Lecture 5

Scattering theory

What is scattering?

\[ A_i (c_{d_1}) + A_2 (c_{d_2}) \rightarrow B_i (c_{d_1}) \]

\( A_i \) and \( B_i \) are some particles or some objects.
\( d_1 \) and \( d_2 \) are degrees of freedom (e.g., momenta, energy, spin, etc.).

There are two ways to approach the problem.

1. Scattering is the transition from \( i \rightarrow f \) and notice momentum can be different but energy is the same = ELASTIC SCATTERING.

2. 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.

2nd approach is to treat the scattering process as scattering off a potential and setup some differential equation.

In \( E \neq E_f \) 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 number 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 \( \sigma = \sigma(\Theta, \Phi) \)

\( d\Omega = 2\pi \sin \Theta d\Theta d\Phi \)

Differential cross-section.

\( \frac{d\sigma}{d\Omega} \) = area/steradian = 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 \( d\Omega \)
\[ \frac{d\sigma}{d\Omega} = \frac{\Delta N}{\Delta \Omega N_i} = \frac{\Delta N}{N_i} = \text{probability of scattering into } d\Omega \]

The total number of scattered particles:
\[ \int dN_s d\Omega = \int N_i \frac{d\sigma}{d\Omega} r^2 d\Omega = N_i \int d\sigma \int d\Omega \]

\[ N_s = N_i \sigma \] where \( \sigma \) = total scattering cross-section

\[ \sigma = \frac{N_s}{N_i} \]

For example: a size of nucleus \( \pi R^2 = 7 \times 10^{-26} \, \text{A}^{2/3} \)

\( A \) is the atomic number.

For A\(^{27}_\text{Al} \) the cross section: 0.588 \( \times 10^{-28} \, \text{A}^2 \)

and for A\(^{197}_\text{Au} \) 2.4 \( \times 10^{-28} \, \text{A}^2 \).

Nuclear cross section \( \sim 10^{-28} \, \text{A}^2 = 1 \text{ barn} \).

Read Section 17.3 if you are involved into scattering projects.

Let's move to quantum mechanics.

\[ \psi_i \sim e^{ikz} \quad \psi_f \sim e^{ikr} \]

\[ f(\theta) \frac{e^{ikr}}{r} \sim \text{spherical wave} \]

\[ \int f(\theta, \phi) = \text{scattering amplitude} \]

incident plane wave

\[ \psi_t \to +e^{ikz} + f \frac{e^{ikr}}{r} \]

\[ \psi_i \to \text{some particle not scattered} \]
To determine $\sigma = \frac{N_s}{N_i}$ we need to find the number of particles.

For monochromatic beams:

\[ J_{\text{inc}} \text{ in the } z \text{ direction: } J_i \sim e^{i\mathbf{p} \cdot \mathbf{r}} \]

incident current density \[ J_i = \frac{i}{\hbar} \frac{\mathbf{p}}{m} \quad (\mathbf{p} = \frac{\mathbf{p}}{m}) \]

Now we calculate current density in $\Gamma$ and into $\bar{\Gamma}$

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

Also this number should be $\sim$ to incident current density $\sigma N_s = J_i \int d\Omega$

\[ r^2 J_s \int d\Omega = J_i \int d\Omega \Rightarrow \frac{d\Omega}{d\Omega} = \frac{r^2 J_s}{J_i} \]

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

\[ J_{s, \mathbf{r}} = \frac{\hbar}{2m} \left( \psi^* \frac{\partial \psi}{\partial \mathbf{r}} - \psi \frac{\partial \psi^*}{\partial \mathbf{r}} \right) \]

\[ \psi = f(0, \varphi) e^{i\mathbf{p} \cdot \mathbf{r}} \quad \psi^* = f(0, \varphi) e^{-i\mathbf{p} \cdot \mathbf{r}} \]

\[ \frac{\partial \psi}{\partial \mathbf{r}} = f(0, \varphi) \left[ \frac{\partial}{\partial r} (i \mathbf{p} \cdot \mathbf{r}) - \frac{1}{r^2} e^{i \mathbf{p} \cdot \mathbf{r}} \right] \]

\[ \frac{\partial \psi^*}{\partial \mathbf{r}} = f(0, \varphi) \left[ \frac{\partial}{\partial r} (i \mathbf{p} \cdot \mathbf{r}) + \frac{1}{r^2} e^{i \mathbf{p} \cdot \mathbf{r}} \right] \]

\[ J_{s, r} = \frac{\hbar}{m r^2} |f(0, \varphi)|^2 \quad \text{and recall } J_i = \frac{\hbar}{m} \quad \text{we get} \]

\[ \sigma = \int d\Omega |f(0, \varphi)|^2 = \int |f|^2 \sin \theta \, d\theta \, d\varphi \quad \text{and} \]

\[ \sigma(\theta) = 2 \pi \int_0^\pi |f|^2 \sin \theta \, d\theta. \]
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 \((\theta, \phi)\).

**Green Functions**

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

**Math detour:** assume \(L\) is a linear operator if \(Ly = f(x)\) we can obtain the solution via G.F.

1. Step 1: obtain the solution of \(Ly = \delta(x-x')\)
2. Step 2: for \(Ly = f(x)\) in the interval \(x \in (a, b]\)

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

Check this:

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

What is \(L\)?

In Q.M. we want to solve

\[
\left( -\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi = E \psi = \frac{\hbar^2 k^2}{2m} \psi \quad \text{or} \quad \frac{\nabla^2 + k^2}{L} \psi = \frac{2m}{\hbar^2} V(x) \psi = U(r) \psi = F(r)
\]

Then \(G(r, r', \theta, \phi)\) is the solution of

\[
\left( \nabla^2 + k^2 \right) G(r, r', \theta, \phi) = \delta(r-r')
\]

So solve this let's try the spherical wave

\[G = \frac{e^{i (l \pi / 2 b) \cdot (1 + r') - (l + 1) \pi / 2 b \cdot (1 - r')}}{2 b \sin \phi} \quad \text{Galilean invariance}\]
\[(\nabla^2 + \kappa^2) G = (\nabla^2 + i\kappa^2) \frac{e^{\pm i\kappa |r-r'|}}{|r-r'|} = -\kappa^2 \frac{e^{\pm i\kappa |r-r'|}}{|r-r'|} + \frac{2\pm i\kappa |r-r'|}{|r-r'|} + 2 \frac{1}{|r-r'|} + \frac{\pm i\kappa |r-r'| - 4\pi \delta(r-r')}{4\pi} \cdot \gamma \cdot \delta(r-r')\]

\[(\nabla^2 + \kappa^2) \frac{\pm i\kappa |r-r'|}{|r-r'|} = \frac{1}{4\pi} \cdot \delta(r-r') \cdot e^{\pm i\kappa |r-r'|}\]

From the definition of \(G(r,r')\)

\[(\nabla^2 + \kappa^2) G(r,r') = \delta(r-r') \]

we can conclude

\[G(r-r') = \frac{e^{\pm i\kappa |r-r'|}}{4\pi |r-r'|}\]

and

\[\delta(r-r') = \delta(r-r') \cdot e^{\pm i\kappa |r-r'|}\]

Correct if \(r = r'\)

Now for the incoming or non-scattered particles \(V = 0\)

\[(\nabla^2 + \kappa^2) \psi = 0 \Rightarrow \psi_0 = e^{ikz} \]

finally

\[\psi(\vec{r}) = e^{ikz} - \frac{1}{4\pi} \int \frac{e^{i\kappa |r-r'|}}{|r-r'|} \psi(r') \, dv'\]

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

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

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

and comparing this expression to:

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

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

We can also try an iterative procedure to solve it.

Replace $r$ by $r'$:

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

(looks like $e^{ikr} + \int G(r-r') \psi(r') e^{ikr'} dv'$

This iterated series is known as Neumann series.

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

Born approximation means cut off the infinite series to the n'th term.

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

First Born approximation.
Suppose \( \psi \) is approximated by \( e^{i k z} \)
meaning \( \psi(r) = \frac{1}{\sqrt{2\pi}} e^{-i \omega r} \frac{e^{i \mathbf{k} \cdot \mathbf{r}}}{k} \). 

1st Born approx: \( \psi(r) = e^{i k z} \) where \( \mathbf{k} = \mathbf{k}_0 \)

\[
\langle \mathbf{r}_1, \varphi \rangle = -\frac{1}{\sqrt{\pi \mathbf{k}_0}} \int \frac{e^{-i \mathbf{k}_0 \cdot \mathbf{r}}}{\mathbf{k} - \mathbf{k}_0} U(r) e^{i \mathbf{k}_0 \cdot \mathbf{r}} d\mathbf{r}
\]

1st Born Approx. \[
\left\{ \begin{array}{l}
\text{Thus scattering amplitude is just Fourier transformation of } U(r) \rightarrow U(\mathbf{k}_0)
\end{array} \right.
\]

\[
\mathbf{k} = \mathbf{k}_0 + \mathbf{s}
\]

\[
\mathbf{s} = 2 \mathbf{k}_0 \sin \frac{\theta}{2}, \quad i \mathbf{n} = 2 \mathbf{k}_0 \cos \theta
\]

\[
\langle \mathbf{r}_1, \varphi \rangle = \frac{1}{\sqrt{\pi \mathbf{k}_0}} \int \frac{e^{-i \mathbf{k}_0 \cdot \mathbf{r}}}{\mathbf{k} - \mathbf{k}_0} U(r) \left( \mathbf{r}_1 \right) \mathbf{r}_1^2 \sin \left( \mathbf{n} \cdot \mathbf{r}_1 \right) d\mathbf{r}_1 d\varphi \frac{d\mathbf{r}_1}{d\cos \theta}
\]

\[
\frac{1}{\sqrt{\pi \mathbf{k}_0}} \int_0^\infty \mathbf{r}_1^2 U(\mathbf{r}_1) d\mathbf{r}_1 \int_0^\infty e^{i \mathbf{n} \cdot \mathbf{r}_1} \sin \left( \mathbf{n} \cdot \mathbf{r}_1 \right) d\mathbf{r}_1 \int_0^{2\pi} d\mathbf{n} \frac{d\mathbf{r}_1}{d\cos \theta}
\]

\[
= 2 \pi \int_0^\infty \mathbf{r}_1^2 U(\mathbf{r}_1) d\mathbf{r}_1 \int \frac{e^{i \mathbf{n} \cdot \mathbf{r}_1} d\mathbf{r}_1}{-\mathbf{n} \cdot \mathbf{n}} = \left[ \frac{\sqrt{\pi}}{\mathbf{k}_0} \int_0^\infty \mathbf{r}_1^2 U(\mathbf{r}_1) \sin (\mathbf{n} \cdot \mathbf{r}_1) d\mathbf{r}_1 \right] - \frac{1}{\sqrt{\pi \mathbf{k}_0}} = -\frac{1}{\mathbf{k}_0} \int_0^\infty \mathbf{r}_1^2 \sin (\mathbf{n} \cdot \mathbf{r}_1) d\mathbf{r}_1
\]
Important features of $f(\theta | \phi)$:
- no dependence on $\phi$
- $f$ is a real function
- $k^2 = \frac{k^2}{k^2 - k_0^2}$ is called momentum transfer
- for small $k$ and $s$ is small, $s(\theta r') \sim s r' \Rightarrow$
  $$f \approx -\frac{2}{s} \int_0^\infty r \, r' \, V(r) \, dr = -\int_0^\infty r'^2 \, V(r') \, dr'$$
- 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: $V(r) = -\frac{Z e^2}{r}$ (positive!)

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

\[ V(r) = -\frac{Z e^2}{r} \left(1 - \frac{e}{r/a}\right) \]

Let's calculate the scattering amplitude for such scattering.
\[ \int e^{-r/\lambda} \left( e^{i \varphi \cdot s} - e^{-i \varphi \cdot s} \right) \, dr \]
\[ = -i \frac{m \varphi e^z}{\hbar^2 s} \int_0^\infty e^{-r/(\lambda + is)} \, dr - \int_0^\infty e^{-r/(\lambda + is)} \, dr \]
\[ = -i \frac{m \varphi e^z}{\hbar^2 s} \left( \frac{1}{(\lambda + is)} \cdot (1) - \left( \frac{1}{(\lambda + is)} \right)^2 \right) \]
\[ = \frac{2m \varphi e^z a^2}{\hbar^2 (a^2 s^2 + 1)} \]

\[ \frac{d\sigma}{d\Omega} = \frac{|f(\varphi)|^2}{\hbar^4} = \frac{4m^2 \varphi^2 e^z a^4}{\hbar^4 (a^2 s^2 + 1)^2} \]

The total cross-section:
\[ \sigma = \int_0^\pi \int_0^{2\pi} \frac{d\sigma}{d\Omega} \sin \theta \, d\phi \, d\theta \]
\[ = 2k \sin \theta/2 \]
\[ = \frac{8\pi m^2 \varphi^2 e^z a^4}{\hbar^4} \int_0^\pi \frac{2 \sin \theta/2}{\left( 1 + k^2 a^4 \sin^2 \theta/2 \right)} \, d\left( \sin \theta/2 \right) \]
\[ = \frac{16\pi m^2 \varphi^2 e^z a^4}{\hbar^4 (1 + k^2 a^4)} \]

(Case: Mathematica or Sympy. Etc.)

If \( a \to \infty \):
\[ V = -\frac{\varphi e^z}{r} \left( 1 + \left( -\frac{r}{a} \right)^4 \right) + \ldots \]

\[ \approx -\frac{\varphi e^z}{r} \langle \frac{a^2 s^2 + 1}{a^2} \rangle \]

In this case, the Rutherford scattering formula
\[ \frac{d\sigma}{d\Omega} \approx \frac{4\pi^2 m^2 \varphi^2 e^z a^4}{\hbar^4 \left( a^2 s^2 + 1 \right)^2} \]

\[ \approx \frac{4\pi^2 m^2 \varphi^2 e^z}{\hbar^4 a^4 s^2 \sin^2 (\theta/2)} \]