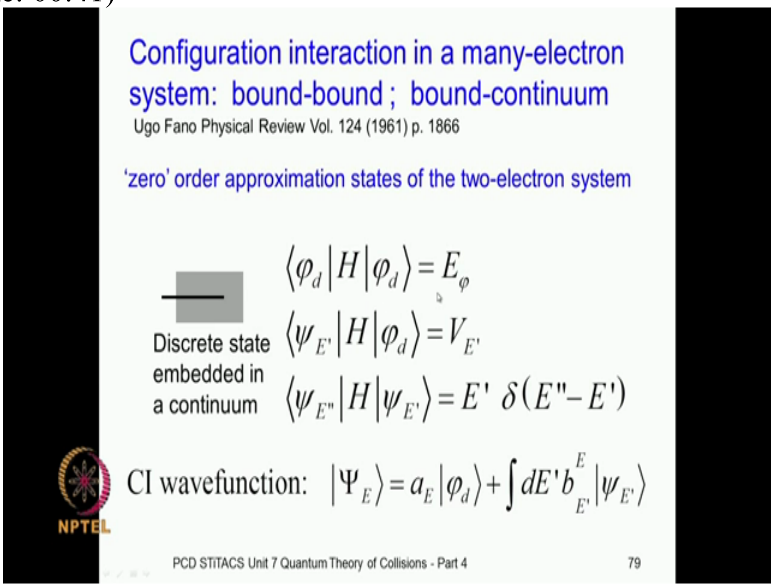
Select/Special Topics in 'Theory of Atomic Collisions and Spectroscopy'
Prof. P.C. Deshmukh
Department of Physics
Indian Institute of Technology-Madras

Lecture 42
Resonance life times

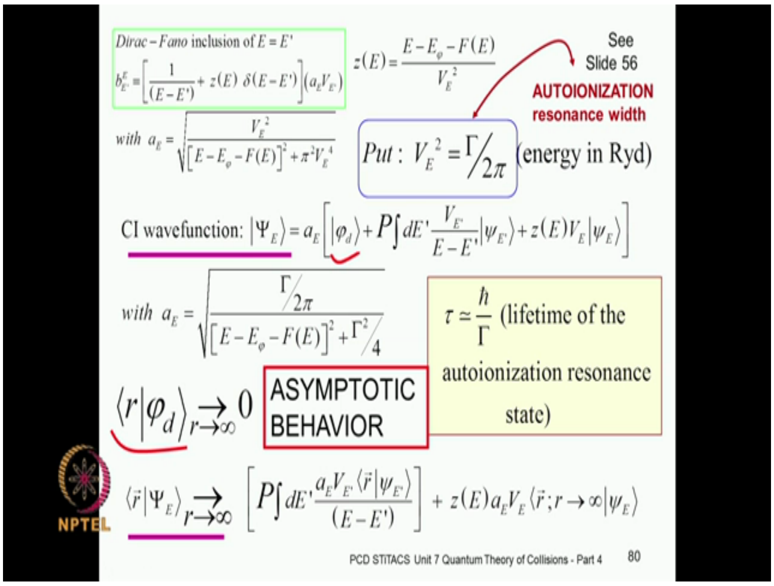
Greetings, so we are coming toward the end of this course. Actually, so, there are just two more classes including today, today and then one more. And we have come a long way in Fano's analysis of the interaction between discrete bound to bound transitions and bound to continuum transitions.

(Refer Slide Time: 00:41)



So, we have a situation in which a bound to bound discrete state is embedded in the continuum and we constructed the energy matrix in our previous class which has these elements right. And then, we set up the configuration Interaction which has got both the components, the discrete as well as the continuum because of the CI. This is a result of the correlation which is ignored in the independent particle approximation.

(Refer Slide Time: 01:17)



And then, we used the Dirac Fano trick of using this Dirac delta function integration whenever the coefficient b would appear in the integrated. So, using that, we agreed that the function z or zee would be would correspond to appropriate boundary condition which is what gave us this form.

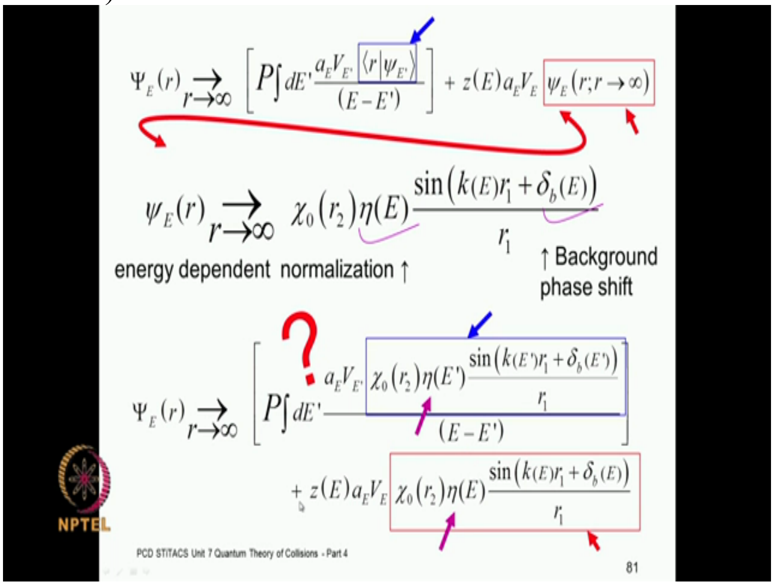
And we found the coefficient aE according to this and I had pointed out that VE has the dimensions of root of energy. So, VE square would be the energy and it would correspond to the energy width of the resonance. So, now, you have the complete configuration interaction wave function. So, it has got a discrete part then, it has got this principal value integration.

And it has got this continuum state with scaled by the factor z, which is coming from the boundary condition. Now, this is the width the gamma, this is the width of the resonance. And as you always have you know its reciprocal scale by the factor h cross, would give you the lifetime of the autoionization state. Now, our interest as we always emphasize in scattering theory, is in seeking asymptotic solutions.

What happens as r tends to infinity, right? That is where you carry out your measurements. Now, this discrete state function, this is the bound state function. So, it would vanish in the asymptotic limit. So, there are 3 terms over here, 1, 2 and 3. Out of which, this term goes to 0 as r tends to infinity, okay. So, we can drop that off, okay.

Now, we are left with these two terms. Out of which this particular one is something that we have some familiarity with from scattering theory, okay. It is the principal value; this is the term that we will have to determine. So, now, the r tending to infinity solution will be given by the remaining two terms. So, these are the two terms which we are now left with for our analysis.

(Refer Slide Time: 03:53)



And now, I have these two terms which describe the asymptotic wave function. So, this is the De Broglie Schrondinger wave function, the coordinate representation of the state vector. And this one coming from scattering theory is the usual sinusoidal function by r plus the usual scattering phase shift which is in this case is the background phase shift.

So, this is known. And what we have over here is pretty much the same except for the fact that this is weighted by this interaction term VE. Now, VE, if you remember is, let me go back to the previous slide, if I have it on this slide or no I do not have it on the slide. I have it on the one prior to this here. VE is nothing but the energy contribution to the energy matrix coming from the interaction between the discrete under continuum, right.

It is this interaction which is resulting in the VE. So, that is the configuration interaction term which is contributing to that. So, let me go back to this slide over here. And here this wave function here is pretty much of this kind except that it is weighted by this configuration interaction VE, right.

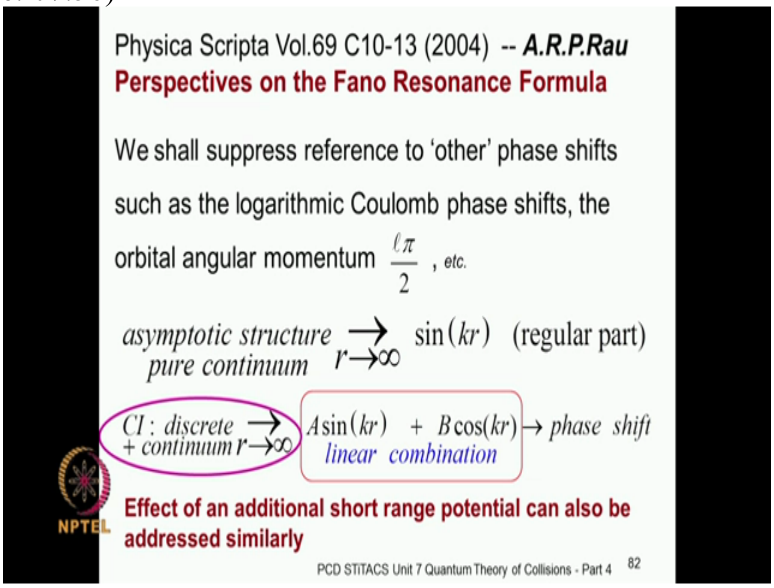
So, this has, this usual sinusoidal behaviour divided by r and then there is a phase shift coming from background, scattering phase shift. Then, there is an energy-dependent normalization. This is the bound state wave function which is normalized independently. It is the square integrable function. So, this is well understood. And this is the background phase shift as I mentioned earlier.

So, we can write these two terms. And look at the second term here, the second term is just what I have written over here. So, what is in this red box comes here with this explicit form inclusive of this energy dependent normalization, the sinusoidal function by r and the background phase shift which is here.

And now, we look at this term out of which aE VE are here, right. The Chi 0 r2 coming from here, comes here. And then, you have got this term which is similar to this except for the fact that now you have this aE VE prime popping up, okay. So, this is what takes care of the configuration interaction but the only thing is that now you have to deal with only the principal value of this integral, okay.

So, one can work out this principal value integration in some details. And all of you would have done this in your Math Physics courses. And instead of going through all those detailed mathematical steps I will comment on the Essential physics which goes into this analysis. And here notice that, this term is over here.

What you should remember that this Eta E is a function this Eta is Energy Dependent Normalization. It is a function of energy and this Eta is the same function of energy. So, if this is known, this is also known, okay. So, that is coming from usual scattering theory. So, these two are essentially the same functions of energy except that the argument is different. So, now, our question is, how to determine this Principal value integral?
(Refer Slide Time: 07:56)



And that is what I will now discuss. And I really like the treatment in this paper which came about 10 years ago by A. R. P. Rau who was, I believe, Fano's first student and he have this paper. The title of this paper is Perspectives on Fano Resonance Formula which he wrote in physica scripta quite recently just 10 years ago considering that Fano's paper is so old; it is relatively recent.

And what Professor Rau suggest is that we focus attention on the essential dynamics which is going into it rather than get lost in notations symbols and other factors which are not contributing to the main terms, which are the focus of our discussion. So, when you write the complete wave function, you will of course have lots of factors. You will have to worry about the Logarithmic Coulomb phase shift.

You will have to worry about the phase shift coming from the orbital angular momentum. There is always this lpi by 2 phase shift which we all know, right? So, all of these terms will be there. And he says that okay, we will remove them from our discussion, to simplify our notation and to simplify our discussion. So, that if we focus on the essential aspects. So, I am following this prescription by Professor Rau.

And what Rau does is to point out that the asymptotic structure of the pure continuum is given by this regular function which is a sinusoidal function, okay. The radial function of course has got that one over r. So, this is the radial function times r okay. Now, this is the pure continuum. Now, we do not have the pure continuum. What we have is a configuration interaction between a discrete and the continuum.

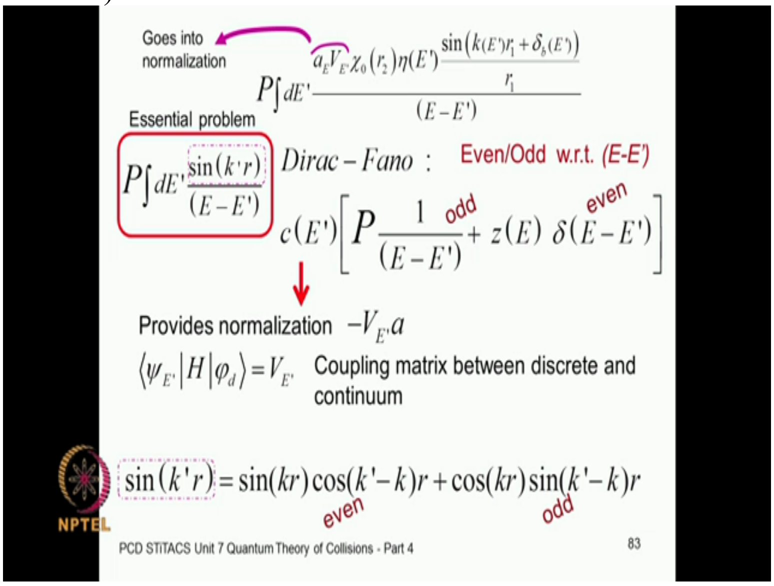
So, now, when you have a superposition of a discrete and continuum, then, the regular part alone will not be able to give you the full wave function. You will need an admixture of the irregular part. So, the solution will be some sort of a linear combination of a sinusoidal and a cosine function. And whenever you have such possibilities, then, you invariably have a phase shift resulting from this, okay.

Which we have seen n number of times in our analysis of Collision Physics, so, this will generate an additional phase shift and this is coming from the interaction between the discrete and the continuum and this is the configuration interaction. So, this results in an additional phase shift so that is what we are going to focus on a discussion on today.

You can also have additional terms in the potential. For example, in more complex forms of the potential, when you take more realistic potentials, many electron system then you know that the s04 symmetry of the Hydrogen atom is broken inside, you know, close to the core. You have got a very complex form of the potential. The potential is no longer 1 over r over the entire region of space.

What one often does in other formalisms like Quantum Defect Theory which is to partition the space in a short-range region and a long-range region. When you do that, you can separate the total phase shift in a short-range part and a long-range part. When you do that again, you will have such a separation which is possible. And you will have additional phase shifts, which result from that.

(Refer Slide Time: 11:35)



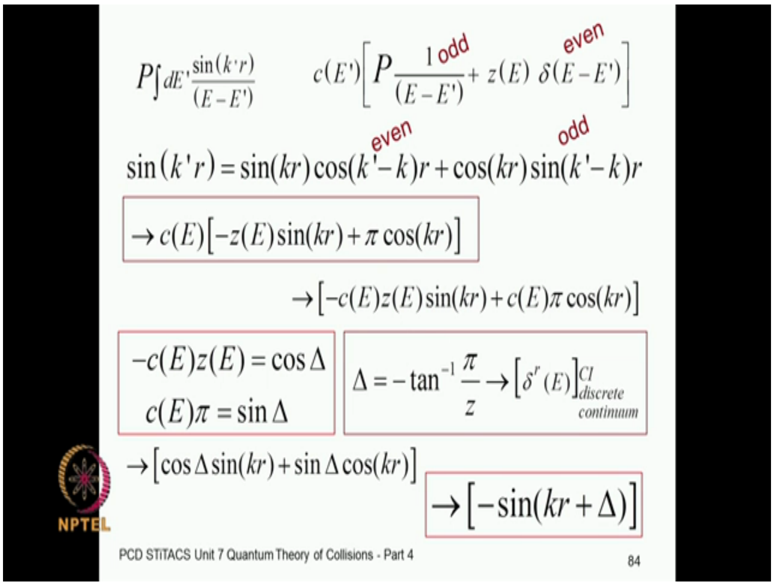
So, our interest is in handling this particular integral. Out of which, this part will go into the normalization, right. As you can see, this is scaling this wave function. And the essential problem is in the evaluation of this integral other than the normalization part which goes into the integration of this function sine over the energy difference, okay. That is the main integral that we have to solve.

And we already know that these integrals can be solved using the Dirac Fano procedure. So, you insert this, prescription which we have used in our discussion, in our previous class. And here, this cE prime has been appended so that it will take care of this normalization, aEV which is coming here, okay. That is, this additional normalization, this one is already there in the other normalization of the scattering solution.

So, this is contained in cE prime, okay. So, now, this normalization has got VE, which is nothing but the coupling matrix between the discrete and the continuum as I have pointed out. Now, this function over here has got two terms: odd and even. So, you can take two other terms like, if you can write your sinusoidal function.

This one in terms of cosine k prime - k and sinek prime - k and this is just a trigonometric identity that you exploit. So, you have got a correspondence from which you can determine the phase shift in terms of the z and c okay. So, that is the trick. That is the essential trick. The rest of it is, just plugging in and evaluating the integrals which are of straightforward procedure.

(Refer Slide Time: 13:38)

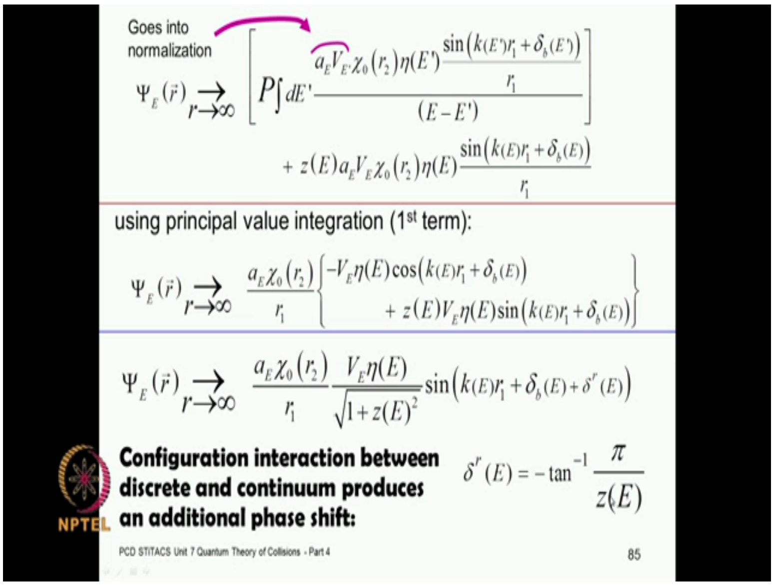


So, using this, you now get, so, this is the expression for the sinusoidal function, in terms of this trigonometric identity. And now the solution is now just a superposition of this sine and cosine and this is this integral is easily solved. The solutions will give you zE and pi factor, okay. And I have just moved this cE inside this, so that I have got cE, zE and sine kr + cE pi times, cosine kr.

And you can see an additional phase shift popping out of this. And you can get it if you introduce this angle delta, this triangular delta as, as I have used. And if you introduce this delta as tan inverse, as negative tan inverse of pi over z, you can write this function as a sinusoidal function with a phase shift.

So, this is the additional phase shift which is resulting from the configuration interaction. Now, this is what we have been expecting that the configuration interaction will essentially generate an additional phase shift. So, that is this delta.

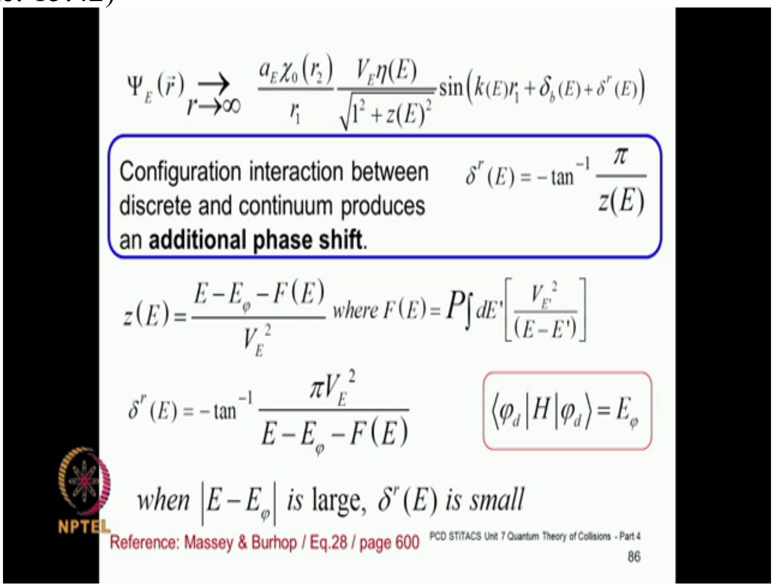
(Refer Slide Time: 14:58)



And the actual function that we wanted to work with was this. So, we used the simple analysis from Rau's paper. So, we use that result and put it over here. Get the solution in terms of the cosine and the sine functions. Get the corresponding phase shift which is nothing but the same, exactly the same expression which is negative of tan inverse pi over z, okay, z we have determined earlier from the boundary condition.

So, this is what the configuration interaction does which is to generate an additional phase shift. So, the configuration interaction results in an additional phase shift which is negative of tan inverse pi over Z.

(Refer Slide Time: 15:42)

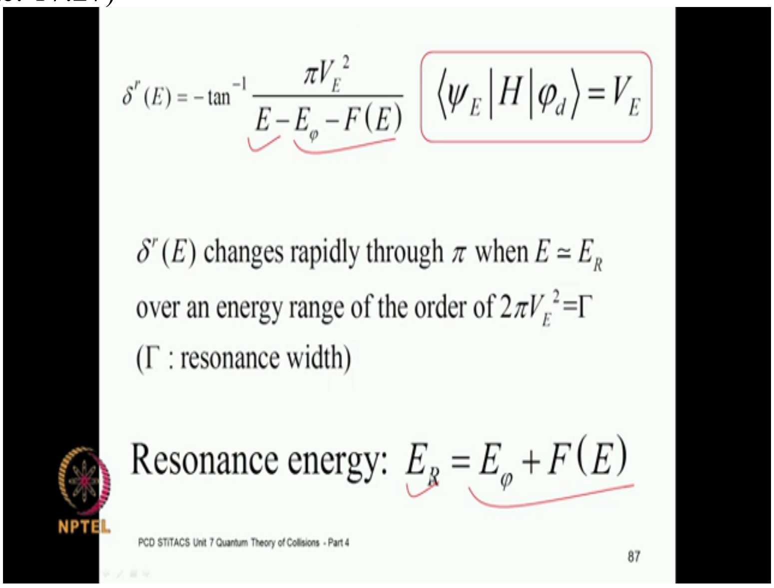


So, this is the additional phase shift and your complete wave function now has got this one. So, we have got the complete solution now, okay. So, the background phase shift was already there. The kr term is always there, right. We are dealing in this case the, we dealt with l = 0 state. So, there is no lpi by 2 phase should. But, otherwise that would also be there. So, in more general forms of the solution, you will see some additional terms.

And then you have got this resonance part. This is coming from the resonant, autoionization, resonant part of the interaction. So, this is the additional phase shift, z we have already introduced earlier, so this is just to summarize the essential results, okay. And notice that you have got the difference between the energy and E phi where E phi is the contribution to the energy matrix from the discrete states, okay. Phi d is the discrete state.

So, the farther E is from E Phi, okay. The lesser the contribution you would expect, as is natural to see, okay. Because if the discrete state is not close enough to the actual resonance processes, the continuum energy is not close enough to the resonant process then, the resident part of the phase shift will become small, ok. So, if E - E Phi is large, the resonant part of the phase shift will become small, alright.

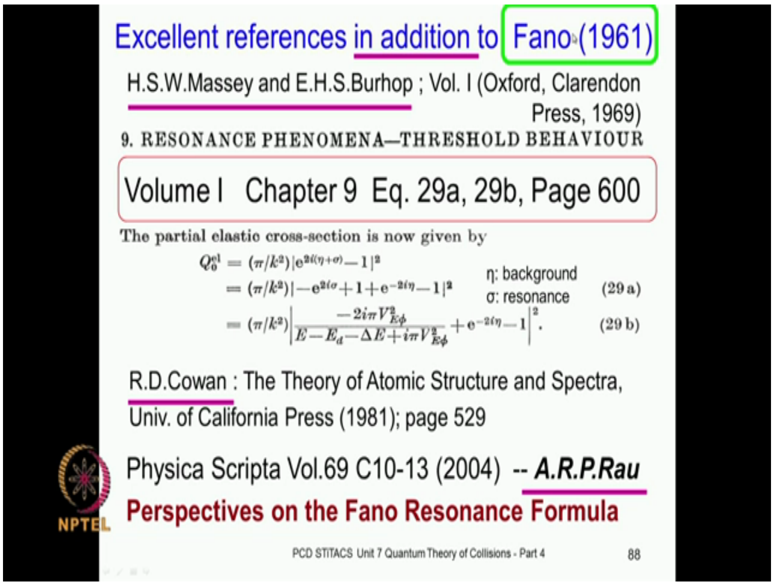
(Refer Slide Time: 17:27)



So, what happens is that, over this width gamma which is, which goes as V square over this width, the resonance part of the phase shift however changes rapidly and it goes through pi, as we have discussed in our previous classes. So, the resonance energy as you see is when this denominator would vanish. So, this is when ER would become EPhi + FE so that becomes the resonant energy.

So, the resonance energy is not necessarily the energy at which the cross-section is maximum or minimum. The criterion for the resonance energy is this. It is it relates to the phase shift and not to the cross section. Cross section and everything else comes as a consequence of that.

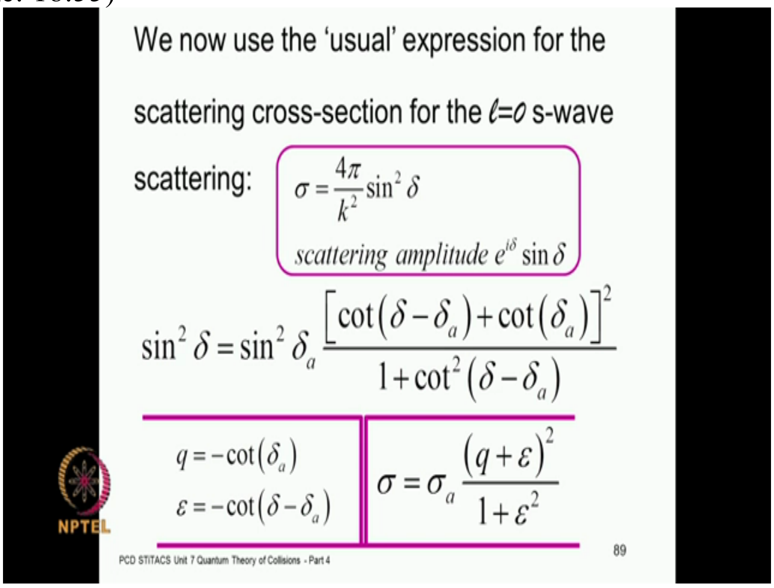
(Refer Slide Time: 18:15)



So, I would like to highlight some important references in this context in addition to Fano's original 1961 paper in which many things have worked out in the appendix of the paper. Massey and Burhop is an excellent source which is chapter 9 in their book which is volume 1 of this, the Carbon's book I have referred to, I have included that reference.

In this paper by Professor Rau, which I cited just a little while ago, so, these are excellent sources for a discussion on this point.

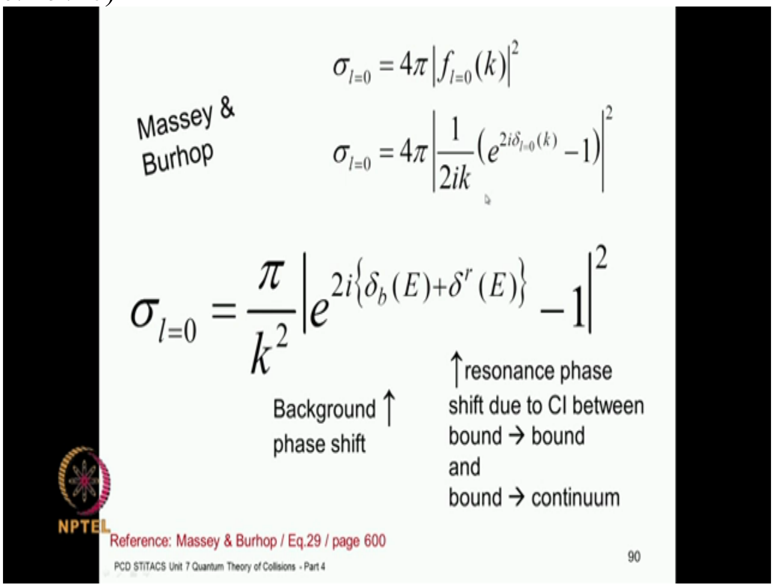
(Refer Slide Time: 18:55)



Professor Rau also points out some very nice things which I am nice to visit. That if you look at the usual expression for the scattering cross section, in terms of the sine squared delta, okay, this is the usual expression. You can use a simple trick to write this sine square delta, in terms of these two co-tangents of two different angles delta - delta a and co-tangent of delta a. So, this is just a trigonometric identity.

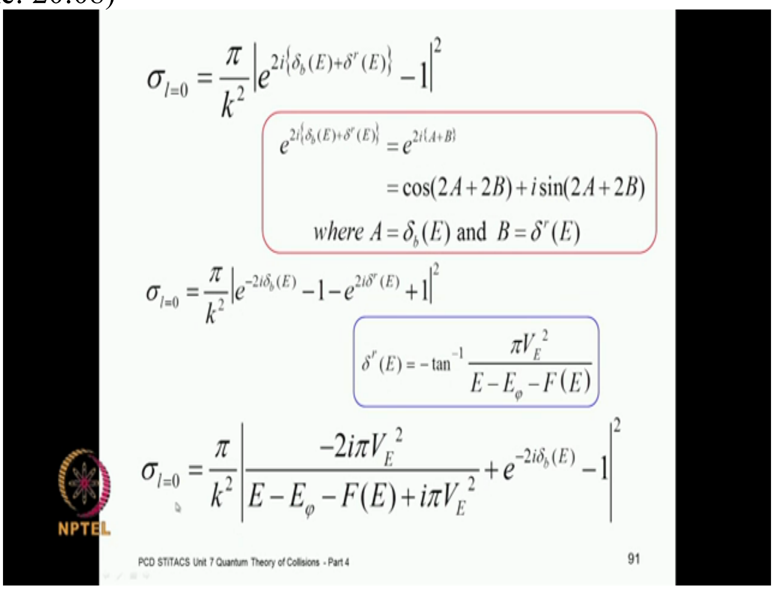
And Massey and Burhop also do a similar thing but in a slightly different way. And using this you can immediately see them relate to the Fano parameters q in epsilon. So, they come so neatly out of this okay, so there are some very nice things which you find in Rau's literature and also it Massey and Burhop.

(Refer Slide Time: 19:46)



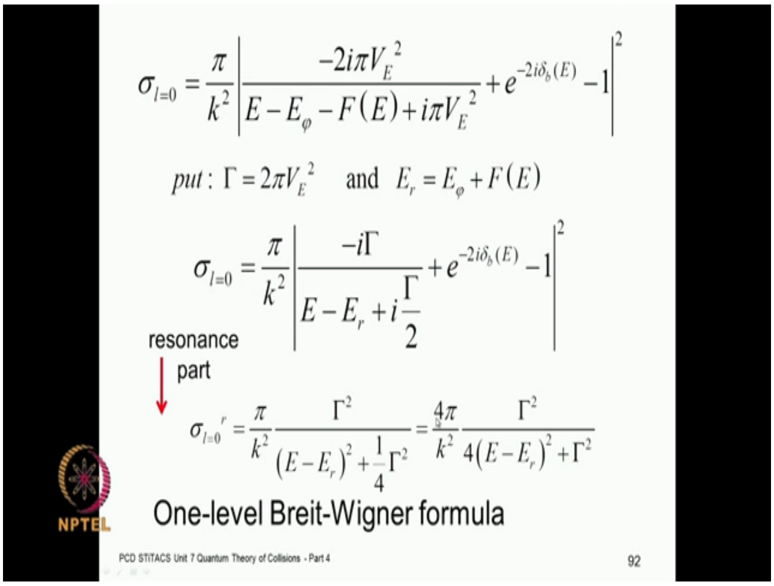
But Massey and Burhop do it in a slightly different way. I will show you how they do it. So, they go; it is essentially the same idea. So, they go back to this expression in terms of the Modulus Square of the Scattering Amplitude. And then, break up the phase shift into the background part and the resonant part, okay as we are quite familiar with already.

(Refer Slide Time: 20:08)



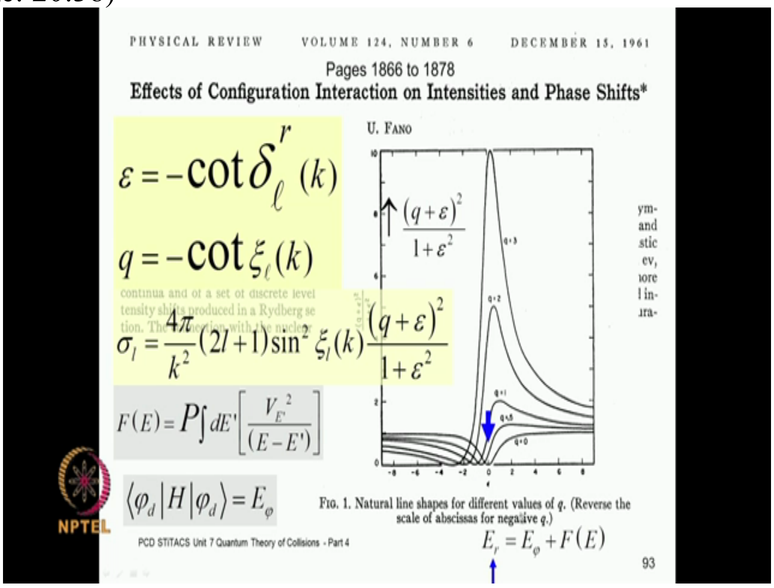
And then, you, they use certain trigonometric identities in terms of, which they write the scattering cross section, this is after doing a little bit of trigonometric manipulation.

(Refer Slide Time: 20:23)



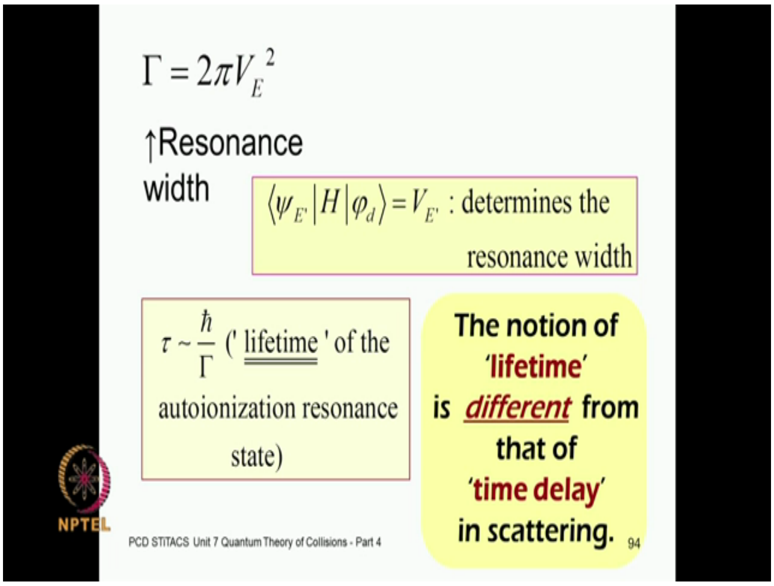
And then, what they find is, that if you ignore the background contribution, you get essentially the Breit-Wigner formula which we have already seen, how it relates to the Fano parameters q in epilson, okay.

(Refer Slide Time: 20:38)



So, these are certain profiles that you get for the scattering cross section. And the scattering cross section actually comes in all kinds of shapes, okay. So, these are the different profiles, naturalized shapes for different values of the q parameter of the Fano’s q parameter. You can get very many different kinds of shapes.And the resonance energy is given by this criterion E Phi + Phi E, as I mentioned earlier.

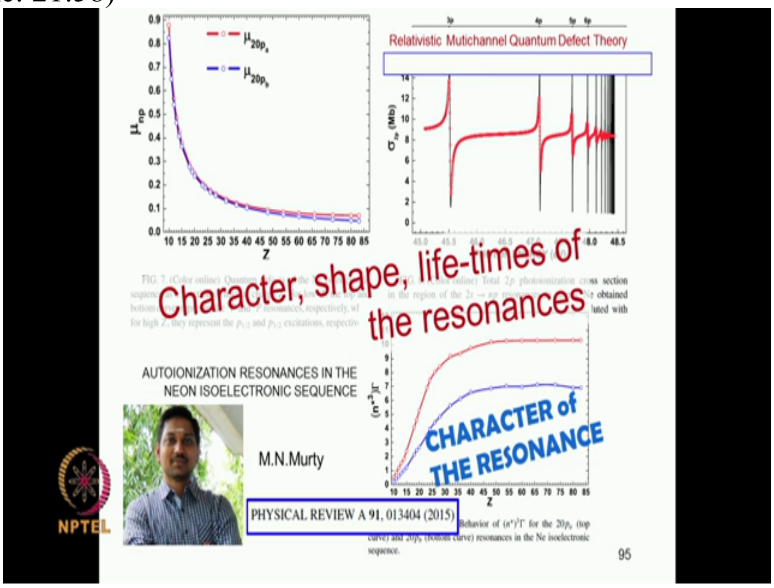
(Refer Slide Time: 21:12)



This is the resonance width, this is the width over which the phase shift changes rapidly through pi. The width is determined by the energy matrix contribution coming from the interaction between the discrete and the continuum. So, that is what determines the width of the resonance.

Lifetime is just the inverse of this width, okay. And one must remember that the idea of lifetime is quite different from the idea of what is called as time delay in scattering, okay. So, I will spend some time discussing the time delay in scattering.

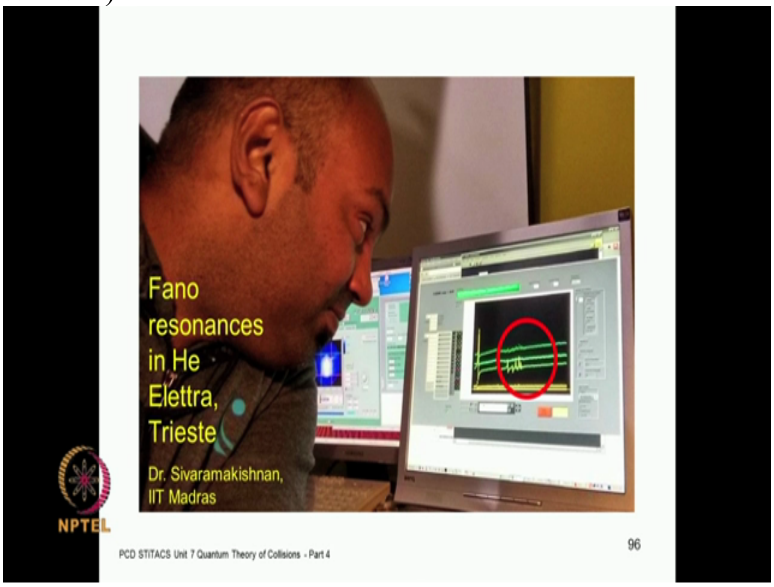
(Refer Slide Time: 21:58)



So, before I do that I would like to show that some of these ideas are of immediate interest, for the analysis of autoionization resonances in a very such group. So, these are, Murthy's results and what there are other additional complexities because we have just dealt with the lifetimes and so on.

But then, what about the character of the resonances and so on; there are many additional complex questions which come up. And those are left for those of you who will reach original literature and move ahead. But these have immediate interest in several research problems.

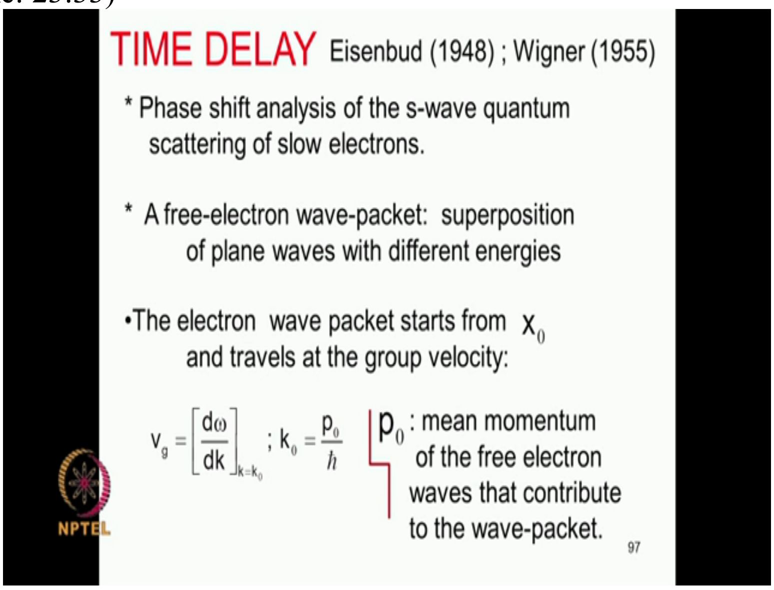
(Refer Slide Time: 22:45)



Here is a figure of Fano resonances Siva's result. So, thank you very much about for lending me in this picture. Siva also told me that the quality of this signal is considered as a measure of how good the set up is. So, the, next generation of the synchrotron is identified by the quality of the spectrum.

So, the Helium spectrum is still used in, in characterizing and in calibrating in particular, all the calibration procedures. So, these are very exciting things and we have people over here to work with these things. So, it is nice to have you all in the audience.

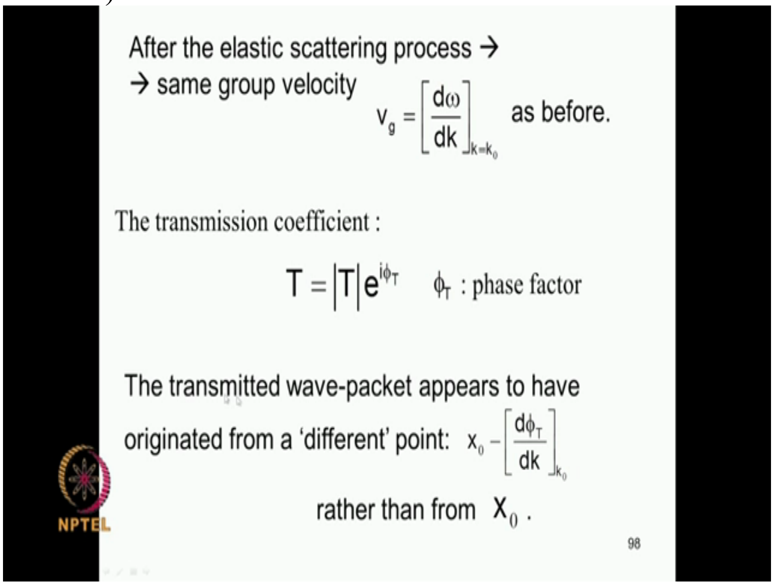
(Refer Slide Time: 23:33)



And I will now come to this time delay in scattering which is an idea, which is different from lifetimes, as I mentioned. And this comes from the analysis of Eisenbud and Wigner. And the original analysis came in the context of phase shift analysis of s-wave scattering, at low energies. So, typically if you have a free electron wave packet, okay, it is a superposition of a number of plane waves. And this wave packet travels at a certain group velocity.

But that group velocity is d omega by dk, as we know from, you know our studies of wave packets. There is a certain mean momentum, okay, which I represent by p0 corresponding to which bottom wave vector k0.

(Refer Slide Time: 24:28)



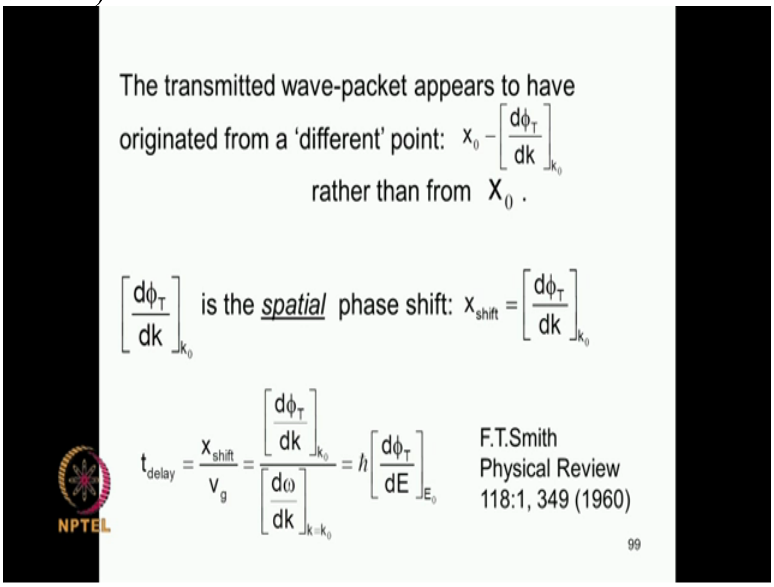
And what happens after the scattering if this wave packet meets an interaction potential, it continues to propagate, it continues to propagate and the same great velocity, the group velocity does not change. There is, it is transmitted through the barrier. So, let us think of a simple one-dimensional case, it goes through that.

But then it spends a little bit of time in the interaction region so that the transmission coefficient will be complex. And there will be a phase delay coming as a result of that. So, Phi is a phase factor and the transmitted wave packet, because of this phase factor, it would appear whenever there is a phase lag, okay.

What is the phase lag represent? It says that, okay if a wave front was to arrive at a certain time, it is arriving either sooner or later. So, there is a phase shift, right? And that means that as if it has originated from a different point of space, that if it were to have originated from a certain source point, if it is arriving earlier, it would appear as if it has arrived from a point, source is not here, but closer.

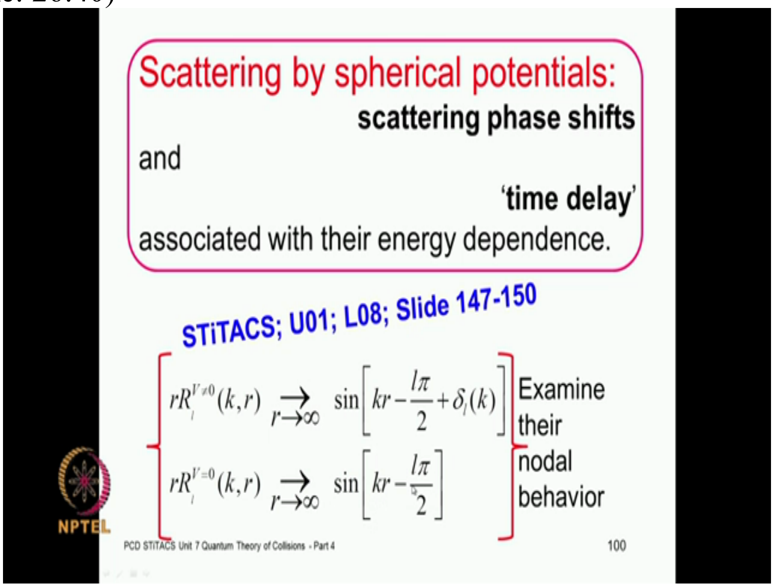
If it is later, it is like coming from a further distance. So there is a spatial phase shift associated with this. And this phase shift it, it would appear as if it is coming from a different point which is d Phi by dk, okay, rather than from x0.

(Refer Slide time: 26:11)



So, then d phi by dk, then, is the spatial phase shift. And if you divide this by the group velocity, you will get the time delay, right. So, the time delay is nothing but this spatial phase shift divided by the group velocity and you can immediately see that this is nothing but the energy derivative of the phase shift. So, this is the time delay in scattering Theory.

(Refer Slide Time: 26:40)

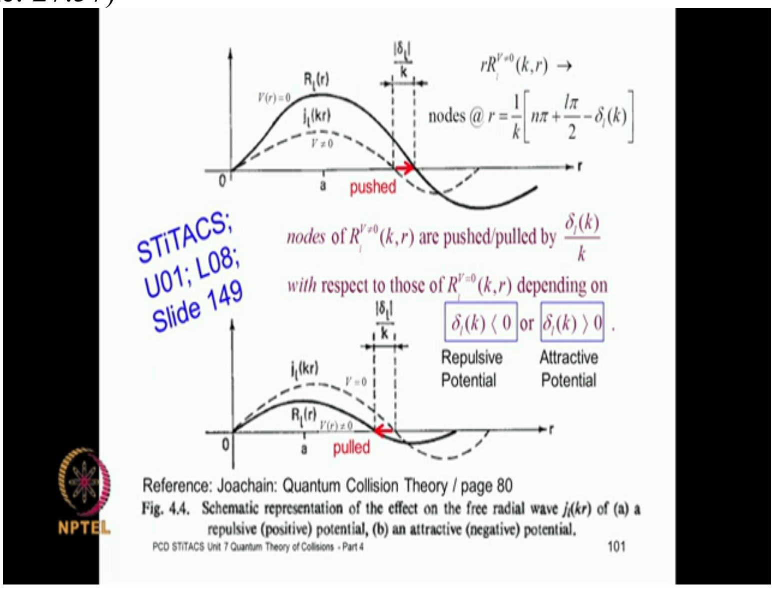


Our interest of course, is scattering in by spherical potentials. And we are in a position to discuss this at some length because we have dealt with this in an earlier unit in considerable detail. And in particular, I will like to draw your attention to the lecture number 8, in unit 1 of this course, okay. And there is a discussion on slide 147 through 150 where you will find these details and you have already been through this.

But let me remind you some of the immediate results which are of interest to us. What we discussed at that point is: that the radial function, if there is a zero potential. So it is like a free particle which is propagating, its solution will go as a sinusoidal function, apart from the angular momentum phase shift, lpi by 2; whereas when you have a potential, there is a phase shift resulting from the scattering potential, right.

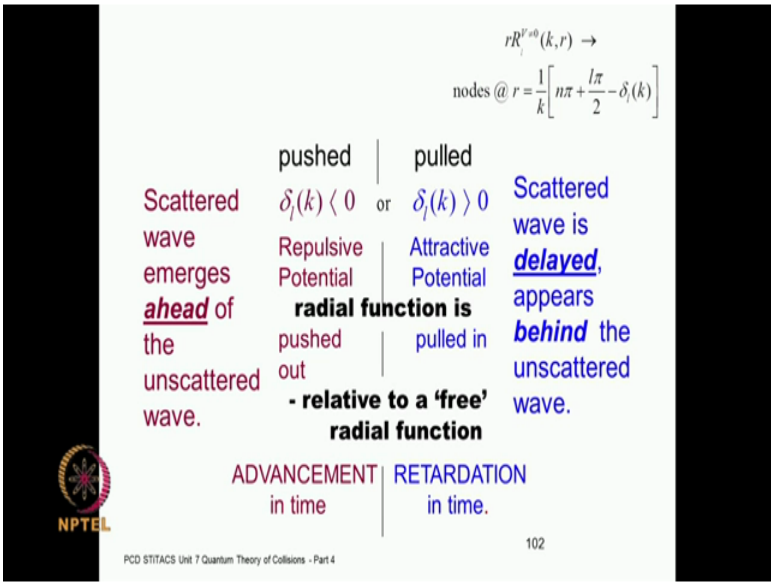
What it does is it changes the positions of the nodes, because the node will come wherever the sinusoidal function goes to zero and the argument of the sinusoidal function being different the position of the nodes is shifted, okay.

(Refer Slide Time: 27:57)



So, we had drawn these pictures from Joechain's book okay and we discuss these solutions that the nodes are either pushed or pulled depending on the potential being either repulsive or attractive. And accordingly, you get a negative phase shift or a positive shift, positive phase shift, ok. So, these details are there in Joechain's book. We discuss them in unit 1.

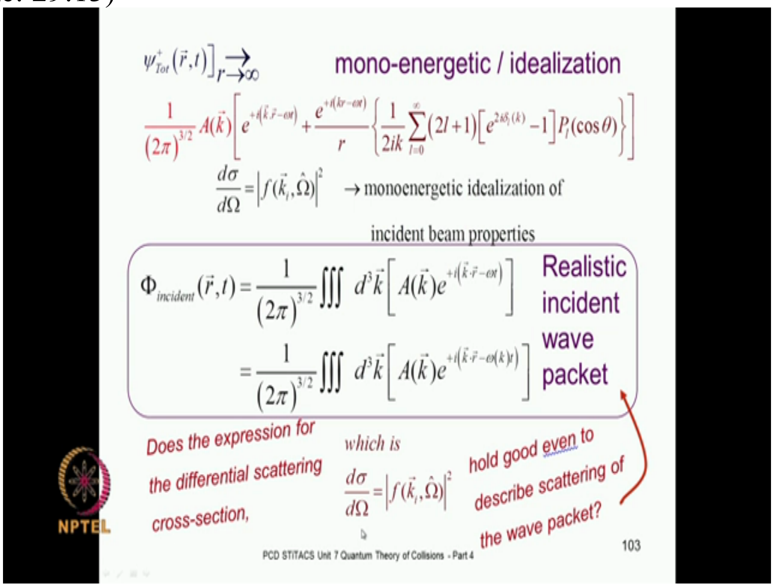
(Refer Slide Time: 28:32)



And this is what happens that the positions of the nodes are given by, what is the value of this, right? Argument of the sine function; And in this case, when it is pushed, when the radial function is pushed, the scattered wave emerges ahead of the unscattered wave. And the unscattered wave is a free particle wave, right.

So, the scattered wave will come ahead of that whereas in this case, is it is delayed it will come behind the unscattered wave. And that is the time delay. So, time delay will be either positive or negative depending on whether it is pushed up hold, okay. So, there is an advancement of time or a retardation of time which goes according to this.

(Refer Slide Time: 29:13)

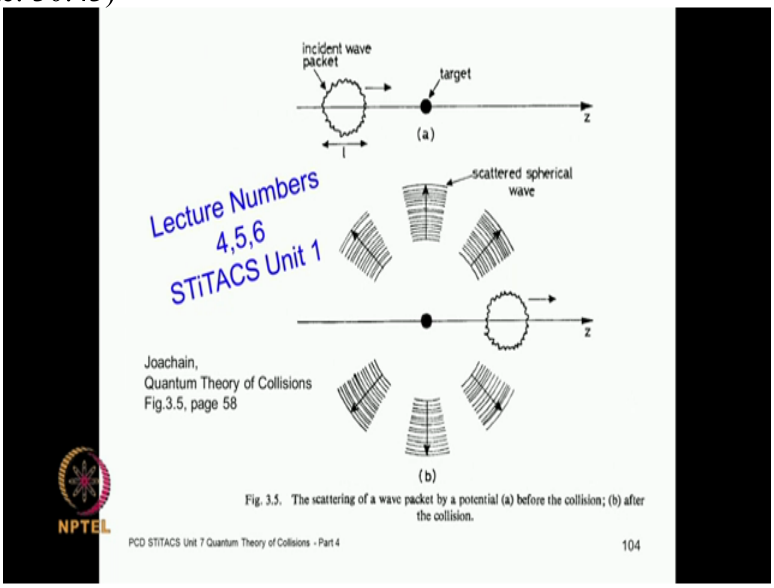


Now, we were very careful about it because we need to treat this as a wave packet, okay; Because the electron is ejected as a wave packet. And we conceded that this particular form of the scattering solution with outgoing wave boundary conditions, okay, inclusive of the time factor. This is written for a strictly mono energetic beam which is an idealization whereas the actual particle will be described by a wave packet.

So, this is a realistic incident packet which is a superposition over a number of different momenta, okay. So, this may have a certain narrow range, but whatever, but it is not sharply mono energetic. So, you have a realistic incident wave packet and we had asked the question if this relation d sigma by d omega being given by the modular square of the scattering amplitude.

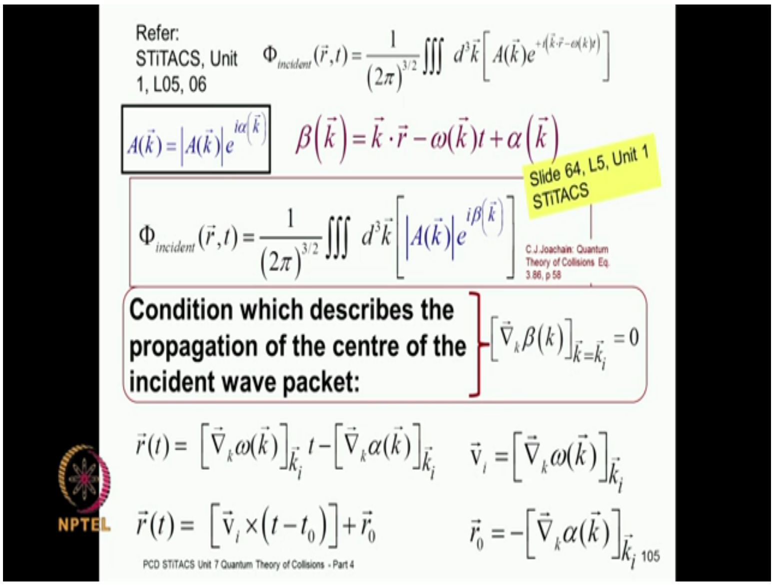
Does it work also for a realistic incident wave packet, when it is described by a superposition of a number of mono energetic waves and not just a mono energetic waves. So, some of you will remember this discussion from Unit 1, okay. But otherwise you can refer back to those lectures.

(Refer Slide Time: 30:43)



And this point was discussed over a number of lectures in that unit lecture number 4, 5 and 6 of Unit 1. So, this is just to remind you where to look back for the details.

(Refer Slide Time: 30:58)

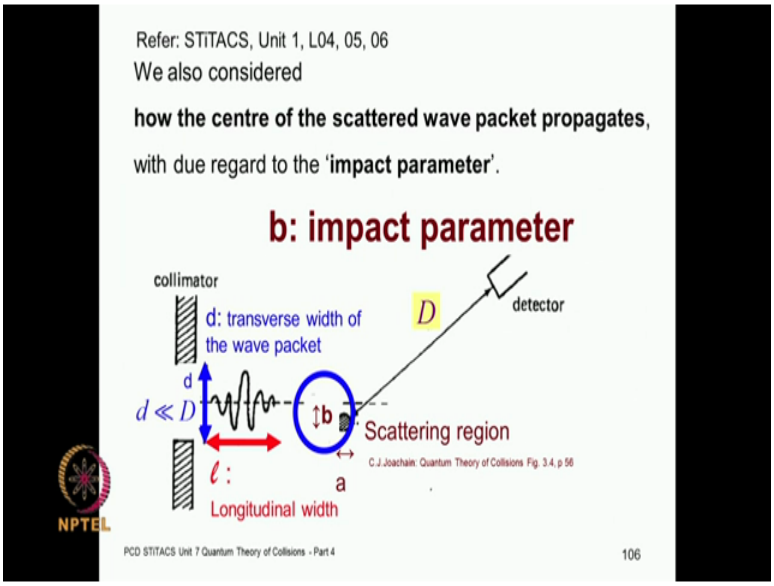


And here if you look at this incident beam, it has got this complex amplitude for each monochromatic wave. So, this e to the i alpha k phase gets added up to this phase so you get a net phase of this function which is given by e to the i beta k. And if beta were to change rapidly with k, okay, there would be so many oscillations that the incident packet would disappear.

So, the condition that it would not happen so that you have scattering at all is that the gradient of beta would be zero, right. So, that is the condition that we discussed. And when we put this condition, we found that the wave packet moves at a certain group velocity which is given by this gradient of Omega with respect to k as we always find, right.

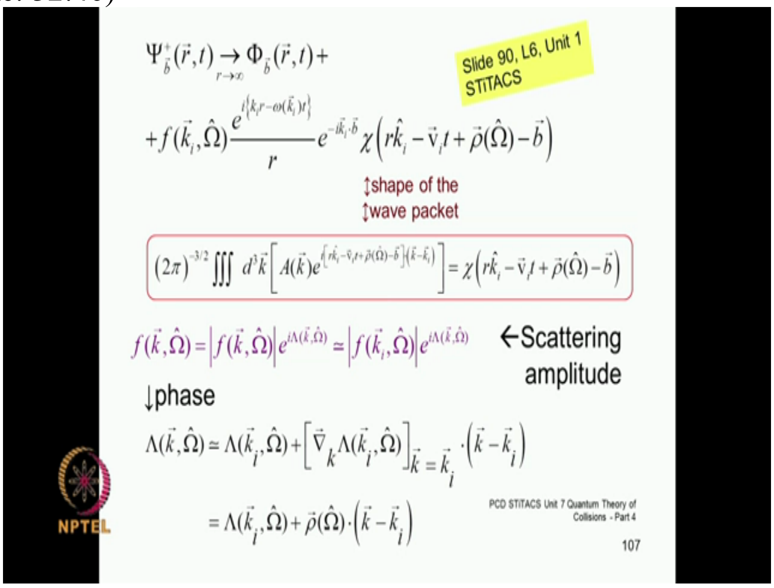
So, this is the relation that we get. And you can write it in terms of, you know, like a kinematic equation r equal to Vt + r0 like in Undergraduate Mechanics courses, right. So, where the velocity is given by this gradient of omega with respect, okay. So, you see that similar relations as we dealt with in the one-dimensional case are present over here as well. So, we get essentially the same kind of consequence.

(Refer Slide Time: 32:31)



We also considered the incident wave packet to come not head-on or the target, but if it is slightly displaced through an impact parameter. And when we consider this.

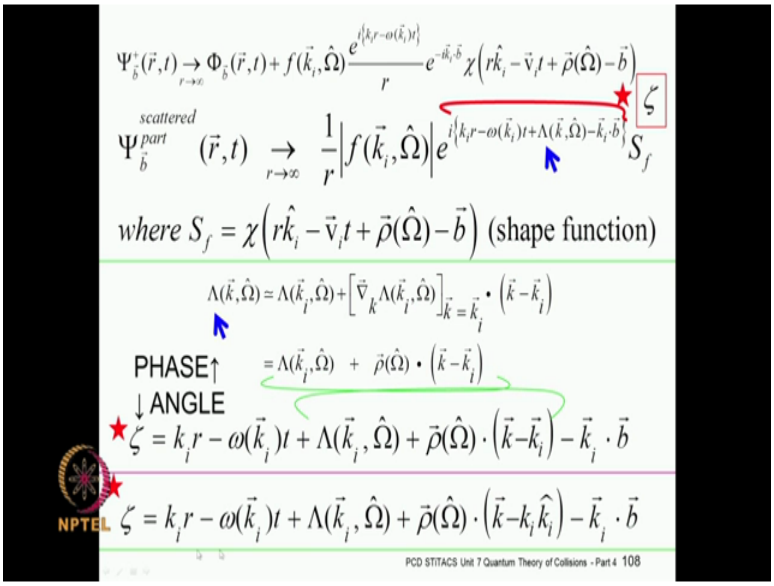
(Refer Slide Time: 32:46)



We found that we can still write the scattering solution in the same form except that we now have an additional function which describes the shape of the wave packet, right. And we found that the scattering amplitude is given by its modulus and a phase factor. And this phase is no longer just the phase of the mean momentum, wave packet with a mean momentum.

sBut you have to expand it around it in a Taylor series, okay. So, you have got the leading term plus the first derivative times the difference of the momentum vectors. So, this is what this gradient of the phase with respect to k is what is written by the by Rho. This is, I am following the notation from Joechain's book, Quantum Collision Theory.

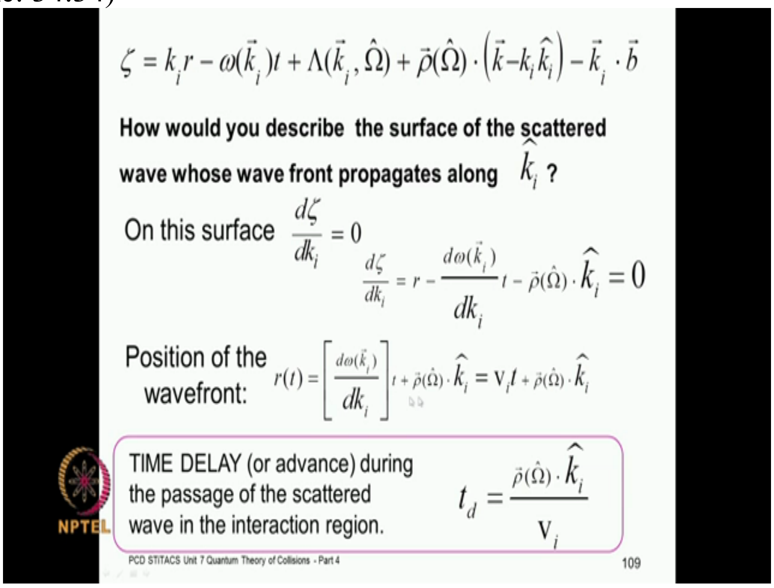
(Refer Slide Time: 33:41)



And now you have got this phase which has been written, which has been expanded about this mean momentum, the phase for the mean momentum; the net phase is this, this is the total phase, right. So, this is the total phase which I call as Zeta and this is the net phase angle of which these this part is given by these two terms; or come they come over here. And over here I simply separate the magnitude of ki from the direction of ki.

So, the last equation is nothing but the one prior to that except for the difference that I have separated the magnitude from the direction of this ki.

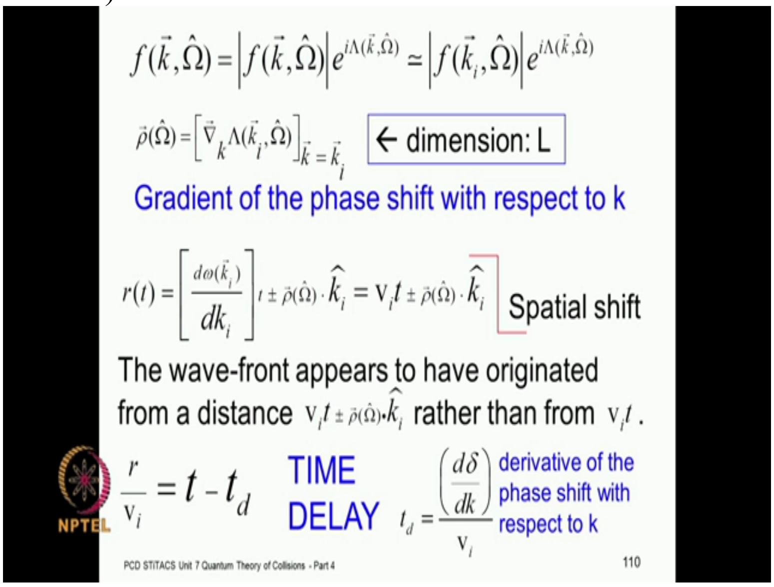
(Refer Slide Time: 34:34)



And I do it for a reason because now you have this as the phase angle and you can ask the question, how would you describe the surface of the scattered wave which is propagating along this particular unit vector, okay? And on the surface you would expect that d Zeta by dk must vanish because that is the criterion for having a surface of constant phase. So, this must be the criterion. So, you can put dPsi by dk = 0. What does it give you?

You just take the derivative of this term with respect to k, put it equal to 0; you get an equation. Again the same kind of kinematic equation and you find that there is a spatial phase shift; you divide the spatial phase shift by the group velocity; you get the time delay, okay. So, this is the time delay and it can also be a time advance, of course. Depending on whether the potential is attractive and repulsive, so this is the time delay in scattering.

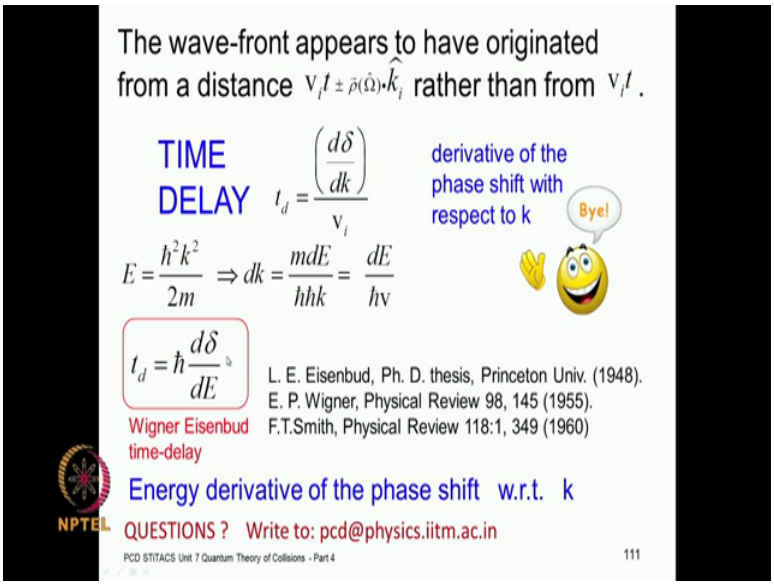
(Refer Slide Time: 35:33)



So, this is essentially coming from the gradient of the phase with respect to k and what happens is that, the wave-front appears to have originated from a different point rather than what would seem like the origin of the wave front, if it were to be travelling only at Vi velocity, Vi over a time t, starting from the origin.

So, the origin is displaced. So, that is the spatial phase shift and corresponding to this phase shift if you divide by the group velocity you will get the time delay, okay. Because any change in phase will then result in the time delay. So, this is the derivative of the phase shift with respect to k. d delta by dk.

(Refer Slide Time: 36:24)



And now, if you recognize the relation between energy and momentum which is h cross square k square by 2m and write this as, d delta by dk, so, this dk now, you write in terms of dE rather than dk. Then, you immediately find that the time delay is nothing but the energy derivative of the phase shift in units of h cross okay.

So, that is the time delay. And this is, analysis originates in the work of Eisenbud and Wigner. Smith has some nice work on this and with that I conclude today's class. In the next class, I will sum up show some applications of the various topics that we have done and that will pretty much conclude the course. Any question.