Lecture 28

Consequences of unitarity of S

recall $|\Psi_\pm(t)\rangle = \Omega_\pm |\Psi^0_\pm(t)\rangle$

$$S = \Omega_+^\dagger \Omega_-$$

$$\langle \bar{p}_1' \bar{p}_2' | S | \bar{p}_1 \bar{p}_2 \rangle = \langle \bar{p}_1' \bar{p}_2' | p_1 p_2 \rangle$$
$$-2\pi i\, \delta(\bar{p}_1' + \bar{p}_2' - \bar{p}_1 - \bar{p}_2)\, \delta(E_1' + E_2' - E_1 - E_2) \times$$
$$\langle \bar{p}_1' \bar{p}_2' \| T(E+i\epsilon) \| \bar{p}_1 \bar{p}_2 \rangle$$

unitarity is the statement

$$S^\dagger S = I$$

using the above this condition can be expressed as

$$\langle \bar{p}_1' \bar{p}_2' | \bar{p}_1 \bar{p}_2 \rangle = \langle \bar{p}_1' \bar{p}_2' | S^\dagger S | p_1 p_2 \rangle =$$
$$\langle \bar{p}_1' \bar{p}_2' | p_1 p_2 \rangle + 2\pi i\, \delta(E' - E)\, \delta(p' - p)\, \langle \bar{p}_1 \bar{p}_2' \| T^\dagger(E+i\epsilon) \| p_1 p_2 \rangle$$
$$-2\pi i\, \delta(E' - E)\, \delta(\bar{p}' - \bar{p})\, \langle \bar{p}_1' \bar{p}_2' \| T(E+i\epsilon) \| p_1 p_2 \rangle +$$
$$(2\pi)^2 \int \delta(E' - E'')\, \delta(E - E'')\, \delta(\bar{p}' - \bar{p}'')\, \delta(\bar{p} - p'')$$
$$\langle \bar{p}_1' \bar{p}_2' \| T^\dagger(E+i\epsilon) \| p_1'' p_2'' \rangle\, d^3 p_1''\, d^3 p_2'' \times$$
$$\langle \bar{p}_1'' \bar{p}_2'' \| T(E+i\epsilon) \| p_1 \bar{p}_2 \rangle$$

This becomes

$$0 = (2\pi i)\,\delta(\bar{p}' - \bar{p})\,\delta(E' - E)\,\times$$

$$\left[\langle \bar{p}_1' \bar{p}_2' \| T^{\dagger}(E+i\epsilon) - T(E+i\epsilon) \| p_1 p_2 \rangle\right] +$$

$$(2\pi)^2 \int \delta(E' - E)\,\delta(\bar{p}' - \bar{p})\,\delta(\bar{p} - \bar{p}'')\,\delta(E - E'')$$

$$\int \langle \bar{p}_1' \bar{p}_2' \| T^{\dagger}(E+i\epsilon) \| \bar{p}_1'' \bar{p}_2'' \rangle\, d^3 p_1''\, d^3 p_2''$$

$$\langle \bar{p}_1'' \bar{p}_2'' \| T(E+i\epsilon) \| p_1 p_2 \rangle$$

note that

$$(T^{\dagger}(E+i\epsilon)) = (V + V(E - H + i\epsilon)^{-1} V)^{\dagger}$$

$$= (V^{\dagger} + V^{\dagger}(E - H^{\dagger} - i\epsilon)^{-1} V^{\dagger}) =$$

$$= V + V(E - H - i\epsilon)^{-1} V$$

$$= T(E - i\epsilon)$$

while the equation above is the general statement of the unitarity condition — it is useful to set

$$\bar{p}_1' = p_1 \qquad \bar{p}_2' = \bar{p}_2$$

The result is (after factoring out $\delta(\bar{p}-\bar{p}')\delta(E-E')$)

$$0 = -(2\pi i)\Big[\langle \bar{p}_1\bar{p}_2 \| T(E+i\epsilon) \| \bar{p}_1\bar{p}_2\rangle - \langle \bar{p}_1\bar{p}_2 \| T(E-i\epsilon) \| p_1 p_2\rangle\Big]$$

$$+(2\pi)^2 \int |\langle p_1'' p_2'' \| T(E+i\epsilon) \| \bar{p}_1\bar{p}_2 \rangle|^2 \times d^3p_1''\, dp_2''\, \delta(p_1''-p_1)\,\delta(E''-E)$$

The term on the last 2 lines is related to the total cross section

$$\sigma_T = \frac{(2\pi)^4 \hbar^2}{V} \int |\langle p_1'' p_2'' \| T(E+i\epsilon) \| p_1 p_2\rangle|^2 \, \delta(\bar{p}''-p)\,\delta(E''-E)\, d^3p_1''\, d^3p_2''$$

using this in the above equation

$$-i\Big[\langle \bar{p}_1\bar{p}_2 \| T(E+i\epsilon) \| p_1 p_2\rangle - \langle \bar{p}_1\bar{p}_2 \| T(E-i\epsilon) \| p_1 p_2\rangle\Big]$$

$$= -\frac{(2\pi)V}{(2\pi)^4 \hbar^2}\sigma_T$$

or

$$\boxed{\sigma_T = \frac{(2\pi)^3\hbar^2}{V} i \left(\langle p_1 p_2 \| T(E+i\epsilon) \| p_1 p_2 \rangle - \langle p_1 p_2 \| T(E-i\epsilon) \| p_1 p_2 \rangle \right)}$$

This is normally expressed in terms of the scattering amplitude

$$F = -(2\pi)^2 \mu \hbar \langle \bar{p}_1' \bar{p}_2' \| T(E+i\epsilon) \| p_1 p_2 \rangle$$

it follows that

$$i \left[\langle p_1 p_2 \| T(E+i\epsilon) \| p_1 p_2 \rangle - \langle p_1 p_2 \| T(E-i\epsilon) \| p_1 p_2 \rangle \right]$$

$$= -\frac{i}{(2\pi)^2 \mu \hbar} \left(F(\bar{k}\bar{k}) - F^*(kk) \right)$$

$$= \frac{2}{(2\pi)^2 \mu \hbar} \operatorname{Im} F(\bar{k},\bar{k})$$

$$\sigma_T = \frac{(2\pi)^3\hbar^2}{V} \times \frac{2}{(2\pi)^2 \mu \hbar} \operatorname{Im} F(\bar{k},\bar{k})$$

$$\boxed{\sigma_T = \frac{4\pi\hbar}{k} \operatorname{Im} F(\bar{k}\bar{k})} \qquad \left(V = \frac{k}{\mu} \right)$$

which relates the total cross section to the imaginary part of the forward ($\bar{k}' = \bar{k}$) scattering amplitude

$$\boxed{\text{Rotationally invariant potentials}}$$

The computational difficulty with the Lippmann Schwinger equation is that it involves 3 dimensional integrals. This can lead to large matrices

$$\int d^3k = \sum_{k_1 k_2 k_3 = 1}^{N} \Delta k_1 \Delta k_2 \Delta k_3$$

this involves N^3 evaluation.

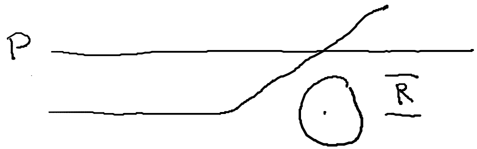
$$\langle \bar{k}_i \| T(E+i\epsilon) \| \bar{k}_j \rangle = \langle \bar{k}_i \| V \| \bar{k}_j \rangle$$

$$+ \sum_{k_x k_y k_z} \underbrace{\langle \bar{k}_i \| V \| \bar{k}'' \rangle \frac{\Delta x k''}{k^2 - k''^2 + i\epsilon}}_{N^3 \times N^3 \text{ matrix}} \langle \bar{k}'' \| T(E+i\epsilon) \| \bar{k} \rangle$$

$$N = 30 \rightarrow N^3 = (30)^3 = 27000$$

size of matrix is (27000 x 27000)

We can take advantage of rotational invariance to simplify the computational problem



L_{max} $|r \times p| < Rp$

If we can express the Lippmann Schwinger equation in an angular momentum basis we expect that for a given p we only need a finite number of L values.

recall that the Lippmann Schwinger equation has the form

$$\langle \bar{r} | (\bar{k}_-) \rangle = \langle \bar{r} | \bar{k} \rangle + \int \langle r | \frac{d^3 r'}{\frac{k^2}{2\mu} - h_0 + i\epsilon} | \bar{r}' \rangle V(r') \langle \bar{r}' | (k_-) \rangle$$

or

$$\langle \bar{k}' || T(E+i\epsilon) || \bar{k} \rangle = \langle \bar{k}' || V || \bar{k} \rangle + \int \langle \bar{k}' || V || \bar{k}'' \rangle \frac{d^3 k''}{\frac{k^2}{2\mu} - h_0 + i\epsilon} \langle k'' || T(E+i\epsilon) || \bar{k} \rangle$$

To take advantage of the spherical symmetry we need to use a different basis

$$|\bar{r}\rangle \to |r \ell m\rangle$$

$$|\bar{k}\rangle \to |k \ell m\rangle$$

$$\langle \bar{r} | \bar{k} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{i\bar{k}\cdot\bar{r}/\hbar} =$$

$$\frac{1}{(2\pi\hbar)^{3/2}} e^{ikr\cos\theta/\hbar}$$

next we expand $e^{ikr\cos\theta/\hbar}$

in terms of Legendre polynomi

$$e^{ikr\cos\theta/\hbar} = \sum_{\ell=0}^{\infty} P_\ell(\cos\theta)\, a_\ell(kr/\hbar)$$

multiply both sides by

$P_{\ell'}(\cos\theta) \sin\theta\, d\theta$ and integrate

from $0 \to \pi$

$$\int_0^\pi e^{ikr\cos\theta/\hbar} P_{\ell'}(\cos\theta) \sin\theta\, d\theta =$$

$$\sum_{\ell=0}^{\infty} \int P_\ell'(\cos\theta)\, P_\ell(\cos\theta) \sin\theta\, d\theta\; a_\ell(kr/\hbar)$$

Let $u = \cos\theta$ $\quad du = -\sin\theta\, d\theta$

$u: 1 \to -1$

This becomes

$$\int e^{ikru/\hbar} P_{\ell'}(u)\, du =$$

$$\sum_{\ell=0}^{\infty} a_\ell\left(\frac{kr}{\hbar}\right) \int_{-1}^{1} P_{\ell'}(u) P_\ell(u)\, du =$$

$$a_{\ell'}\left(\frac{kr}{\hbar}\right) \frac{2}{2\ell'+1}$$

or

$$a_\ell\left(\frac{kr}{\hbar}\right) = \frac{2\ell+1}{2} \boxed{\int_{-1}^{1} e^{ikru/\hbar} P_\ell(u)\, du}$$

The quantity in the red box is an integral representation of a spherical Bessel function

$$j_\ell(x) = \frac{(-i)^\ell}{2} \int_{-1}^{1} P_\ell(u) e^{iux}\, du$$

$$\therefore\ a_\ell\left(\frac{kr}{\hbar}\right) = (2\ell+1)\, i^\ell\, j_\ell\left(\frac{kr}{\hbar}\right)$$

$$\boxed{\langle \vec{r} | \vec{k} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} \sum_{\ell=0}^{\infty} (2\ell+1)\, i^\ell\, j_\ell\left(\frac{kr}{\hbar}\right) P_\ell(\hat{k}\cdot\hat{r})}$$

finally $P_\ell(\hat{k}\cdot\hat{r})$ can be expressed in terms of spherical harmonics

$$P_\ell(\hat{k}\hat{r}) = \sum \frac{4\pi}{2\ell+1} Y_{\ell m}(\hat{k}) Y^*_{\ell m}(\hat{r})$$

$$= \sum \frac{4\pi}{2\ell+1} Y_{\ell m}(\hat{r}) Y^*_{\ell m}(\hat{k})$$

this gives

$$\boxed{\langle \bar{r} | \bar{k} \rangle = \sum \frac{(4\pi)\, i^\ell}{(2\pi\hbar)^{3/2}} j_\ell\left(\frac{kr}{\hbar}\right) Y_{\ell m}(\hat{r}) Y^*_{\ell m}(\hat{k})}$$

the next step is to use this change of basis in the integral equation

$$\langle \bar{r} | (\bar{k}_-) \rangle = \sum_{\ell m} \frac{(4\pi)\, i^\ell}{(2\pi\hbar)^{3/2}} j_\ell\left(\frac{kr}{\hbar}\right) Y_{\ell m}(\hat{r}) Y^*_{\ell m}(\hat{k}) +$$

$$\sum \frac{(4\pi)\, i^\ell}{(2\pi\hbar)^{3/2}} \int \frac{j_\ell(kr/\hbar)}{k^2/2\mu - k'^2/2\mu + i\epsilon} Y_{\ell m}(\hat{r}) Y^*_{\ell m}(\hat{k}) \times$$

$$V(r) \frac{(4\pi)(-i)^{\ell'}}{(2\pi\hbar)^{3/2}} j_{\ell'}\left(\frac{kr'}{\hbar}\right) Y_{\ell' m'}(\hat{k}) Y^*_{\ell' m'}(\hat{r}')$$

$$\langle \bar{r}' | \bar{k}_- \rangle \, d^3r' \, d^3k'$$

first note

$$\int Y_{lem}(\hat{k})\, Y^*_{l'm'}(\hat{k})\, d\hat{k} = \delta_{ll'}\delta_{mm'}$$

so this eliminates the l' and m' sums allowing replacement $l' \to l$ $m' \to m$

$$\langle \bar{r} | \bar{k}^- \rangle = \frac{1}{(2\pi\hbar)^{3/2}} \sum 4\pi i^l j_l\left(\frac{kr}{\hbar}\right) Y^*_{lm}(\hat{r}) Y_{lm}(\hat{k})$$

$$\frac{(4\pi)^2}{(2\pi\hbar)^3} \int \frac{j_l\left(\frac{kr}{\hbar}\right) j_l\left(\frac{kr'}{\hbar}\right)}{\frac{k^2}{2\mu} - \frac{k'^2}{2\mu} + i\epsilon} k^2 dk\, Y^*_{lm}(r)\, V(r')$$

$$\times \int Y_{lm}(\hat{r}) \langle r | k_- \rangle\, d^3r$$

define

$$\boxed{\begin{gathered}\langle rlm | k_- l'm' \rangle = \\ \int d\hat{r}\, d\hat{k}\, Y^*_{lm}(\hat{r}) \langle \bar{r} | \bar{k}_- \rangle Y_{l'm'}(\hat{k}) \\ \langle \bar{r} | \bar{k} \rangle = \sum Y_{lm}(\hat{r}) \langle rlm | k l'm' \rangle Y^*_{l'm'}(\hat{k})\end{gathered}}$$

this can be used to eliminate the spherical harmonics from the above equation

$$\langle r | k_- \rangle_\ell = \frac{4\pi}{(2\pi\hbar)^{3/2}} i^\ell j_\ell\left(\frac{kr}{\hbar}\right)$$

$$- \frac{(4\pi)^2}{(2\pi\hbar)^3} 2\mu \int_0^\infty \frac{j_\ell\left(\frac{k'r}{\hbar}\right) j_\ell\left(\frac{k'r'}{\hbar}\right)}{k'^2 - k^2 - i\epsilon} Y(r') \langle r' | k_- \rangle$$

$$V(r') \times r'^2 dr' \, k'^2 dk'$$

as in the 3 dimensional case we need to compute the greens funct.

$$\int_0^\infty \frac{j_\ell\left(\frac{k'r}{\hbar}\right) j_\ell\left(\frac{k'r'}{\hbar}\right) k'^2 dk'}{k'^2 - k^2 - i\epsilon}$$

(1) $j_\ell(x)$ are odd or even functions of x so $\left(j_\ell(-x) = (-)^\ell j_\ell(x)\right)$

$j_\ell\left(\frac{kr}{\hbar}\right) j_\ell\left(\frac{kr'}{\hbar}\right)$ are even functions of k

$$= \frac{1}{2} \int_{-\infty}^\infty \frac{j_\ell\left(\frac{k'r}{\hbar}\right) j_\ell\left(\frac{kr'}{\hbar}\right) k'^2 dk'}{k'^2 - k^2 - i\epsilon}$$

(2) The spherical bessel functions are entire functions - ie they have no poles in the complex plane

For large k $j_l\left(\frac{kr}{\hbar}\right) \sim \frac{\hbar}{kr}$

so the integral is convergent

(3) $j_l(x) = \frac{1}{2i}\left(h_l^+(x) - h_l^-(x)\right)$

where for large x

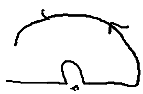
$h_l^\pm(x) \to \frac{e^{\pm ix}}{x}$

(1) to do this integral using the residue theorem start by replacing

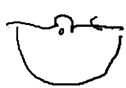
---

---

in the limit that the radius of the small half circle goes to 0 we get the integral on the real axis. To ensure there is no contribution from large half circles



for the $h_\ell^+(\frac{kr}{4})$ integral



for the $h_\ell^-(\frac{kr}{4})$ integral

in replacing j_ℓ by $\frac{h_\ell^+ - h_\ell^-}{2i}$

we introduce poles — in the difference they cancel now we can do the integral

using the residue theorem

$$\frac{1}{2}\int_{-\infty}^{\infty} \frac{j_\ell(k'r/\hbar)\, j_\ell(k'r'/\hbar)}{k'^2 - k^2 - i\epsilon}\, k'' dk'$$

we use the notation

$$\frac{kr_>}{\hbar} = \frac{kr}{\hbar} \quad \text{if } r > r'$$

$$\frac{kr'}{\hbar} \quad \text{if } r' > r$$

$$\frac{kr_<}{\hbar} = \frac{kr}{\hbar} \quad \text{for } r < r'$$

$$\frac{kr'}{\hbar} \quad \text{if } r' < r$$

$r_>$ determines the overall sign in the expression

$$= \frac{1}{2}\int \frac{j_\ell\left(\frac{kr_<}{\hbar}\right)\left(h_\ell^+\left(\frac{kr_>}{\hbar}\right) - h_\ell^-\left(\frac{kr_>}{\hbar}\right)\right)}{(2i)\,(k'^2 - k^2 - i\epsilon)}\, k'' dk'$$

for the $h^+\left(\frac{kr_>}{\hbar}\right)$ integral we close the contour in the upper half plane at pick up a pole at $k' = k$

$$\frac{2\pi i}{4i}\; \frac{j_\ell\left(\frac{kr_<}{\hbar}\right) h_\ell^+\left(\frac{kr_>}{\hbar}\right) k^2}{2k}$$

$$\frac{\pi k}{4} j_e\left(\frac{kr_<}{\hbar}\right) h^{+}\left(\frac{kr_>}{\hbar}\right)$$

for the $h_e^-(kr)$ the integral must be closed in the lower half plane — there are 2 poles — one at $-ik$ an one at 0

$$-\frac{2\pi i}{4i}\frac{(-k^2)}{(-2k)} j_e\left(-\frac{kr_<}{\hbar}\right) h_e^-\left(\frac{-kr_>}{\hbar}\right) =$$

$$\boxed{\frac{\pi k}{4} j_e\left(-\frac{kr_<}{\hbar}\right) h_e^-\left(\frac{kr_>}{\hbar}\right)}$$

next we use

$$j_e\left(-\frac{kr_<}{\hbar}\right) = (-1)^e j_e\left(\frac{kr_<}{\hbar}\right)$$

$$h_e^-\left(-\frac{kr_<}{\hbar}\right) = (-1)^{e+1} h_e^+\left(\frac{kr_>}{\hbar}\right)$$

$$-\frac{\pi k}{4} j_e\left(\frac{kr_<}{\hbar}\right) h_e^+\left(\frac{kr_>}{\hbar}\right)$$

(* there is no contributn from the pole at 0 since $k^2 j_e(k) h_e^{\pm}(k) \to 0$ at the origin we finally get

$$\int_0^\infty \frac{j_\ell\left(\frac{k'r}{\hbar}\right) j_\ell\left(\frac{k'r'}{\hbar}\right) k'^2 dk'}{k'^2 - k^2 - i\epsilon} =$$

$$-\frac{\pi k}{2} j_\ell\left(\frac{kr_<}{\hbar}\right) h_\ell^+\left(\frac{kr_>}{\hbar}\right)$$

$$\boxed{2\mu \int_0^\infty \frac{j_\ell\left(\frac{k'r}{\hbar}\right) j_\ell\left(\frac{k'r'}{\hbar}\right) k'^2 dk'}{k'^2 - k^2 - i\epsilon} \quad \pi k \mu\, j_\ell\left(\frac{kr_<}{\hbar}\right) h_\ell^+\left(\frac{kr_>}{\hbar}\right)}$$

The integral equation becomes

$$\langle r \mid k^- \rangle_\ell = \frac{4\pi i^\ell}{(2\pi\hbar)^{3/2}} j_\ell\left(\frac{kr}{\hbar}\right)$$

$$\frac{(4\pi)^2}{(2\pi\hbar)^3} (\pi \mu k) \int j_\ell(kr_</\hbar)\, h_\ell^+(kr_>/\hbar)\, r'^2 dr'\, V(r') \langle r' \mid k_\ell^- \rangle$$

This is a one variable integral equation for each partial wave

$$= \frac{4\pi i^l}{(2\pi\hbar)^{3/2}} j_l\left(\frac{kr}{\hbar}\right)$$

$$\frac{2\mu k}{\hbar^3} \int j_l\left(\frac{kr_<}{\hbar}\right) h_l^+\left(\frac{kr_>}{\hbar}\right) V(r') \langle r' | k_- \rangle_l \, r'^2 dr'$$

for large this becom

$$\boxed{\longrightarrow \frac{4\pi i^l}{(2\pi\hbar)^{3/2}} j_l\left(\frac{kr}{\hbar}\right) + \frac{2\mu k}{\hbar^3} h_l^+\left(\frac{kr}{\hbar}\right) \int j_l\left(\frac{kr'}{\hbar}\right) V(r') \langle r' | k_- \rangle_l \, r'^2 dr'}$$