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

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Lecture 38

Resonances in Quantum Collisions

Greetings, we are getting close to the point that we will soon have the Breit Wigner relation for Resonances in Collisions. And specifically we will be discussing how the phase shifts behave at a Resonance. So, I will also introduce what exactly do we mean by Resonance? What are the different kinds of Resonances that we talk about? And so on.

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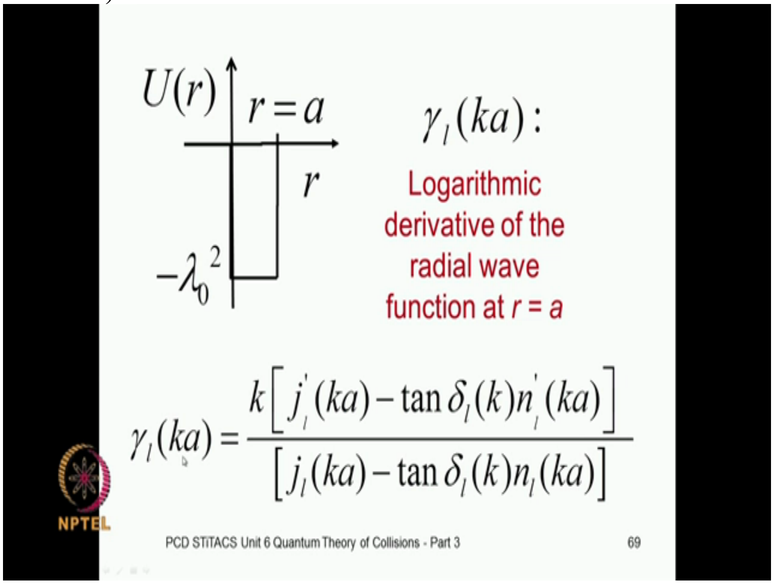

$\gamma_l(ka)$:

Logarithmic derivative of the radial wave function at $r = a$

$$\gamma_l(ka) = \frac{k\left[j_l'(ka) - \tan\delta_l(k) n_l'(ka)\right]}{\left[j_l(ka) - \tan\delta_l(k) n_l(ka)\right]}$$

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So, in our previous class, we consider scattering by a square well and our analysis was based on the, on the, on the continuity of the wave function and the derivative at the boundary. So that was contained in this logarithmic derivative. So, this gamma we have used in our mathematical expressions. So, I will be using it in today's class as well.

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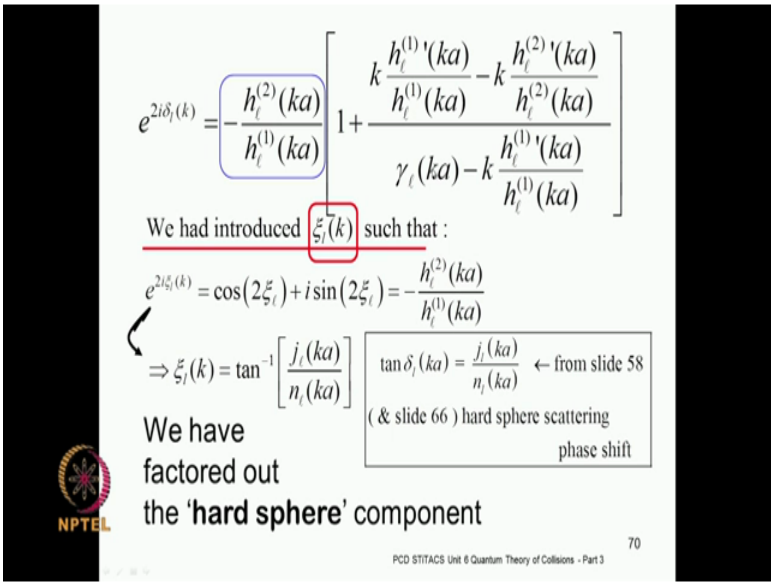

$$e^{2i\delta_\ell(k)} = \boxed{-\frac{h_\ell^{(2)}(ka)}{h_\ell^{(1)}(ka)}}\left[1 + \frac{k\frac{h_\ell^{(1)}{}'(ka)}{h_\ell^{(1)}(ka)} - k\frac{h_\ell^{(2)}{}'(ka)}{h_\ell^{(2)}(ka)}}{\gamma_\ell(ka) - k\frac{h_\ell^{(1)}{}'(ka)}{h_\ell^{(1)}(ka)}}\right]$$

We had introduced $\boxed{\xi_l(k)}$ such that :

$$e^{2i\xi_l(k)} = \cos(2\xi_\ell) + i\sin(2\xi_\ell) = -\frac{h_\ell^{(2)}(ka)}{h_\ell^{(1)}(ka)}$$

$$\Rightarrow \xi_l(k) = \tan^{-1}\left[\frac{j_\ell(ka)}{n_\ell(ka)}\right]$$

$\tan\delta_l(ka) = \frac{j_l(ka)}{n_l(ka)}$ ← from slide 58

(& slide 66) hard sphere scattering phase shift

We have
factored out
the '**hard sphere**' component

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And in terms of this gamma, which comes here, as one of the terms in the denominator which we defined on the previous slide. The scattering phase shift, we wrote as a product of these two factors: One which is in this blue box and the other in this rectangular bracket. So, this separation we expressed in our last class.

Now, what we also do is, to introduce a function Xi of k such that e to the 2i Xi, is given by this ratio minus h2 over h1, h2 is the Hankel function of the second fine kind and h1 is the Hankel function of the first kind. So, the ratio of these two hanker functions with a negative sign is what gives us this ratio. This ratio is then indicated in terms of this angles Xi and the phase shift is now separated in two factors.

One of which is this exponential function of modulus one, right. Now, if you look at this and you set up the you write the Hankel functions: Hankle function of the first kind and Hankle function of the second time in terms of the Bessel function and the Neumann function, okay. Because j + i and j - i are the Hankel functions of first and second kind respectively, right.

So, you can see that this Xi is then nothing but the tan inverse of j over n, the ratio of the Bessel function to the Neumann function. And what is this quantity? Tan over's tan inverse j over n is nothing but the phase shift coming from the hard sphere, okay, so the tangent of the hard sphere scattering. So, this delta is different from this delta, okay.

This delta is the scattering phase shift due to the square well potential that we are talking about, okay which is how we have expressed it. One part of it, which is, the first box in, this blue box; This part which we have written as e to the 2i Xi, this is exactly the same as the scattering phase shift which comes from the hard sphere.

So, this delta is only the hard sphere scattering have used the same symbol because, on slide 66 this ratio represented the tangent of the phase shift due to a hard sphere impenetrable sphere, okay, which has got an infinite barrier. So, that scattering phase shift was given by this ratio and this ratio expresses the tangent of this phase shift Xi which is coming as one of the factors.

Effectively the net phase shift though this is the real phase shift due to the square well potential. This phase shift can now be written as a sum of two parts: one coming from what is in this blue box which is the hard sphere component as we shall call it. And then, there is a remaining part which will depend, which will be very sensitive, to the details of the potential and other, other parameters of the scattering problem.

So, what we have essentially done is to factor out a component which we shall refer to as a hard sphere component. So, mind you, the actual potential is not a hard sphere. The hard sphere results in a total phase shift, scattering phase shift. One part of which is effectively the same as if it is coming from hard sphere scattering and then there is a residual part.

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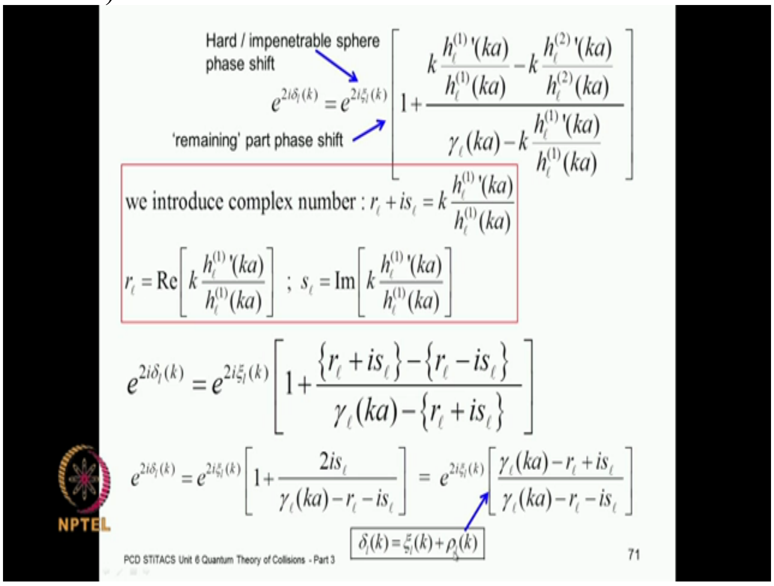

Hard / impenetrable sphere phase shift

'remaining' part phase shift

$$e^{2i\delta_l(k)} = e^{2i\xi_l(k)}\left[1+\frac{k\frac{h_l^{(1)}{}'(ka)}{h_l^{(1)}(ka)}-k\frac{h_l^{(2)}{}'(ka)}{h_l^{(2)}(ka)}}{\gamma_l(ka)-k\frac{h_l^{(1)}{}'(ka)}{h_l^{(1)}(ka)}}\right]$$

we introduce complex number : $r_\ell + is_\ell = k\frac{h_\ell^{(1)}{}'(ka)}{h_\ell^{(1)}(ka)}$

$$r_\ell = \mathrm{Re}\left[k\frac{h_\ell^{(1)}{}'(ka)}{h_\ell^{(1)}(ka)}\right]\ ;\ s_\ell = \mathrm{Im}\left[k\frac{h_\ell^{(1)}{}'(ka)}{h_\ell^{(1)}(ka)}\right]$$

$$e^{2i\delta_l(k)} = e^{2i\xi_l(k)}\left[1+\frac{\{r_\ell+is_\ell\}-\{r_\ell-is_\ell\}}{\gamma_\ell(ka)-\{r_\ell+is_\ell\}}\right]$$

$$e^{2i\delta_l(k)} = e^{2i\xi_l(k)}\left[1+\frac{2is_\ell}{\gamma_\ell(ka)-r_\ell-is_\ell}\right] = e^{2i\xi_l(k)}\left[\frac{\gamma_\ell(ka)-r_\ell+is_\ell}{\gamma_\ell(ka)-r_\ell-is_\ell}\right]$$

$$\boxed{\delta_l(k)=\xi_l(k)+\rho_l(k)}$$

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So, our interest will be very much in the residual part. So, this is the remaining part of the phase shift, okay. So, the 2i Xi is one part of 2i delta. So, Xi is one part of delta. And then, there is another part which is dependent to all the collision details of the real potential and the primary reason of course, is this logarithmic derivative which appears in this term. So, we introduce a complex number r + is.

Now, this is going to be different for every partial wave. There are infinite partial waves. So, we write it specifically for each partial wave. So, there is rl + isl. But for every partial wave, we have a complex number r + is, which is the ratio of the derivative of the Hankel function one to the Hankel function one multiplied by k. So, this is the complex number which we introduce.

And r is now the real part of this complex number s is the imaginary part of this complex number. That is how, we have defined it. And now, we have this 2i delta l, this is the phase shift, delta is the scattering phase shift, which is now written in terms of this hard sphere component Xi and another component.

And because I have now introduced this r and s, I can write these ratios in terms of r and s instead of the hankel functions because here you have defined the r and s, in terms of, the Hankel functions. So, you can invert the relations and write the Hankel functions, in terms of, r and s, okay. And this is what it turns out to be. And you have a very nice relationship emerging from this simplification.

That the scattering phase-shift delta, you can see is now written as a product of e to the 2i Xi and another factor which is in this rectangular box. And this rectangular bracket, you can see is, also of modulus one. So, you can also write it as e to the 2i Rho or something which will be the other part of the scattering phase shift. So, let us see that. So, that other part will be Rho and that is coming from this rectangular box.

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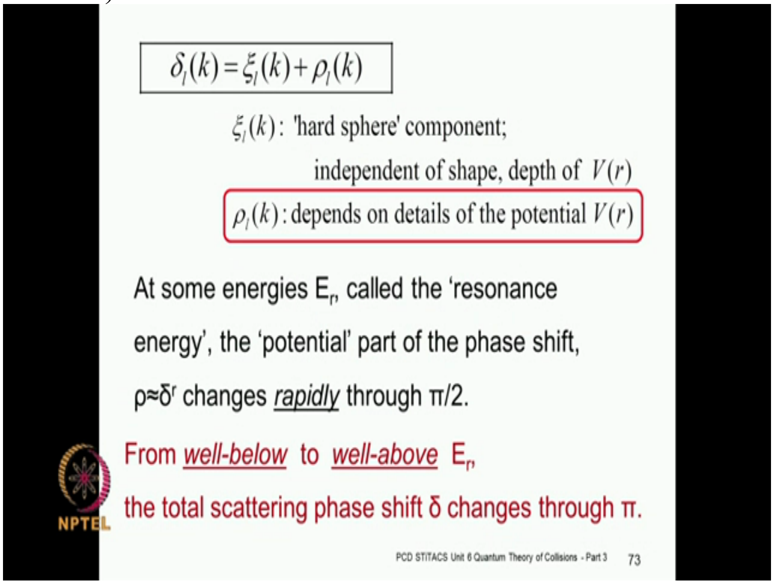

$$\boxed{\delta_l(k)=\xi_l(k)+\rho_l(k)}$$

$\xi_l(k)$: 'hard sphere' component;

independent of shape, depth of $V(r)$

$\boxed{\rho_l(k): \text{depends on details of the potential } V(r)}$

At some energies E_r, called the 'resonance energy', the 'potential' part of the phase shift, $\rho \approx \delta^r$ changes *rapidly* through $\pi/2$.

From *well-below* to *well-above* E_r, the total scattering phase shift δ changes through π.

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So, I will write this relation explicitly over here. So, we have got this e to the 2i delta l at the top of this slide. This second factor is of modulus 1. And we now write the second factor as e to the 2i Rho, because it is of modulus one. So, Rho is another phase shift. Now, Rho is another angle. So, the net phase shifts will be, twice delta is equal to twice Xi + twice Rho or delta = Xi + Rho.

So, that is the relation which is emerging for every partial wave for every lth partial wave. So, delta, we have as a sum of these two phase shifts. So, this part is coming from the hard sphere and it does not matter. The details of the potential then do not matter, okay, because it is just the hard sphere component. The second component Rho is what contains the detailed dynamics of the collision process.

So, so Rho is the one which will determine which will be determined by the details of the potential V. So, here we are. When it depends specifically on the details of the potential, Rho will be very sensitive to this potential. It will be very sensitive to certain dynamical factors which are involved in the collision process and at some particular energies which are, which we shall refer to as the resonance energies.

At these energies, the phase shift Rho, this is the part other than the hard sphere components. So, this will change very rapidly in the vicinity of the resonance. So, it will be extremely sensitive to the resonant, to the resonance phenomenon. And this will change very rapidly. And you will see that it changes very rapidly through pi by 2. But, if you consider a little bit, if you go to slightly lower to lower energies.

And go well above the resonance, then, over this region, then, the phase shift Rho or the consequent phase shift delta will change through pi. So, you will see I will show these figures and that will make this whole thing very clear.

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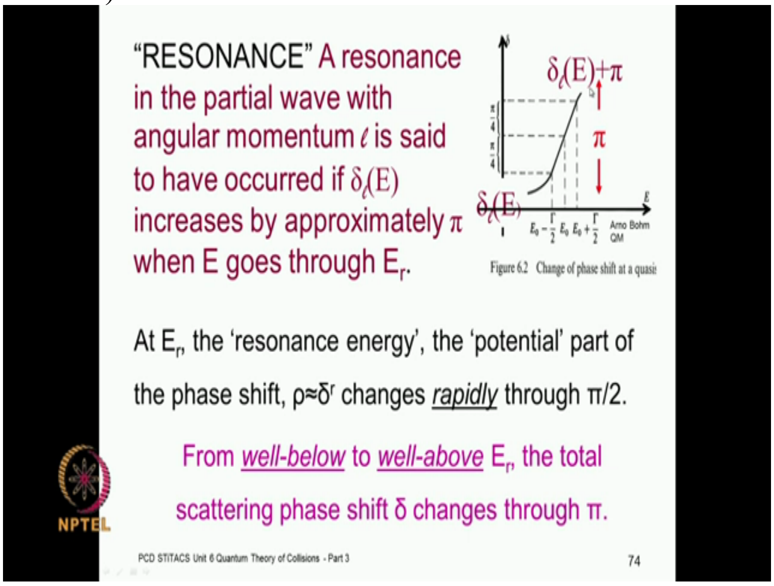

"RESONANCE" A resonance in the partial wave with angular momentum ℓ is said to have occurred if $\delta_\ell(E)$ increases by approximately π when E goes through E_r.

Figure 6.2 Change of phase shift at a quasi

At E_r, the 'resonance energy', the 'potential' part of the phase shift, $\rho \approx \delta^r$ changes *rapidly* through $\pi/2$.

From *well-below* to *well-above* E_r, the total scattering phase shift δ changes through π.

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So, here, is a figure. So, here you have got the phase shift which is changing with energy. E zero is the resonance energy, okay; E0or Er here, it is written as E0, because this figure is from Arno Bohm's book on Quantum mechanics, which is, a very nice book which I recommend for this topic. So, here Er is the resonance energy. And as you see the phase shift changes rather rapidly between here, it goes through pi by 2.

So, from here to here, the net change is pi by 4 + pi by 4. So, there is a pi by 2 change in this region. And there is another pi by 4 change as you go from well below the resonance and go to well above the resonance; there is another pi by 4. So, the net phase shifts change is from delta to delta + pi. So, the net change in the phase shift is pi okay.

That is the angle through which the phase shift changes, as you go across a resonance, okay. And very close to the resonance, in the immediate vicinity of the resonance, the phase shift changes by pi by 2. And that is where it changes rather rapidly. And how rapidly it will happen, will depend on the width of the resonance.

So, gamma is the width. So, half gamma you reduce from E0, you get to the left of this, to the lower energy side and an equal amount on the right of this. So, this is the region where it changes rather rapidly. So, how rapidly it changes, that slope will depend on the actual width of the resonance.

So, this is the net change in the phase shift which goes from whatever value it has delta to delta + pi. So, as you go across a resonance, the net change in the phase shift is pi, very close to the resonance. It goes through pi by 2.

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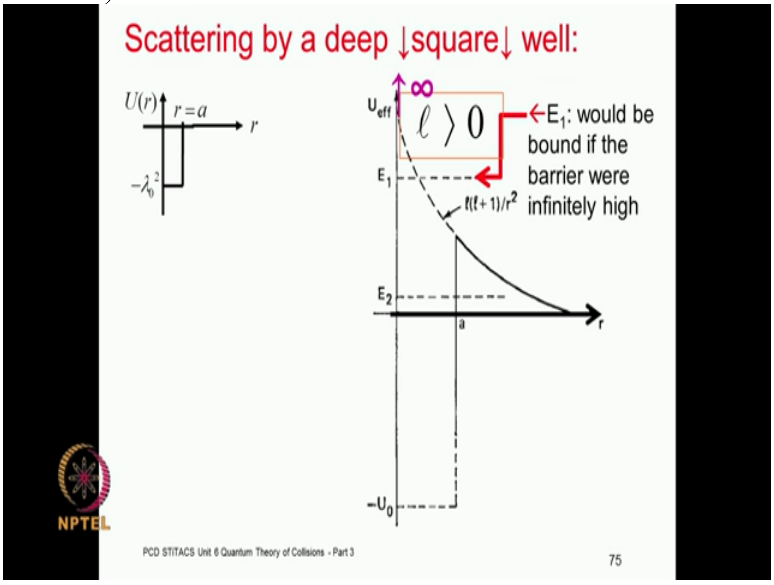

Scattering by a deep ↓square↓ well:

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So, let us consider scattering by a deep square well. And I will consider angular momentum greater than zero. And when you have an angular momentum greater than zero, remember that, when you separate, the Schrodinger equation in the radial part on the angular part, the radial equation will have a constant of separation, which is coming from separating the radial part of the Schrodinger equation from the angular part of the Schrodinger equation.

You would have done that in the first course in Quantum Mechanics. The centrifugal barrier term l into l + 1 by r square term comes out of this separation, okay. Now, this is a centrifugal barrier centrifugal in some sense, it is a pseudo term. It is not the result of a physical interaction like even in the Hydrogen atom, the physical interaction is 1 over r, okay. That is the Coulomb interaction.

But when you write the Schrodinger equation, the radial part of the Schrodinger equation, you will have the net effective potential which is -1 over r which is the Coulomb attraction plus l into l + 1r square, which is the centrifugal term. So, it is not the result of a real physical potential, just the way the pseudo forces are not because of real physical interactions.
They are a result of the fact that we try to do dynamics in some accelerated frame of reference which is why the pseudo forces or the pseudo potentials shape up. And here this term comes up because you have projected the 3-dimensional problem on a 1 dimension which is the r dimension.

You have separated out the spherical harmonics. So, the two dimensions for theta and Phi, the two degrees of freedom that dynamics is separated out. And now, you are left with only a one dimensional Schrodinger equation namely the radial Schrodinger equation. And in this radial charting an equation, you have a centrifugal term which is a pseudo potential kind of thing. And this is repulsive, okay.

So, this goes all the way to the, to infinity as r tends to 0, okay. And the net effective potential will then you know, it will be, but this it starts diminishing as r increases, as r goes to infinity. It will of course go to zero and then the net potential of the square well. If you set up the radial Schrodinger equation for the spherical square well potential, then, you will have a potential which goes like this square.

But then, because of the centrifugal term, you will have a barrier here, okay. So, this is the effective potential as you will see. Now, what is happening is really interesting because, if you have, if you consider collision of a certain projectile, by this potential and let us say that the energy of this projectile is E1. It could be E1, it could be E2, it could be E3 and whatever. So, if you consider a particular energy like E1, as you see in this figure.

Then, you can see that a particle with this energy would not have a chance of being bound, unless the barrier was really high. It needed to be high enough and if the barrier was Infinite then of course you could have trapped it inside, okay. So, this would not be a bound State. What about this state, if the energy is E2? Then it has the possibility of being bound in the inner well.

But, if it tunnels through this barrier region, so, from here to here is the barrier region, right. And if it tunnels through, then it could actually escaped into the continuum with positive energy. So, what is going to happen for a particle with energy E2? It has two possibilities one is that it can be trapped in the inner well and the other is that it can exit into the open continuum and escape to r going all the way to infinity.
It can leak out and go all the way to the asymptotic region r tends to infinity. So, these two possibilities both coexist and it goes back to the classic Young's Double Slit situation. That you have two possibilities and then the amplitudes would interfere just the way they do in the Young's Double Slit experiment, okay.

And then, you have a resonance phenomenon because you have two possibilities which are both possible, both probable, okay. And this is happening because of a particular shape of this potential. If l was zero, okay, the potential would not have the shape and depending on the value of l, l into l +1 by r square will change and the details of this shape will change.

So, here is a resonance phenomenon which is induced by the shape of the potential which is why these resonances or meta stable states are called as shape resonances, okay. So, this is a meta stable state. It will have a certain lifetime okay, because it has the possibility of being bound. But it also has the possibility of being bound in to the continuum.
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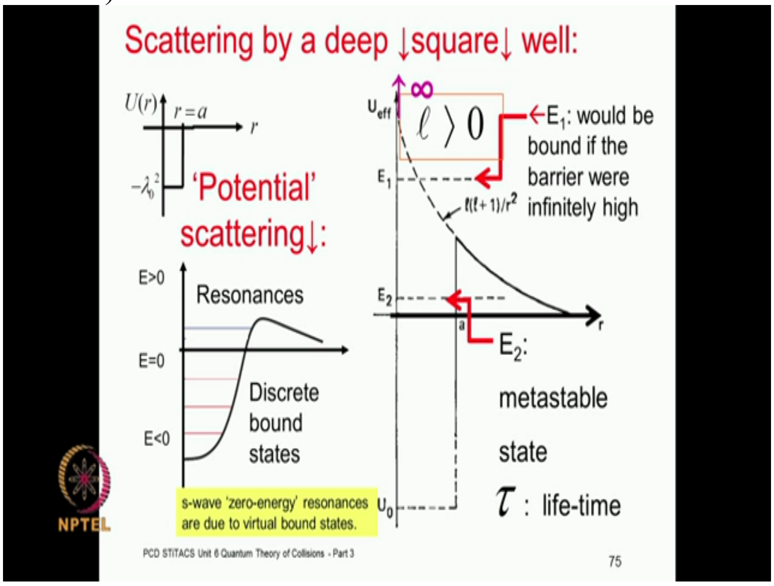

Scattering by a deep ↓square↓ well:

'Potential' scattering↓:

←E_1: would be bound if the barrier were infinitely high

E_2: metastable state

τ : life-time

s-wave 'zero-energy' resonances are due to virtual bound states.

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Now, another potential may not have such sharp boundaries like a square well potential, you may have some sort of it; this is like a harmonic oscillator kind of thing, potential, right. And then you will have some discrete bound states. And then if you have a state over here, which is above E = 0, but not so much that, it is well above the highest value of the potential. So, this is another example of a shape resonance okay.

So, this is for more realistic potentials which are not like having, sharp boundaries like a square well. So, this is an example of a shape resonance. If you remember, we talked about resonances earlier in s-wave scattering. And the s-wave scattering, those were coming because of the virtual bound states, okay.

So, resonances can be because of many, many different reasons; so, the s-wave resonances that we talked about, in the context of the Levinson Levinsons's theorem and so on. So, those who are coming because of zero energy resonances they were because of the virtual bound states or which we often called as a half bound states, okay. But that was not because of a potential shape, okay.

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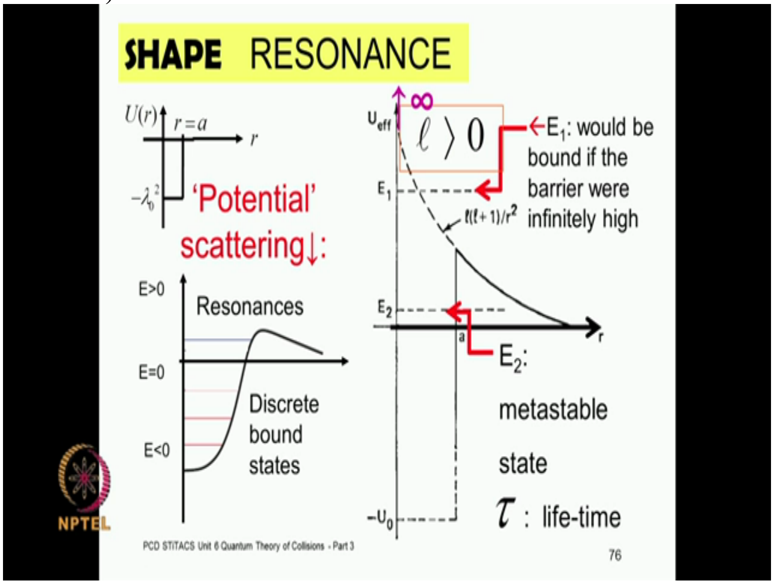

SHAPE RESONANCE

'Potential' scattering↓:

Resonances

Discrete bound states

$\ell > 0$

←E_1: would be bound if the barrier were infinitely high

E_2: metastable state

τ : life-time

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So, here is an example of a shape resonance. So, this is called as a shape resonance specifically because it is determined by the shape of the potential. What exactly is the shape of the potential so that is what determines, the shape resonance.

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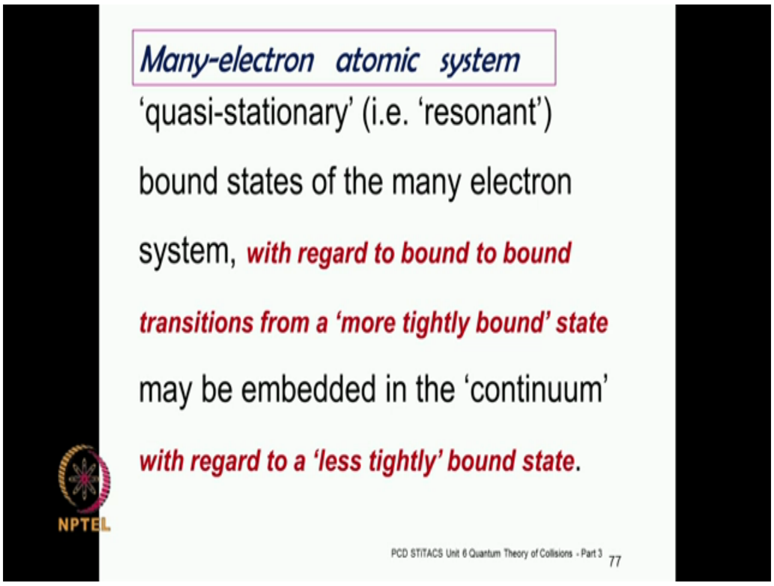

Many-electron atomic system

'quasi-stationary' (i.e. 'resonant') bound states of the many electron system, ***with regard to bound to bound transitions from a 'more tightly bound' state*** may be embedded in the 'continuum' ***with regard to a 'less tightly' bound state.***

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You can have a resonance because of some other situation. And that is typical in a many electron system, because when you have a many electron system, you can have some other kinds of resonances. And these are, if these come about because of certain correlations. And why will there be such a correlation?

Because, the many electron system has got different electrons and all of them do not have the same binding energy. So, you may have a process like in photo ionization or more specifically in atom ionization of as we call it. You may have a photo absorption of a photon which is sufficient to knock out an outer electron okay.

But it does not have enough energy to knock out an inner electron. So, what will happen? It will not be able to knock out an inner electron. It will knock out an outer electron. However, as you sweep on the photon energy, if you are doing spectroscopy and like at a synchrotron light source, you carry out the measurements at different wavelengths of different energies. Then, you may hit upon an energy.

Which is sufficient not to knock out an electron from the inner level, but to raise it to an excited bounce rate and at this energy, you have two processes which are degenerate. One is a bound to bound excitation of an inner electron and a bound to continuum transition of an outer electron which could result in ionization. So, now again you have two possibilities which are degenerate which can coexist.

Which may happen at a particular energy, which is the resonant energy because the bound to bound excitation is possible not at any arbitrary energy but only at specific energies because the bound straight spectrum is this rate so, whenever you have such bound to bound transitions. So, you can have a bound to bound transition from a more tightly bound state.

But if this part of the discrete spectrum is embedded in the continuum of a less tightly bound electron, then you will have a resonance, because again you have two possibilities. And once again you can think about it in terms of, the Young's Double Slit that you will have interference between the two alternatives.

So, this is happening because of electron correlations because the two electrons the dynamics are one electron cannot be completely separated from the dynamics of the other electrons. So, you have other two electron correlation. And as a result of this correlation which is not taken into account in an approximation like the Hartree-fock, okay because in the Hartree-fock, it is a frozen orbital approximation.

It pretends that whatever happens in one orbital has no consequence on any of the other orbital's which remain frozen. But when you go beyond this approximation and think about the electron correlations, then it becomes impossible to separate the dynamics of one electron from that of the other. So, configuration interactions or electron correlations are then responsible for resonances as well.

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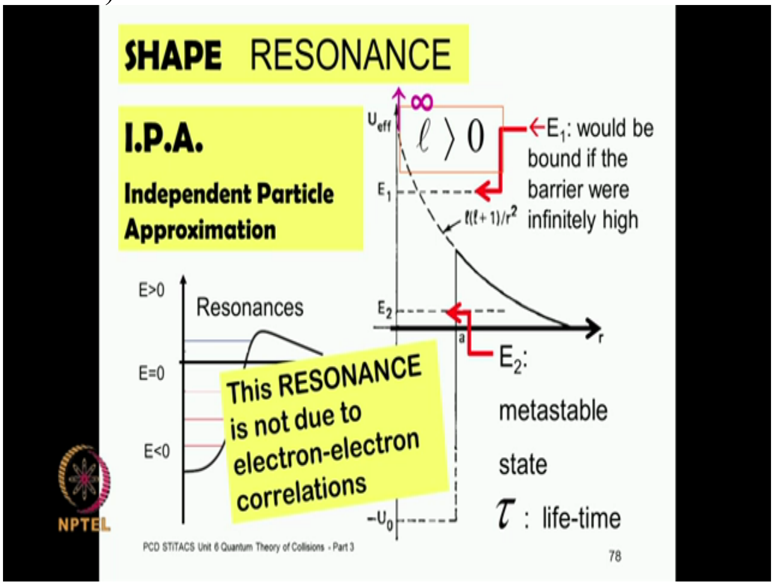

SHAPE RESONANCE

I.P.A.

Independent Particle Approximation

This RESONANCE is not due to electron-electron correlations

E_1: would be bound if the barrier were infinitely high

E_2: metastable state

τ : life-time

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So, you, we first talked about the shape resonance which you can talk about in the framework of the independent particle model because here you are talking only about one single electron, no second electron is involved over here. So, you talk about the shape resonance in the framework of a single particle model.

Of course, electron correlations are there and they complicate this further. But the fundamental process, process does not require correlation. The fundamental process is described in terms of the shape of the potential itself; whereas the other resonance like the

autoionization resonance is essentially a correlation effect. And you will then be talking about a many electron system with at least two electrons. Two is already many, okay.
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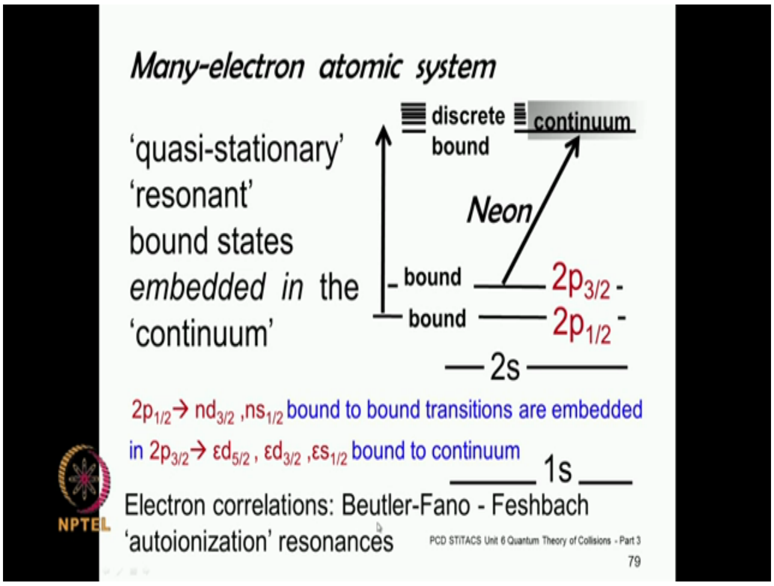

Many-electron atomic system

'quasi-stationary'
'resonant'
bound states
embedded in the
'continuum'

$2p_{1/2} \rightarrow nd_{3/2}, ns_{1/2}$ bound to bound transitions are embedded in $2p_{3/2} \rightarrow \varepsilon d_{5/2}, \varepsilon d_{3/2}, \varepsilon s_{1/2}$ bound to continuum

Electron correlations: Beutler-Fano - Feshbach 'autoionization' resonances

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So, here is it, this is an example of many electrons Atomic System. And let us take the example of Neon, which has got ten electrons. So, 1s2, 2s2, 2p6, that is the usual configuration of the Neon atom. And you have the 1s is filled to 2s filled and the outer 2p. You can have a bound to bound transition over here.

So, these are various bound state excitations possible from the 2p1 half which is more tightly bound than the 2p3 half okay. So, if you have a and a photon energy which is more than the binding energy of the 2p3 half electron, but less than the binding energy of the 2p1 half, so some binding and some photon energy which is greater than the mining energy of 2p3 half.

So, that it can kick out an electron from the 2p3 half into the continuum. It cannot however kick out an electron from the 2p1 half state, which is slightly more tightly bound. However it may be just enough to raise it to a bound excited state like the 4p3 half, the 4d3 half okay. Of course, you have to respect the dipole selection rules.

So, it can from 2p1 half, you can go either to d3 half or 2ns1 half. So, you will have two possibilities over there. And these are the two excitation bound to bound excitation channels which are possible for the bound to bound transition. Whereas the 2p3 half to continuum, you can have various possibilities of getting into the continuum because from 2p3 half, you can get into the d type continuum.

So, d5 half or d3 half and you can of course go to the s half continuum okay. So, these are the different relativistic channels. And I do take into account relativistic splitting of the levels in the, in this discussion because that is fundamental to the understanding of the resonances in this region, okay. So, you have the 2p1 half, 2nd3 half or ns half. So, n are discrete state quantum numbers of excited states.

And this, these bound to bound transitions are embedded, in this bound to continuum. So, continuum state energies are represented by this epsilon bound state energies. I represent by the Principal Quantum Number n, because the bound state energies in Hydrogenic model go as one over n square. So, this is a typical example of an autoionization resonance.

So, you have two possibilities. And there will be interference between the bound to bound States and the bound to continuum. And these states are sometimes referred to as quasi-stationary states or resonance states. And these are, these come into play because you have got one bound state spectrum which is embedded in the continuum with respect to one of the threshold, okay.

So, this is results: the electron correlations cause these resonances which are sometimes referred to as the Beutler-Fano Resonances in Collision Dynamics. They are usually referred to as Feshbach resonances or Fano Feshbach resonances and so on. Or in atomic physics when you're working with outer state, outer electron you typically refer to them as autoionization resonances.

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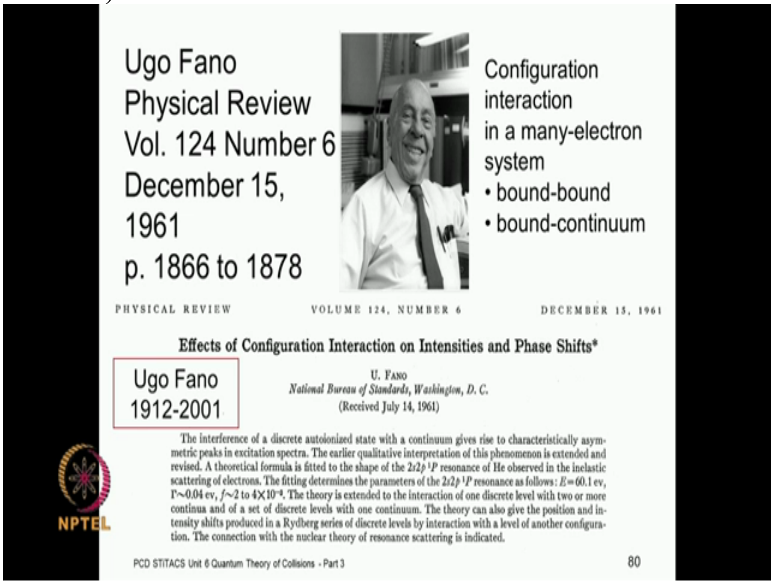

Ugo Fano
Physical Review
Vol. 124 Number 6
December 15,
1961
p. 1866 to 1878

Configuration interaction in a many-electron system
- bound-bound
- bound-continuum

PHYSICAL REVIEW VOLUME 124, NUMBER 6 DECEMBER 15, 1961

Effects of Configuration Interaction on Intensities and Phase Shifts*

Ugo Fano
1912-2001

U. Fano
National Bureau of Standards, Washington, D. C.
(Received July 14, 1961)

The interference of a discrete autoionized state with a continuum gives rise to characteristically asymmetric peaks in excitation spectra. The earlier qualitative interpretation of this phenomenon is extended and revised. A theoretical formula is fitted to the shape of the $2s2p\,^1P$ resonance of He observed in the inelastic scattering of electrons. The fitting determines the parameters of the $2s2p\,^1P$ resonance as follows: $E=60.1$ ev, $\Gamma\sim0.04$ ev, $f\sim2$ to 4×10^{-3}. The theory is extended to the interaction of one discrete level with two or more continua and of a set of discrete levels with one continuum. The theory can also give the position and intensity shifts produced in a Rydberg series of discrete levels by interaction with a level of another configuration. The connection with the nuclear theory of resonance scattering is indicated.

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Now, the classic analysis of this is due to Fano. And I really like to show a picture of this paper, it is a classic paper it came out in 1961, okay, physical review vol 124, Number 6, 1961. And this paper is one of the most cited paper in Physics Literature means you would think that okay.

The papers which are most cited are papers by some, you know, people like Schrodinger, Borne, Bohm, Eisenbud and so on. But this paper is cited across all branches of Physics, Atomic Physics, Condensed matter Physics, Solid-state Physics, Nuclear Physics, okay. And this is a classic paper and it is, I strongly recommend that you go through the original paper itself.

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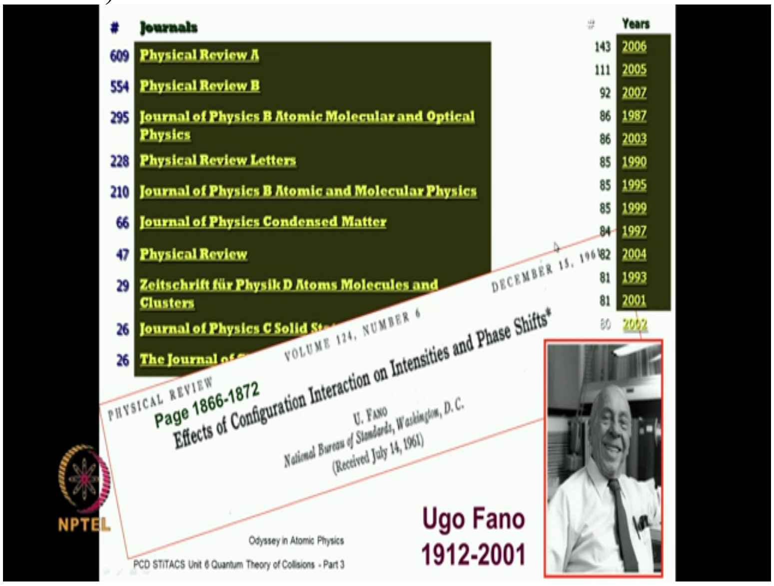

#	Journals
609	Physical Review A
554	Physical Review B
295	Journal of Physics B Atomic Molecular and Optical Physics
228	Physical Review Letters
210	Journal of Physics B Atomic and Molecular Physics
66	Journal of Physics Condensed Matter
47	Physical Review
29	Zeitschrift für Physik D Atoms Molecules and Clusters
26	Journal of Physics C Solid St
26	The Journal of

#	Years
143	2006
111	2005
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Page 1866-1872

Effects of Configuration Interaction on Intensities and Phase Shifts*

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National Bureau of Standards, Washington, D.C.
(Received July 14, 1961)

Ugo Fano
1912-2001

Odyssey in Atomic Physics

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Look at the number of citations in each year like in 2001, it was referred to 81 or 80 times, then 2004, 82 times, in 1997, 84 times, 2006, 143 times. The number of citations, in Physics Rev., are well over 609, thousands of citations, okay. This is absolutely remarkable paper and something that you would love reading.

And when you go through this paper you will really understand why it is so important because it explains the fundamental process of correlations, okay and how these correlations are to be analyzed in terms of configuration interactions and so on.

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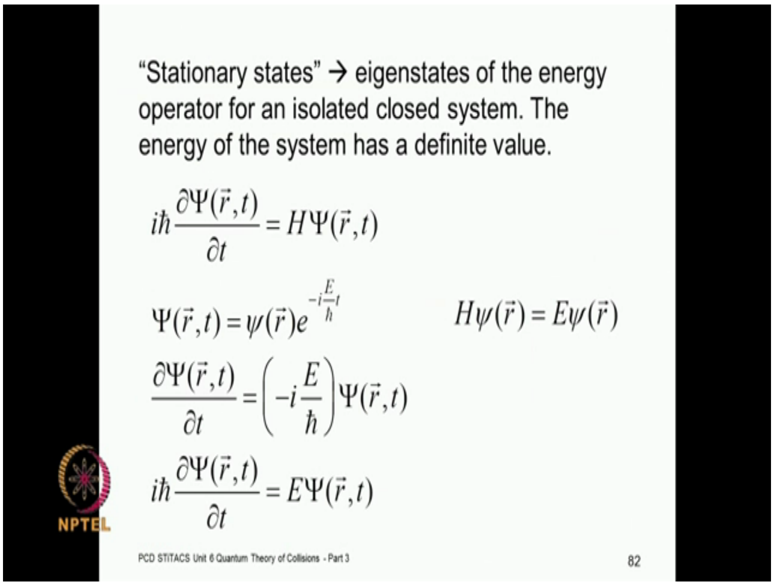

"Stationary states" → eigenstates of the energy operator for an isolated closed system. The energy of the system has a definite value.

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = H\Psi(\vec{r},t)$$

$$\Psi(\vec{r},t) = \psi(\vec{r})e^{-i\frac{E}{\hbar}t} \qquad H\psi(\vec{r}) = E\psi(\vec{r})$$

$$\frac{\partial\Psi(\vec{r},t)}{\partial t} = \left(-i\frac{E}{\hbar}\right)\Psi(\vec{r},t)$$

$$i\hbar\frac{\partial\Psi(\vec{r},t)}{\partial t} = E\Psi(\vec{r},t)$$

So, this is the classic paper and it results in resonances. So, the typical states that we talk about which are non-resonant states. These are the stationary, Eigen states. And if you have an isolated system, then, for an isolated system, you have got the Schrodinger equation, whose solution has got a space dependent factor and a time dependent factor which has got a uniquely defined sharp energy.

This energy E that you find in the solution of the Schrodinger equation is an extremely sharp level. And if any electron gets excited to that state, okay that state being sharp. It will have infinite lifetime and it has no business to that an atom in that type of a state will have no business to decay and come down to a lower energy state okay.

But the reason it has got the sharp energy is because, you have solved the Schrodinger equation for the atom pretending that there is nothing else in the universe that the whole universe is only this. But then there is the rest of the universe and the coupling between the rests of the universe.

And this atom allows for the energy to be transferred from one to the other, okay. And this is just like having what we call as dissipation okay. What we call is friction. The friction when you rub something on a surface, okay, you say that heat is lost or energy is lost. Now, energy cannot really get lost. Where does it go? It gets transformed, okay.

It is not really lost. But then, it gets lost from our bookkeeping because when we set up our equation of motion, we have not taken into account the degrees of freedom coming from the surface interactions. So, these are the unspecified degrees of freedom. And whenever you have these unspecified degrees of freedom, you have the possibility of the system decaying from what you would otherwise expect to be a stationary state.

So, this is not a Stationary state. It becomes a meta stable state because there are these additional degrees of freedom so that the energy can escape to that. So, you have, when you, when you want to rewrite the energy of such a system taking into account the effect of the environment, but not the details of the environment. You can do so by writing these energies as complex numbers, so that they will have a certain width and a certain lifetime.

So, the lifetime comes from that, not from the solution of the Schrodinger equation for an isolated system. The Schrodinger equation for an isolated system will always give you four bound states sharp energy levels which will have infinite lifetimes okay.

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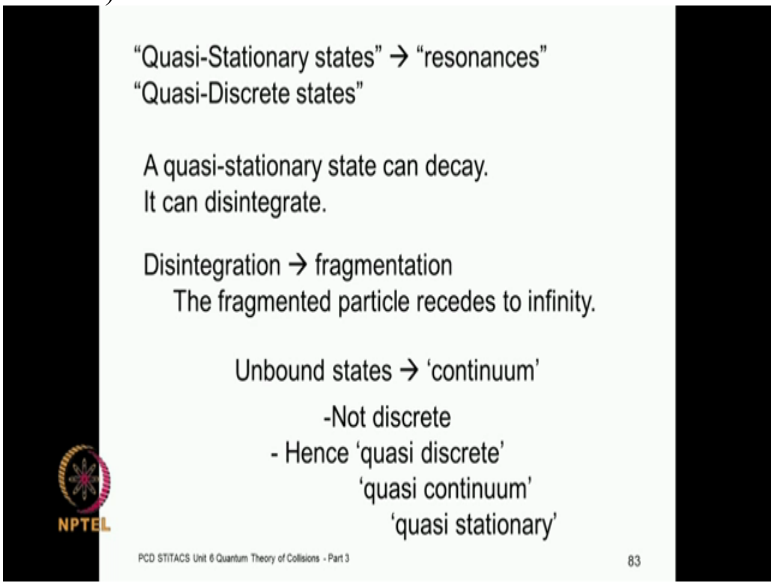

"Quasi-Stationary states" → "resonances"
"Quasi-Discrete states"

A quasi-stationary state can decay.
It can disintegrate.

Disintegration → fragmentation
The fragmented particle recedes to infinity.

Unbound states → 'continuum'
-Not discrete
- Hence 'quasi discrete'
'quasi continuum'
'quasi stationary'

So, now, you will have these costs discrete States because of the presence of the environment in, okay. So, these are quasi-stationary states or resonances or quantity quasi discrete states. They are also called as quasi continuum because they are neither completely bound, nor completely into the continuum okay.

So, you refer to them sometimes as quasi discrete or quasi-stationary, quasi continuum. And all of these terms are used to convey one or the other meaning like in a thesaurus, you have so many different terms, which describe different connotations, different meanings of the term. So, you have these different possibilities. But you are always talking about the same Essential Physics.

So, there is a possibility of disintegration also, because you have one possibility, the continuum channel is degenerated with the bound to bound discrete excitation channel. And the continuum channel will leave you with fragments of the system, which received, which go away from each other into the asymptotic regions far away from each other infinitely far as well.

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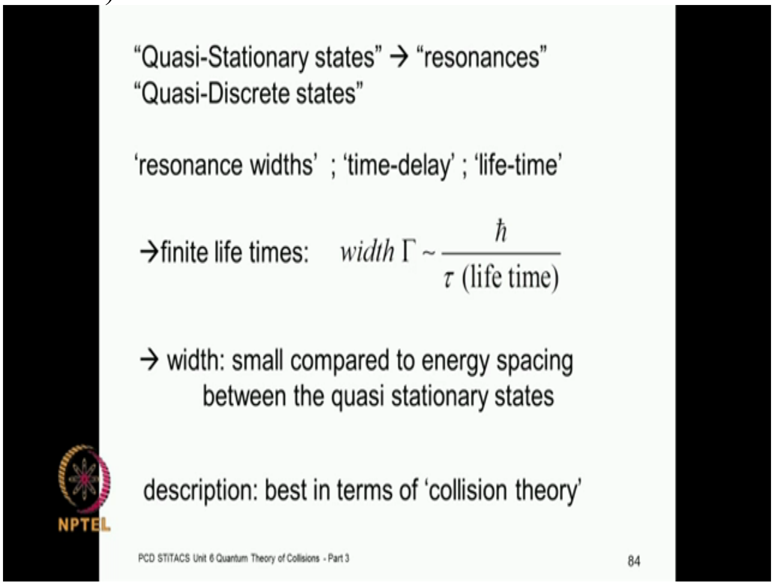

"Quasi-Stationary states" → "resonances"
"Quasi-Discrete states"

'resonance widths' ; 'time-delay' ; 'life-time'

→finite life times: $width\ \Gamma \sim \frac{\hbar}{\tau \text{ (life time)}}$

→ width: small compared to energy spacing between the quasi stationary states

description: best in terms of 'collision theory'

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So, obviously you will now run into resonant widths, time delays, lifetimes and so on, right. So, these are the things that you will now have to be concerned with. So, the lifetime, so, this is like the energy time uncertainty which you are all aware is not the same as the position momentum uncertainty okay. It is coming because of this coupling with the rest of the universe okay. There is no operator for time in Quantum Mechanics.

So, when you write the uncertainty principle for position and momentum, there is an operator for position and for momentum. But, when you write the uncertainty relation energy and time which are also canonically conjugate, you do not write an operator for time, because it is always treated only is a parameter in Quantum Mechanics.

So, you have this width, which is given by a relation, which is like the uncertainty principle. It is in fact often referred to as the uncertainty principle. But it fundamentally it is slightly different from the QP uncertainty because of this real difference because of the fact that time does not have an operator. It is only a parameter.

So, we will continue to refer to it as the uncertainty principle, because it has the same structure and the relationship is again between canonically conjugate variables. And the description of this process is then possible in terms of the Collision Physics, the scattering equations that we have set up the phase shifts and so on.

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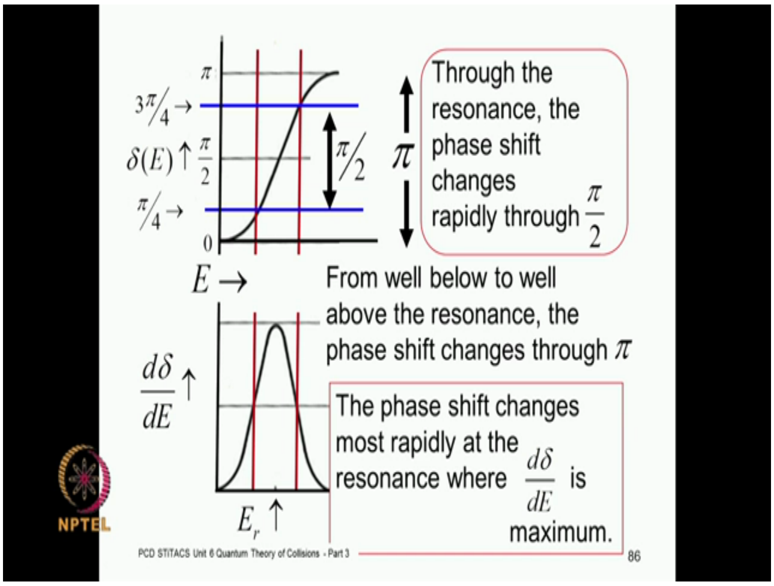

Through the resonance, the phase shift changes rapidly through $\frac{\pi}{2}$

From well below to well above the resonance, the phase shift changes through π

The phase shift changes most rapidly at the resonance where $\frac{d\delta}{dE}$ is maximum.

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So, we will discuss it in terms of the scattering phase shift. So, I mentioned earlier that at a resonance, the phase shift changes rapidly through pi, pi by 2 and from well below the resonance to well above the resonance. The net change in the phase shift is through pi okay. So, across the resonance, you will find that the phase shift changes through pi.

Close to the resonance, it will change rapidly through pi by 2. How rapidly it will change through pi by 2 will depend on the width of the resonance and some other details of the resonance profile, if you look at the derivative of the phase shift with respect to energy okay. So, this is the energy derivative of the phase shift.

This energy derivative of the phase shift, if you see from this profile; so, this is d delta by dE which corresponds to this variation of delta with E, okay. Notice that the phase shift changes most rapidly at the resonance. And here, the rate of change of delta with E becomes 0 okay. It, it is, it becomes flat.
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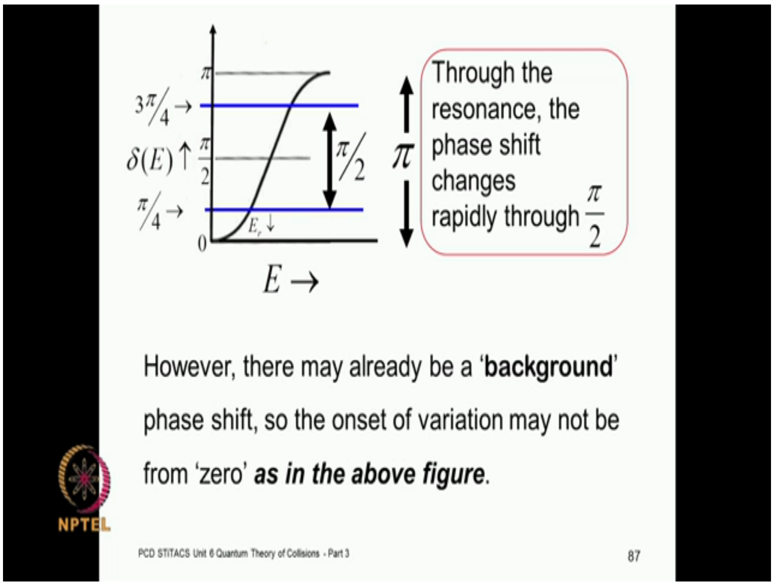

Through the resonance, the phase shift changes rapidly through $\frac{\pi}{2}$

However, there may already be a '**background**' phase shift, so the onset of variation may not be from 'zero' ***as in the above figure***.

So, this is the rate of change of phase shift with energy. The only thing you have to remember is that the change in phase shift which is a change through pi across the resonance.

We have plotted this figure as if we started off from 0. And then, we get to pi, when we go through the resonance.

However, the phase shift at the onset of this resonance may not be necessarily 0. It may already have some value which is coming from the background scattering okay. And then, over and above that background, it will then go through a change in pi, pi by 2, most rapidly at the resonance. But it may have so the zero of the phase shift for a detailed discussion will be offset.

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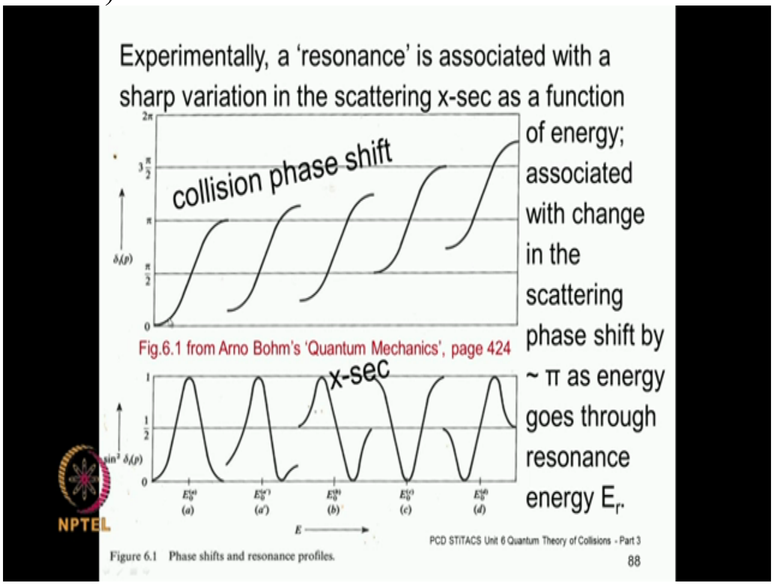

Experimentally, a 'resonance' is associated with a sharp variation in the scattering x-sec as a function of energy; associated with change in the scattering phase shift by ~ π as energy goes through resonance energy E_r.

Fig.6.1 from Arno Bohm's 'Quantum Mechanics', page 424

Figure 6.1 Phase shifts and resonance profiles.

So, that is something that you must remember. So, here is an example of the phase shift, here. So, here, in each case in, there are various figures here. And this is also from Arno Bohm's book. So, here you have the phase shift changing through pi, in all of these five figures, okay. But, the starting phase shift is zero only for the first curve.

For the second, it is somewhat different, for the third again, it is somewhat different, for the fourth is different and for the fifth that is different. So, depending on what value it had from the background scattering, okay because, the collision process we have factored into two processes: one is the hard sphere component okay.

So, delta, the net phase shift is the sum of two angles Xi and Rho. Xi is coming from the hard sphere and there will already be some phase shift because of that. And over and above that, because of the dynamics of the Collision process, you may have an additional phase shift which goes through a change in Phi.

And look at this, that if you have a starting value which is different, then, if you plot the cross section which is like sine square delta for that particular partial wave, of course, these figures will be different for every different value of the l quantum number. Then, the scattering cross section will have very different kind of profiles.

And you will see at a resonance, when the scattering cross section goes all the way to the top or it goes up and then decreases, comes back or it could go to zero, as you see over here okay. So, all these are possibilities. So, resonance does not necessarily mean that the scattering cross section will go to the top and go through the roof.

It can also go through zero. And this will not surprise us because we already know that in Young's double slit experiment, you have got bright fringes, you also have dark fringes, okay. So, that depends on how the phase and the amplitudes, you know, combine to generate the superposition.

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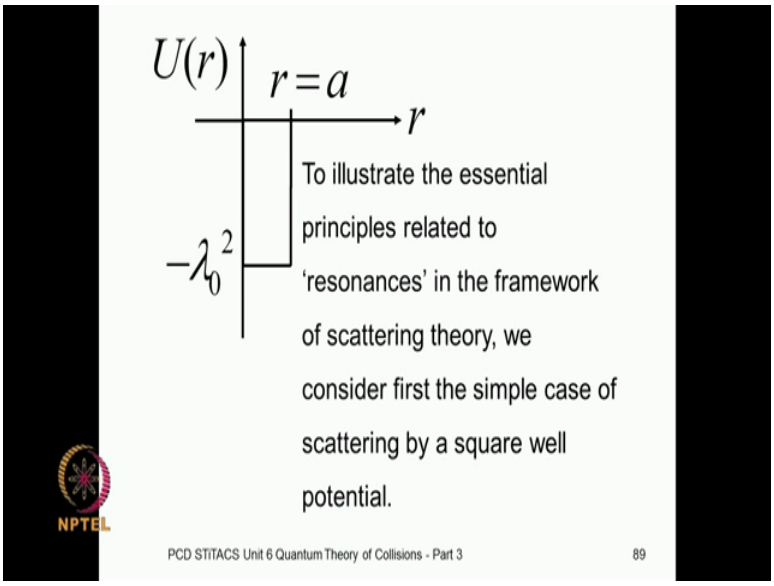

To illustrate the essential principles related to 'resonances' in the framework of scattering theory, we consider first the simple case of scattering by a square well potential.

So, we will take the example of this square well potential and we will discuss our phenomenology in the context of a very simple potential. The actual potentials in that, we have to deal with are much more complex. But this is the easiest example. So, let us take up this example.

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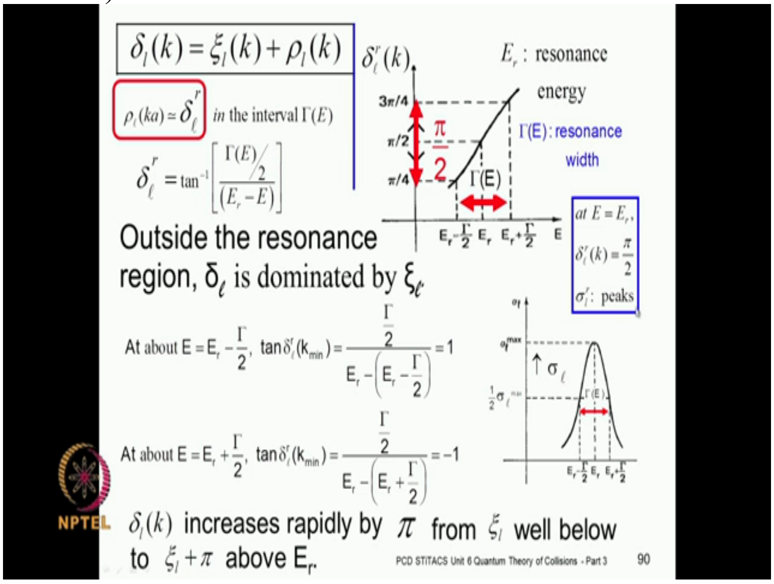

$$\boxed{\delta_l(k)=\xi_l(k)+\rho_l(k)}$$

$\boxed{\rho_l(ka)\simeq\delta_\ell^r}$ in the interval $\Gamma(E)$

$$\delta_\ell^r=\tan^{-1}\left[\frac{\Gamma(E)/2}{(E_r-E)}\right]$$

E_r : resonance energy

$\Gamma(E)$: resonance width

at $E=E_r$, $\delta_\ell^r(k)=\frac{\pi}{2}$ σ_l^r: peaks

Outside the resonance region, δ_ℓ is dominated by ξ_ℓ.

At about $E=E_r-\frac{\Gamma}{2}$, $\tan\delta_\ell^r(k_{min})=\frac{\frac{\Gamma}{2}}{E_r-\left(E_r-\frac{\Gamma}{2}\right)}=1$

At about $E=E_r+\frac{\Gamma}{2}$, $\tan\delta_\ell^r(k_{min})=\frac{\frac{\Gamma}{2}}{E_r-\left(E_r+\frac{\Gamma}{2}\right)}=-1$

$\delta_l(k)$ increases rapidly by π from ξ_l well below to $\xi_l+\pi$ above E_r.

And here, you now have this resonance width. So, this resonance width you have the resonance energy. And depending on the width, you go down, half the width to the lower energy side and half the width, to the upper above this energy, and you define this angle as tan inverse of gamma which is the half-width gamma by 2, over this Er - E, Er is the resonance energy.

So, you define this delta. This is with the superscript r. So, this is what the other phase shift will be in the resonance region, okay. So, your net scattering phase shift is the sum of two powers Xi and Rho, which we saw earlier. When you are at a resonance, this will correspond to the resonance phase shift which is why to emphasize a fact that it is a resonance part.

So, Rho is not always a resonance because resonance will take place only in specific conditions, for resonance are satisfied. It can also be, so both Xi and Rho, in general, are slowly varying functions of energy. But at a resonance, Rho becomes such that it changes rapidly.

And that is when I refer to it as a delta with a superscript r, to remind me that, that is a special case of the resonance feature of the other dynamical phase shift which is Rho. This mouse does not work, okay. So, outside the resonance region, okay, outside the resonance region, the scattering phase shift is dominated by the hard sphere component, okay.

So, what relations do we get at the resonance? If you go to this energy, which is half width below the resonance, the tangent of delta which is defined by this relation becomes +1 as you can see clearly, right. And if you go just as much above the resonance energy, as below like go Er + delta, then the tangent of delta in this case, becomes -1 okay.

So the tan delta becomes +1, at this point. And it becomes -1, at this point. And this is what happens to the cross section itself, okay for this type of behaviour. If it starts off over here, okay. So, this is a typical resonance profile and you have a resonance width. So, the net change in delta will be through an angle which is pi.

What happens at the resonance energy itself? Delta, this resonance phase shift will be pi by 2, okay. It is here, over here, this resonance phase shift is exactly pi by 2, okay. So, it changes through pi by 2 from here to here. At the resonance, this is what is on the vertical axis has got a value which is pi by 2, okay. The net change from well below to well above is through pi. So, now you keep track of the parameters, as we have defined them.
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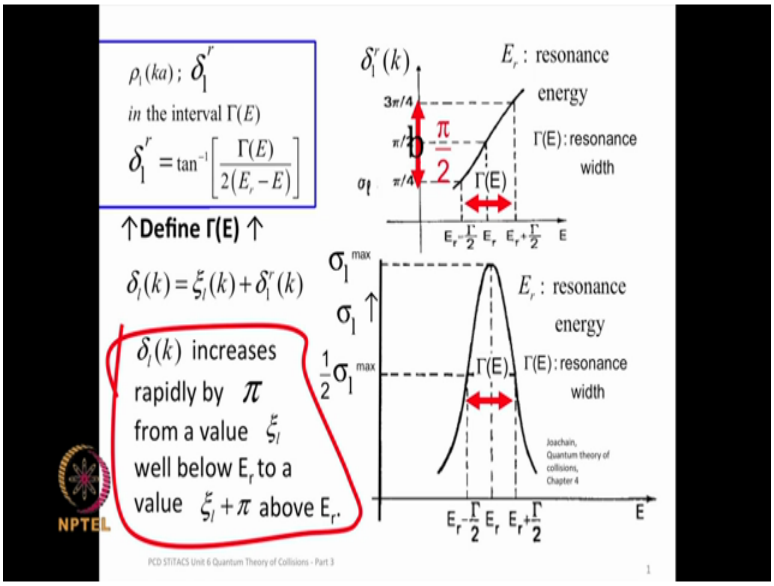

$\rho_1(ka)$; δ_1^r

in the interval $\Gamma(E)$

$$\delta_1^r = \tan^{-1}\left[\frac{\Gamma(E)}{2(E_r - E)}\right]$$

↑Define Γ(E) ↑

$$\delta_l(k) = \xi_l(k) + \delta_1^r(k)$$

$\delta_l(k)$ increases rapidly by π from a value ξ_l well below E_r to a value $\xi_l + \pi$ above E_r.

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And essentially the change in the net phase shift will be from some value to another value which is PI above it okay. So, that is the kind of thing that happens across a resonance, okay.

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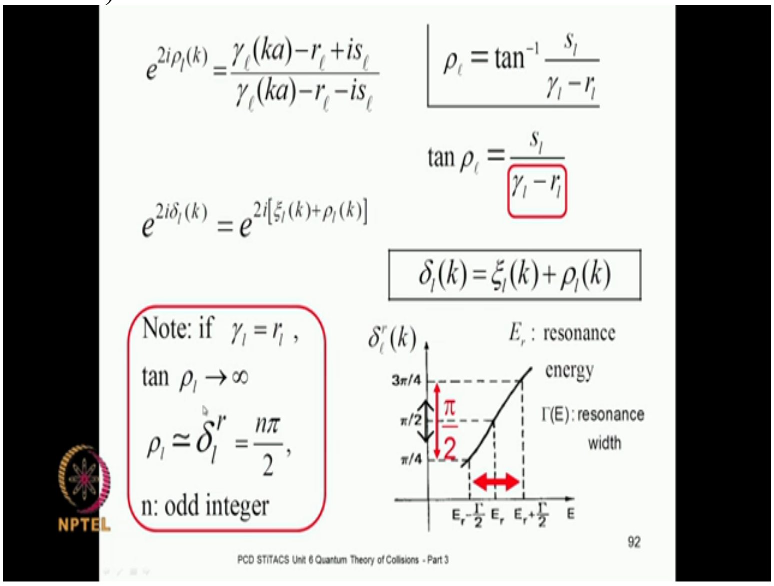

$$e^{2i\rho_l(k)} = \frac{\gamma_\ell(ka) - r_\ell + is_\ell}{\gamma_\ell(ka) - r_\ell - is_\ell}$$

$$\rho_\ell = \tan^{-1}\frac{s_l}{\gamma_l - r_l}$$

$$\tan\rho_\ell = \frac{s_l}{\boxed{\gamma_l - r_l}}$$

$$e^{2i\delta_l(k)} = e^{2i[\xi_l(k) + \rho_l(k)]}$$

$$\boxed{\delta_l(k) = \xi_l(k) + \rho_l(k)}$$

Note: if $\gamma_l = r_l$,

$\tan\rho_l \to \infty$

$\rho_l \simeq \delta_l^r = \frac{n\pi}{2}$,

n: odd integer

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Now, at the resonance, this is the tangent of the second part of the phase shift other than the hard sphere component right.So, see what happens as gamma l becomes equal to r l. The tangent blows up, okay. The tangent of Rho goes, it shoots up to infinity. And the angle Rho itself will be like pi by 2 or 3pi by 2 or 5pi by 2 and so on. So, that is the kind of angular dependence that you get, okay.

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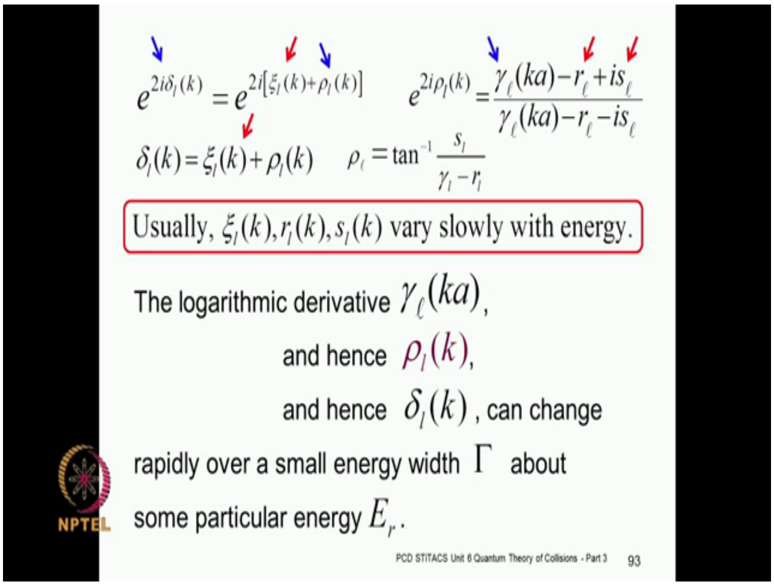

$e^{2i\delta_l(k)} = e^{2i[\xi_l(k)+\rho_l(k)]}$ $\qquad e^{2i\rho_l(k)} = \dfrac{\gamma_\ell(ka)-r_\ell+is_\ell}{\gamma_\ell(ka)-r_\ell-is_\ell}$

$\delta_l(k)=\xi_l(k)+\rho_l(k)$ $\qquad \rho_\ell = \tan^{-1}\dfrac{s_l}{\gamma_l-r_l}$

$\boxed{\text{Usually, } \xi_l(k), r_l(k), s_l(k) \text{ vary slowly with energy.}}$

The logarithmic derivative $\gamma_\ell(ka)$,

and hence $\rho_l(k)$,

and hence $\delta_l(k)$, can change

rapidly over a small energy width Γ about

some particular energy E_r.

So, this is the net phase shift which we have now written as the sum of these two parts. These functions, the hard sphere component and these functions r and s, these usually change with energy. But, only slowly, okay. They are not nothing dramatic is happening to them. What is happening at the resonance is that this gamma, this changes rather dramatically.

And this changes dramatically as a result of which Rho changes dramatically, as a result of which the net phase changes dramatically and the net phase ends up going through a change in Phi, pi, okay. So, the origins are in the details of the dynamics of the Collision process, okay because gamma is the logarithmic derivative of the, of the radial solutions.

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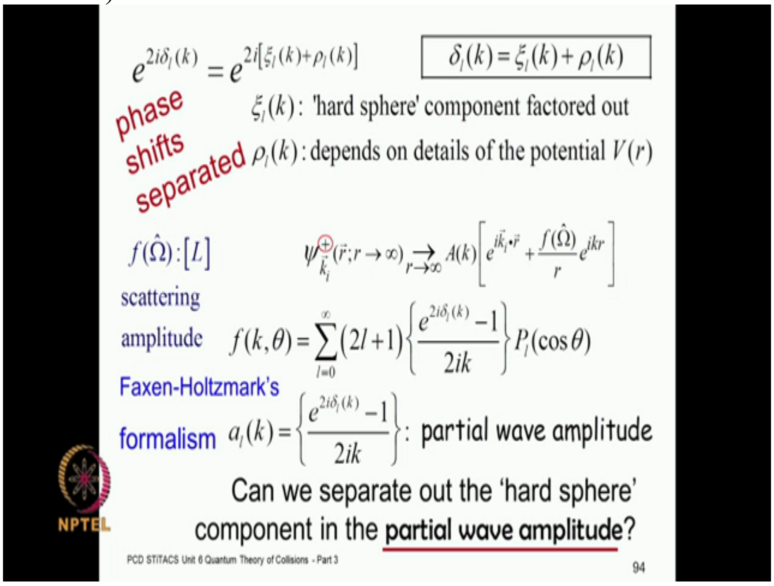

$e^{2i\delta_l(k)} = e^{2i[\xi_l(k)+\rho_l(k)]}$ $\qquad \boxed{\delta_l(k)=\xi_l(k)+\rho_l(k)}$

phase shifts separated

$\xi_l(k)$: 'hard sphere' component factored out

$\rho_l(k)$: depends on details of the potential $V(r)$

$f(\hat\Omega):[L]$

scattering amplitude

$\psi^{(+)}_{\vec{k}_i}(\vec{r}; r\to\infty) \xrightarrow[r\to\infty]{} A(k)\left[e^{i\vec{k}_i\cdot\vec{r}} + \dfrac{f(\hat\Omega)}{r}e^{ikr}\right]$

$f(k,\theta)=\sum_{l=0}^{\infty}(2l+1)\left\{\dfrac{e^{2i\delta_l(k)}-1}{2ik}\right\}P_l(\cos\theta)$

Faxen-Holtzmark's formalism

$a_l(k)=\left\{\dfrac{e^{2i\delta_l(k)}-1}{2ik}\right\}$: partial wave amplitude

Can we separate out the 'hard sphere' component in the partial wave amplitude?

So, now, we have separated the phase shifts into a hard sphere part and another part which depends on the dynamics of the collision process which could become resonant when conditions for resonance are satisfied. And this solution will go into the scattering solution.

So, this is the solution corresponding to the outgoing wave boundary condition. You have got the scattering amplitude.

And the Scattering amplitude is written in terms of what we call as partial wave amplitude, right. So, what comes in this beautiful bracket is what we refer to as partial wave amplitude. E is a partial wave amplitude f is the scattering amplitude. So, what we going to ask, is can we separate out the hard sphere component from the partial wave amplitude?

That a itself if we write it as a sum of two parts one of which is coming from the hard sphere which causes the phase shift Xi, which is the hard sphere phase shift and the other part which will correspond to the dynamics of the collision process. So, we try to separate the hard sphere component from the partial wave amplitude.

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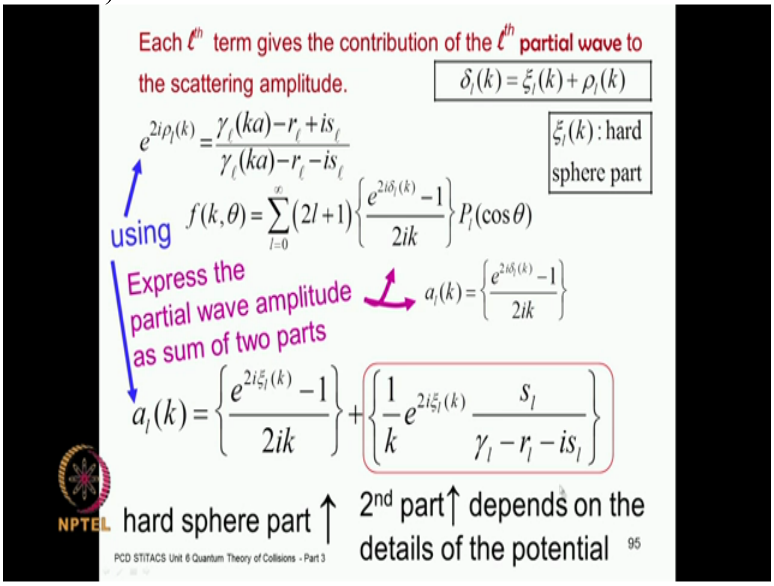

Each ℓ^{th} term gives the contribution of the ℓ^{th} partial wave to the scattering amplitude.

$$\boxed{\delta_l(k)=\xi_l(k)+\rho_l(k)}$$

$\xi_l(k)$: hard sphere part

$$e^{2i\rho_l(k)}=\frac{\gamma_\ell(ka)-r_\ell+is_\ell}{\gamma_\ell(ka)-r_\ell-is_\ell}$$

using

$$f(k,\theta)=\sum_{l=0}^{\infty}(2l+1)\left\{\frac{e^{2i\delta_l(k)}-1}{2ik}\right\}P_l(\cos\theta)$$

Express the partial wave amplitude as sum of two parts

$$a_l(k)=\left\{\frac{e^{2i\delta_l(k)}-1}{2ik}\right\}$$

$$a_l(k)=\left\{\frac{e^{2i\xi_l(k)}-1}{2ik}\right\}+\boxed{\left\{\frac{1}{k}e^{2i\xi_l(k)}\frac{s_l}{\gamma_l-r_l-is_l}\right\}}$$

hard sphere part ↑ 2nd part ↑ depends on the details of the potential

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And indeed it can be done by looking at these complex numbers. So, this is not particularly difficult. So, you write this phase shift Rho, which is now, this second factor. This is the second factor Rho. This is the hard sphere part. The remaining part, the dynamics of the collision is, contained in this factor. And the scattering amplitude is, can be obtained from here. So, the partial wave amplitude, we want to write, as a sum of two parts.

So, this is the usual expression for the partial wave amplitude, right. So, this thing in the beautiful bracket, this is the partial wave amplitude and using this relation, you can write this partial wave amplitude. You can just separate out that part, using this complex numbers. And it comes as a sum of these two parts.

So, this is the hard sphere part and this is coming from the dynamics of the collision process. So, these are the two parts of the partial wave scattering amplitude. So, the second part depends on the details of the potential. The first part is just the hard sphere part okay.

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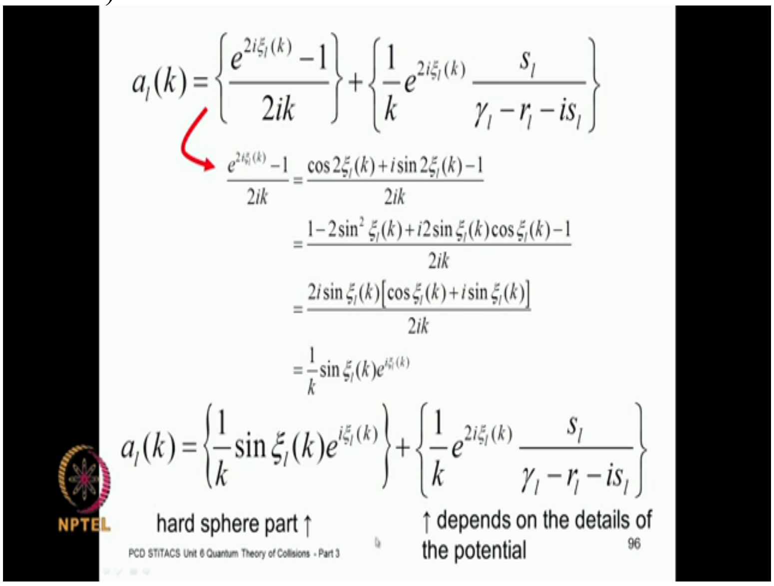

$$a_l(k) = \left\{\frac{e^{2i\xi_l(k)}-1}{2ik}\right\} + \left\{\frac{1}{k}e^{2i\xi_l(k)}\frac{s_l}{\gamma_l - r_l - is_l}\right\}$$

$$\frac{e^{2i\xi_l(k)}-1}{2ik} = \frac{\cos 2\xi_l(k) + i\sin 2\xi_l(k) - 1}{2ik}$$

$$= \frac{1 - 2\sin^2\xi_l(k) + i2\sin\xi_l(k)\cos\xi_l(k) - 1}{2ik}$$

$$= \frac{2i\sin\xi_l(k)\left[\cos\xi_l(k) + i\sin\xi_l(k)\right]}{2ik}$$

$$= \frac{1}{k}\sin\xi_l(k)e^{i\xi_l(k)}$$

$$a_l(k) = \left\{\frac{1}{k}\sin\xi_l(k)e^{i\xi_l(k)}\right\} + \left\{\frac{1}{k}e^{2i\xi_l(k)}\frac{s_l}{\gamma_l - r_l - is_l}\right\}$$

hard sphere part ↑

↑ depends on the details of the potential

So, this the first part you can write in another form in which you find it in many books. So, this is straightforward way of rewriting it. So, I would not comment on this. But you will often find it in this form which is, essentially an equivalent form of writing the partial wave amplitudes.

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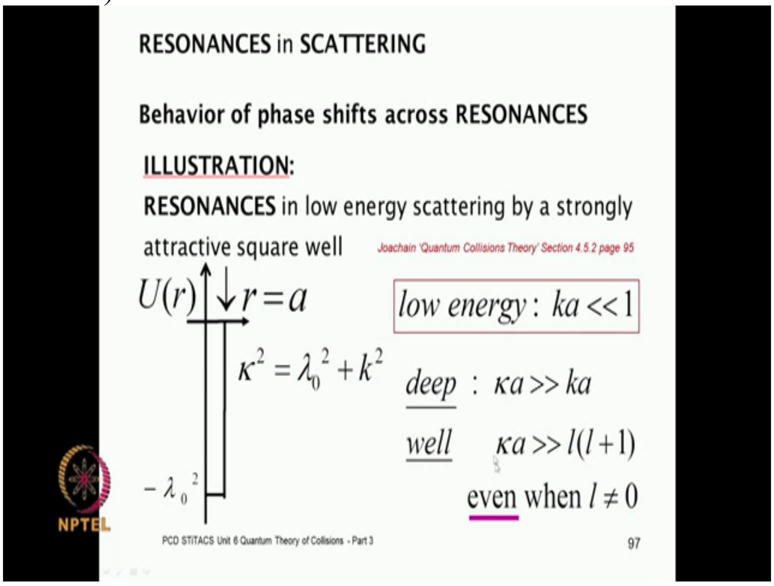

RESONANCES in SCATTERING

Behavior of phase shifts across RESONANCES

ILLUSTRATION:

RESONANCES in low energy scattering by a strongly attractive square well

Joachain 'Quantum Collisions Theory' Section 4.5.2 page 95

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

$\boxed{\text{low energy}: ka << 1}$

deep well : $\kappa a >> ka$

$\kappa a >> l(l+1)$

even when $l \neq 0$

So, now we will consider the behaviour of the phase shifts across the resonance. And we will take the example of a strongly attractive well. So, you have got a well, which is strongly attractive, which is why, I show it by what looks like a deep well just to indicate that, it is strongly attractive, okay. The strongly attractive, the strength, of course, depends on the depth as well as the range of the potential.

But you are only to indicate that we have a strongly attractive well and we have used these relations earlier. So, you define the quantum numbers: kappa square, which is the sum of lambda 0 square and k square is the energy of the projectile. It is actually h cross square k square by 2m, but essentially k square is a measure of the energy right.

So, you have a deep well and the reason I refer to this is a deep well because kappa a, in this case is, much larger this l into l + 1 even when l is not equal to 0. So, as you can see from this right-hand side, the value of this right hand side will increase with the value of l. But we are dealing with such kappa, with such depth. So, that kappa a is always greater than l into l + 1.

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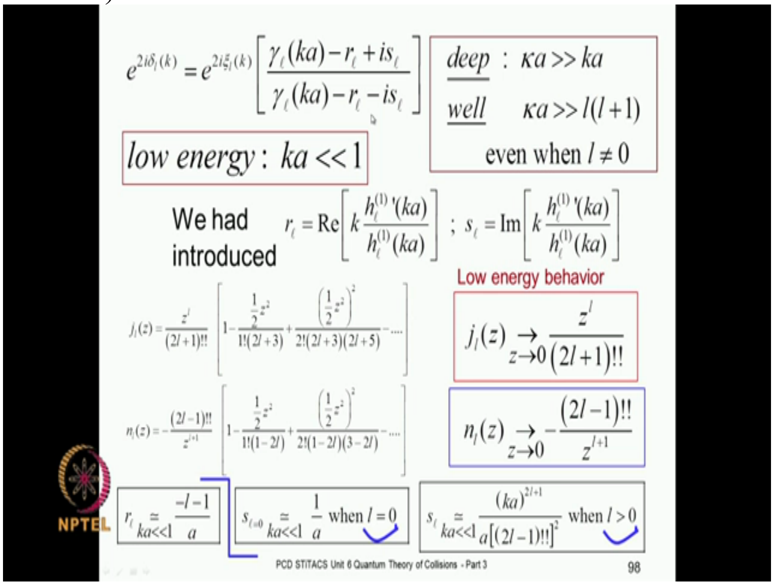

$$e^{2i\delta_l(k)} = e^{2i\xi_l(k)}\left[\frac{\gamma_\ell(ka)-r_\ell+is_\ell}{\gamma_\ell(ka)-r_\ell-is_\ell}\right]$$

$$\boxed{\text{low energy}: ka << 1}$$

$\underline{deep}$: $\kappa a >> ka$

$\underline{well}$ $\kappa a >> l(l+1)$

even when $l \neq 0$

We had introduced $r_\ell = \mathrm{Re}\left[k\frac{h_\ell^{(1)}{}'(ka)}{h_\ell^{(1)}(ka)}\right]$; $s_\ell = \mathrm{Im}\left[k\frac{h_\ell^{(1)}{}'(ka)}{h_\ell^{(1)}(ka)}\right]$

Low energy behavior

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

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

$$n_l(z) = -\frac{(2l-1)!!}{z^{l+1}}\left[1-\frac{\frac{1}{2}z^2}{1!(1-2l)}+\frac{\left(\frac{1}{2}z^2\right)^2}{2!(1-2l)(3-2l)}-....\right]$$

$$\boxed{n_l(z) \xrightarrow[z\to 0]{} -\frac{(2l-1)!!}{z^{l+1}}}$$

$$\boxed{r_\ell \underset{ka<<1}{\simeq} \frac{-l-1}{a}} \quad \boxed{s_{\ell=0} \underset{ka<<1}{\simeq} \frac{1}{a} \text{ when } l=0} \quad \boxed{s_\ell \underset{ka<<1}{\simeq} \frac{(ka)^{2l+1}}{a[(2l-1)!!]^2} \text{ when } l>0}$$

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So, we consider low-energy scattering. And in this, we look at the parameters r and s. These have different values for different partial waves. And you can write these Hankel functions, in terms of the Bessel functions, the Neumann functions. And look at the low-energy behaviour because that is well known.

And from this, you can get the low-energy behaviour of the Hankel functions and get the low-energy behaviour of the terms r and s, okay. So, that is a straightforward analysis which I will not work out in details. But, you can see where it is coming from, okay. So, you have the low-energy behaviour of the Bessel function and the Neumann function.

In terms of which you can describe the low-energy behaviour of the Hankel functions, in terms of, which you can describe the low-energy behaviour of the functions r and s. And in terms of this, you can analyze the phase shifts, the phase shifts Rho. So, you can get these relations that when you are dealing with low energy. So, that k is is much less than 1, okay.

So, this is the low energy domain. And you can get the values for s, when l is 0 and when l is not 0, when l is greater than 0.

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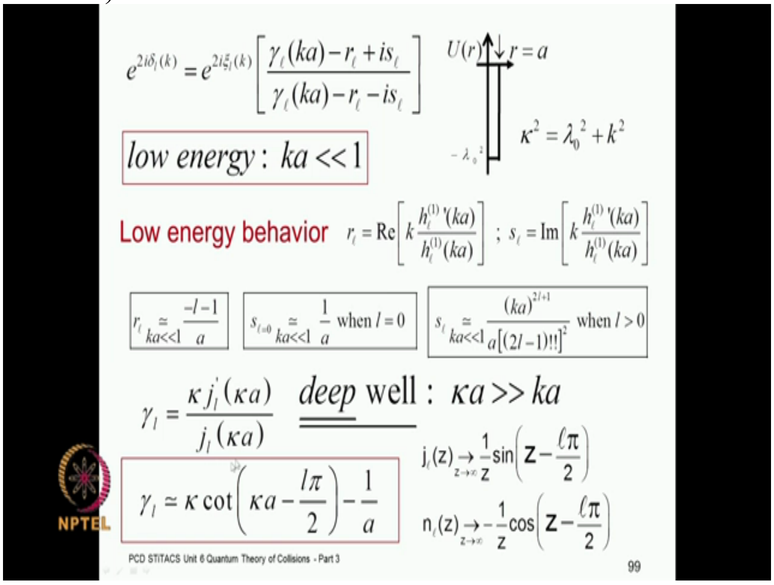

$$e^{2i\delta_\ell(k)} = e^{2i\xi_\ell(k)}\left[\frac{\gamma_\ell(ka)-r_\ell+is_\ell}{\gamma_\ell(ka)-r_\ell-is_\ell}\right]$$

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

$$\boxed{low\ energy:\ ka \ll 1}$$

Low energy behavior $r_\ell = \mathrm{Re}\left[k\frac{h_\ell^{(1)}{}'(ka)}{h_\ell^{(1)}(ka)}\right]$; $s_\ell = \mathrm{Im}\left[k\frac{h_\ell^{(1)}{}'(ka)}{h_\ell^{(1)}(ka)}\right]$

$$\boxed{r_\ell \underset{ka\ll 1}{\simeq} \frac{-l-1}{a}} \quad \boxed{s_{\ell=0} \underset{ka\ll 1}{\simeq} \frac{1}{a} \text{ when } l=0} \quad \boxed{s_\ell \underset{ka\ll 1}{\simeq} \frac{(ka)^{2l+1}}{a[(2l-1)!!]^2} \text{ when } l>0}$$

$$\gamma_l = \frac{\kappa j_l'(\kappa a)}{j_l(\kappa a)} \qquad \underline{\underline{deep}\text{ well}}:\ \kappa a \gg ka$$

$$j_\ell(z) \xrightarrow[z\to\infty]{} \frac{1}{z}\sin\left(z-\frac{\ell\pi}{2}\right)$$

$$\boxed{\gamma_l \simeq \kappa\cot\left(\kappa a-\frac{l\pi}{2}\right)-\frac{1}{a}}$$

$$n_\ell(z) \xrightarrow[z\to\infty]{} -\frac{1}{z}\cos\left(z-\frac{\ell\pi}{2}\right)$$

And you get these values from this by taking the low-energy behaviour. And now you can examine what will be your gamma, because gamma is the one which is going to be a controlling factor okay. So, you find, when you put all of these values of r and s in this relation, gamma which is nothing but this kappa j prime over j. So, this turns out to be given by this k cotangent function -1 over a.

Now, it is this cotangent function, you know, that the tangent function and the cotangent function, they are very sensitive function that there are regions where they just shoot up, right. And any small change in the angle will change their value in such a huge manner that you will have dramatic results. So, that is what you will expect because the key feature in gamma is a cotangent function.

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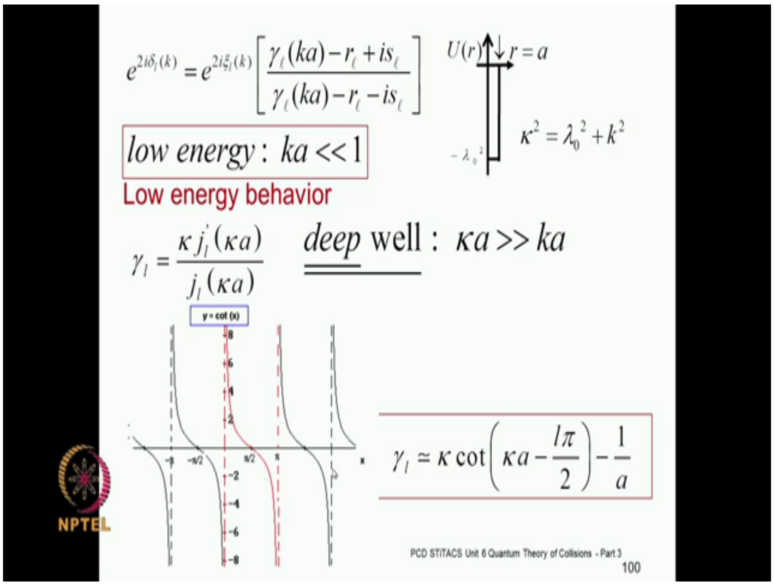

$$e^{2i\delta_\ell(k)} = e^{2i\xi_\ell(k)}\left[\frac{\gamma_\ell(ka) - r_\ell + is_\ell}{\gamma_\ell(ka) - r_\ell - is_\ell}\right]$$

$\boxed{low\ energy:\ ka \ll 1}$

Low energy behavior

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

deep well : $\kappa a \gg ka$

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

$$\boxed{\gamma_l \simeq \kappa \cot\left(\kappa a - \frac{l\pi}{2}\right) - \frac{1}{a}}$$

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So, if you look at the cotangent function, okay. So, this is a cotangent function, okay. And you see that when you are close to these points okay like if the angle is 0 or pi, or 2pi and so on. Any small change in the value of the angle, changes the value of the cotangent dramatically.

And it will change the value of gamma dramatically, which is why, you have such spectacular changes, when there are very small changes in the energy. So, when you go across the resonance, the change in the energy independent parameter may be very small. But the effects on the phase shifts and on scattering cross sections are huge.

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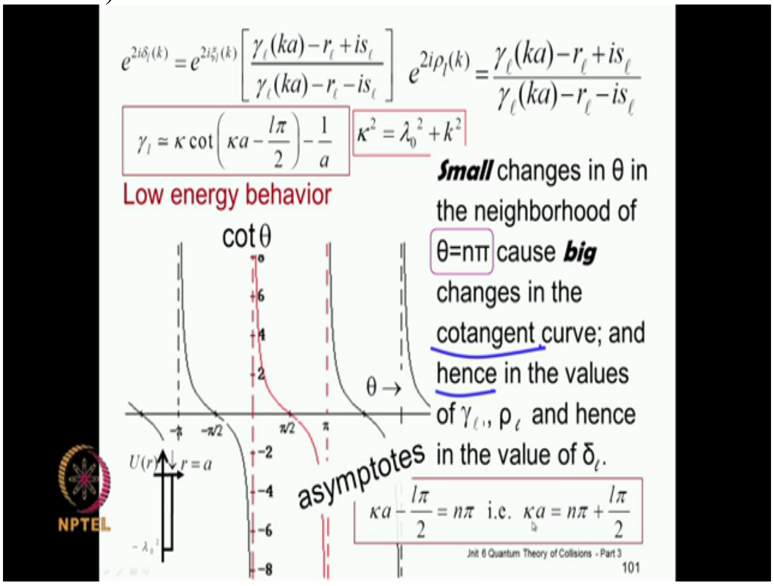

$$e^{2i\delta_\ell(k)} = e^{2i\xi_\ell(k)}\left[\frac{\gamma_\ell(ka) - r_\ell + is_\ell}{\gamma_\ell(ka) - r_\ell - is_\ell}\right] \qquad e^{2i\rho_\ell(k)} = \frac{\gamma_\ell(ka) - r_\ell + is_\ell}{\gamma_\ell(ka) - r_\ell - is_\ell}$$

$$\boxed{\gamma_l \simeq \kappa \cot\left(\kappa a - \frac{l\pi}{2}\right) - \frac{1}{a}} \quad \boxed{\kappa^2 = \lambda_0^2 + k^2}$$

Low energy behavior

Small changes in θ in the neighborhood of θ=nπ cause ***big*** changes in the cotangent curve; and hence in the values of γ_ℓ, ρ_ℓ and hence in the value of δ_ℓ.

$$\boxed{\kappa a - \frac{l\pi}{2} = n\pi \ \text{ i.e. } \ \kappa a = n\pi + \frac{l\pi}{2}}$$

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So, here, look at it over here, that whenever theta, the angle theta is in the neighbourhood of npi okay, whenever it is in the neighbourhood of npi, there are huge changes in the value of the cotangent function. And because of this, gamma changes in a big way. And because this gamma changes, Rho changes and then, the next phase shift delta changes because delta is nothing but Xi + Rho. So, Xi part is not changing very much but the Rho part changes in a very spectacular manner.

So, if you look at the asymptotes of this function, they occur whenever this arguments of the cotangent function. What is argument? This angle is kappa, kappa a - lpi by 2, okay. So whenever this angle kappa a -lpi by 2 is equal to npi that is when you have the asymptotes of the cotangent function, okay. So, kappa a when this condition is satisfied you bring this l pi by 2 to the right. So, kappa a will be npi + lpi by 2.

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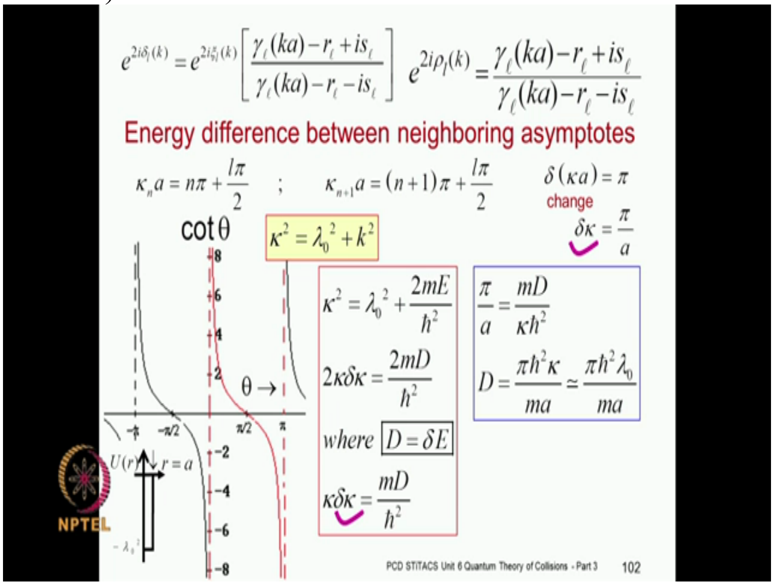

$$e^{2i\delta_l(k)} = e^{2i\xi_l(k)}\left[\frac{\gamma_\ell(ka)-r_\ell+is_\ell}{\gamma_\ell(ka)-r_\ell-is_\ell}\right] \quad e^{2i\rho_l(k)} = \frac{\gamma_\ell(ka)-r_\ell+is_\ell}{\gamma_\ell(ka)-r_\ell-is_\ell}$$

Energy difference between neighboring asymptotes

$$\kappa_n a = n\pi + \frac{l\pi}{2} \quad ; \quad \kappa_{n+1} a = (n+1)\pi + \frac{l\pi}{2} \qquad \delta(\kappa a) = \pi$$

change

$$\delta\kappa = \frac{\pi}{a}$$

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

$$\kappa^2 = \lambda_0^2 + \frac{2mE}{\hbar^2}$$

$$2\kappa\delta\kappa = \frac{2mD}{\hbar^2}$$

where $\boxed{D = \delta E}$

$$\kappa\delta\kappa = \frac{mD}{\hbar^2}$$

$$\frac{\pi}{a} = \frac{mD}{\kappa\hbar^2}$$

$$D = \frac{\pi\hbar^2\kappa}{ma} \simeq \frac{\pi\hbar^2\lambda_0}{ma}$$

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That is what we get. And if you look at neighboring asymptotes, the adjacent asymptotes, then for one kappa a, will be npi + l pi by 2, for the next one which I indicate by a subscript n + 1. Instead of n here, I have n + 1 pi + lpi by 2. So, these are the values of kappa.This is how kappa would change as you go from one asymptote to the next asymptote.

So, what is the net change in kappa a? The net change in kappa a, this is, this delta is not the phase shift. It only represents the change. So, change in kappa a is pi, right. Or change in kappa itself is pi over a, okay. So, now you have kappa square equal to lambda 0 square + k square.

So, from this we can take the derivative. So, you get 2 kappa delta kappa from the left. And this one is just the depth of the potential. So that does not change. And then, you have the 2m over h cross square d, because E is h cross square k square over 2m okay. So, here you get kappa, delta kappa. The two will cancel. So, kappa delta kappa will be md over h cross square.

But now you have a delta kappa from here but you also have a delta kappa from here. So, you can put the two together. And what do you get? You get that pi over a, which is this which is equal to delta Kappa. But this delta Kappa is equal to md over kappa h cross square. So, pi over a, becomes md over kappa h cross square. What is d? d is the energy difference between two edges and resonances.

So, the two adjacent resonances will occur at this energy which will depend, which we have now found to be given by pi h cross square over ma. And it will then be related to the size of the potential lambda 0 is the root of the potential depth in this case okay. The potential depth itself is lambda 0 square. So, it is proportional to the root of the depth of the potential. So this is what you get for the separation between adjacent resonances.
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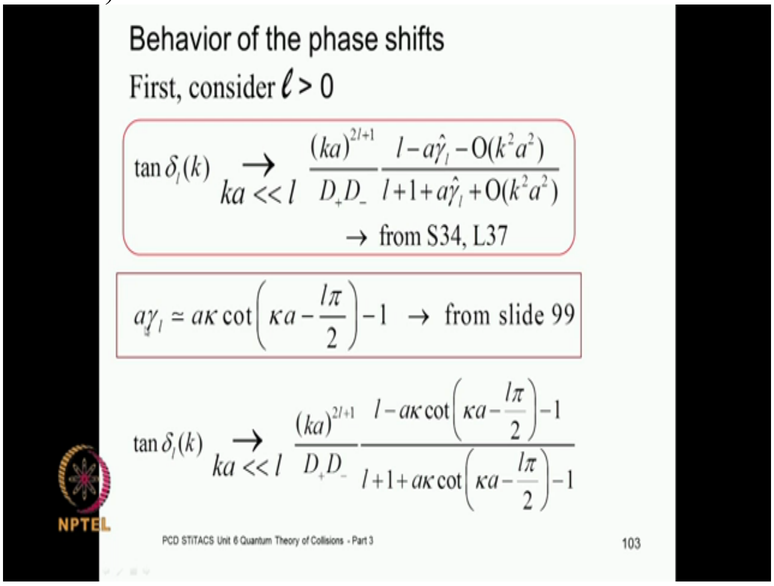

Behavior of the phase shifts

First, consider $\ell > 0$

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

→ from S34, L37

$$a\gamma_l \simeq a\kappa\cot\left(\kappa a - \frac{l\pi}{2}\right) - 1 \rightarrow \text{from slide 99}$$

$$\tan\delta_l(k) \xrightarrow[ka \ll l]{} \frac{(ka)^{2l+1}}{D_+D_-}\frac{l - a\kappa\cot\left(\kappa a - \frac{l\pi}{2}\right) - 1}{l+1+a\kappa\cot\left(\kappa a - \frac{l\pi}{2}\right) - 1}$$

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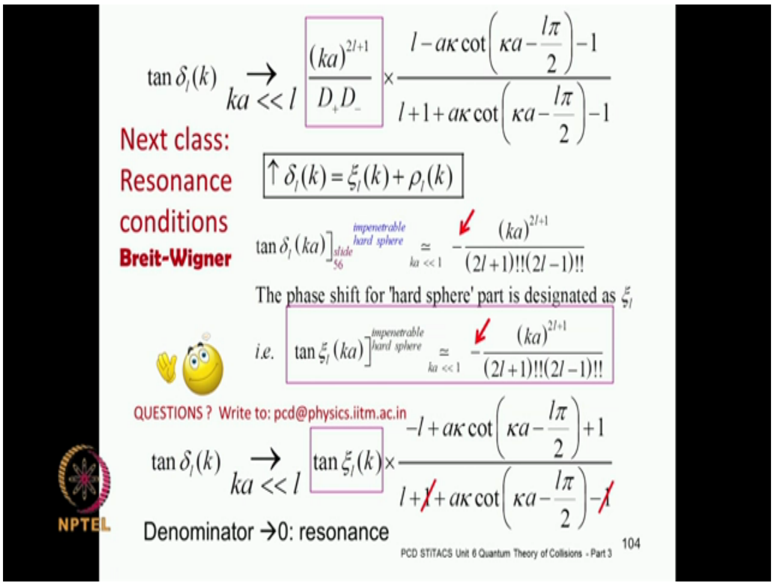
And we will now be interested in examining how the phase shift changes at the resonances. So, this expression we have obtained in one of our earlier classes. So, I will use it directly, okay. And in this notice that there is there is this gamma which we have obtained just few slides prior, prior to this.

And now, you can write this a gamma, okay. This is a gamma. So, we had obtained gammas. So you multiplied by a. You get a gamma right and you can put this a gamma in this expression here. And you get tan delta to be given by this relation, okay. You have neglected certain terms here.
(Refer Slide Time: 59:38)



$$\tan\delta_l(k) \xrightarrow[ka \ll l]{} \boxed{\frac{(ka)^{2l+1}}{D_+D_-}} \times \frac{l - a\kappa\cot\left(\kappa a - \frac{l\pi}{2}\right) - 1}{l + 1 + a\kappa\cot\left(\kappa a - \frac{l\pi}{2}\right) - 1}$$

Next class:
Resonance
conditions
Breit-Wigner

$$\boxed{\uparrow \delta_l(k) = \xi_l(k) + \rho_l(k)}$$

$$\tan\delta_l(ka)\Big]_{\text{slide } 56}^{\text{impenetrable hard sphere}} \underset{ka \ll 1}{\simeq} -\frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!}$$

The phase shift for 'hard sphere' part is designated as ξ_l

$$i.e. \quad \boxed{\tan\xi_l(ka)\Big]^{\text{impenetrable hard sphere}} \underset{ka \ll 1}{\simeq} -\frac{(ka)^{2l+1}}{(2l+1)!!(2l-1)!!}}$$

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

$$\tan\delta_l(k) \xrightarrow[ka \ll l]{} \boxed{\tan\xi_l(k)} \times \frac{-l + a\kappa\cot\left(\kappa a - \frac{l\pi}{2}\right) + 1}{l + \cancel{1} + a\kappa\cot\left(\kappa a - \frac{l\pi}{2}\right) - \cancel{1}}$$

Denominator →0: resonance

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So, this is your expression for tan delta. This phase shift is, has been written as, the sum of these two parts. Remember, that this k a to the power 2 l plus 1 divided by d plus, d minus this factor was nothing but the tangent and the hard sphere scattering phase shift, ok. We have done this earlier.

This is a result from slide number 56 and we have obtained this result earlier. So, this term is nothing but the hard sphere component, ok. This term over here, this term over here is exactly the same over here, with the difference that there is a minus sign here, ok. So, you have to be careful about it. So, take care of this minus sign. And you can write this phase shift.

So, instead of this, you can write this tan of Xi, because it is the same except for the minus sign. And that minus sign you accommodate on in the second term by making this l as minus l. Instead of this minus, a kappa, cotangent function I have got a plus a kappa function and instead of this minus 1 I have got a plus one, okay.

So I have adjusted the minus sign over here. So, you have this net expression for the phase shift, in which, you have one part coming from the hard sphere impenetrable sphere and the remaining part is coming from the dynamics of the actual potential. And that is a part which is of interest in the resonance condition. And you can see where the resonance will take place. The resonance will take place when this denominator will become small, okay.
The cotangent will take all kinds of values, okay. And when the cotangent takes such a value that, a kappa, cotangent theta, where theta is kappa minus l pi by 2, becomes equal to minus of l. That is when you will get a resonance. So, we will discuss those details in the next class. There is any question for today I will be happy to take. Otherwise we will pick up the discussion from this point in the next class. Thank you.