Select/Special Topics in ‘Theory of Atomic Collisions and Spectroscopy’

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Lecture 36
Scattering of partial waves

Greetings, we will have four classes in unit 6 and we will begin to discuss Resonances in Collision phenomena. Resonances are also identified as quasi-stationary states on the principal reference for this unit will be Joachain’s book Chapter 4. Now, today's class, we, we will go a little slow. And essentially what I will do is to remind you about some of the things we studied in an earlier unit, in Unit 1 of this course.

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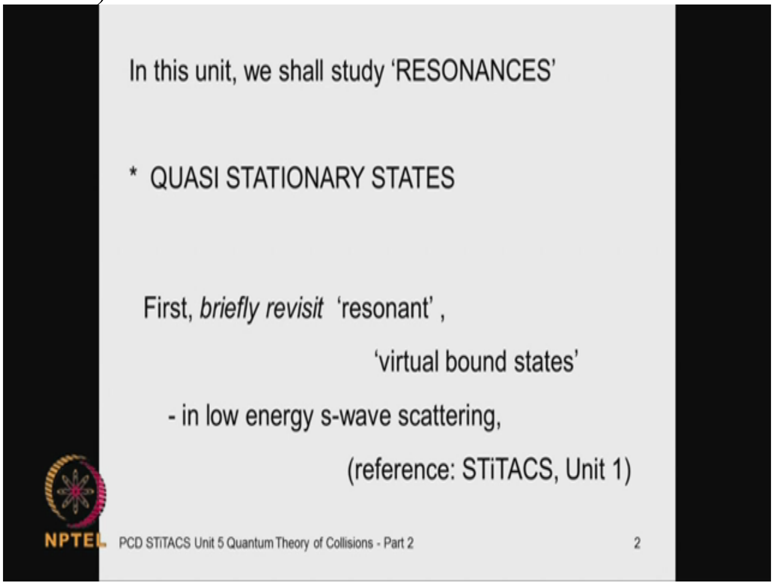

In this unit, we shall study ‘RESONANCES’

* QUASI STATIONARY STATES

First, *briefly revisit* ‘resonant’,
‘virtual bound states’
- in low energy s-wave scattering,
(reference: STiTACS, Unit 1)

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Because we already talked about Resonance states, we talked about the Virtual bound States when we talked about Collisions at low energies, in particular, the s-wave Scattering which we discussed in the Unit 1 of this course. So, I will spend a few minutes re-visiting that and so that it will help us warm up to this topic.

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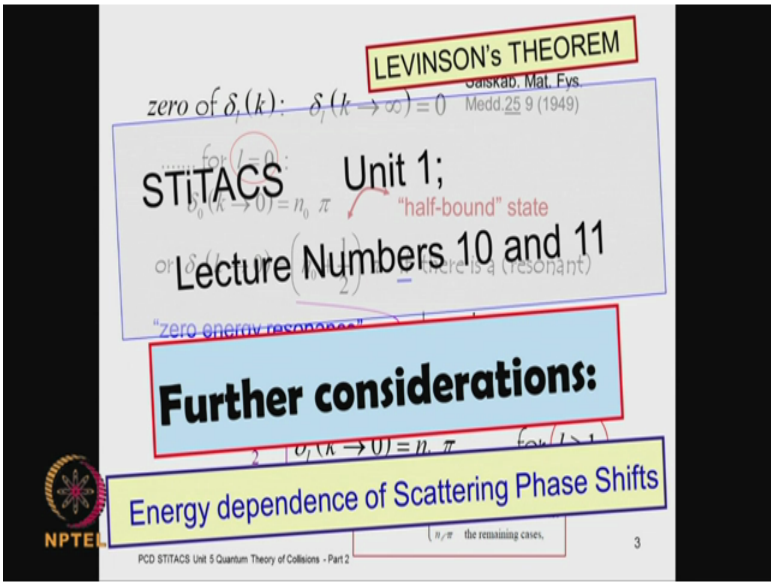

LEVINSON's THEOREM

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

STiTACS Unit 1;

Lecture Numbers 10 and 11

Further considerations:

Energy dependence of Scattering Phase Shifts

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So, in particular, have a look at lecture number is 10 and 11 of unit 1 of this course and what is in the background, in the slide, is the Levinson theorem which we have discussed at considerable length in the previous unit, right. So, we will take our awareness of the Levinson's Theorem for granted for this unit.

So, what we will do is, is to develop some further considerations which go below beyond the immediate consequences of the Levinson's Theorem. And, in particular, we will discuss how the scattering phase shifts depends on energy at low energies. We know the low energy limit which is k tending to zero but when it is not quite 0, but it is still low energy.

And what is its Energy dependence? How does it change? So, we are now getting into some details beyond the Levinson's Theorem.

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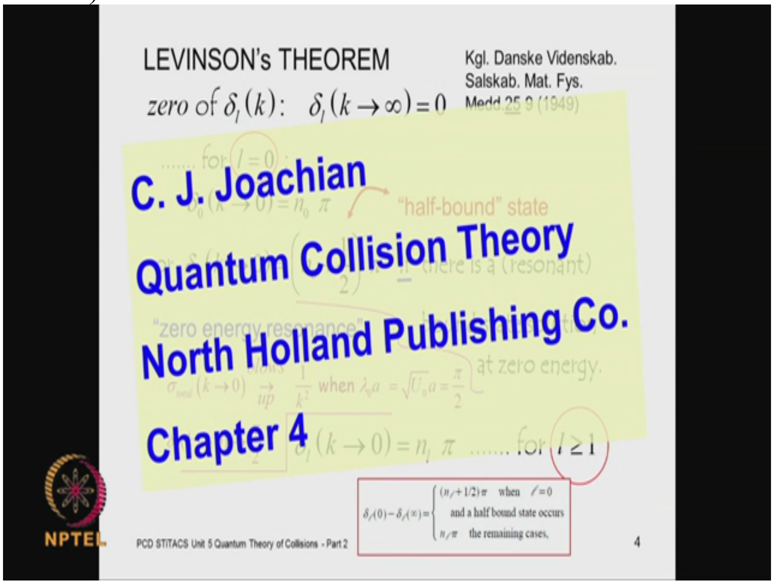

LEVINSON's THEOREM

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

C. J. Joachian

Quantum Collision Theory

North Holland Publishing Co.

Chapter 4

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

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

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And as I mentioned earlier, this is the primary reference for this portion which is a very fine book. I really love this.

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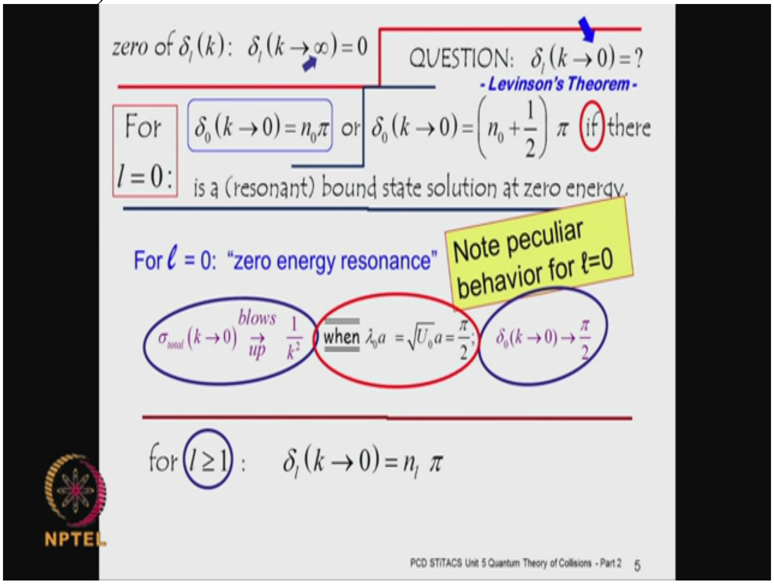

zero of $\delta_l(k)$: $\delta_l(k \to \infty) = 0$

QUESTION: $\delta_l(k \to 0) = ?$

- Levinson's Theorem -

For $l = 0$: $\delta_0(k \to 0) = n_0\pi$ or $\delta_0(k \to 0) = \left(n_0 + \frac{1}{2}\right)\pi$ if there is a (resonant) bound state solution at zero energy.

For $\ell = 0$: "zero energy resonance"

Note peculiar behavior for ℓ=0

$\sigma_{total}(k \to 0) \overset{blows}{\underset{up}{\to}} \frac{1}{k^2}$ when $\lambda_0 a = \sqrt{U_0}a = \frac{\pi}{2}$; $\delta_0(k \to 0) \to \frac{\pi}{2}$

for $l \geq 1$: $\delta_l(k \to 0) = n_l\,\pi$

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So, the phase shifts are measured with reference to a set of zero of the angle. And this zero of the angle is the high energy limit of the phase shift, okay. And as k tends to 0, the phase shift would go to 0 for the lth partial wave.

So, that is the reference level. What happens when k tends to 0? Now that answer is provided by the Levinson’s Theorem, okay. Levinson’s Theorem tells us what happens in the low energy limit which is k tending to zero. So, we know what is at the extreme k tending to zero. And then, as k goes to infinity.

And then we will examine what happens in between and that's where a lot of interesting dynamics is. So, from the Levinson’s Theorem here, we know that for the alert partial wave, if l = 0, when we deal with s-wave scattering and that is the most important contributing to contributor to the collision phenomena at low energies, as we have discussed earlier. This phase shift goes to n times pi where this is the number of bound States.

However, if there is a resonant bound state at that energy, then, it does not go to n0 pi, instead, it goes to n0 + half pi where n0 is the number of bound states which exist at that particular, for that particular potential. For, this is the zero energy resonance. And we have discussed this in our previous unit. We have shown that the phase shift, when you do have a resonant structure, when the strength parameters.

Though we discuss this in the context of a square well potential and the strength of the attractive potential depends on the depth of the potential and the range of the potential. The two together, in fact, it depends quadratically on the range and linearly on the depth. So, u zero a square, is the strength parameter or sometimes it is taken as a root of u 0 times a. So, this is the strength parameter and when this strength parameter becomes pi by 2.

Then, you get the resonant possibility. And the phase shift then, goes to pi by 2. So, this is a virtual bound state, okay. So, at any depth less than this, you would not have a bound state. But then, if you have the depth even a little more than this order, the range, a little more than this, then you will have a bound state.

So, this is the zero energy resonance and at this resonance the cross section blows up. It blows up as 1 over k square. So, you can see that as k tends to 0, it just shoots off. So, what happens if l = 1 or greater than 1, then, the phase shift is always an integral multiple of pi the integer, being the number of bound states, which exists for that particular potential depending on its depth and range.

So, there is a peculiar behaviour for the s phase, as you have noticed which we have discussed in the previous unit.

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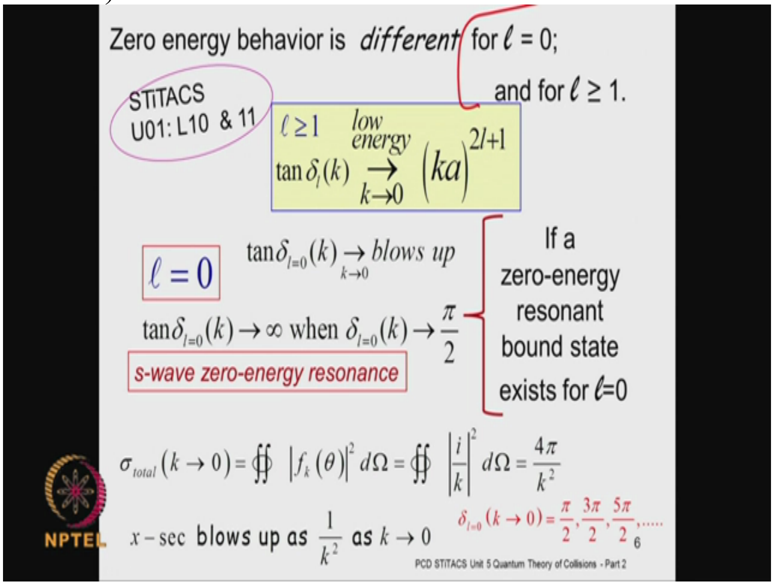

Zero energy behavior is *different* for $\ell = 0$;

and for $\ell \geq 1$.

STITACS
U01: L10 & 11

$\ell \geq 1$ low energy $\tan\delta_l(k) \xrightarrow[k\to 0]{\text{low energy}} (ka)^{2l+1}$

$\boxed{\ell = 0}$ $\tan\delta_{l=0}(k) \underset{k\to 0}{\rightarrow}$ *blows up*

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

s-wave zero-energy resonance

If a zero-energy resonant bound state exists for ℓ=0

$$\sigma_{total}(k \rightarrow 0) = \oiint |f_k(\theta)|^2 d\Omega = \oiint \left|\frac{i}{k}\right|^2 d\Omega = \frac{4\pi}{k^2}$$

$x-\sec$ blows up as $\frac{1}{k^2}$ as $k \rightarrow 0$

$\delta_{l=0}(k \rightarrow 0) = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots\ldots$

And the zero energy behaviour is therefore different for l = 0 and for l greater than or equal to 1. So, I will refer you to the lecture number 10 and 11 of the unit 1 of this course, we have seen in that unit, that the tangent of the phase shift has for its low energy limit the 2l + 1 power dependence on k.

So, as k tends to 0, so, that is just there like a threshold effect okay. And this goes into various, you know, these are results, these results are very general and very powerful go into the framework of what are commonly known as the threshold laws. Wigner made significant contribution to this particular area. So, these are the, this is the threshold behaviour.

And for l equal to zero, the tangent blows up when you have a zero energy resonance, if there is a bound state exactly at that limit okay. Now, we have discussed this: that the cross section goes as 1 over k square. And this phase shift then will be either pi by 2 for the resonant case or it could be 3 pi by 2, or 5 pi by 2. It is not an integral multiple of pi, mind you in this case. But it goes in steps of pi by 2, 3 pi by 2, 5 pi by 2 and so on.

And how large it is depending on how many bound States the potential whole, so just the fact that there is a bar, there is an attractive potential does not mean that you will have a bound state because the potential will have to be sufficiently strong, so that you can have a bound state, okay.The potential being attractive is a necessary condition it is not a sufficient condition for you to get a bound state solution.

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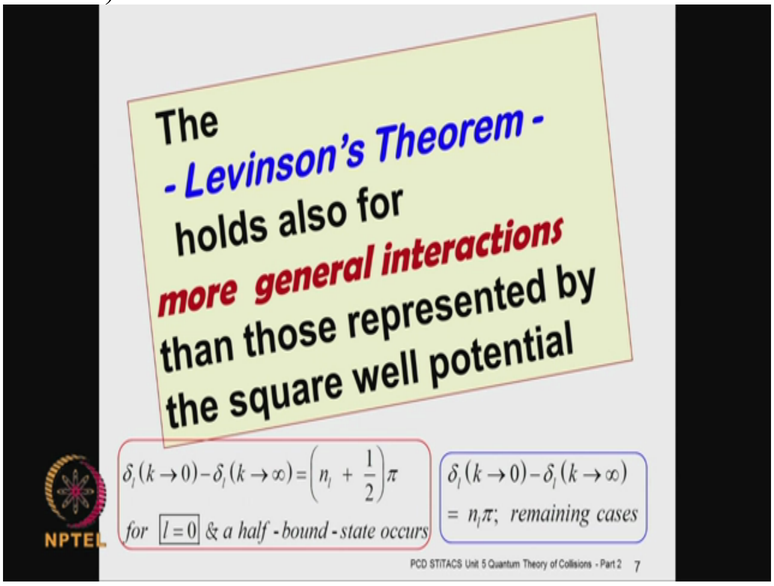

The
- *Levinson's Theorem* -
holds also for
more general interactions
than those represented by
the square well potential

$$\delta_l(k\to 0)-\delta_l(k\to\infty)=\left(n_l+\frac{1}{2}\right)\pi$$

for $\boxed{l=0}$ & a half - bound - state occurs

$$\delta_l(k\to 0)-\delta_l(k\to\infty)$$
$$= n_l\pi;\ \text{remaining cases}$$

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So, this theorem, which is stated so simply that the phase shift is either n pi or n + half pi depending on l being equal to 1 or greater than 1 or equal to 0. We obtained this theorem explicitly for the square well potential. However, it holds also for many general potentials; not just for the square well potential.

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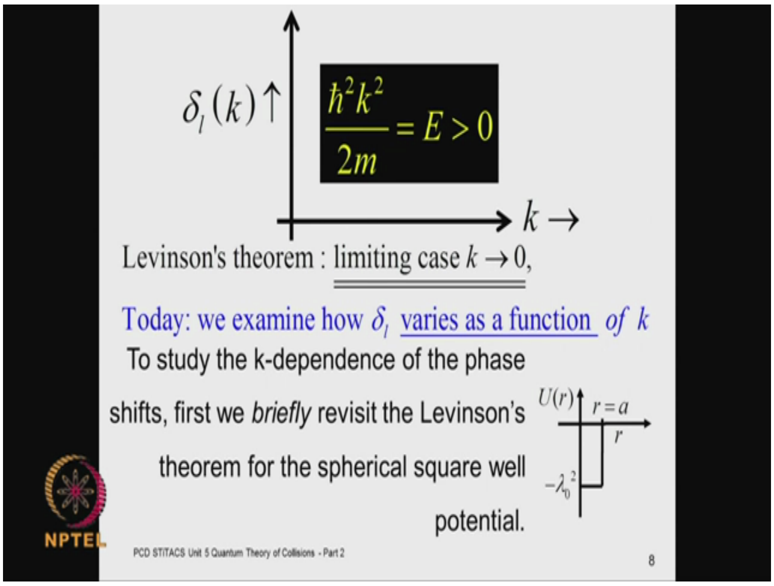

$\delta_l(k)\uparrow$

$$\frac{\hbar^2 k^2}{2m} = E > 0$$

$k \rightarrow$

Levinson's theorem : limiting case $k \rightarrow 0$,

Today: we examine how δ_l varies as a function of k

To study the k-dependence of the phase shifts, first we *briefly* revisit the Levinson's theorem for the spherical square well potential.

So, which is why, it is such a powerful but a theorem. Now, what we will examine is remember limiting behaviour as k tends to 0, okay. What happens as k changes? So, this is k = 0. But, if the k increases gradually and you are still in the low energy regime, okay, you are still in the low energy regime of the collision phenomena, if you plot the phase shift as a function of k. how will this plot look like, okay?

What is the low energy, energy dependence at the phase shift is what we will discuss today. And we will illustrate this by taking the example of the square well potential. So, you have got a depth of minus lambda 0 square. And then, you have a range of r = a. So, this is the square of spherical potential.

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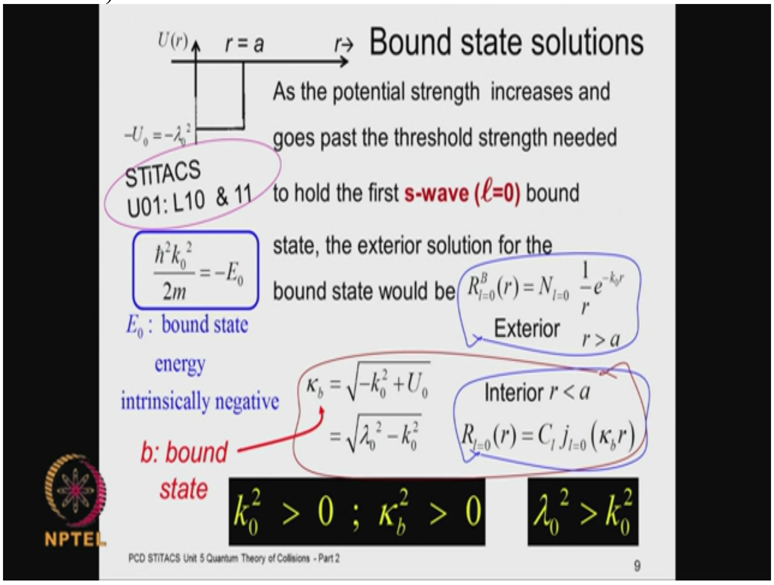

Bound state solutions

As the potential strength increases and goes past the threshold strength needed to hold the first **s-wave (ℓ=0)** bound state, the exterior solution for the bound state would be $R^B_{l=0}(r) = N_{l=0}\frac{1}{r}e^{-k_0 r}$ Exterior $r > a$

STiTACS U01: L10 & 11

$$\frac{\hbar^2 k_0^2}{2m} = -E_0$$

E_0 : bound state energy intrinsically negative

b: bound state

$\kappa_b = \sqrt{-k_0^2 + U_0} = \sqrt{\lambda_0^2 - k_0^2}$

Interior $r < a$ $R_{l=0}(r) = C_l\, j_{l=0}(\kappa_b r)$

$k_0^2 > 0 \;;\; \kappa_b^2 > 0$

$\lambda_0^2 > k_0^2$

And we will re-examine the bound state solutions. The bound state energy is intrinsically negative okay. So h cross square k0 squares by 2m = - E0 because E0 is intrinsically negative. And we will consider first, where l = 0 solutions the S wave scattering and in this case the exterior solution of course will die off exponentially, okay. So, it will have an exponentially decaying solution outside.

And in the interior, you will have the Bessel functions, okay for the solutions. And the Bessel functions, the argument of the Bessel function will be kappa r where kappa will be determined by this k 0 which is the bound state energy and the potential depth, okay. So, these are the two things which will determine the value of Kappa.

So, we have put a subscript b on Kappa to remind us that this is the bound state solution. So, these are the two solutions and you can see that for us in for the geometry that we are dealing with lambda 0 square will be greater than k 0 square so that you will have a bound State there.

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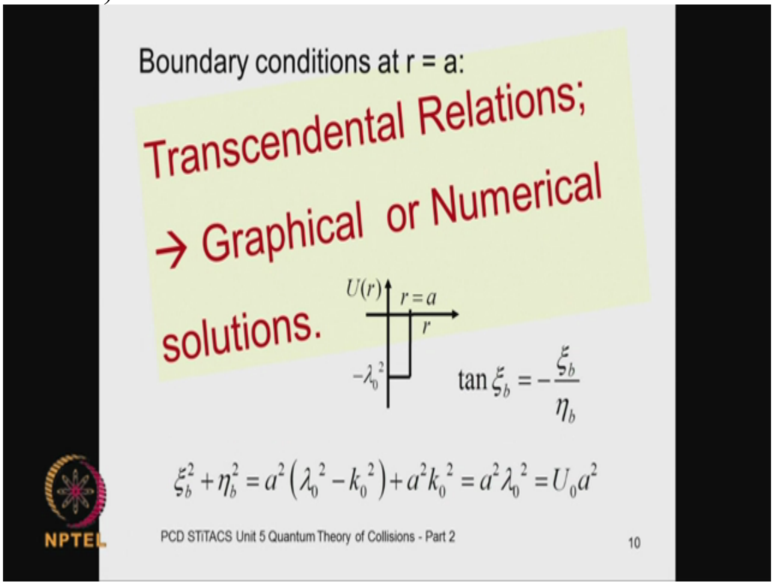

Boundary conditions at r = a:

Transcendental Relations;

→ Graphical or Numerical solutions.

$$\tan\xi_b = -\frac{\xi_b}{\eta_b}$$

$$\xi_b^2+\eta_b^2 = a^2\left(\lambda_0^2-k_0^2\right)+a^2k_0^2 = a^2\lambda_0^2 = U_0a^2$$

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Now, we have discussed these solutions at length in the previous unit. So, I will not re-visit that in any great detail. But you will remember that the bounce rate solutions were obtained at the intersections of these two families of curves, okay. So, there is one solution which is the relationship between Xi and beta.

And then, another set of solutions which is an equation to the circle. And wherever these two curves intersect, we get a solution or this being transcendental relations typically graphical or numerical solutions are obtained.

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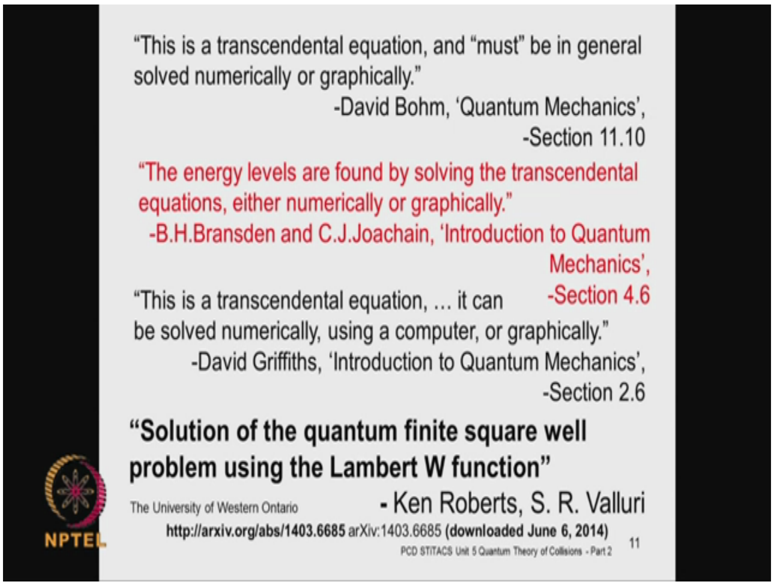

"This is a transcendental equation, and "must" be in general solved numerically or graphically."

-David Bohm, 'Quantum Mechanics',
-Section 11.10

"The energy levels are found by solving the transcendental equations, either numerically or graphically."

-B.H.Bransden and C.J.Joachain, 'Introduction to Quantum Mechanics',
-Section 4.6

"This is a transcendental equation, … it can be solved numerically, using a computer, or graphically."

-David Griffiths, 'Introduction to Quantum Mechanics',
-Section 2.6

"Solution of the quantum finite square well problem using the Lambert W function"

The University of Western Ontario
- Ken Roberts, S. R. Valluri

http://arxiv.org/abs/1403.6685 arXiv:1403.6685 **(downloaded June 6, 2014)**

And I would like to make an interesting observation over here by quoting some writers from books which you would have used. David Bohm's book for example: He says in Section 11 that this is a transcendental equation and must be in general solved numerically or graphically okay. Now, this is David Bohm.

Now, we have Bransden and Joachain and section 4.6. They say the energy levels are found by solving the transcendental equations either numerically or graphically which is pretty much the same thing. Then you have Griffiths, Introduction to Quantum Mechanics. And what does he say?

That this is a transcendental equation it can be solved numerically using a computer or graphically, right? As if there is no other way of doing it. And then I would like you to read this paper by Ken Roberts and Ram Valluri, my good friend at the University of Western Ontario. And I have given the link over here. I strongly recommend that you go through this work.

And they have shown using lambda w functions, how analytical solutions can be obtained for this problem. And this lambda w function is a very powerful technique you can get analytical solutions in many situations. It, they have a very wide range of applications not just in collision problems, but in a very wide variety of problems.

In fact, even for the Coulomb scattering that we discussed yesterday. You can have some applications and photoionization cross-sections you can use them. So, they make use of the poly logarithm functions. And this is very powerful to which Ram has really mastered and strongly recommend that you acquaint yourself with this technique.

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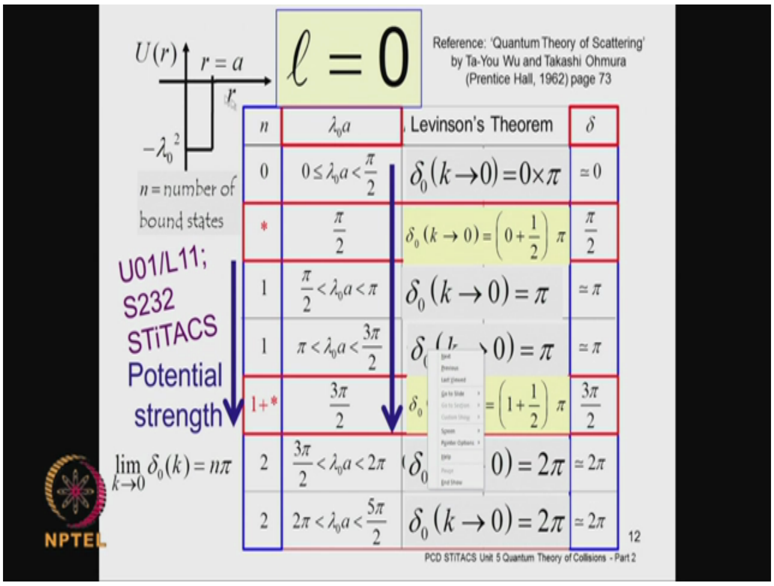

$\ell = 0$

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

n = number of bound states

U01/L11; S232 STiTACS

Potential strength

$\lim_{k \to 0} \delta_0(k) = n\pi$

n	$\lambda_0 a$	Levinson's Theorem	δ
0	$0 \le \lambda_0 a < \frac{\pi}{2}$	$\delta_0(k \to 0) = 0 \times \pi$	$\simeq 0$
*	$\frac{\pi}{2}$	$\delta_0(k \to 0) = \left(0 + \frac{1}{2}\right)\pi$	$\frac{\pi}{2}$
1	$\frac{\pi}{2} < \lambda_0 a < \pi$	$\delta_0(k \to 0) = \pi$	$\simeq \pi$
1	$\pi < \lambda_0 a < \frac{3\pi}{2}$	δ [illegible] $0) = \pi$	$\simeq \pi$
1+*	$\frac{3\pi}{2}$	δ_0 [illegible] $= \left(1 + \frac{1}{2}\right)\pi$	$\frac{3\pi}{2}$
2	$\frac{3\pi}{2} < \lambda_0 a < 2\pi$	δ_0 [illegible] $0) = 2\pi$	$\simeq 2\pi$
2	$2\pi < \lambda_0 a < \frac{5\pi}{2}$	$\delta_0(k \to 0) = 2\pi$	$\simeq 2\pi$

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So, what was the result of the Levinson Theorem? That as lambda 0a is the strength parameter, right? This is lambda 0, is the square root of the depth a, is the range. And as this increases from 0 to pi by 2 then, till it gets to pi by 2, you cannot have any bound state at all. So the number of bound state is 0 and the phase shift will be 0. This is for the S waves.

However, when this strength parameter exceeds pi by 2, then, you have one bound state. And then, the phase shift the low-energy phase shift as k tends to 0 will be equal to pi. And what happens at pi by 2? That is something which I have indicated by this asterisk. That is when you have a virtual bound state. So, that is a resonant bound state, okay. So it is in some sense neither here nor there or in another sense it is here and also there.

And it is like the Schrodinger's scat which is either dead or alive. And the reason this happens is because of Quantum Mechanics, because there is a superposition between the bound state solution and the continuum solution, okay. So, you have a resonant structure over there. And that these two possibilities and that is when you get the resonance. So, you have this you, you have the resonance at pi by 2.

You have it again at 3 pi by 2 when the first box state is already nicely bound. And the next bound state is about to be bound; it is not bound at a depth, slightly below this. And it is bound slightly above this at 3 pi by 2; it is a resonance state, okay. So, this is the picture we get from the Levinson's theorem.

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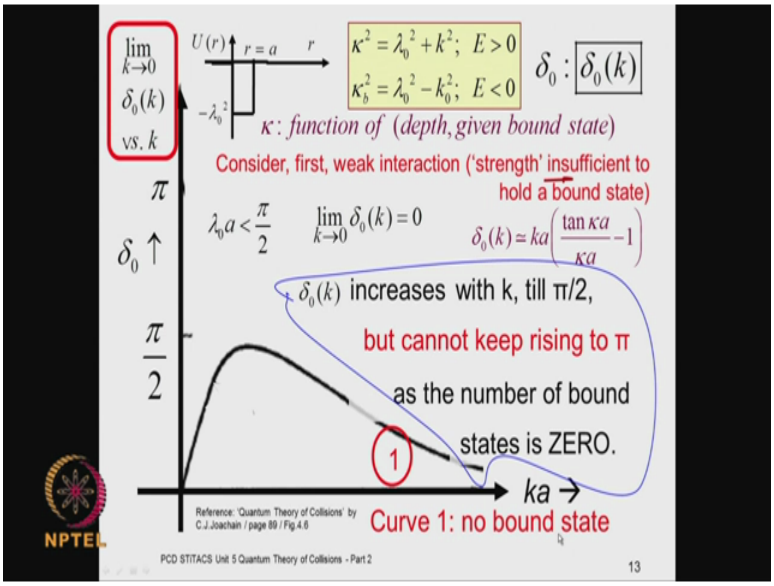

$\lim_{k \to 0} \delta_0(k)$ vs. k

$\kappa^2 = \lambda_0^2 + k^2;\ E > 0$

$\kappa_b^2 = \lambda_0^2 - k_0^2;\ E < 0$

$\delta_0 : \boxed{\delta_0(k)}$

κ: function of (depth, given bound state)

Consider, first, weak interaction ('strength' insufficient to hold a bound state)

$\lambda_0 a < \frac{\pi}{2}$ $\quad \lim_{k \to 0} \delta_0(k) = 0$ $\quad \delta_0(k) \simeq ka\left(\frac{\tan \kappa a}{\kappa a} - 1\right)$

$\delta_0(k)$ increases with k, till π/2,

but cannot keep rising to π

as the number of bound states is ZERO.

Reference: 'Quantum Theory of Collisions' by C.J.Joachain / page 89 / Fig.4.6

Curve 1: no bound state

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So, let us, our interest is in examining how the phase shift changes with case. If you plot delta 0 vs k, not just look at the limiting behaviour k tending to 0, but to what, how does it change with k, as you change k in the low energy domain. So, that is our question here. And we first consider a potential which is a very weak, attractive potential. It is attractive but not sufficiently strong to have even a single bound state, okay.

So, all that attractive feature is not sufficient to bind a particle. And in this case, the phase shift will go to 0, right. So, if you now plot delta 0 vs k, the behaviour is given by this function which we have discussed earlier, it will go to 0 and as you increase k, the phase shift will increase because delta k, ok is given by this ka times tan kappa a by kappa a - 1.

We have derived this relation in the previous unit. So, the phase shift will increase that it cannot keep increasing up to pi, because for the phase shift to be pi, you need the potential to have one bound state, which it does not, because the potential is attractive but not enough attractive to have a bound state. So, the phase shift will not get 2pi.

And what will happen to the phase shift is that it will keep increasing till it gets to pi by 2, and then, start diminishing again because the high energy limit of course is 0, right. So, the phase shift will start increasing and then it will come down. So, you can already expect that the phase shift will have this profile that it will increase from here.

So, this is the curve one. It has got no bound state, zero bound state. And the phase shift increases till it approaches pi by 2 then flips over and then Falls to zero, eventually as k increases. So, that is how the phase shift changes with k. What if the potential has either a little more depth or a little more range then it will pick up a bound state once lambda 0a crosses pi by 2. So, that is the threshold value, right.

So, that is the minimum strength that it should have. So, this is the picture when there is no bound state at all.

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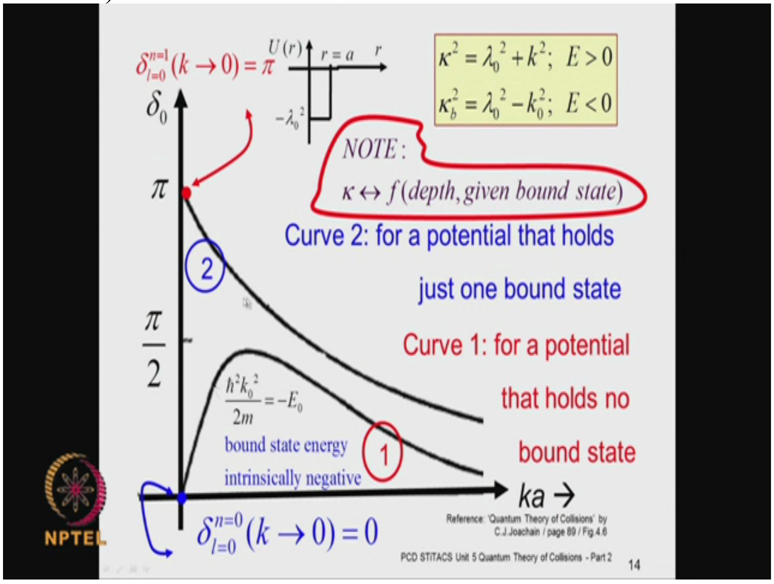

$\delta_{l=0}^{n=1}(k \to 0) = \pi$

$\kappa^2 = \lambda_0^2 + k^2;\ E > 0$

$\kappa_b^2 = \lambda_0^2 - k_0^2;\ E < 0$

NOTE:

$\kappa \leftrightarrow f(\text{depth, given bound state})$

Curve 2: for a potential that holds just one bound state

Curve 1: for a potential that holds no bound state

$\frac{\hbar^2 k_0^2}{2m} = -E_0$

bound state energy intrinsically negative

$\delta_{l=0}^{n=0}(k \to 0) = 0$

Reference: 'Quantum Theory of Collisions' by C.J.Joachain / page 89 / Fig.4.6

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And when you do have one bound state, then, the phase shift as k tends to 0, will be equal to npi, n = 1 now. So, the phase shift will be pi it will begin over here and then it will keep falling. So, the behaviour of the phase shift, the changes in a dramatic manner, in a very dramatic manner depending on the number of bound state.

So, for 0 bound State it goes like this. If you have one bound state it will fall like this. So, these graphs are straight out of Joachain's book. This is in fact figure 4.6 from his book.

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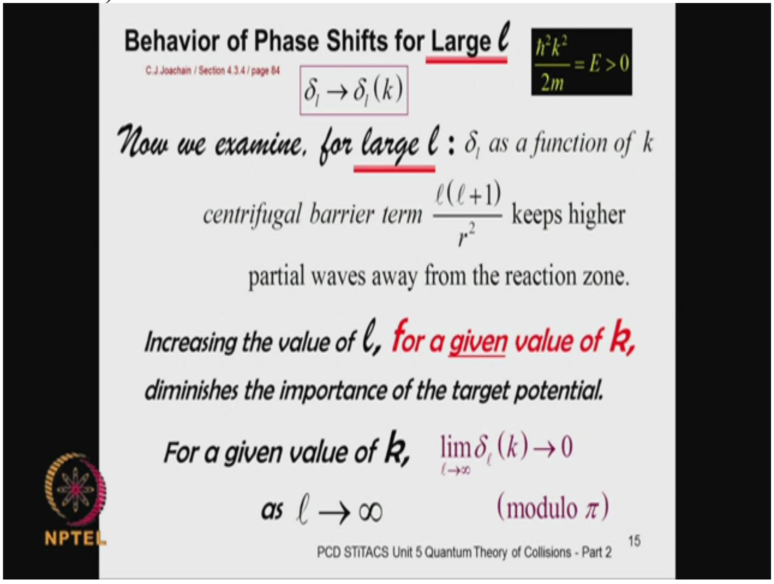

Behavior of Phase Shifts for Large ℓ

C.J.Joachain / Section 4.3.4 / page 84

$\delta_l \to \delta_l(k)$

$\frac{\hbar^2 k^2}{2m} = E > 0$

Now we examine, for large ℓ : δ_l as a function of k

centrifugal barrier term $\frac{\ell(\ell+1)}{r^2}$ keeps higher partial waves away from the reaction zone.

Increasing the value of ℓ, for a given value of k, diminishes the importance of the target potential.

For a given value of k, $\lim_{\ell \to \infty} \delta_\ell(k) \to 0$ as $\ell \to \infty$ (modulo π)

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And now having considered the l equal to zero behaviour, we will now consider the large l, okay. So, let us consider the large l and ask ourselves how will the phase shift change with k the limiting value we already know that as k tends to 0 it will go as npi that is Levinson's theorem. But if you plot delta as a function of k, not just the limiting value k tending to zero, how will the graph of delta versus K look like?

So, that is the question we examined. Now remember, that as l increases, the centrifugal barrier term will become more and more important and it can become so important that, it becomes so much more important than the potential itself, when the potential does not matter, okay. It is there, but it is coming. The total potential is a sum of the centrifugal term plus the physical potential.

The two potentials add up, okay in a radial differential equation for the Schrodinger equation, the two potential add up; one of which becomes a global compared to the other. And the other takes over the dynamics completely. And the physical potential is of no relevance and does not matter if it is square well potential or it has got some shape or no shape or you know whatever it is, it just does not matter.

So, what is going to happen is that if you increase the orbital angular momentum quantum number, then, the target potential becomes less and less significant? And then, we do know that for any given value of k, you can always go to values of l, large enough because in the partial wave analysis l will go all the way from 0 to infinity in the expansion of a plain wave.

You can always go to a value which is large enough and at that value, the potential as if it does not matter. And the phase shift would go to 0 as n tends to infinity for any given value of k, okay. So, that is the large behaviour of the phase shift.

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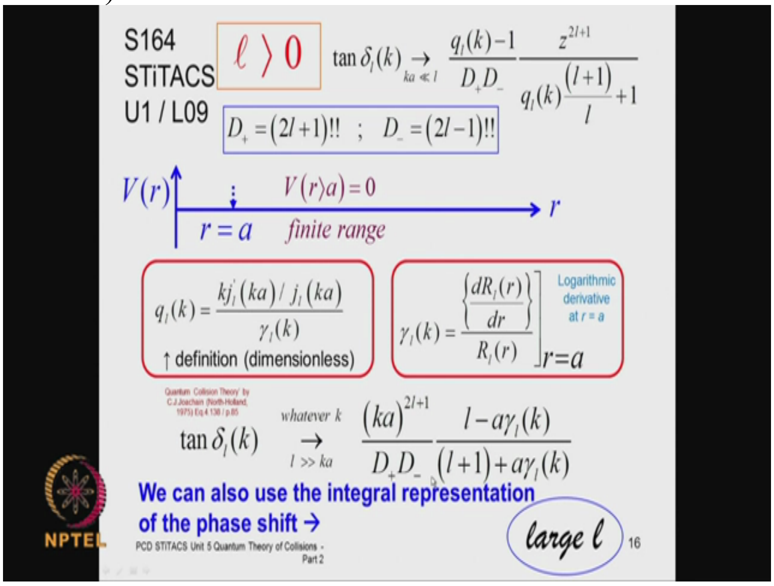

S164
STiTACS
U1 / L09

$$\boxed{\ell \rangle 0}$$

$$\tan\delta_l(k) \xrightarrow[ka \ll l]{} \frac{q_l(k)-1}{D_+D_-}\frac{z^{2l+1}}{q_l(k)\frac{(l+1)}{l}+1}$$

$$\boxed{D_+=(2l+1)!! \;\; ; \;\; D_-=(2l-1)!!}$$

$$\boxed{q_l(k)=\frac{kj_l'(ka)/j_l(ka)}{\gamma_l(k)}}$$

↑ definition (dimensionless)

$$\boxed{\gamma_l(k)=\left.\frac{\left\{\frac{dR_l(r)}{dr}\right\}}{R_l(r)}\right]_{r=a}}$$

Logarithmic derivative at $r = a$

Quantum Collision Theory' by C.J.Joachain (North-Holland, 1975) Eq.4.138 / p.85

$$\tan\delta_l(k) \xrightarrow[l \gg ka]{\text{whatever } k} \frac{(ka)^{2l+1}}{D_+D_-}\frac{l-a\gamma_l(k)}{(l+1)+a\gamma_l(k)}$$

We can also use the integral representation of the phase shift →

large l

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So, let us take some examples here and we have already discussed l equal to 0. So, now we are discussing a greater than 0. So, it will be at least one or more and we have deduced this relation in the previous unit in unit 1 of this course that the tangent of the phase shift is given by this relation.

We had introduced the symbols over here d + and d -. So, these are the double factorial, okay which we have used earlier. We had introduced this dimensionless quantity which is a ratio of kj prime by j. These are the spherical Bessel functions and gamma was the logarithmic derivative of the function inside the potential region. And outside if it has got a strict boundary at r = a.

So, that was the logarithmic derivative. So, gamma is this and this is coming simply from the continuity of the wave function and it is derivative. So, the larger behaviour is given by this relation. No matter what k is, okay. And this will also have a resonant structure, which will depend on this denominator here; because if this denominator vanishes, then, you will expect a resonant behaviour, okay.

So, we will use the integral representation of the phase shift which we have obtained in the previous unit.

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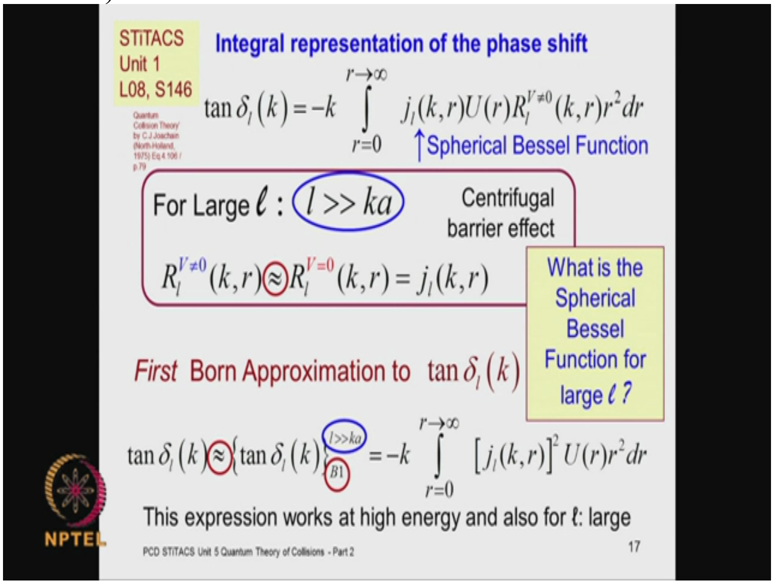

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Quantum Collision Theory by C.J.Joachain (North-Holland, 1975) Eq 4.106 / p.79

Integral representation of the phase shift

$$\tan\delta_l(k) = -k\int_{r=0}^{r\to\infty} j_l(k,r)U(r)R_l^{V\neq 0}(k,r)r^2dr$$

↑Spherical Bessel Function

For Large ℓ : $l \gg ka$ Centrifugal barrier effect

$$R_l^{V\neq 0}(k,r) \approx R_l^{V=0}(k,r) = j_l(k,r)$$

What is the Spherical Bessel Function for large ℓ ?

First Born Approximation to $\tan\delta_l(k)$

$$\tan\delta_l(k) \approx \left\{\tan\delta_l(k)\right\}_{B1}^{l\gg ka} = -k\int_{r=0}^{r\to\infty}\left[j_l(k,r)\right]^2 U(r)r^2dr$$

This expression works at high energy and also for ℓ: large

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This is given in terms of the spherical Bessel function, the potential and the radial solution, I have put v not equal to 0 as a superscript, because, you deal with radial functions of two kinds: One is the solution for the free particle which is the absence of the potential. That is the reference phase and all the phase shifts are measured with respect to the free particle incident beam phase shift, phase value, right.

So, you have the integral representation. This is integration over the entire space 0 through infinity. And then, you have a large value of l. Then, we have noticed that the potential does not matter because of this centrifugal barrier effect. And if the potential does not matter, then, this solution over here, which is actual radial solution for the Schrodinger equation with the potential, with the scattering potential. But then, if all is large, it does not matter.

So, the solution will be pretty much the same as you would have if V is equal to 0. So, the radial solution for V not equal to 0 is pretty much the same as the solution when V is equal to zero which of course is the spherical Bessel function. So, you can put over here for this case when l is large; when l is large, you can use this radial function to be given by the Bessel function.

So, you will have one over here and another Bessel function over here. So, this is like the Born approximation, okay, it is a, right. And you can see that this works at high energy. This works as we discussed in the context of the born approximation. It is a high-energy approximation but the same expression appears even if you are dealing with large l.
So, the large l behaviour is similar to the born approximation at high energy. So, these give you essentially the same kind of relationships. So, here, when l is large you can use the same result. And now, let us plug in the explicit form of the Bessel function. So, what is the spherical Bessel function for larger l.
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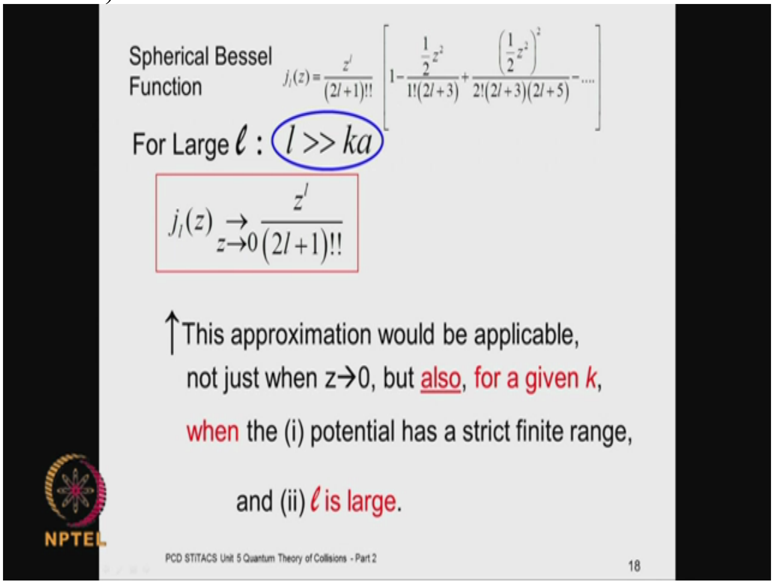

Spherical Bessel Function $j_l(z) = \frac{z^l}{(2l+1)!!}\left[1 - \frac{\frac{1}{2}z^2}{1!(2l+3)} + \frac{\left(\frac{1}{2}z^2\right)^2}{2!(2l+3)(2l+5)} - \ldots\right]$

For Large ℓ : $l >> ka$

$$\boxed{j_l(z) \underset{z\to 0}{\to} \frac{z^l}{(2l+1)!!}}$$

↑This approximation would be applicable, not just when z→0, but also, for a given *k*, when the (i) potential has a strict finite range,

and (ii) ℓ is large.

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So, for large l, what will it be? So, here, this is the policies expansion of the Bessel function in terms of its argument z in our case the z will be ka or kr and so on, right. And here notice, that for any given value of k, if you look at the terms inside this bracket, they are all multiplied by another factor here. But then, inside the bracket, you have l in the denominator. And all of these terms are going to be compared with the number 1.

So, you have got one minus something, plus something, minus something and so on. But each term has got the l in the denominator and the value of l is pretty large. It keeps getting larger as you go to higher terms. But, even the very first term has got 2l + 3 and l is large, no matter what k is. If l goes large enough, okay, you can throw the rest of the terms, okay.

So, what it means is that you can approximate for large l the Bessel function to be given by just this other factor which is outside this bracket multiplying unity over here. And this is nearly equal to z to the power l divided by this 2l + 1, double factorial, okay. So, this approximation would be applicable not just when z = 0 but also for in some given value of k, when l is large.

So, where l is large, you get the same expression that you can use, but for a different reason, okay, the reasons are different for k going to 0. The reasons are that these higher powers of z become increasingly smaller, okay. So, that is the reason for the low energy behaviour.

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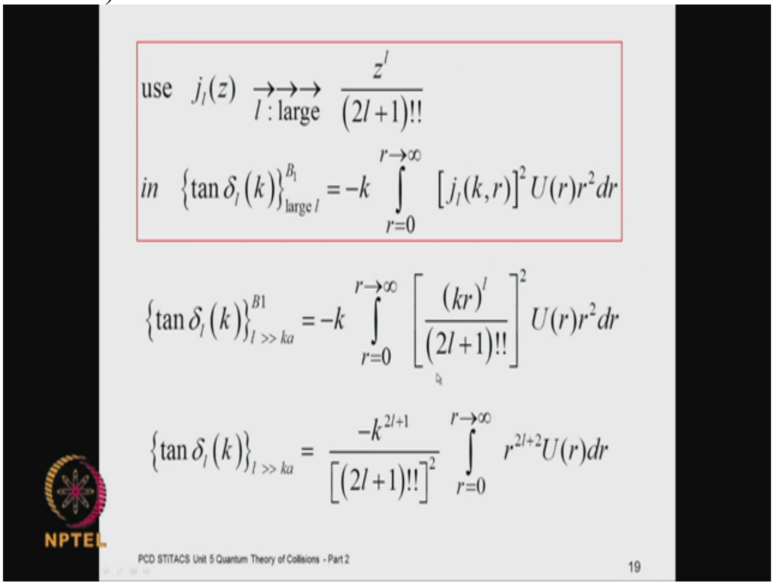

use $j_l(z) \underset{l\,:\,\text{large}}{\longrightarrow\!\!\longrightarrow\!\!\longrightarrow} \dfrac{z^l}{(2l+1)!!}$

$$in \quad \left\{\tan\delta_l(k)\right\}^{B_1}_{\text{large } l} = -k\int_{r=0}^{r\to\infty} \left[j_l(k,r)\right]^2 U(r)r^2dr$$

$$\left\{\tan\delta_l(k)\right\}^{B1}_{l\,\gg\,ka} = -k\int_{r=0}^{r\to\infty} \left[\frac{(kr)^l}{(2l+1)!!}\right]^2 U(r)r^2dr$$

$$\left\{\tan\delta_l(k)\right\}_{l\,\gg\,ka} = \frac{-k^{2l+1}}{\left[(2l+1)!!\right]^2}\int_{r=0}^{r\to\infty} r^{2l+2}U(r)dr$$

So, now our interest is in the large l behaviour and we have justified that this expression for the Bessel function can be used in this context. So, we put this Bessel function, the explicit form of this Bessel function over here. You leave the square of it, okay. So, you put z is kr, you put the square of it which is here kr to the power l upon 2l + 1, double factorial; 2l to the power 2.

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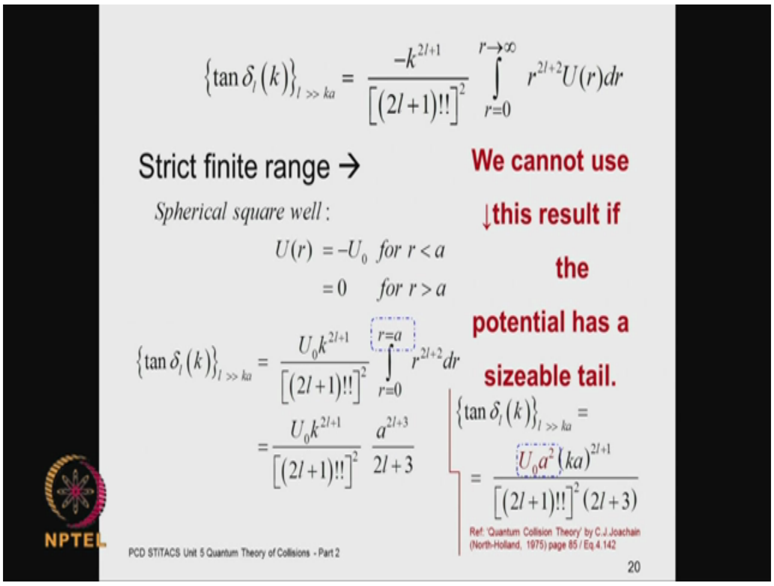

$$\{\tan\delta_l(k)\}_{l>>ka} = \frac{-k^{2l+1}}{[(2l+1)!!]^2}\int_{r=0}^{r\to\infty} r^{2l+2}U(r)dr$$

Strict finite range →

Spherical square well:

$$\begin{aligned} U(r) &= -U_0 \quad \text{for } r<a \\ &= 0 \quad \text{for } r>a \end{aligned}$$

$$\{\tan\delta_l(k)\}_{l>>ka} = \frac{U_0 k^{2l+1}}{[(2l+1)!!]^2}\int_{r=0}^{\boxed{r=a}} r^{2l+2}dr = \frac{U_0 k^{2l+1}}{[(2l+1)!!]^2}\frac{a^{2l+3}}{2l+3}$$

We cannot use ↓this result if the potential has a sizeable tail.

$$\{\tan\delta_l(k)\}_{l>>ka} = \frac{\boxed{U_0 a^2}(ka)^{2l+1}}{[(2l+1)!!]^2(2l+3)}$$

Ref: 'Quantum Collision Theory' by C.J.Joachain (North-Holland, 1975) page 85 / Eq 4.142

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And now you take out whatever does not depend on r, because the integration is with respect to r. So, whatever is not dependent on you pull out of the integration. Now, this is the integral, you have to solve. And in this integral, if you put the square spherical square well which is the potential of finite range, then, you do not have to carry out the integration from r going from 0 through infinity; because the potential has got a finite range only up to a.

And up to a the potential is minus u 0, it is not a function of r for the spherical square well. So, you take it outside the integration. So, u0k to the power 2l + 1 comes here. And you have a simple integral of r to the power 2l + 2 to be evaluated from zero to a. So, you get a to the power 2l + 3 divided by 2l + 3, okay. So that is your tangent of the phase shift in this case.

So, this is a nice result notice that the potential strength parameter appears explicitly and you have got this famous 2l + 1 power of k which appears in the phase shift, okay. Now, we have to be careful because if you have used this result for finite potential. If the potential does not have a finite range and it has got a sizeable tail.

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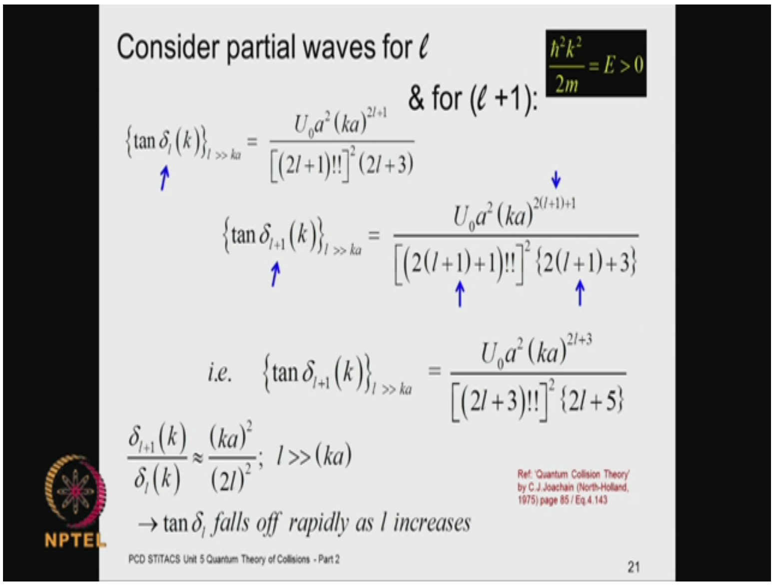

Consider partial waves for ℓ

& for $(\ell+1)$:

$$\frac{\hbar^2 k^2}{2m} = E > 0$$

$$\left\{\tan\delta_l(k)\right\}_{l \gg ka} = \frac{U_0 a^2 (ka)^{2l+1}}{\left[(2l+1)!!\right]^2 (2l+3)}$$

$$\left\{\tan\delta_{l+1}(k)\right\}_{l \gg ka} = \frac{U_0 a^2 (ka)^{2(l+1)+1}}{\left[(2(l+1)+1)!!\right]^2 \{2(l+1)+3\}}$$

$$\text{i.e.} \quad \left\{\tan\delta_{l+1}(k)\right\}_{l \gg ka} = \frac{U_0 a^2 (ka)^{2l+3}}{\left[(2l+3)!!\right]^2 \{2l+5\}}$$

$$\frac{\delta_{l+1}(k)}{\delta_l(k)} \approx \frac{(ka)^2}{(2l)^2}; \quad l \gg (ka)$$

$\rightarrow \tan\delta_l$ *falls off rapidly as l increases*

Ref: 'Quantum Collision Theory' by C.J.Joachain (North-Holland, 1975) page 85 / Eq 4.143

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And you will have those cases like in a Coulomb potential or something, then, you cannot use this. Let us consider two partial waves, 2 partial waves with adjacent quantum numbers for the orbital angular momentum. So, one is got an orbital angular momentum l, the next one is l +1. So, we will write this expression for both, okay, tan delta l which we just obtained. And we will also write the corresponding expression if the angular momentum was l + 1.

So, wherever you have l over here, you will write l + 1. So, you had l over here. So, now, we have written a +1 over here. You had 2i over here. So, you have 2l + 1 over here. And we do the same thing over here, okay. So, this is the corresponding expression for l + 1. And if you, you can determine the value explicitly. So, you have 2l + 5 in the denominator and 2l + 3 power of ka.

So, if you take the ratio of these two angles then notice that it falls pretty rapidly as l increases because the ratio goes as 1 over s square. And this is what one would expect because it is completely in line with our understanding of the fact that as the centrifugal barrier becomes strong, then, the higher partial waves can be ignored, okay.

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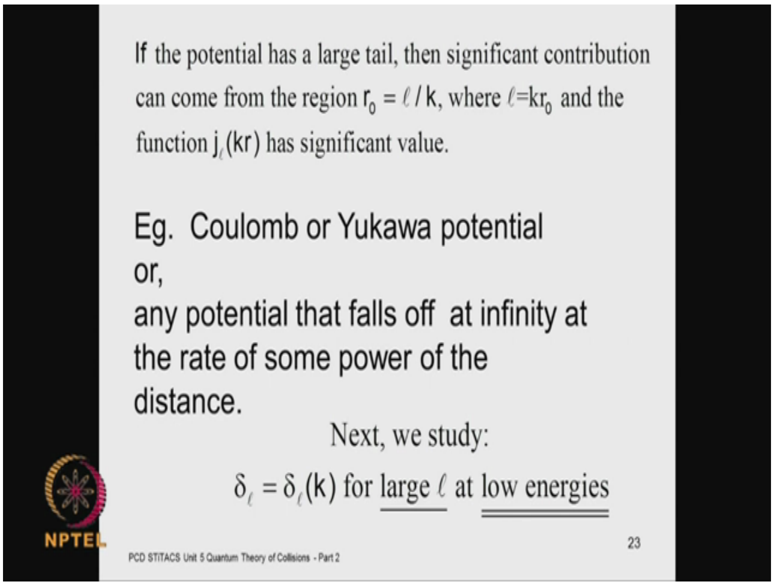

If the potential has a large tail, then significant contribution can come from the region $r_0 = \ell / k$, where $\ell = kr_0$ and the function $j_\ell(kr)$ has significant value.

Eg. Coulomb or Yukawa potential
or,
any potential that falls off at infinity at the rate of some power of the distance.

Next, we study:

$\delta_\ell = \delta_\ell(k)$ for $\underline{\text{large } \ell}$ at $\underline{\underline{\text{low energies}}}$

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So, all that is fine, the only thing is that if the potential has got some strength even as you go as far as l over k, then, you may have some significant contributions to scattering. So, otherwise you can use this, in those situations, where the potential has got a finite range. So, any potential which has got a tail like the Yukawa potential or the Coulomb potential, you will not use this particular approximation.

So, we will study the behaviour of the phase shifts as a function of k for large l and at lower energies.

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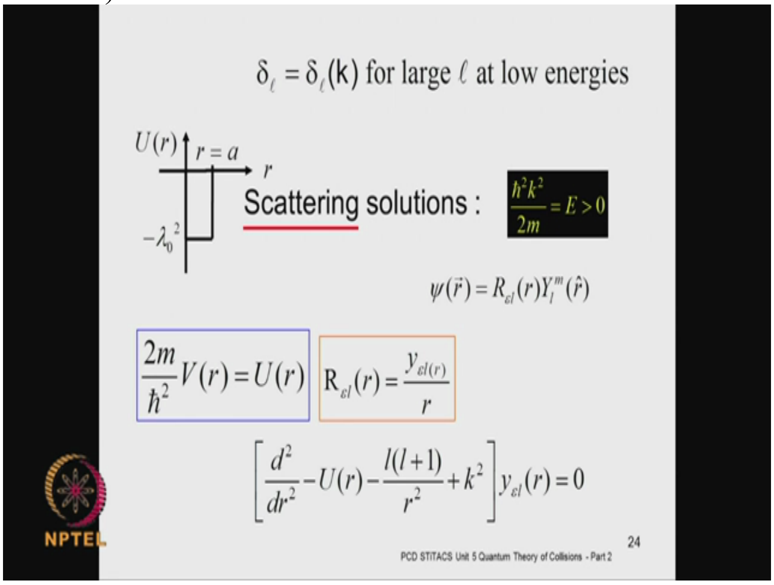

$\delta_\ell = \delta_\ell(k)$ for large ℓ at low energies

Scattering solutions : $\frac{\hbar^2 k^2}{2m} = E > 0$

$$\psi(\vec{r}) = R_{\varepsilon l}(r) Y_l^m(\hat{r})$$

$$\boxed{\frac{2m}{\hbar^2} V(r) = U(r)} \quad \boxed{R_{\varepsilon l}(r) = \frac{y_{\varepsilon l(r)}}{r}}$$

$$\left[\frac{d^2}{dr^2} - U(r) - \frac{l(l+1)}{r^2} + k^2\right] y_{\varepsilon l}(r) = 0$$

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So, the scattering solutions, we consider. And the Scattering solutions, we can again rewrite, by Schrodinger's equation for the reduced potential u instead of v, so that we get rid of the m and h cross and so on. We set up the differential equation for y instead of r, okay. But the information in the differential equation for y is essentially the same as that in the Schrodinger's equation.

So, this is the effective, effective leader Schrodinger's equation or what comes straight out of the Schrodinger's equation.

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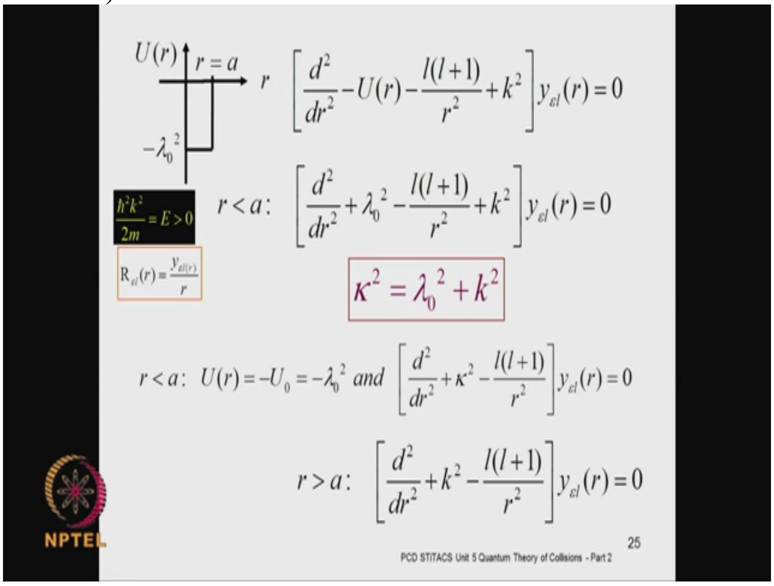

$$\left[\frac{d^2}{dr^2}-U(r)-\frac{l(l+1)}{r^2}+k^2\right]y_{\varepsilon l}(r)=0$$

$$\frac{\hbar^2k^2}{2m}=E>0$$

$$r<a:\ \left[\frac{d^2}{dr^2}+\lambda_0^2-\frac{l(l+1)}{r^2}+k^2\right]y_{\varepsilon l}(r)=0$$

$$R_{\varepsilon l}(r)=\frac{y_{\varepsilon l(r)}}{r}$$

$$\boxed{\kappa^2=\lambda_0^2+k^2}$$

$$r<a:\ U(r)=-U_0=-\lambda_0^2 \text{ and } \left[\frac{d^2}{dr^2}+\kappa^2-\frac{l(l+1)}{r^2}\right]y_{\varepsilon l}(r)=0$$

$$r>a:\ \left[\frac{d^2}{dr^2}+k^2-\frac{l(l+1)}{r^2}\right]y_{\varepsilon l}(r)=0$$

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And we have to examine its solutions. So, you have the solution for r less than a will be given by this; because the potential in this case is minus lambda 0, okay. And for r greater than 0, the potential is 0. So, there is no term corresponding to the potential. And instead of this, kappa square, kappa is determined by the depth of the potential and the energy both.

But outside this region, the depth of the potential does not matter, because the potential itself does not matter. There is no potential outside r = a, right. So, these are the two solutions, two equations for the two regions of space.

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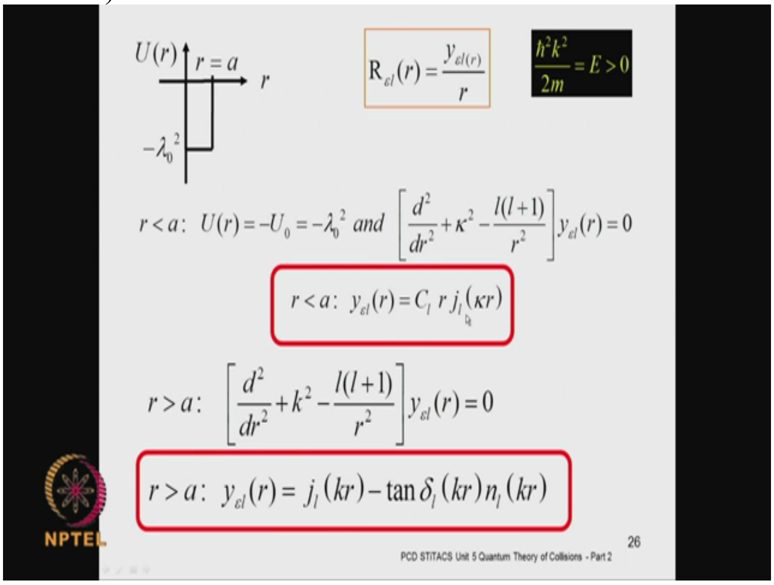

$$R_{\varepsilon l}(r)=\frac{y_{\varepsilon l(r)}}{r}$$

$$\frac{\hbar^2k^2}{2m}=E>0$$

$$r<a:\ U(r)=-U_0=-\lambda_0^2 \text{ and } \left[\frac{d^2}{dr^2}+\kappa^2-\frac{l(l+1)}{r^2}\right]y_{\varepsilon l}(r)=0$$

$$\boxed{r<a:\ y_{\varepsilon l}(r)=C_l\, r\, j_l(\kappa r)}$$

$$r>a:\ \left[\frac{d^2}{dr^2}+k^2-\frac{l(l+1)}{r^2}\right]y_{\varepsilon l}(r)=0$$

$$\boxed{r>a:\ y_{\varepsilon l}(r)=j_l(kr)-\tan\delta_l(kr)n_l(kr)}$$

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And we can find the solution. So, for the inner region you have got r times j, as the solution. And outside the region, the potential will generate a phase shift. And the solution will be written as a superposition of two linearly independent functions. You can as usual use the Bessel function and the Neumann function.

You can also do it in some other basis, if you like. But essentially the two pieces of which will be, which will be superposed, will be superposed by a coefficient which will be determined by the scattering phase shift because that is what is generating the potential, the scattering phase shift itself, right. So, this is the solution for r greater than e. And so, there is a this relationship between kappa and lambda 0.

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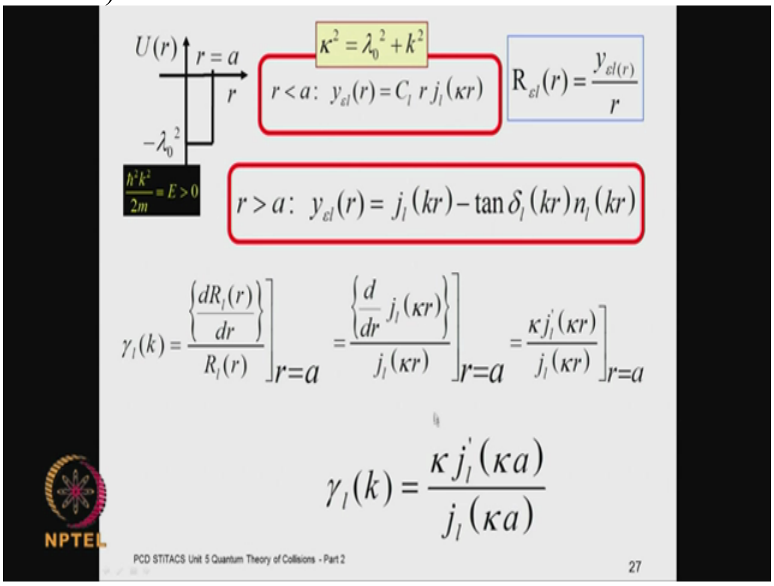

$\kappa^2=\lambda_0^2+k^2$

$r<a:\ y_{\varepsilon l}(r)=C_l\, r\, j_l(\kappa r)$

$R_{\varepsilon l}(r)=\frac{y_{\varepsilon l}(r)}{r}$

$r>a:\ y_{\varepsilon l}(r)=j_l(kr)-\tan\delta_l(kr)\,n_l(kr)$

$$\gamma_l(k)=\left.\frac{\left\{\frac{dR_l(r)}{dr}\right\}}{R_l(r)}\right]_{r=a}=\left.\frac{\left\{\frac{d}{dr}j_l(\kappa r)\right\}}{j_l(\kappa r)}\right]_{r=a}=\left.\frac{\kappa j_l'(\kappa r)}{j_l(\kappa r)}\right]_{r=a}$$

$$\gamma_l(k)=\frac{\kappa j_l'(\kappa a)}{j_l(\kappa a)}$$

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So, these are the two solutions for the two different regions of space. The solution, however, will have to be continuous at the boundary, at r = a. So, the usual way of setting this up is to get the logarithmic derivative and then explore the continuity of the logarithmic derivative itself. And whatever be the value of this derivative from inside, it will have to be the same as you get from the outside.

And you can for the outside; you have got the solution explicitly. So, you can see that this is kappa j prime kappa r by j kappa r, okay. Kappa is coming from the depth under energy itself. So, this is the logarithmic derivative.

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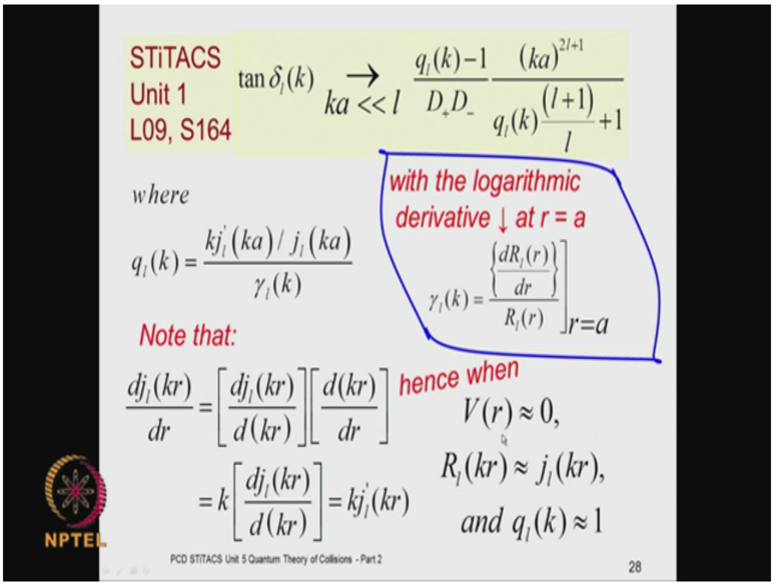

STiTACS
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$$\tan\delta_l(k)\xrightarrow[ka<<l]{}\frac{q_l(k)-1}{D_+D_-}\frac{(ka)^{2l+1}}{q_l(k)\frac{(l+1)}{l}+1}$$

where

$$q_l(k)=\frac{kj_l'(ka)/j_l(ka)}{\gamma_l(k)}$$

with the logarithmic derivative ↓ at r = a

$$\gamma_l(k)=\left.\frac{\left\{\frac{dR_l(r)}{dr}\right\}}{R_l(r)}\right]_{r=a}$$

Note that:

$$\frac{dj_l(kr)}{dr}=\left[\frac{dj_l(kr)}{d(kr)}\right]\left[\frac{d(kr)}{dr}\right]=k\left[\frac{dj_l(kr)}{d(kr)}\right]=kj_l'(kr)$$

hence when

$$V(r)\approx 0,\quad R_l(kr)\approx j_l(kr),\quad and\ q_l(k)\approx 1$$

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And we have expressed this logarithmic derivative. We had introduced this dimensionless parameter q because it offers a good deal of mathematical convenience. It is in fact the logarithmic derivative itself, if the solutions were just the free particle waves. So, that is in the numerator, you just have to remember that the derivative is with respect to r.

And therefore there will be an extra factor of k, when you write, the take the derivative, right with respect to r; because argument is kr and not r. So, when the potential is zero, the factor q, will be equal to 1 because these two will become equal. That is how we have defined it, okay.
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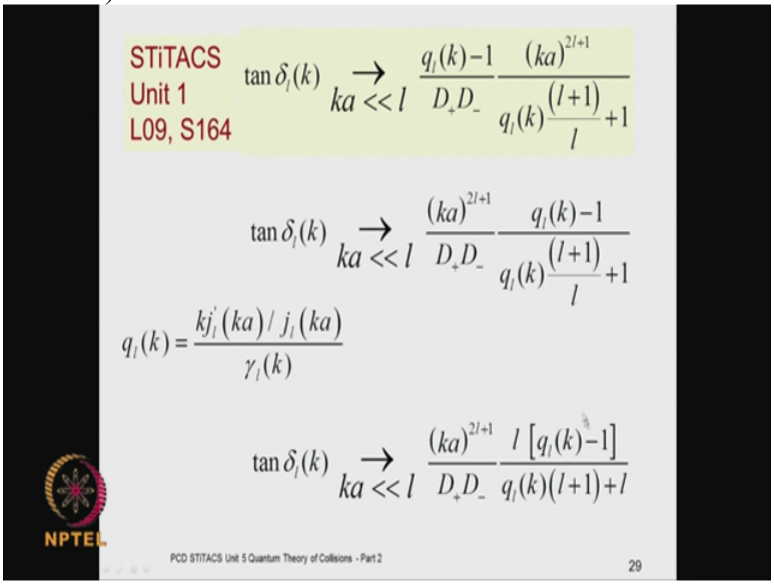

STiTACS
Unit 1
L09, S164

$$\tan\delta_l(k)\xrightarrow[ka<<l]{}\frac{q_l(k)-1}{D_+D_-}\frac{(ka)^{2l+1}}{q_l(k)\frac{(l+1)}{l}+1}$$

$$\tan\delta_l(k)\xrightarrow[ka<<l]{}\frac{(ka)^{2l+1}}{D_+D_-}\frac{q_l(k)-1}{q_l(k)\frac{(l+1)}{l}+1}$$

$$q_l(k)=\frac{kj_l'(ka)/j_l(ka)}{\gamma_l(k)}$$

$$\tan\delta_l(k)\xrightarrow[ka<<l]{}\frac{(ka)^{2l+1}}{D_+D_-}\frac{l\left[q_l(k)-1\right]}{q_l(k)(l+1)+l}$$

PCD STiTACS Unit 5 Quantum Theory of Collisions - Part 2

So, this is what we have got so far. And you can rearrange the terms and put it in a somewhat simple form, right. So, you now have l into this l. which is in the denominator here. I have multiplied this one by l. So, I get l + 1 + over here. And this l is now in the numerator.
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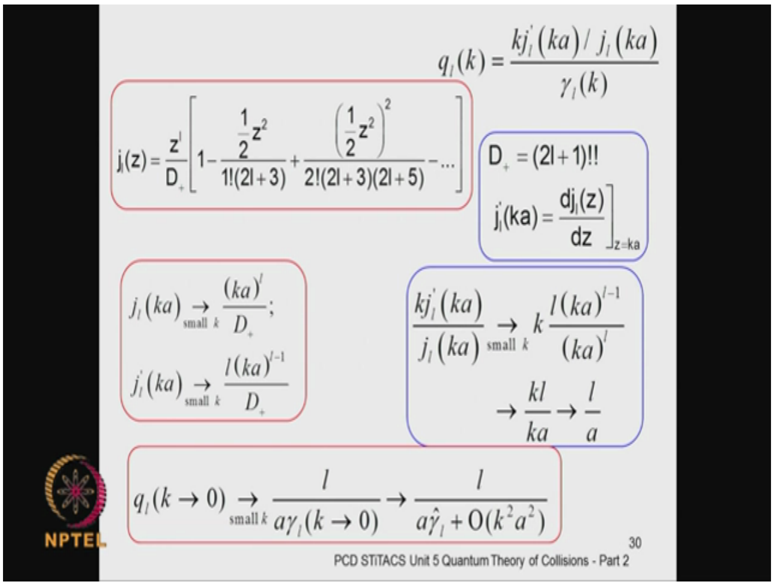

$$q_l(k) = \frac{k j_l'(ka)/j_l(ka)}{\gamma_l(k)}$$

$$j_l(z) = \frac{z^l}{D_+}\left[1 - \frac{\frac{1}{2}z^2}{1!(2l+3)} + \frac{\left(\frac{1}{2}z^2\right)^2}{2!(2l+3)(2l+5)} - \dots\right]$$

$$D_+ = (2l+1)!!$$

$$j_l'(ka) = \left.\frac{dj_l(z)}{dz}\right]_{z=ka}$$

$$j_l(ka) \xrightarrow[\text{small } k]{} \frac{(ka)^l}{D_+};$$

$$j_l'(ka) \xrightarrow[\text{small } k]{} \frac{l(ka)^{l-1}}{D_+}$$

$$\frac{k j_l'(ka)}{j_l(ka)} \xrightarrow[\text{small } k]{} k\frac{l(ka)^{l-1}}{(ka)^l} \to \frac{kl}{ka} \to \frac{l}{a}$$

$$q_l(k \to 0) \xrightarrow[\text{small } k]{} \frac{l}{a\gamma_l(k \to 0)} \to \frac{l}{a\hat{\gamma}_l + O(k^2a^2)}$$

So, this is a little bit of rearrangement we have made use of the explicit form of the Bessel functions. We have taken the derivatives appropriately. And by putting this these the ratio of the derivative and the function itself at the Bessel function, you find that this ratio becomes l over a. So, now, what does it give us for q? q is this.

So, q you can get this numerator now goes as l over a and you will now get this q, the dimensionless quantity which we defined to be l over a gamma and gamma we will take the limiting value of gamma k tends to 0 + some other terms which we have ignored. And those will be of the order of t a square, okay.

The terms that we have ignored but then we take the limiting value of gamma which is represented by this gamma carrot or gamma hat right.

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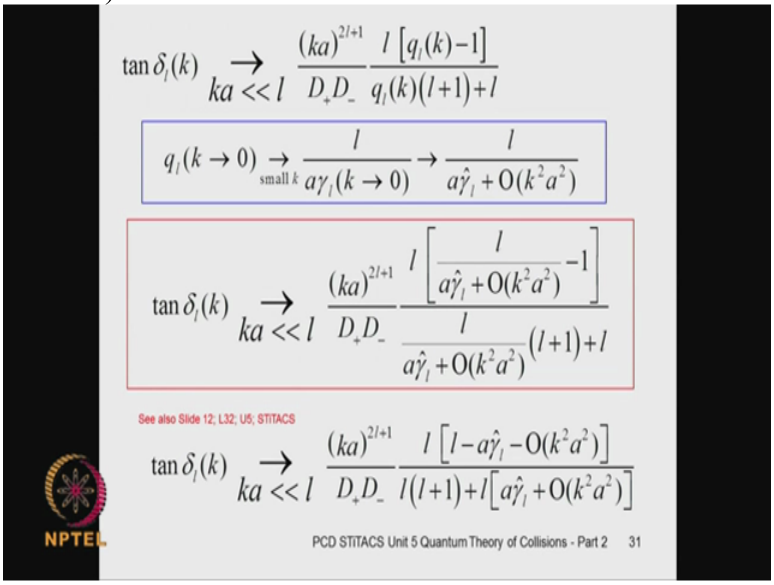

$$\tan\delta_l(k) \xrightarrow[ka \ll l]{} \frac{(ka)^{2l+1}}{D_+D_-}\,\frac{l\,[q_l(k)-1]}{q_l(k)(l+1)+l}$$

$$q_l(k \to 0) \xrightarrow[\text{small } k]{} \frac{l}{a\gamma_l(k \to 0)} \to \frac{l}{a\hat{\gamma}_l + O(k^2a^2)}$$

$$\tan\delta_l(k) \xrightarrow[ka \ll l]{} \frac{(ka)^{2l+1}}{D_+D_-}\,\frac{l\left[\frac{l}{a\hat{\gamma}_l + O(k^2a^2)} - 1\right]}{\frac{l}{a\hat{\gamma}_l + O(k^2a^2)}(l+1)+l}$$

See also Slide 12; L32; U5; STiTACS

$$\tan\delta_l(k) \xrightarrow[ka \ll l]{} \frac{(ka)^{2l+1}}{D_+D_-}\,\frac{l\,[l - a\hat{\gamma}_l - O(k^2a^2)]}{l(l+1)+l[a\hat{\gamma}_l + O(k^2a^2)]}$$

So, this is the result we have, okay. So, this is the limiting behaviour of the dimensionless parameter q. What is ignored is the tangent of the first shift so far are these terms of the order of ka square. Other than that, all the terms are taken care of. So, I will like you to recognize that there will be a certain resonance condition.

And at the resonance, if the terms that we have ignored will they may be of any importance and we had some discussion on this in the previous units. So, I am going to stop here at this point so that when we come for the next class, we have brushed up some of these considerations.

But essentially, we know the terms as we get, we know what the resonant condition for l greater than 0 will be, okay; for l = 0, we already discussed. We know that, what approximations we have made; because over here, we have ignored terms of the order of k square a square. Now, you can again find some common terms and simplify this. So, there was an extra factor of l, which was needless. So, we can get rid of it.

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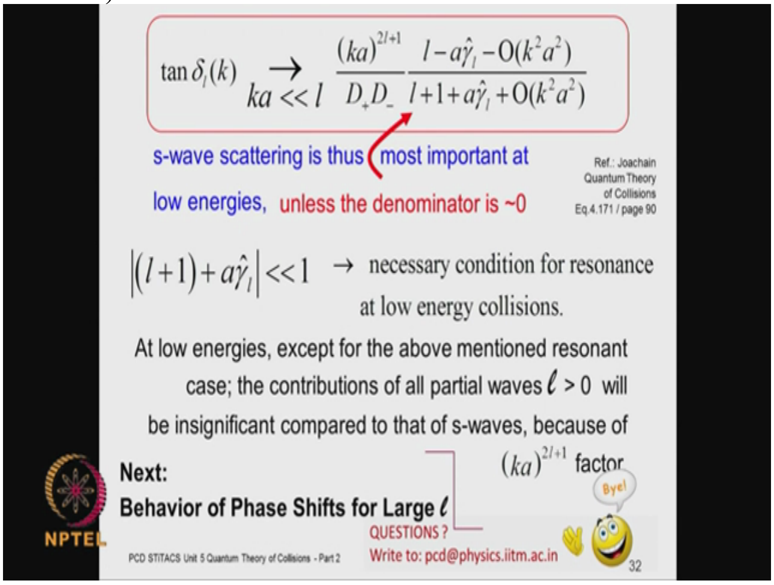

$$\boxed{\tan\delta_l(k) \xrightarrow[ka \ll l]{} \frac{(ka)^{2l+1}}{D_+D_-}\frac{l - a\hat{\gamma}_l - O(k^2a^2)}{l + 1 + a\hat{\gamma}_l + O(k^2a^2)}}$$

s-wave scattering is thus most important at low energies, unless the denominator is ~0

Ref.: Joachain
Quantum Theory
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$|(l+1) + a\hat{\gamma}_l| \ll 1$ → necessary condition for resonance at low energy collisions.

At low energies, except for the above mentioned resonant case; the contributions of all partial waves $\ell > 0$ will be insignificant compared to that of s-waves, because of $(ka)^{2l+1}$ factor

Next:
Behavior of Phase Shifts for Large ℓ

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

PCD STiTACS Unit 5 Quantum Theory of Collisions - Part 2

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So, we already know that the s wave scattering is the most important one because you see that the phase shift goes as 2l + 1 and as l increases, it will become smaller and smaller, right. So, that is the importance of the centrifugal barrier effect unless of course you have a resonance, okay. So, all this is fine but when you do have a resonance which you may have because depending on the range of the potential.

And the logarithmic derivative you may hit a value of l that for some partial wave, you may hit a resonance. And the necessary condition for resonance now is that the denominator goes to 0 or it becomes much smaller than 1 okay. That is now the condition for resonance. So, the resonance in the lth partial wave will take place, when you have this condition satisfied that this denominator is much smaller than 1.

And this is a good approximation. The only thing is, it ignores is terms of order k square, a square. So, all the contributions from higher partial waves can be ignored. You can work only with S waves except when the resonance condition is satisfied. And we have found what the resonance condition is that this modulus of l + 1 + a gamma must be not less than 1, okay. all right, if there is any question I will be happy to take. Otherwise, we continue from here, in the next class.