

## Lecture 5

### Scattering theory

What is scattering.

$$A_1(\alpha_1) + A_2(\alpha_2) + \dots \rightarrow B_i(\beta_i)$$

$A_i$  and  $B_i$  are some particles or  
some objects

$\alpha_i$  and  $\beta_i$  are degrees of freedom  
e.g. momentum, energy, spin etc.

- There are two ways to approach the problem.

Scattering is the transition from  $|i\rangle \xrightarrow{H} |f\rangle$   
Notice momentum can be different but  
energy is the same = ELASTIC SCATTERING.

We can apply our time dependent perturbation  
theory, and use the Fermi golden rule

$$\Gamma = \frac{2\pi}{\hbar} |\langle f | H^{(1)} | i \rangle|^2 \rho_f(E)$$

density of final states.

- 2<sup>d</sup> approach is to treat the scattering  
process as scattering off a potential  
and setup some differential equation.

In  $E_i \neq E_f$  the scattering is called  
INELASTIC.

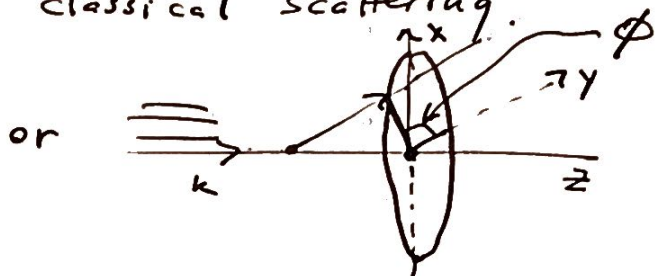
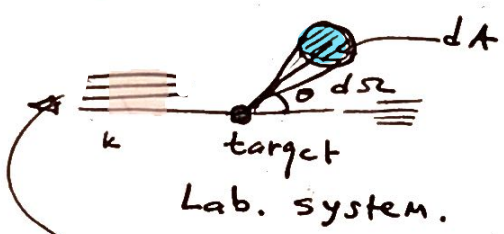
This process is the most important  
since it allows to probe excitation spectrum  
of an object in question.

→ In quantum scattering we calculate a probability  
of certain final states given the initial  
state and the perturbation hamiltonian.

The aim is to deduce the details of internal workings of the object in question.

More specifically we want to connect a cross-section (will define later) and wave function.

Brief reminder about classical scattering.



A parallel beam of particles.

Some particles are scattered but some transmitted.

Number of incident particles crossing unit area per time = FLUX

$\Delta N_s$  is the # of particles scattered into  $d\Omega$

so :  $\Delta N_s \sim N_i d\Omega$  or

$dN_s = \frac{d\sigma}{d\Omega} \cdot N_i d\Omega$  where  $\sigma = \sigma(\theta, \varphi)$   
 $d\Omega = 2\pi \sin\theta d\theta$

differential cross-section.

$[\frac{d\sigma}{d\Omega}] = \frac{\text{Area}}{\text{steradian}} \equiv \text{SI units}$

or  $\Delta \sigma = (\frac{d\sigma}{d\Omega}) d\Omega$  is the area.

which incident particles strike per target particle in order to scatter into  $d\Omega$

$$\frac{d\sigma}{d\Omega} d\Omega = \frac{\Delta N_s}{d\Omega N_i} d\Omega = \frac{\Delta N_s}{N_i} \equiv \text{probability of scattering into } d\Omega$$

The total number of scattered particles:

$$\int dN_s d\Omega = \int N_i \frac{d\sigma}{d\Omega} d\Omega = N_i \int d\sigma d\Omega$$

$$N_s = N_i \cdot \sigma \quad \text{where } \sigma \equiv \text{TOTAL SCATTERING CROSS-SECTION}$$

$$\sigma = \frac{N_s}{N_i}$$

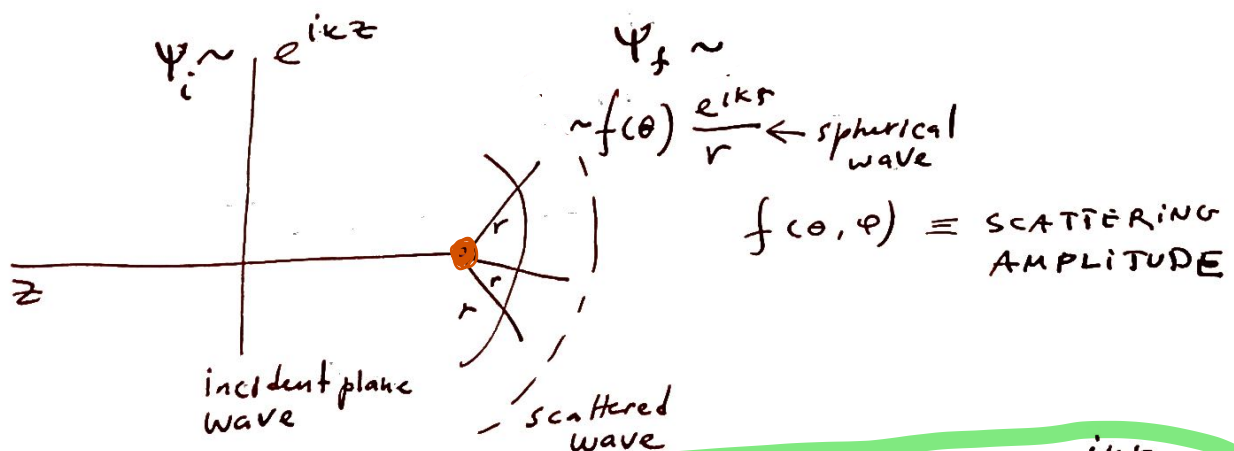
For example: a size of nucleus  $\pi R^2 = 7 \cdot 10^{-26} A^{2/3}$   
 $A$  is the atomic number.

for  $Al^{27}$  the cross section:  $0.588 \cdot 10^{-28} \text{ m}^2$   
 and for  $Au^{197}$   $2.4 \cdot 10^{-28} \text{ m}^2$ .

Nuclear cross section  $\sim 10^{-28} \text{ m}^2 = 1 \text{ barn}$ .

Read section 17.3 if you are involved into scattering projects.

Lets move to quantum mechanics



So the total  $\psi_{r \rightarrow \infty} \sim e^{ikz} + f \frac{e^{ikr}}{r}$

$\uparrow$  some particles are not scattered

$\uparrow$  some are

To determine  $\sigma = \frac{N_s}{N_i}$  we need to find the number of particles:

For monochromatic beam:

$J_{inc}$  in the  $z$  direction  $\psi_i \sim e^{ikz}$   
 Current density  $|\vec{J}_{inc}| = \frac{\hbar(k)}{m}$  ( $j = q \vec{v} \cdot \vec{m} \cdot n$ )

Now we calculate current density in  $\vec{r}$  and into  $dA$

Number of scattered  $\Delta N_s = J_s \cdot dA = r^2 J_s \cdot d\Omega$

Also this number should be  $\sim$  to incident current density

$\Delta N_s = J_i d\sigma$



$r^2 J_s d\Omega = J_i d\sigma \Rightarrow \frac{d\sigma}{d\Omega} = r^2 \frac{J_{s,r}}{|J_i|}$

From basic quantum mechanics we know that any current density can be expressed in terms of  $\psi$  and  $\frac{\partial \psi}{\partial x}$

$J_{s,r} = \frac{\hbar}{2mi} \left( \psi_s^* \frac{\partial \psi_s}{\partial r} - \psi_s \frac{\partial \psi_s^*}{\partial r} \right)$

$\psi_s = f(\theta, \varphi) \frac{e^{ikr}}{r}$        $\psi_s^* = f(\theta, \varphi) \frac{e^{-ikr}}{r}$   
 $\frac{\partial \psi_s}{\partial r} = f(\theta, \varphi) \left[ \frac{e^{ikr}}{r} (ikr) - \frac{1}{r^2} e^{ikr} \right]$   
 $\frac{\partial \psi_s^*}{\partial r} = f(\theta, \varphi) \left[ \frac{e^{-ikr}}{r} (-ikr) - \frac{1}{r^2} e^{-ikr} \right]$

$J_{s,r} = \frac{\hbar k}{mr^2} |f(\theta, \varphi)|^2$  and recall  $J_i = \frac{\hbar k}{m}$  we get

$\frac{d\sigma}{d\Omega} = r^2 \frac{J_{s,r}}{J_i} = r^2 \frac{\frac{\hbar k}{mr^2} |f(\theta, \varphi)|^2}{\frac{\hbar k}{m}} = |f(\theta, \varphi)|^2$

$\sigma = \int d\Omega |f(\theta, \varphi)|^2 = \int |f|^2 \sin\theta d\theta d\varphi$  and

$\sigma(\theta) = 2\pi \int_0^\pi |f|^2 \sin\theta d\theta$

Note, since in quantum mechanics we cannot discuss a path of the quantum object we can only talk about probability of scattering of the incoming particle at the angle  $(\theta, \varphi)$ .

Comment: of course one can develop a new way called the Path Integral formalism.

Green's Functions

Green's functions is the way to transform the Sch. eqn. into an integral equation.

Math detour: assume  $\hat{L}$  is a linear operator

if  $\hat{L}y = f(x)$  we can obtain the solution via G.F. source is  $\delta$ -like

step 1: obtain the solution of  $Ly = \delta(x-x')$

step 2: for  $Ly = f(x)$  in the interval  $x \in [a, b]$

$$y(x) = \int_a^b G(x, x') f(x') dx'$$

any arbitrary source

check this:

$$Ly(x) = L \int_a^b G(x, x') f(x') dx' =$$

What's L?  $G(x, x') = \delta(x-x') \rightarrow \int_a^b \delta(x-x') f(x') dx' = f(x)$

in QM we want to solve

$$\left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \Psi = E \Psi = \frac{\hbar^2 k^2}{2m} \Psi \quad \text{or}$$

$$\underbrace{(\nabla^2 + k^2)}_L \Psi = \underbrace{\frac{2m}{\hbar^2} V(r)}_{U(r)} \Psi = U(r) \Psi = F(r)$$

then  $G(r, r')$  is the solution of

$$(\nabla^2 + k^2) G(r, r') = \delta(r-r')$$

So solve this lets try the spherical wave

$$G(r, r') = \frac{e^{\pm i k |r-r'|}}{|r-r'|} \quad \leftarrow \text{Galilean invariance}$$

$$\begin{aligned}
 (\nabla^2 + k^2) G(r, r') &= (\nabla^2 + k^2) \frac{e^{\pm ik|r-r'|}}{|r-r'|} = \\
 &= -\frac{k^2 e^{\pm ik|r-r'|}}{|r-r'|} + \frac{e^{\pm ik|r-r'|}}{|r-r'|} \underbrace{\left( \nabla^2 \frac{1}{|r-r'|} + \right)}_{-4\pi \delta(r-r')} \\
 &+ k^2 \frac{e^{\pm ik|r-r'|}}{|r-r'|} = -\frac{e^{\pm ik|r-r'|}}{4\pi \delta(r-r')}
 \end{aligned}$$

$$(\nabla^2 + k^2) \frac{e^{\pm ik|r-r'|}}{|r-r'|} \cdot \frac{1}{-4\pi} = \delta(r-r') \cdot e^{\pm ik|r-r'|}$$

from the definition of  $G(r, r')$

$$(\nabla^2 + k^2) G(r, r') = \delta(r-r') \quad \text{we can conclude}$$

$$G(r-r') = -\frac{e^{\pm ik|r-r'|}}{4\pi |r-r'|}$$

and

$$\delta(r-r') = \delta(r-r') e^{\pm ik|r-r'|}$$

Correct if  $r=r'$

Now for the incoming or non scattered particles  $v=0$

$$(\nabla^2 + k^2) \psi = 0 \Rightarrow \psi_0 = e^{ikz} \quad \text{finally}$$

$$\psi(\vec{r}) = e^{ikz} - \frac{1}{4\pi} \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} U(\vec{r}') \psi(\vec{r}') dV'$$

here we only used + sign for  $r \rightarrow +\infty$ .

The scattered amplitude is made of spherical waves arising at each point of  $r'$  space.

the amplitude of those waves is  $U(\vec{r}')\psi(\vec{r}')$

All those waves are interfering to produce the total scattered wave at  $\vec{r}$ .

Physical meaning:



We can simplify the equation for  $\psi(r)$  at  $r \rightarrow \infty$

$$\psi(r) = e^{ikz} - \frac{1}{4\pi} \frac{e^{ikr}}{r} \int e^{-ikr'} \underbrace{U(r') \psi(r')}_{\text{which is just the Fourier transform of } U(r) \psi(r')}$$

which is just the Fourier transform of  $U(r) \psi(r)$

and comparing this expression to the previously derived:

$$\psi(r) = e^{ikz} + f(\theta, \phi) \frac{e^{ikr}}{r} \Rightarrow$$

$$f(\theta, \phi) = -\frac{1}{4\pi} \int e^{-ikr} U(r) \psi(r) dV$$

looks easy but remember  $\psi(r)$  is still not known!

We can also try an iterative procedure to solve it:

(1) replace  $r$  by  $r'$ :  $\psi(r') = e^{ikz'} - \frac{1}{4\pi} \int \frac{e^{ik|r'-r''|}}{|r'-r''|} U(r'') \psi(r'') dV''$

and (2) plug this into  $\psi(r) = \dots$

$$\psi(r) = e^{ikz} \leftarrow \text{incident beam} - \frac{1}{4\pi} \int \frac{e^{ik|r-r'|}}{|r-r'|} U(r') e^{ikz'} dV' \leftarrow \text{single scattering by } U(r')$$

$$- \left( -\frac{1}{4\pi} \right)^2 \iint \frac{e^{ik|r-r''|}}{|r-r''|} U(r'') \frac{e^{ik|r-r''|}}{|r-r''|} U(r') e^{ikz'} dV' dV''$$

(looks like  $e^{ikz} + \int G(r-r') U(r') e^{ikr'} dV'$ )

$$- \iint G(r-r') U(r) G(r-r'') \psi(r'') U(r'') dV' dV''$$

This iterated series is known as Neumann Series

NEXT: how to find  $\psi(r)$ .

Both approximation means cut off the infinite series to the  $n$ th term.

scattering of the scattered wave by  $U(r'')$ !

DOUBLE SCATTERING

MAX BORN APPROXIMATION

First Born approximation.

Suppose  $\psi$  is approximated by  $e^{ikz}$

meaning  $g(\mathbf{r}) \equiv |\psi - e^{ikz}| \ll |e^{ikz}| = 1$

1st Born approx:  $\psi = e^{ikz}$  where  $k = k_0$

$$f(\theta, \varphi) = -\frac{1}{4\pi} \int e^{-i\mathbf{k}\cdot\mathbf{r}} U(\mathbf{r}) e^{i\mathbf{k}_0\cdot\mathbf{r}} d\mathbf{r}$$

$$= -\frac{1}{4\pi} \int e^{-i\vec{s}\cdot\vec{r}} U(\mathbf{r}) d\mathbf{r}$$

$\vec{s} = \mathbf{k} - \mathbf{k}_0$

1st Born Approx.

Thus scattering amplitude is just Fourier transformation of  $U(\mathbf{r}) \rightarrow U(\mathbf{k})$



$s = 2k \sin \theta/2$  ;  $\vec{s}\cdot\vec{r} = sr \cos \theta$

$$f = \frac{1}{4\pi} \int_0^\infty \int_0^\pi \int_0^{2\pi} e^{-isr' \cos \theta'} U(r') r'^2 \sin \theta' dr' d\theta' d\varphi'$$

$$= -\frac{1}{4\pi} \left[ \int_0^\infty r'^2 U(r') dr' \int_0^\pi e^{isr' \cos \theta'} \sin \theta' d\theta' \int_0^{2\pi} d\varphi' \right]$$

$$= 2\pi \int_0^\infty r'^2 U(r') dr' \int_{-1}^1 e^{isr'x} dx =$$

$$= \left[ \frac{4\pi}{s} \int_0^\infty r' U(r') \sin(sr') dr' \right] \cdot \left( -\frac{1}{4\pi} \right) =$$

$$= -\frac{1}{s} \int_0^\infty r' \sin(sr') dr' = f(s)$$

$\vec{s} \equiv \mathbf{k} - \mathbf{k}'$   
so called transferred momentum.



Important features of  $f(\theta, \phi)$ :

- no dependence on  $\phi$
- $f$  is a real function
- $\hbar \bar{s} = \hbar (\bar{k} - \bar{k}_0)$  - is called MOMENTUM TRANSFER

- For small  $\bar{k}$ ,  $\bar{s}$  is small  
 $\sin(sr') \sim sr' \Rightarrow$

forward scattering  $\rightarrow f \approx -\frac{1}{s} \int_0^\infty r \cdot r U(r) dr = - \int_0^\infty r'^2 U(r') dr'$

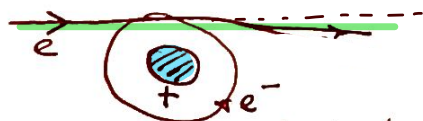
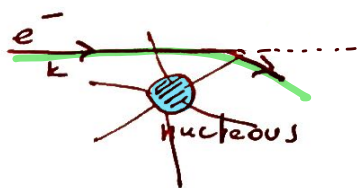
large angle scattering - for large momentum transfer  $s$   
 $f(\theta)$  is small.

STUDY PROBLEM #3 page 428 and SECTION 17.6.2.1

Scattering from Coulomb Potential

If we have no electrons and nucleus is a point charge:  $V(r) = -Ze^2/r$   
 (POSITIVE!)

When we add up an electron, it will screen the Coulomb potential.



$$V(r) = -\frac{Ze^2}{r} e^{-r/a}$$

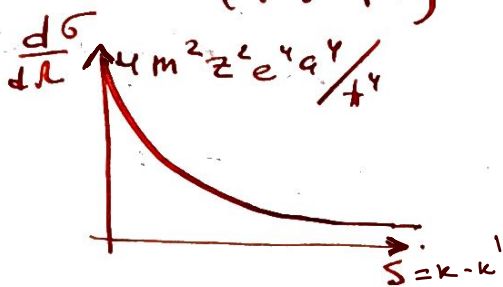
screened potential.

cut-off radius

Let's calculate the scattering amplitude for such scattering.

in nuclear physics, it is known as Yukawa potential

$$\begin{aligned}
 f(\theta) &= -\frac{imZe^2}{\hbar^2 s} \int_0^{\infty} e^{-r/a} \left( \frac{e^{isr} - e^{-isr}}{\uparrow \sin(sr)} \right) dr \\
 &= -\frac{imZe^2}{\hbar^2 s} \int_0^{\infty} e^{-r(\frac{1}{a} - is)} dr - \int_0^{\infty} e^{-r(\frac{1}{a} + is)} dr \\
 &= \frac{-imZe^2}{\hbar^2 s} \left( \frac{1}{i(\frac{1}{a} - is)} \cdot (+1) - \frac{(-1)}{(\frac{1}{a} + is)(-1)} \right) = \\
 &= \frac{2mZe^2 a^2}{\hbar^2 (a^2 s^2 + 1)} \Rightarrow \frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{4m^2 Z^2 e^4 a^4}{\hbar^4 (a^2 s^2 + 1)^2}
 \end{aligned}$$



The total cross-section:

$$\sigma = \int_0^{\pi} \int_0^{2\pi} \frac{d\sigma}{d\Omega} \sin\theta d\theta d\phi$$

$$\begin{aligned}
 &= \frac{4m^2 Z^2 e^4 a^4}{\hbar^4} \int_0^{\pi} \frac{2 \sin\theta/2 \cdot \cos\theta/2}{[1 + 4k^2 a^2 \sin^2\theta/2]^2} d\theta \int_0^{2\pi} d\phi \\
 &= \frac{8\pi m^2 Z^2 e^4 a^4}{\hbar^4} \int_0^{\pi} \frac{2 \sin\theta/2}{(1 + 4k^2 a^2 \sin^2\theta/2)^2} d\theta
 \end{aligned}$$

$$\begin{aligned}
 &= \frac{16\pi m^2 Z^2 e^4 a^4}{\hbar^4 (1 + 4k^2 a^2)} \quad (\text{use mathematics or sympy. etc}) \\
 &\quad \int_0^{\pi} \frac{d(\sin\theta/2)}{(1 + 4k^2 a^2 \sin^2\theta/2)} \quad \cos\frac{\theta}{2} d\theta = d\sin\frac{\theta}{2} \cdot 2 =
 \end{aligned}$$

Now, if  $a \rightarrow \infty \Rightarrow V = -\frac{Ze^2}{r} \left( 1 + \left( -\frac{r}{a} \right) \right) + \dots$   
 $\xrightarrow{a \rightarrow \infty} -\frac{Ze^2}{r}$  ← Unscreened Coulomb potential

famous in this case  
 Rutherford  
 scattering  
 formula

$$\begin{aligned}
 \frac{d\sigma}{d\Omega} &= \frac{4 \cdot Z^2 e^4 m^2 a^4}{\hbar^4 (a^2 s^2 + 1)^2} \approx \\
 &\approx \frac{4 \cdot Z^2 e^4}{\hbar^4} \frac{1}{s^4} = \frac{4m^2 Z^2 e^4}{\hbar^4 k^4 \sin^4(\theta/2)}
 \end{aligned}$$