

Select/Special Topics in ‘Theory of Atomic Collisions and Spectroscopy’
 Prof. P.C. Deshmukh
 Department of Physics
 Indian Institute of Technology-Madras

Lecture 11
 Levinson’s theorem

Greetings, so today we will discuss the Levinson’s theorem and we got very close to that in the previous class in talking about the scattering phase shifts. And what the Levinson’s theorem does is to relate the scattering phase shifts at low energy in the limit energy going to zero to the number of bound states that an attractive potential can hold.
 (Refer Slide Time: 00:43)

For $l=0$, $\alpha_{l=0} = -(l+1) = -1$
 considering the next order term in $(ka)^4$ *resonant part*

$$\tan \delta_{l=0}(k) \xrightarrow{k \rightarrow 0} \frac{1}{-3(ka)}$$

$$\lim_{k \rightarrow 0} a_0(k) = \lim_{k \rightarrow 0} \frac{\tan \delta_0(k)}{k} = -\alpha$$

definition: scattering length

$$\lim_{k \rightarrow 0} \alpha \rightarrow \frac{1}{k^2} \text{ as } k \rightarrow 0,$$

scattering length diverges as $\frac{1}{k^2}$

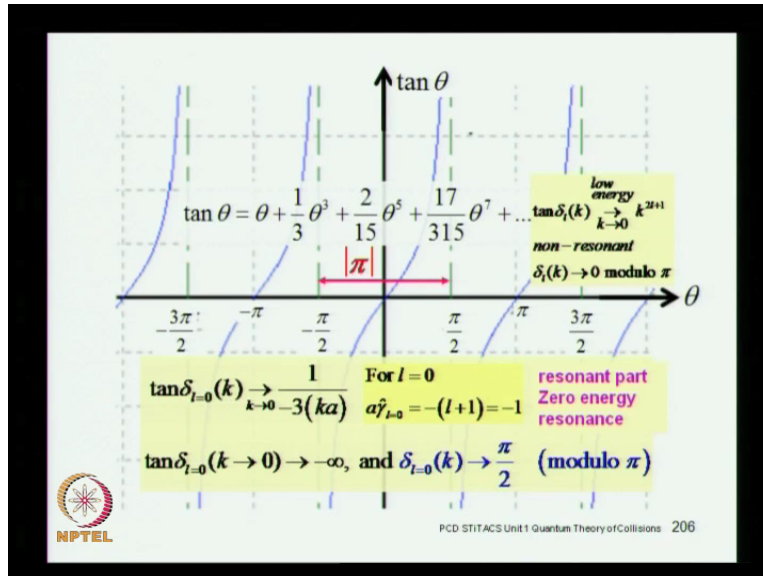
$\tan \delta_{l=0}(k) \rightarrow \text{blows up}$ as $k \rightarrow 0$

$\tan \delta_{l=0}(k) \rightarrow \pm \infty$ when $\delta_{l=0}(k) \rightarrow \pm \frac{\pi}{2}$

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 205

So, let me quickly recapitulate some important results. We considered the resonant part of the S wave scattering in the previous class okay. So, there is a non resonant part and there is a resonant part. So, in the resonant part we considered higher order terms k to the power 4 and we found that the tangent of the phase shift blows up as inverse k as k tends to 0 the $\tan \delta$ blows up right.

And if you look at the scattering length the scattering length goes as 1 over k squared because it is $\tan \delta$ over k and δ itself goes as 1 over k , so the scattering length goes as 1 over k square and because the scattering wave wavelength goes as 1 over k square the $\tan \delta$ goes blows up. And when the $\tan \delta$ goes up to infinity the δ itself the phase shift is like π by two multiples of π by 2 modulo π of course right.
 (Refer Slide Time: 01:54)



So, this is the typical tangent curve and let us have a look at this so you notice that the tangent of an angle blows up at π by 2, 3π by 2 and so on. In half integer multiples of π by 2 that is when the tangent of the angle blows up and the low energy non resonant part, we have already seen the phase shift goes there as k to the $2l+1$, so it will tend to 0, so that phase shift ends to 0, modulo π in the non resonant region.

But then in the resonant part something happens that the tangent of the phase shift blows up it does not go to 0 instead it blows up and what it does is happens when the phase shift is π by 2 or plus or minus π . Now this is a very peculiar effect and it is happening because of a resonance effect and we will discuss why this resonance takes place. And notice that the tangent curve reverses its sign at π by 2.

(Refer Slide Time: 03:10)

And this is the expression for the scattering amplitude and the partial wave amplitude which we have seen before. Now let us evaluate the partial wave amplitude when delta is π by 2 so

this is where the resonance takes place right. So, as delta approaches pi by 2 then the partial wave amplitude which is this S matrix element S_{l-1} over $2ik$ gives the partial wave amplitude?

So, this is now $\cos 2\delta$ and at $\delta = \pi/2$ and $2\delta = \pi$ and you see quickly that the partial wave amplitude itself goes to i over k .
(Refer Slide Time: 04:00)

$l=0 \quad a_0(k \rightarrow 0) \rightarrow \left[\frac{\cos \pi + i \sin \pi - 1}{2ik} \right] \delta_0 = \frac{i}{k}$
 For $l=0$
 $a_{l=0} = -(l+1) = -1$ **resonant part**
Zero energy resonance
 $f_k(\theta) = \sum_{l=0}^{\infty} (2l+1) a_l(k) P_l(\cos \theta) \rightarrow f_k(\theta): \text{scattering amplitude}$
 $a_l(k) = \frac{[e^{2i\delta_l(k)} - 1]}{2ik} = \frac{[S_l(k) - 1]}{2ik} \rightarrow a_l(k): \text{partial wave amplitude}$
 \Rightarrow
 $\sigma_{tot}(k \rightarrow 0) = \iint |f_k(\theta)|^2 d\Omega = \iint \left| \frac{i}{k} \right|^2 d\Omega = \frac{4\pi}{k^2} \quad [f_{k \rightarrow 0}(\theta)]_{l=0} = \frac{i}{k}$
 $x\text{-sec blows up as } \frac{1}{k^2} \left(\text{i.e. as } \frac{1}{k} \right) \text{ as } k \rightarrow 0$ **"Zero energy resonance"**
 $\delta_{l=0}(k \rightarrow 0) = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \dots$
 NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 208

Now as partial wave amplitude goes as i over k you can also get what the scattering amplitudes will do it, will also go i over k for $l=0$ okay. Because that is the only thing which is contributing to the scattering amplitude in low-energy scattering only the $l=0$ is important. And this goes as i over k .

And the sketching cross section itself will go as 1 over k square because it is the integral over all angles and the scattering amplitude is independent of angle. So, all you have to do is to integrate all the angles that gives you the factor 4π . So, the cross section blows up as 1 over k square and this is the zero energy resonance which happens at δ equal to $\pi/2, 3\pi/2, 5\pi/2$ and so on.
(Refer Slide Time: 05:00)

LEVINSON'S THEOREM Kgl. Danske Videnskab.
Selskab. Mat. Fys.
Medd. 25 9 (1949)

reference zero of $\delta_l(k)$: $\delta_l(k \rightarrow \infty) = 0$

..... for $l=0$:

$\delta_0(k \rightarrow 0) = n_0 \pi$ ↗ "half-bound" state

or $\delta_0(k \rightarrow 0) = \left(n_0 + \frac{1}{2}\right) \pi$ ↖ if there is a (resonant)

"zero energy resonance" ↗ bound state solution

$\sigma_{tot}(k \rightarrow 0) \xrightarrow{\text{blows up}} \frac{1}{k^2}$ ↖ when $\lambda_0 a = \sqrt{U_0} a = \frac{\pi}{2}$ at zero energy.

$\delta_0(k \rightarrow 0) \rightarrow \frac{\pi}{2}$ ↖ $\delta_l(k \rightarrow 0) = n_l \pi$ for $l \geq 1$

$$\delta_l(0) - \delta_l(\infty) = \begin{cases} (n_l + 1/2)\pi & \text{when } l=0 \\ & \text{and a half bound state occurs} \\ n_l \pi & \text{the remaining cases.} \end{cases}$$

NPTEL STITACS Unit 1 Quantum Theory of Collisions 209

So, the question is why does this happen and this is connected to a theorem which was set up by Levinson in 1949 and what it does was to take the zero of the phase shift at high energy. In the high energy limit as k tending to infinity so that is only the reference. So, phase shifts are measured with reference to this as the zero of the phase shift.

So, with this as the reference level let us first state it for S wave scattering which is for $l = 0$. And the state the Levinson's theorem applies for $l = 0$ and also for other values of l . So, let me first state it for $l = 0$ the theorem is the following that for $l = 0$ as k tends to 0. The S wave phase shift goes to $n \pi$ or $n_0 \pi$ the subscript zero corresponds to the angular momentum quantum number which is $l = 0$.

So basically δ_0 goes as $n_0 \pi$ in the low energy limit or else it goes to $n_0 + \text{half times } \pi$ if there is a resonant bound state okay. In the event there is a resonance, there is a resonant bound state solution then the phase shift does not go to $n_0 \pi$ okay. Now this is the Levinson's theorem.

Now to indicate the fact that the reference of the phase shift δ_l is 0 at k tending to infinity this theorem is sometimes stated like this that the difference in these phase shifts the shift of the l th partial wave at 0 energy with reference to what it is at k tending to infinity is equal to either $n \pi$ or $n + \text{half } \pi$, $n + \text{half } \pi$ is relevant only in the case of S waves and only when there is a resonance.

(Refer Slide Time: 07:05)

Square well attractive potential

$U(r) = -\beta^2$ for $r < a$
 $= 0$ for $r > a$


$y_{al(r)} = rR_{al}(r)$

$\left[-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \left\{ V(r) + \frac{\hbar^2 l(l+1)}{2m r^2} \right\} - E \right] y_{al}(r) = 0$

$\left(-\frac{2m}{\hbar^2} \right) \times \quad \ell = 0$

$U(r) = \frac{2m}{\hbar^2} V(r) \quad \left[\frac{d^2}{dr^2} + \{ -U(r) \} + \frac{2m}{\hbar^2} E \right] y_{al}(r) = 0$

$\frac{2mE}{\hbar^2} = -\gamma^2 \quad \left[\frac{d^2}{dr^2} + \{ -U(r) \} - \gamma^2 \right] y_{al}(r) = 0$

 discrete bound state

PCD STITACS Unit 1 Quantum Theory of Collisions 210

So, this is the statement of the Levinson's theorem and to illustrate this I will consider a square well attractive potential okay. So, this is just to illustrate us Levinson's theorem although it is applicable for any kind of attractive potential. But it is easiest to demonstrate it for the square well attractive potential it is a very simple potential as you can see. And the potential has got a depth of $-\beta^2$ up to a range $r = a$ beyond that it is 0.

So, that is the nature of the potential we are going to work with. If you now set up the Schrodinger equation for this potential and you write the Schrodinger equation and rewrite it, rewrite a differential equation for the function y which is r times the capital R which is the radial solution to the Schrodinger equation. Then specialize it for the S waves which is for $l = 0$ and then write it in terms of the reduced potential which is U .

Which is only scaled real potential V by a factor of $2m$ over \hbar cross square. Then it simply looks the differential equation looks in a neater form. So, that is the only reason to carry out this transformation. So, you get a differential equation for the function y okay. And for this function we have put $l = 0$. Consider first discrete bound state solutions. So, the energy is intrinsically negative for discrete bound states okay.

And this explicit intrinsically negative energy is what has been written as minus gamma square so that its explicit negative nature is now manifest okay. So, this is your differential equation for y which is little r with the distance times capital R which is the solution to the original Schrodinger equation.

(Refer Slide Time: 09:08)

Bound states of the SPHERICAL well attractive potential

$\ell = 0 \quad y_{a(r)} = rR_{a(r)}$

$$\left[\frac{d^2}{dr^2} + \{-U(r)\} - \gamma^2 \right] y_{a(r)} = 0$$

discrete bound state $E = -\gamma^2$

$$U(r) = -\beta^2 \text{ for } r < a$$

$$= 0 \text{ for } r > a$$

$$\left[\frac{d^2}{dr^2} + \beta^2 - \gamma^2 \right] y_{a(r)} = 0 \text{ for } r < a \quad y_{a(r)} = A \sin(r\sqrt{\beta^2 - \gamma^2})$$

$$\left[\frac{d^2}{dr^2} - \gamma^2 \right] y_{a(r)} = 0 \text{ for } r > 0 \quad y_{a(r)} = B e^{-\gamma r}$$

Continuity at $r = a \Rightarrow \tan(a\sqrt{\beta^2 - \gamma^2}) = -\frac{\sqrt{\beta^2 - \gamma^2}}{\gamma}$
tan θ properties.....

NPTEL STITACS Unit 1 Quantum Theory of Collisions

211

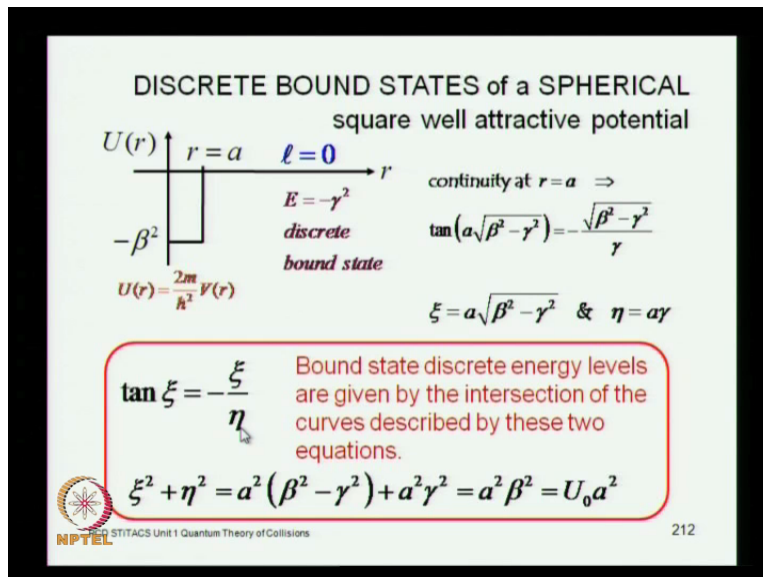
So, now you know this what the solutions are, now this differential equation for r less than a is minus beta square. So you can solve this very easily okay, this will be a sinusoidal function right. For U which is the constant over this entire range from 0 to a. And outside it is an exponentially damped function okay. So, outside the well it will be an exponentially damped state because it is a bound state.

So, it can certainly penetrate through the potential a little bit but then the amplitude will damp out. So, it will damp out as e to the minus gamma. So, these are the solutions of these two differential equations for the range r less than a and r greater than a. But at r = a, the wave function and also its derivative must be continuous. So, you just impose the boundary conditions of the continuity of the wave function as well as its derivative.

And you can get the derivative of the sine function as well as the e to the minus gamma r function very easily. And from these continuity equations you get a relation which is tangent of this angle equal to minus of root beta square minus gamma square over gamma. So, that is an automatic consequence of the continuity at r = a. So, you need to study the properties of the tangent function okay.

Let us say have a look at how the tangent function behaves and from this behaviour we will learn a lot.

(Refer Slide Time: 10:58)

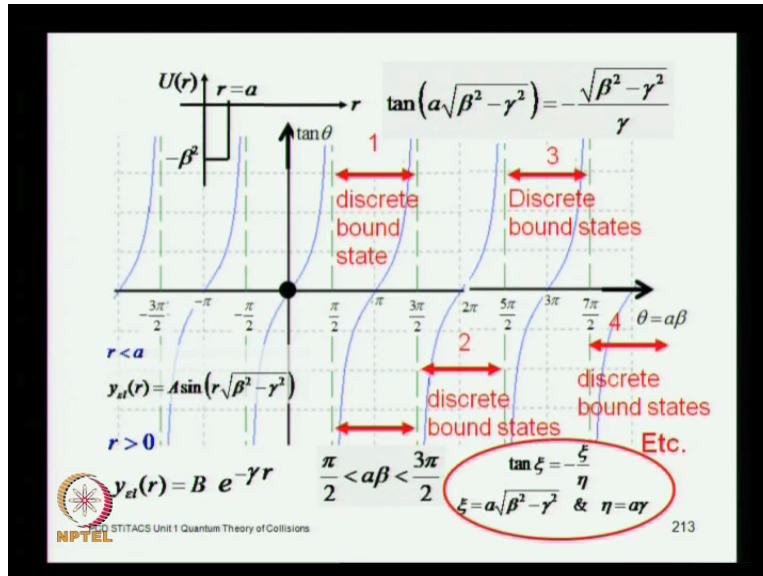


So, the bound states are given by this solution which is tangent of the single equate tangent of this angle and this angle is determined by properties of beta, beta is determined by the depth of the potential right. That is what determines the depth of the potential and what is gamma? Gamma is the energy parameter okay.

Gamma or Eta are the energy parameters, a is the range of the potential. So, your equation which is tan theta equal to minus this angle over gamma can be written as this ratio can be written as Xi over Eta and if you look at the relationship between Xi and Eta then the relationship is given by Xi square + Eta square becomes equal to constant which is determined completely by the properties of the potential.

a is the range of the potential and U0 is the depth okay. So, U0 a square is what determines the strength of the potential, how deep is it? That is U0 and how far does it have an influence that is the range of the potential. So, U0 a square is the strength of the potential and Xi square plus Eta squared equal to U0 a square is what must also be satisfied and the other relation that must be satisfied is a tan Xi and -Xi over Eta these are equal right.

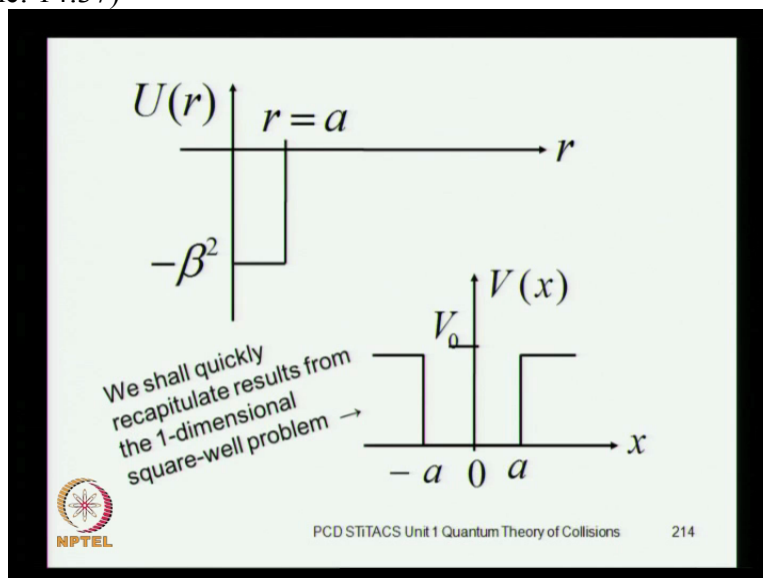
So, the bound state discrete energy levels are then given by the intersection of these curves. So, this is a relationship between Eta and Xi which describes a certain family of curve. Here is another relation between Xi and Eta which is another family of curves right. And the intersection of these two will give you the solutions to the discrete bound state energy. (Refer Slide Time: 13:10)



Now what happens; is because of this peculiar nature of the relationship between Xi and Eta the solutions being given for the r less than a region and are greater than a region by these two solutions. Inside the well it is sinusoidal outside the well it is exponentially done. So, that is the nature of the square well potential. And in this range between $\pi/2$ and $3\pi/2$ you get one bound state.

In the region between $3\pi/2$ and $5\pi/2$ you get 2 bound states, between $5\pi/2$ and $7\pi/2$ you get 3 bound states and as a beta increases the number of bound states increases but not continuously only where it crosses $\pi/2$ then $3\pi/2$ then $5\pi/2$. So, it must go through this $\pi/2$ or $3\pi/2$ or $5\pi/2$ to pick up the next bound state. Now that is that has to happen and the number of bound States increases as you go from left to right in this figure.

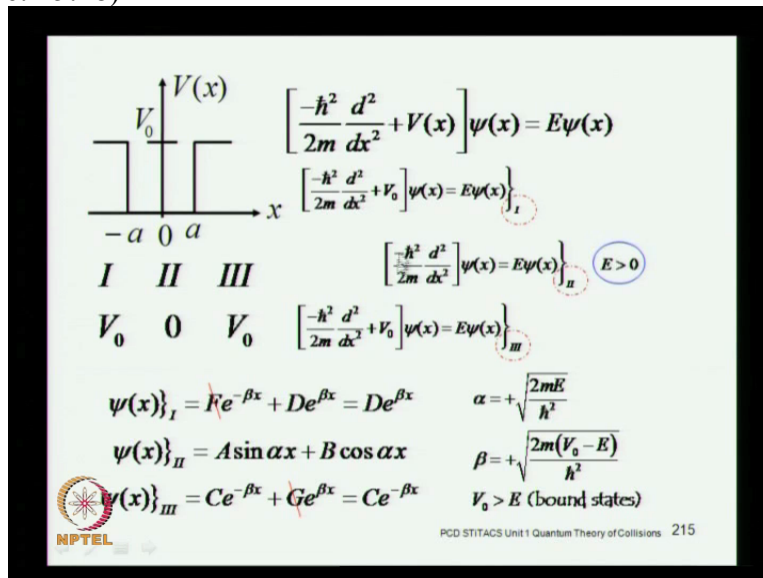
(Refer Slide Time: 14:37)



And to understand it I will take you back to what you probably studied in your first course in quantum mechanics and we will just do very quickly a one dimensional square well okay. Just to recapitulate the method and you will see that it is exactly the same algebra which is used over here. So, we will very quickly do a one dimensional square well.

So you have got a square well potential in one dimension along the x axis. The potential is V_0 in the region $-a$ to $+a$ okay. The potential is 0 in this region I am sorry and it is V_0 in the region less than $-a$ on the left of this and it is equal to a constant V_0 for x greater than a . So, that is the nature of the one dimensional square well that we will consider.

(Refer Slide Time: 15:28)



So, there are 3 regions the potential is V_0 in region 1 and 3 it is 0 in the region 2 that is the square well you set up the Schrodinger equation for this one dimensional problem. You have solutions to the Schrodinger equation in the 3 regions. In region 1 and 3 the potential is V_0 , in the region 2 the potential is 0. So, you solve these differential equations okay. And you solve this differential equation for e greater than 0 and you can solve for e less than 0 okay.

Depending on what kind of solution you are looking for, for bound state solutions or for continuum solutions. And then if you look at this expression you find that in region 1 the coefficient F must be 0 because in region 1, x is negative and this term will blow up. Whereas in region 3 the Ge to the βx will blow up. So, G coefficient must be 0. So, the solution in region 1 is only De to the βx .

So, mathematics gives you two solutions but physical boundary conditions tell you that one of these coefficients must be 0. And this is the nature of the solution when you have bound states. When the V_0 which is 0 in the well when this is greater than e okay. Because in the

well the potential is 0 and for bound states E is less than V_0 which is less than E less than 0 okay. So, the bound state solutions will be intrinsically of negative energy. (Refer Slide Time: 17:18)

$$V(x)$$

$$\psi(x)\}_I = De^{\beta x}$$

$$\psi(x)\}_II = A \sin \alpha x + B \cos \alpha x$$

$$\psi(x)\}_III = Ce^{-\beta x}$$

@ $x = a$:
 $A \sin \alpha a + B \cos \alpha a = Ce^{-\beta a}$
 $A \alpha \cos \alpha a - B \alpha \sin \alpha a = -\beta C e^{-\beta a}$

@ $x = -a$:
 $-A \sin \alpha a + B \cos \alpha a = D e^{-\beta a}$
 $A \alpha \cos \alpha a + B \alpha \sin \alpha a = \beta D e^{-\beta a}$

$\alpha = +\sqrt{\frac{2mE}{\hbar^2}}$
 $\beta = +\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$
 $E < V_0$ (bound states)

NPTEL
 PCD STITACS Unit 1 Quantum Theory of Collisions 216

So, these are the solutions now and these are the 3 regions solution in region 1, solution in region 2 and solution in region 3. Now what do you do, the solution must be continuous at both the boundaries at $x = -a$ and $x = +a$. So, the wave function must be continuous and the derivative of the wave function should also be continuous. So, this is the continuity of the wave function at $x = a$.

And this is the continuity to the wave function at $x = -a$, the two relations one coming from the continuity of the wave function and the other coming from continuity of the derivative of the wave function. Because this is a second order differential equation, so the first sort of that you know derivative should also be continuous. So the Schrodinger wave function is of course an analytical function and these are the two relations.

(Refer Slide Time: 18:16)

$V(x)$ vs x diagram showing regions I, II, III with $V_0, 0, V_0$ respectively.

@ $x = a$: $A \sin \alpha a + B \cos \alpha a = C e^{-\beta a}$
 $A \alpha \cos \alpha a - B \alpha \sin \alpha a = -\beta C e^{-\beta a}$

@ $x = -a$: $-A \sin \alpha a + B \cos \alpha a = D e^{-\beta a}$
 $A \alpha \cos \alpha a + B \alpha \sin \alpha a = \beta D e^{-\beta a}$

$2A \sin \alpha a = (C - D) e^{-\beta a}$
 $2A \alpha \cos \alpha a = \beta (D - C) e^{-\beta a}$
 $2B \cos \alpha a = (C + D) e^{-\beta a}$
 $2B \alpha \sin \alpha a = \beta (C + D) e^{-\beta a}$

$\alpha = +\sqrt{\frac{2mE}{\hbar^2}}$
 $\beta = +\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$
 $V_0 > E$ (bound states)

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 217

From which you can get the relationships between the different coefficients and you can solve these equations by combining. If you subtract this equation from the one at the top you get twice a sine alpha a, because this term will cancel this you get C - D e to the -beta a. So, these are the usual things that you do in your first course in quantum mechanics. And you can easily get these relations which must be simultaneously satisfied right. (Refer Slide Time: 18:45)

$V(x)$ vs x diagram showing regions I, II, III with $V_0, 0, V_0$ respectively.

$2A \sin \alpha a = (C - D) e^{-\beta a}$
 $2A \alpha \cos \alpha a = \beta (D - C) e^{-\beta a}$
 $2B \cos \alpha a = (C + D) e^{-\beta a}$
 $2B \alpha \sin \alpha a = \beta (C + D) e^{-\beta a}$

$\alpha = +\sqrt{\frac{2mE}{\hbar^2}}$
 $\beta = +\sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$
 $V_0 > E$ (bound states)

$A = 0$ and $C = D$ whence
 $2B \cos \alpha a = 2C e^{-\beta a} \Rightarrow \alpha \tan \alpha a = \beta$
 $2\alpha B \sin \alpha a = 2C \beta e^{-\beta a}$

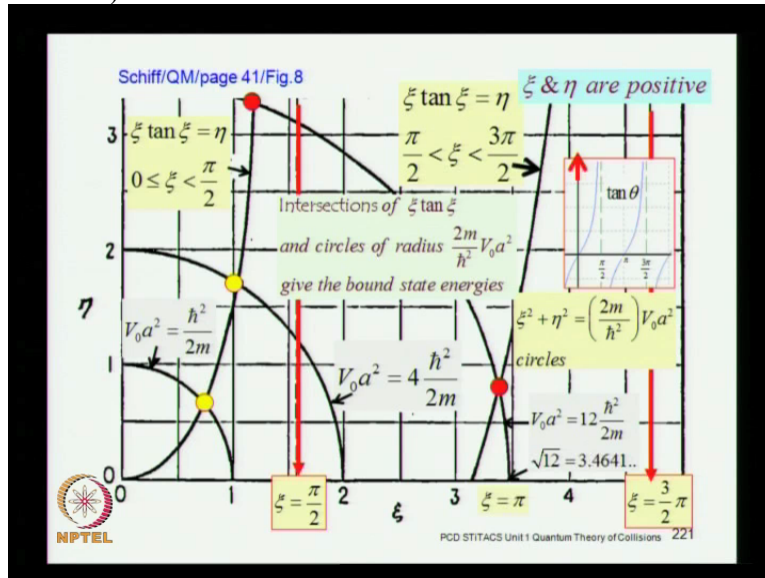
$B = 0$ and $C = -D$ whence
 $2A \sin \alpha a = 2C e^{-\beta a} \Rightarrow \frac{1}{\alpha} \tan \alpha a = -\frac{1}{\beta}$
 $2\alpha A \cos \alpha a = -2C \beta e^{-\beta a}$ i.e. $\alpha \cot \alpha a = -\beta$

NPTEL PCD STITACS Unit 1 Quantum Theory of Collisions 218

And when you satisfy these equations you get certain solutions you get one class of solutions if $A = 0$ and $C = D$, if $A = 0$ then the right hand side should also be 0 that makes $C = D$. And if $C = D$ then this is what happens that $C + D$ becomes $2C$ and $2B \cos \alpha a$ becomes $2C e$ to the $-\beta a$ okay. Likewise $2\alpha B \sin \alpha a$ becomes this is $C + D$ becomes $2C$, so it is $2C \beta e$ to the $-\beta a$.

So, this is one class of solutions that you get what essentially it means is that if $2\alpha B \sin \alpha a = 2C \beta e$ to the $-\beta a$, the solution is completely, you know you can strike off

And the second its range which is a, these are the two parameters and these two parameters completely define the potential. And they define actually the capability of the potential to hold a bound state which is why it is called as the strength parameter. And this as you can see is an equation to a circle between Xi and Eta which Xi squared + Eta squared is equal to constant then it is an equation to a circle.
 (Refer Slide Time: 23:01)



So the solutions are given by the intersections of the relations $\xi \tan \xi = \eta$ and circles defined by $\xi^2 + \eta^2 = \text{constant}$. And there are a number of circles which are drawn over here you can see this is one circle, second circle, third circle. And these circles are of three different radii $\xi = 1$, $\xi = 2$, $\xi = 3.5$ right this is actually 3.46 it is the square root of 12 which has been used in this figure.

This is a figure which I have taken some Schiff quantum mechanics. So this is the reference for this figure this is straight out of Schiff's book and you will get solutions whenever these circles intersect the relationship when each $\eta = \xi \tan \xi$. Now this is how the $\tan \theta$ figure looks like and if you multiply $\tan \theta$ by θ you get $\xi \tan \xi$ right. So, the tangent of the angle multiplied by the angle itself is what gives use $\xi \tan \xi$.

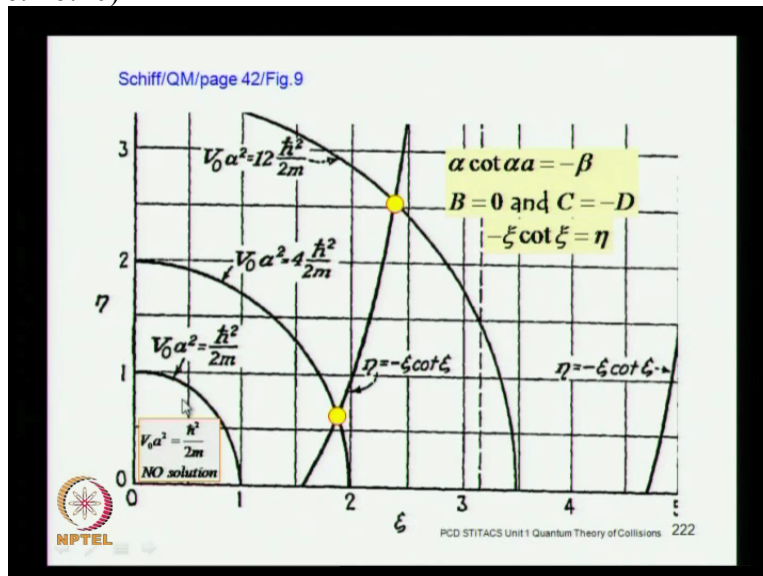
And this has been plotted on the y axis. So, this is not exactly the tangent curve this is $\tan \xi$ multiplied by ξ . And this curve intersects this circles and variable it intersects is where you will have a bounce rate. So, now notice that the radius of the circle is determined by the strength of the potential because this is drawn for $V_0 a^2$ a square equal to $\frac{\hbar^2}{2m}$ that is when ξ will be equal to 1 right.

This is drawn for $\xi = 2$ which is when $V_0 a^2$ will be = 4 times this right. So, that is how you are getting the different radii and they correspond to a different strength of the

potential. And the intersections of these circles with the $\eta = \xi \tan \xi$ gives you the solutions. So, here are the solutions you get the first solution over here. The second intersection is what you get over here. Then you get two bound states for this circle okay.

You get two bound states for the circle whereas for these two circles you get only one bound state because the potential must cross a certain minimum strength. A potential of an arbitrarily less strength will not be able to hold a bound state. Only if it becomes sufficiently deep or sufficiently you know wide range a is the parameter.

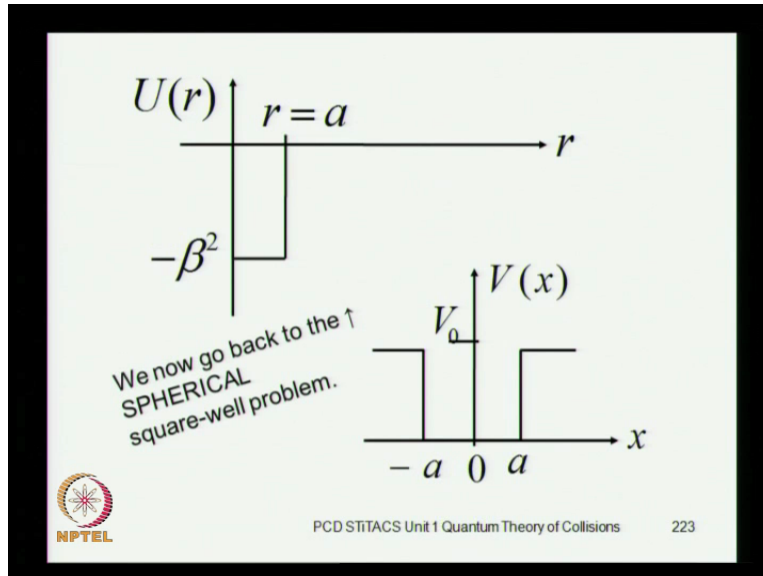
$V_0 a^2$ a square actually it depends linearly on the depth and quadratically on the width okay. So, the potential becomes stronger quadratically by the width and linearly by the strength, so for a square well of course. But other potentials have got more complicated forms but this is how you get different number of bound states depending on you know what its strength is. (Refer Slide Time: 26:40)



And there is another separate family of solutions which I mentioned when you get $B = 0$ and $C = -D$ you get the second family of solutions. And in this case also you get one solution for these two values of the strengths okay. So, each circle represents a particular strength of the potential. And depending on what is the radius or what is the value of the strength of the potential you get those many bound states.

So, notice that if $V_0 a^2$ is equal to $h^2 / (2m)$ for the first circle which has been drawn for $\xi = 1$ there is no bound state at all okay. So, the potential has got a depth, it does got a range but it does not mean that it can hold the bound state it cannot. So, unless the potential is sufficiently deep, so that this parameter crosses $\pi / 2$ okay, it cannot hold a bound state.

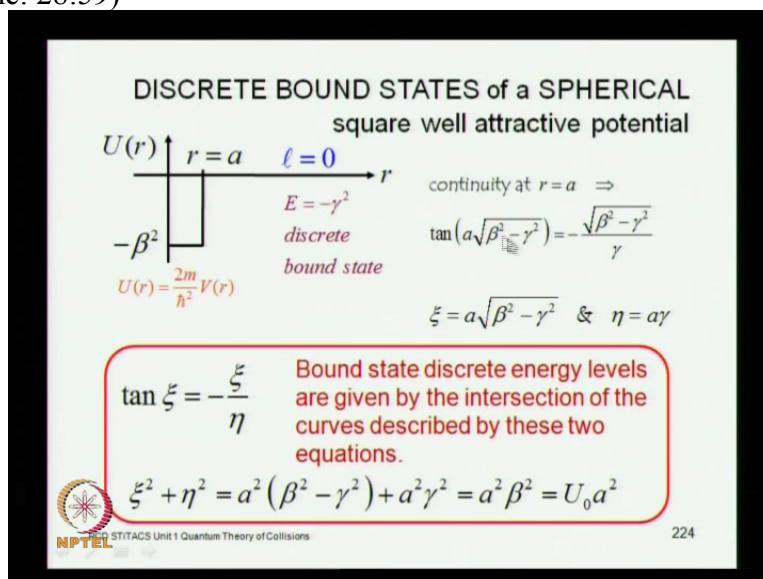
(Refer Slide Time: 27:39)



So, now we go back to our problem of the square well potential yes (Question time: 27:39 not audible) yeah yeah that can hold upon bound state in other set of solutions a = yeah here yes yes how will define how will you know that actual set of equation well that does not you will know it from the parity of the solution. The actual solution itself will come from different boundary conditions.

And from that you will get the nature of the solution because in one case you have got one set of the constants which goes to 0. In the other case it is the other set of concepts which goes to zero. So, you can get solution from one or the other but never simultaneously from both because sure but there are two linearly independent solutions.

So, you get solutions from one or the other not from both. You can get solutions from both if the boundary conditions are satisfied for both.
(Refer Slide Time: 28:59)

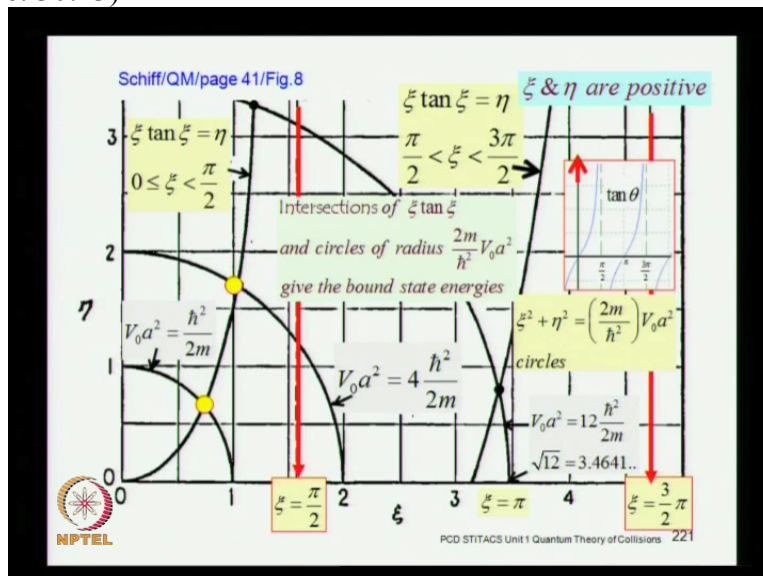


So, for the spherical square well now we are not talking anymore about the one dimension square well. But let us go back to the spherical square well we have already seen that the continuity of the solutions at $r = a$, requires us to have the solutions satisfy this relationship between ξ and η .

Where ξ and η are determined by the potential strength parameter which is related to β and a and the energy of the solution and the consideration which is coming from γ , energy is minus γ square for bound states okay. It is intrinsically negative, so it has been chosen to be minus γ square.

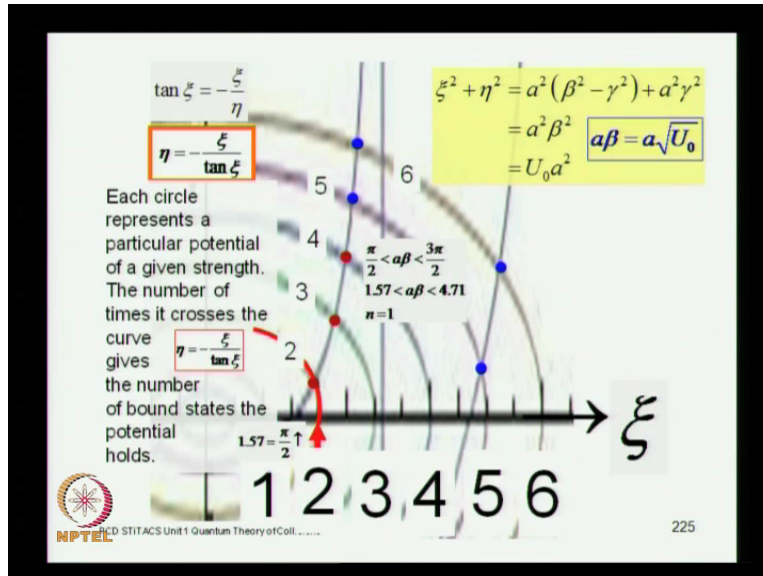
So, here again we find that ξ square + η square equal to the strength of the potential this is again an equation to a circle. So, it is a very similar situation as we have seen in the previous case. But for a one dimension square well we had $\xi \eta \xi$ whereas in this case it is η times $\xi = -\xi$. So, this relationship the family of curves this time is different okay.

(Refer Slide Time: 30:13)



So, if you remember here this relation was $\xi \tan \xi = \eta$, this was the relation for a one dimension square well okay. Now it is not $\xi \tan \xi = \eta$.

(Refer Slide Time: 30:31)



It is Eta times Xi = -Eta or Eta = - Xi over tan Xi okay, Eta must be = -Xi over tan Xi right, so that is the relation. So, if you plot Eta versus Xi, you get a family of curves and these curves are drawn over here. So, this is one curve which describes the relationship between Eta and Xi.

Then this is the part of the curve in this part of the value of the angles Xi. Angles Xi are indicated in radians in this. And there are circles also drawn which are given by Xi square + Eta square equal to the strength of the potential under a circles drawn with different strength parameters for different values of the radius. So, here is the circle drawn for radius Xi = half, this is for Xi =1, this is for Xi = 2 and so on right.

So, there are a number of different circles and each circle represents a particular strength of the potential. Now this is the value of pi by 2 and notice that this is 1.57, on this axis right. So, this is pi by 2 and below pi by 2 this curve is negative the tangent residue this curve is negative Xi over tan Xi okay. The - Xi over tan Xi is negative, now because this is negative you do not have any solution for anything less than this.

For any value of Xi less this you do not have a solution. And you will get the first solution only after the value of Xi crosses pi by 2. So, the solutions will come from the intersections of these two curves. And the number of times you have a crossing of a particular strength with this family of curves is the number of bound states that potential will hold okay, so now if you take the circle with radius 2 okay.

Now the circle with radius 2 has got a value which is greater than pi by 2, pi by 2 is 1.57, so this is more than pi by 2 and for this you will have one crossing and that the solution you get right. What happens is Xi is equal to 3, if the radius is equal to 3 you have increased the

strength of the potential either through U_0 or through a , it does not matter what, okay. You can increase it any way either by making it deeper or wider or both.

But if it now becomes given by $U_0 a^2 = 3$, no or the square of 3, the radius is 3 then again you have got 1 crossing. What about 4? What do you expect? Again you have a single crossing right. Now here notice that you have got only a one bound state the first bound state you get only after crossing π , π by two. So, for anything less than π by 2 the number of bound state is 0.

There is no crossing for these smaller circles after the circle became large enough, so that it crossed π by 2 you get one bound state and you continue to get one bound state till you hit 3π by 2 okay. So, here this is 3, this is 4 but it is still less than 3π by 2 and you get only one crossing, so you get only one bound state. Now what happens if the radius is 5? Now it has crossed 3π by 2 okay.

And because it is because 3π by 2, you will get 2 bound states because it crosses at 2 points the same circle crosses the curve is χ_i versus, η versus χ_i where the relationship is given by the equation that must be satisfied by the equation of continuity at the boundary right. The wave function must be continuous, the derivative must be continuous.

So, this condition must be satisfied and you get 2 bound states for $\chi_i = 5$. And for $\chi_i = 6$ again you will get 2 bound states okay, and it will remain the same number till you get to 5π by 2. When you cross 5π by 2 then you will get the next bound state. Because we have seen that at π by 2, you get a resonant bound state.

Every time you get π by 2, 3π by 2, 5π by 2 you get resonant bound States this is what we have seen earlier. So, in this range from 3π by 2 to 5π by 2 you get 2 bound states thanks to Pranav and Sayantan who did the calculations and the graph for me. And these are the graphs which have been used over here.

(Refer Slide Time: 36:38)

Now consider the scattering states for positive energy okay. Now energy is not intrinsically negative it is intrinsically positive okay. These are the solutions for the scattering of the continuum states and for this the solutions of course are different because the boundary conditions are different. And you set up the Schrodinger equation once again. (Refer Slide Time: 38:31)

The slide contains the following content:

$U(r)$ vs r graph: $U(r) = -\beta^2$ for $r < a$, $U(r) = 0$ for $r > a$. $\ell = 0$, $\frac{2mE}{\hbar^2} = k^2 > 0$. $y_{a\ell}(r) = rR_{\ell}(r)$.

$U(r) = \frac{2m}{\hbar^2} V(r)$

$\left[\frac{d^2}{dr^2} + \{-U(r)\} + k^2 \right] y_{a\ell}(r) = 0$

$\left[\frac{d^2}{dr^2} + \beta^2 + k^2 \right] y_{a\ell}(r) = 0 \quad r < a \quad y_{a\ell}(r) = C \sin(r\sqrt{\beta^2 + k^2})$

$\left[\frac{d^2}{dr^2} + k^2 \right] y_{a\ell}(r) = 0 \quad r > a \quad y_{a\ell}(r) = D \sin(kr + \delta_0(k))$

Continuity at $r = a \Rightarrow$

$C \sin(a\sqrt{\beta^2 + k^2}) = D \sin(ka + \delta_0(k))$

$C\sqrt{\beta^2 + k^2} \cos(a\sqrt{\beta^2 + k^2}) = Dk \cos(ka + \delta_0(k))$

NPTEL STITACS Unit 1 Quantum Theory of Collisions 228

We consider $\ell = 0$ and for continuum states the energy goes as k^2 and for this the solutions are different for $r < a$ and for $r > a$. For $r < a$, you have got sinusoidal solutions and for $r > a$, you do not have exponentially damped solutions anymore because these are continuum solutions, these are not bound, so they are oscillatory okay, and that is the reason you get sinusoidal solutions.

But the sinusoidal solutions will have a phase shift okay. That is a phase shift of the partial wave, the partial wave under consideration is $\ell = 0$, which is the S wave. So, that is denoted by the phase shift δ_0 because with respect to the continuum solutions for free particles the solutions in the presence, the scattering solutions in the presence of a potential are the same except for a phase shift and the phase shift is δ_0 it is $\frac{1}{2}\pi$ as we know right.

But $\ell = 0$ and then in addition to $\frac{1}{2}\pi$ there is a phase shift which is introduced by the potential which is the scattering phase shift δ_0 . So that is the δ_0 , that we now have in the solution in the asymptotic region $r > a$, now we impose the boundary conditions at $r = a$.

So, these two solutions must be equal and the derivatives must also be equal. So, the derivative will give you the cosine term. In both multiplied by the factor which multiplies r , so in this case it is $\beta^2 + k^2$ in this case it is k right. So, these are the two

equations which result from the continuity of the wave function and continuity of its derivative.

(Refer Slide Time: 40:27)

Slide 229 contains the following equations:

$$C \sin(a\sqrt{\beta^2 + k^2}) = D \sin(ka + \delta_0(k))$$

$$C\sqrt{\beta^2 + k^2} \cos(a\sqrt{\beta^2 + k^2}) = Dk \cos(ka + \delta_0(k))$$

$$\frac{1}{\sqrt{\beta^2 + k^2}} \tan(a\sqrt{\beta^2 + k^2}) = \frac{1}{k} \tan(ka + \delta_0(k))$$

$$= \frac{1}{k} \times \frac{\tan(ka) + \tan(\delta_0(k))}{1 - \tan(ka)\tan(\delta_0(k))}$$

$$\frac{k}{\sqrt{\beta^2 + k^2}} \tan(a\sqrt{\beta^2 + k^2}) - \frac{k}{\sqrt{\beta^2 + k^2}} \tan(a\sqrt{\beta^2 + k^2}) \tan(ka) \tan(\delta_0(k)) = \tan(ka) + \tan(\delta_0(k))$$

$$-\tan(\delta_0(k)) \left\{ 1 + \frac{k}{\sqrt{\beta^2 + k^2}} \tan(a\sqrt{\beta^2 + k^2}) \tan(ka) \right\} = \tan(ka) - \frac{k}{\sqrt{\beta^2 + k^2}} \tan(a\sqrt{\beta^2 + k^2}) \tan(ka)$$

NPTEL logo and footer: PCD STITACS Unit 1 Quantum Theory of Collisions 229

So, these two solutions must be the, these two equations must be satisfied and when you divide the first equation by the second, you get the relationship between the two tangents okay. And then you can manipulate this result by a little bit of very simple algebra by doing cross multiplication and rearranging the terms.

So, I will not go through these steps in detail it is very straightforward. All you are doing is you know rearranging the terms.

(Refer Slide Time: 41:16)

Slide 230 contains the following equations:

$$-\tan(\delta_0(k)) = \frac{\tan(ka) - \frac{k}{\sqrt{\beta^2 + k^2}} \tan(a\sqrt{\beta^2 + k^2})}{1 + \frac{k}{\sqrt{\beta^2 + k^2}} \tan(a\sqrt{\beta^2 + k^2}) \tan(ka)}$$

$$\tan(\delta_0(k)) = \frac{k \tan(a\sqrt{\beta^2 + k^2}) - \sqrt{\beta^2 + k^2} \tan(ka)}{\sqrt{\beta^2 + k^2} + k \tan(a\sqrt{\beta^2 + k^2}) \tan(ka)}$$

$$\frac{\tan(\delta_0(k))}{k} = \frac{\tan(a\sqrt{\beta^2 + k^2}) - \frac{\sqrt{\beta^2 + k^2}}{k} \tan(ka)}{\sqrt{\beta^2 + k^2} + k \tan(a\sqrt{\beta^2 + k^2}) \tan(ka)}$$

$$\alpha = -\lim_{k \rightarrow 0} \frac{\tan \delta_0(k)}{k}$$

scattering length

$$-\alpha = \frac{a \tan(a\beta) - \beta a}{\beta a}$$

$$\alpha = a - \frac{\tan(a\beta)}{\beta}$$

NPTEL logo and footer: PCD STITACS Unit 1 Quantum Theory of Collisions 230

So, that you get the tangent of the phase shift okay, which is tan delta. So, tan delta is what you are looking for, so you rearrange the terms and you find that can delta is given by this relation you can write it change the sign as well and you get the tan delta to be given by this ratio okay.

It is just a rearrangement of the terms. So, this is the final expression for tangent of the phase shift that you get and you can take this k from right to the left by dividing both sides by k. So, the first term becomes tangent of this angle and the second term you have got this beta square + k square square root divided by k. Now notice the tan delta by k in the limit k going to 0, gives you the scattering length okay.

So, we about an expression for the scattering length and the scattering length being given by this relation in the limit k going to 0, you let k going to go to 0, so this first term becomes tangent of a root beta. The second term becomes minus of this root beta square + k square over k in k going to 0 will become beta a okay.

Because you have got a tan ka over here which goes to ka in the limit k going to 0 okay, tan theta goes to theta in a limit theta going to 0, so ka goes to ka and that k cancels this k right. So you get this numerator in the denominator you root beta square over here and then you get from which you get beta. So, alpha becomes equal to a - tan alpha beta by beta. So that is the expression you get for the scattering length.
(Refer Slide Time: 43:16)

Reference: 'Quantum Theory of Scattering' by Ta-Yu Wu and Takashi Ohmura (Prentice Hall, 1962) page 73

n	βa	Levinson's Theorem	δ
0	$0 \leq \beta a < \frac{\pi}{2}$	$\delta_0(k \rightarrow 0) = 0 \times \pi$	$= 0$
*	$\frac{\pi}{2}$	$\delta_0(k \rightarrow 0) = \left(0 + \frac{1}{2}\right) \pi$	$\frac{\pi}{2}$
1	$\frac{\pi}{2} < \beta a < \pi$	$\delta_0(k \rightarrow 0) = \pi$	$\approx \pi$
1	$\pi < \beta a < \frac{3\pi}{2}$	$\delta_0(k \rightarrow 0) = \pi$	$\approx \pi$
1+*	$\frac{3\pi}{2}$	$\delta_0(k \rightarrow 0) = \left(1 + \frac{1}{2}\right) \pi$	$\frac{3\pi}{2}$
2	$\frac{3\pi}{2} < \beta a < 2\pi$	$\delta_0(k \rightarrow 0) = 2\pi$	$= 2\pi$
2	$2\pi < \beta a < \frac{5\pi}{2}$	$\delta_0(k \rightarrow 0) = 2\pi$	$= 2\pi$

$\alpha = -\lim_{k \rightarrow 0} \frac{\tan \delta_0(k)}{k}$
 $-\frac{1}{\alpha} = \lim_{k \rightarrow 0} k \cot \delta_0(k)$
 $\alpha = a - \frac{\tan(a\beta)}{\beta}$
 $\lim_{\beta \rightarrow 0} \alpha = a - \frac{\tan(a\beta)}{\beta} = a - \frac{a\beta}{\beta} \rightarrow 0$

NPTEL

And you can now make a table which I have borrowed from Wu and Ohmura very nice book quantum theory of scattering which I strongly recommend. And you, this table give you the number of bound states to the first column. Then here you have got the potential strength parameter. We have defined it as U0 a square this is the square root of U0 which is beta. And this is the square root of a square which is a.

So, this is essentially the strength parameter this gives you this k cot delta it tells you how the parameter x changes in this domain as beta a changes from 0 to pi by 2. This tells you how the scattering wavelength changes in this corresponding region of the potential strength as it

changes from 0 to pi by 2. And you get the phase shift which goes to 0 when the number of bound states is 0.

Then when the phase shift is pi by 2 that is when you get the first resonant bound state. That is when the electron is just about to be bound because it is resonantly bound and that is what I have indicated by this asterisk over here. So this is what is sometimes referred to as the half bound state. Because it is resonantly bound for any depth less than this it will not be bound for slightly more than this depth it will get bound.

Then you have if the strength parameter increases beyond pi by 2 till it gets to pi the number of bound States remains 1. In fact it remains 1 even when the strength exceeds pi till it gets to 3 pi by 2. Because still gets to 3 pi by 2 the next state does not get bound we have seen that in the solution. That the next bound state is what you get when the depth parameter, the strength parameter changes from pi by 2 to 3 pi by 2 that is when you get the next bound state.

And at this the phase should become 3 pi by 2 so the phase shift goes from 0 or it is pi by 2 or it is pi or 3 pi by 2 or it is 2 pi in this case when the number of bound state is 2 when this parameter exceeds 3 pi by 2 and so on. So, essentially this is a manifestation of the Levinson's theorem that the phase shift for S waves is an integer multiple of pi in this case right.

So, it is either 0 pi or pi or 1 pi or 2 pi and so on. Where the number multiplying pi is the number of bound states or else it is if you have a resonant bound state then it is half integer multiples of pi like 0 plus half times pi because this will become pi by 2 the phase shift becomes pi by 2 or 3 pi by 2 or 5 pi by 2 and so on right.
(Refer Slide Time: 46:44)

LEVINSON'S THEOREM

$zero\ of\ \delta_l(k): \delta_l(k \rightarrow \infty) = 0$

..... for $l=0$:

$\delta_0(k \rightarrow 0) = n_0 \pi$ ↖ "half-bound" state

or $\delta_0(k \rightarrow 0) = \left(n_0 + \frac{1}{2}\right) \pi$ if there is a (resonant)

"zero energy resonance" bound state solution

$\sigma_{total}(k \rightarrow 0) \xrightarrow{\text{blows up}} \frac{1}{k^2}$ when $\lambda_0 a = \sqrt{U_0} a = \frac{\pi}{2}$ at zero energy.

$\delta_0(k \rightarrow 0) \rightarrow \frac{\pi}{2}$ Yes! for $l \geq 1$

$\delta_l(k \rightarrow 0) = n_l \pi$ for $l \geq 1$

Kgl. Danske Videnskab. Selskab. Mat. Fys. Medd. 25 9 (1949)

QUESTIONS? Write to: pcd@physics.iitm.ac.in

STITACS Unit 1 Quantum Theory of Collisions

233

So, that is the basic resonance theorem that for S waves the phase shift the zero energy phase shift is either an integer multiple of π or it is a half integer multiple of π when there is a resonance okay. So, this is the resonance, this is the Levinson's theorem and when you have a resonance you will have zero energy resonance the cross section goes as 1 over k square as we have seen.

And this is a very powerful theorem it is valid not just for $l = 0$, but for any value of l the phase shift is the zero energy phase shift is always equal to $n\pi$ it is only in the case of zero energy zero $l = 0$ partial waves which is the S wave scattering that you have these resonant bound states. In which case the phase shift becomes half integer multiples of π okay.

So, if there are any questions I will be happy to take of course this theorem we have demonstrated for a square well potential but it is valid for other attractive potentials no matter what the shape of the attractive potential and what Sayantan and Pranov are working on the bound states of a cylindrical potential okay. It could be any, any potential it does not matter what is the nature of the potential.

It does not even have to have a very simple geometry it may have some you know very complicated dependence on r . Any physical potential will eventually go to zero it has no effect, no influence at infinity. So, it will have a certain range there may be a sharp cutoff or it may taper off rather slowly.

So, no matter what it is, if you have an attractive potential then it will have bound states subject to certain conditions which are discussed over here in terms of the strength of the potential parameter. For square wells it is very easy to define the strength because it is just U_0 a square you cannot define it in very simple terms like U_0 a square for other shapes of the potential so easily.

Nevertheless the idea of a strength over the potential is valid for any attractive potential because given it an attractive potential it is not guaranteed that the bound state will exist. And some minimal conditions some threshold conditions will need to be satisfied and depending on when that condition is satisfied you will have a bound state.

And if you make the potential deeper or stronger than that it does not automatically mean that you will have the next bound state because another threshold condition will have to be satisfied to pick the next bound state. So, we have found that for the square well potential the next bound state can result only when the strength parameter increases such that our parameter goes to the next half integer multiple of π by 2 .

So, it from $\pi/2$ to $3\pi/2$ you have got only one bound state. From $3\pi/2$ to $5\pi/2$ you get the next bound state okay. So, that the Levinson's theorem and in the next class we will we will discuss some further aspects of low energy scattering in particular I will introduce the effective range formalism developed by Schwinger, Betti and so on.

Thank you there is any question I will be happy to take (Question time: 50:28, not audible) you are calculating δ by just putting β a condition into the $\tan \delta$ yeah. As k tends to zero typically the phase shift goes as k^{2l+1} . So, it goes to zero and it goes to zero in integral multiples of π okay, so it goes to zero is an integral multiples of π the cross section goes to zero as the phase shift goes to zero right.

But the number of times this happens this value of the integer must change as the potential to get stronger because the potential has already crossed $\pi/2$ it has to cross $\pi/2$ to pick the first bound state. If it does not cross $\pi/2$ it cannot hold a bound state okay. So, this really enables you to provide an absolute value to the phase shift. So, it is not just 0 modulo π but what is the coefficient of π is determined by the number of bound states it holds.

Because the number of bound states is equal to 0 up to $\pi/2$, it is 1 between $\pi/2$ and $3\pi/2$ and only after $3\pi/2$ it becomes twice π after $5\pi/2$ it will become 2π that is what makes it $n + \text{half times } \pi$. But then the phase shift in between as k tends to zero in the non resonant region it must go to 0 modulo π , so it will go as zero π , 1 π , 2 π , 3 π and so on okay.

So, typically the phase shift zero energy phase shift is equal to $n\pi$ where n is the number of bound states. It is a very powerful theorem and it has got many applications in nuclear physics and atomic physics. Thank you.