the electron. That acts to confine the wave.

Once you have confined this wave, what will happen; I can have a time-dependent situation, where the shape of the goes on changing. And that is what happens in spectroscopic experiments. If you are doing spectroscopic experiments, you are actually changing the shape of this wave by external influence. But, we are not going to think about that today. What we want to think about is the situation, where I have standing waves. Suppose the electron – you think of the electron; it can have the wave associated with it forming a standing wave. And what can you say? You can say, the simplest possible standing wave pattern would have no nodes. The next one would have 1 node; the next one would have 2; the next would have 3, 4 etcetera. How many standing wave patterns can it form? Infinite number. And each such standing wave pattern is what you are referred to as an atomic orbital.

Remember these; this time the waves are actually in 3 dimensions; the hydrogen atom is a 3 dimensional object; it is not 2 dimensional. So, the waves are in 3 dimensions. So, if you think of nodes, what would you say the dimension of the node is? See you will look at what happened. If we had a string which is 1 dimensional, node is a point 0 dimensional; for a membrane, which is 2 dimensional, node is a line.

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So, if we had waves in 3 dimensions, naturally, the nodes will be 2 dimensional. So, what would you expect as far as the hydrogen atom is concerned? Maybe a node could be a plane, because a plane is a 2 dimensional thing; or, it could be... A node could be a

surface of a sphere, because mathematically speaking, surface of a sphere also is 2 dimensional. Even though it is excess in 3 dimensional space, you see mathematically, it is a 2 dimensional thing.

Therefore, it is possible to have standing wave patterns. And what are the standing wave patterns? They are atomic orbitals. The simplest possible standing wave pattern actually gives you s orbital, because the shape is well-known. I have not represented it here, but we will discuss it later during the course. This is a p orbital of the hydrogen atom; it has 1 node as you are very likely to know. This is a d sub-square orbital; it also has nodes, but it has two nodes. Then, you can have d x y; again, this is 3 d z square and 3 d x y. These are having two nodes each. This is a f z cube; it has 3 nodes. Then, another one, which may be referred to as g z to the power of 4; it has four nodes. So, what are they? They are nothing but standing wave patterns. In quantum mechanics of course, these are referred to as atomic orbitals or as stationary states of the system. I think I will stop.