

**Basic Quantum Mechanics**  
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**Module No. # 09**

**The JWKB Approximation & Applications**

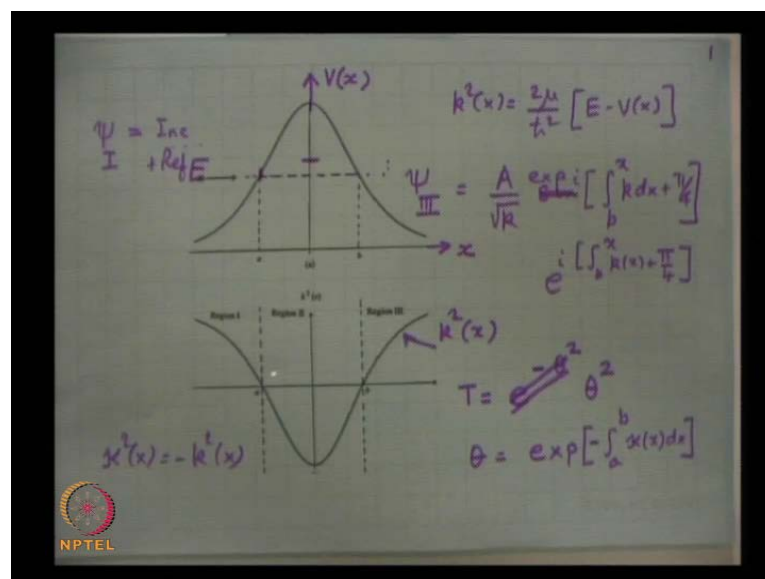
**Lecture No. # 5**

**JWKB Approximation: Justification of the Connection Formulae**

We have been discussing the JWKB approximation and I have given the solutions of the JWKB, in the JWKB approximation of the differential equation. Today, we will continue our discussions on that. We will consider one small problem in tunneling probability calculation. Actually, we will assign a problem and then we will discuss the generality of the WKB approximation. And, we will show that it can be used to solve a general class of differential equations.

Finally, we will give a heuristic treatment of the justification for the connection formulae. So, first we will start with the tunneling through the barrier problem, which we had discussed in considerable detail. And, we had considered a potential energy variation, which was something like this.

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So, this is the  $V$  of  $x$ , a particle of energy  $E$  of mass  $\mu$  is incident and this is the energy level and there were two turning points. Now, the  $k^2$  of  $x$ ;  $k^2$  of  $x$  is equal to  $2\mu$  by  $\hbar^2$  cross  $E$  minus  $V$  of  $x$ . So, since it is the inverse of minus sign of  $x$ , so  $k^2$  of  $x$ , this is the variation of  $k^2$  of  $x$ . And,  $x$  is equal to  $a$  and  $x$  is equal to  $b$  are the turning points.

So, here you will have oscillatory solutions, here you have exponential solutions and here you have again oscillatory solutions. So, what we did was in region three, we gave as, we wrote down a solution like this:  $A \exp\left(\int_b^x k dx + \frac{\pi}{4}\right)$

Actually we wrote the solution. We can write down the solution as sin and cosine. So, instead, what we did was we consider an outgoing plane wave. So, we had exponential  $i$  times this. So, actually I should write it down as  $E$  to the power of  $i \int_b^x k dx + \frac{\pi}{4}$  and wrote it as cosine plus sin. Then, used each of them to hop from this turning point here and then we looked at the turning point  $x$  is equal to  $A$ . And then, when we hopped through this turning point and obtained solutions here. and, the region, the solution and the region 1 was expressed as an incident wave plus as a reflected wave. And, we compared the coefficients and we found out that the transmission coefficient was equal to  $e$  to the power of minus  $\theta^2$ , where  $\theta$  was equal to exponential.

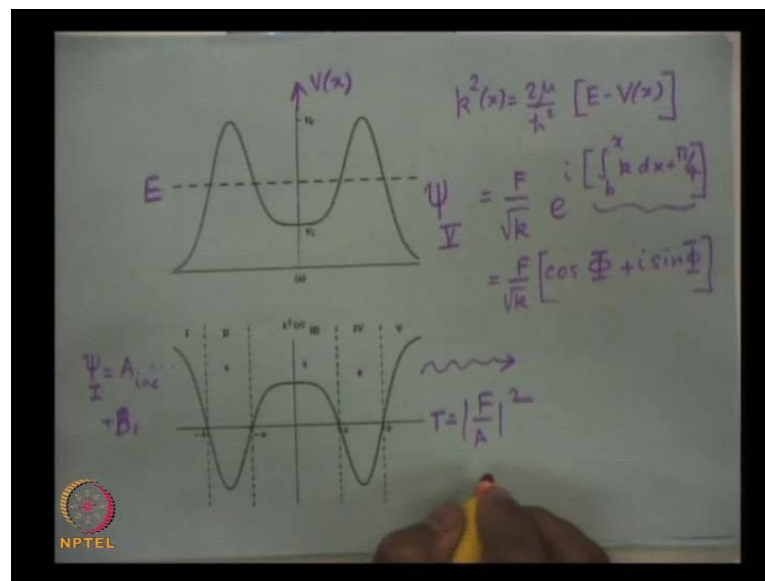
So, I am sorry, the transmission coefficient was  $\theta^2$  and  $\theta$  was equal to exponential minus  $a$  to  $b$   $\kappa$  of  $x dx$  because in the region of  $a$  to  $b$ ,  $k^2$  of  $x$  is negative. And so, therefore, we define  $\kappa^2$  of  $x$  which was equal to minus  $k^2$  of  $x$ .

And, using that, and therefore using this relation we discuss the two, three problems; one, the tunneling through a parabolic barrier, then we discussed the tunneling through the triangular barrier and also to the  $\alpha d k$  problem. But, I wanted to tell you today that, if we have a double potential like this and which has two peaks like the one that I have shown here and I assume the energy  $E$  and the  $V$  of  $x$  is variation like this. Then the corresponding  $k^2$  of  $x$ , which is given by  $k^2$  of  $x$  is once again  $2\mu$  by  $\hbar^2$  cross  $E$  minus  $V$  of  $x$ . And, it will be something like this. So, there will be four turning points now.

Now, then what we have to do is, we have to first start with the solution in the region five. So,  $\psi$  in region five will be an outgoing wave. So, we write down this as  $F e^{i \int_b^x k dx} + \frac{\pi}{4}$ . So, I write the solution here, which I write as  $F \sqrt{k}$ , cosine of the same argument, cosine of this argument. So, let us suppose this is, say I write as  $\Phi + i \sin \Phi$ .

And then, use connection formulae to go to the region four, then we look toward the turning point  $a$  and I go over to the region three and then we look to turning point minus  $a$ . And then, use the connection formulae to get to region two and then to region one. It is a very systematic process, very straight forward process. And, I would urge all of you, who want to learn the tricks of using the connection formulae, work this out yourself. It will help you to use the WKB JWKB approximation with tremendous efficiency and simplicity. It is very simple. You just have to get used to using these connection formulae.

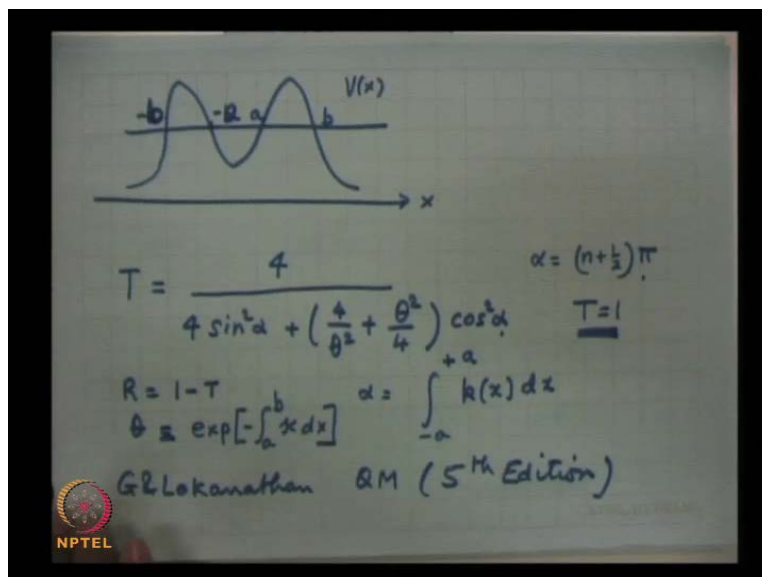
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And, finally in region one, you express the solution as  $A$  times the coefficient of the incident wave plus  $E$  to the... and then you have the  $B$ , which is the coefficient to the reflected wave. And then, you will have  $F$  by  $A$  whole mod square will be tunneling probability. And, if you calculate that, you will find that the tunneling probability comes out to be... Let me write this expression. The, if you have a double humpty and these are

the two turning points minus a minus b, plus a and plus b. This is the  $V$  of  $x$  variation, this is the  $V$  of  $x$  variation as a function of  $x$ .

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The slide shows a handwritten diagram of a potential energy curve  $V(x)$  on a coordinate system with  $x$  on the horizontal axis. The curve has two turning points at  $x = -a$  and  $x = b$ . Below the diagram, the following formulas are written:

$$T = \frac{4}{4 \sin^2 \alpha + \left( \frac{4}{\theta^2} + \frac{\theta^2}{4} \right) \cos^2 \alpha} \quad \alpha = \left( n + \frac{1}{2} \right) \pi \quad T = 1$$

$$R = 1 - T \quad \theta = \exp \left[ - \int_a^b \kappa(x) dx \right] \quad \alpha = \int_{-a}^b k(x) dx$$

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So, if you work this out and I would urge all of you to work this out. The tunneling probability comes out to be  $4$  by  $4 \sin^2 \alpha$  plus  $4$  by  $\theta^2$  square plus  $\theta^2$  square by  $4 \cos^2 \alpha$ . And then, similar expression for  $T$ ; and, you will find that  $R$  plus  $T$  is equal to one, so that the reflection coefficient is  $1$  minus  $T$ .

What are the values of  $\alpha$  and  $\theta$ ? The value of  $\alpha$  is minus  $a$  to plus  $a$ . **sorry**. This is minus  $a$  and this is minus  $b$ . I am **sorry**. So, you have here; **let me** let me do this here. So, this is minus  $a$  and this is minus  $b$ . I hope all of you can see this. **All of you can see this**. So, the transmission coefficient becomes, so the  $\alpha$  is equal to minus  $a$  to plus  $a$ . And, between minus  $a$  plus  $a$ ,  $k$  square of  $x$  is positive. So, this is  $k$  of  $x$   $dx$ . And then,  $\theta$  is defined to be equal to exponential minus  $a$  to  $b$   $\kappa$   $dx$ . As I mentioned to you, you first start with an outgoing plane wave here, outgoing wave here, then you hop to this region, then you hop to this region, then you hop to this region, then you hop to this region. And, in each hopping, you use the **W** JWKB connection formulae.

The remarkable feature of this simple formula is that, when  $\alpha$  is equal to  $n$  plus half  $\pi$ , **when  $\alpha$  is equal to  $n$  plus half  $\pi$** , then  $\cos^2$  is equal to  $0$ ,  $\sin^2 \alpha$  is  $1$ . So,  $T$  is equal to  $1$ . These are known as the **Fabry-Perot transmission resonances**. **Fabry-Perot transmission resonances**. And, no matter what the shape of the potential

variation be. The transmission coefficient is unity. These corresponds to, **these corresponds**, this is alpha is equal to n plus half pi. These are the Eigen values corresponding to the **well**.

So, those energy Eigen values which form for this particular well, you have transmission resonances. These are the modes, which resonate back and forth between the well. And, you **have an** unity transmission coefficient. So, to conclude that, for a double well, double hump potential well of the type shown here, you have, **sorry**, double. So, the... I would advice all of you to work out step by step, the tunneling probability.

It is the details, if you are unable to do that, the details are given in our book by myself and professor Lokanathan on Quantum Mechanics fifth edition. So, the details are there also, but I would like to, like you to work this out. And, obtain an analytical expression for the tunneling probability. And, this tunneling probability becomes equal to 1, irrespective of the shape of the potential structure when alpha becomes equal to n plus half pi. And, those are known as the Fabry-Perot transmission resonances.

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$$k^2(x)$$

$$\frac{2}{\sqrt{k}} \sin \left[ \int_a^x k dx + \frac{\pi}{4} \right] \Rightarrow \frac{1}{\sqrt{x}} \exp \left[ - \int_0^x x dx \right]$$

$$\frac{1}{\sqrt{k}} \cos \left[ \int_x^a k dx + \frac{\pi}{4} \right] \Rightarrow \frac{1}{\sqrt{x}} \exp \left[ + \int_0^x x dx \right]$$

$$\frac{d^2 \psi}{dx^2} + k^2(x) \psi(x) = 0$$

$$x \approx a \quad k^2(x) \approx -\alpha (x-a)$$

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Now, we then, we then go over to calculating justifying the connection formulae. **Justifying the connection formulae**. For example, if you have a k square of x variation like this, **this** is the k square of x variation, **k square of x variation**. And, you have a 0, so that on the right side of the turning point, you have exponential solution. And, on the left side, k square of x is positive. So, we have sin and cosine solution. And, we had said

without proof that  $2$  by root  $k$ , let us suppose the turning point is  $x$  is equal to  $a$ , then  $2$  by root  $k$  sin of  $x$  to a  $k$  d  $x$  plus  $\pi$  by  $4$ . It goes over to an exponentially decaying solution; minus exponential minus  $a$  to  $x$  kappa d  $x$ . And similarly, we had  $1$  over root  $k$  cos of  $x$  to a  $k$  d  $x$  k of  $x$  d  $x$  plus  $\pi$  by  $4$ . It goes over to the exponentially amplifying solution; so,  $1$  over root  $k$  exponential plus integral  $a$  to  $x$  kappa of  $x$  d  $x$ .

Now, I want to justify this. Now, near the turning point, near the turning point I can assume that the variation of  $k$  square of  $x$  is linear. So, the equation that we wanted, that we have been wanting to solve is  $d^2 \psi$  by  $d x$  square plus  $k$  square times  $\psi$  of  $x$  is equal to  $0$ .  $k$  square of  $x$ , actually  $k$  square of  $x$ .

Now, we assume that in the vicinity of the turning point. So, at  $x$ , around  $x$  is equal to  $a$ , we assume that  $k$  square of  $x$ . In this case, it is decreasing function of  $x$ . So, we say that this is equal to minus  $\alpha$  of  $x$  minus  $a$  approximately, so that in the vicinity of the turning point, we assume a linear variation for  $k$  square of  $x$ .

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$$\frac{d^2 \psi}{dx^2} - \alpha(x-a) \psi(x) = 0$$

$$z = \alpha^{1/3}(x-a) \quad \frac{d\psi}{dx} = \frac{d\psi}{dz} \cdot \alpha^{1/3}$$

$$\boxed{\frac{d^2 \psi}{dz^2} - z \psi(z) = 0} \quad \text{AIRY Equation}$$

$$k^2(z) = -z$$

$$z \geq 0 \quad k^2(z) = z$$

$$k(z) = \sqrt{z}$$

$$\frac{d^2 \psi}{dz^2} - k^2(z) \psi(z) = 0$$

$$\frac{1}{\sqrt{x}} \exp\left[\pm \int k(z) dz\right]$$

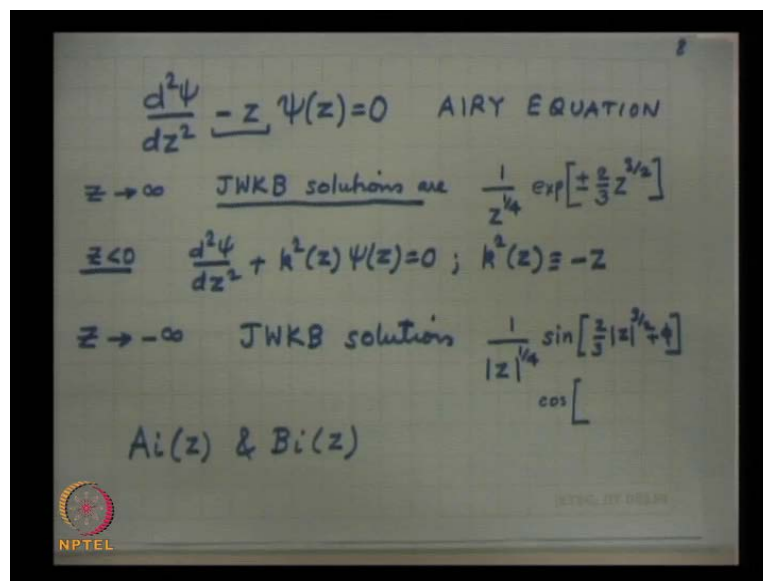
$$\frac{1}{z} \exp\left[\pm \frac{2}{3} z^{3/2}\right]$$

So therefore, my Schrodinger equation or the wave equation becomes  $d^2 \psi$  by  $d x$  square minus  $\alpha$  into  $x$  minus  $a$   $\psi$  of  $x$  is equal to  $0$ . Now, I make a transformation I make a transformation that  $z$  is equal to  $\alpha$  raised to the power of  $1$  by  $3$  into  $x$  minus  $a$ . Then  $d \psi$  by  $d x$ , then  $d \psi$  by  $d x$  will be  $d \psi$  by  $d z$  into  $d z$  by  $d x$ . That is,  $\alpha$  to the power of  $1$  by  $3$ , then  $\alpha$  to the power of  $2$  by  $3$  and then you will have  $x$  minus  $a$  is  $z$  by  $\alpha$  to the power of  $1$  by  $3$  and so on. You do that and you

will obtain  $\frac{d^2 \psi}{dz^2} - z \psi = 0$ . This equation, this equation is known as the Airy equation after the name of the British astronomer G. B. Airy.

This is and the solution of this, the rigorously correct solution of these equations is known as the Airy functions. Now, first let me write down. So, here in this case  $k^2$  of  $z$  is equal to  $-z$ . So, for  $z$  greater than 0, I must write  $k^2$  of  $z$  is equal to  $-z$ . And,  $k^2$  of  $z$  will be equal to  $-z$ . So that, for  $z$  greater than 0, this equation becomes  $\frac{d^2 \psi}{dz^2} - z \psi = 0$ . Now, since  $k^2$  of  $z$  is equal to  $-z$ , so  $k$  of  $z$  is square root of  $-z$  and square root of  $-z$  is equal to  $z$  to the power of  $1/4$ . Now, the WKB solutions of this equation are  $\frac{1}{z^{1/4}} \exp\left[\pm \frac{2}{3} z^{3/2}\right]$  exponential plus minus integral  $z^{3/2} dz$ . So, if I integrate this  $z^{3/2} dz$ , this will be exponential plus minus  $\frac{2}{3} z^{3/2}$ . And, outside it will be  $z$  to the power of  $1/4$ .

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Handwritten notes on a slide showing the Airy equation and its solutions:

$$\frac{d^2 \psi}{dz^2} - z \psi = 0 \quad \text{AIRY EQUATION}$$

For  $z \rightarrow \infty$ , JWKB solutions are  $\frac{1}{z^{1/4}} \exp\left[\pm \frac{2}{3} z^{3/2}\right]$

For  $z < 0$ ,  $\frac{d^2 \psi}{dz^2} + k^2(z) \psi = 0$ ;  $k^2(z) = -z$

For  $z \rightarrow -\infty$ , JWKB solution  $\frac{1}{|z|^{1/4}} \sin\left[\frac{2}{3} |z|^{3/2} + \phi\right]$

$\cos\left[\right]$

$Ai(z) \text{ \& } Bi(z)$

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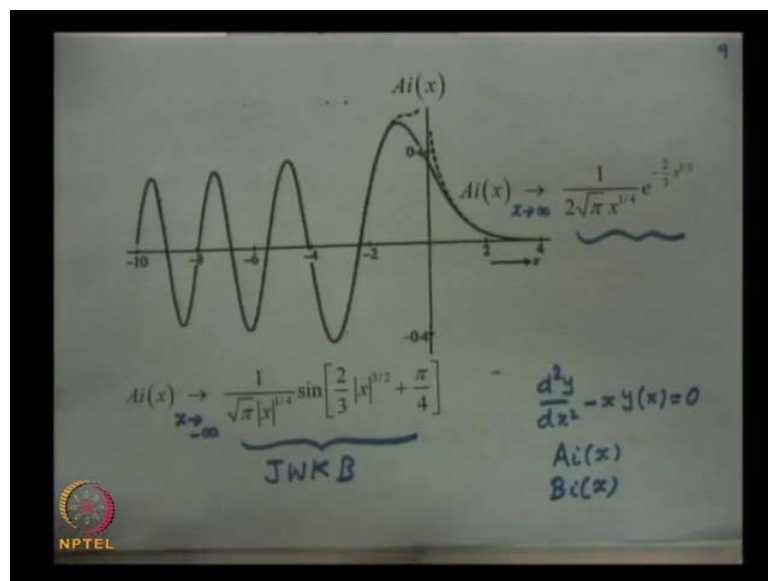
Therefore, therefore, the, of this equation  $\frac{d^2 \psi}{dz^2} - z \psi = 0$ . As  $z$  tends to infinity, the JWKB solutions are  $z$  tends to plus infinity. JWKB solutions are plus minus  $\frac{1}{z^{1/4}}$  exponential plus minus  $\frac{2}{3} z^{3/2}$ ; small  $z$  everywhere.



Now, for  $z$  less than 0, this is positive. Minus  $z$  is positive. So, I must write it as  $d^2 \psi$  by  $dz^2$ , plus  $k^2$  of  $z$  is equal to  $\psi$  of  $z$  equal to 0, where  $k^2$  of  $z$  is defined to be equal to minus of  $z$ . And then, as  $z$  tends to minus infinity,  $z$  tends to minus infinity, the JWKB solution are the JWKB solutions are  $1$  over  $\text{mod } z$  because now it becomes minus  $z$  mod  $z$   $1$  to the power and then sin or cosine, sin and similarly cosine and two-third plus minus you can have, mod  $z$  to the power of  $3/2$  plus  $\phi$ . And, similarly you can have the cos solutions.

So, the... So, of this equation, of this is the, as I mentioned this is the Airy equation. This is the Airy equation and obvious Airy equations. The WKB solutions are exponential this and that. Now, of the Airy equation, the rigorously correct solutions are denoted by  $A_i$  of  $z$  and  $B_i$  of  $z$ . These are known as the airy functions, which are related to Bessel functions. which are related to Bessel functions.

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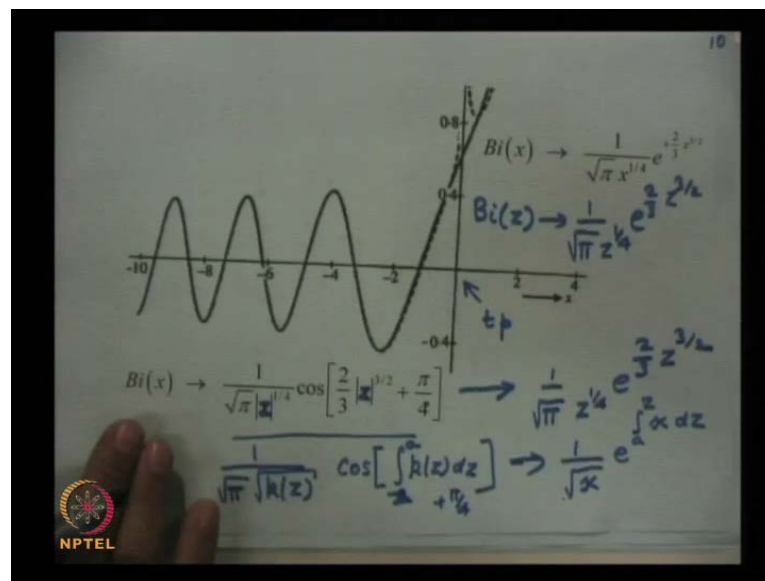


Now, the airy functions are the this solid line. You see, actually this is not in terms of  $z$ . This is the solution of the equation  $d^2 y$  by  $dx^2$  minus  $x y$  of  $x$ . So, please replace  $z$  by  $x$ . So, of  $A_i$  of  $x$ , the two independent solutions are  $A_i$  of  $x$  and  $B_i$  of  $x$ . And,  $A_i$  of  $x$  has a asymptotic form as  $x$  tends to minus infinity, which is given by this. This I am not proving. But, it can be obtained from the asymptotic forms of the Bessel functions, which must be known to all of you.



Similarly, as  $x$  tends to plus infinity, this is the asymptotic form. If you can read properly, this is exponential minus 2 by 3  $x$  to the power of 3 by 2. Now, these asymptotic forms are the JWKB solutions **are the JWKB solutions**. And so, therefore the sin term goes over to this term.

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Let me first also show you the  $Bi$  function. The other independent solution of this equation is the  $Bi$  function, which are known as the Airy  $Bi$  function. And, the asymptotic form is a cos plus pi by 4 as  $x$  tends to minus infinity. And, these asymptotic forms are plotted if you can see this as a dash line. You see the asymptotic solutions, which are just WKB solutions, they go to infinity at  $x$  is equal to 0; because this is the turning point;  $x$  is equal to 0 is the turning point.

So, here also the asymptotic solutions are shown by the dash line. And, they go to 0. And, the asymptotic solutions are the JWKB solutions. Here, the asymptotic solutions of  $Bi$  of  $x$  is actually, I should have written  $Bi$  of  $z$  goes over to 1 over root pi  $z$  to the power of 1 by 4  $e$  to the power of 2 by 3  $z$  to the power of 3 by 2. And, this also, I should have written  $z$ .

So, these are the same solutions that we had **written** down earlier. You see, exponential plus minus 2 by 3  $z$  to the... So, one can say that cos plus pi by 4 goes over to 1 over

$\sqrt{\pi} z$  to the power of  $1/4$   $e$  to the power of  $2/3$   $z$  to the power of  $3/2$ . This suggests, **this suggests** that, since these are the WKB solutions, therefore  $1/\sqrt{\pi k}$  of  $z$ , under  $\sqrt{k}$  of  $z$   $\cos$  of  $\int k \, dz$ . In this case, the turning point is at 0. So, from turning point say **say**  $z$  to  $a$ , that is 0. And, the turning point is, say  $a$ . This plus  $\pi/4$  goes over to an exponentially amplifying solution. So, this is under root of  $\kappa z$   $e$  to the power of  $\int_0^z$ .

In this case, therefore  $a$  to  $z$   $\kappa z \, dz$ ; so, this is the, we have **we have** tried to justify the connection **formulae** because what we did was, we assumed **the** in the vicinity of the turning point, the solution to be the variation to be linear. When we assume the  $k$  square of  $x$  variation to be linear, then the solutions are rigorously  $A$  of  $x$  and  $B$  of actually not  $x$ ,  $B$  of  $z$ ; where  $z$  is equal to  $\alpha$  to the power of  $1/3$  into  $x - a$ . Then, these are the WKB solutions. And, we showed by comparing the WKB solutions with the actual, with the exact asymptotic forms. We found that the  $\sin$  from  $x$  to  $a$  plus  $\pi/4$  will go over to an exponentially decaying solution and the  $\cos$  term will go over to an exponentially amplifying solution.

So, this is the justification. We assume this to be linear, then the solutions become Airy functions. And, by looking at the asymptotic forms and comparing it with the WKB solutions, we write the connection **formulae**. And, as we have seen **for** to use these connections **formulae**, we will get exact results for the harmonic oscillator problems. And, even for the linear potential, **if** this gives very accurate results. We calculated the tunneling probability using the life time of alpha particle decay and showed the extreme variation. And, there are many comparisons that have been made to compare the validity of the JWKB approximation. And, it has been found as long as  $k$  square of  $x$ ; that is, the potential energy variation is reasonably smooth, then JWKB approximation gives a fairly accurate solution.

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$$p(x) \frac{d^2 y}{dx^2} + q(x) \frac{dy}{dx} + r(x) y(x) = 0$$

$$\frac{d^2 y}{dx^2} + f(x) \frac{dy}{dx} + g(x) y(x) = 0$$

$$\psi(x) = y(x) \exp\left[\frac{1}{2} \int f(x) dx\right]$$

$$\frac{d^2 \psi}{dx^2} + k^2(x) \psi(x) = 0$$

$$k^2(x) \equiv g(x) - \frac{1}{2} \frac{df}{dx} - \frac{1}{4} f^2(x)$$

We finally, end up by saying that a general differential equation of the type  $p$  of  $x$   $d^2 y$  by  $dx^2$  plus  $q$  of  $x$   $dy$  by  $dx$  plus  $r$  of  $x$   $y$  of  $x$   $dx$  equal to 0. I can always write this. I can always write this in the form of  $d^2 y$  by  $dx^2$ , plus  $f$  of  $x$   $dy$  by  $dx$ , plus  $g$  of  $x$   $y$  of  $x$ . Obvious that,  $f$  of  $x$  is equal to  $q$  by  $p$  and  $g$  of  $x$  is  $r$  by  $p$ .

Then, we make two transformations. We make that, let us suppose that  $\psi$  of  $x$  is equal to  $y$  of  $x$  exponential half integral  $f$  of  $x$   $dx$ . I leave this as an exercise for you. And, if you assume  $\psi$  of  $x$  to be given by this and then you differentiate this and use this equation, you will find that  $d^2 \psi$  by  $dx^2$  satisfies this equation;  $k^2$  square of  $x$   $\psi$  of  $x$  is equal 0, where  $k^2$  square of  $x$  is now defined as  $g$  of  $x$  minus half  $d f$  by  $dx$  minus 1 by 4  $f^2$  square of  $x$ .

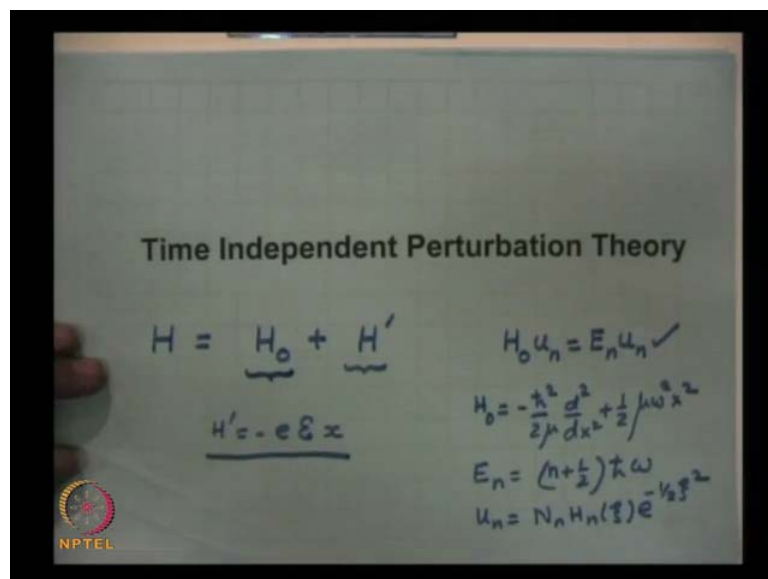
So, what I was trying to tell you is that any second order differential equation of the type shown here, can always be transformed to any equation of this type. Any secondary second order differential equation of this form can always be transform to an equation, rigorously to an equation of this type. And then, we can use the WKB the w k b solutions to obtain approximate solutions of this equation. In fact, one can take the Bessel equation as an example and obtain solutions and they are, they often agree quite well with the exact solutions.

So, first you take, you look at any second order differential equation, try to transform it. Transformed airy differential equation of this type can be transformed to an equation of

this type. And then, **then** one can obtain the WKB solution of that. So, in principle, we have given a recipe for obtaining a JWKB solution of a second order general; second order differential equation of this type. And hence, therefore **w k** JWKB approximation forms of very powerful method for solving the second order differential equations.

That concludes our discussion on the WKB approximation, in which to summarize this is a very powerful method for solving a second order differential equation. In which,  $k^2$  of  $x$  is assume to be a smoothly varying function. It should not be very rapidly varying. It should not have too many zeroes because if it has too many zeroes, then you have to hop from one turning point to the other. But that, in principle, is possible as long as the variation of  $k^2$  of  $x$  is **fairly** smooth. And therefore, it has been extensively used not only in Quantum Mechanics, but in Wave Guide theory in Plasma Physics and in **in** many other areas; diverse area of Physics and Engineering.

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**Time Independent Perturbation Theory**

$$H = \underbrace{H_0} + \underbrace{H'}$$

$$\underline{H' = -eEx}$$

$$H_0 u_n = E_n u_n \checkmark$$

$$H_0 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} \mu \omega^2 x^2$$

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega$$

$$u_n = N_n H_n\left(\frac{x}{\sqrt{\hbar / \mu \omega}}\right) e^{-\frac{1}{2} x^2 / (\hbar / \mu \omega)}$$

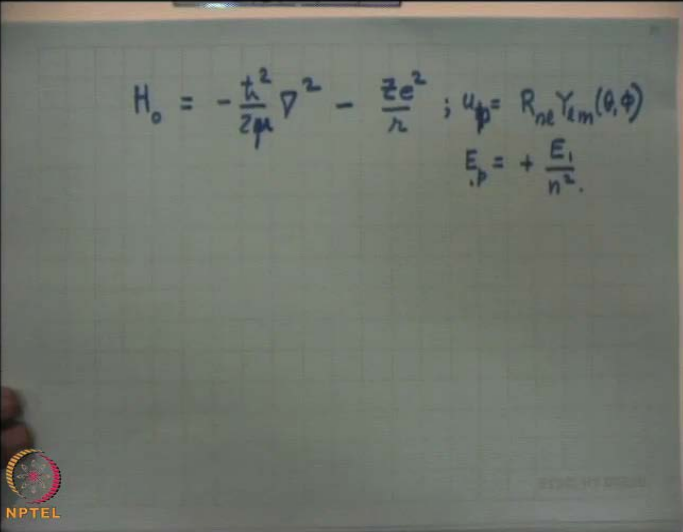
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Our next lecture, in this lecture itself we will continue our discussions on developing and approximate method and that will be the Perturbation theory. We will continue our discussions on yet another very powerful approximate method. And, the method is known as the Time Independent Perturbation Theory. So, we have here in the Time Independent Perturbation Theory. We write the Hamiltonian as a sum of two parts;  $H$  is equal to  $H$  naught plus  $H$  prime.

Now,  $H_0$  is the Hamiltonian for which I know the solutions. So,  $H_0 u_n$  is equal to  $E_n u_n$ . For example,  $H_0$  may be the harmonic oscillator problem, like  $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2$ . Now, ... we know the solutions. So, what are  $E_n$  and  $u_n$ ? The  $E_n$ , we know that is equal to  $n + \frac{1}{2} \hbar \omega$  and  $u_n$ s are the normalized Hermite gauss functions **the Hermite gauss function** or  $H_0$  maybe the Hamiltonian, corresponding to the Hydrogen atom problems.

Now, therefore  $H_0$  is the **is the** portion of the Hamiltonian for which the solutions are known. Then, we add to it another term. And then, we try to calculate the effect of this term. So, for example, we have a charged oscillator. We put it in an electric field. And then, there is a Hamiltonian, which is something like minus, say  $e$  times the electric field times  $x$ .

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$$H_0 = -\frac{\hbar^2}{2m} \nabla^2 - \frac{Ze^2}{r}; u_{nlm} = R_{nl} Y_{lm}(\theta, \phi)$$

$$E_{nl} = -\frac{E_1}{n^2}$$

So, this is the perturbation or, you may have something like the  $H_0$  may represent the hydrogen atom problem, in which it is given by  $-\frac{\hbar^2}{2m} \nabla^2 - \frac{Ze^2}{r}$ . This is  $V$  of  $r$ . So, for this problem, we know that  $u_n$ s are equal to  $R_{nl} Y_{lm}$ . Actually, these are three subscripts here. These are **these are** the wave functions. **These are the wave functions.**

This  $n$  and this  $n$  are different. So, this maybe something like say, we may write as  $u_{nlm}$  or  $u_{pnlm}$ . **u p**  $u_{pnlm}$  is a combined form of these three. And, the  $E_{pnlm}$ , the energy Eigen values

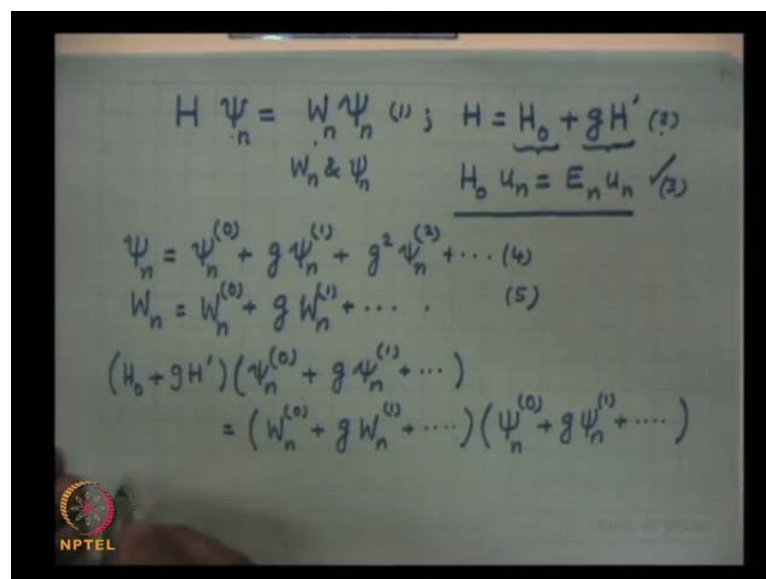
corresponding to be real state will be something like, the energy for the first state divided by  $n$  square. And,  $E_1$  is about minus 13.6 electron  $\mu$ . So, I know the Eigen values and Eigen functions corresponding to  $H$  naught.

Now, I put the hydrogen atom in an electric field. And, they will be a perturbation or in a magnetic field. There will be a they will be an additional term, which will represent the interaction with the electric field and the magnetic field.

So, what will be the effect on the energy Eigen values? This is an extremely important problem in Quantum Mechanics as well as in Atomic and Molecular Spectroscopy. So, and, in any, in most problems of interest, you cannot obtain a direct solution of the, a closed form solution of the Schrodinger equation. And, you have to apply an approximate method. One approximate method, we have already discussed. And, that was the JWKB method in which  $k$  square of  $x$  was assumed to be as slowly varying function.

Here, what we assume is that we have a solution, which is known to us, which is closed to the electric or magnetic field is weak enough, so that it makes a small change in the Eigen value structures of  $H$  dot. So, what we do is the method the method involves in writing the... Let me write it on a fresh page.

(Refer Slide Time: 38: 14)



The image shows a whiteboard with handwritten mathematical derivations for perturbation theory. The equations are as follows:

$$H \psi_n = W_n \psi_n^{(1)}; \quad H = H_0 + g H' \quad (2)$$

$$W_n \psi_n \quad H_0 u_n = E_n u_n \quad (3)$$

$$\psi_n = \psi_n^{(0)} + g \psi_n^{(1)} + g^2 \psi_n^{(2)} + \dots \quad (4)$$

$$W_n = W_n^{(0)} + g W_n^{(1)} + \dots \quad (5)$$

$$(H_0 + g H')(\psi_n^{(0)} + g \psi_n^{(1)} + \dots)$$

$$= (W_n^{(0)} + g W_n^{(1)} + \dots)(\psi_n^{(0)} + g \psi_n^{(1)} + \dots)$$

An NPTEL logo is visible in the bottom left corner of the whiteboard image.

So, our objective is to solve this equation;  $H\psi$  is equal to  $W\psi$ . Where  $H$ , I write as  $H_0$  and I introduce a parameter  $g$ , if for example,  $H'$  is due to the perturbation, due to the electric field, so it maybe the parameter is something like the strength of the electric field. So that, when the electric field goes to 0, you have the original Hamiltonian. So,  $g$  is a parameter, which is assumed to be less than one.

So, what we do is, we make a parametric expansion of  $\psi$  and  $W$ . So, our objective is to obtain a specific state. Let us suppose, the  $n$ th state. So, our objective is to find  $W_n$  and  $\psi_n$ . However, we know the Eigen values and Eigen functions of the operator  $H_0$ . So, the solutions of this are known. So,  $H_0 u_n$  is equal to  $E_n u_n$ . So, this we know.

So, therefore let me state the problem clearly. The hydrogen atom is put in an electric field or in a magnetic field. Because of the presence of the magnetic field, it causes an additional term; it results in an additional term in Hamiltonian. If I exclude this term **if I exclude this term**, then I know the solution of the Eigen value equation corresponding to  $H_0$ .

This may be something like the hydrogen atom problem or the harmonic oscillator problem or a particle in a box problem. So, these solutions, the solution of the Eigen value equation corresponding to  $H_0$  are known to us. Our objective is that when we apply this perturbation, what will be the value of  $W_n$  and what will be the value, what will be the corresponding Eigen function?

So, what we do is, we introduced the parameter  $g$  as I mentioned. And then, make a parametric expansion; that is, write  $\psi_n$  is equal to  $\psi_n^0$  plus  $g\psi_n^1$  plus  $g^2\psi_n^2$  etcetera. And similarly, we write  $W_n$  is equal to  $W_n^0$  plus  $gW_n^1$  plus  $g^2W_n^2$  and so on. And, I substitute this. So, this let be equation 1, this be equation 2, this be equation 3, this be equation 4 and this be equation 5.

So, we substitute 2, 4 and 5 in equation 1. So, we get, please see this.  $H_0$  plus  $gH'$  multiplied by  $\psi_n^0$  plus  $g\psi_n^1$  plus  $g^2\psi_n^2$ . Let me neglect the higher order terms right now. **It** is equal to bracket  $W_n$  is  $W_n^0$ ; the **zeroeth** order term plus the first order term multiplied by  $\psi_n^0$  plus  $g\psi_n^1$  plus this.



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$$\begin{aligned}\psi_n &= \psi_n^{(0)} + g \psi_n^{(1)} + g^2 \psi_n^{(2)} + \dots \quad (4) \\ W_n &= W_n^{(0)} + g W_n^{(1)} + \dots \quad (5) \\ (H_0 + g H')(\psi_n^{(0)} + g \psi_n^{(1)} + \dots) &= (W_n^{(0)} + g W_n^{(1)} + \dots)(\psi_n^{(0)} + g \psi_n^{(1)} + \dots) \\ H_0 \psi_n^{(0)} + g(H_0 \psi_n^{(1)} + H' \psi_n^{(0)}) + g^2 \dots &= W_n^{(0)} \psi_n^{(0)} + g(W_n^{(0)} \psi_n^{(1)} + W_n^{(1)} \psi_n^{(0)}) + g^2 \dots\end{aligned}$$

Now, I multiply this out and collect power, collect terms of different powers of  $g$ . So, you have the term which is independent of  $g$  is,  $H$  naught  $\psi_n$  0 plus  $g$  will be  $g$  will be  $H$  naught  $\psi_n$  1  $H$  naught  $\psi_n$  1 plus  $H$  prime  $\psi_n$  0, plus terms which are proportional to  $g$  square, plus terms which are proportional to  $g$  cubed and so on. This will be equal to the first term will be is equal to  $W_n$  0  $\psi_n$  0 plus the term which is proportional to  $g$ ,  $W_n$  0  $\psi_n$  1 plus  $W_n$  1  $\psi_n$  0, plus term which are proportional to  $g$  square, plus terms which are proportional to  $g$  cube.

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$$\begin{aligned}H_0 \psi_n^{(0)} &= W_n^{(0)} \psi_n^{(0)} \Rightarrow W_n^{(0)} = E_n \text{ \& } \psi_n^{(0)} = u_n \\ \text{Zeroth order equation} \\ H_0 u_n &= E_n u_n \\ H_0 \psi_n^{(1)} + H' u_n &= E_n \psi_n^{(1)} + W_n^{(1)} u_n \\ \psi_n^{(1)} &= \sum_m a_m^{(1)} u_m \\ \sum_m a_m^{(1)} E_m u_m + H' u_n &= E_n \sum_m a_m^{(1)} u_m + W_n^{(1)} u_n \\ u_k^* \int u_k^* u_m d\tau &= \delta_{km}\end{aligned}$$

Now,...  $g$  tends to 0. And, there is always possible because we let the, let us suppose the external electric thing goes to 0. So, then all the terms cancel out. And, we had the zeroth order equation,  $H \psi_n^0$  is equal to  $W_n^0 \psi_n^0$ . This is the zeroth order equation. Zeroth order equation. And, this is the same Eigen value equation, as for the  $H$  naught because for  $H$  naught, we wrote  $H \psi_n$  is equal to  $E_n \psi_n$ . So, therefore we first consider non-degenerate states. And, I will tell you the difficulty that we encounter, when we consider degenerate states.

So,  $n$  is equal to 1 is this state or  $n$  is equal to 0, then  $n$  is equal to 1 or  $n$  is equal to 1 and so on. Each state is a non-degenerate state. Then, I can write this down immediately that  $W_n^0$  is equal to  $E_n$  and  $\psi_n^0$  is equal to  $\psi_n$ . This is the zeroth order solution; which is obvious because there is no electric field or magnetic field or something, there is no perturbation.

Now, then we have, so we said that this term is equal to this term. So, then these two terms cancel out. Then, we divide the whole equation by  $g$ . So, this goes out, this goes out, this goes out, this becomes  $g$  square,  $g$  square and  $g$ .

So, if I now make  $g$  tends to 0, then this is the first order term. So, the first order term becomes, you see becomes,  $H \psi_n^1$  plus  $H' \psi_n^0$ ; which we have written as  $\psi_n^1 W_n^0$  is  $E_n \psi_n^1$  plus  $W_n^1 \psi_n^0$ . This is my first order equation. This is my first order equation.

Similarly, I can write down my second order equation also. But, we will restrict ourselves to only first order perturbation theory; because in most analysis, one uses first order perturbation theory. Then, what I do is that, we have we have already assumed that the, we are considering the perturbation to the  $n$ th state whose Eigen function is known.  $\psi_n^1$ , I do not know. But, I know that  $\psi_n$  form a complete set of functions. Therefore, let us expand it.  $\psi_n^1$ , we can always expand  $\psi_n^1$  as  $\sum a_n^1 \psi_n$ ; superscript present that, we are considering first order of perturbation, times  $\psi_n$ .

So, multiply this  $H$  naught,  $a_n$  is a constant. So,  $H \psi_n^1$  is equal to  $E_n \psi_n^1$ . So,  $H$  naught operating on this will give me summation  $a_n^1 E_n \psi_n$ , plus  $H' \psi_n^0$  is equal to  $E_n \sum a_n^1 \psi_n$ . Actually, I am expanding. So, I must put it here as  $m$  because this is the dummy variable. So, this is  $\sum a_m^1 E_m \psi_m$ . I am considering the

perturbation to the  $n$ th state. So,  $m, n$  is fixed. So, this is  $a_{m-1} E_n a_{m-1}$  and  $u$  is of  $m-1$  plus  $W_{n-1}$   $u$  is of  $n$ .

Now, I multiply by  $u_k^*$  and integrate. And, I know that these Eigen function for the **non- orthonormal** set; that is,  $u_k^* u_m d\tau$  is equal to the **chronicle** delta function. Remember that the harmonic oscillator functions also satisfy this orthonormality relation, where the integration is over the dash space.

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The slide contains the following handwritten equations:

$$\sum_m a_m^{(0)} E_m \delta_{km} + H'_{kn} = E_n \sum_m a_m^{(1)} \delta_{km} + W_n^{(1)} \delta_{kn}$$

$$H'_{kn} = \int u_k^* H' u_n d\tau = \langle k | H' | n \rangle$$

$$a_k^{(1)} E_k + H'_{kn} = E_n a_k^{(1)} + W_n^{(1)} \delta_{kn}$$

Case I:  $k = n$

$$W_n^{(1)} = H'_{nn} = \int u_n^* H' u_n d\tau = \langle n | H' | n \rangle$$

$k \neq n$

$$H'_{kn} = (E_n - E_k) a_k^{(1)}$$

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So, therefore if I multiply the entire equation by  $u_k^*$ , so we multiply the entire equation by  $u_k^*$  on the left and then integrate. So, the first term will become summation  $a_{m-1} E_m \delta_{km}$  plus  $H'_{kn}$  is equal to  $E_n$  summation  $a_{m-1} \delta_{km}$  plus  $W_{n-1} \delta_{kn}$ ; where,  $H'_{kn}$  is known as the **k n th** matrix element; is the  $u_k^* H' u_n d\tau$ . Symbolically, this is more convenient to write this as  $k H'$  prime **ket**  $n$ . This is **the k nth** matrix element of this.

So, therefore if I sum the series, only the  $m$  equal to  $k$  term survives. And, so we have a  $k-1 E_k$  plus  $H'_{kn}$  is equal to  $a_n a_{k-1}$ ; because only the  $m$  equal to  $k$  term will survive and  $W_{n-1} \delta_{kn}$ . So, case 1, if I assume that  $k$  is equal to  $n$ . That, I multiply by  $u_n^*$  only. So, this term and this term cancel out. This becomes 1.

And then,  $W_{n-1}$  becomes  $H'_{nn}$ . So, this is the first order perturbation to the energy. So, this is  $u_n^* H' u_n d\tau$ . And symbolically, it is  $n H'$  prime  $n$  in the

bracket notation. When,  $k$  is not equal to  $n$ , then you will have this term goes to zero. And, if I take, if I take the others, so  $H'_{kn}$  is equal to  $E_n - E_k$  into  $a_{k1}$ .

So, you can use this, you can use this to calculate  $a_{k1}$ , which will be equal to  $H'_{kn}$  divided by  $E_n - E_k$ . So, we have the coefficients because  $\psi_{n1}$  was equal to  $a_{k1} u_k$ . Actually, we had written  $a_{m1} u_m$ . This is a dummy variable. So, it does not really matter. But, here, and this I will discuss it greater detail in my next lecture. One see is that if,  $k$  is not equal to  $n$ , but  $E_n$  is equal to  $E_k$ ; that is, if we have, let us suppose if 2 4 degenerate state, that is about, this is the ground state, this is a 2 4 degenerate state. So, this is  $u_0$ .

This is  $u_1$  and  $u_2$ .  $u_1$  and  $u_2$  belong to the same energy state. So, that is a degenerate state. Then, this tells us that  $H'_{kn}$  must be 0. And, this I will explain it in greater detail in my next lecture.

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$$(E_n - E_k) a_{kn}^{(1)} = H'_{kn}$$

$$H'_{12} = 0$$

That, you see in degenerate state, if let us suppose  $u_0$  is a ground state and the second state is 2 4 degenerate, then  $u_1$  is a possible wave function,  $u_2$  is a possible wave function; any linear combination is also a possible wave function. So, if that is so, then this relation  $E_n - E_k$  times  $a_{k1}$  is equal to  $H'_{kn}$ , says that I must choose such linear combination for which  $H'_{kn}$ , that is  $H'_{12}$  must be 0. That is the representation should be such that, the  $H'$  in the subspace generated by the

degenerate state vectors. ...the  $H'$  must be diagonal. And then, only the diagonal elements will give the energy Eigen values.

So, with that, if you have not followed this, we will give more illustrations. We will have, so the basic formulation is completed; that the first zeroth order term is equal to  $E_n$ , of course. So, these are the  $E_0$  and  $E_1$  and things like that. This we know. Then, the first order correction  $W_{n1}$  is equal to; you just have to calculate the matrix element. First, we will do for non-degenerate states. And then, we will say, what precaution do we have to take for degenerate state perturbation theory. Thank you.