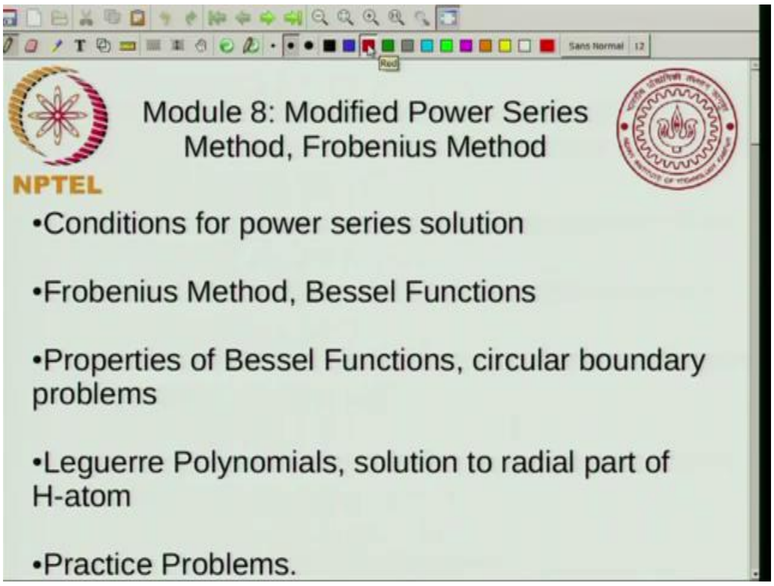
Mathematics for Chemistry
Prof. Madhav Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Module - 08
Lecture - 40
Practice Problems

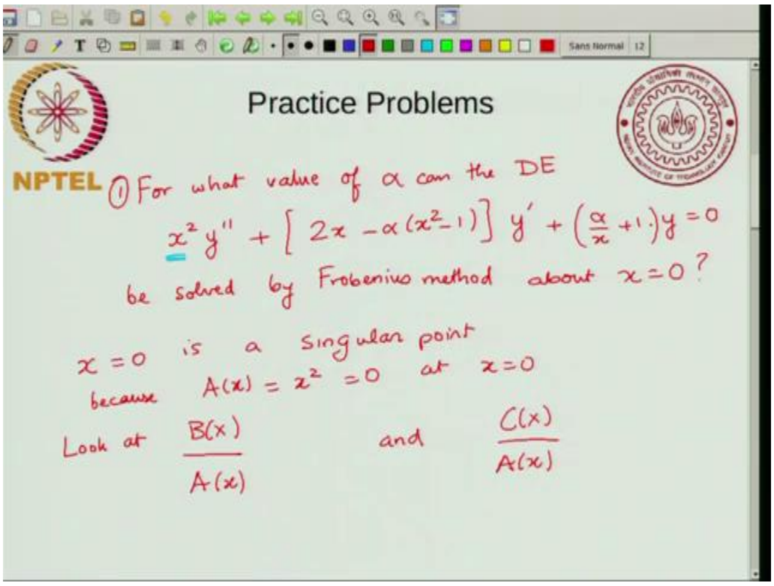
(Refer Slide Time: 00:17)



So we will conclude this module and this course with some practice problems. Now before I start the practice problems, I just want to mention that you know where we have done this Frobenius method and it is a very general method and there are a very large number of problems that can be solved using the Frobenius method. You can write down any number of differential equations and try to solve them using the Frobenius method you can write down a differential equation by yourself make sure that it is that you can solve it using the Frobenius method and try to go ahead and solve it.

So, in that sense I do not want to; I would not be doing those kind of practice problems, what I will just show you I will just show you a couple of examples where of fairly straightforward practice problems that that you can get, but you know for those who are interested in learning more and getting used to these you can you can make up all kinds of practice problems or you can even look them up in various books.

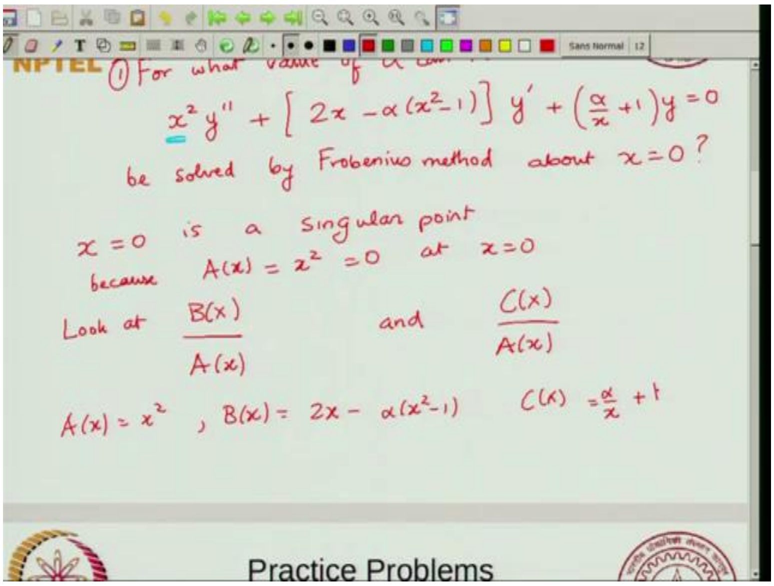
(Refer Slide Time: 01:21)



So, let me do; I will do a couple of short practice problems. So, the first one is has to do with the use of the Frobenius method. So, I will just state the problem. So, for what value of alpha can the differential equation x square y double prime plus 2 x minus alpha x square minus 1 y prime plus alpha by x plus 1 y equal to 0? So, we solved by Frobenius method about x equal to 0. So, basically why I am asking that for what should be the condition on alpha? So that, you can use the Frobenius method to solve about x equal to 0; now you can clearly see that x equal to 0 is a singular point because A of x equal to x square equal to 0 at x equal to 0.

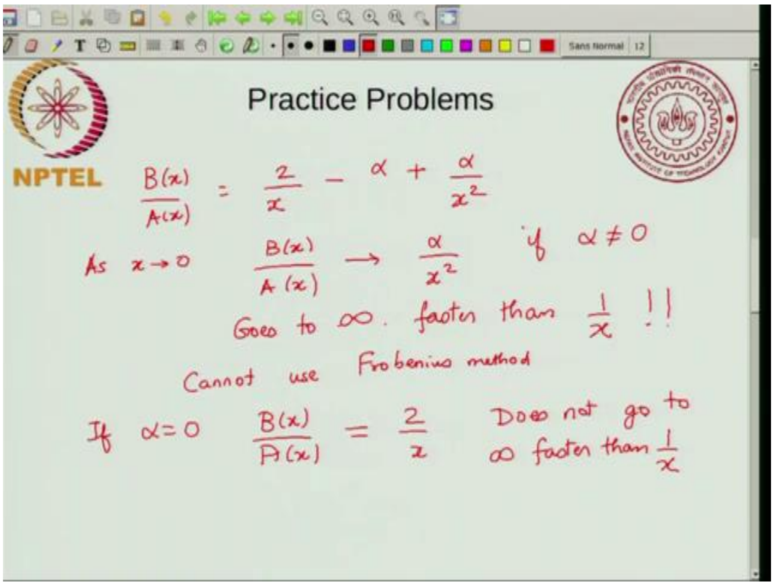
So, clearly since this same that is multiplying y double prime is x square and that goes to 0 at x equal to 0. So, x equal to 0 is a singular point. So, then what should you do you look at D of x divided by A of x and C of x divided by A of x.

(Refer Slide Time: 03:25)



So, B of x is basically 2 x minus alpha x square minus 1 C of x is alpha by x plus 1 and A of x is x square. So, we look at these 2 and then we decide whether you can use the Frobenius method and what should be the condition on alpha twin in order to use the Frobenius method. So, let me just write that you have A of x equal to x square B of x is equal to 2 x minus alpha x square minus 1 and C of x is equal to alpha by x plus 1.

(Refer Slide Time: 03:48)

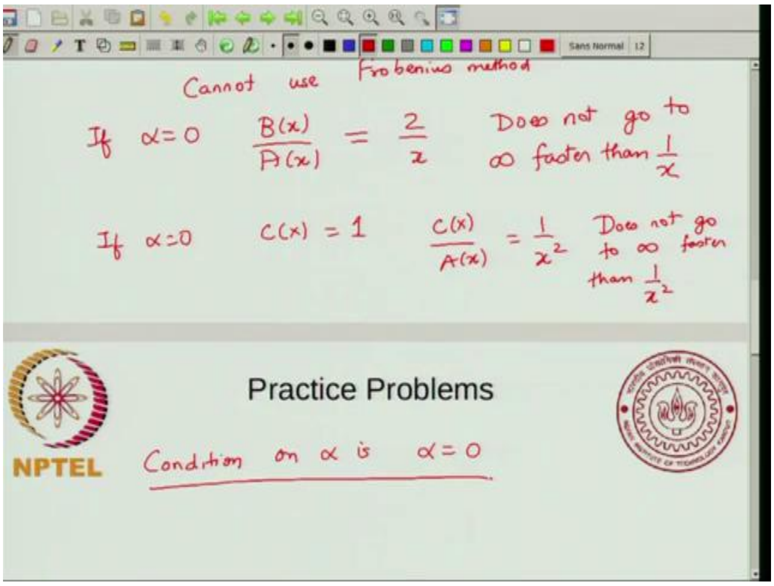


So, suppose I look at B of x divided by A of x. So, that is equal to; so, 2 by x minus alpha times alpha plus alpha divided by x square. So, you have 3 terms.

So, I just opened the alpha times x square minus 1 and I got these 3 terms. So, I divided by x square. So, you get at this, now I deliberately wrote this in this form and you can immediately see you can immediately see the advantage of this. So, as x tends to 0 B by x divided by A by x tends to alpha by x square if alpha is not equal to 0. So, as x goes to 0 alpha by x square is much greater than 2 by x. So, this goes as 1 by x this goes as a constant whereas, this is going to infinity. So, alpha by x square is the largest term as x goes to 0. So, if alpha is not equal to 0 then B by x by A by x goes as alpha by x square. So, this goes to 0 faster than 1 by x. So, this goes to 0 faster than one by x and so, you cannot use the Frobenius method. So, that immediately says that cannot use Frobenius method.

So, when can you use a Frobenius method? If alpha equal to 0 then B by x B of x divided by A of x goes as 2 by x. So, this does not go to 0. So, this does not go to 0 then go to 0 goes to infinity does not go to infinity faster than 1 by x. So, if alpha equal to 0, it appears that at least at least the B by x by a by x is fine what about the C by x by A by x. So, C of x is alpha by x plus 1 can now alpha equal to 0 then it is just 1.

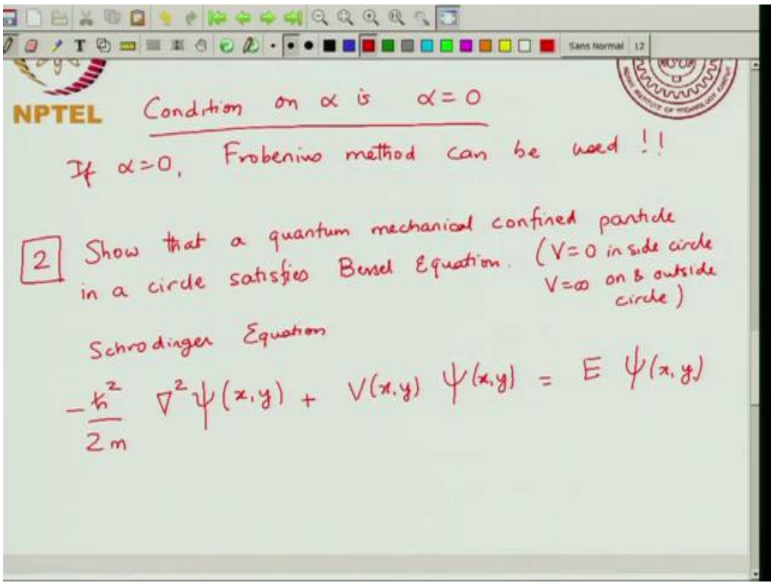
(Refer Slide Time: 06:31)



So, if alpha equal to 0, C of x equal to 1 and what you get C of x divided by A of x equal to 1 by x square and this does not go to 0 faster than 1 by x square. So, it goes to 0 as fast as 1 by x square, but not faster, similarly this goes; go to infinity I am sorry, I am making this mistake repeatedly, but it should be go to infinity.

So, C by x by A by x does not diverge faster than 1 by x square, similarly B by x by A by x does not diverge faster than 1 by x.

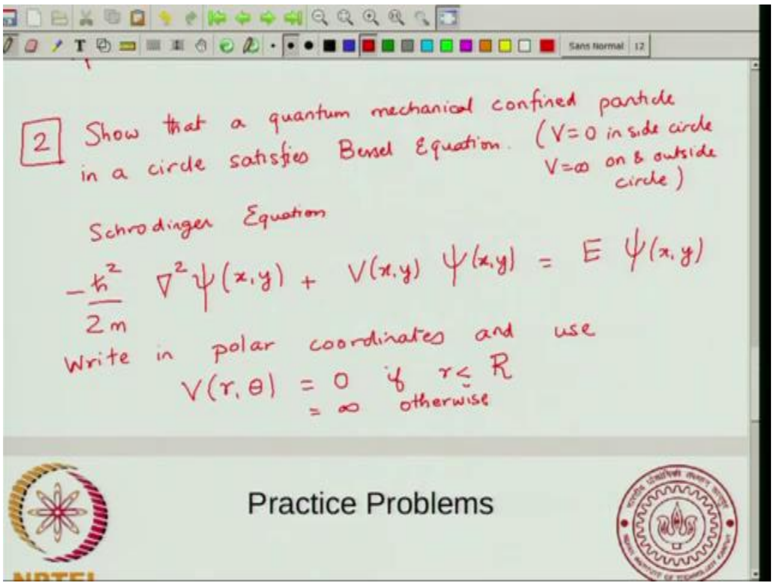
(Refer Slide Time: 07:20)



So, the solutions; so the condition on alpha is alpha equal to 0. So, if you want to use the Frobenius method then alpha has to be equal to 0. So, if alpha equal to 0, Frobenius method can be used. So this was the first problem, now the second problem and here we will focus on setting up the problem. So, show that quantum mechanical confined particle in a circle satisfies Bessel equation. So, the particle in a circle, the typical quantum mechanical particle in a circle satisfies special equation and you know I have not stated the entire question, but you should say that V equal to 0 inside circle V equal to infinity on and outside circle.

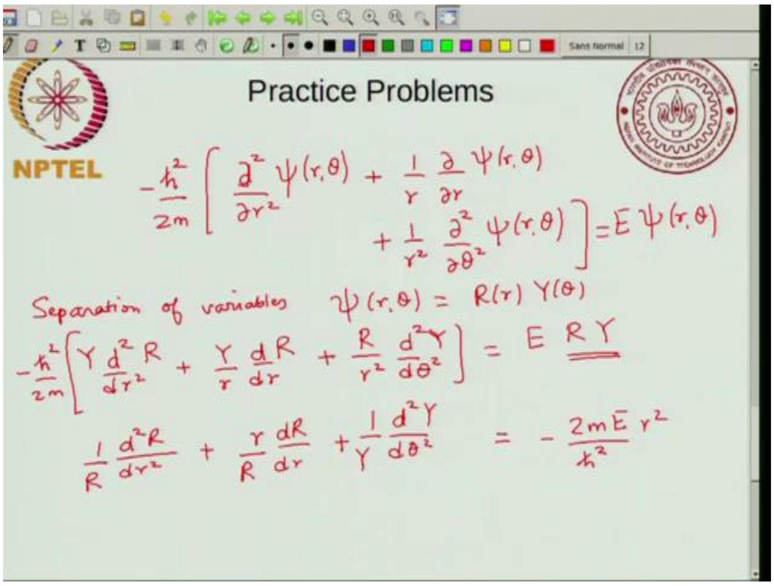
So, that is the condition just like the particle in a box you can have particle in a circle and what I am asking you is to show that this satisfies Bessel equation something that looks like a Bessel equation. So, your Schrodinger equation, now we have minus h bar square by 2 m. Now you have a Laplacian in a; you have a Laplacian, I will just write it as del square psi and psi is a function of x y. So, I will write this plus V of x y psi of x y is equal to E times psi of x y. So, this is the Schrodinger equation.

(Refer Slide Time: 10:04)

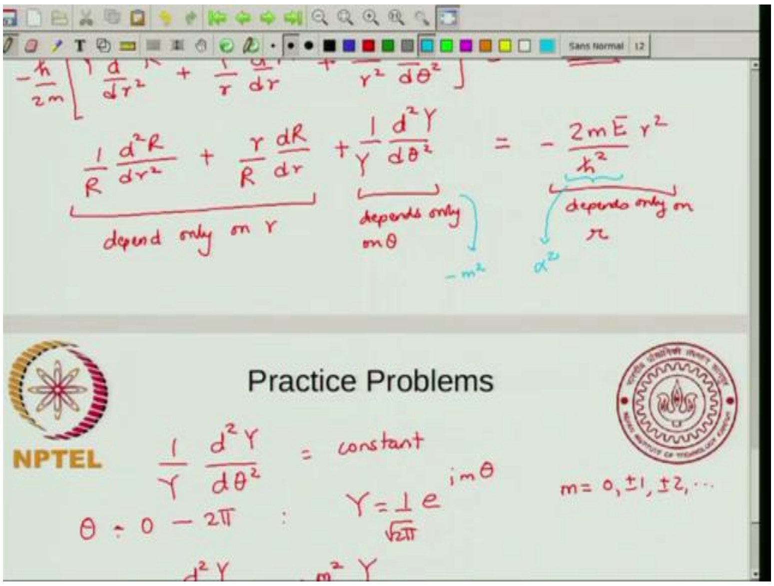


Now, what we do is we will write this in. So, write it in write in polar coordinates in it and use V of V of r theta equal to 0 if r is less than some radius I will call the radius as capital r and equal to infinity otherwise. So, if r is greater than that radius then it goes to infinity. So, what we do is just like in the particle in a box what you need to do is to write this Laplacian in polar coordinates and you need to set V equal to 0 inside the box.

(Refer Slide Time: 10:59)



(Refer Slide Time: 14:08)



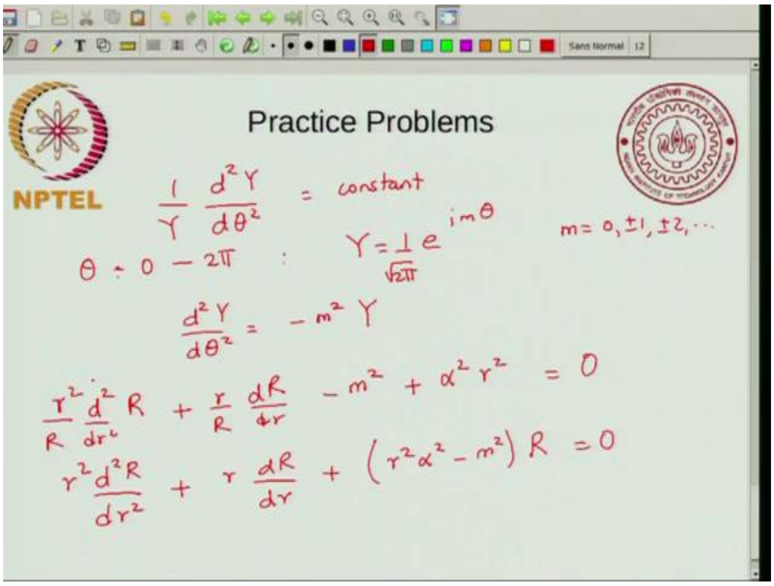
So, what you will get is minus h cross square by 2 m now you will get the Laplacian in polar coordinates we have already seen that. So, we have d square or dou square by dou r square of psi. Now psi is a function of r theta plus 1 by r dou by dou r of psi of r theta plus one by r square dou square by dou theta square psi of r theta is equal to E times psi of r theta. So, this is the Schrodinger equation that you have and now suppose you do a separation of variables. So, separation of variables, so, what you will say is psi of r theta is equal to I will say R of r times I will just say Y of theta.

Now, when I substitute in this, what I will get is minus h cross square by 2 m, now I will get d square by d r square of r and you will have the Y outside plus y by r d by d r of R and then you have plus Y by or rather in this case, you will get R by r square d square by D theta square of Y, Y is only a function of theta and this should be equal to E times R times Y and if you divide by this if you; let us say you multiplied by r square. So, suppose I multiplied by r square and divide by R Y divided by capital R times capital Y then what I will get is the following I will and let me take this 2 m E by h cross square on the right.

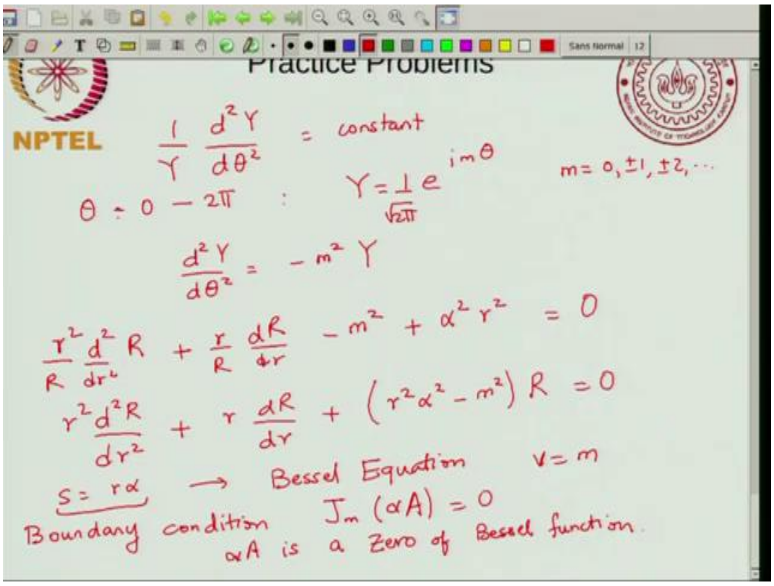
So, what I will get is minus 2 m E by h bar square and I will multiply by r square. So, I will just multiply by r square. So, I will have this and I have divided by R Y. So, I would not have the R Y term and what I get here is d square r by d r square times 1 by r plus r times d r by d r and divided by r plus d square y by d theta square times 1 by Y. So, what you have? So, you get an equation of this form. So, we just rewrote the Schrodinger equation of the separating variables, now what is the advantage of this is that these 2 terms depend only on r this depends only on theta and the right hand side depends only on r.

So; that means, this theta dependence has to be a constant because if we, if it is a function of theta then the right hand side; there is no function of theta, left hand side cannot be a function of theta. So, this has to be a constant.

(Refer Slide Time: 14:48)



(Refer Slide Time: 18:13)



So that means, you immediately get d square Y by d theta square into 1 by Y equal to constant and we have seen this earlier we have seen this earlier when we were do when we are dealing with spherical harmonics since theta goes from 0 to 2 pi. We can write this in the following form y is equal to E to the I m theta and there is a factor of one by root 2 pi, but I would not bother that.

So, if I can write 1 by root 2 pi E to the I m theta where m is equal to 0 plus minus 1 plus minus 2 and so on. So, we have this and then you can immediately see that d square Y by d theta square is just minus m square Y, it is just minus m square Y. So, now, you can take this and you can substitute in this equation and you can replace this whole quantity by just minus m square. So, what you are going to do is to replace this by minus m square and for convenience let me just call this alpha square, I will just call it alpha square it is a positive number. So, then what I will get is I can write my equation in the following form. So, this equation I can write as 1 by r d square by d r square of r plus what I have is r by r d r by d r.

So, that will be as it is. So, r by r d r by d r and then and then what you have is this quantity is just minus m square. So, then I just write this as m square. So, this is just minus m square. So, what you have here is just minus m square and this and I will I will bring the alpha to the; to this side. So, I will just write it as alpha square r square alpha square r square. So, plus alpha square r square equal to 0, so suppose I just multiply by capital R then what I will get is d square R by d r square plus r d r by d r k plus r square, I will alpha square minus m square times r equal to 0 I just check once again make sure I got all the factors. So, oh when I multiply by r square there should be an r square here sorry there should be an r square here there should have been an r square here that is good. So, you have an r square here and you have this r square here.

So, just to say it again, so, I wrote I multiplied out by r square I should have an r square here. So, I forgotten to write that, but now we can see that once we put that then you get this exactly like the; so if you want you can just make a change of variables from you can just put s equal to r alpha if you want you do not have to do it so, but if you do that then you can immediately see that you will get a an you will get a Bessel equation v equal to m you can get a Bessel like equation and when we would have expected this because what because the problem that we have the quantum mechanical particle confined to a circle is just like a circular drum.

So, you have a Schrodinger wave equation with the with the drum boundary conditions and incidentally you can verify that if R is actually limit change the change the label for the radius I will just call it a is the label for the radius you can verify that that the boundary condition will basically be related to j m of alpha a equal to 0. So, basically alpha will be related to the roots of the Bessel function so; that means, alpha A should be A is a 0 of the Bessel function. So this is how you get; you solve the problems with circular boundary conditions and indeed it is because the 0s appear at distinct levels at distinct points that you actually get the quantization of this circular of this particle on a circle.

So, with this, I will stop here. So, I will stop and I hope I have been able to show you some of the nice applications of the Frobenius method in chemical problems through this and I hope that through this course, we have been going quite fast, we have been doing lot of topics. But hopefully if you have taken this entire course and you will feel confident enough to practice all these problems or to practice more problems on your own and to go ahead and try to actually solve try to solve various drop problems in especially in quantum chemistry with this knowledge of a mathematics.

Thank you.