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

Lecture 45 Ionization and Excitation of Atoms by Fast Charged Particles

Greetings, So, we have the second guest lecture today by Professor Steve Manson and today he will talk about Collisions, Quantum Collisions. See. Hey! Thank you. Today's talk will be a little bit different. Today's class will be a little bit different in the sense that it will be much more quantitative. What I want to talk about today is Charged Particle Collisions particularly with atoms. Although what I say is going to be fairly general and can be applied to molecules as well.

But I will aim at the demonstration of what goes on in a simple system. Now, why are we interested in Charge particles of Impinging on atoms? Well, for a number of reasons. First of all, Scat and photo ionization are probably two of the major processes that go on in the Universe. You know, the Universe is much bigger than a few miles above the crust of the earth.

It is most of the universe has lots of charged particles coming out and into and interacting with all kinds of things. And so, to understand what goes on, we need to understand Charged Particle Collisions. Furthermore, there are all kinds of applications, fluorescent lighting for example, charged particles that Ion on that ionize and excite and the resulting radiation is what you see.

Well actually a lot of the radiation you do not see, but never mind that. However, unlike photons charged particles have a very strong interaction with the targets. And that is something that leads to be looked at carefully. So, what I would like to do is start out with a relatively simple problem, a Structure less Charged Particle interacting with a hydrogen atom in its ground state.

I mean, that is I say, Structure less what I mean is a Bare Nucleus because I am not going to get into that today. Supposing you have a Collision where the projectile brings in its own electrons; that makes it much more complicated. We are not going to talk about today. What I want to talk about is complicated enough and aside from doing the derivation of what what the probability.

What the cross section looks like. What I want to focus on is the approximations made and what the implication of the approximations are; because you know it is easy to do the mathematical derivation, I mean, we have you know various packages that will essentially do it for you. But they would not interpret it for you and that is the important thing.

One of the things we do as physicists is, you take a problem and you say okay, what methodology shall I use to solve this problem? In other words, what methodology should I use that has the essential physics of the particular problem? That is what you have to worry about. And in order to know, what has the essential physics, you have to know a) the essential physics of the problem and b) the essential physics of the method.

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I am not going to talk about the problem now. I want to talk about the method right now, All right. Let us see, Chalk. Scattering mean I am told that you have sort of a background in at least Elastic Scattering. We know that the wave function let us say, just for potential Scattering, the Elastic Scattering of a particle off some central force goes as r goes to infinity.

That is get very far away as e to the ik z + f of theta and phi e to the ikr over r where my force is centered at r = 0. (Refer Slide Time: 5:25)



This, if this is the asymptotic form of the wave function, asymptotic form gets much messier if r is not, they are not going to infinity. Then, the differential scattering cross section is equal to 0. That is pretty good. So, that does not sound too hard. Too hard you get a wave function that has that asymptotic form and then you just pull out that f and you take the epsilon square. Oh, we can do that. f star times f you know.

Where we are pros at dealing with complex things and get well. Not quite that easy. The way you get this is by looking at the probability current density. And for the incident wave let us just you know plane wave coming in. And the scattered wave and it turns out that you know the probability current density you just get from the continuity equation, for the Schrodinger equation.

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It relates the time derivative of Psi star Psi or which is the probability per unit volume to the probability current density actually. If I call Rho as Psi star Psi then del Rho dt + del not s is

equal to zero. That just says that the total probability over all space remains constant that is that is all. What that is and but this thing here is the so-called probability current density. Very often students look at that and say Oh, my god! That is so complicated but it is really quite trivial.

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If it is a charged particle and you multiply by the charge q put it in here and I put it in here and this is just the Charge Density. That has nothing. And this is the Current Density, you know that. So, these are so without the q these are just general concepts that we use in quantum mechanics which represent the same kind of thing except probability. You know, Charge density sounds so easy.

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And probability density sounds so hard. But it is really not okay. So, you do this and actually what you get for me. If I call this the incoming wave and the scattered wave what I get is that

s incoming is equal to, Well, all I care is the magnitude, is h bar k over m and s scattered as r goes to infinity. It is actually a very complicated expression.

But most of it goes away as r goes to infinity you get h bar k over m f absolute squared over r squared and the cross section the differential cross section is almost a ratio of these two things. But you have to do one more thing; you have because it is there is in the definition of the cross section on the bottom. It is a number of particles per unit area or probability for your area.

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On top it is a probability with the unit time in there as well, on the top it is the same thing but per unit solid angle. And so, you have to get area for solid angle that gives you, you r squared and that is why everything just cancels out. And you just get the effort the f absolute square. Again, I am assuming that this is review I hope it is a review, because this is hardly a derivation.

I am just trying to remind you of some things that I hope you already know, okay. Now, let us get to our problem. What we want to try to solve is a Charged particle striking a Hydrogen atom. And when I particularly, you see, this is Potential scattering just get Elastic scattering what I particularly want to focus on is Inelastic scattering, where it gives some energy to the

Hydrogen atom. (Refer Slide Time: 10:08)



And if let us say, if the Hydrogen Atom starts in the ground state it ends up excited, okay. Well, how do we solve it? Well, First, we got to write down the equation that we want to solve. And that is the Schrodinger equation which I am going to write in this form. Remember now, we have two electrons the electron coming in and the Hydrogen Atom electron.

So, notice I multiply the Schrodinger equation by a minus sign because I always like the first term to be positive. I I just I just feel better like that it is like in mathematics, having an eye on the bottom I never like an eye on the bottom I was like to get rid of it and put the eye on top. I know it is a quirk.

Anyway, 1 square + del 2 squared + e squared over r1 + e squared over r2 - e squared of r2Psi, I should make this a capital Psi of r1 and r2 equals 0. Oh, no it is not. I forgot something did not I? I will squeeze it in here. That is important move everything over to this side this is simply the Schrödinger equation for two electrons.

Now, I got to solve that with the right boundary conditions. It will come in a moment to what the right boundary conditions are. But now, I am going to make my first approximation. You know that electrons are identical. So, we have no way of knowing if this happens or if this happens. And however, if my electron is very fast compared to the velocity of the bound electron, the chances of exchange are very small.

So, my first approximation is, no exchange. And that implies that this will be reasonable as long as the incident electron is going much faster than they or has much higher energy is another way of saying it than the atomic electron, Okay. That is it you see saying, what

saying no exchange that we do with that exchange does not carry with it immediately. The idea of where that approximation is good.

That is, now this is the point that I want you to think about. So, if I am sending in a3 eV electron or say at 10eV electron, when the hydrogen atom is bound by 13.6eV, this is a crummy approximation. I would have to put exchange. Now, putting exchange in is not terribly difficult, but it just makes the equations much messier and it is harder to see what is going on.

That is why I like to leave it out to begin with. All right now. It is partial differential equation. Again two ways we know of solving partial differential equations separation of variables. We do not know how to do this. Guessing I do not have any good guesses, we have to approximate, Okay.

Now, one of the postulates of quantum mechanics is that you can expand any wave function in any complete set, right. Unfortunately, complete sets in this case are infinite. So we take a finite set. However, let me just write it down in principle what we would do. (Pafer Slide Time: 15:11)

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I take Psi r1 and r2 I am going to write it some remember it is a two particle, so I am going to do it in two particles and I am going to write this Psi n of r1. Actually of r2 I think. I did yeah fn of r1.Since I am not allowing exchange here r1 is I am going to use to the incident particle and r2 for the bound electron this without exchange they become in principle distinguishable, okay.

I am free to pick my set. Since I know that I am dealing with a Hydrogen atom, I am going to pick these to be the Eigen functions of the hydrogen atom. Those you know. And these I am

going to leave for the moment. These are the way the functions representing the continuum electron the scatter the incident and scatter electron.

However, before I can begin to even approximately solve a partial differential equation, unlike an ordinary differential equation there is something crucial that I need, Boundary conditions. If you remember back, to when you took a course in the mathematical methods of physics, you cannot even begin to solve a partial differential equation even approximately unless you pick boundary conditions.

Because you get different solutions on the different cases and you see it is easy when it is a bound state the boundary conditions everything goes to 0 at infinity. You bang, that is no problem. But here, everything does not go to 0. And what does the asymptotic form of this wave function have to look like. Well, this tells me something about that.

It is equal to or it goes to what e to the ik dot r1 times Psi0 of r2. This is a plane wave on the ground state of Hydrogen Atom. That is what you had at infinity plus where see what does this represent from what we talked about here this represents the hydrogen atom in various states and waves coming out.

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However the k is different in other words here k was rk squared was 2mE of h bar squared.

That is the energy of the incident electron. (Refer Slide Time: 18:18)

Here when the electron has lost some energy kn squared is equal to 2 me minus en over h bar squared. The excitation energy to a particular state of the hydrogen I mean. So, this is just definition so far. But now, we mentioned something else. Supposing the hydrogen atom was not in ground state, supposing it is in some excited state and the electron comes in.

Can it knock it down and the electrons come out with more energy absolutely? That is called a super Elastic Collision. And just falls automatically or out of this formalism. However, in this case, it is just a little bit easier to think of it in the hydrogen in the ground state but it could be in any state.

And you can add or subtract energy. And this way and this actually happens not that much. The reason is that usually excited states decay fairly quickly. So, in order to see this kind of thing you have to have a really, really high density of charged particles or you know everything will decay. (Refer Slide Time: 20:33)



Or you have to have a met stable state. That will work, okay. So, you need boundary conditions like this. So, that tells me what the f ends are. In other words, f0 has this in it. Plus Psi and Psi0 e to the ik and but all the others just have this. So, since I want to focus on Inelastic Collisions, Fn goes as r goes to infinity e to the ikn r1over r1 sine n of r2 and now I have a boundary condition or boundary conditions.

Oh, by the way. There is one more thing that I want to mention. Let us assume that I can solve this. A really bad assumption but let us assume that I can. Then, from what we did before the sigma n d omega be equal to what? Would it be I am sorry, I I forgot something here. Would it be and I forgot it here too. That is important. I mean, so, it looks like the Elastic scattering case.

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Is it just the Fn squared? No, why not? Because remember, when I wrote down what the probability current density was, it had this h bar k, well here. I have the h bar k n in the ratio

still have the h bar k for the incident wave. So, what you get is kn over k fm the absolute square. All right. Now, I got to bite the bullet and actually calculate this Fn which is not easy. Let us say, how am I going to do it? (Refer Slide Time: 22:47)



Well, let me take this form plug it in here, okay. You see the reason I do it this way, why do I pick this fixed and this I have not fixed; because I know first of all asymptotically, what the wave function is going to be and asymptotically I am going to have these by themselves here. And this also why do not I just take something like plane waves or no work because I cannot take an infinite set.

And because I know that I am not going to be able to do an infinite set. So, I want to determine these to get the best I can, with a finite set. And so, let me get the equations now that govern Fn. yeah so, what I do, I simply take this and plug it in here. So far there were no approximations except for the exchange business, All right. I am going to plug in. But before I do that I wanted to note something. (Refer Slide Time: 24:09)



Note that I know what equation that is a solution to its Hydrogen. So h bar squared over 2m del 2 squared plus En - e squared over r2 all right. I mean it is just a rendering of the Schrodinger equation, for the Hydrogen atom, okay. (Refer Slide Time: 24:39)



Now, here is what I am going to do. I am going to plug this into here and then multiply by Psi n of r2 star and integrate this it means the same thing. I would like to do it this way because there is less writing. But it is exactly the same thing. Let us see what happens then. What I am going to get is sigma of n Psi star r2 make sure I have got this right.

Well, no I am just now plugging that in and multiplying times h bar squared over 2m del 1 squared + E - En by the way I have made a mistake here that is a + sign in it + e squared over r2 yeah. (Refer Slide Time: 27:01)

Because if I multiply everything by -1 that gets multiplied also Fn of r1 is equal to what is on the other side well let me write what is on the other side, this way, I am moving some stuff to the other side. It ise e square over r12 - e squared over r1. See all I have done here is, I taken part of this and plugged in here and that is how I got the this and this together on this to give me the En. That is the way I got the En here. (Refer Slide Time: 27:32)



That is r1 that is r1 and that is r1. No, that is gone. Yeah that is what it looks like I am sorry the r2 is gone from here. But here is everything else you see, okay to get rid of this now, okay. No I have you multiplied by the star yet okay now I multiply by Psi and star and I integrate this just gives me one and I get what I get h bar squared over 2m del 1 squared + E - En, Fn of r1 is equal to he integral of I multiply one side by Psi and star. (Refer Slide Time: 29:02)

And the got to multiply the other side Psi star of r2 e squared over r12 - e squared over r1 Psi of r1 and r2 dr to erase a little bit here. So, you can actually see this. And now what this is? Is basically just a transformation of this equation that of a race. Now, multiply through by h pi by 2m / h bar squared and this becomes what I called kn squared. (Refer Slide Time: 31:00)



And what I get is then 1 square + kn squared fn of r1 yeah good equals to 2m h bar squared integral e square root of r 1; 2 minus e squared of r one Psi n star of r2. Now again, this is simply a transformation of the Schrodinger equation, nothing else. It leaves something to be desired if you actually want to solve it from the following point of view. First of all, there are an infinite number of these terms that already is a downer.

Secondly, in order to solve the equation you need to know the right hand side and the right hand side has what is unknown to begin with. So what I have is exact but in this moment it is

not very helpful yet. So, what, so what can I do? Well, what I can do is, say all right let me take some 0th order approximation here.

That I will get a first order approximation can go back and I can do iteration and I can do this approximation at various levels. For example, remember, the expansion for this which I just erased. Well I can pick instead of an infinite number of terms, of finite number of terms. That will help a lot, you know. You know, so, if I take capital Psi sigma n = 0 to some capital N that infinity of Psi n of r2 Fn of r1.

Then if I plug this in here, I will have on this side, the fn's here. The fn's and good actually in principle solve. This is messy but it is solvable. When I take those terms, bunch of terms there, that is known as a Close Coupling Expansion. You can solve this analytically but you can do it numerically, got to do it by iteration.

But it is solvable so by doing this by taking a finite number of terms. You are saying that the higher part for your purposes is unimportant. And one has to consider under what conditions the higher part will be unimportant or if these not affect the part that you're looking at. But you can even take something more. Supposing, in lowest order, what will happen? Electron will miss.

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So, if there were no interactions at all what would P si? Psi would just be e to the ik dot r1 Psi 0 of r 2. Ooh, that looks like something I just might be able to deal with. So my philosophy is this. Going to start with this as my 0th all the wave function, plug that in here. I am going to get the fn out. Then I can get a new side I next door the next order plug that in.

This, in a general sense is known as the Born approximation, it is not the usual way of deriving it. But I like this way because you can see exactly the approximations that are being

made. So, you are not approximating, no scattering that is my 0th order approximation and I am going on. And in principle, if I carry this out to infinite order, it will be exact. I would not carry it out the infinite.

So, I take this plug it in now. Again let us think about this. Under what conditions is this, a reasonable approximation? That is important, very important to think about. Well, I am guessing because I know something about how physics works the longer time the incident electron spends around the hydrogen atom.

The more likely it is to do something, okay. I am starting off with a zero is 0th with approximation that it does nothing. So, how do you get it to spend less time, have a fast collision, high energy collisions? So, this just think about the physics of the situation is, a high-energy phenomenon; a high-energy approximation.

This should be good at higher energies, all right. It is still non-trivial to do. Because, then my equation becomes what? del square + kn Fn r1 is equal to h bar squared 2m over hbar squared the integral e squared over r12 e squared or e to the ik dot r1. I am plugging this into that Phi and star of r2 zero of r2 is that everything make sure, yeah, sr2 okay. Now, I am not going to make another approximation.

Yet, but I am going to restrict myself I want to consider specifically inelastic collisions what inelastic collisions mean in this case n is not equal to 0 because if n = 0 then it stays in the ground state. And that is okay. This is important, because look at this integral over r2 with this term here. (Refer Slide Time: 37:56)



We have, I forget about this term. All I have these are the only two things I depended on r2. When I integrate over r2 that gives 0 because the wave functions for different states of the hydrogen atom are orthogonal, so for n not equal to 0, I can forget about that term, all right. (Refer Slide Time: 38:30)

Solve them so, then, del square kn squared Fn r1 is 2m h bar squared the integral of e to the i well pull out the e squared as well; e to the ik dot r1 yeah I know make sure I am not making any mistakes. Oh, yeah. Over r12 and Psi n star of r2 Psi 0 of r2 dr2, believe it or not we can actually solve this equation. You use what is called the greens function of this, I do not have time to go into deriving the Green's function. (Refer Slide Time: 41:50)

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But the actual solution then is Fn of r1 = 2pi me squared over h bar squared the integral e to the ikn 0, or let me write this as r, I get too many r - r1 right; e to the ik dot r1. Oh sorry this double integral now make sure I am getting this right Psi n star of r2 Psi 0 of r2 dr2 dr1 and

this is the exact solution of that. And you see I have this, this Green's function business, integrate over it and then just everything else here.

Fortunately, I know something about how this works. And I can take the asymptotic form of it because for large enough r and r is greater than r. This just becomes R and this becomes a little bit more complicated but when we put it all together what I get is Fn r = 2pi. I am sorry but for large r why do I just want it why do not I just actually solve for fn why do I want it for large r.

Remember it is for large are that it has the form fn times e to the ikn r over r. And all I am looking for is that little f, I mean I could do a lot more, but it is much harder. So, this is just the asymptotic form for large r which I take the large r here. As I go along I lose things like the age which what happens when you get old you lose things a double integral of e to the ik -kn dot r over; I am sorry but not over anything. (Refer Slide Time: 45:04)

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Oh actually it is a minus sign here. Let me rewrite this a little bit because I did you give myself enough room. Fm or it is actually the Green's function has a minus sign it should have been a minus sign there too actually and there is something there is something funny, yes. There is something very funny I lost that too. You know okay. Over r12 Psi n star of r2 Psi 0 of r2 dr1 dr2 times e to the ikr over r.

And I wrote it this way particularly because then this is my scattering amplitude the Fn. And if I can calculate that, I can calculate the cross section, when I only have five minutes to do it. So, what I do is, I change I make a change of variables I change the variable, well. First of all, I define capital K and that is generally called the momentum transfer. Although it is actually h-bar times capital K which is the momentum transfer; because h bar k

is the momentum of the incident particle. h bar kn is the momentum of the scattered particle.

So, that is the difference. That just makes things a little bit easier. And then I change variables for r, I change it to r12. It is a simple change Jacobian near the transformation is one I would have done it. But I do not have time to at the moment. (Refer Slide Time: 47:30)

But if I, but in any case just looking at this: Then the differential scattering cross section is what it is kn over k times, this absolute square which is 4pi squared m squared e to the fourth over h bar to the fourth double integral of e to the i okay ik dot r of r12 Psi zero of r2 Psi n star r2 dr1 dr2 square.

Now, what I was saying here is that we just look at a piece of this. The integral of 1: I am sorry that is I have lost something somewhere. Yes I have where is it that is r1 and I am integrating over that and so 1 over r12 e to the ik dot r1 Psi 0 of r2 Psi n star of r2 dr1. I can make that that substitution here. And I simply get here, I get 4 pi over k squared e to the i actually -i k dot r2 and Psi 0 of r2 Psi n star of r2.

Yeah let us up, sorry this. So, that must square of my matrix element absolute square or just the absolute value of the matrix element then is 4pi over k squared. The integral of a now we're going to write it in a particular way now Psi n star of r2 e to the -ik dot r2 Psi 0 of r2 dr2 absolute value.

So look at what that means. I have reduced this whole mess to a matrix element between the ground state of the hydrogen atom and the excited state of e to the - ik dot r2. You will if you look this up, you will sometimes see it as e to the plus e to the ik dot r2; but it does not really matter because you are taking the absolute square so you can do it either way.

In other words, then if I, if I call this epsilon n 0 okay, the momentum transfers what I am going to get is: sigma the omega is equal to whole bunch of constants for pi, the kn epsilon n 0 k absolute square. And I am going over time but I would not go over time much I promise there are various properties associated with; but the crucial thing here is that the cross section depends only well not only it depends on the incident energy.

Because you have this kn over k here. But in a real recite from that it depends only on this momentum transfer. This is a characteristic of the Born approximation, only on the momentum transfer. So you have taken a very messy problem and said okay. I take this plane wave I take the matrix out with this integral.

Now supposing you have something more complicated than a hydrogen atom. Well, whatever the wave functions are makes this, make sure this by the way this matrix element is very easy to take. What you do is you expand this in a series just like the series that you expand it in for a plane wave of scattering.

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And since these things have spherical harmonics associated with it you only get a few terms. And this is a very quick and dirty view of how you do charge particle scattering. Now all this work is just for doing it in the Born approximation although what we really did is called the first Born approximation because what you can actually do is, actually get you can solve this where you can do this integral numerically if you have to.

And you can iterate and get the second Born approximation etc it is very messy. But it is not. It is perfectly doable but within the Born approximation, the first Born approximation which is applicable again, the high-energy collisions you can get very, very good answers. When I say very good answers mean it agrees rather nicely with experiment in many, many cases I guess since I have gone over time I should stop here.