Select/Special Topics in
'Theory of Atomic Collisions and Spectroscopy'
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Lecture 01
Introductory Lecture - Course Overview

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Greetings, welcome to this course on theory of atomic collisions and spectroscopy. So, I will make an attempt to provide you with an overview of what to expect in this course and I would like to remind you of something that we would have referred to in one of our earlier courses in atomic physics which is a quote from a very distinguished physicist who ventured to speculate on what would one leave behind for posterity.

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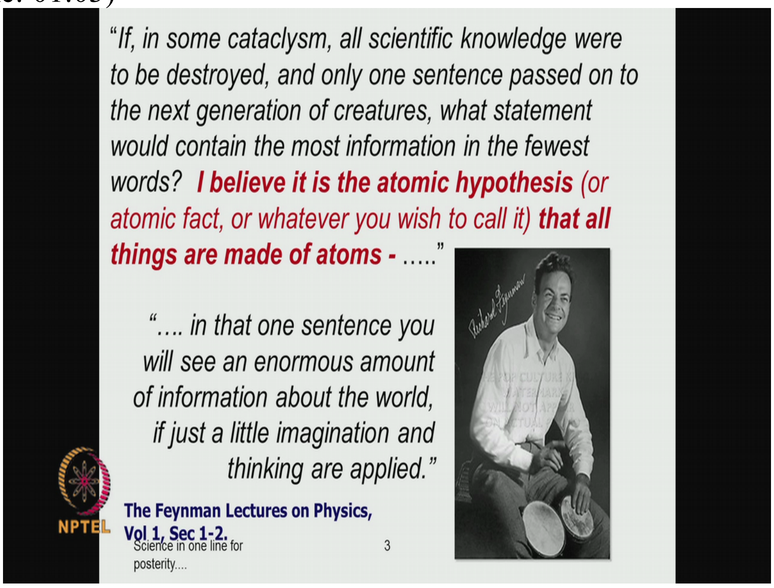

If you could write and describe science and only one line if everything else were to perish, now this almost sounds like a very arrogant attempt as to how could one thing that you can even attempt to do that. But the person who did it was fully qualified to make such an attempt it was none other than Richard Feynman and this is a quote from Feynman lectures and what he says in this is that.

If in some Cataclysm all scientific knowledge were to be destroyed and only one sentence passed on to the next generation of creatures, what statement would contain the most information in the fewest words. Now Feynman goes on to answer this and he says that it is the atomic hypothesis that all things are made of atoms now that is his answer.

And he goes on to clarify that in that one sentence you will see an enormous amount of information about the world if just a little imagination but of course it is not the imagination of an ordinary man it is the imagination of someone like Feynman if you add a little bit of imagination then you know one could extract a lot of science.

Now it is very fascinating to you know speculate on this question why would Feynman choose this particular atomic hypothesis to be the one line in which he could transfer the most information for posterity. And I really do not know what Feynman's reasons were but if we if we sit together and apply our minds then I think one could guess that okay by studying the physics of atoms one could really get a lot of information.

And it does require a little bit of imagination as Feynman say is very neatly in this quote but you could extract quantum mechanics, you could extract relativity out of it, you could extract quantum statistics out of it and so much of the fundamentals of science could come out of atomic physics. Which is what makes this subject so fascinating, so complete and so important.

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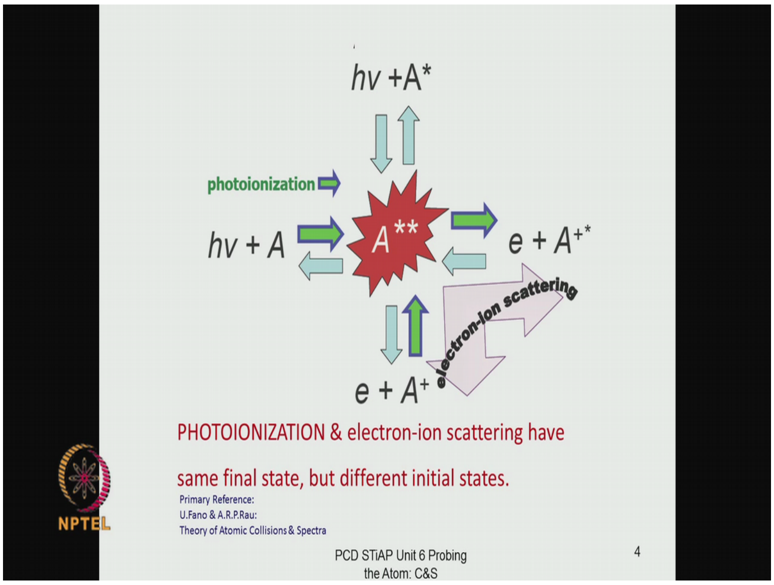

So, having said that I would think that okay it is very important to study atomic physics in one's graduate studies in physics and one could study it in a variety of ways because you have an atom and then you can use certain kinds of probes. And you can either use electromagnetic radiation which is here so h nu is a photon and if A is a neutral atom.

Then you could have a photon atom interaction to probe the atom and see what kind of results you would get or you could also target this using an electron and you can do scattering. This is what typically one would call a scattering and these details I have dealt with in different at a different point of this course and one of the previous courses as well.

So, I am not getting into those details but the point that I want to highlight over here that photon matter interaction and quantum collisions are the two fundamental probes, to probe an atomic system. And the atomic system is then the fundamental thing which is of most importance if we go by Feynman's code.

And this kind of interaction makes the subject of collisions and spectroscopy extremely important. These two processes collisions and spectroscopy when you are probing with electromagnetic radiation you do spectroscopy and these two processes are in fact related to each other through time reversal symmetry. So, I think these are issues of details which I will not get into in this introductory class.

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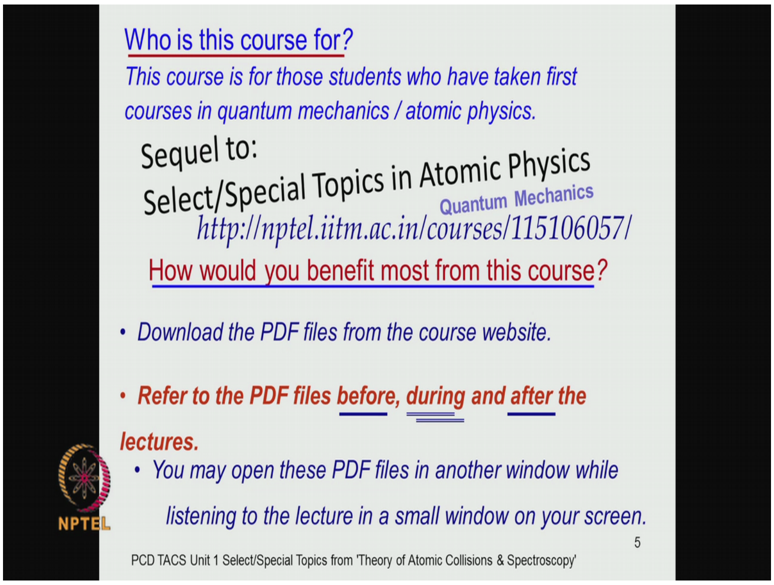

So, let me give you a general overview of this course and first of all I would like to tell you who this course is for and this course is developed as a sequel to another course which I offered for the NPTEL which is on select or special topics in atomic physics. And as such this course can also be considered as the select topics in quantum mechanics.

And this is not surprising because quantum mechanics and atomic physics grew hand in hand in the 20th century. So, all developments and atomic physics and all developments in quantum mechanics and atomic physics went progressed together in the early days of quantum theory.

Which is why an introductory course in atomic physics strongly overlaps with an introductory course in quantum mechanics, so anybody who has taken an introductory course in quantum mechanics or atomic physics is well suited to take this course which we are described, which we are introducing in today's class which is on select or special topics in the theory of atomic collisions and spectroscopy.

Now I would like to point out how to benefit most from this course because I have used PowerPoint slides to discuss various materials. It takes good amount of time to prepare those slides but the advantage is that the corresponding PDF files can be prepared and these are uploaded at the course website.

So, you can download these PDF files and that is the first recommendation I will like to make that download these PDF files from the course website and you can use these PDF files before viewing the video lecture, during the time that you are viewing the lecture or after it, because then all of that material is available.

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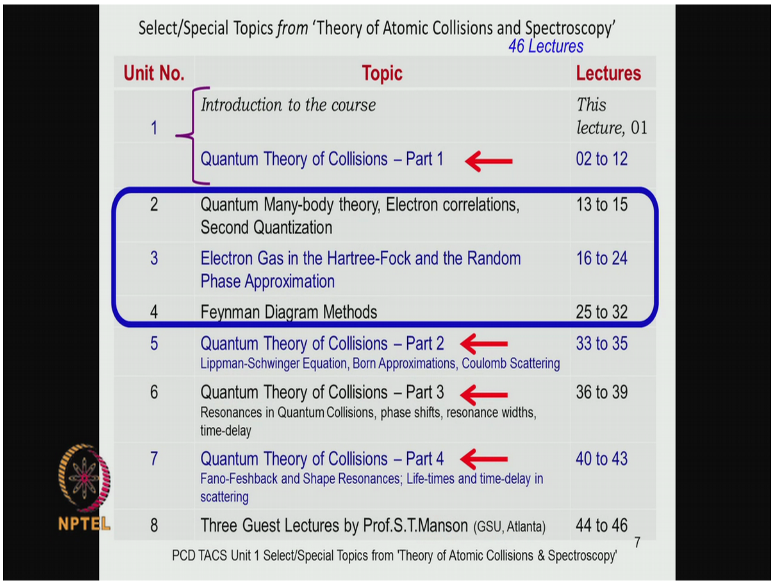
Select/Special Topics *from* 'Theory of Atomic Collisions and Spectroscopy'
46 Lectures

Unit No.	Topic	Lectures
1	*Introduction to the course*	*This lecture, 01*
	Quantum Theory of Collisions – Part 1	02 to 12
2	Quantum Many-body theory, Electron correlations, Second Quantization	13 to 15
3	Electron Gas in the Hartree-Fock and the Random Phase Approximation	16 to 24
4	Feynman Diagram Methods	25 to 32
5	Quantum Theory of Collisions – Part 2 Lippman-Schwinger Equation, Born Approximations, Coulomb Scattering	33 to 35
6	Quantum Theory of Collisions – Part 3 Resonances in Quantum Collisions, phase shifts, resonance widths, time-delay	36 to 39
7	Quantum Theory of Collisions – Part 4 Fano-Feshback and Shape Resonances; Life-times and time-delay in scattering	40 to 43
8	Three Guest Lectures by Prof.S.T.Manson (GSU, Atlanta)	44 to 46

The other advantage is that you do not have to take notes while going listening to the lecture because all the PDF files have got the complete description of the topic and you will have them handy already. So, you can just pay attention on the discussion itself and go through the lectures. So, this course is, there will be 46 lectures in this course including this lecture which is the introductory lecture.

And then we will have a number of units in the first unit I will introduce quantum theory of collisions this will be a second part of what we did in the earlier course in atomic physics. So, some background will be assumed about collision physics. In the second unit we will do quantum many-body theory, discuss second quantization methods so that we can address the subject of electron correlations in many electron systems.

In the third unit we will go beyond the Hartree Fock method because the Hartree Fock which gives you an excellent starting point but then for detailed calculations and detailed analysis of atomic structure and dynamics you need to take into account electron correlations which are excluded in the Hartree Fock formalism. And to be able to do that there are a number of ways of doing it one of the very powerful ways of doing it is the linearization technique.

And this can be done using a variety of ways. One of the formalism is due to Bohm and Pines which is known as a Random Phase Approximation and this name applies to other methods of linearization techniques in this particular context. So we will discuss the Bohm Pines method in unit 3. Then we will also introduce Feynman diagrammatic methods and get into the ring diagrams which correspond to the linearization technique which is also used in Bohm and Pines.

Then we will get back to quantum collisions and do a few problems which are of major importance like the Lippman Schwinger equation, the Born approximation. We will also do the Coulomb Scattering and we will then deal with resonances in quantum collisions. And then we will do a Fano analysis using the final shape parameters of the Fano Fechbach resonances.

We will deal with lifetimes and time delays in scattering and also in the photoemission process. Then we have one unit in which we will have some guest lectures by my long time research collaborator professor S.T. Manson, he has given three lectures which will be appended to this course toward the end.

In which he will show some applications of you know the techniques which have been introduced in this course. So, these this is the general overview of the course. So, now let me give you one specific information that the unit 2, 3 and 4 which is on quantum many-body theory and many electron methods.

So these three units can be done even toward the end of the course, so not necessarily after unit one. So, if you want you can jump from unit 1 to unit 5 and so on okay. When the whole course is ready you could do that but you can do it in any sequence. So, these three form one sort of group and then the other units which have in which I deal with quantum theory of collisions part 1, part 2, part 3 and part 4. They can also be done together in one go.

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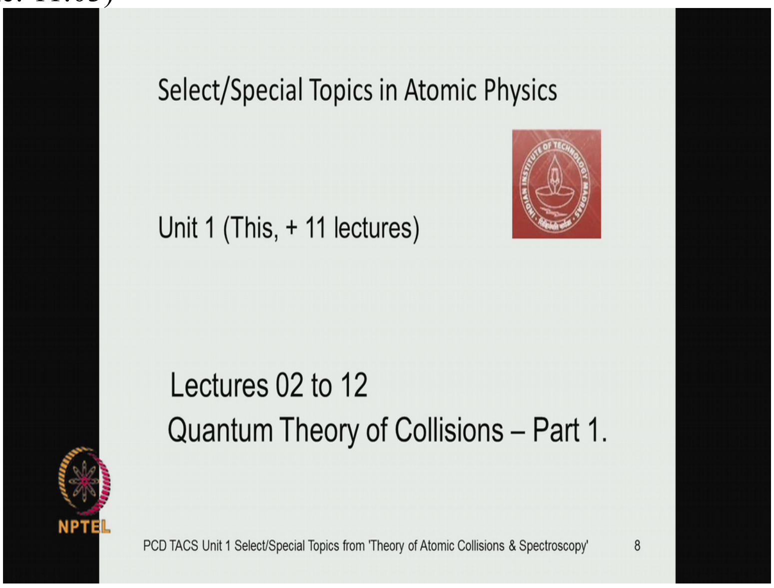

So, in part 1 of the quantum collision theory;

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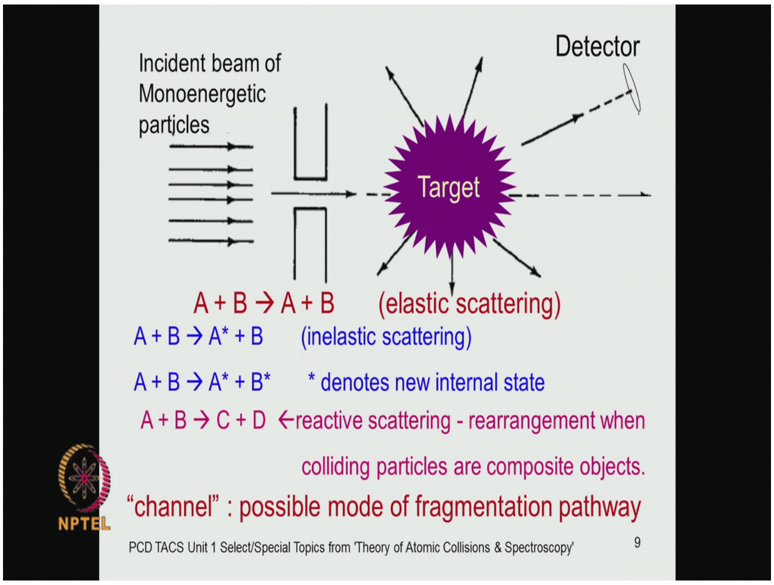

I will basically describe the collision process deal with different kinds of collisions inelastic collisions. Then we will even talk about reactive scattering, inelastic collisions, elastic collisions and so on. And then we will discuss what our collision pathways? What are different collision channels?

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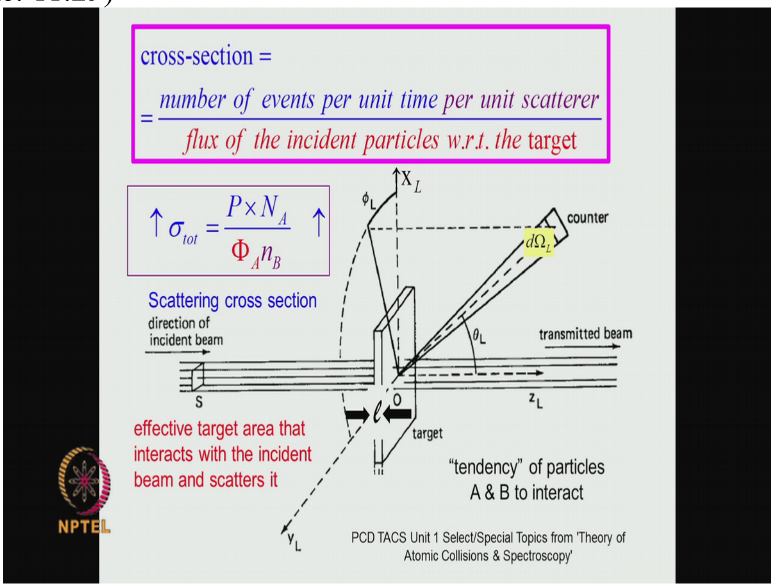

So we will introduce the vocabulary of doing collision physics we will define the cross section carefully as the number of events per unit time per unit scatter. It is the ratio of this to the flux of incident particles with respect to the target. So, starting with the fundamentals of what exactly is a scattering cross section. We will develop the formalism;

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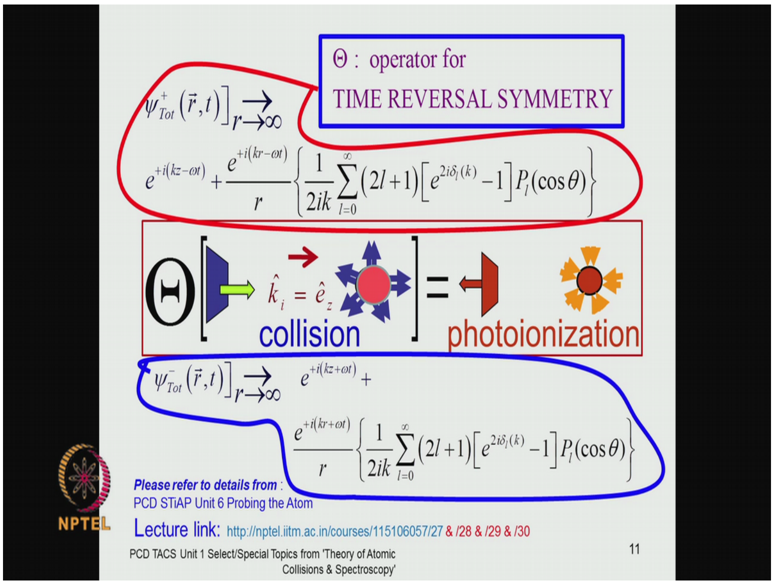

We will refer to this relationship between collisions and photo ionization. Which is through time reversal symmetry we have done this somewhat extensively in the previous course which is also an NPTEL course which is a special topics in atomic physics and this was done in unit 6 of that but we will use some of these results in this course as well. So, we will make use of the relationships between the solutions to the quantum problem for collisions and for photo ionization.

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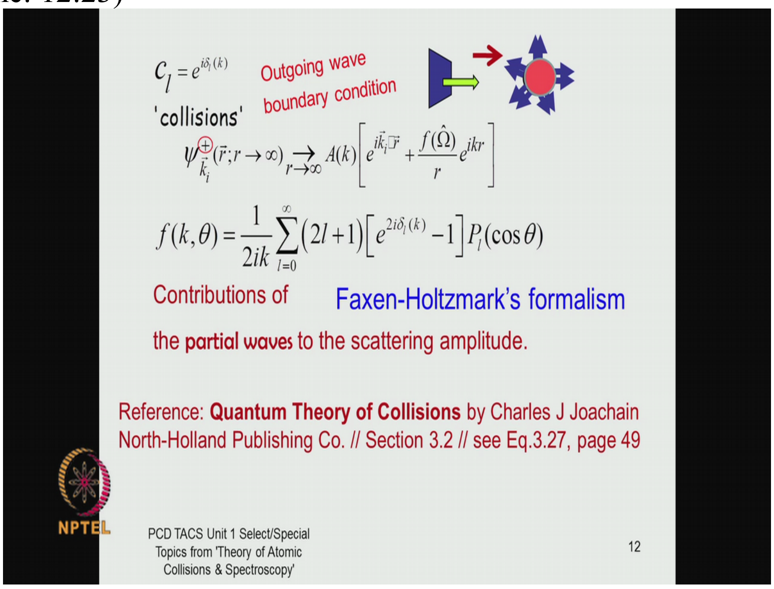

Via the time reversal symmetry and then do formal collision physics without going away boundary conditions so, we will develop the Faxen Holtzmark's mark equation for the scattering amplitude and so on.

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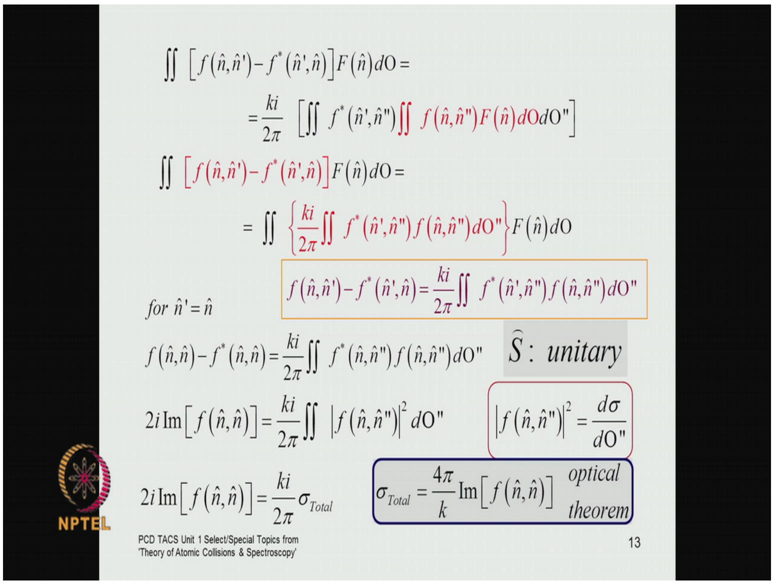

So, we will introduce all of these parameters or phase shifts. We will do the optical theorem; we will discuss the unitarity of the S operator, the sketching operator. And as you see from these slides there are a number of mathematical equations and it would take you some time to take notes which you do not have to.

Because all of this is available in the PDF file which is why I said at the very outset that a good idea to take this course is to download those PDF files at the very beginning and keep them handy you can even have them in one window and listen to the video lecture in another window.

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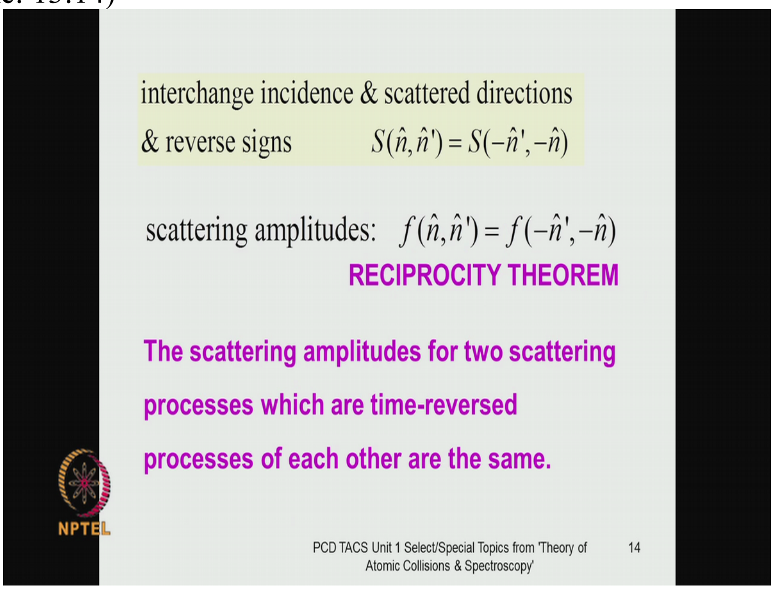

We will also do what is known as the reciprocity theorem. This also reflects on the time reversal symmetry. So, all this will be done in unit 1.

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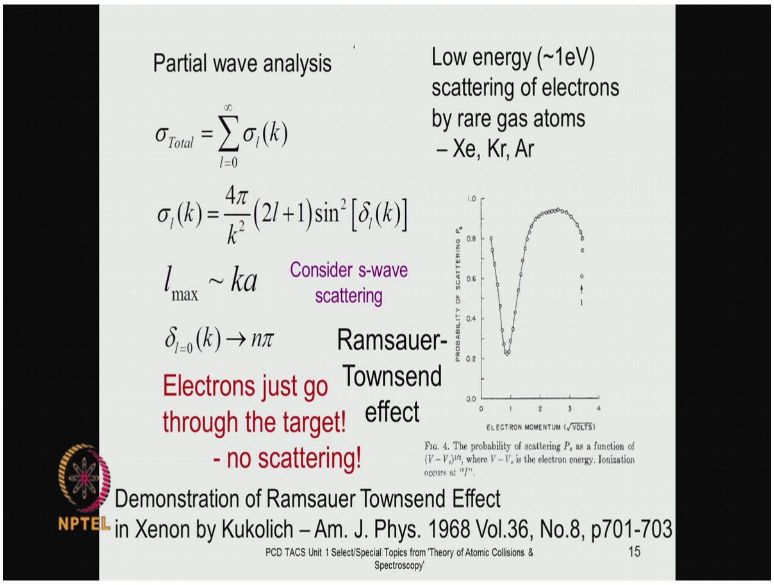

We will deal with some special cases in which you have a target, you have an incident beam of projectiles but if you look at the scattered flux it would appear under certain conditions as if there was no scattering at all. As if the scattering has disappeared as if the target has vanished. And this is what is referred to as the Ramsauer Townsend Effect as to why you have this effect. So, we will look into some detailed aspects of this.

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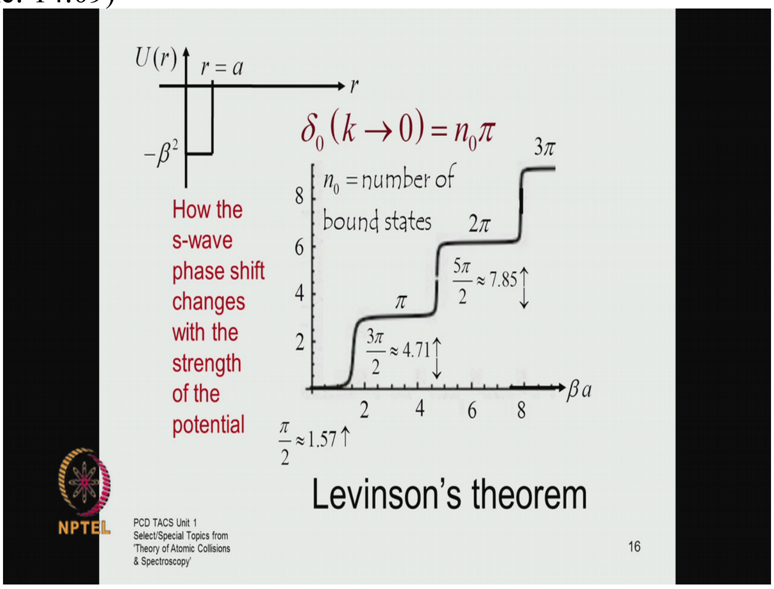

This has closed bearing on also related theorem which is known as the Levinson theorem which we will discuss and it will deal with what is the scattering phase shift at the threshold and how it is related to the number of bound states of an attractive potential because it will have a certain finite number of bound states so that is the question we will address in this.

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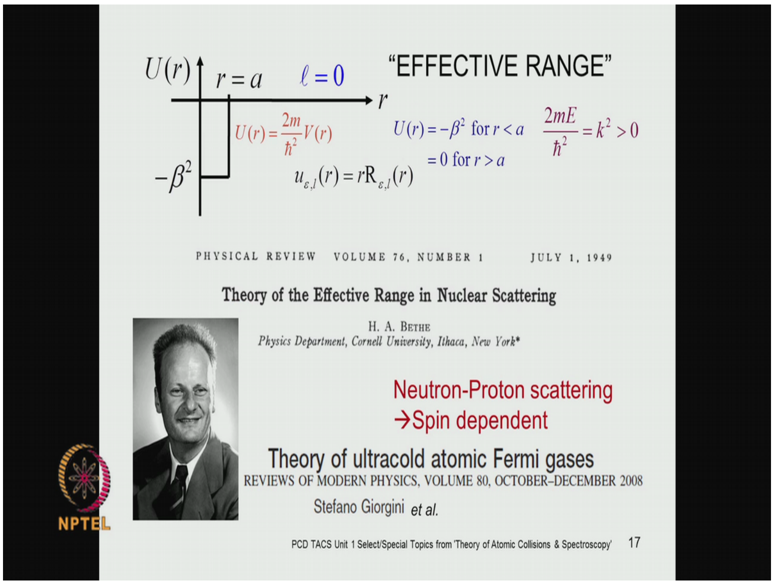

And we will also introduce the effective range theory which was developed by Bethe. It will have some applications and some problems of current interest. In which you will find this to have interesting applications is on cold atoms and Bose Einstein condensation including the condensation of Fermi mixtures.

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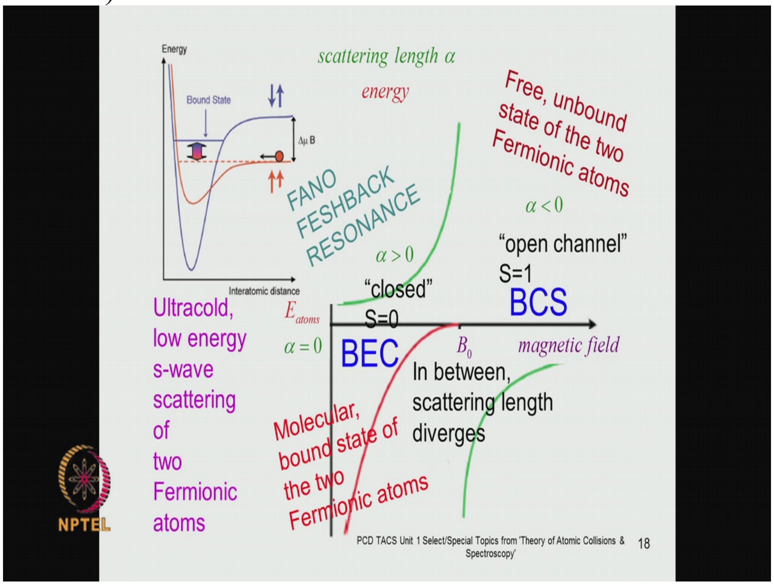

In which you use these techniques and discuss this transformation from a BCE to a BCS state and so on. So some of these are done via and exploiting the physics of the Fano Feshbach Resonances so some of these things will be introduced in this unit.

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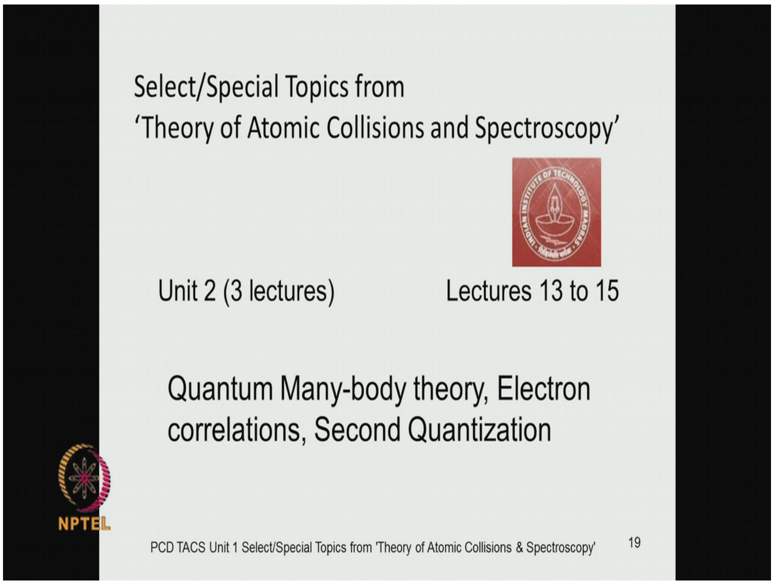

Then we get into the formalism of many electron theories and in particular we will introduce the second quantization method which is a very powerful language to deal with the many electron problems. And it gives you a very nice handle on developing techniques which go beyond the Hartree Fock.

So, the Hartree Fock remains within the domain of the single particle approximation although of course it does deal with the N electron system. But it deals only with the anti-symmetric nature so it takes into account the Fermi Dirac statistics, the Fermi Dirac correlations but not the Coulomb correlation. So, those are the ones which methods of second quantization will help us address.

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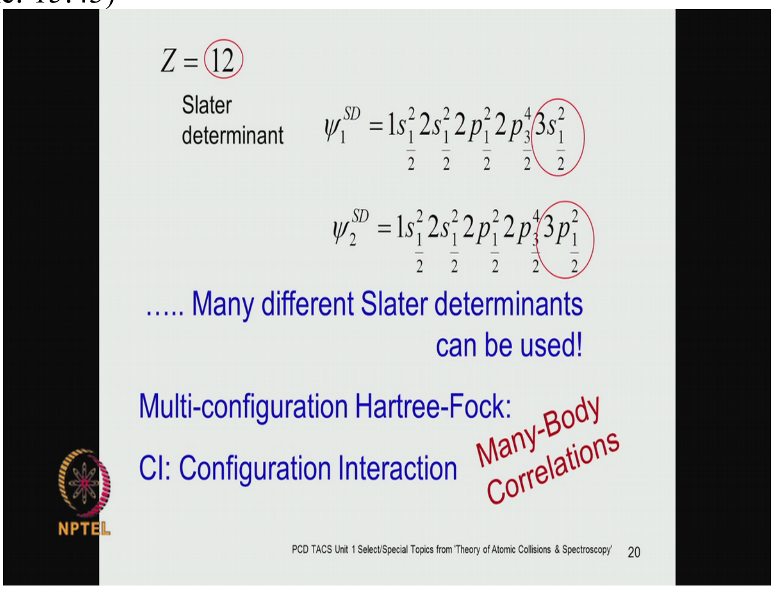

So, we will take up some examples of what a configuration interaction will do so that a single Slater determinant of the Hartree Fock will not be a sufficient description of the N electrons state. You need multi configurational Hartree Fock or multi configuration Dirac Hartree Fock, if you were to be using relativistic wave functions.

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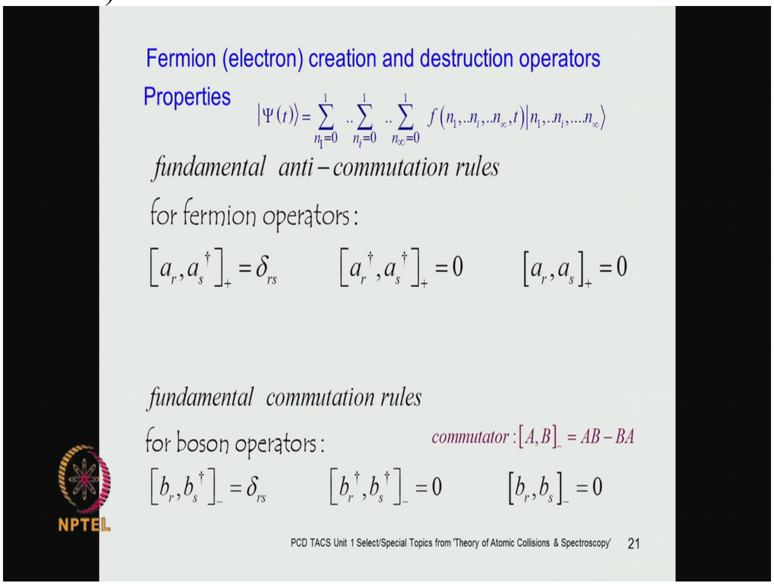

And the second quantization methods give you a very nice handle on addressing such configuration interactions which are involved in electron correlations. So, the second quantization methods, you know the fundamental quantities for these are the Fermion and Boson electron creation and destruction operators. So, the whole formalism is developed in terms of the second quantization operators.

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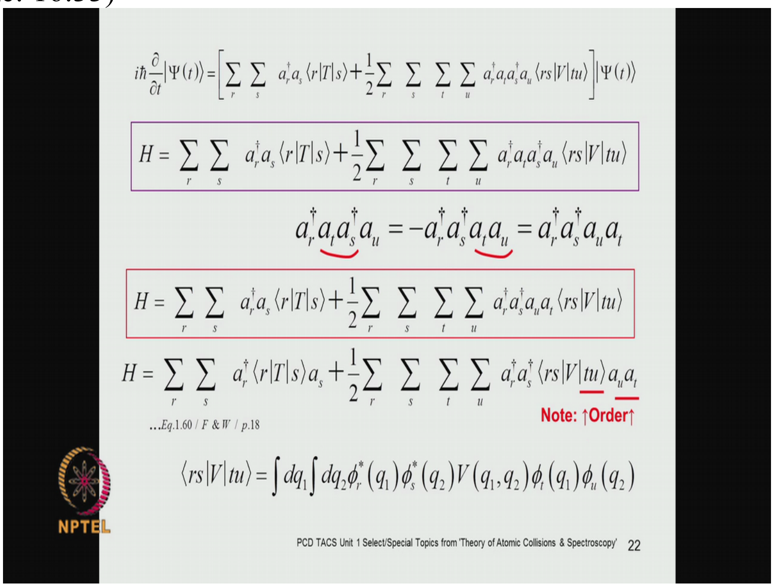

And we will develop a handle on this. We will write the many electrons Hamiltonian in terms of the second quantization operators.

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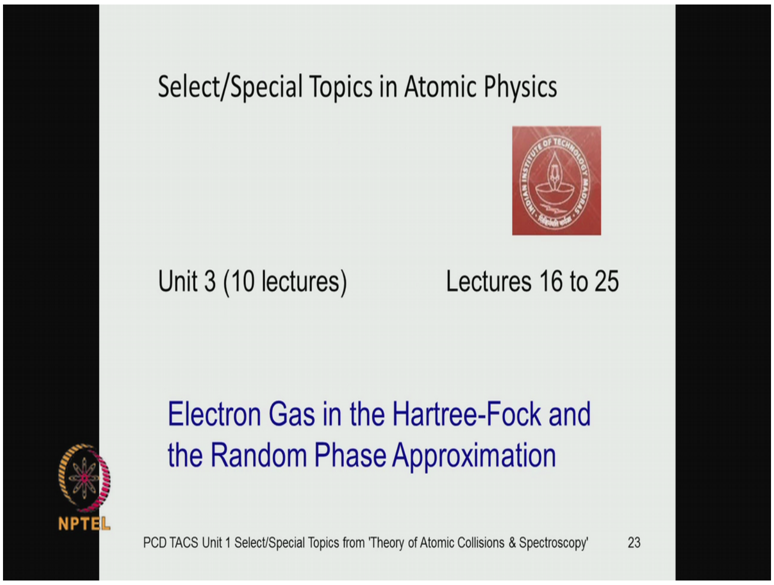

And then I will get into the details of the Random Phase Approximation which is to go beyond the Hartree Fock. And then we will take the classic example of the electron gas in the random phase approximation. So, the Hartree Fock we have already done in the previous course and we will now consider the electron gas in the random phase approximation.

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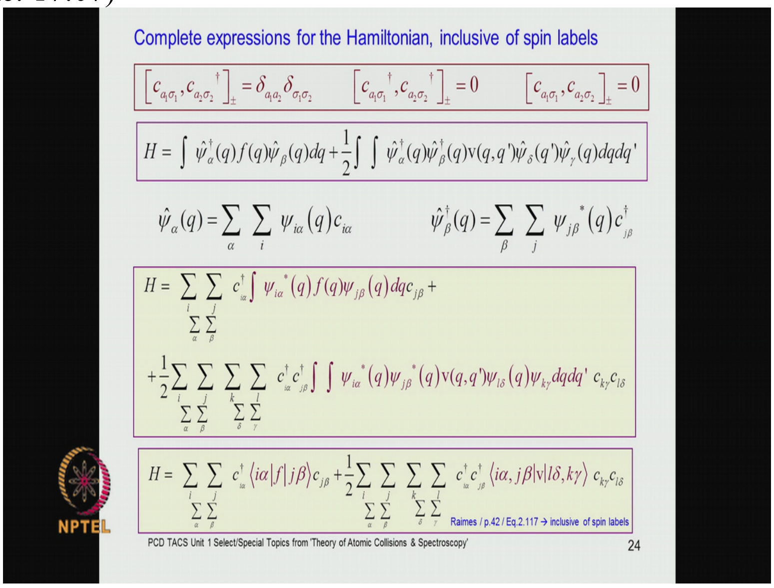

Now here again we will develop the complete expressions of the Hamiltonian including the spin labels using second quantized formalism. Using the field operators and also or the equivalently the creation and destruction operators.

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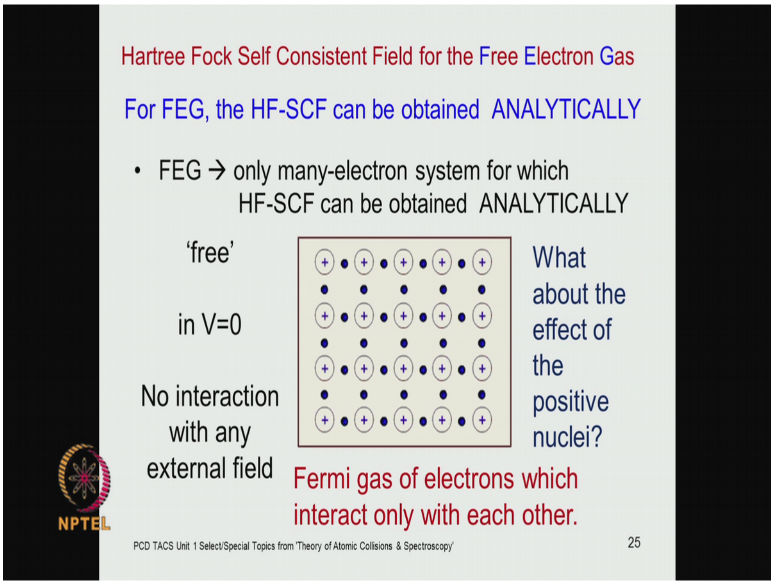

And we will deal with; we will follow the Bohm Pines method in which what they did was to address the question of the electron gas in condensed matter. In which you have got electron gas which is smeared out in a metal for example. But there also is a positive charge so what they did was to smear out that positive charge throughout the volume of the metal.

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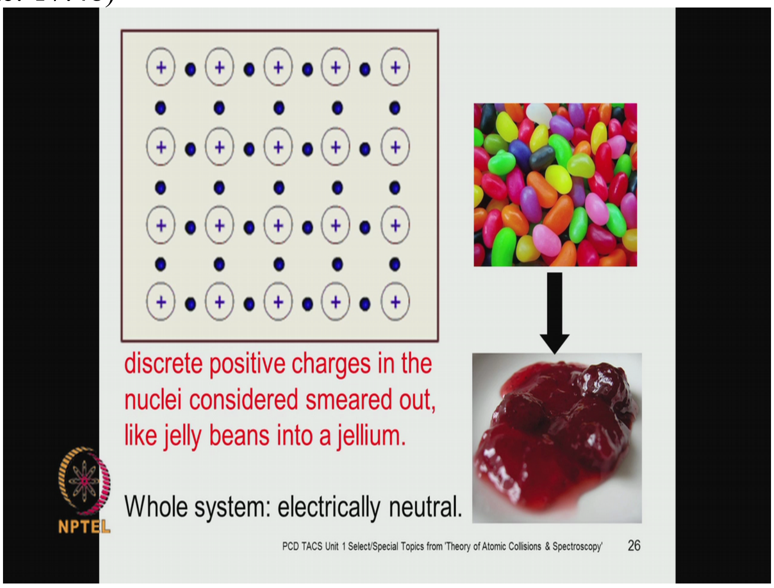

And that is what is called as a Jellium potentials. So, as if whatever charge was concentrated in the nuclei is smashed out and then you smear it out in the entire region of space. So, that is the system that is the electron gas in Jellium potential. The reason to do that is so that you deal with an electrically neutral system.

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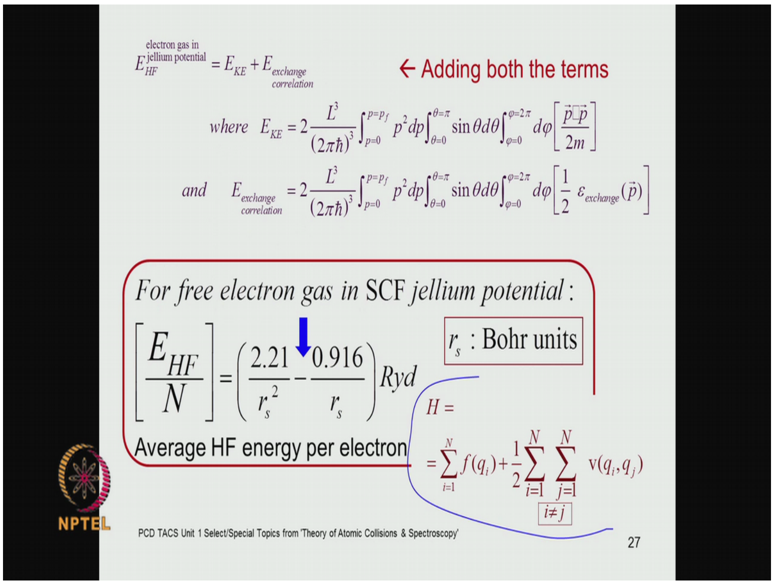

And using this method you can first address the dynamics of this system in the Hartree Fock approximation in which you get a certain expression for the energy per particle which turns out to be what you find on the screen which is 2.21 upon rs square and .916 upon rs, rs is like the average radius of an electron if you presume that all of these N electrons occupy a total amount of space of the condensed matter block itself.

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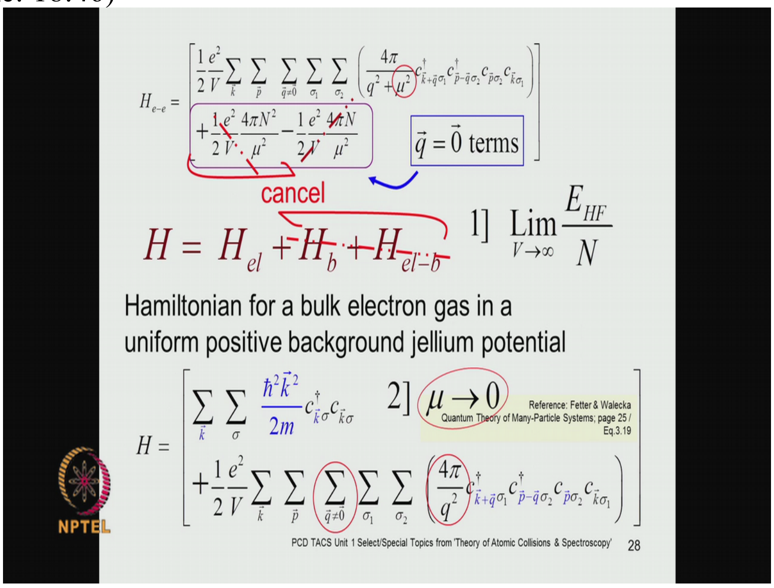

So, this is the expression that you get in the Hartree Fock approximation. But then you can go ahead and do it using the random phase approximation and to be able to do that you use the methods of second quantization. And keep track of all the interactions because the total Hamiltonian you can write in various pieces the electron, electron part, the electronic part.

Then you have got the background which is the jellium and then there is also the interaction between the background and the electron system which is between the jellium and the electronic system. And then you have to find out which if there is any cancellation of the terms and so on. So, we will do this part carefully.

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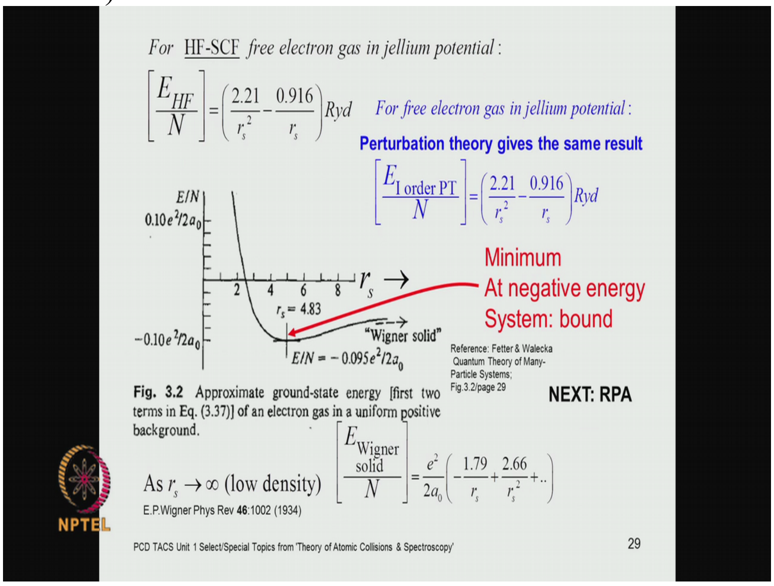

And then we will ask if there are any corrections to the Hartree Fock expression and we do find that yes indeed.

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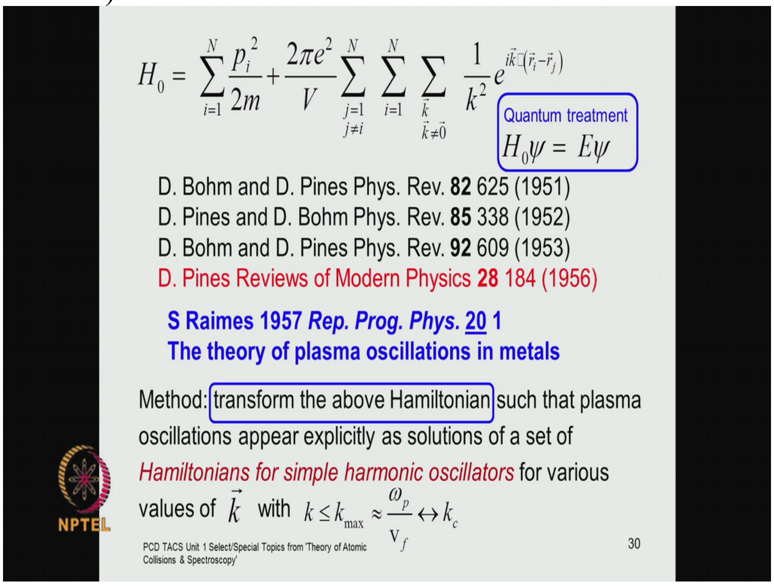

We do get corrections and these are the; this was the technique which was introduced by Bohm and Pines in the 1950's. So, there were very nice papers in the physical review during that period Raimes has got a nice review in the reports on progress in physics and of course the book by Raimes, which I like to refer to is a very good source for reading this particular information. So, what this technique?

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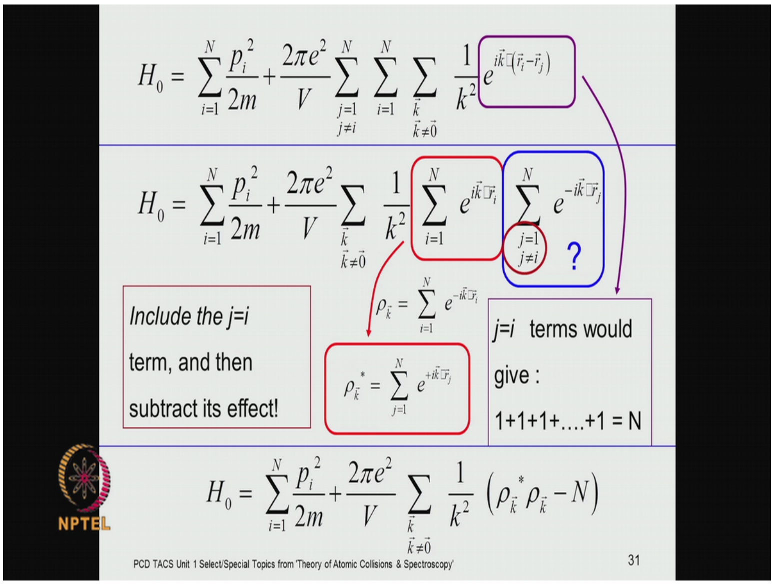

What the Bohm Pines technique does is to transform the Hamiltonian into a set of new coordinates and new momenta. So, this is a method of coordinate transformation, canonical transformation of the Hamiltonian written in terms of new coordinates and momenta. This has to be done very systematically.

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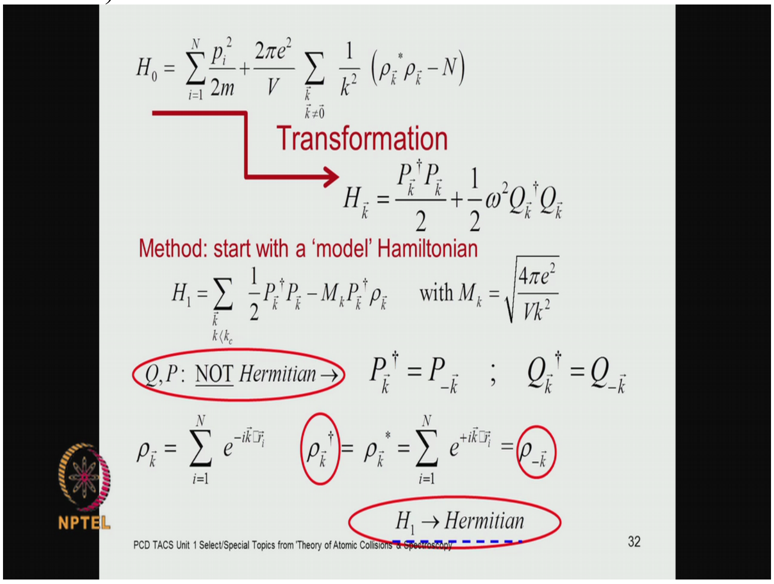

So, Bohm Pines came up with some very innovative transformation techniques and to set of new coordinates and momenta.

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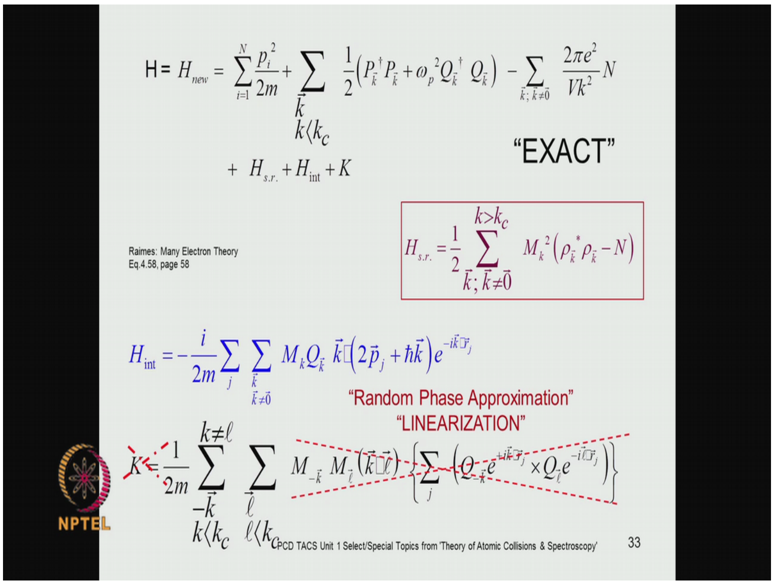

In terms of which they were able to rewrite the new Hamiltonian in a set of completely new transformation which describes the original system however in terms of canonical transformations to new coordinates and momenta. So, when you do that you do get plenty of terms and they are quite complicated to handle.

But you can carry out certain approximations and using these approximations the final form of the Hamiltonian becomes very handy and it is very easily amenable to physical analysis.
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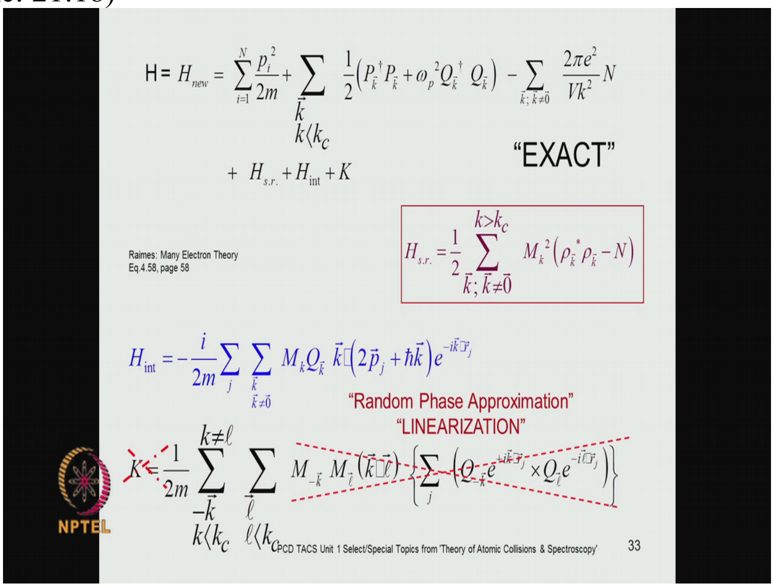

And that is done using this method of Bohm Pines and the approximation which is made is that of linearization. So, there are certain quadratic terms over here. So, the Q's so there is a Q here and a Q here so, there are quadratic terms in Q and these are the ones which are left out in a linearization process and one can argue as to what is the justification for this linearization. So, we will discuss all of these aspects and details in this unit.
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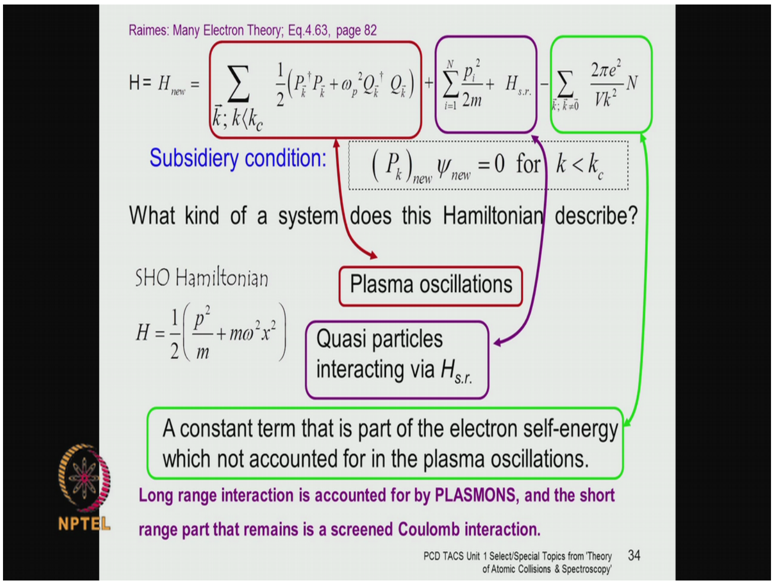

And we will introduce the random of phase approximation so, in the new set of coordinates and momenta generalized coordinates and new momenta the Hamiltonian for the many electron system in the background of Jellium potential can be written in three pieces one which looks like the Hamiltonian for an oscillator which gives you the explanation for the plasma oscillations you get in a many electron system.

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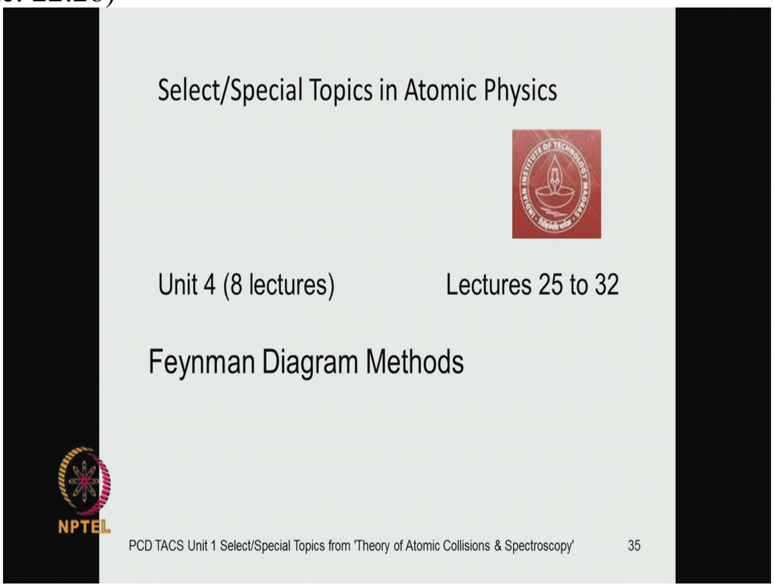

Then you have short-range interaction between these quasi particles and then you also have a part which is coming from the self energy of the electrons. So, we will conclude this discussion with the final result that we get from the Bohm Pines method of canonical transformations.

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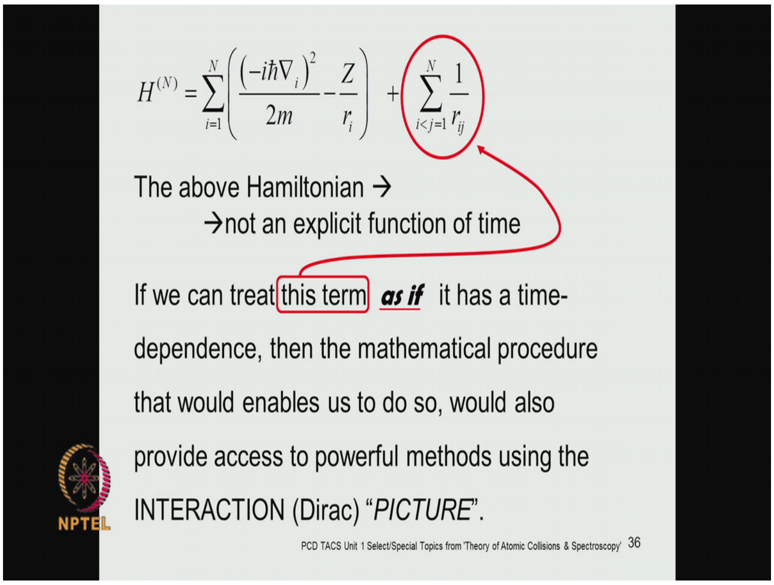

Then we will introduce the Feynman diagram methods and for that we will essentially make use of the interaction picture, quantum mechanics in the interaction picture. So, we will introduce the Dirac picture description of a many electron Hamiltonian.

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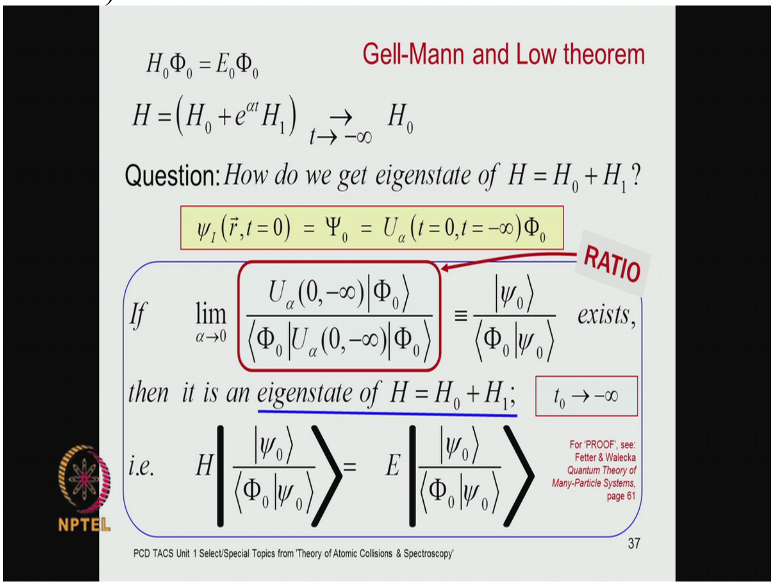

And then we will make use of the Gell-Mann and Low theorem to relate the solutions inclusive of the correlations of the many electron system. In terms of a solvable part which excludes the electron-electron interactions. So, it is some sort of a perturbative approach but it is quite different also and it allows us to use this chronological evolution of the system from an uncorrelated system to a correlated system.

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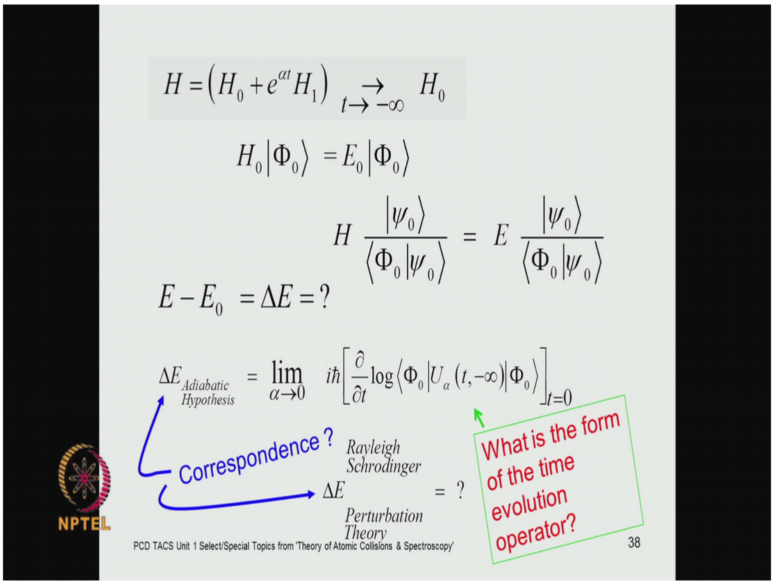

So, that we can see exactly what is the role of these correlations and how are these to be addressed. So, you can approach this from the point of view of an adiabatic hypothesis in which you introduce the electron-electron correlations adiabatically through a mathematical switch. But then you can compare the results with what you can get through the formal Reyleigh Schrodinger perturbation theory.

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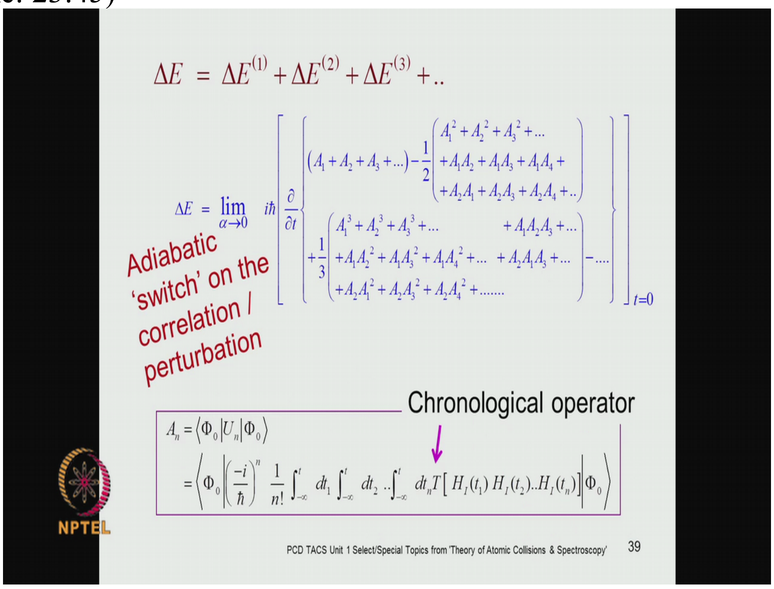

And when you develop this formalism it turns out that the; you really get infinite terms and a multiplicity of them. So, there are just too many terms the whole description becomes quite complicated. You have the chronological operator which orders all the operators with the latest operators to the left and so on. So, this so the whole analysis is quite complicated.

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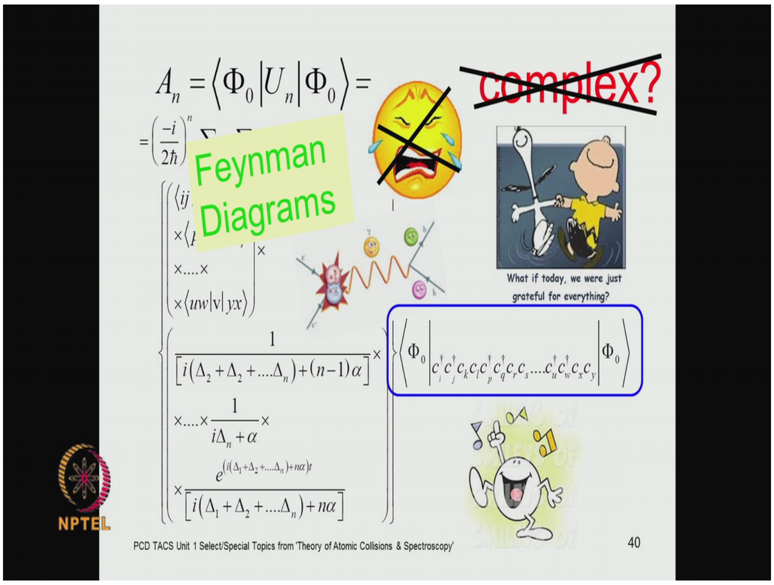

But then it is a Feynman diagrams which make them easy to analyze okay. Because all of these terms you can handle in a very compact and beautiful manner in a very elegant manner by introducing Feynman diagrams which is what we will do in this unit.

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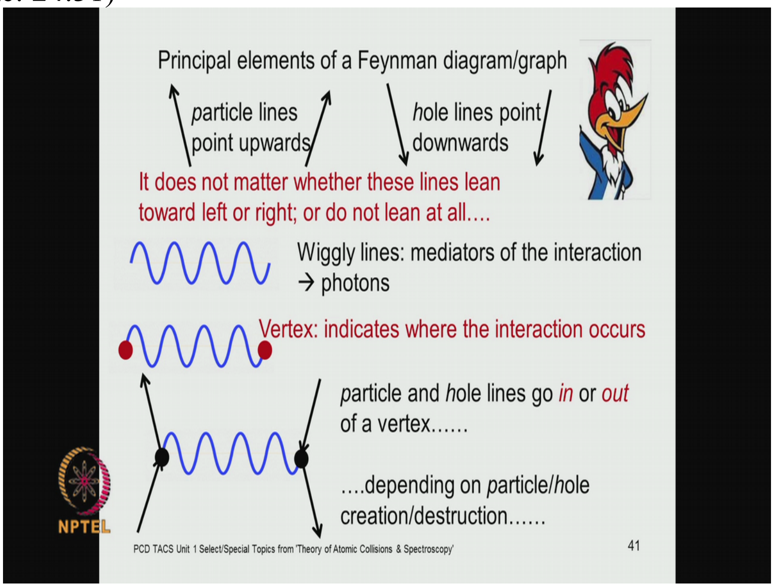

So, we will define these diagrams they are based on certain conventions. So, an arrow pointing upward or downward has got a different meaning whether these are the particle lines or the hole lines of course it depends on what kind of convention you have for the time axis whether time is flowing from the bottom to the top are from left to right. So, there are certain conventions which you have to define.

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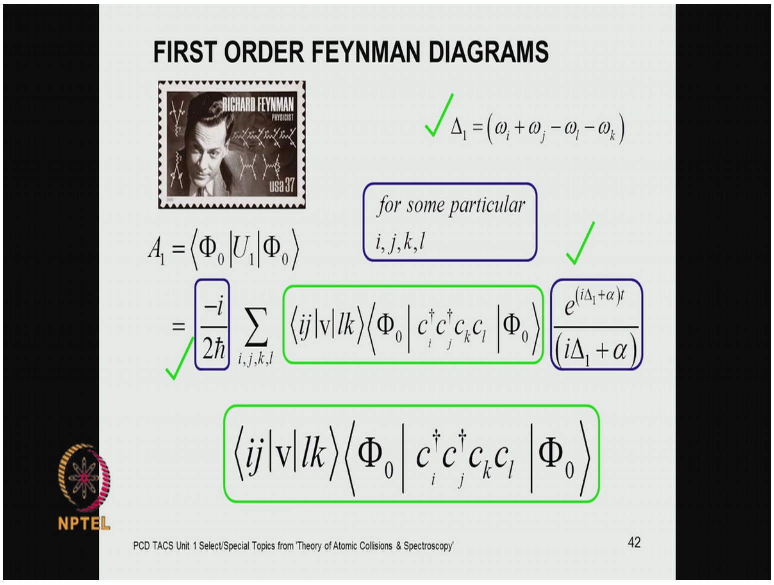

And then you can define the particle creation and destruction in terms of these arrows which go into a vertex are out of a vertex and so on. So, we will define these conventions and then they will help us analyze the terms which go into the many-body electron correlation.

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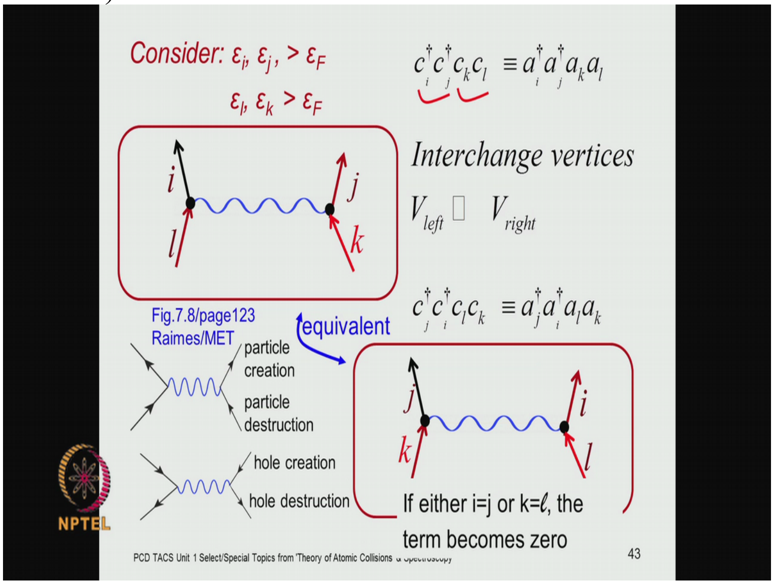

So, that we can describe them in terms of these very nice very beautiful elegant pictures known as Feynman diagrams. So, we will spend some time discussing the first our order diagrams.

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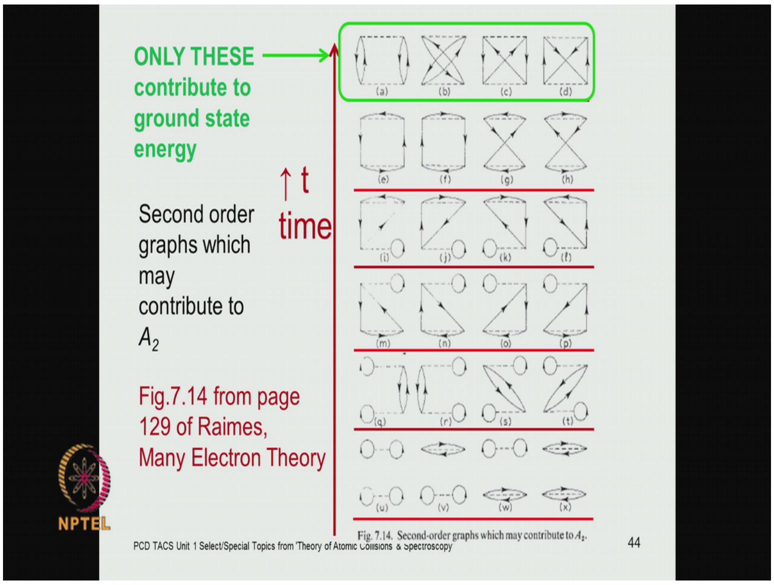

Then we will also introduce the second order diagrams and also the third order diagrams. So, that we get some sort of a familiarity with this technique we will also learn to recognize which diagrams are equivalent, which are not equivalent, which are the fundamental ones, which need to be used which are connected, which are not connected.

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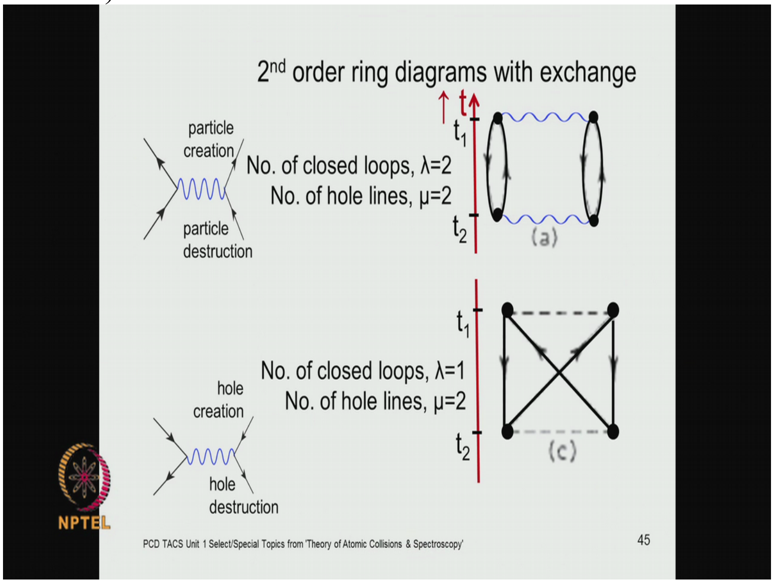

And then how when you do many body theory you can select a group of diagrams to address. So that you can restrict your attention to certain correlations which you think are important for your study and the RPA the random phase approximation comes through one of these techniques or retaining only these ring diagrams and the corresponding exchange. So, some of these things we will discuss in the context of the Feynman diagrams.

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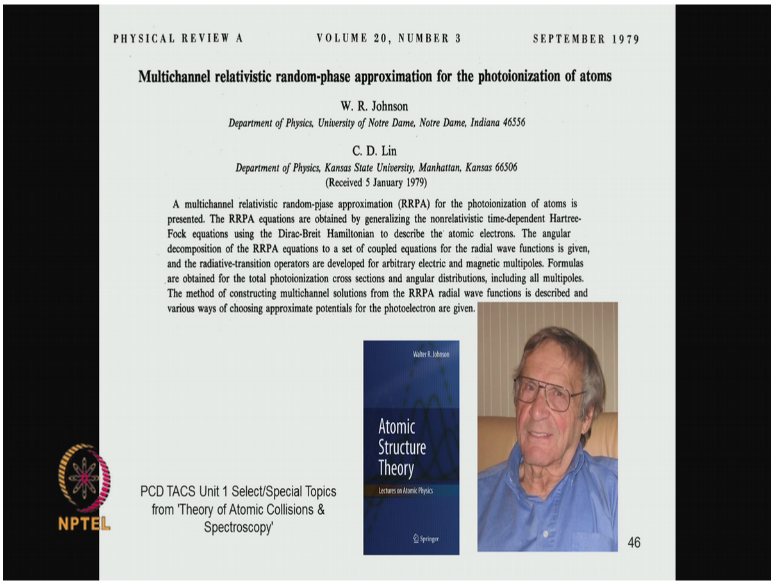

I will also spend some time in describing yet another way of getting the RPA like I mentioned there is a Bohm Pines method of getting the random phase approximation. There is basically it is a linearization technique. So, even in the diagrammatic perturbation theory, if you keep the ring diagrams again you get an equivalent or what is RPA.

But you can get it also by carrying out a linearization of the time dependent Dirac Hartree Fock and this is the technique that was done that was used by Dalgaarno and Victor for the non relativistic many body problem and by Dalgarno and Walter Johnson for the relativistic case which is known as a linearization of the time dependent Dirac Hartree Fock method or which is equivalently called as the relativistic random phase approximations. So, I will provide some introduction to that.

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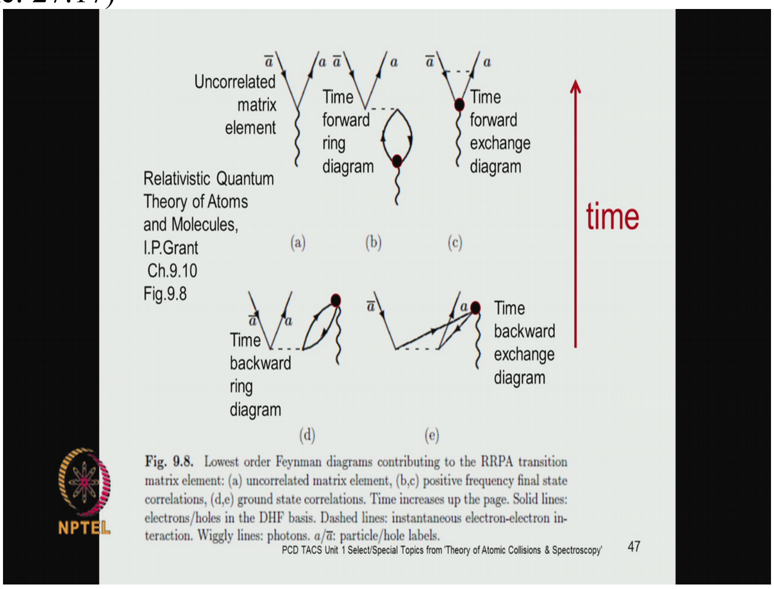

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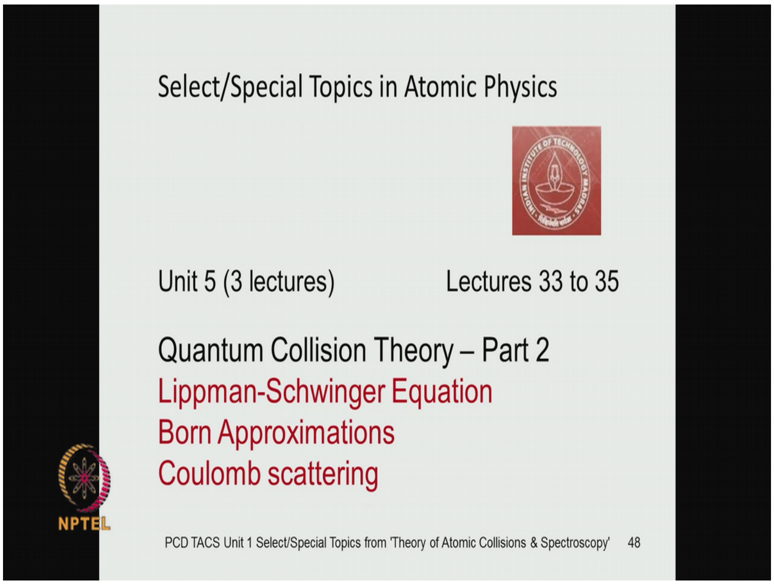

And then you get the relativistic RPA diagrams which as you can see from this are again basically focused on the ring diagrams which is a central feature of the RPA. In the unit 5 we will you get back to quantum collisions and I like I said that in principle one can study this after the first unit in which we would have studied the Levinson's theorem and so on.

So, in this unit we will introduce the Lippman Schwinger equation which is the integral equation of potential scattering. We will also do the Born approximations.

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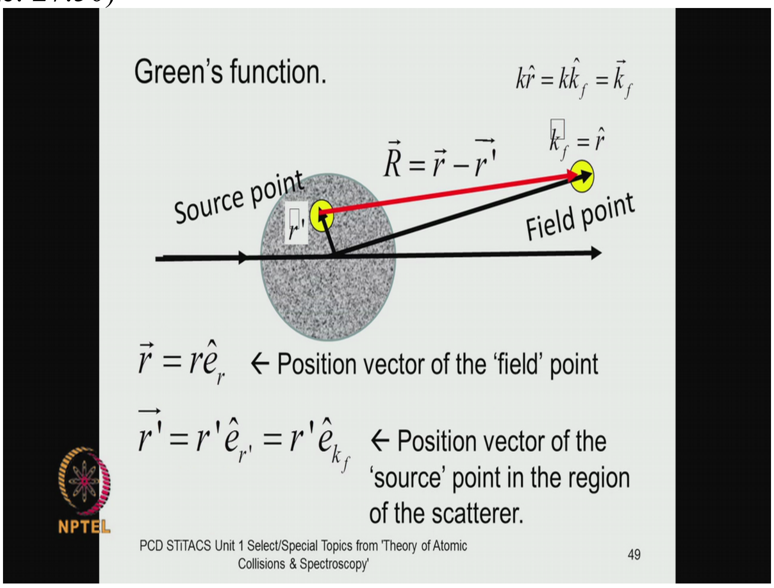

We will also do Coulomb scattering. So, we will introduce methods in which the Green's functions are used. So, there is a certain causality which is referred to over here.

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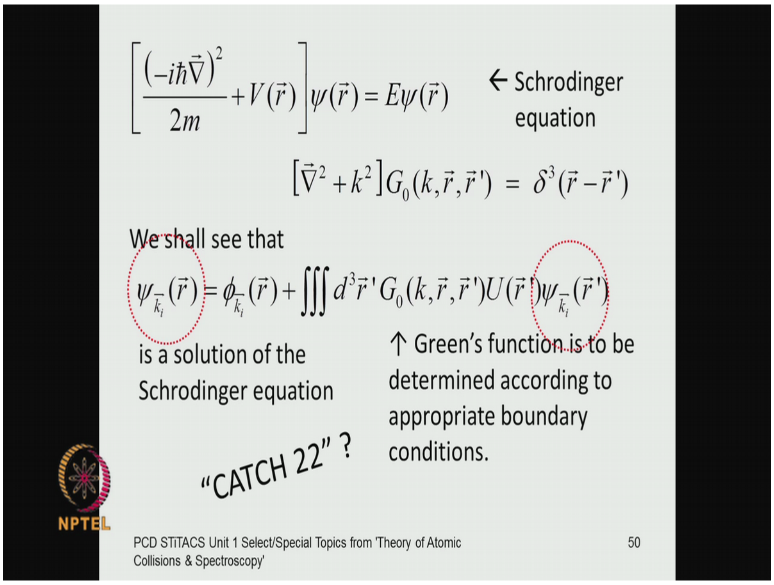

We will write the Lippman Schwinger equation and we will find that it is amenable to an iterative solution because unless you make some approximation you cannot go too far with the Lippman Schwinger equation itself because it generates a catch-22 type of situation because you get a solution in terms of the problem. So, to be able to handle that you can develop certain approximation methods.

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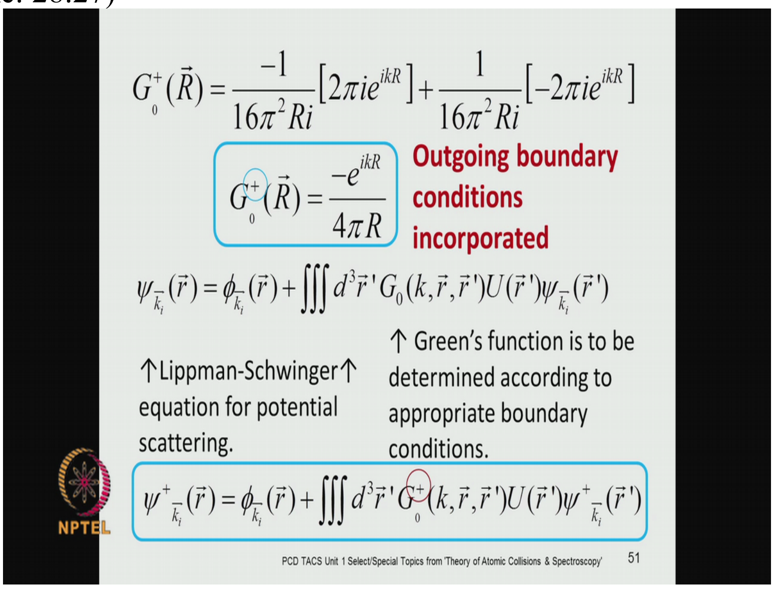

And these approximation methods with reference to appropriate boundary conditions of the collision problem they let you choose what would be the appropriate Green's function that goes in the integral expression of the Lippman Schwinger equation.

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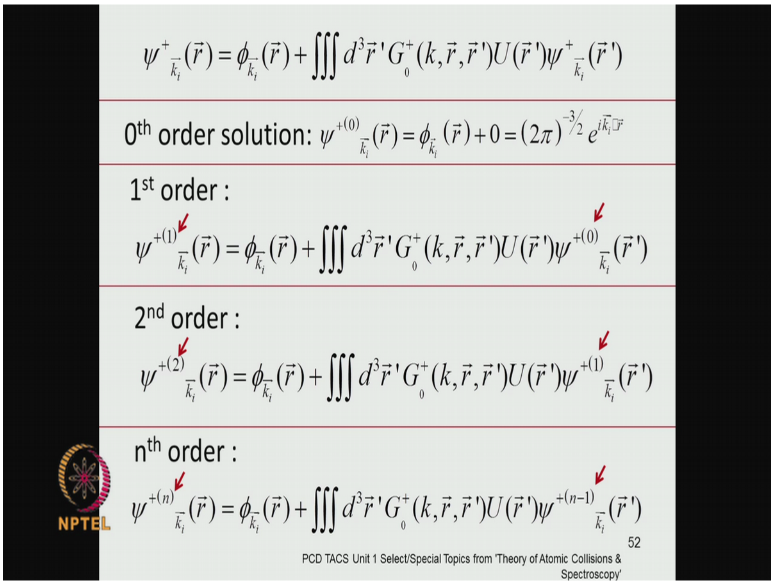

So, when you choose the property in Green's function you get a series of approximation which are known as the Born approximation. So, there is a first order Born approximation the second order Born approximation and then nth ordered Born approximation. So, you will be introduced to this Born series of approximations.

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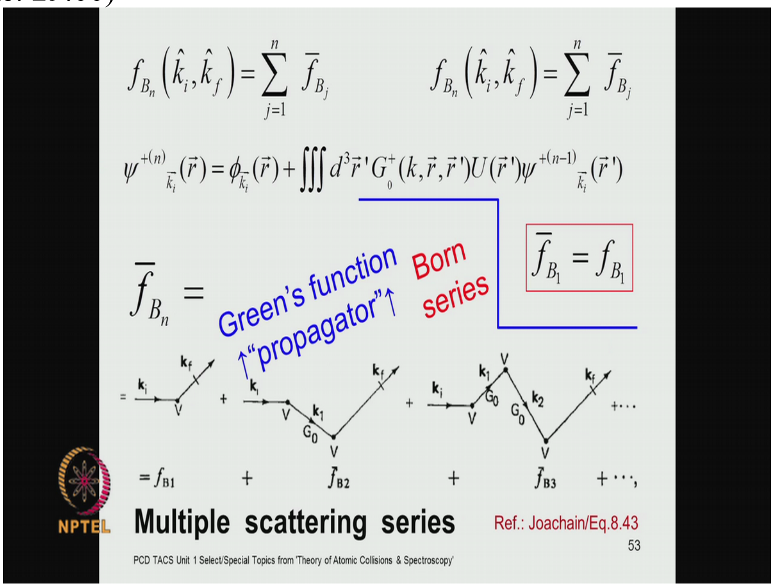

So, we will spend some time discussing this and as you see most of this discussion will be based on Joe Shane's book quantum collision theory.

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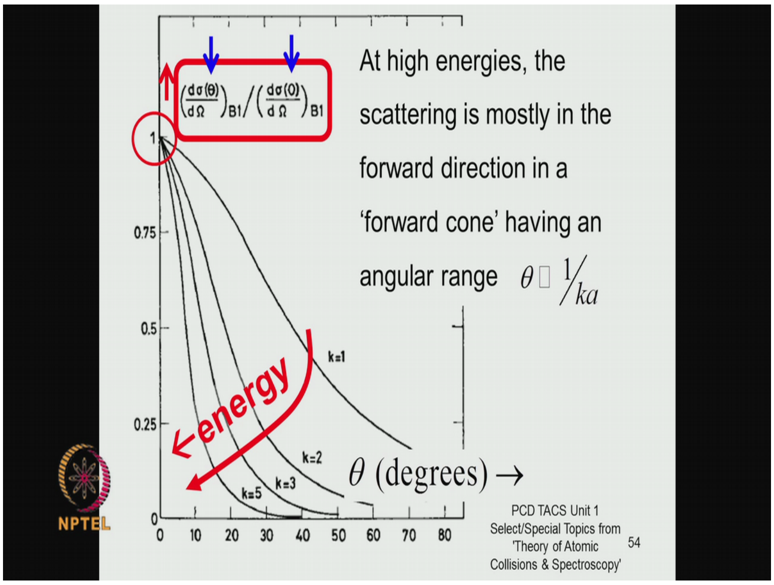

And we will also discuss what happens in the Born approximations, How is it suitable in the high energy? What happens is the high energy range is the first Born approximation good enough.

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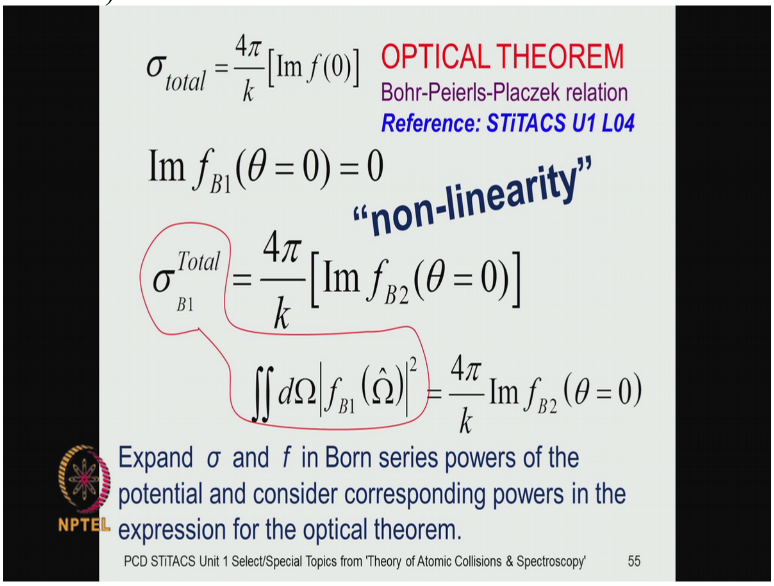

Is the optical theorem satisfied in the Born approximation or do you get a certain non linearity over there. So, all of these questions we will take up in this unit.

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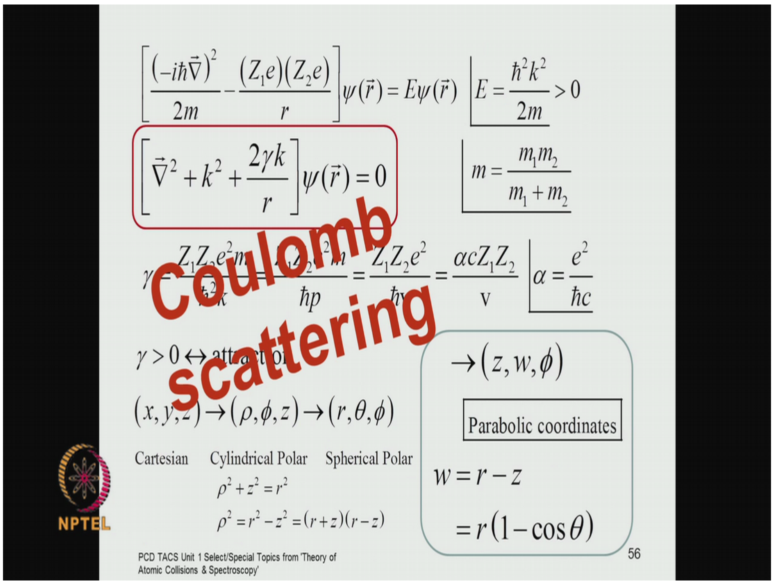

We will also discuss Coulomb scattering and the Coulomb problem is a very peculiar problem because the usual methods which we discuss in quantum collisions do not apply directly to the 1 over r potential. So, this problem is addressed using a new set of coordinate system known as the parabolic coordinates.

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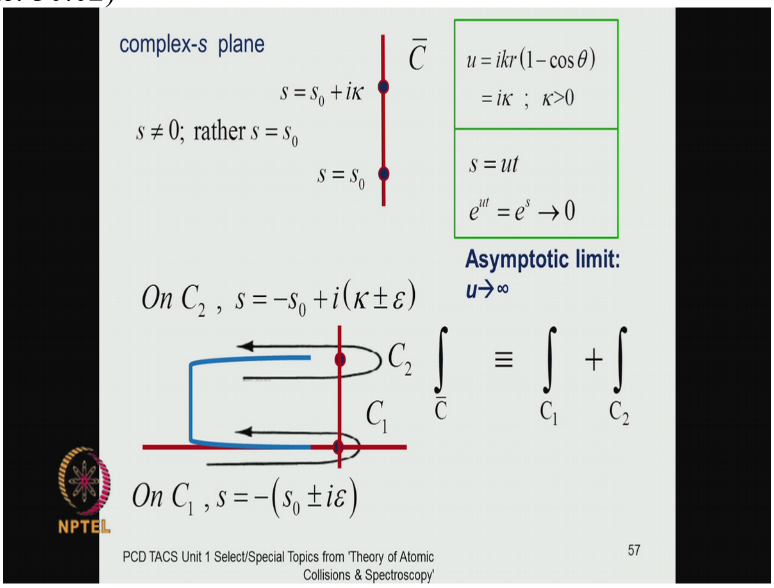

So we will solve the problem of Coulomb scattering in parabolic coordinates using methods of contour integration and branch cuts.

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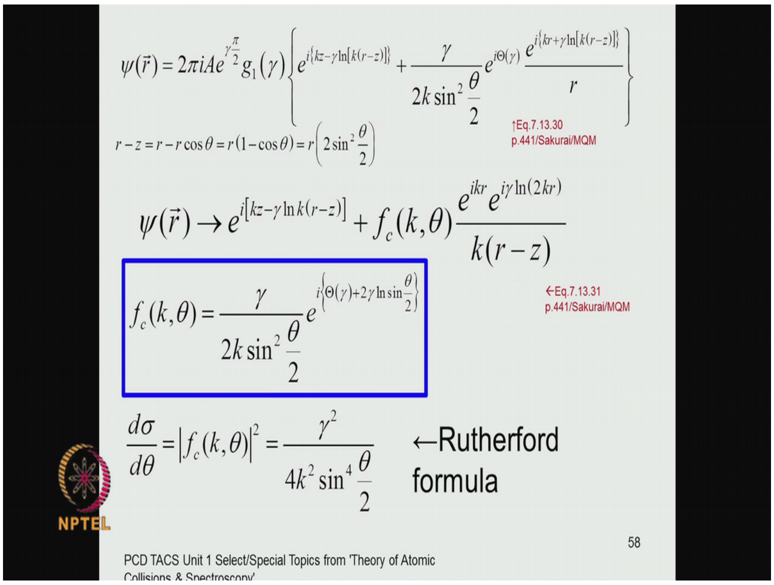

So, we will get the solutions which will give us the Coulomb logarithmic phase shift and also the expression for the scattering cross section. Which turns out to be the same as you get in the Born approximation or for that matter also in classical mechanics. So, it turns out that so this is interesting coincidence that you get the same result for the scattering cross section in classical mechanics in the Born approximation and also in the complete quantum mechanical solution to the Coulomb problem.

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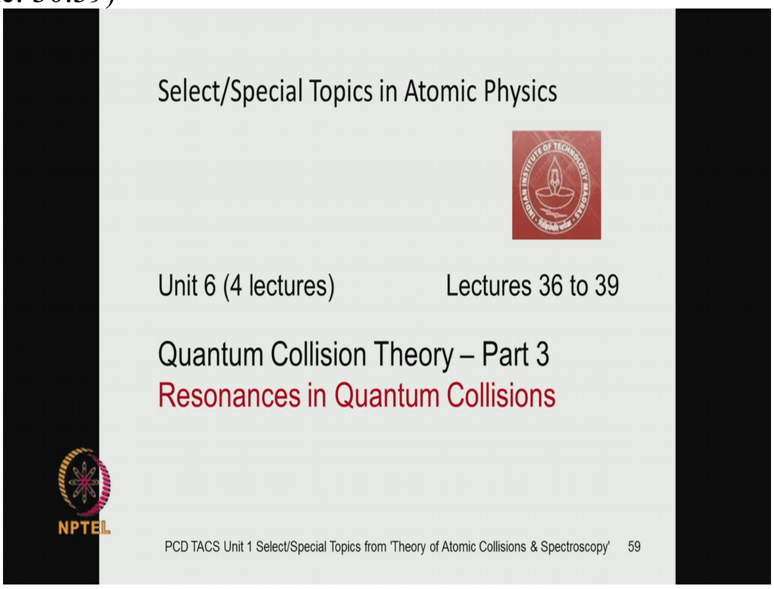

So, that will bring us to the next unit which will be on resonances in quantum collisions.

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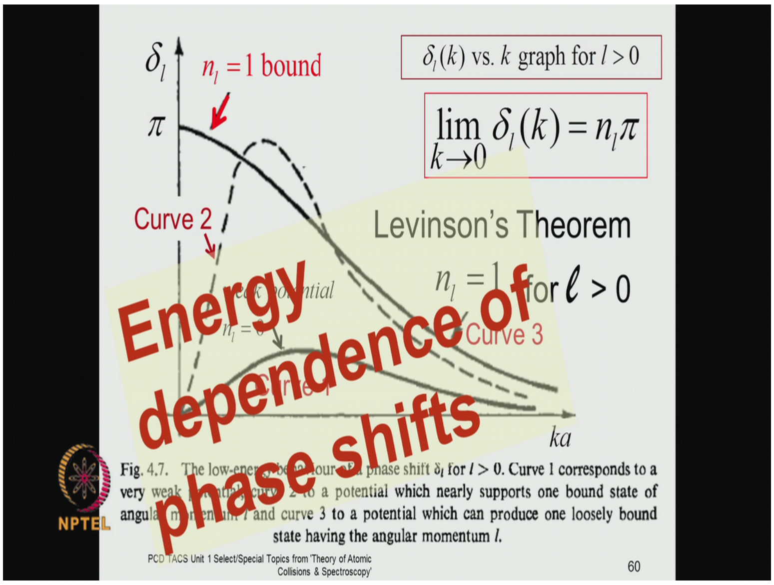

Because what happens is when you do a phase shift analysis the phase shifts, the scattering phase shifts they change somewhat rapidly in the vicinity of a resonance. So, we will discuss the energy dependence of the phase shifts.

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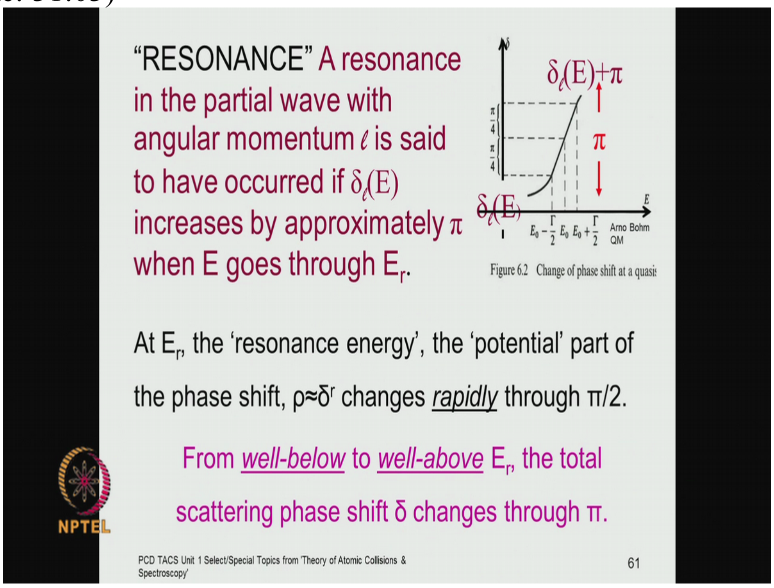

And we will see that these phase shifts they change rather rapidly in the vicinity of resonance and so if you have a resonance at this energy then from slightly below the resonance to slightly above the resonance the phase shift undergoes a major change through pi. So, we will discuss and try to understand resonances in terms of how the scattering phase shift changes in the vicinity of resonance.

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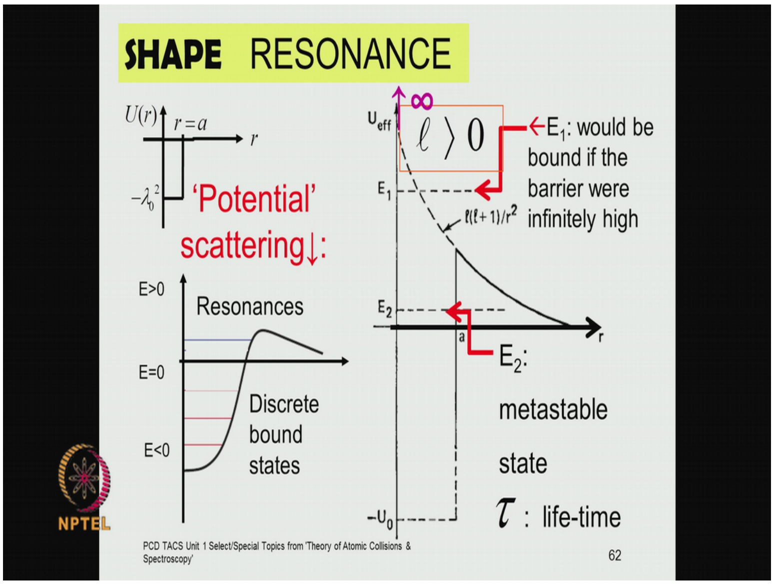

We will also discuss resonances of different kinds. So, broadly speaking there categorized either a shape resonances or as Fano Feshbach resonances. So we will describe both of them the shape resonances are because of the nature of the shape of the potential itself.

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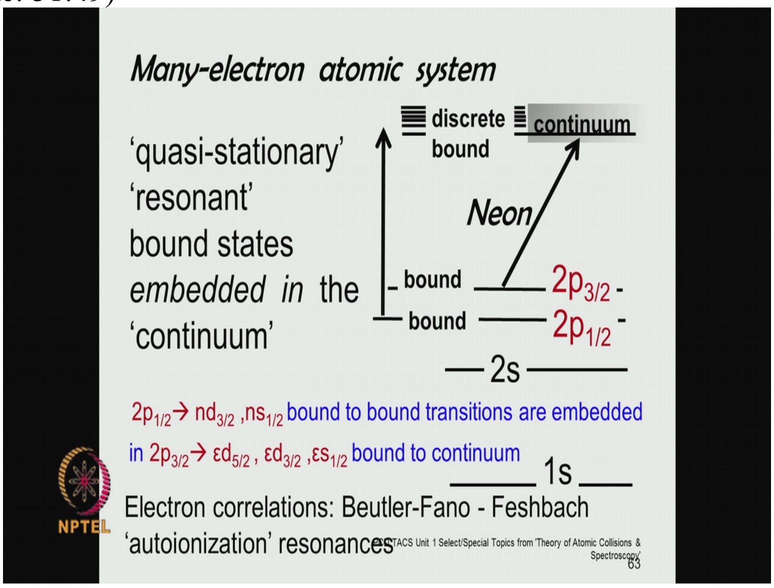

And the Fano Feshbach resonance takes place when you have a quasi-stationary state. You have got a discrete state which is embedded in the continuum. So, you have got a resonance between a bound state, bound to bound excitation and a bound to continuum transition like ionization as you could have in the Butler Fano resonance or the autoionization resonances.

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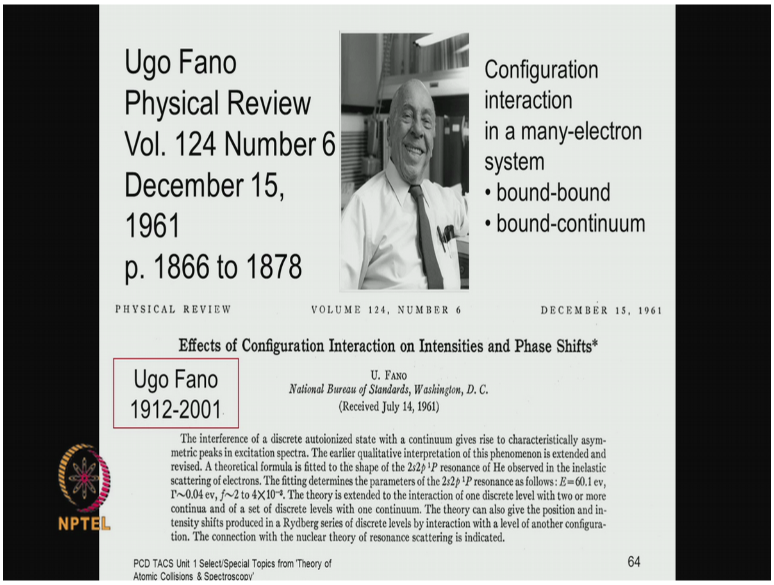

So, in particular I think this is a topic which I hope all of you will enjoy very much because we will work through Fano's very famous paper this has received more citations and a lot of other papers which perhaps you might know better. But then the actual citations to this paper are far too many.

This is a very important paper in physics not just in atomic physics but it has got applications across physics in various disciplines Condensed matter physics, Molecular physics whatnot.

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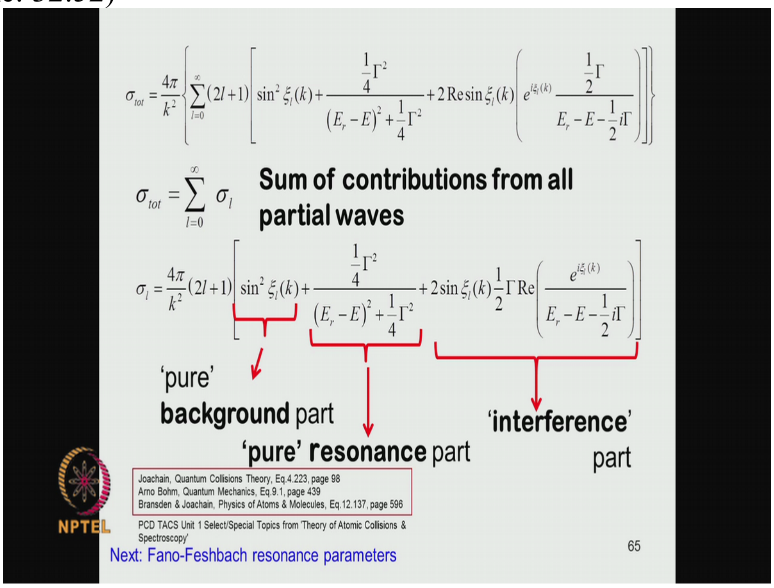

So, we will deal with this paper so we will arrive at a general expression for the Bright Wigner formula for resonances. In which the scattering cross section for the lth partial wave can be written separately in terms of the background part, the resonance part and the interference part between the resonance part and the background part.

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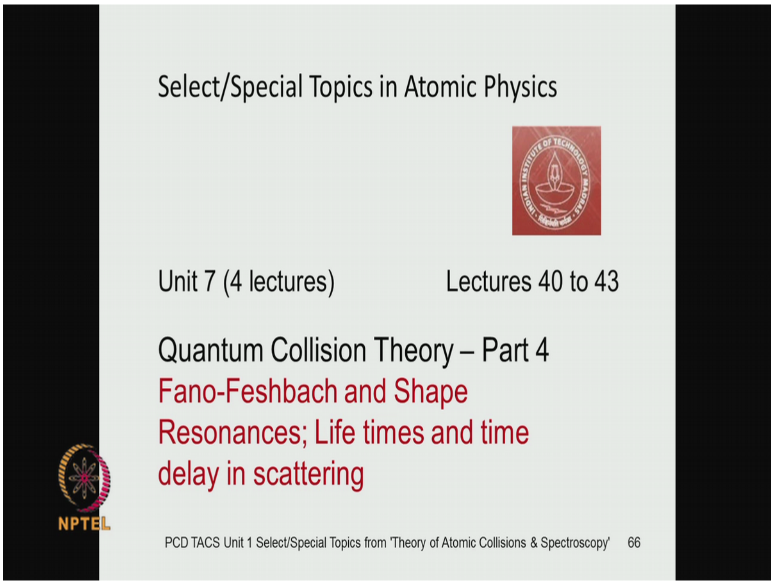

And then we will do what is known as a shape analysis of these resonance profiles. So, that can be done using Fano's methods.

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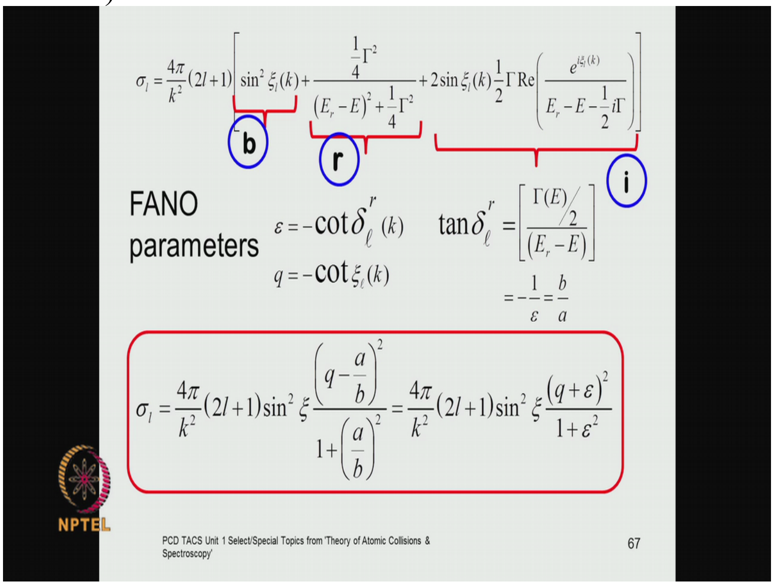

Fano introduce these parameters which are famously knows as Fano's q in epsilon parameters. So, we will introduce this and show the equivalence with the Bright to Wagner formula.

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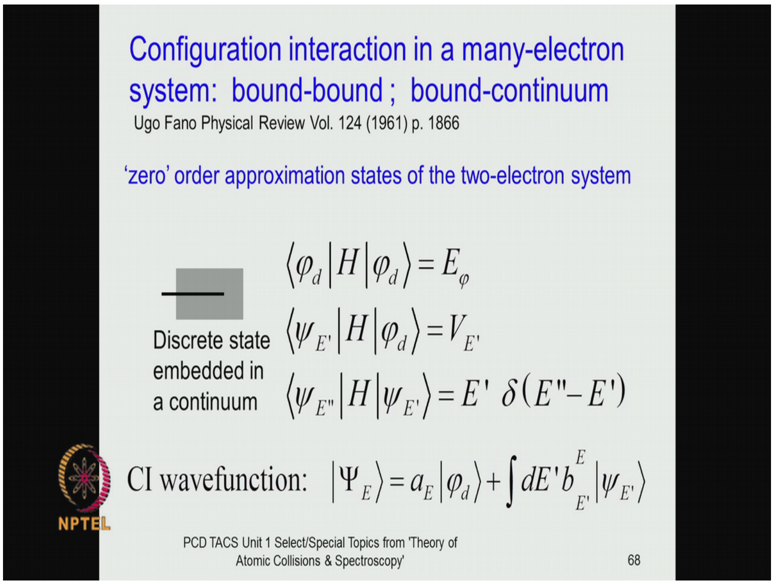

And in terms of this we will discuss the autoionization resonances between the bound to bound and mounted continuum transitions.

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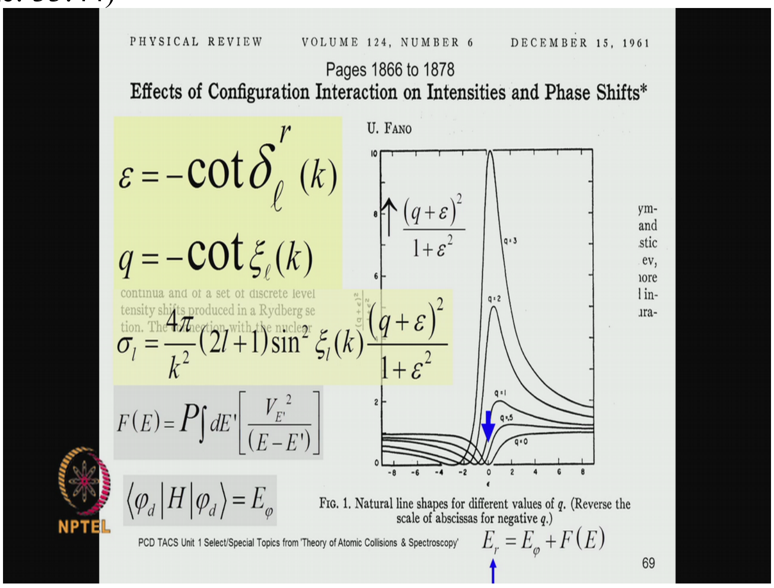

So, the shape of a resonance can be just about anything, these are not always symmetric lines across the resonance energy on either side of the resonance energy. You typically have symmetry. So, we will talk about it.

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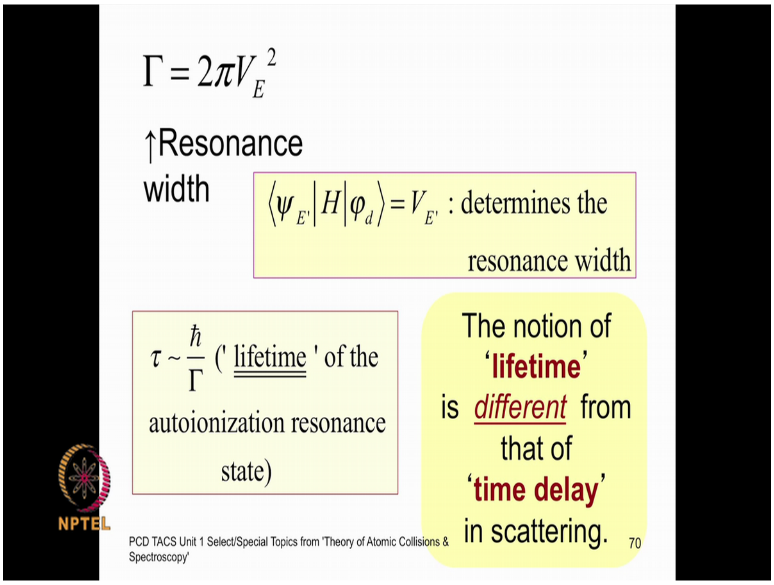

Then we will have, we will introduce the idea of time delay in scattering which is different from that of lifetime of a resonance state. So, you will have the time delay in scattering.

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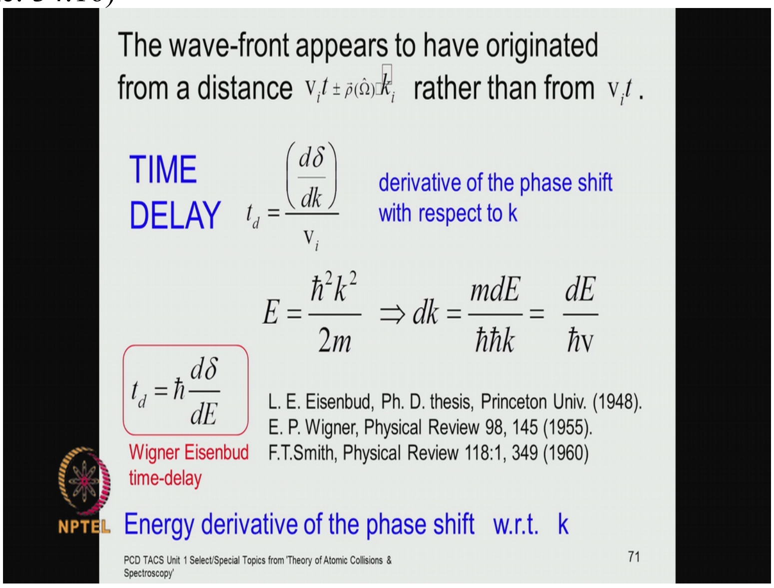

This is also known as the Wigner Eisenbud time delay because the original formalism was done by Eisenbud and Wigner around 1950 and there are important contributions by Smith and others. So, we will introduce time delay in scattering.

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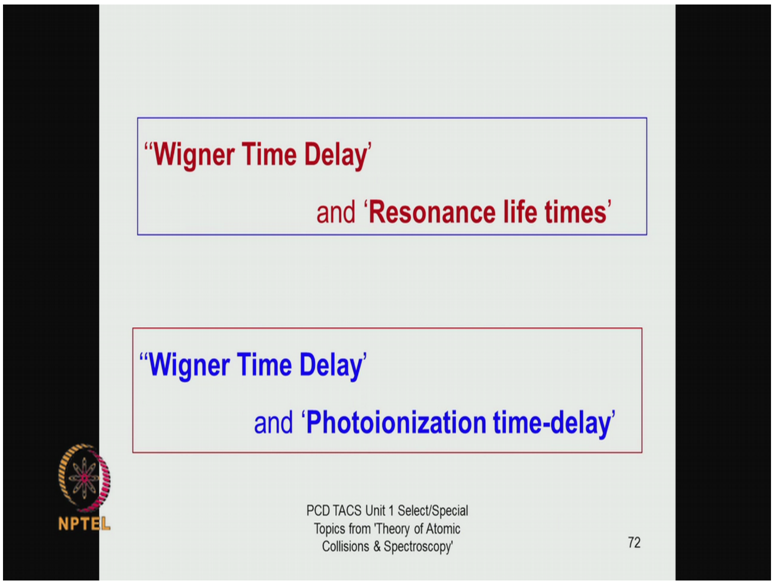

Which is typically known as the Wigner time delay? And we will relate the Wigner time delays with resonance lifetimes and in the context of the Wigner time delay we will also discuss the time delay in photo emission process or photoionization processes. So, these are the topics that we will cover in this unit.

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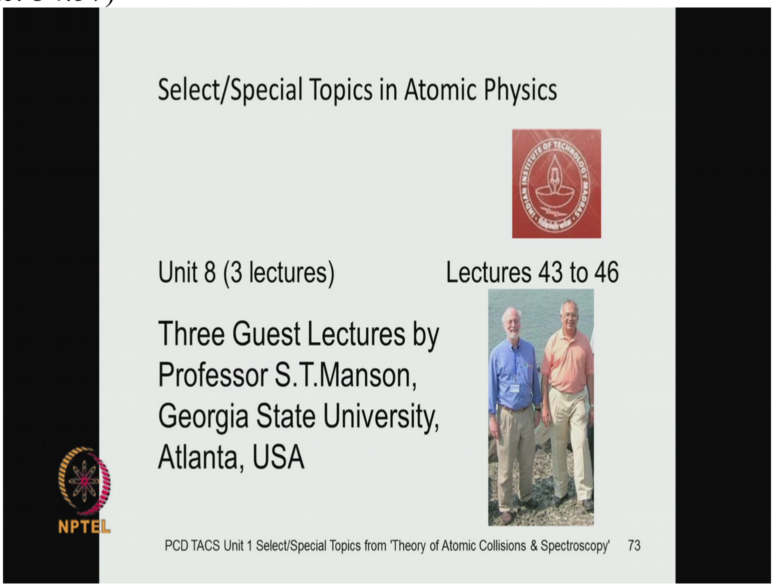

And that will bring us to the guest lectures in the last unit. These guest lectures are delivered by Professor Steve Manson of the Georgia State University and Steve has delivered three lectures.

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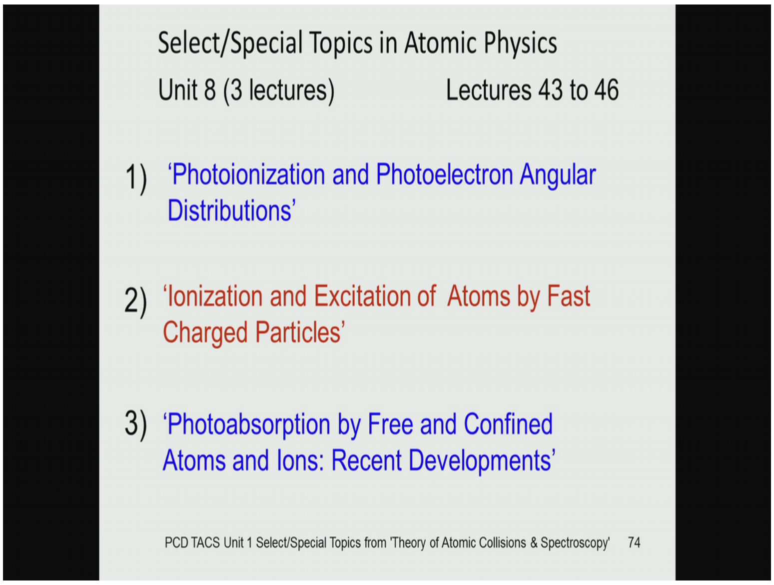

These three lectures are on photo ionization of Photoelectron Angular distributions, the lecture two is on Ionization and Excitation of Atoms by Fast Charged Particles and the third lecture is on Photoabsorption by Free and Confined Atoms and he will give you an overview of some other recent developments.

So there will be these three lectures end in the last unit. So, that pretty much sums up an overview of what this course will turn out to be. And I hope that you will benefit from it and the basic idea which I would like to emphasize over here having said that okay it is important to study atomic physics means following the spirit of Feynman Quote that is the most important thing that he would like to leave for posterity.

And how one can really get so much of other knowledge in science by extending atomic physics into other areas then what this course attempts to do is to give you the tools to study atomic physics. So, you need to study atomic physics, atomic structure then atomic dynamics collisions, how an atom is probed using particles or electromagnetic radiation okay.

So, the tools that are necessary, is what I shall attempt to provide in this course. So, thank you very much.

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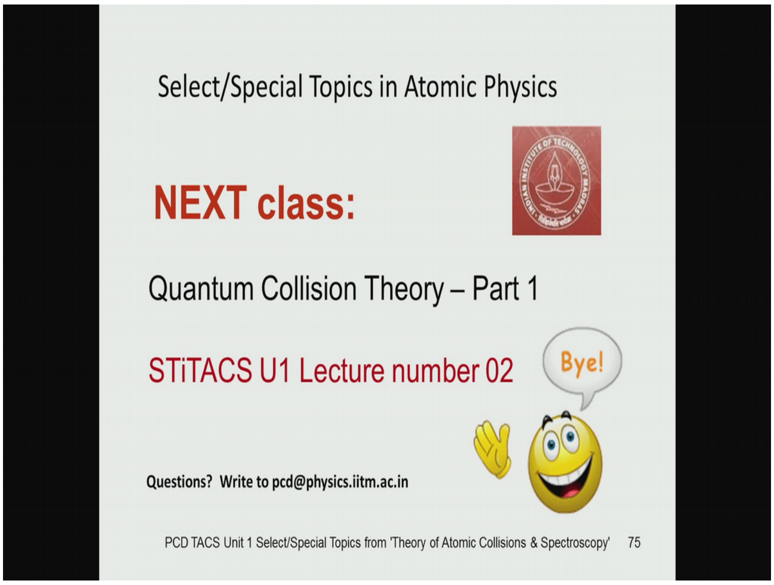

And we will begin the next lecture with the first lecture of quantum collision physics. Thank you very much.