Implementation Aspects of Quantum Computing

Prof. Debabrata Gowswami
Department of Chemistry
Indian Institute of Technology, Kanpur

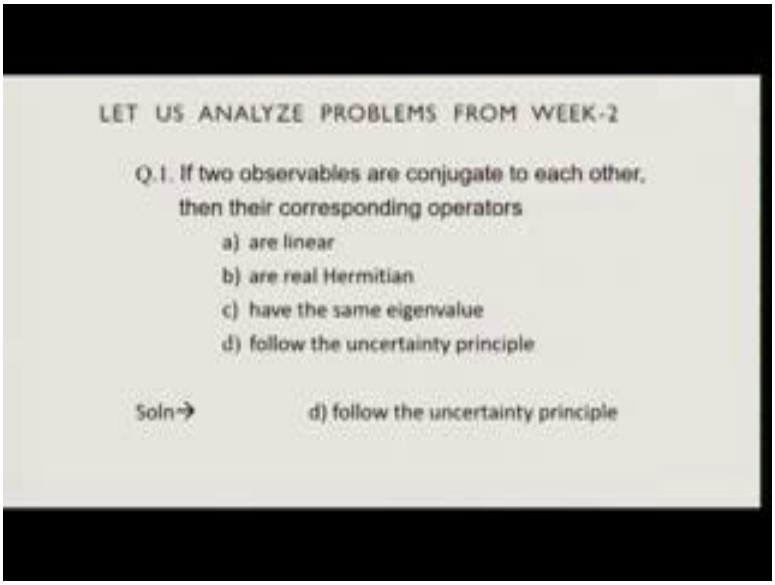
Lecture - 25
Reviewing Concepts and Clarifying Problems – 1

In this lecture we will go back to some of the issues that we have been discussing earlier and have formed the basis of many of the implementation that we have been doing in the recent times. While we looked at the problem sets and the solutions and we looked at what the students are saying about the discussion which are happening on the internet, it has become clear that a little bit of background material revise is very important as we go along, because we have been looking at implementation aspects, where many of these aspects which we are currently describing needs to have a relook.

In this lecture we will look back at some of the problems that we have already given to you. And then while discussing those problems or looking at those problems we will be reviewing the concepts that have laid the foundation of the implementation aspect that we are looking at in the present lectures. In terms of reviewing the concepts, let us see how do we go about doing this.

In some previous lecture, we have already looked at solution of problems from a certain week, the first week solutions were already looked at. This particular reviewing session would therefore, start with looking at the analysis of problems from week 2 because we have not done any of that before.

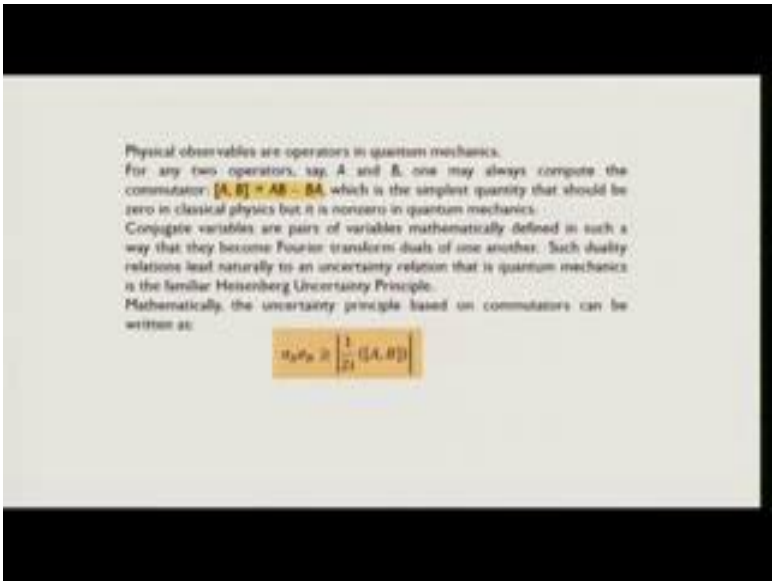
(Refer Slide Time: 01:42)



In that regard, let us look at the problem from the very beginning of week 2, and while doing that as I promise we will be also reviewing the concepts that we have either missed or needs a little bit more clarification.

The first question in week 2 was concerning the uncertainty principle and the observables and how they appear as conjugates at that time. In order to look at the solution, which is basically saying that the observables are conjugates to each other, then their corresponding operators are going to follow the uncertainty principle. This is what the concept was.

(Refer Slide Time: 02:32)

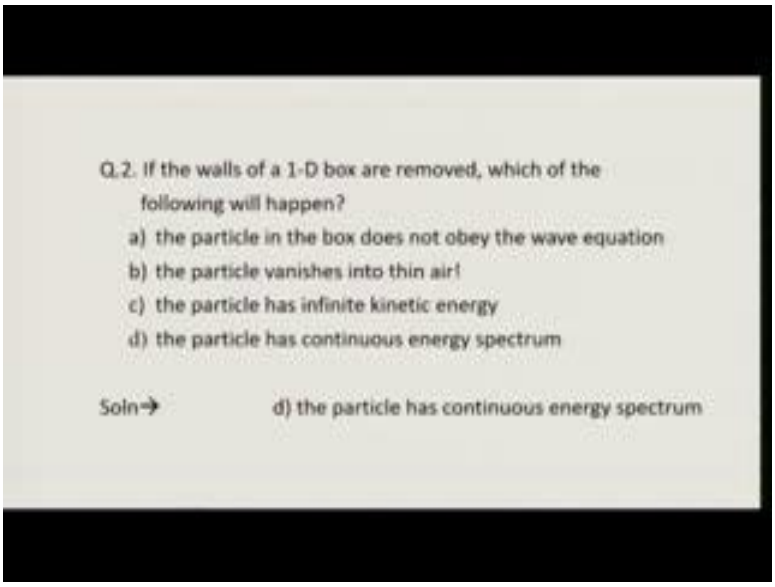


Now in order to look at the concept let us see what the physical observables the way we have defined them in quantum mechanics. The physical observables are operators for any 2 operators say A and B, one may always compute the communicator A B, which is basically the difference of the product in the 2 different ways. If they are commuting, which is the simplest quantity and is 0 for classical physics, but it is often non 0 in quantum mechanics. Conjugate variables are pairs of variables that are mathematically defined in such a way that they become furrier transform duels of one another. Such duality relations lead naturally to an uncertainty relation that is the quantum mechanics familiar features that we have discussed, which is the Heisenberg uncertainty principle.

Mathematically the uncertainty principle is based on commutators and it can be written as the variance from the actual value of the true observables, which will be always following the inequality that have written here. And as you all know, the variance of these are defined with respect to the operators that we are measuring. And in most cases in quantum mechanics, we also have realized that the operators that we are using are going to be having real values because the observables are always going to real values. They are often Hermitian and other kinds of things which we have discussed earlier in this previous concept.

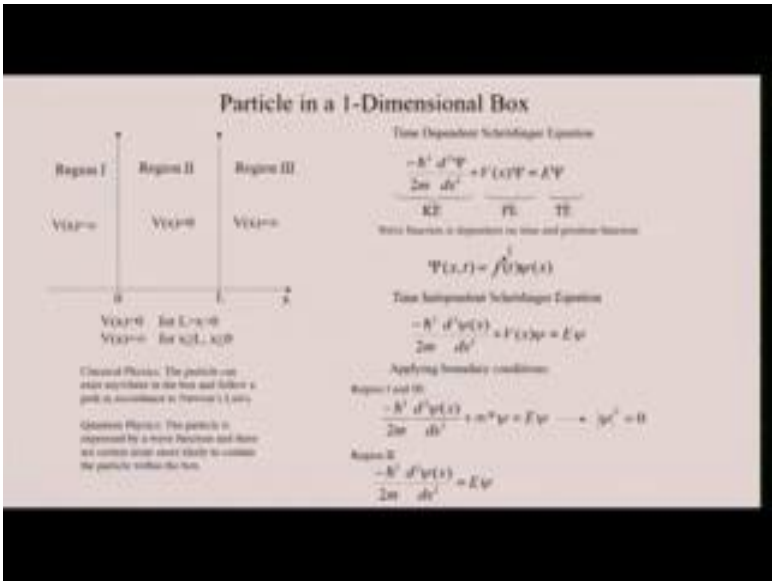
With this, we have re visited the uncertainty principle part a little. Let us now go back and see what happens when we go to the particle in a box problem.

(Refer Slide Time: 04:32)



This is a concept problem from the particle in a box, where it is asked when the walls of the 1-D box are removed, which of the following will happen? The concept of these problems is to realize that how important the walls of the particle in a box are, when we are going to answer this question. Now the solution has been given as the particle is going to have continuous energy spectrum.

(Refer Slide Time: 05:05)



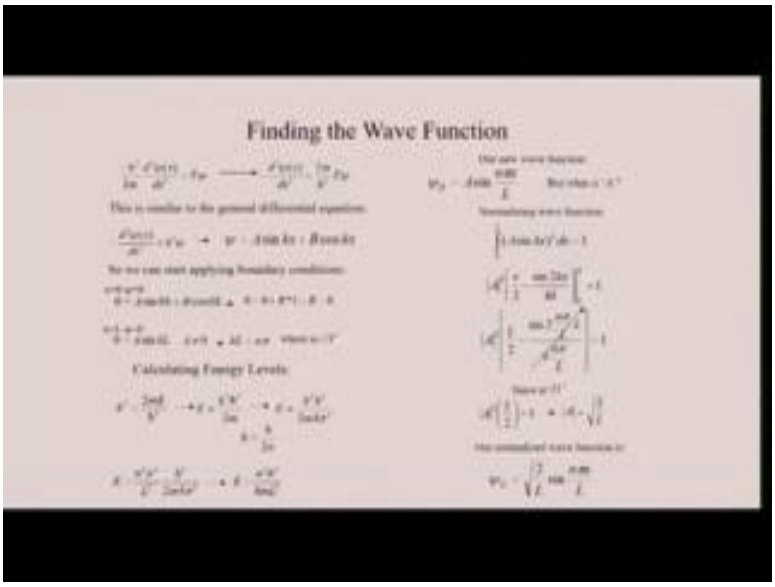
Now, to understand that let us revisit particle in a 1-Dimensional box and see how this can be looked at. Roughly speaking we can define 3 regions, although region 1 and region 3 are the same, where our potentials are infinity; is the region 2 were we have 0 potential and that is where the particle is suppose to reside. According to classical physics, the particle can exist anywhere in the box and follows a path in accordance to Newton's laws. However, as we have noted in quantum physics or quantum mechanics as we have been studying, the particle is expressed by wave function and there are certain areas more likely to contain the particle within the box.

We can start by looking at the time dependent Schrodinger equation, which contains the kinetic energy part, the potential energy part which gives rise to a total energy; some of the 2 giving raise a total energy. And the wave function is dependent on time and position function. However, when we integrate the time out, then the time part is not going to be important we have only going to look at the position distribution. And the time independent Schrodinger equation therefore, forms the part which we are looking at, in this case.

And in this case its only one variable. We have this time independent Schrodinger equation on which we can apply the boundary conditions and what we will find that

region 1 and 3 has infinity in terms of its potential. This will basically have no wave function, no probability of finding the particle at all. The particle is essentially a constraint in region 2 where the potential is absent is 0.

(Refer Slide Time: 07:03)

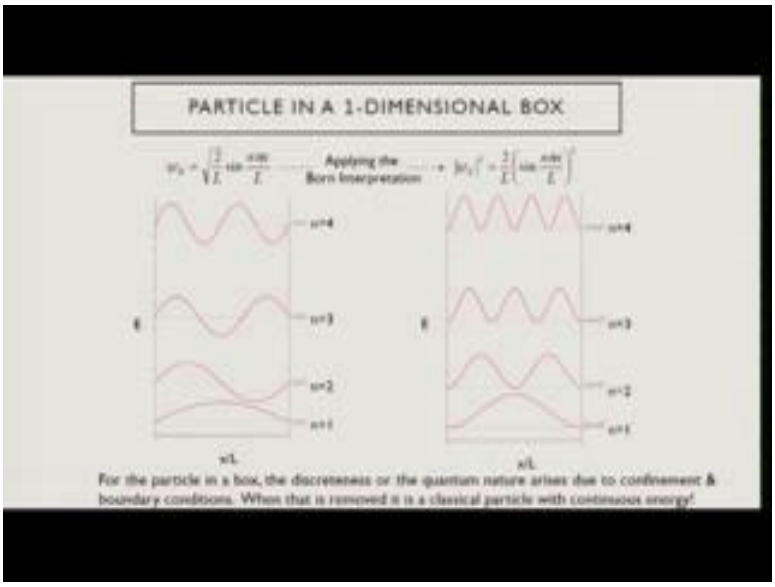


We can use this to find the wave function of this solution and this is similar to the general deferential equation or the wave equation and we have a generalized solution which is a sin and co sin function of which will give the solution and we can then apply the boundary condition which is that at both X is equal to 0 and X is equal to L, our wave function has to vanish so psi has to go to 0. We can apply that and for both the cases and what we find is, there are 2 conditions that we can apply and then we can find the energy levels. And we often use H over 2 pi as our H cross, and we can finally get to our energy levels which is E equal to N square H square over 8 M L square; L being the length of the box and M being the mass of the particle.

Our new wave function will have the sign function part because there co sin part has gone to 0, but what is the part which we can normalize and if we normalize we get A equal to root 2 over L. Our normalize wave function is given here. In this way, the particle in a box solution is done. Previous styles when we looked at it, we basically assumed that you were already knowing these solutions, but with time of evolution of

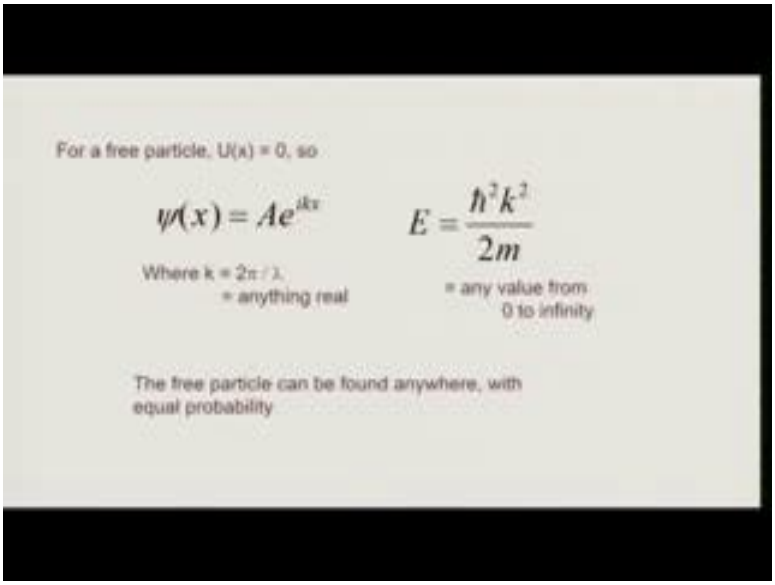
these course we have come to realize it is better that we also sometimes give you the background materials that it can become clear as we go along.

(Refer Slide Time: 08:51)



What we realize is that there are these wave functions which are discrete at discrete energy states and that exist only within the box. And the square of the wave function gives raise to the probability of finding the particle. This is the interpretation which we talked about earlier, which is known as the born interpretation, and for the particle in the box the discreetness or the quantum nature arises due to the confinement and boundary conditions that is what we found out.

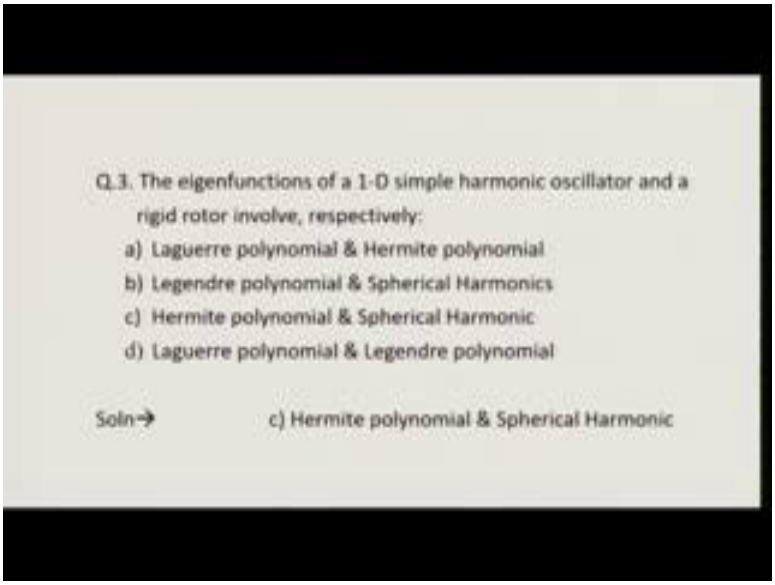
(Refer Slide Time: 09:29)



But when it is removed, it is a classical particle with continuous energy which means we have a free particle where our energy is potentially 0. We just get this solution, which is a free wave function, which can have any direction. The particle can go anywhere, it can be found anywhere with equal probability as well as the energy values can take any values continuous values from 0 to infinities.

So that is what the solution to the problem was that when we removed the constrain of the particle box, then the particle becomes a free particle and it can be found anywhere with equal probability as well as with continuous energy. This is our revisit to the particle in a box.

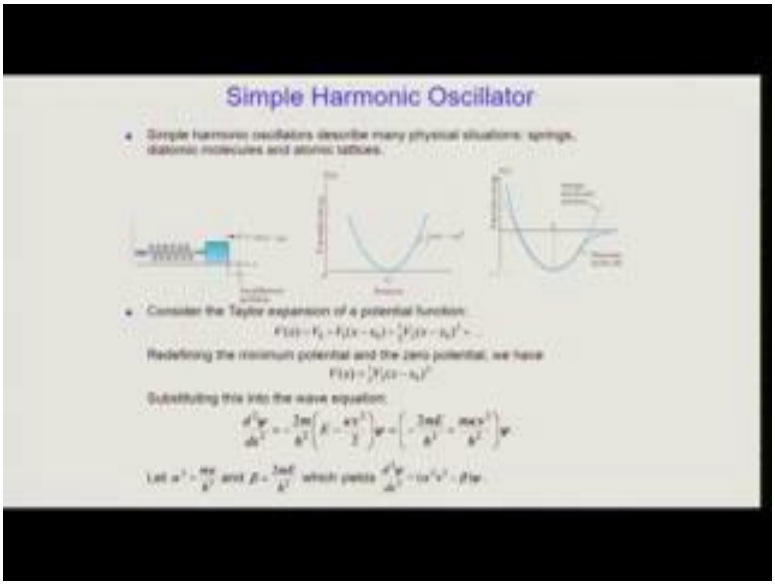
(Refer Slide Time: 10:16)



In the next problem, enable us to revisit the harmonic oscillator and the rigid rotor part. The question essentially asked as to the form of the solution for the Eigen functions of the 1-D simple harmonic oscillators and the rigid rotor would involve what kind of polynomials. Now this is possible to be known if you have an idea, would have the solutions for these Eigen functions of simple harmonic oscillator and rigid rotor are.

The solution is given here because that is what we had told you before, but I do not think we had really gone through again the details of these solutions of the harmonic oscillator or the rigid rotor which we now show you for clarity.

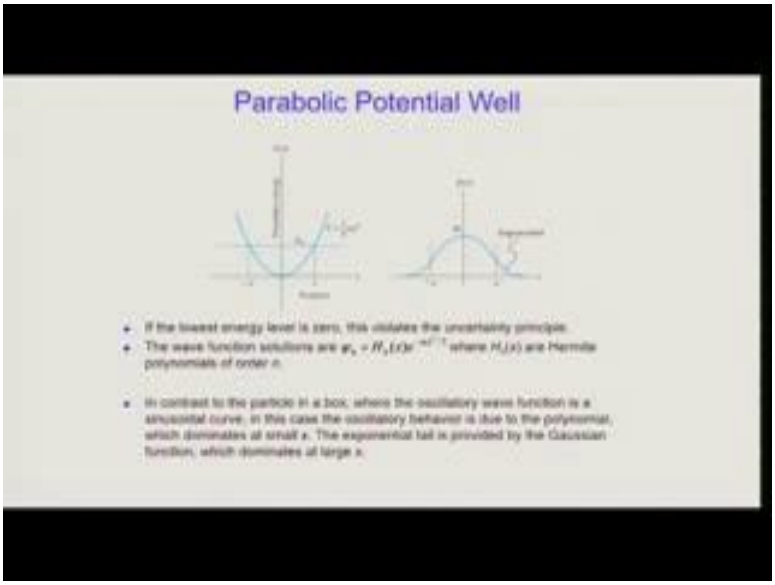
(Refer Slide Time: 11:05)



A simple harmonic oscillator is simply a particle, which is held, which has a spring constant K and is undergoing a displacement in terms of the applied force F. The force is the restoring force. The force is the restoring force which is trying to bring back the particle to its position and we get this potential with respect to position which is quadratic in nature. And we can do a tailor expansion of the potential function to redefine the minima of the potential. And the 0 potential we find that the potential can be written in terms of half V 2 X minus X 0 square, and when we substitute these to the wave equation we are able to get this wave equation solution that we are used to.

This sort of brings you back to the original problem that we have talked about. And here we have therefore given you the values of the beta as well as the alpha which are often used in these contexts. This is a very good depiction of a diatomic molecule in many ways the bottom of the potential for a diatomic molecule roughly follows the simple harmonic motion which we show in this particular graph for you.

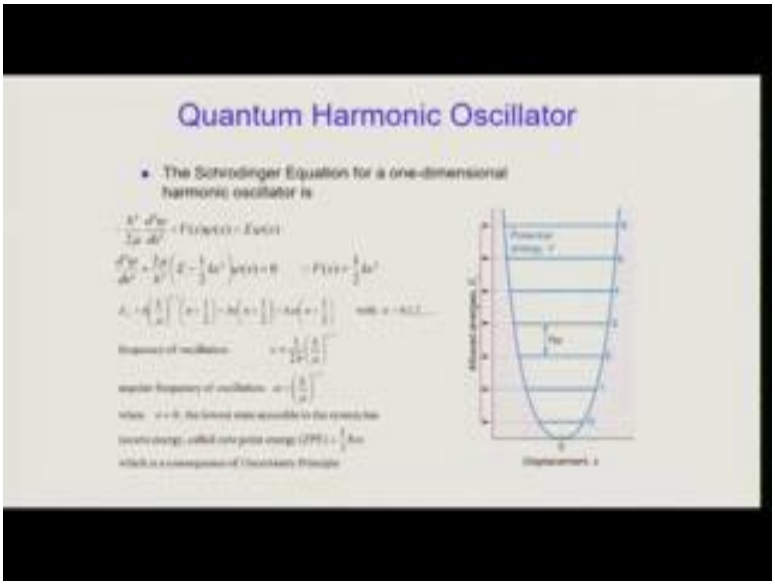
(Refer Slide Time: 12:28)



This parabolic potential well enables us to bound the system and if the lowest energy level of the system is set to 0 it would violate the uncertainty principle because, it is not possible to have a system completely well defined because in this particular case when it is only under vibrational mode, all the other motion processes can go to 0 and it will violate, the principle that it can be defined in a specific position. So that is why it has to have a certain value, and the wave functions solutions are in terms of the Hermit polynomial which is psi N H N X E to the power minus alpha X square over 2 which is where it is shown; where the H N X is the hermit polynomial of order N.

In contrast to the particle in a box problem, where the oscillator wave function is sinusoidal curve, in this case the oscillatory behavior is due to the polynomial which dominates at small X. The exponential tail is provided by the Gaussian function which dominates at large X. And so there is a competition between the 2 which makes this wave function look the way it is.

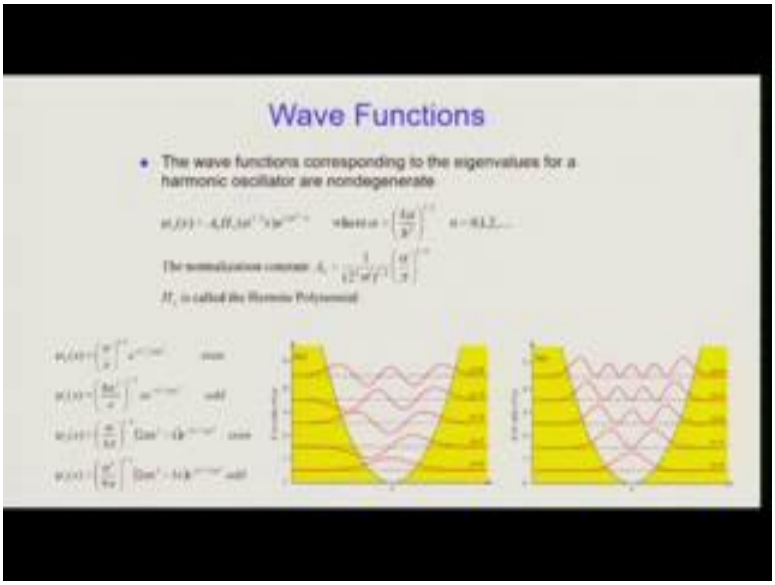
(Refer Slide Time: 13:56)



In order to understand it a little better, let us look up the quantum harmonic oscillator in slightly more detail here. The Schrodinger equation for a 1-Dimensional harmonic oscillator can be written in the simplest possible form, in 1-Dimensions just this X is the dimension here one displacement, and we can write the Schrodinger equation which can be than re written to solve for the problem. And the V as we know is already we have seen in the earlier cases is half K X square, because my restoring force is minus K X.

The energy for this can be found out to be H cross omega N plus half with N going from 0 to all the way up, but because half H cross omega is always going to be there, there is a 0 point energy. The frequency of oscillation is 1 over 2 pi root force constant K over mu, mu is the reduce mass of the system. The angle of frequency of the oscillation omega is basically 2 part omega, and when we look at the 0 point energy it is as I mention half H cross omega. And this sort of provides the fact that we can have the 0 point energy in this case to be non 0 because of the consequence that you have to follow the uncertainty principle, you cannot determinately say where the particle is at any point of time.

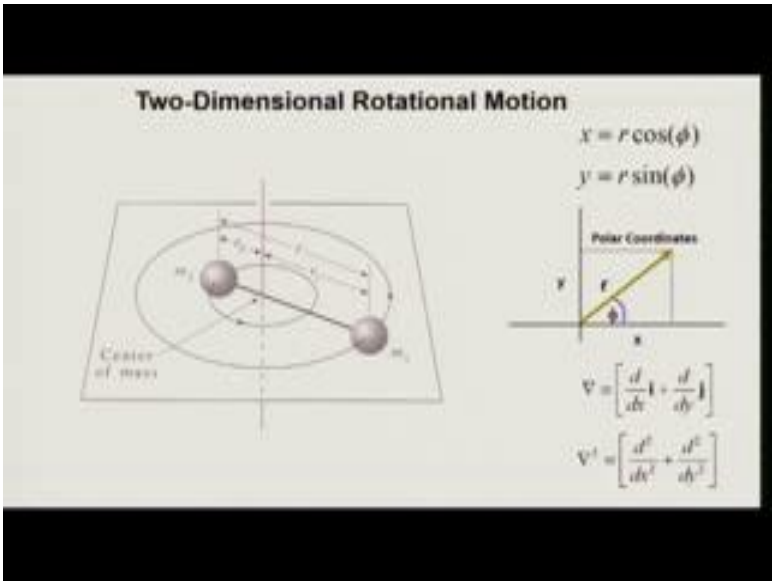
(Refer Slide Time: 15:37)



The wave functions corresponding to the Eigen values for the harmonic oscillator are non degenerate and they have the form as we have been saying earlier also. This type with a polynomial as well as a Gaussian function exponential which happens to be a Gaussian and these polynomials are known as the hermit polynomial.

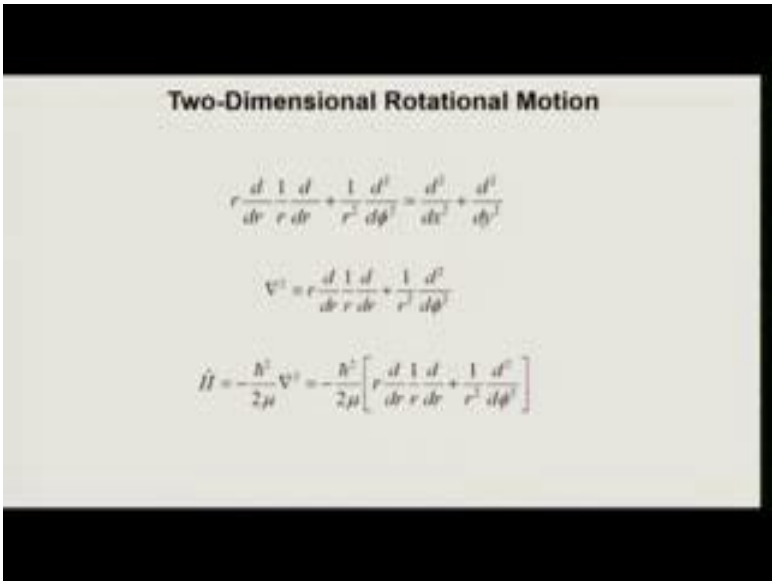
There is a normalization factor also N which is been shown here and we find that each of these wave functions go between even odd even odd kind of a feature. All the even ones are even functions, whereas all the odd N values are odd functions. That is how these wave functions are. And we can see that it here in terms of the picture that we have shown here.

(Refer Slide Time: 16:23)



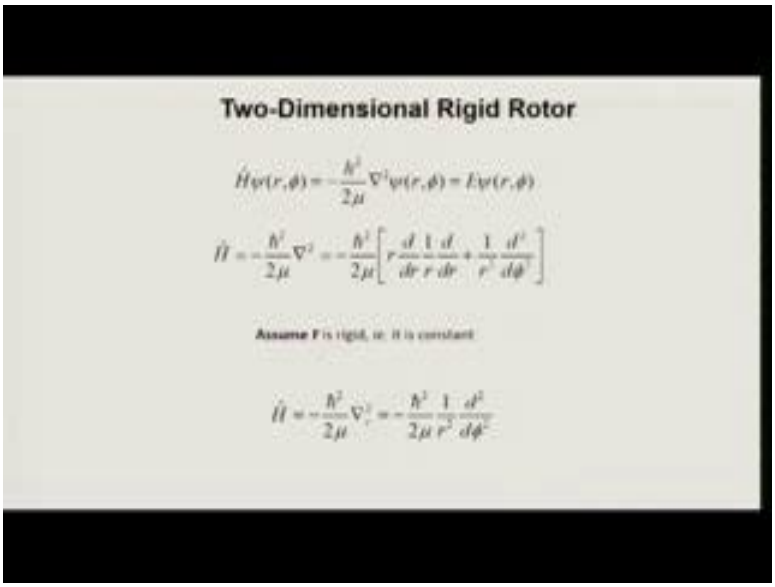
Once we know that the harmonic oscillator problem is a hermit polynomial, now let us look into the rotational motion problem. And as we know the smallest; I mean the first possible rotational rigid root of problem would be a 2 dimensional rotation because whenever we rotate we involve 2 dimensions. Here is the picture which shows that 2 particle which are rotating, it has a center of mass and now this is a center of mass problem in contrast to the reduce mass problem that we saw in the last problem of the vibrating particle, vibrating system which was simple harmonic oscillator. And here in this case the center of mass problem would be represented in terms of the 2 dimensional rotation with the easiest to deal with this in terms of polar coordinates, because the for rigid rotor, the R which is the radial distance is going to be constant. The radius is not going to change, so one of the coordinates can be easily handle compare to the other.

(Refer Slide Time: 17:33)



The 2 dimensional rotation motions can be written in terms of the radial coordinates, and the Hamiltonian can therefore be written in terms of the radial coordinates. And the particle is constraint its rotation and there is no external potential working on it.

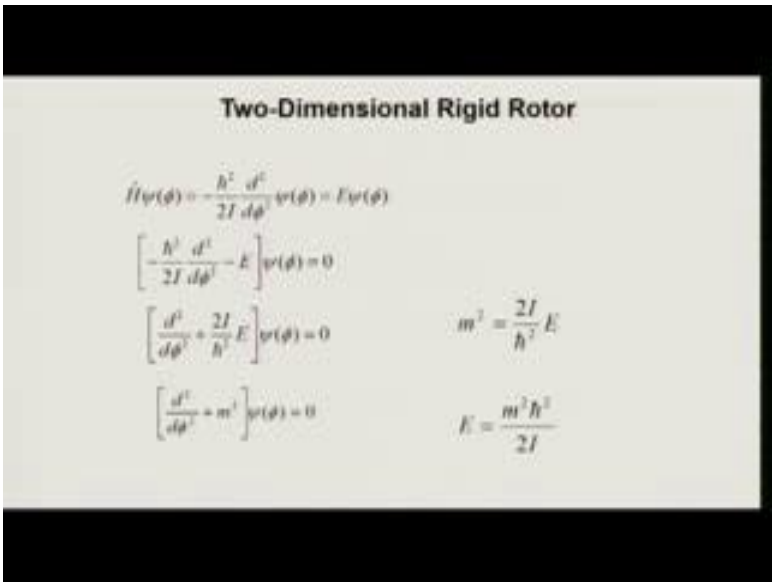
(Refer Slide Time: 17:46)



It is just their kinetic energy of the system, so it is H cross 2 mu central mass minus H

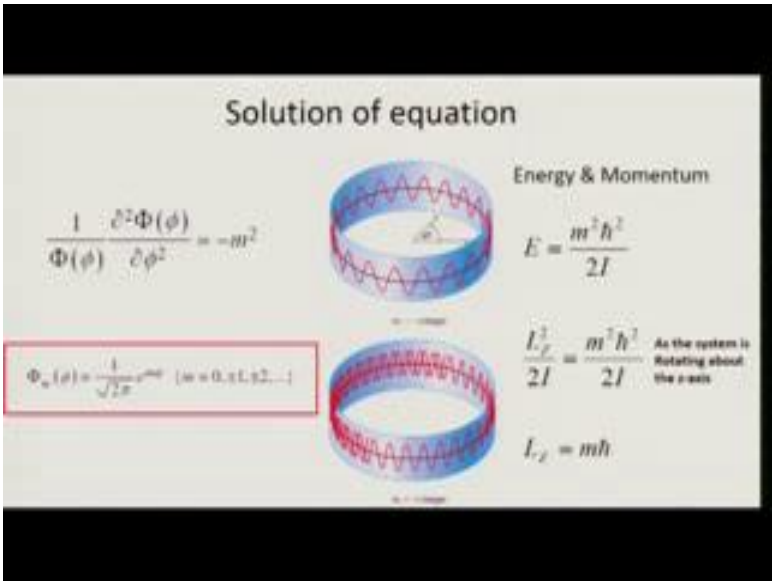
cross 2 mu L square, which is going to be written in terms of the angular coordinates, which is what is written. And since the R is going to be rigid that it is the rigid rotor, so it is going to be constant. We are only going to have the variation coming due to the phi angle the angular motion. And therefore, although it is a 2 dimensional problem it reduces to a single dimensional nature.

(Refer Slide Time: 18:31)



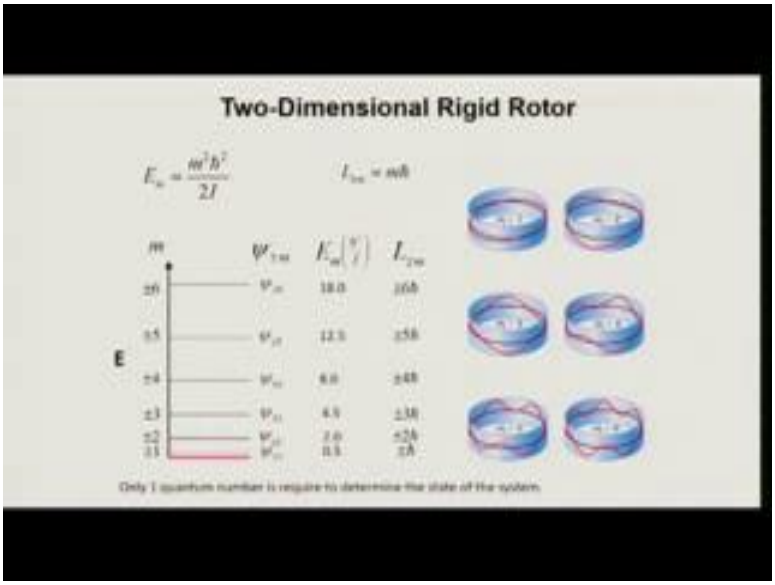
Then we can solve the single dimensional problem by using the Schrodinger equation, and once we apply the S psi equal to E psi form here and in this case the variable is on the phi which is the rotating angle then we can find how this constrain is going to work, because at every 2 pi the particle is going to retrace its parse and that is its constrain. So we can put the boundary conditions and we can find out how the energy and the quantum numbers vary for these kinds of problems. The quantum number is N and this is the rotational rigid rotor problem.

(Refer Slide Time: 19:10)



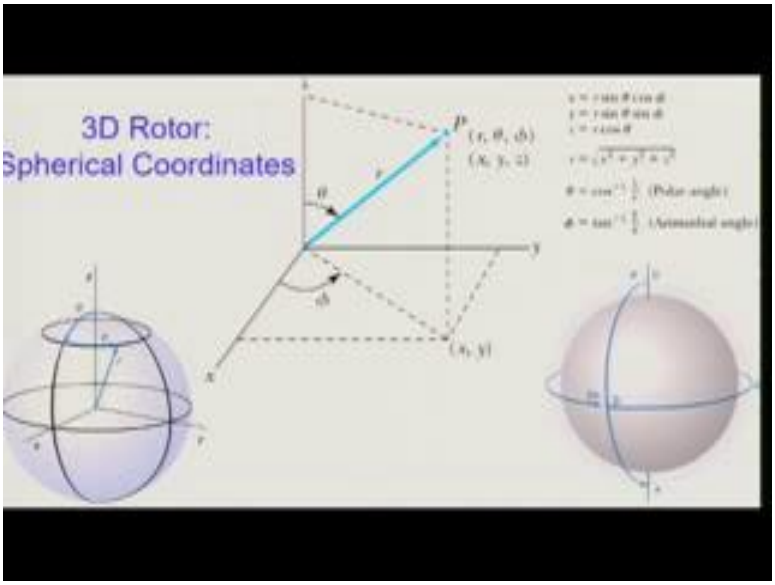
The solution can be taken in terms of this form. And the solution of this is phi, this is the angular part of the motion which is been shown the wave function, angular wave function. And the corresponding energy and momentum can be found out by this process where the energy is M squad H squad over 2 I,I is the momentum of inertia of this system. And since it is rotating about the Z axis then it is the L Z square is the good angular momentum, so it is L Z is the one which is conserved so it is M M H cross is the L Z operator.

(Refer Slide Time: 22:02)



For the 2 dimensional rigid rotor we have this solution that we are already familiar with, but here we have try to showed you how to get to it. And what we find is that it is dependent on the angular momentum and the operator for that is L Z M where we are getting all these values from. Only 1 quantum number is required in this case to determine the state because the radial part is constant and we have kept it as a constant. This is the solution that we have used.

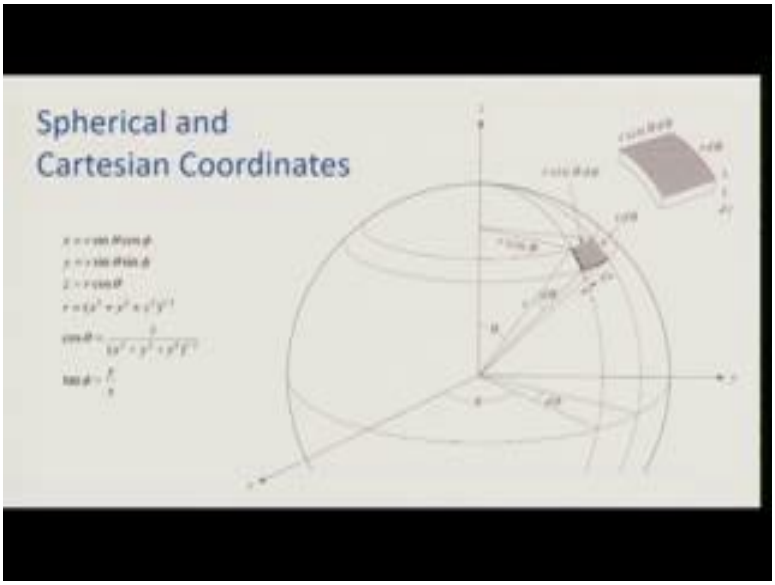
(Refer Slide Time: 20:33)



And when instead of using 2 dimensional motions if it is allowed to move in all the 3 dimensions then it a 3D rotor and we have to use spherical coordinates. And in terms us spherical coordinates it is curious to note that while 2 pi is the motion that we need to do for the rotation constrain to be put in, along the other dimension all you need to do is to move which is the theta angle that corresponds to just a pi rotation which can then generate all the rest of the motions which is what is being shown here in these 3 dimensional cartoons.

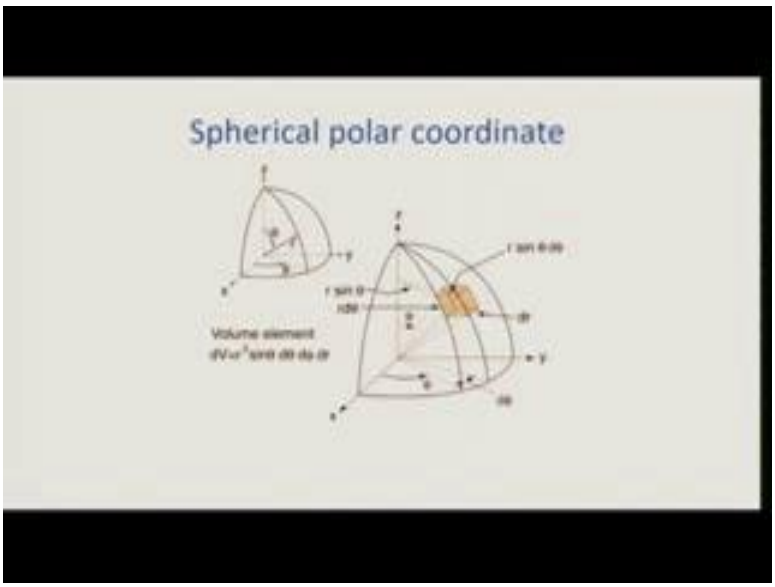
And the theta angle is constrain to go between 0 and pi, whereas the 5 angle is going to go between 0 2 to pi. And the radial part, the radius R is going to be given by the 3 coordinates root of that and we can use this to get to our coordinate system.

(Refer Slide Time: 21:35)



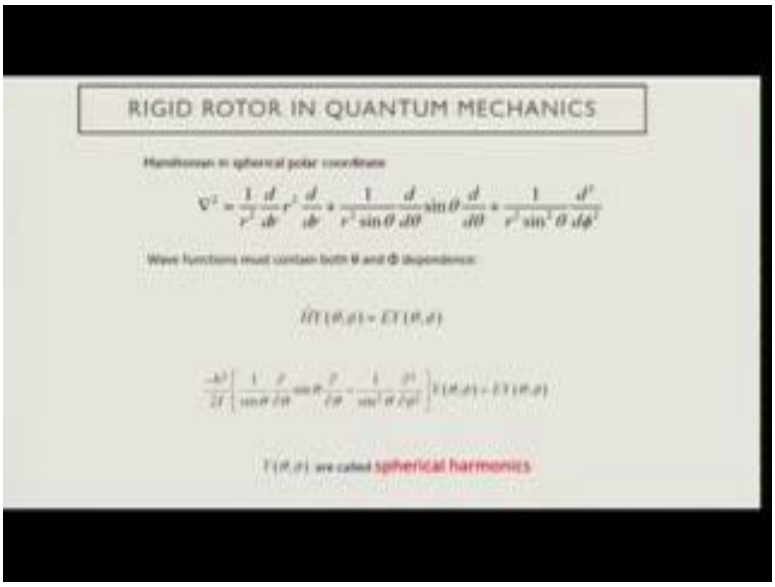
And the parallel between the spherical and the Cartesian coordinate can be utilized to get to know the volume element, which is being described here. And we can make a parallel between this which is being shown in this graph, where we have made the volume element which is being created because of this motion and the D theta, D R and D 5 are the dimensions that we are looking at when we do the volume element.

(Refer Slide Time: 22:08)



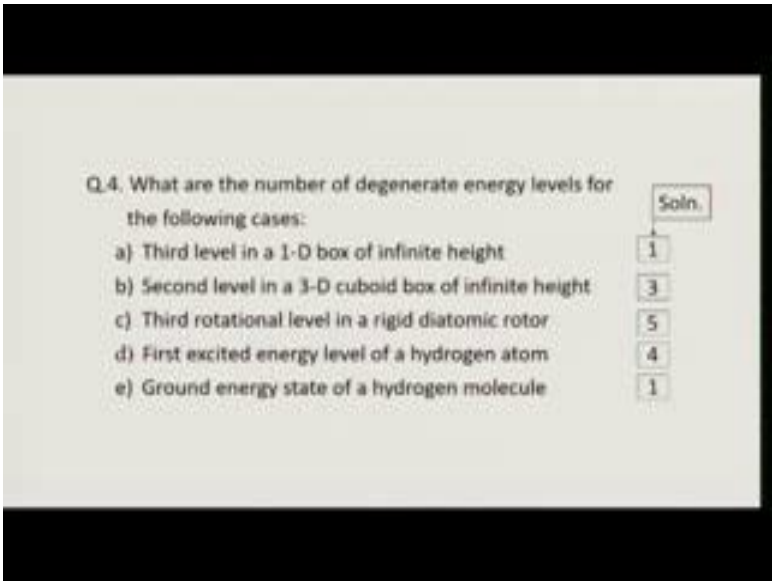
The spherical polar coordinates minimum volume element would therefore, be given by this D B where it can have this elements which is been looked at; R D theta, R sin theta, D phi and as result we get and D 5, so we get R square sin theta D, 5 D theta and D R.

(Refer Slide Time: 22:38)



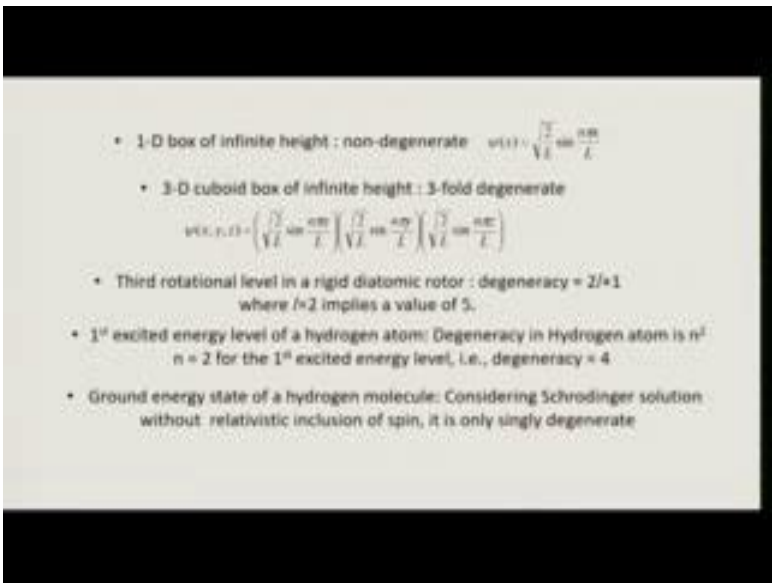
The rigid rotor in quantum mechanics can be written in this form where the spherical coordinates Hamiltonian would be having the form which is given here, the wave function must contain both theta and pi now, because we are now having 2 different coordinates. And when you solve for this, we will be getting the solution which is why theta and 5 which are known as spherical harmonics. And this is the solution which was given to this problem when it was been asked and this background information is something which I thought is important for you to at least be able to be familiarized yourself to go along with this.

(Refer Slide Time: 23:20)



The next question, concept of degeneracy of the energy levels were been asked and looked at in order to ensure that you understand how this is done. All these different cases that have been studied has been looked at 1-D box, 3D cuboids box, third rotational level in a rigid diatomic rotor, first excited energy level of a hydrogen atom and ground energy state of a hydrogen molecule.

(Refer Slide Time: 23:56)



How do you address this? This is to essentially look at what are the possible degeneracy's that can arise in each of these problems. For a 1-D box of infinite high, there is only one possibility of getting the answer, because the numbers of parameters available are only as gone to be one which is 1-Dimensional X, and it is a single process so it is non degenerate set. The 3D cuboids box of infinite length would have 3 parameters left, 3 parameters dependence because it is a 3D condition it is X Y Z which is there and it is 3 fold degenerate and will be having the degeneracy as 3.

The third rotational level in a rigid diatomic rotor, will have a degeneracy of 2 L plus 1, because each of the L values which is corresponding to the theta rotation can take 2 plus 1 values because for each L value which can go from 0 to N minus 1 there are correspondingly minus L through 0 to plus L number of degeneracy. And so for a third rotational level of a rigid diatomic rotor L is equal to 2 0 1 2 and our degeneracy is going to be 2 times 2 plus 1 which is 5.

The first excited level of a hydrogen atom would correspond to the degeneracy, because we know that for the hydrogen atom which is coming later in this review also where we look at the development and treatment of the hydrogen atom. The degeneracy of the hydrogen atom is N squared. And so for this particular case which is the first excited energy level of hydrogen, where N starts from the first case N equal to 2, and we have a degeneracy of 4. The ground energy state of a hydrogen molecule would be singly degenerate when we consider that Schrodinger solution without relativistic inclusion of spin, because in our particular case of solution of the Schrodinger equation we only have 3 quantum number; N, L and M l. For this particular case, when we do not include the spin part it will only be singly degenerate, because for a given N value, the ground state of the system we will only have N equal to 1 will only have one particular degeneracy which is N squared 1 squared is 1.

Based on this what we have done is, we have managed to reflect some of the initial parts of the discussion that we have been looking at. As we go along because we have only covered say 4 of the different concepts that we tested in week 2 problem set. We will be looking back and reviewing the rest of the problems in the subsequent lecture. Where we will be able to see how many more of those concept that are necessary to be looked at

once again, because at the time of implementation all of these are being assumed to be known to you, when we are going through the steps.

This particular process right now that we are going through is very critical for you to be able to understand and be able to address all the problems that we are currently doing and be able to understand the principle of the implementations that we are doing in terms of quantum complete. See you in the next lecture.