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

Lecture 34 Born Approximation

Greetings, so we have the second lecture of the unit 5 and this will be on the Born approximations notice that there is a plural s at the end because it is not just one approximation but a series of approximations that is why it is referred to as a Born approximations. Now before I get into this I will like to remind you that I did you know rush through several portions in the previous class in the last class.

For example when we wanted to estimate the asymptotic distance okay and then I had a few slides with these blue arrows on the side (Refer Slide Time: 01:09)



And I just want to remind you that there is very simple reorganization of terms okay. And there is no big physics or mathematics which is no trick which is involved in this. It is just rearrangement nothing else. (Refer Slide Time: 01:22)



And as part of this technology enhanced learning NPTEL program one advantage that I can take off is that the PDF which has all of these details is available at the course webpage. So, you can download it and go through all the intermediate steps which I have rushed through but there is nothing very big about any of these steps but they are all available in the PDF file and the course webpage.

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So, we went through this to get an estimate of this e to the ik r by r which we have used in our

previous class and then we put it into the Lippmann Schwinger equation. (Refer Slide Time: 02:02)

Born approximations Iterative solutions of the Lippman Schwinger equation $\psi^{+}_{\vec{k}_{i}}(\vec{r}) = \phi_{\vec{k}_{i}}(\vec{r}) + \iiint d^{3}\vec{r}' G^{+}_{0}(k,\vec{r},\vec{r}')U(\vec{r}')\psi^{+}_{\vec{k}_{i}}(\vec{r}')$ "CATCH 22 Zero^{eth} order solution: $\psi_{(0)} = \phi_{\vec{k}_i}(\vec{r}) + 0 = (2\pi)^{-3/2} e^{i\vec{k}_i \cdot \vec{r}}$ PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 45

And this is where we begin our discussion for today's class. So, the Lippmann Schwinger equation had one difficulty which is that it was it offered as a formal solution but not a particularly useful one because of what I call as the CATCH 22 situation. And I have explained the term CATCH 22.

It has become commonly accepted in the English language in the colloquial way because of this famous novel and there was this movie which was made on this and some of you may have seen the movie that you I do not want to go into the story of the movie because that will take us much to away from the discussion of the Born approximations.

Well it is very nice story and it argues that okay there was somebody who said that okay he needed you know some waivers and he argued that he should get that waiver because he was not mentally alert enough to take care of those situations. And then the administration argued that if he is in such a frame of mind that he can plan such a strategy then he cannot have any issue and he would actually be mentally alert.

So, that is the kind of situation that that you try to pose a problem okay or solve a problem but then the solution and the problem become integral parts of each other and you there is no getting away from that. So, that is the; what I call is a CATCH-22 situation. So, you have any problem in physics when you seek a solution.

And then you want to have an unknown left hand side which is to be described by an equation. And on the right hand side it is necessary that everything on the right hand side is known and only in terms of that can you determine the left hand side ever right. Now how can you do that if the right hand side has the very same function which you hand on the left hand side. So, this is the CATCH-22 situation we have to find way of coming out of this.

So, this is what the Born approximations will help us to achieve. So, let us see how to go about doing that as a 0th-order solution what we propose is that we just put in the incident plane wave which we know okay there is nothing unknown about this. And we plug it in over here, so this looks like ad hoc but then there is some sort of merit to it because what it does to the right hand side is that you have the incident plane wave over here.

But then it appears again over here but in the second term it incorporates various things what does it incorporate it has got the potential okay. So, that is the quantity of interest it also has got the Green's function with appropriate boundary conditions right. So, there is some information which has gone into the second term regardless of the fact that you have made an approximation to that.

So, this is just a start this is not the end of it because you can always improve upon it. So, you can take it as an early solution and then make an effort to improve upon it this is the kind of thing we do also in the Hartree Fock self-consistent field method when you do not have a solution you propose some sort of a solution. And then iterate on it till you get convergence right. So, it is something of this kind.

So, you propose this as a 0th order solution and now everything on the right hand side is known because this solution is now replaced by this incident wave incident plane wave and now everything on the right hand side is known. So, in terms of which you can actually evaluate the left hand side. So, that is the strategy of the Born approximation. (Refer Slide Time: 06:20)

$$\psi^{+}_{\vec{k}_{i}}(\vec{r}) = \phi_{\vec{k}_{i}}(\vec{r}) + \iiint d^{3}\vec{r}'G_{0}^{+}(k,\vec{r},\vec{r}')U(\vec{r}')\psi^{+}_{\vec{k}_{i}}(\vec{r}')$$
Oth order solution: $\psi^{+(0)}_{\vec{k}_{i}}(\vec{r}) = \phi_{\vec{k}_{i}}(\vec{r}) + 0 = (2\pi)^{-3/2} e^{i\vec{k}_{i}\cdot\vec{r}}$
1st order :
$$\psi^{+(1)}_{\vec{k}_{i}}(\vec{r}) = \phi_{\vec{k}_{i}}(\vec{r}) + \iiint d^{3}\vec{r}'G_{0}^{+}(k,\vec{r},\vec{r}')U(\vec{r}')\psi^{+(0)}_{\vec{k}_{i}}(\vec{r}')$$
2nd order :
$$\psi^{+(2)}_{\vec{k}_{i}}(\vec{r}) = \phi_{\vec{k}_{i}}(\vec{r})^{\flat} + \iiint d^{3}\vec{r}'G_{0}^{+}(k,\vec{r},\vec{r}')U(\vec{r}')\psi^{+(1)}_{\vec{k}_{i}}(\vec{r}')$$
nth order :
$$\psi^{+(n)}_{\vec{k}_{i}}(\vec{r}) = \phi_{\vec{k}_{i}}(\vec{r}) + \iiint d^{3}\vec{r}'G_{0}^{+}(k,\vec{r},\vec{r}')U(\vec{r}')\psi^{+(n-1)}_{\vec{k}_{i}}(\vec{r}')$$
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Now having done this you can improve upon it because this is our 0th order solution as we just discussed but then you can go further because you can go to the next higher order

solution. If you take the first order solution so here the superscript is 0, so watch it very carefully okay.

So, the notation is that this is the 0th order solution which is nothing but the incident plane wave. And now you go for the first order solution this is the superscript one in which you put the 0th order term here okay. And now you can go further because in terms of this 0th order solution which you already know is the incident plane wave you can evaluate the first order term.

And now you can put this first order term over here in place of this. So, the correct complete solution is Psi superscript + okay that is the correct solution. We are approximating it now by Psi superscript + but with the superscript 1 which was our first order correction. So, we pick the first order correction from here put it over here and now again you have got a right hand side which is not perhaps the exact solution nevertheless.

It is better than what you started out with okay. And you can make subsequent sale you know approximations following essentially the same logic. So, you get the first order correction the second order correction you can get a third and fourth order correction and in general the nth order solution which is indicated by the superscript n will have the n minus 1 at solution of the previous step which will be plugged in over here okay.

So, that is the plan of this series of approximation which is why this called as the Born approximations as a plural, so that you have got a series of approximation and you can go to nth order you can go to infinite order in principle right. So, the exact solution will require infinite order.

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But then you can go as far as you need to and also as far as you possibly can depending on a given situation. So, let us have a look at the second-order solution. So, you have got the superscript 2 over here the superscript 1 which is n - 1 in this case right 2 -1 and this is your second order solution. Now let us write it a little more fully because the first order solution itself had the 0th order term plus this correction right.

So, the first order term consisted of these two terms which I have now put in place of this explicitly. So, now you have got one term over here a second term which is coming from this integration and then you have got this term and then a third term which will have two integrations 1 over r prime and the other over r double prime. So, each is a triple integral but then there will be 3 + 3, 6 integrations in the third term.

So, in general if you look at the nth order term the potential itself like this is the second order term sorry, I let me go back so in the second order term this is the second order term the potential appears here and it also appears here, so it appears twice okay. And for a weak potential the powers as you have more and more powers of the potential the subsequent terms in the Born approximation series you will hopefully become smaller and smaller. (Refer Slide Time: 10:16)



And that is what makes it possible to use this approximation in a very constructive manner. So, this is the general structure of the second order term. So, let us write these terms explicitly. So, these are the three terms the first is nothing but the incident plane wave. Second has got the potential once and the third term will have the potential twice one is here and the second is here.

Make sure that you have the appropriate dummy label of integration okay. An integration variable it is a dummy label it gets integrated out but then it has to be appropriate for each

integrand okay. So, make sure that you do not make any careless mistake about it. So, there are these three terms and let us now focus our attention on the integrants. What is it that you are integrating out?

So, let us look at them and in this integrand. So, let us look at the second term this we know this is the plane wave incident plane wave right. And then the other part or the main essential part of the integrand is this GU right. So, that is like the heart of the integral because you have this term of course it is a part of the integrand. The integrand you can think of the integrand as factored into this piece and then into this piece.

So, this is what is in the blue box is then like the heart of the integral and it is often refer to as the kernel of the integral. So, it is not as the integrand itself, but it is the main part of the integrand. So, you have identified the kernel in this term and then there is likewise in the third term this is the one if you agree that okay.

This is something that is known we already know what it is. And then the remaining part of the integration which really has got the heart of the integral or the kernel of the integral that is what is in this red box okay.

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So, let us write these terms clearly now, so these are the three terms we have identified the three kernels and these are written as K1 and K2. So, K1 kernel is this one GU, K2 is this GU GU okay. But then the argument of this U is r prime, the argument of this U is r double prime. So, you have to be very careful about that okay. So, this is the recognition of the essential core of the integrand which is the kernal.

And we now write this kernel which is the one with subscript 1 has got the potential once and the one with subscript 2 has got the potential twice once here and again over here okay. The

arguments of the kernel again you have to be careful because this one will depend on r and r prime this one will depend on r and r double prime, r single prime gets integrated out okay. So that is the kernel that we will be using. (Refer Slide Time: 13:32)

$$\psi^{+(2)}_{\vec{k}_{i}}(\vec{r}) = \begin{cases} \phi_{\vec{k}_{i}}(\vec{r}) + \text{Kernel} \\ + \iiint d^{3}\vec{r}'[K_{1}(k,\vec{r},\vec{r}')]\phi_{\vec{k}_{i}}(\vec{r}') \\ + \iiint d^{3}\vec{r}''[K_{2}(k,\vec{r},\vec{r}')]\phi_{\vec{k}_{i}}(\vec{r}') \end{cases}$$

$$\phi_{0}(\vec{r}) = \phi_{\vec{k}_{i}}(\vec{r})$$

$$\phi_{1}(\vec{r}) = \iiint d^{3}\vec{r}'[K_{1}(k,\vec{r},\vec{r}')]\phi_{\vec{k}_{i}}(\vec{r}')$$

$$\phi_{2}(\vec{r}) = \iiint d^{3}\vec{r}''[K_{2}(k,\vec{r},\vec{r}')]\phi_{\vec{k}_{i}}(\vec{r}')$$

$$\psi^{+(2)}_{\vec{k}_{i}}(\vec{r}) = \phi_{0}(\vec{r}) + \phi_{1}(\vec{r}) + \phi_{2}(\vec{r})$$

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So, this is the second order term and you can now write in the second order term as the sum of three parts one is here, second is this integral and the third is this integral. So these three pieces can be written as Phi0, Phi1 and Phi2 and then you can write the second order solution as the sum of these three terms Phi0 + Phi1 + Phi2 okay. (Refer Slide Time: 14:14)

$$\psi^{+(2)}_{\vec{k}_{i}}(\vec{r}) = \phi_{0}(\vec{r}) + \phi_{1}(\vec{r}) + \phi_{2}(\vec{r})$$

$$\psi^{+(n)}_{\vec{k}_{i}}(\vec{r}) = \sum_{m=0}^{n} \phi_{m}(\vec{r})$$

$$\psi^{+(n)}_{\vec{k}_{i}}(\vec{r}) = \sum_{m=0}^{\infty} \phi_{m}(\vec{r})$$
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So, you can in the nth order solution you will have n terms and you can go to n + 1 with order or even infinite order if you like. So, the nth order solution will be a sum of similar terms and now you know how to come up with these terms. How to come up with the next term, so the n + the nth term will have all of these terms n + 1 terms Phi m going from 0 to n, so there will be n + 1 terms over there right. And your solution is the one with superscript plus which will actually require you to go all the way to infinity okay only then you will have the complete solution. So, that is the; this procedure of getting an approximate solution to the scattering problem using the Lippmann Schwinger equation and making an approximation appropriately depending on the powers of the potential.

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$$f(\hat{k}_{i},\hat{k}_{f}) = -2\pi^{2} \iiint d^{3}\vec{r} \cdot \phi_{\vec{k}_{f}}(\vec{r} \cdot)U(\vec{r} \cdot)\psi^{+}_{\vec{k}_{i}}(\vec{r} \cdot) = -2\pi^{2} \left\langle \phi_{\vec{k}_{f}} \middle| U \middle| \psi^{+}_{\vec{k}_{i}} \right\rangle$$

$$\psi^{+}_{\vec{k}_{i}}(\vec{r}) = \sum_{m=0}^{\infty} \phi_{m}(\vec{r})$$

$$1^{\text{st}} \text{ order:} \quad f_{B_{1}}(\hat{k}_{i},\hat{k}_{f}) = -2\pi^{2} \left\langle \phi_{\vec{k}_{f}} \middle| U \middle| \psi^{+(0)}_{\vec{k}_{i}} \right\rangle$$

$$2^{\text{nd}} \text{ order:} \quad f_{B_{2}}(\hat{k}_{i},\hat{k}_{f}) = -2\pi^{2} \left\langle \phi_{\vec{k}_{f}} \middle| U \middle| \psi^{+(1)}_{\vec{k}_{i}} \right\rangle$$

$$f_{B_{n}}(\hat{k}_{i},\hat{k}_{f}) = \sum_{j=1}^{n} \overline{f}_{B_{j}}$$

$$geties$$

$$\overline{f}_{B_{j}} = -2\pi^{2} \left\langle \phi_{\vec{k}_{f}} \middle| UG_{0}^{+}U....G_{0}^{+}U \middle| \phi_{\vec{k}_{i}} \right\rangle$$

$$U \text{ appears } j \text{ times and } G_{0}^{+} \text{ appears } (j-1) \text{ times}$$

$$geties$$

So, this is this whole scheme is called as a Born approximation and that will give you an approximate expression of the scattering amplitude. So, the scattering amplitude which we know is this integral Phi kf this is the final state momentum in the scattered state and this is the initial momentum and you need to evaluate this matrix element. So, here the superscript is plus but you will be making an approximation to this.

So, you value in this matrix element and the corresponding scattering amplitude at various levels of approximation the first order, the second order and so on. So, this is your complete expansion and if you put this term over here, your scattering amplitude will be a sum of a number of these matrix elements as you can see directly right because in this vector you will have n number of vectors for the nth order solution.

So, you will have the first order solution, so this is when you get a solution at this level where you have only the first power of you have a solution which you call as the first order Born approximation to the scattering problem. So, this is your first order Born approximation then you have the second order Born approximation.

And then you have a sum of all these terms so the nth order scattering amplitude will be a some of these n matrix elements okay. And these this is what you call as a Born series. So,

this is after Max Born and here I have written this f with a bar on top of it but you can immediately see that.

So, far as the first born approximation is concerned it is already this right. So, here in this if you look at the jth term in the scattering amplitude then the potential U will appear j times and G0 the greens function will appear j -1 time okay. So, as you can see very clearly from this.

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So, this is what we have got and if we look at the nth order solution, so this is the main story but essentially the Born series is then a some of these all these terms. And you can represent them by diagrams notice that in the second order term the potential will appear twice. So, it is as if you have got a particle which is incident in this state finally it gets out in this momentum kf which is the same as in here.

So, the final state momentum is always kf but intermittently it can get multiply scattered okay. So, that is represented pictorially, so as if the particle get scattered in the scattering region get scattered by some other part in the source region again and then again and depending on how many times the potential term appears in the Born series it gets multiplied scattered.

So this is essentially it is a multiple scattering series and you can represent this pictorially as well. So, these are the G0 is of course the greens function of the propagator. (Refer Slide Time: 18:29)

1st order
Born:

$$f_{B_{1}}(k,\vec{\Delta}) = -2\pi^{2} \langle \phi_{\vec{k}_{f}} | U | \phi_{\vec{k}_{i}} \rangle$$

$$f_{B_{1}}(k,\vec{\Delta}) = -2\pi^{2} \iiint d^{3}\vec{r} \phi_{\vec{k}_{f}}^{*}(\vec{r}) U(\vec{r}) \phi_{\vec{k}_{i}}(\vec{r})$$

$$\vec{\Delta} = \vec{k}_{i} - \vec{k}_{f} \quad : \text{momentum transfer}$$

$$f_{B_{1}}(k,\vec{\Delta}) = -\frac{2\pi^{2}}{(2\pi)^{3/2}(2\pi)^{3/2}} \iiint d^{3}\vec{r} \ e^{-i\vec{k}_{f}\cdot\vec{r}} U(\vec{r}) e^{+i\vec{k}_{i}\cdot\vec{r}}$$

$$f_{B_{1}}(k,\vec{\Delta}) = -\frac{1}{4\pi} \iiint d^{3}\vec{r} \ U(\vec{r}) e^{+i\vec{k}_{i}\cdot\vec{r}}$$

$$= -\frac{1}{4\pi} \iiint d^{3}\vec{r} \ U(\vec{r}) e^{+i\vec{\Delta}\cdot\vec{r}}$$

And let this now focus our attention on the first order Born approximation. So, here this delta is the momentum transfer it is the difference between these two vectors the initial state momentum and the final state momentum. You can always write it along with the h cross if you like so these are the k vectors and h cross k is the momentum right.

So, delta which is ki - kf is the momentum transfer and this is the scattering amplitude in the first Born approximation. So, you will need to evaluate this integral and you can manipulate these terms because this is nothing but a plane wave with momentum kf this is the complex conjugate.

So, this comes with a minus sign here and this one on the right comes with a plus sign and then you have the difference ki - kf which is the momentum transfer. So, that this is the integral that you have to determine now this looks like a very familiar expression okay. You can see what it is and it will already occur to you how to evaluate this. (Refer Slide Time: 19:45)

$$f_{B_{1}}(k,\vec{\Delta}) = -\frac{1}{4\pi} \iiint d^{3}\vec{r} \ U(\vec{r})e^{+i\vec{\Delta}\cdot\vec{r}}$$

$$f_{B_{1}}(k,\vec{\Delta}) = -\frac{m}{2\pi\hbar^{2}} \iiint d^{3}\vec{r} \ V(\vec{r})e^{+i\vec{\Delta}\cdot\vec{r}}$$
Fourier transform of the potential
$$\tilde{V}(\vec{\Delta}) = \iiint d^{3}\vec{r} \ V(\vec{r})e^{+i\vec{\Delta}\cdot\vec{r}}$$

$$f_{B_{1}}(k,\vec{\Delta}) = -\frac{m}{2\pi\hbar^{2}}\tilde{V}(\vec{\Delta})$$
The 1st Born scattering amplitude is proportional to the Fourier transform of the potential

You can also write it in terms of the real potential because the difference between the reduced potential and the real potential was only in terms of this m and h cross and so on. So, you can scale it appropriately write it in terms of this. What is your conclusion that the scattering amplitude in the first Born approximation is essentially the Fourier transform of the potential right.

So, that is a very useful and a very powerful result all you have to do is to; you if you have some form of the potential in mind put it over there get its Fourier transform and that will give you the scattering amplitude. So, this is the result in the first Born approximation. In the first born approximation the scattering amplitude is proportional to the Fourier transform of the potential.

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Now having done this let us go ahead and see what it gives us for the scattering cross section. The differential cross section is nothing but the modulus square of the scattering amplitude so you can go ahead and get that okay. And notice that because it goes as the modular square if there was any sign involved in V like an attractive potential would come with a minus sign and a repulsive potential will come with a plus sign.

If there was any sign which you needed to worry about the information about that sign would become irrelevant when you take the modulus square right. The result is that the differential cross section remains the same regardless of the potential being attractive or negative it does not matter whether it is plus or minus you get essentially the same result. So, this is a very interesting feature of the first born approximation. (Refer Slide Time: 21:32)

 $f_{B_{1}}(k,\vec{\Delta}) = -\frac{1}{4\pi} \iiint d^{3}\vec{r} \ U(\vec{r})e^{+i\vec{\Delta}\cdot\vec{r}}$ $\sigma_{B_{1}}^{Total} = \iint d\Omega \ \frac{d\sigma(\hat{\Omega})}{d\Omega}\Big]_{B_{1}} = \int_{\phi=0}^{2\pi} d\phi \int_{\theta=0}^{\pi} \sin\theta d\theta \Big| f_{B_{1}}(\hat{\Omega} = \hat{k}_{f})\Big|^{2}$ $\vec{\Delta} = \vec{k}_{i} - \vec{k}_{f} \text{ momentum transfer ; choose } \hat{e}_{z} = \hat{\Delta}$ $\sigma_{B_{1}}^{Total} = 2\pi \int_{\theta=0}^{\pi} \sin\theta d\theta \Big| f_{B_{1}}(\hat{\Omega} = \hat{k}_{f})\Big|^{2}$ For a spherically symmetric potential: $f_{B_{1}}(k,\Delta) = -\frac{1}{4\pi} (2\pi) \int_{r=0}^{\infty} r^{2} U(r) dr \int_{\theta=0}^{\pi} \sin\theta d\theta e^{+ir\Delta\cos\theta}$ PCD STITACS Unit 5 Quantum Theory of Collisions - Part 2 $f_{B_{1}}(k,\Delta) = -\frac{1}{4\pi} (2\pi) \int_{r=0}^{\infty} r^{2} U(r) dr \int_{\theta=0}^{\pi} \sin\theta d\theta e^{+ir\Delta\cos\theta}$

So, here you have the Fourier transform and this appears as a volume integral you can simplify this integration because you know that so far as the total cross section is concerned it is a double integral not a triple integral it is the differential cross section is over all the angles and you can carry out this angle integration over the azimuthal angle and over the polar angle theta going from 0 to 2pi.

As azimuthal angle going from 0 to 2pi and this is the differential cross section which is the modulus square of the scattering amplitude. So, this integration will give you the total cross section you can always choose one axis of symmetry which will give you a factor of 2 pi when you integrate over the azimuthal angle right.

From symmetry you get that result directly and then you have got an angle dependent scattering amplitude which you will have to evaluate in this theta integral. So, if you have a spherically symmetric potential then this integration which is a triple integral right the scattering amplitude is a triple integral.

So, you have one integration over the axis of symmetry which gives you a factor of 2pi so you have got this -1 over 4 pi here one integration over the azimuthal angle around the axis of symmetry gives you a factor of 2 pi then you have integration over the remaining two degrees of freedom r going from 0 through infinity and theta going from 0 to pi okay. So, those are the two integrals that you now have to determine. (Refer Slide Time: 23:31)



One of which is already determined in this 2 pi. So, this 2 pi in this 4pi will give you a factor of 1 over 2 and with that 1 over 2 we write the scattering amplitude as minus half and then you have got a radial integral under integration over the polar angle theta. Now this looks like a integration that you have done what do you call it like ajardines right.

So, might as well put a new variable there like carry out the integration over cosine theta instead of theta and that makes it easy, so I will not spend much time discussing this. So, you have got the integration for this new variable which is cosine theta going from - 1 to +1 and then you carry out this integration.

So, you get put the limits okay you get this familiar form so this is the usual integration that you would have done, so many times. And now what do you get you are left with a radial integral from 0 through infinity. The integration over theta has now been carried out okay. There is an r square here there is a 1 over r here, so you get only 1 power of r right.

And everything else is now taken care of your instead of using the exponential form you have written it as a sinusoidal function. (Refer Slide Time: 24:50)

$$f_{B_{1}}(k,\Delta) = -\frac{1}{\Delta} \int_{r=0}^{\infty} rU(r)\sin(r\Delta) dr \quad \overline{U(\vec{r}) = \frac{2m}{\hbar^{2}}V(\vec{r})}$$

$$\sigma_{B_{1}}^{Total} = \iint d\Omega \frac{d\sigma(\hat{\Omega})}{d\Omega} \Big]_{B_{1}} = \int_{\phi=0}^{2\pi} d\phi \int_{\theta=0}^{\pi} \sin\theta d\theta \Big| f_{B_{1}}(k,\Delta) \Big|^{2}$$

$$momentum \ transfer = h\vec{\Delta} \qquad \Delta = \left|\vec{k}_{i} - \vec{k}_{f}\right| = 2k \sin\frac{\theta}{2}$$

$$\sin\theta d\theta = \frac{\Delta d\Delta}{k^{2}}$$

$$range \ of \ \theta: 0 \ to \ \pi$$

$$range \ of \ \Delta: 0 \ to \ 2k$$

$$\sigma_{B_{1}}^{Total} = \frac{2\pi}{k^{2}} \int_{\Delta=0}^{2k} \left| f_{B_{1}}(\Delta) \right|^{2} \Delta d\Delta$$
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$$\sigma_{B_{1}}^{Total} = \frac{2\pi}{k^{2}} \int_{\Delta=0}^{2k} \left| f_{B_{1}}(\Delta) \right|^{2} \Delta d\Delta$$

So, this is the integration that you have to carry out in the first born approximation. The momentum transferred is h cross delta this diagram you would have drawn a number of times in a number of different situations I think most commonly in x-ray diffraction when you use this Ewald's Sphere kind of right.

So, you have got the net momentum transfer which is ki - kf, so this is the difference vector. And then you have got an isosceles triangle over here, so here you have got a right angle triangle of which this side has got a magnitude of delta over 2, this side has got a magnitude of k which is the angle opposite to the 90 degrees to the right angle right. And this, the third side will be k times sine of half theta right.

So, from this Pythagoras theorem you can use that and what it gives you for delta or is this 2k sine theta by 2 and you have the Pythagoras theorem which relates the squares of these sides. So, you get you get a relation for delta square or half delta square but then if you differentiate that you will get a 2 delta d delta so using that you will get sine theta d theta equal to delta d delta over k square.

What is the range of theta, theta goes from 0 to pi and theta = 0 is forward scattering, theta = pi is backward scattering. So, the difference vector k will go from 0 to 2 k right, so the range of delta itself will be 0 to 2k. So, if you carry out the integration instead of theta you carry it over k here you can transfer the integration. So, this is the Ewald's Sphere this is in three dimensions okay.

We have drawn the figure on a plane and this is now your total cross section in the Born approximation the first one approximation. And you need to evaluate this integral instead of integration over theta you can integrate over the momentum transfer delta which will have a minimum value of 0 corresponding to forward scattering and 2k corresponding to backward scattering right. So you integrate from 0 to 2k all right. (Refer Slide Time: 27:25)

$$f_{B_{1}}(k,\Delta) = -\frac{1}{\Delta} \int_{r=0}^{\infty} rU(r)\sin(r\Delta) dr$$

$$\Delta = |\vec{k}_{i} - \vec{k}_{f}| = 2k \sin\frac{\theta}{2}$$

$$\sigma_{B_{1}}^{Total} = \frac{2\pi}{k^{2}} \int_{\Delta=0}^{2k} |f_{B_{1}}(\Delta)|^{2} \Delta d\Delta$$
High energy limit
$$\sigma_{B_{1}}^{Total} \xrightarrow{\simeq} \frac{2\pi}{k^{2}} \int_{\Delta=0}^{\infty} |f_{B_{1}}(\Delta)|^{2} \Delta d\Delta$$

$$\phi_{B_{1}}^{Total} \xrightarrow{\simeq} \frac{2\pi}{k^{2}} \int_{\Delta=0}^{\infty} |f_{B_{1}}(\Delta)|^{2} \Delta d\Delta$$

$$\sigma_{B_{1}}^{Total} \lim_{k \to \infty} \rightarrow^{b} 0 \dots as \frac{1}{k^{2}}; i.e. as \frac{1}{E}$$
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So, these are our main results and now let us look at the high energy limit which is where the Born approximation is very commonly used and everybody believes and rightly so far most situations although there are some exceptions on which I will comment later. If you now look at the high energy limit now energy goes as quadratically with k right, h cross square k square by 2m is the energy.

So, the high energy limit will be obtained by carrying out this integration with this limit k going to infinity. So, here you have this 2pi over k square integration going from 0 through infinity. Now what do you see there is a 1 over k square here on 1 over k square as k tends to infinity will give you a 0.

So, that is your result that the Born approximation, first born approximation cross section will in the limiting case if you go to high enough energies it will go to 0 and the rate at which it will go to 0 is 1 over k square or 1 over energy, so it will fall as 1 over e. So, this is your first one approximation scattering amplitude. (Refer Slide Time: 28:51)

$$f_{B_{1}}(k,\Delta) = -\frac{1}{\Delta} \int_{r=0}^{\infty} rU(r)\sin(r\Delta) dr$$
Screened
coulomb
potential
$$U(\vec{r}) = -U_{0} \frac{e^{-\alpha r}}{r} = -U_{0} \frac{e^{-\tau/a}}{r} ; \quad \alpha = \frac{1}{a}$$
REAL: what about the optical theorem?
$$f_{B_{1}}(k,\Delta) = \frac{U_{0}}{\Delta} \int_{r=0}^{\infty} e^{-\alpha r} \sin(r\Delta) dr \qquad \overset{\text{Ref:Eq.8.82}}{\overset{\text{Dechain}}{\overset{\text{Dechain}}{\overset{\text{Outhom Theory of Collisions}}{\overset{\text{Outhom Theory of Collisions}}{\overset{\text{Outhom Theory of Collisions}}{\overset{\text{Outhom Theory of Collisions}}} f_{B_{1}}(k,\Delta) = \frac{U_{0}}{\Delta} \int_{r=0}^{\infty} e^{-\alpha r} \frac{(e^{ir\Delta} - e^{ir\Delta})}{2i} dr$$

Now let us take the case of Coulomb potential but in particular let just take the case of the screen Coulomb potential. And when you adjust when you tune the screening parameter in the Yokawa potential or in the screen potential screen Coulomb potential you can always take the limit and find what would be the value for the Coulomb potential itself okay.

So, let us determine this for the screened Coulomb potential. So, this is the Yokawa type screened Coulomb potential. And you can write it in terms of this parameter alpha or its inverse it's the same. So, you have the screen Coulomb potential and now you should immediately recognize that when you put this potential over here. This will give you a real number right.

There is nothing over here which has a chance of giving you anything imaginary now what happens to the optical theorem? Because in the optical theorem we discussed earlier in the previous set of classes that the scattering cross section goes as the imaginary part of the forward scattering amplitude right. And they mention apart no matter what angle in this case actually goes to 0.

So, obviously you know that the optical theorem is not going to be valid at least in its form in the form in which we have established it in the case of the first Born approximation okay. So, we already expect that we will have difficulty with the optical theorem. And now let us get rid of this r, now you have this expression for the first Born approximation scattering amplitude.

So, you have to determine this integral now which is again you would have carried out integrations of functions this is a product of two functions of this kind quite routinely it is

easy as to do it if you put this in the exponential form and take the sum of two integrals that is

much easier, so these are usual tricks. (Refer Slide Tim<u>e: 31:06</u>)



And if you carry out this integration which you can work out very easily the result is that the first Born approximation scattering amplitude for the screen Coulomb potential goes as U0 over delta square + alpha square. Now this is a very important result the differential cross section will go as a modulus square, so you get U0 square and the square of this denominator okay. It is the same for the attractive and for the repulsive potential as we commented earlier okay.

(Refer Slide Time: 31:42)

$$f_{B_1}(k,\Delta) = \frac{U_0}{\Delta^2 + \alpha^2}$$

$$U(\vec{r}) = \frac{2m}{\hbar^2} V(\vec{r})$$

$$U(\vec{r}) = -U_0 \frac{e^{-\alpha r}}{r}$$

$$f_{B_1}(k,\Delta) = \frac{2m}{\hbar^2} \frac{Z_1 Z_2 e^2}{\Delta^2 + \alpha^2} = \frac{Z_1 Z_2 e^2}{\frac{\hbar^2}{2m} \Delta^2 + \frac{\hbar^2}{2m} \alpha^2}$$

$$\Delta = \left|\vec{k}_i - \vec{k}_f\right| = 2k \sin\frac{\theta}{2} ; \quad \Delta^2 = 4k^2 \sin^2\frac{\theta}{2} = 4\frac{E}{\hbar^2} \sin^2\frac{\theta}{2}$$

$$f_{B_1}(k,\Delta) = \frac{Z_1 Z_2 e^2}{\frac{\hbar^2}{2m} 4\frac{E}{\hbar^2} \sin^2\frac{\theta}{2} + \frac{\hbar^2}{2m} \alpha^2} = \frac{2Z_1 Z_2 m e^2}{4E \sin^2\frac{\theta}{2} + \hbar^2 \alpha^2}$$
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And now if you use these forms you plug in the explicit form of the scattering potential, so instead of the reduced potential you use the real potential. And if this is some sort of a screened Coulomb interaction between; so this is scatting between a charge Z1 e times which is being scattered or interacting with another charge Z2 e.

Then you will have this Z1 Z2 e square and then you will have the other terms in which we now find this h cross and m because we are using the real potential not just the reduced potential U. So, we already using that Ewald's construction we have shown that this delta is twice k sine theta by 2 right.

From that previous diagram for the Ewald's construction and delta square which comes over here in the denominator we can find it in terms of k square which we can write in terms of e and h cross square. So, we can put all the terms together and write it in a form and you probably begin to recognize this result.

Because it is very familiar it is something that you would have seen earlier and it comes as a surprise that you are you seem to be heading toward a classical result as you can see that you are heading toward that okay. (Refer Slide Time: 33:19)

$f_{B_{1}}(k,\Delta) = \frac{2m}{\hbar^{2}} \frac{Z_{1}Z_{2}e^{2}}{\Delta^{2} + \alpha^{2}} = \frac{Z_{1}Z_{2}e^{2}}{\frac{\hbar^{2}}{2m}\Delta^{2} + \frac{\hbar^{2}}{2m}\alpha^{2}} \frac{U(\vec{r}) = \frac{2m}{\hbar^{2}}}{U(\vec{r}) = -U_{0}}$	$V(\vec{r})$ $\frac{e^{-\alpha r}}{r}$
$f_{B_1}(k,\Delta) = \frac{Z_1 Z_2 e^2}{\frac{\hbar^2}{2m} 4 \frac{E}{\hbar^2} \sin^2 \frac{\theta}{2} + \frac{\hbar^2}{2m} \alpha^2} = \frac{2Z_1 Z_2 m e^2}{4E \sin^2 \frac{\theta}{2} + \hbar^2}$	$2\alpha^2$
$\frac{d\sigma}{d\Omega}\Big]_{B_1} = \left[\frac{2Z}{\Delta^2 + \alpha^2}\right]^2 = \frac{4Z^2}{\alpha^2 \left(4k^2 \sin^2 \frac{\theta}{2} + \alpha^2\right)^2}$	$\frac{n^2}{2m}$
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So, if you see this is very interesting situation and I have just rewritten this for this alpha is coming from the Yukawa potential this is the one which scales the Coulomb by the exponential term. And instead of putting it in these me and h cross and so on. I write it in terms of these atomic you unit for length which is a0. So, in terms of a0 it is for Z square for an electron proton scattering.

So Z1 and Z2 are both equal in this case so you get a factor of Z square instead of Z1, Z2 okay. And now you have this a0 square and you have this term here. (Refer Slide Time: 34:12)

$$\frac{d\sigma}{d\Omega}\Big|_{B_{1}} = \frac{U_{0}^{2}}{(\Delta^{2} + \alpha^{2})^{2}} \qquad \Delta = \left|\vec{k}_{i} - \vec{k}_{f}\right| = 2k\sin\frac{\theta}{2}$$
range of θ : 0 to π
range of Δ : 0 to 2k
$$\sigma_{B_{1}}^{total} = \iint \sin\theta d\theta d\phi \frac{U_{0}^{2}}{(\Delta^{2} + \alpha^{2})^{2}}$$

$$\sigma_{B_{1}}^{total} = \frac{2\pi U_{0}^{2}}{k^{2}} \int_{0}^{2k} \frac{\Delta d\Delta}{(\Delta^{2} + \alpha^{2})^{2}} = \frac{4\pi U_{0}^{2}}{\alpha^{2}(\alpha^{2} + 4k^{2})}$$
For C

Now this is the differential cross section you can integrate it to get the total cross section integrate over all the angles right. So, integration over theta and Phi and the range of integration will be for theta going from 0 to pi corresponding to the momentum transfer going from 0 to twice k. (Refer Slide Time: 34:41)



So, this is the total cross section in the Born approximation and here is how it will behave okay. So, first thing to note is that the total cross section are this energy is not 0 whereas the imaginary part of the forward scattering amplitude is 0. So, the optical theorem is let down in the first Born approximation.

Now if you plot this it gives us some interesting characteristic features of the barn approximation, so here is one. So, this is the differential cross section plotted in units of U0 square a4. So, that is just some scaling so do not worry too much about it and here it is plotted as a function of the momentum transfer okay.

And this is measured in terms of 1 over a so this is some sort of a range which is involved in in scaling down the Coulomb potential by the Yukawa factor okay. So, this is how the differential cross-section behaves in general. (Refer Slide Time: 35:51)



Now let me show you another plot which is really very interesting which is here okay. Now this is a similar plot but it has been here you see curves for different values of k. So, this is for k = 1, this is for k = 2, k = 3, k = 5 and so on. But what are you plotting you are plotting a ratio okay. This is a ratio of the differential cross section in the first Born approximation at an arbitrary angle theta okay that is in the numerator.

And what is in the denominator is the differential cross section in the first Born approximation not at an arbitrary angle but in the forward scattering direction at theta = 0 okay. So, this tells us to what extent scattering in other angles is important relative to scattering in the forward direction.

So, this ratio what you are plotting is a measure of the importance of scattering in different directions compared to the scattering in the forward direction. And notice that here if you go to high energy you know this is k = 1, k = 2, k = 3, so as you go inward energy is increasing as you go in this direction and as you go to the high energy limit which is what we considered almost and this is plotted as a function of the angle theta right.

So, what you find is that almost all the scattering is in the forward direction because this ratio is equal to unity over here okay. So, at the high energy limit almost all the scattering is in the forward direction. So, forward direction means it will go in some small cone in the forward direction right. So, you will have a direction of incidence and you will have a small measure of cone and that cone will become smaller and smaller as the energy increases or the range increases. So, you can expect it to go as 1 over ka some sort of an order of magnitude estimate for this angle and





So, this is the result that you get that at high energies almost all the scattering is in the forward direction. Now this angle is about is of the order of 1 over ka and this is the kind of code in which most of the high energy scattering takes place. Now this is a good result very useful one. And you can see because delta is 2k sine theta by 2 this we know from the previous analysis of the Ewald's diagram.

Then delta over 2k will be of the order of sine theta over 2 or right and theta over 2 you know when this angle is small this sine of this angle is nearly equal to the angle itself. Which is of the order of 1 over ka, so you get a factor of 1 over 2ka for delta over 2k right. (Refer Slide Time: 39:01)



So, you get 1 over twice ka over here and in the high energy Born approximation you get your this result we have seen earlier we have written it in terms of this Bohr radius a0 also. (Refer Slide Time: 39:20)



And what we get is if you look at the limit alpha going to 0 or a goes to infinity which is when the Yokawa potential will go to the Coulomb potential right. So, as the Yokawa potential goes to the Coulomb potential this term alpha square vanishes and then you get the sine square theta by 2 but then you have not another power of 2 over here and that is essentially the classical result okay.

In classical Rutherford scattering okay that is exactly the result that you get. And this is rather exciting that the Born approximation or the Coulomb potential obtained from the Yukawa potential by taking the limit of this alpha going to zero you get you recover the classical Rutherford result. (Refer Slide Time: 40:16)

So, this is the problem with the optical theorem that we had noticed that the imaginary part of the forward scattering amplitude actually goes to 0 okay. But then if you determine the scattering amplitude using this integration of the differential cross section right, you do get nonzero scattering amplitude. But then if you determine the Born approximation scattering amplitude in the second Born approximation it turns out.

And I will not work that out in any detail over here but then you do get the total cross section to be given by 4 pi over k times the imaginary part of the forward scattering amplitude but in the second Born approximation. So, there is some sort of a non-linearity over here and this is sometimes referred to as a nonlinear nature of the Born approximation or the Born series of approximations.

And it is only with reference to what you expect from the optical theorem and you can still write an expression which is somewhat similar to the Born approximation and you can expand the scattering amplitude and the scattering cross section in different powers of the potential.

And then look at the corresponding powers of if you make a comparison of corresponding powers then you see that there is this non-linearity pops out of that. So, this is a straightforward extension which I will not discuss any further. (Refer Slide Time: 41:48)



The only thing I will like to remind you or make a comment on that one expects the Born approximation from all this discussion that it will work at high energy. And at high energy then the particle comes at such immense energy that it sees the target potential interacts with it get scattered off and there will be no effect of the electron correlations.

Because if the target consists of many electrons which it almost always does when you do atomic scattering then you know very well that the single particle approximation does not describe the atom fully correctly right. Because it leaves out, what does leave out it leaves out, the Coulomb correlation.

These Coulomb correlations are left out and you do not expect these correlations to play any important role in high-energy scattering because you think that okay is going to come so fast that it will not be disturbed by the correlations which will be so weak and so insignificant that they would not matter.

In other words your one would be tempted to conclude that in high energy the independent particle approximation and the Born approximation will always be valid and it is not a bad approximation as such it is not a bad conclusion in most situations it holds. However there are certain considerations due to which you cannot really get rid of the consequences of correlations.

And as a matter of fact it turns out that as has been discussed in this reference here that the independent particle approximation in x-ray photoemission, so that is high-energy photoemission. In that it turns out that it is all means if it all the Born approximation was it is almost always an exception and not quite a rule.

And this is because of certain correlations that you really cannot completely get rid off so the independent particle approximation actually breaks down so one has to be concerned about some of these things I can show you one of the results like if you were to look at the Born approximation result what you would expect this line over here.

But this line is not what explains the experimental result which is well away from this Born approximation or independent particle approximation result and you have these additional features. So, this is just a comment for further studies and something that you might want to keep back of your mind.

But other than that for most applications the Born approximation and the independent particle approximation is an excellent approximation in the high energy range and with that I will conclude this class over here. In the next class I will discuss coulombs scattering you will remember that the methods that we discussed earlier was not directly applicable for the Coulomb case.

And it needed a different approach. So that is the one I will discuss in the next class there is any question for today I will be happy to take.