Lecture 5

Scattering theory

What is scattering.

$$A_1(\alpha_1) + A_2(\alpha_2) + \quad \rightarrow B_1(\beta_1)$$

A_i and B_i are some particles or some objects

α_i and β_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

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

density of final states.

- 2^d approach is to treat the scattering process as scattering off a potential and setup some differentiall equation.

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

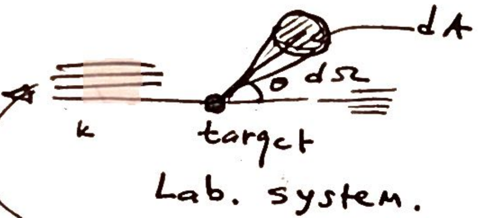
This process is the most important since it allows to probe excitation spectrum of an object in question.

→ 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.



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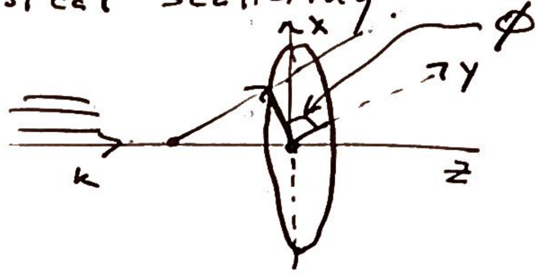


A parallel beam of particles.

Some particles are scattered but some transmitted.

Number of incident particels crossing unit area per time = FLUX

ΔN_s is the # of particles scattered into $d\Omega$

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

$$dN_s = \frac{d\sigma}{d\Omega} \cdot N_i \, d\Omega \qquad \text{where } \sigma = \sigma(\theta, \varphi)$$

$$d\Omega = 2\pi \sin\theta \, d\theta$$

↑ differential cross-section.

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

or $\Delta\sigma = \left(\frac{d\sigma}{d\Omega}\right) d\Omega$ is the area ~~of~~ which incident particles strike per target particle in order to scatter into $d\Omega$

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

The total number of scattered particles:

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

$N_s = N_i \cdot \sigma$ where $\sigma \equiv$ 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.

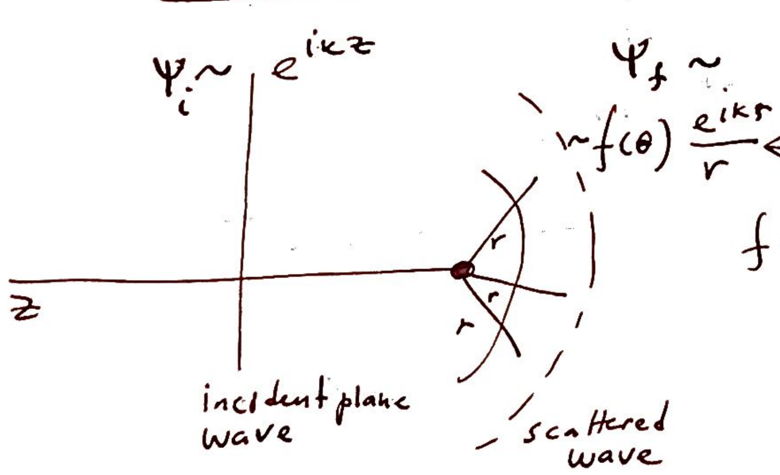
for Al^{27} the cross section: $0.588 \cdot 10^{-28}\, m^2$

and for Au^{197} $2.4 \cdot 10^{-28}\, m^2$.

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

Read Section 17.3 if you are involved into scattering projects.

Lets move to quantum mechanics



$f(\theta, \varphi) \equiv$ SCATTERING AMPLITUDE

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

↑ some particles are not scattered

↖ 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 $\psi_i \sim e^{ikz}$

incident current density $|\bar{J}_{in}| = \frac{\hbar |k|}{m}$ $\quad (j = q \overbrace{v \cdot m}^{p=\hbar k} \cdot n)$

Now we calculate current density in $\bar{r}$ 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 ~ 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 ψ and $\frac{\partial \psi}{\partial x}$

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

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

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

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

$\sigma = \int d\Omega \, |f(\theta,\varphi)|^2 = \iint |f|^2 \sin\theta \, d\theta \, d\varphi$ 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 (θ, φ).

Green Functions

Green 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.

step1: obtain the solution of $Ly = \delta(x-x')$

step2: for $Ly = f(x)$ in the interval $x \in [a,b]$

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

check this:

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

$G(x,x') = \delta(x-x')$

$$= \int_a^b \delta(x-x') f(x') dx' = f(x).$$

what's L?

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

$$G \sim \frac{e^{\pm ik|r-r'|}}{|r-r'|} \text{ — Galilean invariance}$$

$$(\nabla^2+k^2)G = (\nabla^2+k^2)\frac{e^{\pm ik|r-r'|}}{|r-r'|} =$$

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

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

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

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

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

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

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

Correct if $r=r'$

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

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

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

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

▶ The scattered amplitude is made of spherical waves arising at each point of r' space.
the amplitude of those waves is $U(r')\psi(r')$
All those waves are interfering to produce the total scattered wave at $\bar{r}$.

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

$$\psi(r) = e^{ikz} - \frac{1}{4\pi}\frac{e^{ikr}}{r}\int e^{-ikr'}\underbrace{U(r')\psi(r')}\,dv'$$

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

and comparing this expression to:

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

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

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

We can also try an iterative procedure to solve it.

replace r by r' : $\psi(r') = e^{ikz'} - \frac{1}{4\pi}\int \frac{e^{ik|r'-r''|}}{|r'-r''|}\cdot U(r'')\psi(r'')\,dv''$ and plug this into $\psi(r) = \ldots$

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

$$-\left(-\frac{1}{4\pi}\right)^2\iint \frac{e^{ik|r-r'|}}{|r-r'|}U(r)\,\frac{e^{ik|r-r''|}}{|r-r''|}\cdot U(r'')\psi(r'')\,dv'dv''$$

(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

scatterings of the scattered wave by $V(r'')$!

DOUBLE SCATTERING

NEXT: how to find $\psi(r)$.
Born approximation means cut off the infinite series to the n^{th} term.

BORN APPROXIMATION

First Born approximation.

Suppose ψ is approximated by e^{ikz}

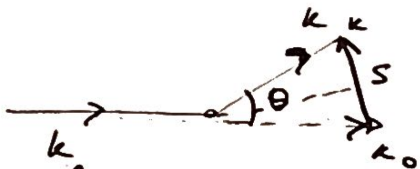
meaning $g(r) = |\psi - e^{ikz}| << |e^{ikz}| = 1$

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

$$f(\theta,\varphi) = -\frac{1}{4\pi}\int e^{-ikr}\, U(r)\, e^{ik_0 r}\, dV$$

$$= -\frac{1}{4\pi}\int e^{-i\underbrace{\bar{s}}_{\bar{k}-\bar{k}_0}\cdot\bar{r}}\, U(r)\, dV$$

1st Born Approx. { Thus scattering amplitude is just Fourier transformation of $U(r) \rightarrow U(k)$



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

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

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

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

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

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

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

- no dependence on φ
- f is a real function
- $\hbar \vec{s} = \hbar(\vec{k}-\vec{k_0})$ - is called MOMENTUM TRANSFER

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

$$f \cong -\frac{g}{s}\int_0^\infty r \cdot r\, U(r)\, dr = -\int_0^\infty r'^2 U(r')\, dr'$$

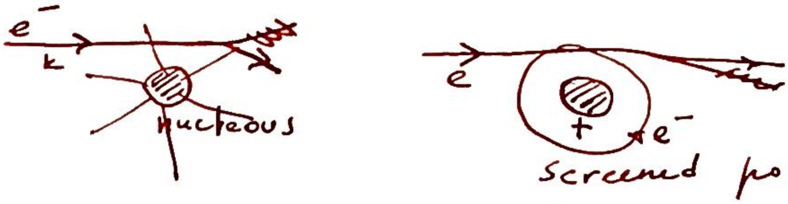
- for large momentum transfer s $f(\theta)$ is small.

STUDY PROBLEM #3 page 428 and Section 17.6.2.1

<u>Scattering from Coulomb Potential</u>

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

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



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

screened potential.

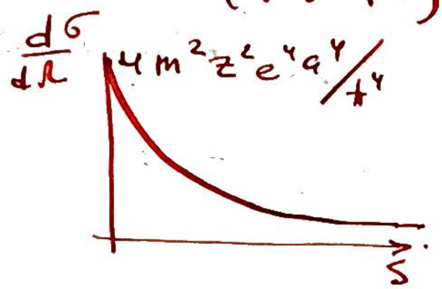
Lets calculate the scattering amplitude for such scattering.

$$f = -\frac{imZe^2}{\hbar^2 s}\int_0^\infty e^{-r/a}\left(\underbrace{e^{isr}-e^{-irs}}_{\uparrow \sin(sr)}\right)dr$$

$$= -\frac{imZe^2}{\hbar^2 s}\int_0^\infty e^{-r(\frac{1}{a}-is)}\,dr - \int_0^\infty e^{-r(\frac{1}{a}+is)}\,dr$$

$$= \frac{-imZe^2}{\hbar^2 s}\left(\frac{1}{(\frac{1}{a}-is)}\cdot(+1) - \frac{\cancel{(-1)}}{(\frac{1}{a}+is)\cancel{(-1)}}\right) =$$

$$= \frac{2mZe^2a^2}{\hbar^2(a^2s^2+1)} \Rightarrow \frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{4m^2Z^2e^4a^4}{\hbar^4(a^2s^2+1)^2}$$



The total cross-section:

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

$$= s = 2k\sin\theta/2 = \frac{8\pi m^2Z^2e^4a^4}{\hbar^4}\int_0^\pi d\theta\,\frac{2\sin\theta/2\cdot\cos\theta/2}{[1+4k^2a^2\sin^2\theta/2]^2} = \cancel{(d\cos\theta/2)}\quad \cos\frac{\theta}{2}d\theta = d\sin\frac{\theta}{2}\cdot 2 =$$

$$= \frac{8\pi m^2Z^2e^4a^4}{\hbar^4}\int_0^1 d\left(\sin\frac{\theta}{2}\right)\frac{2\sin\theta/2}{\left(1+4k^2a^2\sin^2\frac{\theta}{2}\right)}$$

$$= \frac{16\pi m^2Z^2e^4a^4}{\hbar^4(1+4k^2a^2)}$$ (use mathematica or sympy. else)

if $a\to\infty \Rightarrow V = -\frac{Ze^2}{r}\left(1+\left(-r/a\right)\right)+\dots$

$$\underset{a\to\infty}{\cong} -\frac{Ze^2}{r} \Leftarrow$$ unscreened Coulomb potential

in this case $\frac{d\sigma}{d\Omega} = \frac{4m^2Z^2e^4\cancel{a^4}}{\hbar^4}\frac{1}{\left(\frac{a^2s^2}{a^2}+\frac{1}{a^2}\right)^2} \cong$

$$\approx \frac{4m^2Z^2e^4}{\hbar^4}\frac{1}{s^4} = \frac{m^2Z^2e^4}{4\hbar^4k^4\sin^4(\theta/2)}$$

the Rutherford scattering formula