Select/Special Topics in Atomic Physics

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Lecture - 26

Probing the Atom
Collisions and Spectroscopy - Boundary Conditions

Greetings, we begin with a new unit today, this is our 6th unit. And we will begin to discuss the methods that we have to probe an atom, that you have got an atom and you want to carry out some experiments on the atom. So, that you can explore some properties, which the atom has… Now, whether the target is an atom or an ion or a molecule or a cluster or any microscopic quantum system or even extended condensed matter.

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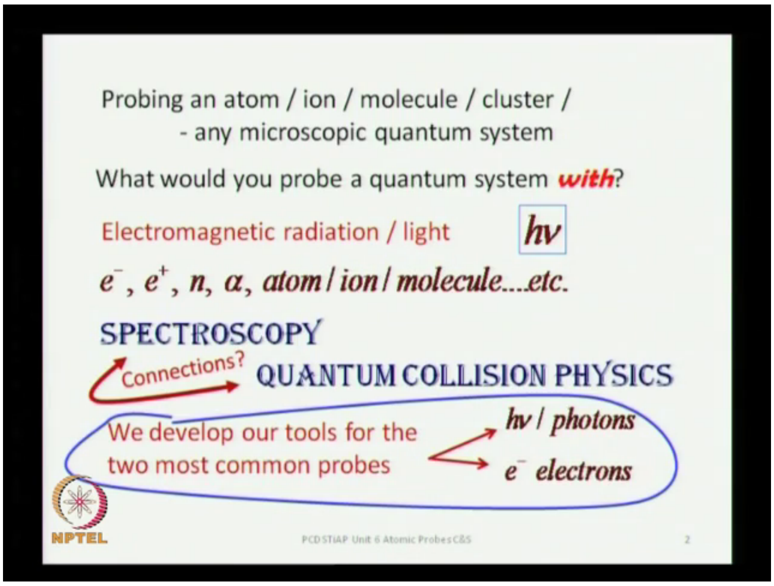

Probing an atom / ion / molecule / cluster /
- any microscopic quantum system

What would you probe a quantum system ***with***?

Electromagnetic radiation / light $\boxed{h\nu}$

e^-, e^+, n, α, *atom / ion / molecule….etc.*

SPECTROSCOPY

Connections?

QUANTUM COLLISION PHYSICS

We develop our tools for the two most common probes

$h\nu$ / *photons*

e^- *electrons*

PCDSTiAP Unit 6 Atomic Probes C&S

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You are going to need some tools to probe the target with, and the techniques that you set up in atomic physics are then used in other areas of condensed matter. Because, when several atoms come together, two or more you have molecules and then you have more atoms coming together, you have clusters and extended, condensed matter. So, the question is what do you probe the quantum system with, you need a tool, you need to probe and that probe can certainly be electromagnetic radiation, you can shine light on it bottom of frequency.

The other thing you can do is to bombard it with particles, like if there is no light in this room and you want to figure out what is on this desk, the first thing you would do is to switch on the lights, and see that this is what there is on the desk. But, if there is no power that happens in Chennai, then you feel for it you touch it, and by touching it or by firing something at it by looking at the scattering and so on. Your then able to make out what object is over there, so there are different tools which are available for you to probe quantum systems.

And your probe can be an electron, it can be a positron, it can be a neutron, it can be a alpha particle, an atom, it can be another ion, it can be a molecule, it can be your hand, which is a combination of, so many atoms and molecules and everything. So, what we will do is when you investigate your target using light, then you are doing spectroscopy, or else you are doing collisions. The question that we will discuss in today's class, in the next couple of classes is whether, there are connections between spectroscopy and collision physics.

And if yes, what are these connections, and it will turn out that these processes are related to each other through time reversal symmetry. And that is why you can carry out information that you get from spectroscopy into collision physics and vice a versa. So, that is something that we are going to learn amongst many other things as we discuss, this unit and later units. So, what we will do is, we will develop our tools for the two most common probes, one is light electromagnetic radiation and the other, which is a prototype of a projectile, which is fired at the target in a collision experiment.

And regardless of what kind of projectile you might choose for a given experiment, we will develop our tools for electrons. And then the same techniques with appropriate modifications can be extended, and developed further when you are dealing with other probes, so these are the basic ingredients of collision physics. So, we will investigate these two probes in particular, and if you have an excited state of a quantum system, then it can take decay through a radiative channel, not necessarily it can decay also through non- radiative channels, but that is a matter of detail. But, quite often it would radiate energy and this would come out as light, so this is how the quantum system interacts with electromagnetic radiation it, actually emits electromagnetic radiation, when it decays through a radiative channel.

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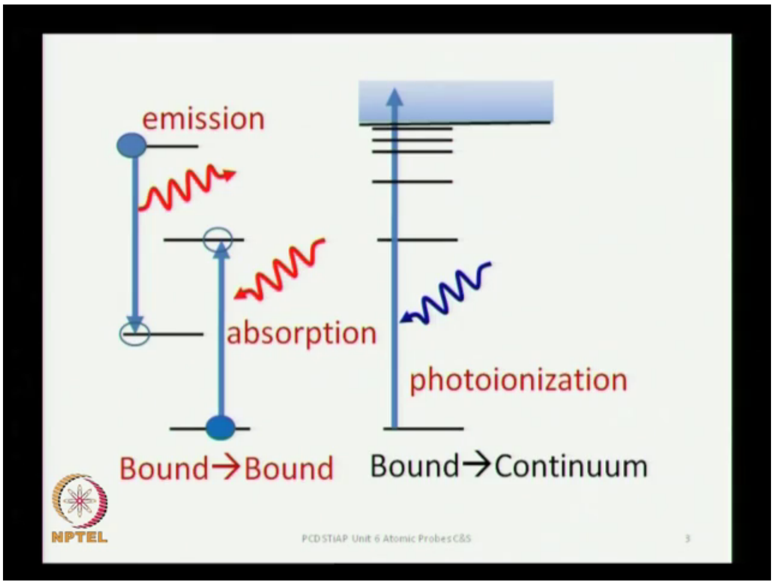

emission

absorption

photoionization

Bound→Bound

Bound→Continuum

Then it can also observe light and the result of absorption, can be an excitation of the quantum atomic system to an excited state, that is one consequence of absorption of radiation. Or you have a number of quantum states, which is a discrete part of the spectrum, but the discrete part of the spectrum, it converges to what you call is a red bursaries limit, beyond which is ionization continuum. So, your 0 of the energy scale is at the limit of, this is the red bursaries limit that is your 0 of the energy scale, all the discrete states are bound states, so those are negative energy state.

Everything above it are positive energy states and that is a continuum, there is nothing discrete about those energy levels. You have some energy and an energy level which is infinite to simile higher than that, is also within the Eigen spectrum of your quantum system, which is why we emphasize that discreteness is not the signature of quantum mechanics. And these continuum states are as much as a part of your quantum Eigen value spectrum, as the discrete bound states patron. So, you can have a transition into the continuum, and when that happens the electron goes into the continuum, so what is left behind is an ion.

So, if you have a neutral atom, which observes energy and the electron is knocked down into the continuum, what is left behind is an ion, so this process is what you call as photoionization. So, essentially you can have either a bound to bound transition, from one bound state to another bound state, or you can have a bound to continuum transition. Of course, it could happen that a bound to bound transition is degenerate with bound to continuum, and when that happens you have resonances.

Because, it is like two processes which are accessible to the system at the same energy, because they are degenerate and then it is almost like a Young's Double-slit experiment. That you have got the possibility of light going through slit one or through slit two.

Student: ((Refer Time: 07:41))

The degeneracy is in these two processes, one is a bound to bound process, a transition from a bound state to a another bound state, the other process is bound to continuum. So, some electron in a many electronic system, may have a transition into the continuum at the same energy at which some other electron can undergo a transition from bound to bound. And then you have a degeneracy, because there are two processes, which can take place at the same energy.

And this is what I was comparing with Young's Double-slit experiment, in which you have two possibilities that light can go either from slit one or from slit two, when only one slit is open, you get a certain intensity distribution pattern. But, when both the slits are open you get interference and that is the signature of quantum mechanics, because that is what requires the principal of super position. So, that is a fundamental requirement in quantum mechanics, that you have the possibility in this case, you have a bound to bound process which is degenerate with the bound to continuum and both can take place. And you will then see interference which manifest as certain resonances, but these are questions of details, but these are the various processes which can take place, when a quantum system interacts with electrometric radiation.

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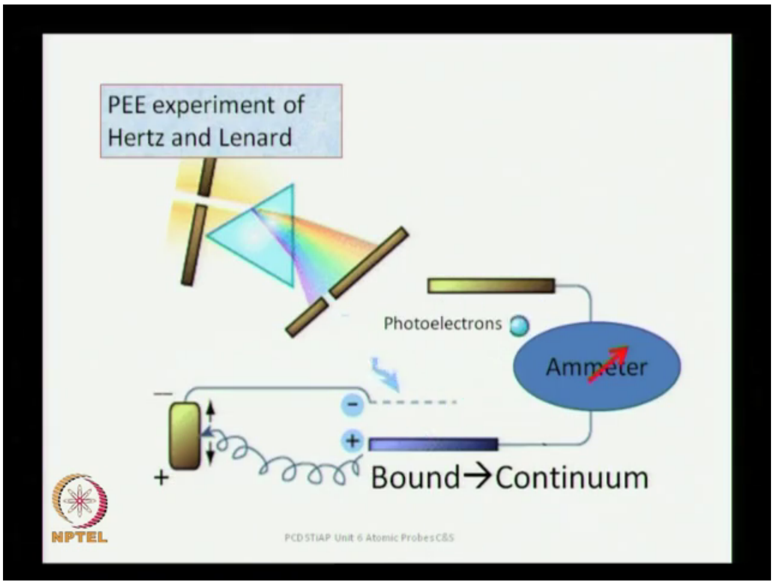
PEE experiment of Hertz and Lenard

So, this is a typical laboratory photoelectric effect experiment, which all of you would have done presumably that you have got a light source, you separate the frequencies by some sort of a prism or whatever. And then you have a metal plate from which electrons are knocked out, this is photo ionization, so electrons are knocked out. And then you can major the kinetic energy of the electrons using this retardation potential applied by a d c source.

So, that is the typical photoelectric effect experiment that you would have done, and essentially these electrons, which are coming out as a result of photo absorption, or what you call as photoelectrons. So, now, the question is what properties of the photoelectron can you measure, because the photoelectron is coming out, because of a certain transition from bound to continuum. And you can measure what is the probability that this process takes place, and that probability is then measured is appropriate units; and other terms to which the probability is proportional.

And then it is referred to as measurement of photo ionization cross section, you can also measure in which direction is the electron going, with reference to the direction of the electromagnetic radiation. The incident direction with reference to its direction of photo ionization, the electric intensity vector will have a certain direction. So, with reference to these two directions, what is the direction in which the photoelectron will come out, so when you study that, you measure the angular distributions.

And you would obviously, be interested in carrying out a complete experiment, you want to measure as much about this process as you can. So, you look for those processes, which are compatible with each other and that will give you a complete set of compatible observations, for the photoelectric effect measurement. So, you can measure the cross sections which is the transition probability, you can measure the angular distribution of the photoelectrons. And then there are some other properties which are also compatible with this, but I will not get into those details at this stage not yet.

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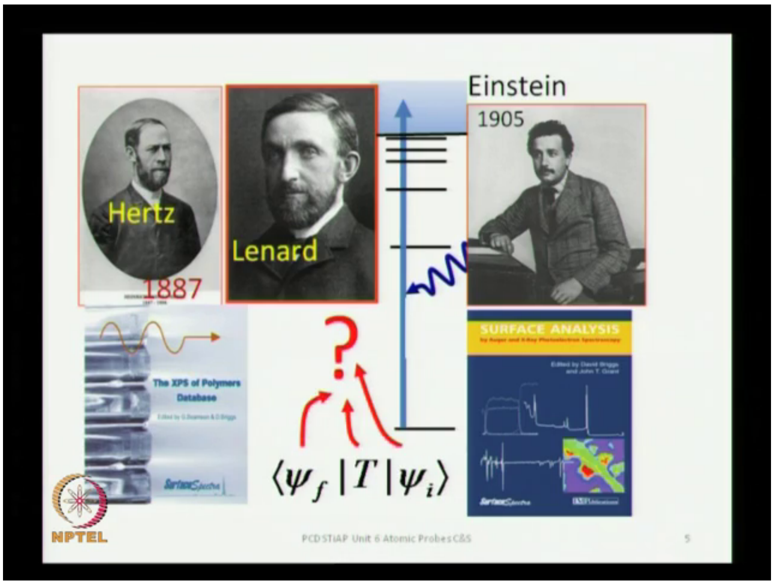

So, this experiment was first done by Hertz and Lenard in 1887, the explanation came in 1905 and it was Einstein's explanation, which really marked the beginnings of quantum mechanics, much more than Planck's interpretation. Almost 5 or 6 years before that, because Einstein really recognized the quantization of the electromagnetic field, which Plank had not. So, this is the photo ionization experiment and this is one tool that you can use, this has now developed into a very powerful tool to study condensed matter, you do surface analysis using photoelectrons.

And there are huge conferences international conferences and so on, which take place in this field and what you are doing is looking at a transition from a certain initial state to a certain final state. This is a matrix element of the transition, T is the transition matrix operator it is the physical interaction between the quantum system and the probe, which is responsible for this transition. And you could ask how do you describe the initial state, how do you describe the final state, and how do you represent the interaction itself, which is responsible for this transition.

And it is not easy to get exact solutions for this we already know that, so one has to make approximations to all of this, you make approximations to the initial state, you make approximations to the final state, you make approximations to the coupling. Represent all of this as best as you can, and that is what you do to find out what is this matrix element, which will be a measure of the probability amplitude. It will then it is modular square will give you the transition probability itself, and that will in some way be proportional to the intensity of that particular transition. So, these are the questions that you need to take up.

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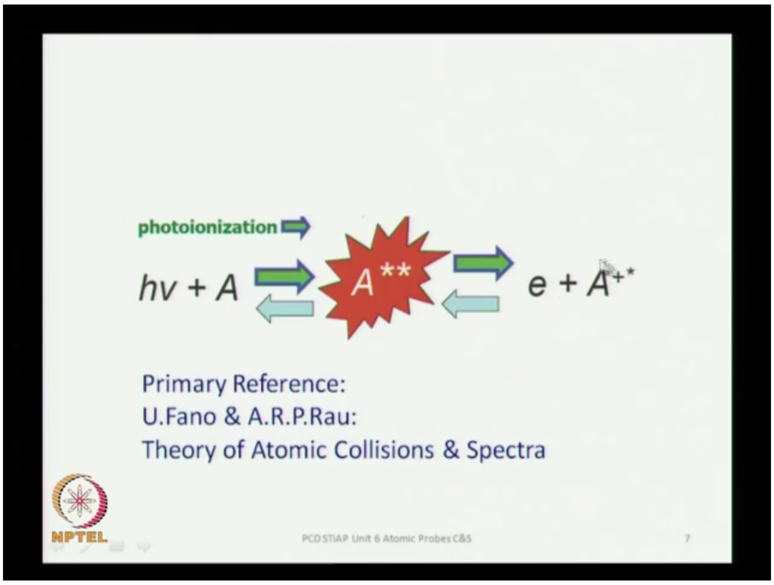

Primary Reference:
U.Fano & A.R.P.Rau:
Theory of Atomic Collisions & Spectra

And if you look at the photo ionization experiment, this is a typical event that you have got a photon, which is observed by a neutral atom. You have the formation of an excited state, and this excited state is represented by putting these two asterisks on A, which can then decay into an electron and an ion, which may also be in an excited state or it could be in a ground state. So, for the sake of generality I have placed an asterisk over here and two asterisks over here.

It is just suggestive of the fact that you may have different states of excitation, it is not that you have a unique excitation channel, so you have the photo ionization event, which is described like this. Now, this process of course, can take place backward as well, so there is no reason for the reverse process to take place. So, that is also governed by conservation laws and this can in fact take place, the other thing is that, if you look at the end product, what is this end product it is an electron and an ion.

You have got in your final state an electron and an ion, these two objects one is an electron and the other is an ion, these two objects are completely different from what you had in the initial state. In the initial state you had a photon and a neutral atom, so neither of their ingredients of the initial state or present in the final state and the products of the reaction did not exist in the initial state.

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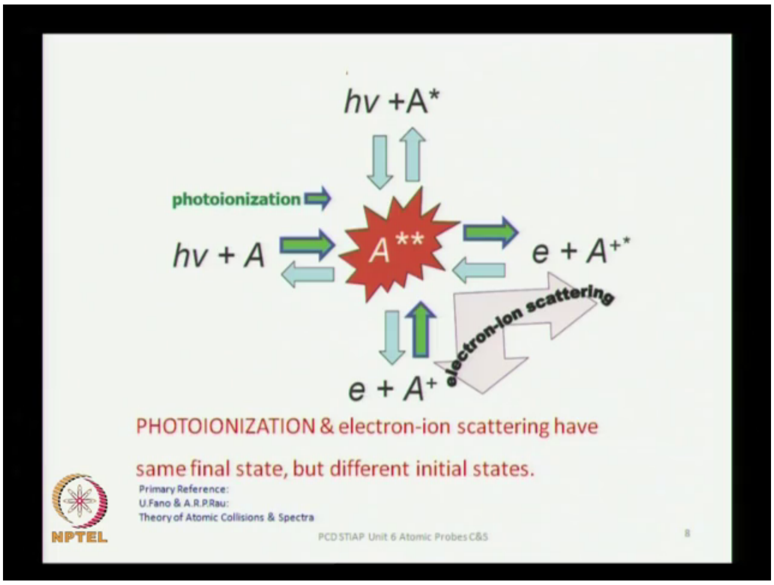

PHOTOIONIZATION & electron-ion scattering have same final state, but different initial states.

Primary Reference:
U.Fano & A.R.P.Rau:
Theory of Atomic Collisions & Spectra

But, can you not do an electron ion scattering experiment like this, you can begin with an initial state in which you have an ion. So, ion is your target and you fire electrons at it and this electron gets scattered, what do you have in the final state, you have an electron and you have an ion. So, the same final stage you can get, either through electron ion scattering also photon ionization, these are completely different processes, but they have got the same final state.

So, you can have different, this process will also be reversible, you can also have another channel over here. And an electron and ion can proceed in a reaction channel, from the bottom to the toper or from left to right or right to left or top to bottom any which way. So, there are all kinds of possibilities, which exist in process of this kind, so now here you have a representation of an electron ion scattering.

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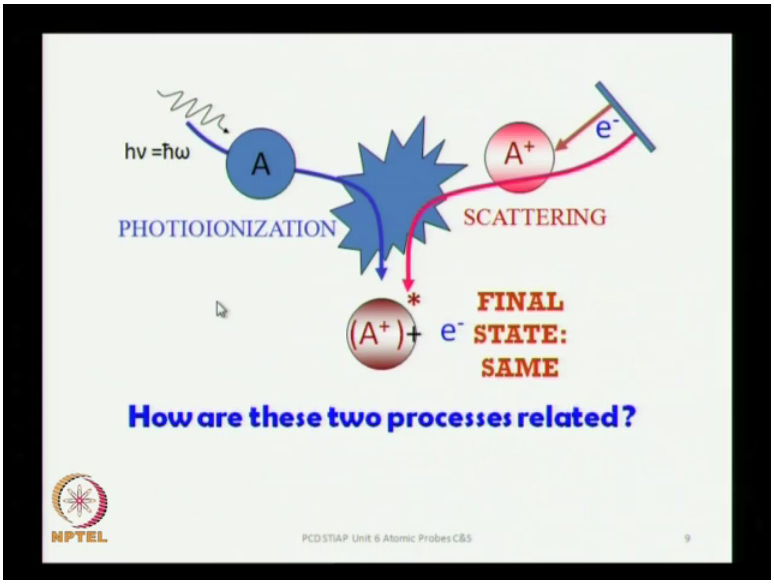

How are these two processes related?

You have an electron incident beam of plain waves, electrons, which are scattered by an ion, giving you a final state which is an ion possibly in an excited state not necessarily, although it could be. And an electron, but you can also get this same final state by the absorption of a photon by a neutral atom. So, how are these two processes related are they related at all and if so what is the relationship.

So, we need to investigate symmetries and atomic processes, and the symmetry that will be of importance in this case is the time reversal symmetry, we will eventually get to that, but before that we need to develop our tools for collision itself. So, what is peculiar to a collision experiment, because it is very important that you relate this quantum mechanics to an experiment, because that is what quantum mechanics is for, that is a very purpose of quantum mechanics.

So, you have got a target some atom and then you fire projectiles at it, the projectile that I am considering is a beam of mono energetic electrons and I have setup this experiment. So, I know where my target is, I know my electron gun is over here, and the electrons are coming only this way. And for the purpose of this experiment I know for a fact, that these electrons are coming from here to here, and certainly not from here to here, because that is how you have setup the experiment.

You can certainly set up the experiment in which you have the electron gun over here, but then this would be your entrance channel, and that would be unique. So, your entrance channel has got a unique direction in collisions, this scattered particles could then go in various directions, in almost any directional. All though the probability that they will go in different directions need not be uniform, it may show some an isotropy, so that is again a matter of detail that we will discuss once we get there.

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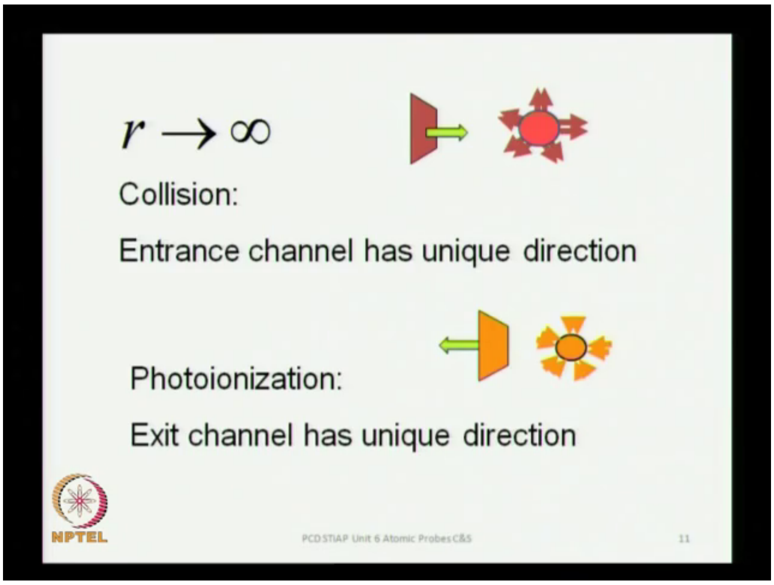

$r \rightarrow \infty$

Collision:

Entrance channel has unique direction

Photoionization:

Exit channel has unique direction

Whereas, in photoionization what do we have, we have got an atom and this atom has absorbed light and then an electron is knocked out into the continuum, and the detector would detect it. So, where have you kept the detector, the detector is here that side, and if you have detected the photoelectron, you know what the photoelectron is. If the photoelectron has been detected over here, then in this particular event, this electron had has gone only this way and not in any other, because this is the detector which has detected it.

So, it is the exit channel which has got a unique direction, so the boundary conditions for collisions and photo ionization are different, and we are going to discuss the boundary conditions for these two processes. One is called as the outgoing wave boundary conditions, the other is called has the ingoing wave boundary conditions, so we will study. The question is where was the photoelectron at T less than 0, if photo ionization took place at T is equal to 0 sometime, so that is your clock and you set T equal to 0 at that.

Where was the photoelectron, it did not exist as an electron, it does not exist as a free particle, so it just was not there it is a very similar to beta decay, in a beta decay when the nucleus gets it decays through a beta decay channel. An electron comes out it is not that the electron existed as an electron inside the nucleus, before the decay took place at T less than 0, if that is when the beta decay took place. So, this is a very similar to that and you, therefore do not really have an electron which existed as an independent free particle before T less than 0. So, you are going to generate some boundary conditions, which will simulate this effect.

So, you simulate it by seeing that it does not exist as a free electron, and if you have ingoing spherical wave, so that the flux going any in all directions, one going in this direction cancels, that going in the other direction right, one going in this direction cancels this flux going upward. So, that there is no net flux, but such an ingoing spherical wave could represent an electron in the initial state. So, this will become more clear, when we represent it using appropriate mathematical tools, so these boundary conditions are different.

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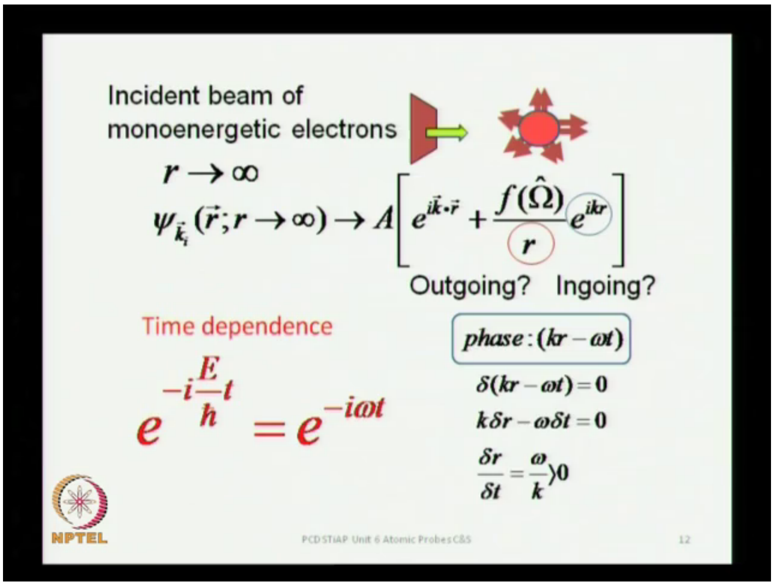

Incident beam of monoenergetic electrons

$$r \rightarrow \infty$$

$$\psi_{\vec{k}_i}(\vec{r}; r \rightarrow \infty) \rightarrow A\left[e^{i\vec{k}\cdot\vec{r}} + \frac{f(\hat{\Omega})}{r} e^{ikr}\right]$$

Outgoing? Ingoing?

Time dependence

$$e^{-i\frac{E}{h}t} = e^{-i\omega t}$$

$$\boxed{phase : (kr - \omega t)}$$

$$\delta(kr - \omega t) = 0$$

$$k\delta r - \omega \delta t = 0$$

$$\frac{\delta r}{\delta t} = \frac{\omega}{k} \rangle 0$$

NPTEL

And before we do that, we will first discuss collisions, which is where we really developed the machinery, so the first part of this unit will be on collisions and then we will go over to photoionization. So, this is the kind of the wave function that you will expect to get, because in the incident beam of mono energetic electrons will be represented by a plain wave. And then you have a scattered wave, which will go as each of the i k r over r multiplied by some function, which is a function of angles.

So, here you have got e to the i k r in the denominator you have put in 1 over r and that is a good thing to do, because the intensity will go as amplitude square, certain intensity will go as 1 over r square. And if it is spreading out in all the different directions, then the surface area of a sphere is goes as r square, so the flux in any solid angle will be conserved. So, the 1 over r takes care of that, then you have this e to the i k r, so 1 over r, we know what is the role of this 1 over r. What about each of the i k r, is it a spherical outgoing wave or is it an incoming, in this context incoming and ingoing are used synonymously.

So, now each of the i k r is it going in or is it going out, how do you decide whether it is going in or out, sin of what?

Student: k dot r

What about e to the i k dot r, let us look at the spherical wave later, look at the first one e to the i k dot r, which way is it going.

Student: ((Refer Time: 24:48))

If k, if you choose a coordinate system in which your z is along the direction of k, e z is along k, then k dot r will be k r cos theta, r cos theta will give you the z coordinate, so you have e to the i k z. Now, is it going along the positive z direction or is it going backward.

Student: ((Refer Time: 25:19))

How do you know that

Student: Actually through the phase constant, the phase is concerned, so if we derivative with respect to k, which can find out the relation (( )) of omega and r t, omega by (( )).

So, now do the same for the each of the i k r, because whether it is going along the positive z direction or opposite to that, whenever you talk about travelling waves, a travel must involve time. It has to proceed from t 1 to t 2 and where was it at t 1 and where is it at t 2 is what will determine. So, without reference to time, you cannot really answer these questions at all, and depending on how the time dependence is indicated based on that, you can determine, if this is going along the positive z axis or it could also go along the negative z axis.

Because, it depends on how you have defined your time axis, so you have to indicate that, so here in our time dependence Schrodinger equation, the stationary states are represented by e to the minus i omega t. So, there is a time dependence, so the net phase for the spherical wave is k r minus omega t, ((Refer Time: 26:45)) this is e to the i k r, this is e to the minus i omega t. So, the next phase is k r minus omega t, this is the minus sign here, so now you ask how does the surface of constant phase propagate, what is that that determines the surface of constant phase.

For the surface of constant phase the variation the change in k r minus omega t must be 0, so k delta r minus omega delta t must be 0 and delta r by delta t is positive, because omega in k are intrinsically positive. So, if delta r and delta t, this ratio is positive, then as time increases r must increase delta r is r 2 minus r 1, r 2 is where the surface is at time t 2, r 1 is where the surface was at time t 1, so r 2 minus r 1, which is delta r that must be positive, which means that this surface of constant phase is propagating outward.

So, this is an outgoing wave with reference to the time dependence, which must be considered, so this is your typical collision experiment the fiction, that you have got a plane incident wave which is moving from left to right, and this is the direction of the z axis that we have chosen in our diagram. And then you have scattered waves, but then there will be an amplitude function, which depends on the angle and in general, it could depend on angles because there is no reason that scattering would be essentially as a tropic it may or may not be.

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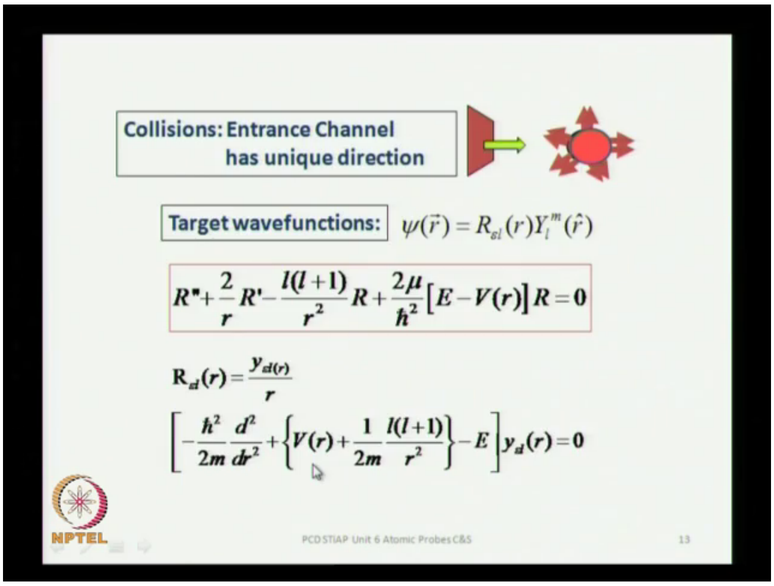

Collisions: Entrance Channel has unique direction

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

$$\boxed{R'' + \frac{2}{r}R' - \frac{l(l+1)}{r^2}R + \frac{2\mu}{\hbar^2}\left[E - V(r)\right]R = 0}$$

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

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

So, now let us look at the target wave functions, what we have learned so far is that, in a collision experiment you have got a unique entrance channel, you have got scattered waves and the target wave functions, which is an atomic system for our consideration. You can represent this, you can factor the radial dependence from the angular dependence as you always do, the angular part you have solved the problem as spherical harmonics. So, those solutions are available at your disposal at your fingertips and then you look at the solutions to the radial part.

So, you separate out the radial part of the wave function, and find that it must satisfy a certain radial differential equation, so this is your radial Schrodinger equation. So, now it is convenient to write the radial function as a ratio of i over r, so you just factor out 1 over r out of it. This is just a matter of mathematical elegance, and this condition requires a certain equation to be satisfied by y that differential equation, but y must satisfy is what you have over here. So, this is the differential equation that y must satisfy, all you do is to substitute this y over r get the first derivative, the second derivative plug it in and then cancel out the common terms this is what you get.

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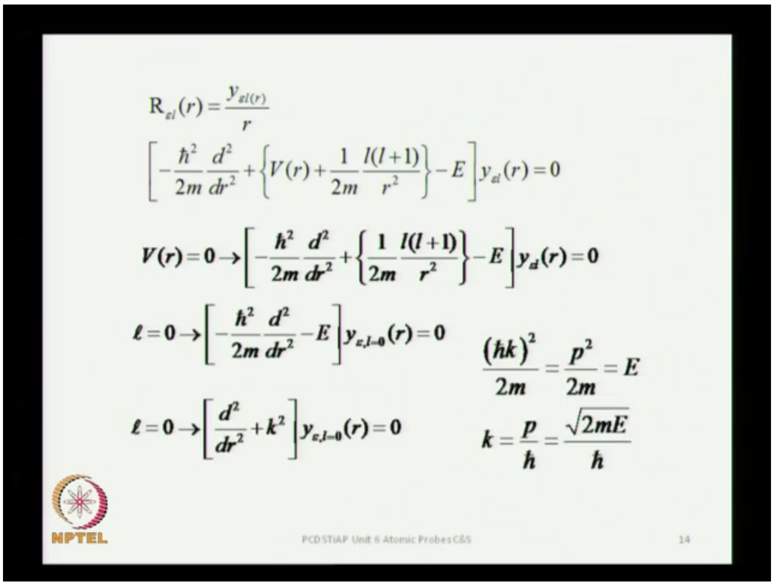

$$R_{\varepsilon l}(r) = \frac{y_{\varepsilon l(r)}}{r}$$

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

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

$$\ell = 0 \rightarrow \left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} - E\right] y_{\varepsilon,l=0}(r) = 0 \qquad \frac{(\hbar k)^2}{2m} = \frac{p^2}{2m} = E$$

$$\ell = 0 \rightarrow \left[\frac{d^2}{dr^2} + k^2\right] y_{\varepsilon,l=0}(r) = 0 \qquad k = \frac{p}{\hbar} = \frac{\sqrt{2mE}}{\hbar}$$

So, this is the differential equation that must be satisfied by y, so it has it is contents are completely based on the radial Schrodinger equation, it has got all the strength of the Schrodinger equation. And to get an idea of our solutions, we will deal with some peculiar cases, let us consider V equal to 0 that is also a spherical potential, it is got the same value in all directions. So, 0 potential you already know the solutions, when there is no potential, you have a free particle and the solution to the Schrodinger equation for a free particle is the plane wave, e to the i k dot r, you already know the solution.

So, we will deal with V of r equal to 0 is a special case, for which we know the solution, so in this equation, in this differential equation I put V equal to 0, so I get the equation without the potential now, so this is the equation for the free particle. Further more I take another special case in which I deal only with l equal to 0, the S waves; l equal to 0 is S, l equal to 1 is P and then you have D and F and so on. So, we will deal with just the S wave solutions that is the simplest one that is the, so that you can throw off the centrifugal term altogether; the l into l plus 1 by r square term can be thrown for l equal to 0.

So, now you have got a very simple differential equation, which is not only these two terms the kinetic energy term, and you can solve this differential equation in your mind and you know what the solutions are. So, the reason to do this, it turns out to be extremely advantageous, because you can get solutions to higher l values, for l equal to 1, you are certainly interested in solutions for l equal to 1, 2, 3, 4 everything. But, it will turn out that all of those solutions can be obtained from the l equal to 0 solution, so this is like a generic solution. So, this is the most important case and it is very simple, so this is the equation for l equal to 0, the solution you can write in terms of k.

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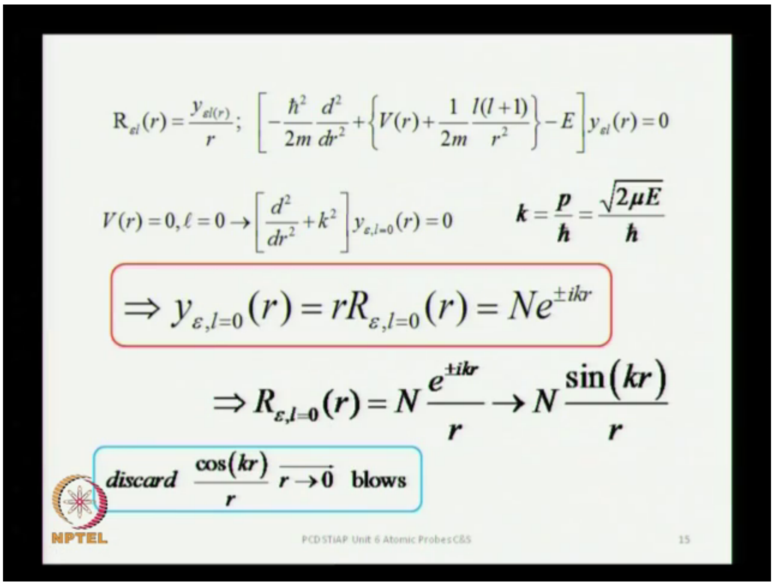

$$R_{\varepsilon l}(r)=\frac{y_{\varepsilon l(r)}}{r};\quad \left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+\left\{V(r)+\frac{1}{2m}\frac{l(l+1)}{r^2}\right\}-E\right]y_{\varepsilon l}(r)=0$$

$$V(r)=0,\ell=0\rightarrow\left[\frac{d^2}{dr^2}+k^2\right]y_{\varepsilon,l=0}(r)=0 \qquad k=\frac{p}{\hbar}=\frac{\sqrt{2\mu E}}{\hbar}$$

$$\boxed{\Rightarrow y_{\varepsilon,l=0}(r)=rR_{\varepsilon,l=0}(r)=Ne^{\pm ikr}}$$

$$\Rightarrow R_{\varepsilon,l=0}(r)=N\frac{e^{\pm ikr}}{r}\rightarrow N\frac{\sin(kr)}{r}$$

$$\boxed{discard\ \frac{\cos(kr)}{r}\ \xrightarrow[r\rightarrow 0]{}\ \text{blows}}$$

And this solution is essentially this e to the plus or minus i k r, this is the solution to the differential equation for Y. Now, this e to the i k r is a combination of cosine and sin functions, out of which since the radial function is, this solution divided by r there was 1 over r, and this cosine k r over r would blow up as r goes to 0, that is not what you want. So, you throw the cosine part of the solution and your solution is really sin k r over r multiplied by some normalization consent, so that is your solution you already have your radial solution for l equal to 0 for the free particle.

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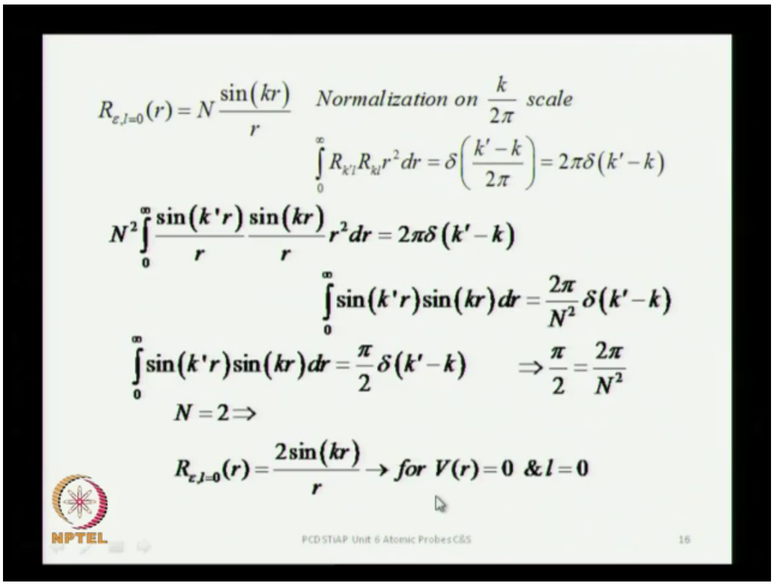

$R_{\varepsilon,l=0}(r) = N\frac{\sin(kr)}{r}$ *Normalization on* $\frac{k}{2\pi}$ *scale*

$$\int_0^\infty R_{k'l}R_{kl}r^2dr = \delta\left(\frac{k'-k}{2\pi}\right) = 2\pi\delta(k'-k)$$

$$N^2\int_0^\infty \frac{\sin(k'r)}{r}\frac{\sin(kr)}{r}r^2dr = 2\pi\delta(k'-k)$$

$$\int_0^\infty \sin(k'r)\sin(kr)dr = \frac{2\pi}{N^2}\delta(k'-k)$$

$$\int_0^\infty \sin(k'r)\sin(kr)dr = \frac{\pi}{2}\delta(k'-k) \qquad \Rightarrow \frac{\pi}{2} = \frac{2\pi}{N^2}$$

$N = 2 \Rightarrow$

$$R_{\varepsilon,l=0}(r) = \frac{2\sin(kr)}{r} \rightarrow for\ V(r)=0\ \&\ l=0$$

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So, this cannot be normalized, because these are non-squared integral functions, normalization involves integration over whole space of psi star psi d v, now if psi is e to the i theta, psi star is e to the minus i theta, psi star psi gives you 1. And then what your doing is adding up those volume elements delta v over the whole space or going from 0 through infinity, so the integral blows up. So, these wave functions are normalized using the delta function integration, which I mentioned in unit 1.

And the direct delta normalization for two different radial functions, one with k and the other with k prime, this is called as normalization on the k over 2 pi scale, so the radial functions are normalized on the k over 2 pi scale. So, this integral is twice pi derived delta k prime minus k and since, ((Refer Time: 34:59)) this is n sin k r over r you get n square sin k prime r over r, the integrant is a product of this function with another one. And then you have got the volume element, which the radial volume element is r square d r, in the spherical polar coordinate system. So, this is your integration, note is that this r square will cancel the 1 over r and the 1 over r over here.

So, what you have is just an integration from 0 through infinity of a product of these two sin function, given by this derived delta normalization. Now, you can carry out this integration explicitly, and this integration sin k prime r sin k r d r. The expressive mathematical integration of this will of course, give you the delta function, which is pi by 2, which means that this 2 pi over N square must be equal to pi over 2 and that tells you what the normalization constant is. So, what is a normalization constant, it must be equal to 2, the normalization constant N must be equal to 2.

So, the radial function this is the normalized function, normalized according to the derived delta, normalization over the k over 2 pi scale. So, this radial function is twice sin k r over r, this is for the free particle V r equal to 0, this is the S wave solution for l equal to 0.

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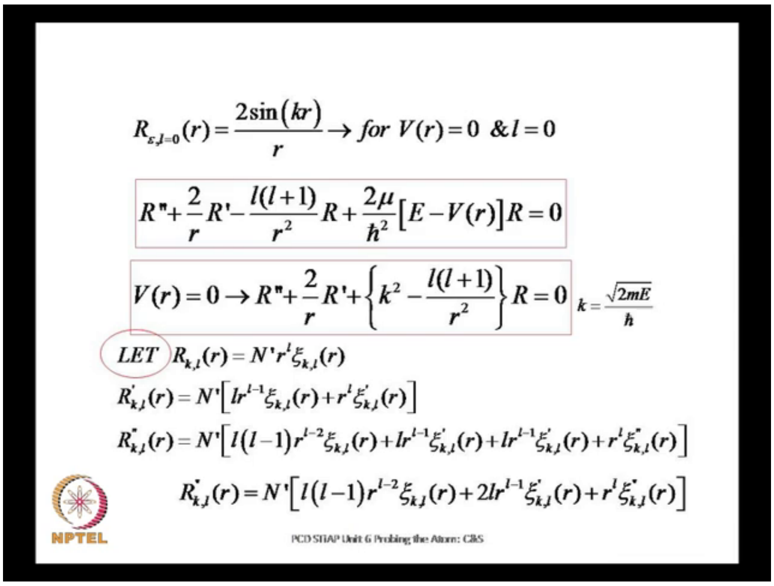

$$R_{\varepsilon,l=0}(r)=\frac{2\sin(kr)}{r}\rightarrow for\ V(r)=0\ \&\ l=0$$

$$\boxed{R''+\frac{2}{r}R'-\frac{l(l+1)}{r^2}R+\frac{2\mu}{\hbar^2}\left[E-V(r)\right]R=0}$$

$$\boxed{V(r)=0\rightarrow R''+\frac{2}{r}R'+\left\{k^2-\frac{l(l+1)}{r^2}\right\}R=0}\ k=\frac{\sqrt{2mE}}{\hbar}$$

$LET\ R_{k,l}(r)=N'r^l\xi_{k,l}(r)$

$$R'_{k,l}(r)=N'\left[lr^{l-1}\xi_{k,l}(r)+r^l\xi'_{k,l}(r)\right]$$

$$R''_{k,l}(r)=N'\left[l(l-1)r^{l-2}\xi_{k,l}(r)+lr^{l-1}\xi'_{k,l}(r)+lr^{l-1}\xi'_{k,l}(r)+r^l\xi''_{k,l}(r)\right]$$

$$R''_{k,l}(r)=N'\left[l(l-1)r^{l-2}\xi_{k,l}(r)+2lr^{l-1}\xi'_{k,l}(r)+r^l\xi''_{k,l}(r)\right]$$

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So, we have got this for our interest is of course, is in the full problem not in these special cases, so we have to go from the special case to the general case. So, we will do it again in steps what we will do is, we will now retain the centrifugal potential term. So, that l is not equal to 0 anymore, but we will still deal with V equal to 0 and then at a later stage of course, we have to put in the target potential. So, this is your radial equation for the free particle, but for all values of l including l equal to 0, but also higher values of l.

So, what I propose is let this radial solution be given by this, essentially what I have done is I know that there is a certain r dependence of the function, from this r dependence I factor out r to the power l. And then there is some residual r dependence, I have no idea what that is, whatever it is, it is called as psi of r, so the radial function keep track of the subscripts, it will depend parametrically on the energy, and therefore on k. It will depend parametrically on the l quantum number, because it is different for different l values and then this is actually a function of r, of which the r to the l dependence is factored out the remaining residual r dependence in psi of r and then there is some normalization which I have written as N prime, whatever it is.

Because, once you have any function to the differential equation that multiplied by any constant is also a solution, so N prime is some normalization constant. And for this I can find what the first derivative of r is by taking the derivative of a product of these two functions r to the l and psi, I can likewise get the second derivative. And then put the function and the first derivative and the second derivative respectively over here, this is where the function comes, this is where the first derivative comes, this is where the second derivative comes.

And I will get a differential equation that must be satisfied by the function psi of r by after you cancel out the common terms. So, you can simplify combine various terms of these, there are two terms of this kind which combine over here to give this l r to the power l minus 1 psi time with a factor of 2. So, that is just a matter of simple substitution.

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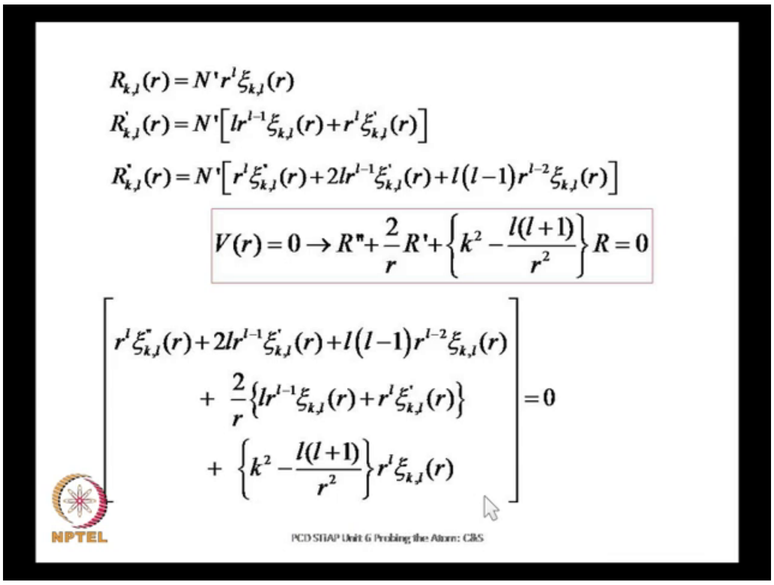

$$R_{k,l}(r) = N' r^l \xi_{k,l}(r)$$

$$R'_{k,l}(r) = N'\left[l r^{l-1}\xi_{k,l}(r) + r^l \xi'_{k,l}(r)\right]$$

$$R''_{k,l}(r) = N'\left[r^l \xi''_{k,l}(r) + 2l r^{l-1}\xi'_{k,l}(r) + l(l-1) r^{l-2}\xi_{k,l}(r)\right]$$

$$\boxed{V(r) = 0 \rightarrow R'' + \frac{2}{r}R' + \left\{k^2 - \frac{l(l+1)}{r^2}\right\}R = 0}$$

$$\left[\begin{array}{l} r^l \xi''_{k,l}(r) + 2l r^{l-1}\xi'_{k,l}(r) + l(l-1) r^{l-2}\xi_{k,l}(r) \\ \quad + \dfrac{2}{r}\left\{l r^{l-1}\xi_{k,l}(r) + r^l \xi'_{k,l}(r)\right\} \\ \quad + \left\{k^2 - \dfrac{l(l+1)}{r^2}\right\} r^l \xi_{k,l}(r) \end{array}\right] = 0$$

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And the differential equation that psi must satisfy is this, so this is something that you can work out take your time to do it, it will take you about anywhere between 17 to 19 seconds. Or whatever time it does when you do this at home, which your of course, expected to do.

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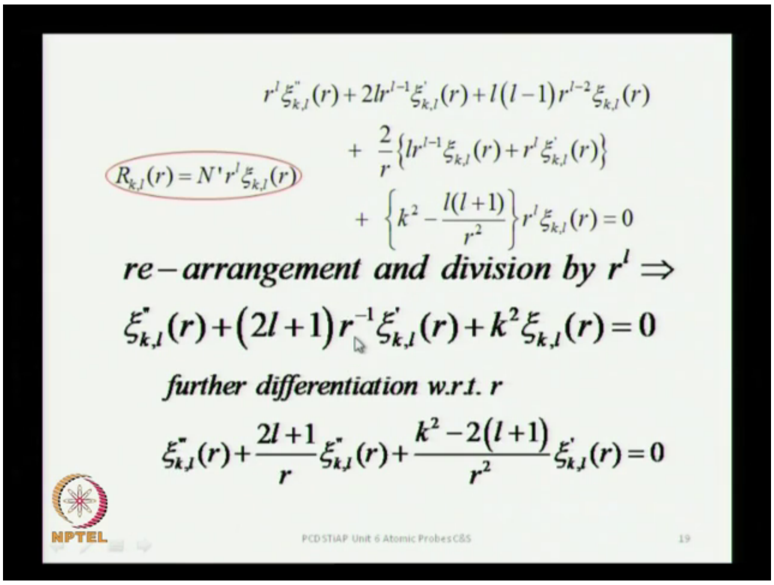

$$r^l \xi''_{k,l}(r) + 2l r^{l-1} \xi'_{k,l}(r) + l(l-1) r^{l-2} \xi_{k,l}(r)$$

$$+ \frac{2}{r}\left\{ l r^{l-1} \xi_{k,l}(r) + r^l \xi'_{k,l}(r) \right\}$$

$$+ \left\{ k^2 - \frac{l(l+1)}{r^2} \right\} r^l \xi_{k,l}(r) = 0$$

$$\boxed{R_{k,l}(r) = N' r^l \xi_{k,l}(r)}$$

$$re-arrangement\ and\ division\ by\ r^l \Rightarrow$$

$$\xi''_{k,l}(r) + (2l+1) r^{-1} \xi'_{k,l}(r) + k^2 \xi_{k,l}(r) = 0$$

further differentiation w.r.t. r

$$\xi'''_{k,l}(r) + \frac{2l+1}{r} \xi''_{k,l}(r) + \frac{k^2 - 2(l+1)}{r^2} \xi'_{k,l}(r) = 0$$

So, you rearrange the terms cancel out the common terms divide by r to the l, the differential equation that psi must satisfy it is a very simple equation, and you understand precisely how we have got it. This differential equation has got all the strength of the Schrodinger equation, let us come straight out of it, so far is it is physical content is concerned, it is as good as a Schrodinger equation itself. Now, we borrow some tricks, which have been developed by mathematicians and these are very powerful tricks, very elegant tricks, very simple tricks.

The whole reason to do this is because we want to get the solution for an arbitrary l, we have got the explicit solution for a l equal to 0. So, now we are trying to look for some mechanism to get a solution for the next l from the previous l, and if we could do that, then we could get the solution for l equal to 1 from the solution for l equal to 0, which we have with us and then for l equal to two from l equal to 1 and so on. And then we have the general solution, so we are going to look for some recursion relations, and the way mathematicians develop these recursion relations, they often go to higher order differential equations.

So, here you have got a second order differential equation in psi, you go to the third order differentiate the whole equation one more time, so you get psi triple prime, a prime denotes differentiation with r in our notation here. So, this is the third derivative of psi with respect to r and then you take the derivative of these terms you have got a 1 over r here, so that will give you 1 over minus 1 over r square you will get it psi double prime over here. So, you keep track of all the terms, combine common terms and then you get a differential equation for psi, which is the third order differential equation for psi.

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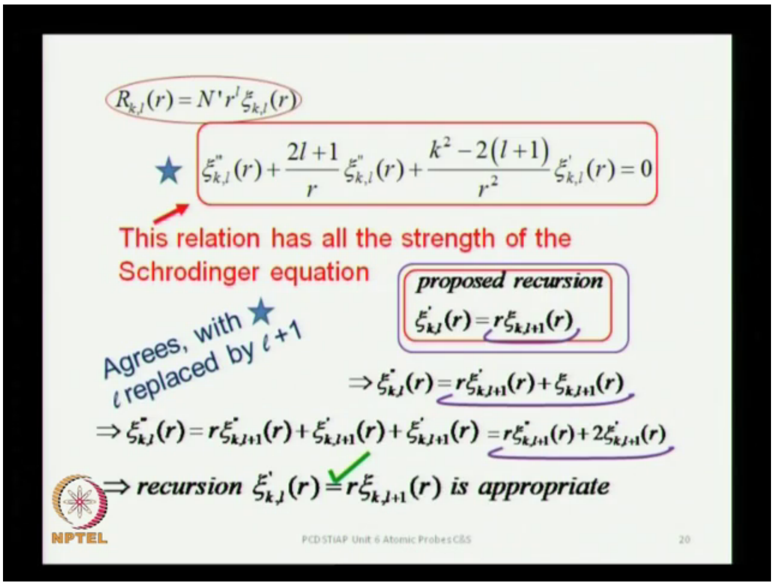

$R_{k,l}(r) = N' r^l \xi_{k,l}(r)$

★ $\boxed{\xi'''_{k,l}(r) + \frac{2l+1}{r}\xi''_{k,l}(r) + \frac{k^2 - 2(l+1)}{r^2}\xi'_{k,l}(r) = 0}$

This relation has all the strength of the Schrodinger equation

proposed recursion

$\xi'_{k,l}(r) = r\xi_{k,l+1}(r)$

Agrees, with ★ l replaced by $l+1$

$\Rightarrow \xi''_{k,l}(r) = r\xi'_{k,l+1}(r) + \xi_{k,l+1}(r)$

$\Rightarrow \xi'''_{k,l}(r) = r\xi''_{k,l+1}(r) + \xi'_{k,l+1}(r) + \xi'_{k,l+1}(r) = r\xi''_{k,l+1}(r) + 2\xi'_{k,l+1}(r)$

$\Rightarrow$ *recursion* $\xi'_{k,l}(r) \overset{\checkmark}{=} r\xi_{k,l+1}(r)$ *is appropriate*

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Now, this third order differential equation for psi, the 3 psi by d r 3, it has all the strength of quantum mechanics. Now, what we are going to do is propose a recursion relation in which the next value for l equal to l plus 1, look at the subscript here, the prime meters which were denoted as subscripts, energy is a prime meter, which is represented by k is h cross square k square by 2 m for the free particle. And then the other prime meter is l which is coming from the centrifugal term in the Schrodinger equation. So, the solution for psi for the next l, if it is related to the solution for the previous l through this relation, which is psi prime k l equal to r time psi k l plus 1, if this relation is valid.

We are not assuming that it is valid, we are enquiring if it is a valid recursion relation, nothing stops you from making an enquiry that is what study is about, so we enquire if this recursion relation will turn out to be a valid relation, so how do you check it out. So, you take the second derivative from this, so the second derivative is r times psi prime plus psi fair enough. Now, you can take the third derivative do the same thing, and now you have got this you can combine these terms, these two terms are the same.

So, you get a twice psi prime over here and now, you can take this term which is r psi for psi prime, you can take this term for psi double prime and this term for psi triple prime. And put them back in this equation, in which you do not change these numbers, so if you did that do you get a consistent result with the relation for psi prime, what do you meant by consistent relation. Because, what you have in this red loop is a differential equation for the third derivative of psi, and there are terms in the second derivative and also in the first derivative, and the sum of these three terms appropriate factors is equal to 0.

So, now it turns out that, if you replace ((Refer Time: 45:42)) this triple derivative, this double derivative and this derivative with theses three terms, you find that along with these factors, you recover the same differential equation. But, l replaced by l plus 1 which is fine, which means that your recursion relation is quite appropriate, now that is a great help. Because, you have already got the solution for l equal to 0 and then from that recursion relation you can get the solutions for higher values of l, so this recursion relation is quite appropriate that is our conclusion.

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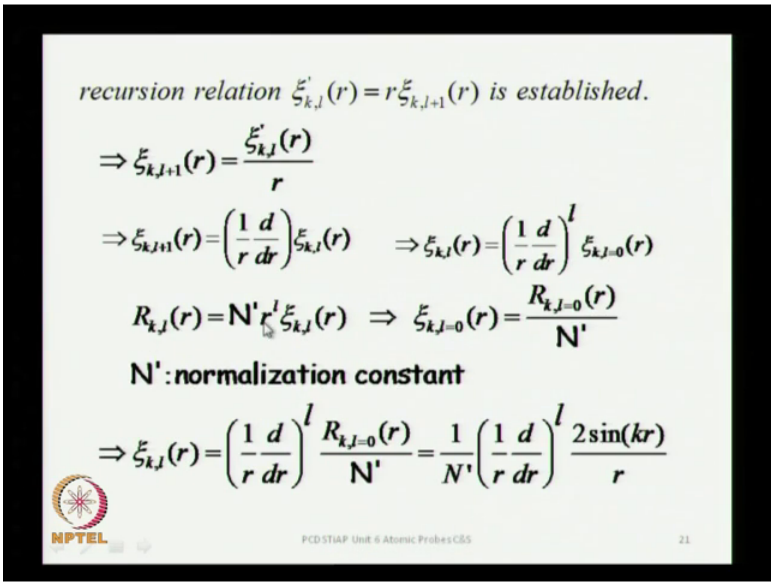

recursion relation $\xi'_{k,l}(r) = r\xi_{k,l+1}(r)$ *is established.*

$$\Rightarrow \xi_{k,l+1}(r) = \frac{\xi'_{k,l}(r)}{r}$$

$$\Rightarrow \xi_{k,l+1}(r) = \left(\frac{1}{r}\frac{d}{dr}\right)\xi_{k,l}(r) \qquad \Rightarrow \xi_{k,l}(r) = \left(\frac{1}{r}\frac{d}{dr}\right)^{l}\xi_{k,l=0}(r)$$

$$R_{k,l}(r) = \mathrm{N}' r^{l}\xi_{k,l}(r) \Rightarrow \xi_{k,l=0}(r) = \frac{R_{k,l=0}(r)}{\mathrm{N}'}$$

N': normalization constant

$$\Rightarrow \xi_{k,l}(r) = \left(\frac{1}{r}\frac{d}{dr}\right)^{l}\frac{R_{k,l=0}(r)}{\mathrm{N}'} = \frac{1}{N'}\left(\frac{1}{r}\frac{d}{dr}\right)^{l}\frac{2\sin(kr)}{r}$$

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We will use it to get solutions for the higher l values, and this relation you divide you take r on this side, so psi for the l plus 1, this is the solution for the next value of l, this is given by the derivative of the previous value for l divided by r. So, what is your prescription how you get the solution for l plus 1 from l, you take the solution for l and operate on this by 1 over r d over d r, so that is your operator. So, the solution for the l itself is obtained from the solution for l equal to 0 by operating by this operator l times, that is your prescription.

And now you have solved the whole problem, because you have got the solution for l equal to 0, and now you can operate on that solution l times by the operator 1 over r d by d r. So, this is your solution now, the solution for l equal to 0 is this r divided by some normalization whatever it is, and what you have to do is to operate on this solution for l equal to 0 l times a 1 over r d over d r to the power l, this is what will give you the solution for l. And then the radial solution itself is obtained by multiplying this by r to the power l, because that is what we had earlier factored out.

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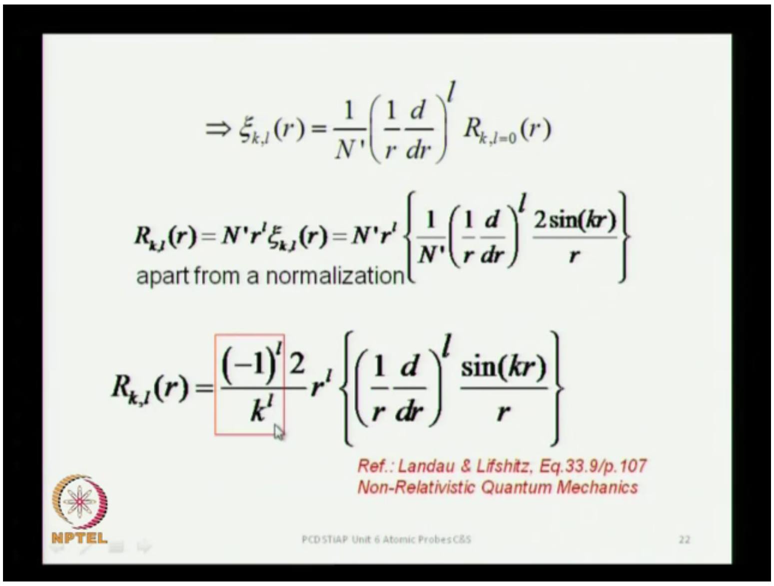

$$\Rightarrow \xi_{k,l}(r) = \frac{1}{N'}\left(\frac{1}{r}\frac{d}{dr}\right)^{l} R_{k,l=0}(r)$$

$$R_{k,l}(r) = N' r^{l} \xi_{k,l}(r) = N' r^{l} \left\{\frac{1}{N'}\left(\frac{1}{r}\frac{d}{dr}\right)^{l} \frac{2\sin(kr)}{r}\right\}$$

apart from a normalization

$$R_{k,l}(r) = \frac{(-1)^{l}\,2}{k^{l}} r^{l} \left\{\left(\frac{1}{r}\frac{d}{dr}\right)^{l} \frac{\sin(kr)}{r}\right\}$$

Ref.: Landau & Lifshitz, Eq.33.9/p.107
Non-Relativistic Quantum Mechanics

So, this is your prescription which is to operate l times by the operator 1 over r d over d r, apart from some normalization, there will be some normalization caution, which can be always be plugged in. The normalization which is used is minus 1 to the l k to the l and this is for a certain reason, which will become clear very shortly that normalization we only know has to be independent of r, it can depend on l and k parametrically. So, this is what is chosen and why this is chosen will become clear, and this will be your solution for all the partial waves.

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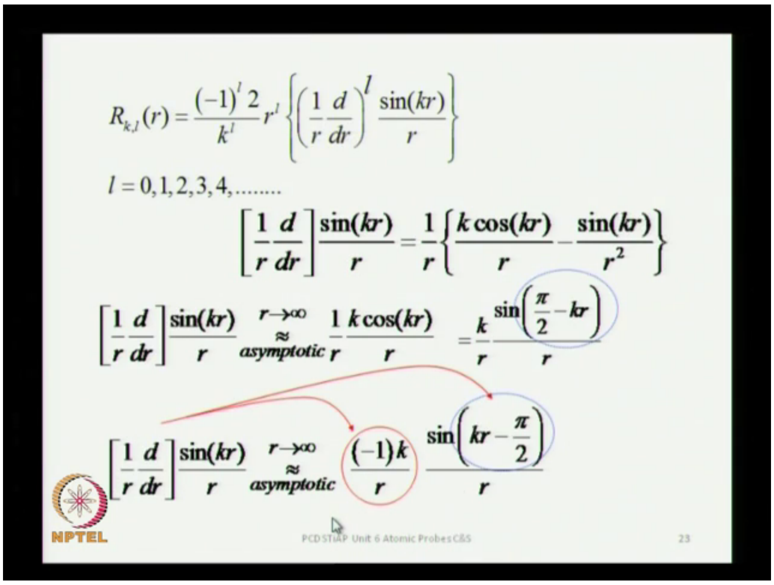

$$R_{k,l}(r) = \frac{(-1)^l 2}{k^l} r^l \left\{ \left(\frac{1}{r} \frac{d}{dr} \right)^l \frac{\sin(kr)}{r} \right\}$$

$l = 0,1,2,3,4,\ldots\ldots$

$$\left[\frac{1}{r} \frac{d}{dr} \right] \frac{\sin(kr)}{r} = \frac{1}{r} \left\{ \frac{k\cos(kr)}{r} - \frac{\sin(kr)}{r^2} \right\}$$

$$\left[\frac{1}{r} \frac{d}{dr} \right] \frac{\sin(kr)}{r} \underset{asymptotic}{\overset{r \to \infty}{\approx}} \frac{1}{r} \frac{k\cos(kr)}{r} = \frac{k}{r} \frac{\sin\boxed{\left(\frac{\pi}{2} - kr \right)}}{r}$$

$$\left[\frac{1}{r} \frac{d}{dr} \right] \frac{\sin(kr)}{r} \underset{asymptotic}{\overset{r \to \infty}{\approx}} \boxed{\frac{(-1)k}{r}} \frac{\sin\boxed{\left(kr - \frac{\pi}{2} \right)}}{r}$$

For l equal to 0, 1, 2, 3 no matter what, this is your most general solution, now let us see what 1 over r d over d r does to this, this is your l equal to 0 solution, sin k r over r what does 1 over r d over d r do to this. So, you take the derivative of sin k r over r, the derivative is k cos k r over r minus sin k r over r square, now why are you doing this, to investigate collision phenomena. And what is a collision phenomenon, what does it involve, you got a target you have an incident beam of electrons.

Then this gets scattered and then you are going to carry out measurements of the scattered particle by having some detector where are you placing this detector, how close to the target, it is certainly has to be well beyond the scattering region. You are detector has to be well away from it, so for all practical purposes it is at infinity, it is in the asymptotic region, it could be for a given experiment, it could be 10 centimeters, if the range of interaction is only a few form is or few ions toms.

But, then for our practical purposes, the region you are really interested in this experiment is that you perform the measurements, you carry out your detection at a distance which is sufficiently far from the scattering region. It cannot be a part of the scattering potential region, so it is situated well away from the r equal to 0 place. And what is the meaning of well away, well away does not mean 10 centimeters or 10 kilometers, it means it is sufficiently far well beyond the target potential, the region of influence of the scattering potential.

That region is effectively, so far as this purpose is concerned at infinity, it is a very large distance, it is much larger than any other region, you have to be concerned about for the analysis of this experiment.

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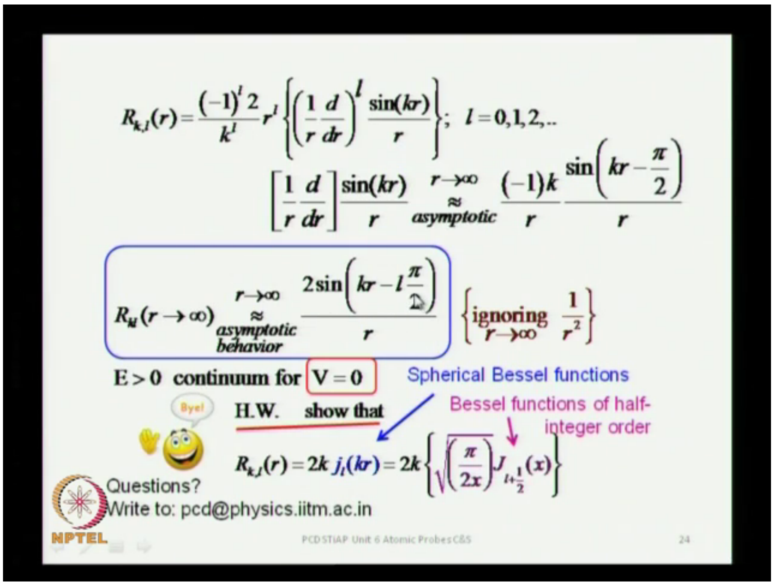

$$R_{k,l}(r)=\frac{(-1)^l 2}{k^l}r^l\left\{\left(\frac{1}{r}\frac{d}{dr}\right)^l\frac{\sin(kr)}{r}\right\};\ l=0,1,2,..$$

$$\left[\frac{1}{r}\frac{d}{dr}\right]\frac{\sin(kr)}{r}\ \underset{asymptotic}{\overset{r\to\infty}{\approx}}\ \frac{(-1)k}{r}\frac{\sin\left(kr-\frac{\pi}{2}\right)}{r}$$

$$\boxed{R_{kl}(r\to\infty)\ \underset{\substack{asymptotic\\behavior}}{\overset{r\to\infty}{\approx}}\ \frac{2\sin\left(kr-l\frac{\pi}{2}\right)}{r}}\ \left\{\underset{r\to\infty}{\text{ignoring}}\ \frac{1}{r^2}\right\}$$

$\mathrm{E}>0$ continuum for $\boxed{\mathrm{V}=0}$

Spherical Bessel functions

Bessel functions of half-integer order

H.W. show that

$$R_{k,l}(r)=2k\,j_l(kr)=2k\left\{\sqrt{\left(\frac{\pi}{2x}\right)}J_{l+\frac{1}{2}}(x)\right\}$$

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

And if it is so far, then 1 over r square term will be negligible compared to the 1 over r term, so in this solution you can throw off the second term, which is sin k r over r square, that is what you get from the derivative. But, in the asymptotic region well away from the scattering region, the solution is then only 1 over r k cos k r over r. But, your solution for l equal to 0 was a sin function, the solution that your getting has got a cosine function, but what the heck it would be nice, if it is the same.

And the cosine function is in fact, the same as the sin function except for a phase shift, so plug in that phase shift, so this will be sin of pi by 2 minus k r. So, that it also becomes a sinusoidal function, but your original function was a function of k r and not minus k r, so change the sin of this angle. So, instead of pi by 2 minus k r, make it k r minus pi by 2 that will pick up a minus 1 sin here, and now you have got a prescription that the effect of this operator 1 over r d over d r is essentially this, you get the same solution sign k r over r, with the difference that the function must be multiplied by minus times minus 1 times.

It must be multiplied by k, it must be divided by r and the angle the phase must drop by pi by 2, now this is the result of the operator 1 over r d by d r, effectively the operator 1 over r d over d r is equivalent to multiplication by minus k over r. And simultaneous change of the phase shift from k r to k r minus pi by 2 and to get the lth solution, you have to do this l times. So, every time you do this there will be a phase shift of pi by 2, so every time you do this the phase shift will keep dropping by pi by 2, so your r angle over here will be k r minus l pi by 2.

You have ignored o1 over r square term every time, you have ignored 1 over r square compared to 1 over r, and this is your solution for E greater than 0, these are the positive energy states, the scattering states for a free particle. And this is where I will conclude today's class that this is your most general solution, now you will see that this choice of normalization is rather convenient, this r to the l will cancel the 1 over r to the l coming out of this.

This 1 over k to the l that we had included in the normalization will cancel the k to the power l, because every time you take a derivative, you are going to multiple by a factor of k, when you do it l times you will get k to the l. So, that k to the l will be cancelled by this 1 over k to the l, so now your solution after the cancellation of this r to l and k to l and minus 1 to the l is twice sin k r minus l pi by 2 over r; this is your solution for an arbitrary value of r. So, is there any questions I will be happy to take otherwise, we proceed from here in the next class.