COLLEGE OF ARTS AND SCIENCES
HOMER L. DODGE
DEPARTMENT OF PHYSICS AND ASTRONOMY
The UNIVERSITY of OKLAHOMA

Quantum Mechanics 2

CH. 6 SCATTERING THEORY LECTURE NOTES

STUDENT
Taylor Larrechea

PROFESSOR
Dr. Bruno Uchoa

3-30-22

Scattering Theory

1.) Lippman Schwinger Equation

The Hamiltonian of the scattering problem can be written as:

$$\mathcal{H} = \mathcal{H}_0 + V$$

where $\mathcal{H}_0 = P^2/2m$. For elastic processes, the energy is conserved. This way, we are looking at solutions of the Schrödinger equation for Hamiltonian (4) that have the energy of a free particle.

If $|\varphi\rangle$ is an eigenstate of the free Hamiltonian,

$$\mathcal{H}_0|\varphi\rangle = E|\varphi\rangle \qquad (5)$$

we need to solve:

$$(\mathcal{H}_0 + V)|\psi\rangle = E|\psi\rangle$$

Where both $\mathcal{H}_0$ and $\mathcal{H}_0 + V$ have a continuous spectrum we are looking for solutions of (6) that have the same eigenvalues of (5), such that $|\psi\rangle \to |\varphi\rangle$ when $V \to 0$.

Ansatz (1)

Let's suppose that

$$|\psi\rangle = \frac{1}{E-\mathcal{H}_0} V|\psi\rangle + |\varphi\rangle \qquad (\mathrm{I})$$

It's clear that

$$(E-\mathcal{H}_0)|\psi\rangle = V|\psi\rangle + (E-\mathcal{H}_0)|\varphi\rangle$$

then (I) satisfies the Schrödinger equation. However, (I) is still ill defined because of $\frac{1}{E-\mathcal{H}_0}$ term, which is singular.

The method of projecting out states, in static perturbation theory does not work in a continuous spectrum. The regularization is done by introducing a small complex part to the energy.

$$|\psi\rangle = |\varphi\rangle + \frac{1}{E-\mathcal{H}_0} V|\psi^{(\pm)}\rangle \qquad (\mathrm{II})$$

where the co-ordinate representation is

$$\langle \vec{x} | \psi^{(\pm)} \rangle = \langle \vec{x} | \varphi \rangle + \int \langle \vec{x} | \frac{1}{E - \mathcal{H}_0 \pm i0_x} | \vec{x}' \rangle \langle \vec{x}' | V | \psi^{(\pm)} \rangle \qquad (\text{III})$$

We can then go on to say

$$\langle \vec{x} | \varphi \rangle = \frac{e^{i(\vec{k}\cdot\vec{x})}}{(2\pi)^{3/2}}$$

In momentum space we have

$$\langle \vec{p} | \psi^{(\pm)} \rangle = \langle \vec{p} | \varphi \rangle + \frac{1}{E - \hbar^2 \varphi^2/2m \pm i0_x} \langle \vec{p} | V | \psi^{(\pm)} \rangle$$

4-4-22

Previous class

The Lipmann-Schwinger Equation is

$$\langle \vec{x} | \psi^{\pm} \rangle = \langle \vec{x} | \varphi \rangle + \int d^3\vec{x}' \langle \vec{x} | \frac{1}{E - \mathcal{H}_0 \pm i0_+} | \vec{x}' \rangle \times \langle \vec{x} | \hat{V} | \psi^{\pm} \rangle \qquad (*)$$

We then go on to define : Greens Function (kernel of Integral Eq. (1))

$$G_\pm(\vec{x}, \vec{x}') = \frac{\hbar^2}{2m} \langle \vec{x} | \frac{1}{E - \mathcal{H}_0 \pm i0_+} | \vec{x}' \rangle$$

Writing this in momentum space we have

$$G_\pm(\vec{x}, \vec{x}') = \frac{\hbar^2}{2m} \int d^3p' \, d^3p'' \langle \vec{x} | \vec{p}' \rangle \langle \vec{p}' | \frac{1}{E - p'^2\hbar^2/2m \pm i0_x} | \vec{p}'' \rangle \langle \vec{p}'' | \vec{x}' \rangle$$

Since

$$\langle \vec{p}' | \frac{1}{E - p^2\hbar^2/2m \pm i0_+} | \vec{p}'' \rangle = \frac{\delta^3(\vec{p}' - \vec{p}'')}{E - p'^2\hbar^2/2m \pm i0_+}$$

We now have our Green Function change to

$$G_\pm(\vec{x}, \vec{x}') = \frac{\hbar^2}{2m} \int d^3\vec{p}' \, d^3\vec{p}'' \frac{e^{i\vec{p}'\cdot\vec{x}'}}{(2\pi)^{3/2}} \frac{e^{-i\vec{p}''\cdot\vec{x}'}}{(2\pi)^{3/2}} \times \frac{\delta^3(\vec{p}' - \vec{p}'')}{E - p'^2\hbar^2/2m \pm i0_+}$$

$$= \frac{\hbar^2}{2m} \int \frac{d^3\vec{p}'}{(2\pi)^3} \frac{e^{i\vec{p}'\cdot(\vec{x} - \vec{x}')}}{E - p'^2\hbar^2/2m \pm i0_+}$$

To solve this integral we use

$$E = \hbar^2 k^2/2m$$

Our Geen's Function becomes

$$G_\pm(\vec{x},\vec{x}') = \frac{\hbar^2}{2m}\frac{1}{(2\pi)^3}\int d^3q \, \frac{e^{i\vec{q}\cdot(\vec{x}-\vec{x}')}}{K^2-q^2\pm i0_+}\,\frac{2m}{\hbar^2}$$

$$= \frac{1}{(2\pi)^3}\int_0^\infty dq\, q^2 \int_0^{2\pi} d\phi_q \int_0^{2\pi} \sin(\theta_q)\, d\theta_q \cdot \exp(iq|\vec{x}-\vec{x}'|\cos(\theta_q))$$

We then make a change of variables

$$\mu_q \equiv \cos(\theta_q) \quad , \quad d\mu_q = -\sin(\theta_q)\, d\theta_q$$

We then have

$$G_\pm(\vec{x},\vec{x}') = \frac{1}{(2\pi)^2}\int_0^\infty dq\, q^2 \int_{-1}^{1} d\mu_q \, \frac{\exp(iq|\vec{x}-\vec{x}'|\mu_q)}{K^2-q^2\pm i0_+}$$

$$= \frac{1}{(2\pi)^2}\int_0^\infty dq\, \frac{q^2}{K^2-q^2\pm i0_+}\,\frac{e^{iq|\vec{x}-\vec{x}'|}-e^{-iq|\vec{x}-\vec{x}'|}}{iq|\vec{x}-\vec{x}'|}$$

$$= \frac{1}{2(2\pi)^2}\frac{1}{|\vec{x}-\vec{x}'|}\int_{-\infty}^{+\infty} dq\, \frac{q}{K^2-q^2\pm i0_+}\left\{e^{iq|\vec{x}-\vec{x}'|} - e^{-iq|\vec{x}-\vec{x}'|}\right\}$$

We then define some poles to be

$$\bar{q}^2 = K^2 \pm i0_+ \implies \bar{q} = \pm\sqrt{K^2\pm i0_+} = \pm(K\pm i0_+)$$

G_+ has two poles, at

$$\bar{q} = \begin{cases} +K + i0_+ \equiv K_+ \\ -K - i0_+ \equiv -K_+ \end{cases}$$

G_- has two poles, at

$$\bar{q} = \begin{cases} +K - i0_+ \equiv K_+ \\ -K + i0_+ \equiv -K_+ \end{cases}$$

We then have a Green's Function that says

$$G_+(\vec{x},\vec{x}') = -\frac{1}{8\pi^2}\frac{1}{i|\vec{x}-\vec{x}'|} \times \left\{ \oint_{-\infty}^{+\infty} dq\, \frac{q e^{iq|\vec{x}-\vec{x}'|}}{q^2-K_+^2} - \oint_{-\infty}^{+\infty} dq\, \frac{q e^{-iq|\vec{x}-\vec{x}'|}}{q^2-K_+^2} \right\}$$

$$= -\frac{2\pi i}{8\pi^2 i|\vec{x}-\vec{x}'|} \times \left\{ \operatorname*{Res}_{K+i0_+}\left(\frac{q e^{iq|\vec{x}-\vec{x}'|}}{q^2-K_+^2}\right) + \operatorname*{Res}_{-K-i0_+}\left(\frac{q e^{-iq|\vec{x}-\vec{x}'|}}{q^2-K_+^2}\right)\right\}$$

$$= -\frac{2\pi i}{8\pi^2 i|\vec{x}-\vec{x}'|}\left\{\frac{Ke^{iK|\vec{x}-\vec{x}'|}}{2K} - \frac{(-K)e^{iK|\vec{x}-\vec{x}'|}}{2K}\right\} = -\frac{e^{iK|\vec{x}-\vec{x}'|}}{4\pi|\vec{x}-\vec{x}'|}$$

We can then go on to show that

$$G_\pm(\vec{x},\vec{x}') = \frac{1}{4\pi|\vec{x}-\vec{x}'|} e^{\pm ik|\vec{x}-\vec{x}'|} \qquad (2)$$

Which is the Green's Function of the Helmholtz equation

$$(\nabla^2 + k^2)\, G_\pm(\vec{x},\vec{x}') = \delta^{(3)}(\vec{x}-\vec{x}')$$

We can then rewrite the integral in eq (1) as

$$\langle \vec{x}|\psi^{(\pm)}\rangle = \langle \vec{x}|\varphi\rangle - \frac{2m}{\hbar^3}\int d^3\vec{x}'\, \frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{4\pi|\vec{x}-\vec{x}'|} \times \langle \vec{x}'|V|\psi^{(\pm)}\rangle$$

Where the first term is the incident wave and the second the scattered wave.

<u>Asymptotic</u> <u>Behavior</u>

$\langle \vec{x}|\psi^{(\pm)}\rangle = \psi^\pm(\vec{x})$ is a superposition of the incoming wave plus a term that results from the scattering. At long distances we want to show that the second term behaves as a spherical wave,

$$\frac{e^{\pm ikr}}{r}$$

When the scattering potential is local,

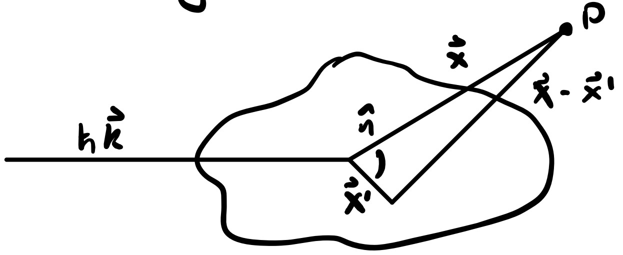
$$\langle \vec{x}|\hat{V}|\vec{x}'\rangle = V(\vec{x})\,\delta(\vec{x}-\vec{x}')$$

$$\Rightarrow \qquad \langle \vec{x}'|\hat{V}|\psi^{(\pm)}\rangle = \int d^3\vec{x}''\langle \vec{x}|\hat{V}|\vec{x}''\rangle\langle \vec{x}''|\psi^{\pm}\rangle = V(\vec{x}')\langle \vec{x}'|\psi^{(\pm)}\rangle$$

and therefore,

$$\langle \vec{x}|\psi^{(\pm)}\rangle = \langle \vec{x}|\varphi\rangle - \frac{2m}{\hbar}\,x \times \int d^3\vec{x}'\, \frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{4\pi|\vec{x}-\vec{x}'|} \times V(\vec{x}')\langle \vec{x}'|\psi^{(\pm)}\rangle \qquad (3)$$

The typical geometry of a scattering experiment is



$$\alpha = \angle(\vec{x},\vec{x}')\ ,\quad |\vec{x}'| << |\vec{x}|\ ,\quad |\vec{x}| \equiv \hat{n}\ ,\quad |\vec{x}'| \equiv \hat{n}'$$

We can then go on to say

$$|\vec{x}-\vec{x}'| = n\sqrt{1+(n'/n)^2 - 2n'/n\cos(\alpha)} \approx n\left(1 - n'/n\cos(\alpha)\right)$$
$$= n - n'\cos(\alpha) = n - \hat{n}\cdot\vec{x}'$$

Where $\hat{n} = \frac{\vec{x}}{|\vec{x}|} = \frac{\vec{x}}{n}$.

<u>Definition</u>: $\vec{k}' \equiv k\hat{n}$

we then have

$$e^{\pm ik|\vec{x}-\vec{x}'|} \approx e^{\pm ikn}e^{\mp i\vec{k}'\cdot\vec{x}'} \tag{4}$$

For large n. Replacing (4) into (3) we have,

$$\langle \vec{x}|\psi^{\pm}\rangle = \langle \vec{x}|\vec{k}\rangle - \frac{2m}{\hbar^2}\frac{e^{\pm ikn}}{4\pi n}\int d^3\vec{x}' \frac{V(\vec{x}')}{1 - \frac{\hat{n}\cdot\vec{x}'}{n}} e^{\mp i\vec{k}'\cdot\vec{x}'}\langle \vec{x}|\psi^{\pm}\rangle$$

Then in leading order for $1/n$,

$$\langle \vec{x}|\psi^{\pm}\rangle \xrightarrow[n\to\infty]{} \langle \vec{x}|\vec{k}\rangle - \frac{2m}{\hbar^2}\frac{e^{\pm ikn}}{4\pi n}\times\int d^3\vec{x}'\, V(\vec{x}')e^{\mp i\vec{k}'\cdot\vec{x}'}\langle \vec{x}|\psi^{\pm}\rangle$$
$$= \frac{1}{(2\pi)^{3/2}}\left\{e^{i\vec{k}\cdot\vec{x}} + \frac{e^{\pm ikn}}{n}f^{\pm}(\vec{k},\vec{k}')\right\}$$

Where

$$f^{\pm}(\vec{k},\vec{k}') = -(2\pi)^{3/2}\frac{2m}{4\pi\hbar^2}\times\int d^3\vec{x}'\, e^{\mp i\vec{k}'\cdot\vec{x}'}\langle \vec{x}'|\psi^{\pm}\rangle V(\vec{x}')\langle \pm\vec{k}'|\vec{x}'\rangle(2\pi)^{3/2}$$

Hence,

$$f^{\pm}(\vec{k},\vec{k}') = -2\pi^2\cdot\frac{2m}{\hbar^2}\langle \pm\vec{k}'|V|\psi^{\pm}\rangle \tag{4}$$

which is referred to as the scattering amplitude.

<u>4-6-22</u>

<u>The Differential Cross Section</u>:

If the flux of incoming particles is N and dN_s the number of scattered particles per unit time in the solid angle $d\Omega$ at polar co-ordinates (θ,φ), then dN_s is proportional to N and

$$dN_s = \sigma(\theta,\varphi)\, N\, d\Omega$$

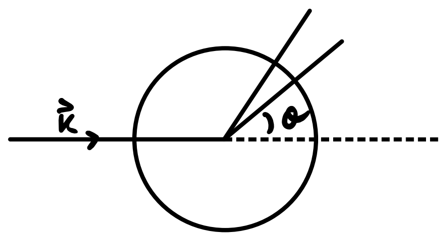
where $\sigma'(\theta,\varphi)$ is the differential scattering cross section. The total number of scattered particles is:

$$N_s = \int dN_s = \int_{4\pi} \sigma'(\theta,\varphi)\, N\, d\Omega$$

where

$$\sigma'_T = \int_{4\pi} \sigma'(\theta,\varphi)\, d\Omega$$

is the total scattering cross section. Diagramatically this looks like



calling

$$V(r) = \frac{e^{ikr}}{r} f(\vec{k},\vec{k}')$$

the scattered wave, the flux of scattered particles per unit time can be calculated from the current,

$$\vec{J}_s = \frac{-i\hbar}{2m}\left[V^* \vec{\nabla} V - V \vec{\nabla} V^*\right] \qquad (1)$$

In spherical co-ordinates

$$\vec{\nabla} \equiv \frac{\partial}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial}{\partial \theta}\hat{\theta} + \frac{1}{r\sin(\theta)}\frac{\partial}{\partial \varphi}\hat{\varphi}$$

In leading order in $1/r$,

$$\vec{J}_s \xrightarrow{r\to\infty} \frac{\hbar k}{m} \frac{|f(\theta,\varphi)|^2}{r^2}\hat{r} + \mathcal{O}(1/r^3)$$

Since $d\Omega = dA/r^2$ therefore

$$dN_s = \vec{J}_s \cdot d\vec{A} = \frac{\hbar k}{m}\frac{|f(\theta,\varphi)|^2}{r^2} r^2\, d\Omega = \frac{\hbar k}{m}|f(\theta,\varphi)|^2\, d\Omega$$

The flux on incoming waves per unit time can be calculated with

$$\psi = e^{ikz}$$

From (1),

$$|\vec{J}_i| = \frac{\hbar k}{m}$$

we then have

$$\frac{dN_s}{N} = \sigma(\theta,\varphi)\, d\Omega = \frac{|J_s| r^2 d\Omega}{|\vec{J}_i|} = |f(\theta,\varphi)|^2 d\Omega$$

we can then further say

$$\Rightarrow \qquad \sigma(\theta,\varphi) = |f(\theta,\varphi)|^2 = |f(\vec{k},\vec{k}')|^2$$

<u>First Born Approximation</u>

Expanding the Lippman Schwinger equation to first order in the potential, we need to compute the scattering amplitude by iteration.

Replacing

$$\langle \vec{x}' | \psi^{\pm} \rangle = \langle \vec{x}' | \varphi \rangle = \frac{e^{i\vec{k}\cdot\vec{x}}}{(2\pi)^{3/2}}$$

we get in first order

$$f^{+(1)}(\vec{k},\vec{k}') = -(2\pi)^{3/2} \frac{2m}{4\pi\hbar^2} \int d\vec{x}'\, V(\vec{x}') \cdot e^{-i\vec{k}'\cdot\vec{x}'} \cdot \frac{e^{i\vec{k}\cdot\vec{x}'}}{(2\pi)^{3/2}}$$

$$= -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3\vec{x}'\, e^{i(\vec{k}-\vec{k}')\cdot\vec{x}'} V(\vec{x}')$$

which is the Fourier Transform of $V(\vec{x})$ times constants. For a spherically symmetric potential,

$$V(\vec{x}') = V(r) \quad , \quad r = |\vec{x}'|$$

$$\Rightarrow \qquad (\vec{k}-\vec{k}')\cdot\vec{x}' = r\,|\vec{k}-\vec{k}'| \cos(\theta)$$

we then have

$$f^{+(1)}(\vec{k},\vec{k}') = -\frac{1}{4\pi} \cdot \frac{2m}{\hbar^2} \int_0^\infty dr\, r^2 \int_0^{2\pi} d\varphi \times V(r) \int_0^{\pi} \frac{d\theta \cdot \sin(\theta)}{dr} e^{i|\vec{k}-\vec{k}'| r \cdot \cos(\theta)}$$

$$= -\frac{1}{2} \frac{2m}{\hbar^2} \int_0^\infty dr\, r^2 V(r) \times \frac{1}{ir|\vec{k}-\vec{k}'|} \left(e^{i|\vec{k}-\vec{k}'|r} - e^{-i|\vec{k}-\vec{k}'|r} \right)$$

$$= \frac{-2m}{\hbar^2 |\vec{k}-\vec{k}'|} \int_0^\infty dr\, r V(r) \sin(|\vec{k}-\vec{k}'| r)$$

we then Finally have

$$f^{(1)}(\vec{k},\vec{k}') = \frac{-2m}{\hbar^2|\vec{k}-\vec{k}'|}\int_0^\infty dr\; r\, V(r)\sin(|\vec{k}-\vec{k}'|r) \qquad (2)$$

Example: Yukawa Potential

The potential is

$$V(r) = V_0\frac{e^{-\mu r}}{r}$$

where $1/\mu$ is the range of the potential, with

$$V(r) \to 0 \quad \text{for} \quad r \gg \frac{1}{\mu}$$

which yields

$$f^{(1)}(\vec{k},\vec{k}') = -\frac{2m}{\hbar^2}\frac{V_0}{|\vec{k}-\vec{k}'|}\underbrace{\int_0^\infty \frac{e^{-\mu r}}{r}\sin(|\vec{k}-\vec{k}'|r)\times r\,dr}_{I}$$

For I we then have

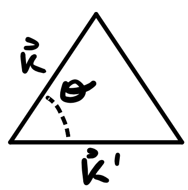
$$I = \frac{1}{2i}\int_0^\infty dr\left[e^{i|\vec{k}-\vec{k}'|r-\mu r} - e^{-i|\vec{k}-\vec{k}'|r-\mu r}\right]$$

$$= \frac{1}{2}\left[\frac{1}{|\vec{k}-\vec{k}'|+i\mu} + \frac{1}{|\vec{k}-\vec{k}'|-i\mu}\right] = \frac{|\vec{k}-\vec{k}'|}{|\vec{k}-\vec{k}'|^2+\mu^2}$$

This then implies

$$\Rightarrow \qquad f^{+(1)}(\vec{k},\vec{k}') = \frac{-2mV_0}{\hbar^2}\frac{1}{|\vec{k}-\vec{k}'|^2+\mu^2}$$

we then define $\vec{q} = \vec{k}-\vec{k}'$ with geometry



$$\vec{k}-\vec{k}' = \vec{q} \Rightarrow \left(\frac{q}{2}\right) = k\sin\left(\frac{\theta}{2}\right)$$

we can then say

$$q^2 = 4k^2\sin^2(\theta/2) = 2k^2(1-\cos(\theta))$$

We can then say

$$f^{+(1)}(\vec{k},\vec{k}') = -\frac{2m}{\hbar^2} V_0 \frac{1}{2k^2(1-\cos(\theta))+\mu^2}$$

Therefore the differential scattering cross section becomes

$$\sigma(\theta,\varphi) = \left(\frac{2mV_0}{\hbar^2}\right)^2 \frac{1}{[2k^2(1-\cos(\theta))+\mu^2]^2} = \left(\frac{2mV_0}{\hbar^2}\right)^2 \frac{1}{[4k^2\sin^2(\theta/2)+\mu^2]^2}$$

In the limit where $\mu \to 0$, and

$$V_0 \to ZZ'e^2$$

the Yukawa potential becomes the Coulomb potential, where Z is the atomic number of the nucleus and Z' the atomic number of the incident particle.

The differential scattering cross section is

$$\sigma(\theta,\varphi) = \frac{(2m)^2(ZZ'e^2)^2}{\hbar^4} \frac{1}{16k^4\sin^4(\theta/2)}$$

which is the same as the Rutherford formula for classical scattering.

<u>Born Approximation In Higher Order</u>

<u>Definition</u>: Scattering Matrix

$$T|\varphi\rangle = V|\psi^{\pm}\rangle$$

Multiplying the L.S equation by V we get

$$V|\psi^{\pm}\rangle = V|\varphi\rangle + V\frac{1}{E-\mathcal{H}_0+i\varepsilon}V|\psi^{\pm}\rangle'$$

$\Rightarrow$

$$T = V + V\frac{1}{E-\mathcal{H}_0+i\varepsilon}T \tag{3}$$

The scattering amplitude can be written as

$$f(\vec{k},\vec{k}') = -\frac{1}{4\pi}(2\pi)^3 \cdot \frac{2m}{\hbar^2}\frac{\langle\vec{k}'|T|\varphi\rangle}{\langle\vec{k}'|T|\vec{k}\rangle}$$

We can then say

$$T = V + V\frac{1}{E-\mathcal{H}_0+i\varepsilon}V + V\frac{1}{E-\mathcal{H}_0+i\varepsilon}V\frac{1}{E-\mathcal{H}_0+i\varepsilon}V$$

The scattering amplitude can be equivalently expanded

$$f(\vec{k},\vec{k}') = \sum_{n=1}^{\infty} f^{(n)}(\vec{k},\vec{k}')$$

where n is the order of the expansion in the potential. We have

$$f^{(1)}(\vec{k},\vec{k}') = -\frac{1}{4\pi}(2\pi)^3 \frac{2m}{\hbar^2} \langle \vec{k}'|V|\vec{k}\rangle$$

Where the above is the First Born Approximation. The second order is

$$f^{(2)}(\vec{k},\vec{k}') = \frac{-1}{4\pi}(2\pi)^3 \frac{2m}{\hbar^2} \times \langle \vec{k}'|V \frac{1}{E-\mathcal{H}_0+i\varepsilon} V|\vec{k}\rangle .$$

In co-ordinate representation this is

$$f^{(2)}(\vec{k},\vec{k}') = -\frac{1}{4\pi}(2\pi)^3 \frac{2m}{\hbar^2} \int d^3\vec{x}'\, d^3\vec{x}''\, \langle \vec{k}'|\vec{x}'\rangle V(\vec{x}')\langle \vec{x}'|\frac{1}{E-\mathcal{H}_0+i\varepsilon}|\vec{x}''\rangle V(\vec{x}'')\langle \vec{x}''|\vec{k}\rangle$$

$$= -\frac{1}{4\pi}\frac{(2m)}{\hbar^2} \int d^3\vec{x}'\, d^3\vec{x}''\, e^{-i\vec{k}'\cdot\vec{x}'} V(\vec{x}') \left[\frac{2m}{\hbar^2} G(\vec{x}',\vec{x}'')\right] V(\vec{x}'') e^{i\vec{k}\cdot\vec{x}''}$$

4-11-22

Partial Waves Decomposition

Free particles have a well defined angular momentum, since the kinetic energy commutes with angular momentum operators, forming a set of compatible operators,

$$\{\mathcal{H}_0, L^2, L_z\}$$

If we disregard the spin, the basis that diagonalizes those operators is

$$|E,\ell,m\rangle$$

Which describe spherical wave states. In this basis,

$$|\vec{k}\rangle = \sum_{\ell,m} \int dE\, |E,\ell,m\rangle\langle E,\ell,m|$$

where

$$\langle \vec{k}|E,\ell,m\rangle = \frac{\hbar}{\sqrt{mk}}\, \delta\left(\frac{\hbar^2 k^2}{2m} - E\right) Y_m^{\ell}(\hat{k}) \tag{1}$$

(see Sakurai). We can equivalently say

$$|\vec{x}\rangle = \sum_{\ell,m} dE\, |E,\ell,m\rangle\langle E,\ell,m|$$

we then finally have

$$\langle \vec{x} | E, l, m \rangle = \frac{i^l}{\hbar} \sqrt{\frac{2mk}{\pi}}\, j_l(kr)\, Y^l_m(\hat{n}) \tag{2}$$

where $j_l(x)$ is a spherical Bessel function. Let us now assume that $V \neq 0$, where

$$V(\vec{x}) = V(r)$$

is a central potential. By symmetry, the scattering matrix $\hat{T}$ commutes with L^2 and L_z, since:

$$T = V + V \frac{1}{E - \mathcal{H}_0 + i\varepsilon} V + V \frac{1}{E - \mathcal{H}_0 + i\varepsilon} V \frac{1}{E - \mathcal{H}_0 + i\varepsilon} V + \dots$$

Hence, we expect that

$$\langle E', l', m' | T | E, l, m \rangle = T_l(E, E') \delta_{l,l'} \delta_{m,m'}$$

The scattering amplitude

$$f(\vec{k}, \vec{k}') = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \vec{k}' | T | \vec{k} \rangle = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \sum_{ll'} \sum_{mm'} \int dE\, dE'$$

Evaluating we then have

$$= \langle \vec{k}' | E', l', m' \rangle \langle E', l', m' | T | E, l, m \rangle \langle E, l, m | \vec{k} \rangle$$

$$= -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \sum_{ll'} \sum_{mm'} \int dE\, dE' \times \frac{\hbar^2}{m\sqrt{kk'}} \delta\left(\frac{\hbar^2 k^2}{2m} - E'\right) T_l(E, E')$$

$$\times \delta_{l,l'} \delta_{m,m'} \delta\left(\frac{\hbar^2 k^2}{2m} - E\right) Y^{l'}_{m'}(\hat{k}') \times Y^{l*}_m(\hat{k})$$

$$= -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \sum_l \frac{\hbar^2}{mk} T_l(E, E') \Big|_{E = \frac{\hbar^2 k^2}{2m}} \times \sum_m Y^{l*}_m(\hat{k}') Y^l_m(\hat{k})$$

$$= -\frac{4\pi^2}{k} \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} P_l(\hat{k}, \hat{k}') \times T_l(E, E') \Big|_{E = \frac{\hbar^2 k^2}{2m}}$$

Definition:

$$\cos(\alpha) \equiv \hat{k} \cdot \hat{k}' \qquad f_l(k) \equiv -\frac{\pi}{k} T_l(E, E') \Big|_{E = \frac{\hbar^2 k^2}{2m}}$$

where $f_l(k)$ is the partial wave amplitude.

Therefore,

$$f(\vec{n},\vec{k}') = f(\cos(\alpha)) = \sum_{l=0}^{\infty} (2l+1)\, f_l(k)\, P_l(\cos(\alpha))$$

<u>Physical Meaning of $f_l(k)$</u>

At long distances,

$$\langle \vec{x} | \psi^+ \rangle \xrightarrow{r \to \infty} \frac{1}{(2\pi)^{3/2}} \left[e^{ikz} + f(\cos(\alpha)) \frac{e^{ikr}}{r} \right]$$

Expanding in partial waves

$$e^{ikz} = \sum_{l=0}^{\infty} (2l+1)\, i^l j_l(kr)\, P_l(\cos(\alpha))$$

and

$$f(\cos(\alpha)) \frac{e^{ikr}}{r} = \sum_{l=0}^{\infty} (2l+1)\, j_l(k)\, P_l(\cos(\alpha)) \frac{e^{ikr}}{r}$$

Since

$$j_l(kr) \xrightarrow{k \to \infty} \frac{e^{i(kr - l\pi/2)} - e^{-i(kr - l\pi/2)}}{2ikr}$$

and $i^l = e^{i\pi/2 l}$, then we have

$$e^{ikz} = \sum_{l=0}^{\infty} (2l+1) \left[\frac{e^{ikr} - e^{-i(kr - l\pi)}}{2ikr} \right] \times P_l(\cos(\alpha))$$

The complete function becomes:

$$\langle \vec{x} | \psi^{\pm} \rangle \xrightarrow{r \to \infty} \frac{1}{(2\pi)^{3/2}} \times \sum_{l=0}^{\infty} (2l+1) \frac{P_l(\cos(\alpha))}{2ik} \times \left\{ [r + 2ik f_l(k)] \frac{e^{ikr}}{r} - \frac{e^{-i(kr - l\pi)}}{r} \right\}$$

When $V=0$, a plane wave can be seen as a superposition of an emerging Spherical wave

$$\frac{e^{ikr}}{r}$$

and an incident Spherical wave $-e^{-i(kr - \pi l)}$, for each l. The presence of the scattering center just modifies the coefficient of the emergent wave,

$$1 \to 1 + 2ik \cdot f_l(k)$$

If the probability is conserved

$$\vec{\nabla} \cdot \vec{j} = -\partial |\psi|^2 / \partial t = 0$$

Through Gauss' Theorem,

$$\int_V dv\, \vec{\nabla}\cdot\vec{j} = \int_{\partial V} \vec{j}\cdot d\vec{s} = 0$$

Therefore the flux of probability that enters the volume is the same that leaves. Hence, the co-efficient of $\frac{e^{ikn}}{n}$ is the same in absolute value as the co-efficient of e^{-ikn}/n.

<u>Defining</u>:

$$S_\ell(k) \equiv 1 + 2ik\cdot f_\ell(k)$$

The potential only changes the phase of the emerging wave,

$$S_\ell(k) = e^{2i\delta_\ell}$$

<u>Definition</u>: δ_ℓ is the phase shift

We then have:

$$f_\ell(k) = \frac{S_\ell(k)-1}{2ik} = \frac{e^{2i\delta_\ell}-1}{2ik} = \frac{e^{i\delta_\ell}}{k}\,\frac{e^{i\delta_\ell}-e^{-i\delta_\ell}}{2i} = \frac{e^{i\delta_\ell}}{k}\sin(\delta_\ell) = \frac{1}{k\cot(\delta_\ell)-ik}$$

The amplitude of scattering is

$$f(\cos(\alpha)) = \sum_{\ell=0}^{\infty}(2\ell+1)\frac{e^{i\delta_\ell}}{k}\sin(\delta_\ell)P_\ell(\cos(\alpha))$$

where $\delta_\ell \in \mathbb{R}$. The unitarity of $\delta_\ell(k)$ follows from rotational invariance of the potential and conservation of probability.

The differential cross section,

$$\sigma(\alpha) = |f(\cos(\alpha))|^2$$

The total scattering cross section is

$$\sigma_T = \int_{4\pi}\sigma(\theta,\varphi)\,d\Omega = \int |f(\cos(\alpha))|^2\,d\Omega$$

$$= \frac{1}{k^2}\cdot 2\pi\int_{-1}^{1} d(\cos(\alpha))\sum_{\ell,\ell'}(2\ell+1)(2\ell'+1)e^{i\delta_\ell}e^{-i\delta_{\ell'}}\sin(\delta_\ell)\sin(\delta_{\ell'})P_\ell(\cos(\alpha))P_{\ell'}(\cos(\alpha))$$

From the orthogonality of Legendre Polynomials,

$$\int_{-1}^{1}dx\, P_\ell(x)P_{\ell'}(x) = \frac{2\delta_{\ell,\ell'}}{2\ell+1}$$

we then Finally have

$$\sigma'_T = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2(\delta_l)$$

We can also compute:

$$\mathrm{Im}(f(\cos(\omega))) = \sum_{l=0}^{\infty}(2l+1)\frac{\sin(\delta_l)}{k}\,\mathrm{Im}(e^{i\delta_l}) \times P_l(1)$$

Since $P_l(1) = 1$

$$\mathrm{Im}(f(\cos(\omega)=1)) = \sum_{l=0}^{\infty}(2l+1)\frac{\sin^2(\delta_l)}{k} = \frac{k}{4\pi}\sigma'_T$$

Finally we have

$$\mathrm{Im}(f(\cos(\omega)=1)) = \frac{k}{4\pi}\sigma'_T$$

which is known as the optical theorem

4-13-22

Scattering of Identical Particles

The Hamiltonian of two interacting particles is:

$$\mathcal{H} = -\frac{\hbar^2}{2m_1}\vec{\nabla}_1^2 - \frac{\hbar^2}{2m_2}\vec{\nabla}_2^2 + V(|\vec{x}_1 - \vec{x}_2|)$$

Next we change the variables to the center of mass,

$$\vec{X} = \frac{m_1\vec{x}_1 + m_2\vec{x}_2}{m_1+m_2}$$

and the relative co-ordinate

$$\vec{r} \equiv \vec{x}_1 - \vec{x}_2 \,, \quad r \equiv |\vec{x}_1 - \vec{x}_2|$$

The transformation gives

$$\mathcal{H} = \frac{-\hbar^2}{2(m_1+m_2)}\nabla_X^2 - \frac{\hbar^2}{2\mu}\nabla_r^2 + V(r)$$

The First term gives the Kinetic equation of the center of mass, whereas the relative Kinetic energy, with

$$\mu = \frac{m_1 m_2}{m_1+m_2}$$

the reduced mass.

Separating the wavefunctions

$$\psi(\vec{x},\vec{r}) = \varphi(\vec{x})\,\psi(\vec{r})$$

the second term satisfies the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\psi(\vec{r}) = E\,\psi(\vec{r})$$

Where E is the energy in the CM frame.

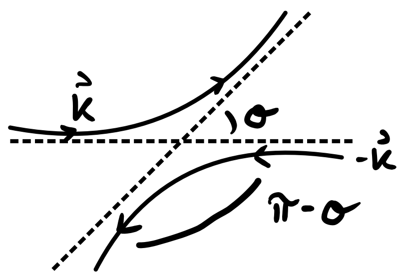
In the scattering problem, the wavefunction is of the form

$$\psi(\vec{r}) = \psi_i(\vec{r}) + \psi_s(\vec{r})$$

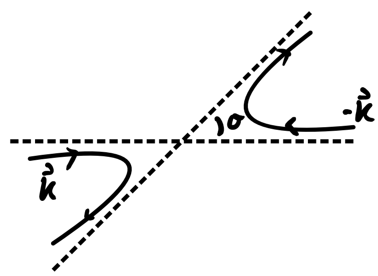
Where $\psi_i(\vec{r})$ is the incident wave and $\psi_s(\vec{r})$ is the scattered one.

For identical particles, we have two equivalent processes:

Process 1



Process 2



For spinless particles the wavefunction is symmetric $\Rightarrow$ the asymptotic solution is a solution in the form

$$e^{i\vec{k}\cdot\vec{r}} + e^{-i\vec{k}\cdot\hat{r}} + [f(\theta)+f(\pi-\theta)] \times \frac{e^{ikr}}{r}$$

where $\vec{r} \equiv \vec{x}_1 - \vec{x}_0$. The differential scattering cross section is

$$\sigma(\theta,\varphi) = |f(\theta)+f(\pi-\theta)|^2 = |f(\theta)|^2 + |f(\pi-\theta)|^2 + 2\,\mathrm{Re}\left(f(\theta)f^*(\pi-\theta)\right)$$

For $\theta = \pi/2$ we get constructive interference. $\sigma(\theta=\pi/2) = 4|f(\theta)|^2$

If the spatial part of the wave function is anti symmetric, we get:

$$e^{i\vec{k}\cdot\vec{n}} + e^{-i\vec{k}\cdot\vec{n}} + \left[f(\theta) - f(\pi-\theta)\right]\frac{e^{ikn}}{n}$$

For spin-1/2 electrons, the triplet state is symmetric in spin (Anti-Symmetric in space), and the singlet is Anti-symmetric in spin and symmetric in space.

<u>Symmetric for scattering Processes</u>

Suppose the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + V$$

(where V is the scattering potential) is invariant under a symmetry operation (unitary)

$$U\mathcal{H}_0U^+ = \mathcal{H}_0 \quad , \quad UVU^+ = V$$

The scattering matrix

$$T = V + VG_0V + VG_0VG_0V + \ldots\ldots$$

is also invariant,

$$UTU^+ = T \quad \text{or} \quad U^+TU = T$$

Defining the kets

$$|\tilde{k}\rangle \equiv U|\vec{k}\rangle \quad , \quad |\tilde{k}'\rangle \equiv U|\vec{k}'\rangle$$

we have

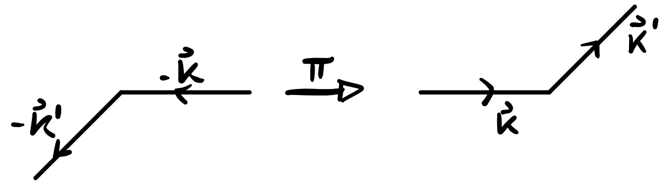
$$\langle\tilde{k}'|T|\tilde{k}\rangle = \langle\vec{k}'|UTU|\vec{k}\rangle = \langle\vec{k}'|T|\vec{k}\rangle$$

For a parity operator, π

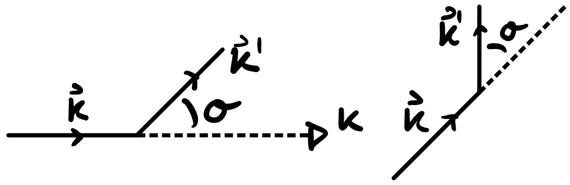
$$\pi|\vec{k}\rangle = |-\vec{k}\rangle \quad , \quad \pi|\vec{k}'\rangle = |-\vec{k}'\rangle$$

The invariance of $\mathcal{H}_0$ and V under parity means that

$$\langle-\vec{k}'|T|-\vec{k}'\rangle = \langle\vec{k}'|T|\vec{k}\rangle$$



For a central potential, the system has rotational symmetry, angular momentum is conserved.



Since T depends only on the relative orientations of $\vec{k}$ and $\vec{k}'$.

For anti-unitary operators, such as time reversal, Θ

$$\Theta \mathcal{H}_0 \Theta^{-1} = \mathcal{H}_0$$

$$\Theta V \Theta^{-1} = V$$

But

$$\Theta \frac{1}{E-\mathcal{H}_0+i\varepsilon} \Theta^{-1} = \frac{1}{E-\mathcal{H}_0-i\varepsilon}$$

This implies $\Theta T \Theta^{-1} = T^{\dagger}$. Also if

$$|\tilde{\alpha}\rangle = \Theta|\alpha\rangle \quad , \quad |\tilde{\beta}\rangle = \Theta|\beta\rangle$$

For anti-unitary operators ($\Theta^2 = -1$),

$$\langle\alpha|\beta\rangle = \langle\tilde{\beta}|\tilde{\alpha}\rangle = \langle\tilde{\alpha}|\tilde{\beta}\rangle^* \qquad (1)$$

Since an anti-unitary operator can be written as

$$\Theta = UK$$

Where K is charge conjugation

$$|\alpha\rangle = \sum_a |a\rangle\langle a|\alpha\rangle \longrightarrow \sum_a \langle a|\alpha\rangle^* U|a\rangle = \sum_a \langle \alpha|a\rangle U|a\rangle \equiv |\tilde{\alpha}\rangle$$

And

$$|\tilde{\beta}\rangle = \sum_a \langle\beta|a\rangle U|a\rangle \Rightarrow \langle\tilde{\beta}| = \sum_a \langle a|\beta\rangle\langle a| U^{\dagger}$$

We then have

$$\langle\tilde{\beta}|\tilde{\alpha}\rangle = \sum_{a',a} \langle a'|\beta\rangle\langle a'|U^{\dagger}U|a\rangle\langle\alpha|a\rangle = \sum_a \langle\alpha|a\rangle\langle a|\beta\rangle = \langle\alpha|\beta\rangle$$

Recovering (1). In the case where

$$|\alpha\rangle = T|\vec{k}\rangle \quad , \quad \langle\beta| = \langle\vec{k}'|$$

Then we have,

$$|\tilde{\alpha}\rangle = \Theta T|\vec{k}\rangle \quad , \quad |\tilde{\beta}\rangle = \Theta|\vec{k}'\rangle$$

We then can say

$$|\tilde{\alpha}\rangle = \Theta T|\vec{k}\rangle = (\Theta T \Theta^{-1})\Theta|\vec{k}\rangle = T^{+}|-\vec{k}\rangle \tag{2}$$

And for $|\tilde{\beta}\rangle$

$$|\tilde{\beta}\rangle = \Theta|\vec{k}'\rangle = |-\vec{k}'\rangle \tag{3}$$

From (1), (2), and (3). We can say $\langle\alpha|\beta\rangle^*$ becomes

$$\langle\alpha|\beta\rangle^* = \langle\beta|\alpha\rangle = \langle\vec{k}'|T|\vec{k}\rangle = \langle\tilde{\alpha}|\tilde{\beta}\rangle = \langle-\vec{k}'|T|-\vec{k}'\rangle$$

or

$$\langle\vec{k}'|T|\vec{k}\rangle = \langle-\vec{k}|T|-\vec{k}'\rangle$$

under time reversal. Combining time reversal and parity,

$$\langle\vec{k}'|T|\vec{k}\rangle \overset{\Theta}{=} \langle-\vec{k}'|T|-\vec{k}'\rangle \overset{\Pi}{=} \langle\vec{k}|T|\vec{k}'\rangle$$

Therefore, the scattering amplitude gives

$$f(\vec{k},\vec{k}') = f(\vec{k}',\vec{k})$$

Meaning

$$\sigma(\vec{k}\to\vec{k}') = \sigma(\vec{k}'\to\vec{k})$$

Which is called detailed balance. For particles with spin

$$\Theta|j,m\rangle = i^{2m}|j,-m\rangle$$

For free particles with kets $|\vec{k},j,m\rangle$,

$$\langle\vec{k}',j,m'|T|\vec{k},j,m\rangle = i^{2(m-m')}\langle-\vec{k},j,-m|T|-\vec{k}',j,-m'\rangle$$

Applying parity we get

$$= i^{2(m-m')}\langle\vec{k},j,-m|T|\vec{k}',j,-m'\rangle$$

In such a way that

$$|\langle\vec{k}',j,m|T|\vec{k},j,m'\rangle|^2 = |\langle\vec{k},j,-m|T|\vec{k}',j,-m'\rangle|^2$$

For unpolarized states,

$$\sigma(\vec{k} \to \vec{k}') = \frac{1}{2j+1} \sum_{M,M'} |\langle \vec{k}', j, M' | T | \vec{k}, j, M \rangle|^2$$

$$= \frac{1}{2j+1} \sum_{M,M'} |\langle \vec{k}, j, -M' | T | \vec{k}', j, -M \rangle|^2$$

$$= \sigma'(\vec{k}' \to \vec{k})$$

where we have recovered the detail balance.

4-18-22

<u>Brief Summary of Scattering Theory</u>

Lipmann Schwinger Equation

$$|\psi^\pm\rangle = |\varphi\rangle + \frac{1}{E - \mathcal{H}_0 \pm i\varepsilon} \hat{V} |\psi^\pm\rangle \tag{1}$$

where

$$\langle \vec{p}' | \frac{1}{E - \mathcal{H}_0 \pm i\varepsilon} | \vec{p} \rangle = \frac{\delta^{(3)}(\vec{p} - \vec{p}')}{E - \frac{p^2}{2m} \pm i\varepsilon}$$

where the real space representation is

$$G_\pm(\vec{x}, \vec{x}') = \frac{\hbar^2}{2m} \langle \vec{x} | \frac{1}{E - \mathcal{H}_0 \pm i\varepsilon} | \vec{x}' \rangle = -\frac{e^{\pm ik|\vec{x} - \vec{x}'|}}{4\pi |\vec{x} - \vec{x}'|} \tag{3D}$$

Lipmann Schwinger Equation (In Real Space)

$$\langle \vec{x} | \psi^\pm \rangle = \langle \vec{x} | \varphi \rangle + \frac{2m}{\hbar^2} \int dx' \, G_\pm(\vec{x}, \vec{x}') \times \langle \vec{x}' | V | \psi^\pm \rangle \tag{2}$$

For large r, away from the scattering potential ($x \gg x'$),

$$\langle \vec{x} | \psi^\pm \rangle \xrightarrow{r \to \infty} \langle \vec{x} | \vec{k} \rangle - \frac{2m}{\hbar^2} \frac{e^{\pm ikr}}{4\pi r} \int d^3\vec{x}' \, V(\vec{x}') \times e^{\mp i\vec{k}' \cdot \vec{x}'} \langle \vec{x}' | \psi^\pm \rangle$$

$$= \frac{1}{(2\pi)^{3/2}} \left[e^{i\vec{k} \cdot \vec{x}} + \frac{e^{\pm ikr}}{r} f^\pm(\vec{k}, \vec{k}') \right]$$

where

$$f^\pm(\vec{k}, \vec{k}') = -(2\pi)^{3/2} \frac{2m}{4\pi \hbar^2} \times \int d^3\vec{x}' \, V(\vec{x}') \, e^{\mp i(\vec{k}' \cdot \vec{x}')} \times \langle \vec{x}' | \psi^\pm \rangle$$

$$= -\frac{1}{4\pi}(2\pi)^3 \frac{2m}{\hbar^2} \langle \vec{k}' | V | \psi^{\pm} \rangle$$

where

$$T = V + VG_0V + VG_0VG_0V + \ldots\ldots$$

is the Scattering matrix.

<u>Differential Scattering Cross Section</u>

The differential scattering cross section is

$$\sigma(\theta,\varphi) = |f(\vec{k},\vec{k}')|^2$$

where the total is found by

$$\sigma_T = \int d\Omega \; \sigma(\theta,\varphi)$$

<u>1st Born Approximation</u>

The First Born Approximation tells us

$$\langle \vec{x}' | \psi^{\pm} \rangle \rightarrow \langle \vec{x}' | \vec{k} \rangle = \frac{e^{i\vec{k}\cdot\vec{x}}}{(2\pi)^{3/2}}$$

or equivalently

$$\langle \vec{k}' | T | \vec{k} \rangle = \langle \vec{k}' | V | \vec{k} \rangle$$

we can then say

$$f^{(1)}(\vec{k},\vec{k}') = \frac{-2m}{\hbar^2 |\vec{k}-\vec{k}'|} \int_0^\infty dr \; r \, V(r) \sin(|\vec{k}-\vec{k}'| r)$$

<u>Partial Wave Decomposition</u>

$f(\vec{k},\vec{k}')$ is

$$f(\vec{k},\vec{k}') = f(\cos\theta) = \sum_{l=0}^{\infty} (2l+1) f_l(k) P_l(\cos\theta)$$

where

$$f_l(k) \equiv \frac{-\pi T_l(E,E')}{k}$$

and

$$\langle E', l', m' | \hat{T} | E, l, m \rangle = T_l(E,E) \delta_{ll'} \delta_{mm'}$$

At long wavelength

$$\langle \vec{x} | \psi^+ \rangle \xrightarrow{r \to \infty} \frac{1}{(2\pi)^{3/2}} \sum_{l=0}^{\infty} (2l+1) \frac{P_l(\cos\theta)}{2ik} \times \left[(1 + 2ik f_l(k)) \frac{e^{ikr}}{r} - e^{-i(kr - \pi l)} \right]$$

Where

$$f_l(k) = \frac{e^{i\delta_l}}{k} \sin(\delta_l)$$

Which then tells us

$$\Rightarrow \qquad f(\cos\theta) = \sum_{l=0}^{\infty} (2l+1) \frac{e^{i\delta_l}}{k} \sin(\delta_l) P_l(\cos\theta)$$

with δ_l the phase shift.

<u>Scattering And Angular Momentum channels</u>

The scattering of a particle through a central potential satisfies the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial r^2} + V_{ef}(r) \right] u_l(r) = \frac{\hbar^2 k^2}{2m} u_l(r)$$

where $u_l(r) = r A_l(r)$ with $A_l(r)$ the radial part of the wavefunction and

$$V_{ef}(r) = V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}$$

is the effective potential.

At Low energy, when

$$\frac{\lambda}{2\pi} = \frac{1}{k} \gg R$$

with R the range of the potential, the $l=0$ channel dominates, since the l to decay exponentially inside the centrifugal barrier at low energy ($k \to 0$) and Long wavelengths in the opposite regime,

$$\frac{\lambda}{2\pi} = \frac{1}{k} \ll R$$

Lastly,