Lecture 18

We have shown that the wave function for a scattering process can be written:

$$\psi_{k,\,phys}(r,\theta) = \sum_{l=0}^{\infty} a_l P_l(\cos\theta)\, R_{kl}(r)$$

where R_{kl} solves the radial equation with asymptotic behaviour:

$$R_{kl} \overset{r\to\infty}{\sim} \frac{2\sin(kr - \frac{l\pi}{2} + \delta_l)}{r}$$

and $P_l(\cos\theta)$ has the standard normalisation.

Moreover, a_l can be expressed in terms of the phase shift δ_l as:

$$a_l = (i)^l \frac{2l+1}{2k} e^{i\delta_l}$$

$$= \frac{2l+1}{2k} e^{i(\delta_l + \frac{l\pi}{2})}$$

The same form of the wave function holds when the particle is free ($V(r) = 0$) but with $\delta_l = 0$.

So far, we know nothing about δ_l. So we start by estimating δ_l for large l using the WKB approximation.

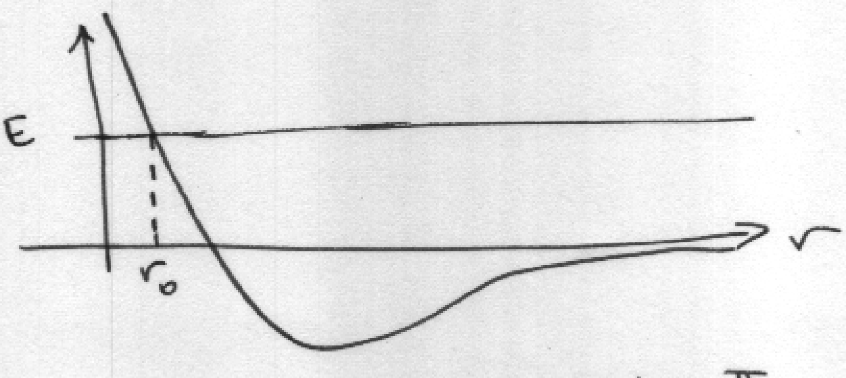
For this, let us re-visit ~~the~~ WKB approximation in the context of radial motion in 3 dimensions.

The WKB wave function for angular momentum quantum number l and potential $V(r)$ should naively ~~have~~ have a phase:

$$\frac{1}{\hbar}\int p\,dx = \frac{1}{\hbar}\int\sqrt{2m\left(\frac{\hbar^2k^2}{2m} - \frac{\hbar^2 l(l+1)}{2mr^2} - V(r)\right)}\,dr$$

$$= \int\sqrt{k^2 - \frac{l(l+1)}{r^2} - \frac{2mV(r)}{\hbar^2}}\,dr$$

~~However~~ ~~In~~ At a situation with a turning point r_0 on one side and unbounded motion on the other:



we should also add $-\frac{\pi}{4}$ to the phase on the RHS (recall the matching conditions!).

However the phase so obtained does not agree with that from the <u>free</u> spherical wave. The latter gives:

$$j_l(kr) \sim \frac{2\sin\left(kr - \frac{l\pi}{2}\right)}{r}$$

$$= \frac{e^{i\left(kr - \frac{l\pi}{2}\right)}}{ir} - \frac{e^{-i\left(kr - \frac{l\pi}{2}\right)}}{ir}$$

Thus the e^{ikr} part is multiplied by

$$\frac{e^{-i\frac{l\pi}{2}}}{ir} = \frac{e^{-i\left(\frac{l+1}{2}\right)\pi}}{r}$$

This phase should be reproduced if we evaluate, for $V(r) = 0$, the quantity:

$$\frac{1}{\hbar}\int_{r_0}^{r} p\,dx - \frac{\pi}{4} \qquad \text{as} \quad r \to \text{large}.$$

However we get:

$$\frac{1}{\hbar}\int_{r_0}^{r} p\,dx = \int_{r_0}^{r} \sqrt{k^2 - \frac{l(l+1)}{r^2}}\,dr \qquad \left(r_0 = \frac{k}{\sqrt{l(l+1)}}\right)$$

$$\simeq kr - \sqrt{l(l+1)}\,\frac{\pi}{2} - \frac{\pi}{4}$$

So the phase is $e^{-\frac{i\pi}{2}\left(\sqrt{l(l+1)} + \frac{1}{2}\right)}$!

The discrepancy does not matter too much because the validity of WKB requires $l \gg 1$:

$$\frac{d}{dx}\left|\frac{\hbar}{p}\right| \ll 1 \Rightarrow \frac{d}{dr}\left|\frac{\hbar r}{l}\right| \ll 1 \Rightarrow \left|\frac{\hbar}{l}\right| \ll 1$$

so $l \gg 1$.

For large l, $\sqrt{l(l+1)}+\frac{1}{2}$ and $l+1$ are almost equal. Nevertheless, this fact suggests that in 3d, the WKB momentum should be taken as

$$p = \sqrt{2m\left(E - \frac{\hbar^2(l+\frac{1}{2})^2}{2mr^2} - V(r)\right)}$$

In this case $\frac{1}{\hbar}\int p\,dx - \frac{\pi}{4}$ indeed has the phase $-\frac{i}{2}(l+1)\pi$ in the free case as required.

Now δ_l is given is given by the phase difference of the interacting and free theory:

$$\delta_l \simeq \left[\int_{r_0}^{r}\sqrt{k^2 - \frac{(l+\frac{1}{2})^2}{r^2} - \frac{2mV(r)}{\hbar^2}}\,dr - \int_{r_0}^{r}\sqrt{k^2 - \frac{(l+\frac{1}{2})^2}{r^2}}\,dr\right]_{r\to\infty}$$

(we assume $r_0 \simeq \frac{l+\frac{1}{2}}{k}$ in both integrals, which should be approximately true)

Notice that each of the integrals is divergent as $r \to \infty$ but the difference can be convergent. In fact for large l, the turning point r_0. (which solves $k^2 - \frac{(l+\frac{1}{2})^2}{r^2} - \frac{2mV(r)}{\hbar^2} = 0$) is also quite large. Then $V(r)$ can be taken small throughout the integration region and:

$$\sqrt{\left(k^2 - \frac{(l+\frac{1}{2})^2}{r^2} - \frac{2mV(r)}{\hbar^2}\right)} - \sqrt{\left(k^2 - \frac{(l+\frac{1}{2})^2}{r^2}\right)}$$

$$\simeq - \frac{m}{\hbar^2} \frac{V(r)}{\sqrt{k^2 - \frac{(l+\frac{1}{2})^2}{r^2}}}$$

so $$\delta_l \simeq -\frac{m}{\hbar^2} \int_{r_0}^{\infty} \frac{V(r)\,dr}{\sqrt{k^2 - \frac{(l+\frac{1}{2})^2}{r^2}}}$$

This is convergent if $V(r) \sim \frac{1}{r^n}$ as $r \to \infty$ with $n > 1$. We will assume this is true for the moment.

To estimate the magnitude of δ_l, let us assume $V(r) = \frac{V_0}{r^n}$ for some n.

Then $$\delta_l \simeq -\frac{mV_0}{\hbar^2} \int_{r_0}^{\infty} \frac{dr}{r^n \sqrt{k^2 - \frac{(l+\frac{1}{2})^2}{r^2}}}$$

$$= -\frac{mV_0}{\hbar^2} \int_{r_0}^{\infty} \frac{dr}{r^{n-1} \sqrt{k^2 r^2 - (l+\frac{1}{2})^2}}$$

Now use $r_0 \simeq \frac{l+\frac{1}{2}}{k}$ to get:

$$\delta_l \sim \frac{-mV_0}{\hbar^2 (l+\frac{1}{2})} \int_{r_0}^{\infty} \frac{dr}{r^{n-1}\sqrt{\left(\frac{r}{r_0}\right)^2 - 1}}$$

$$= \frac{-mV_0}{\hbar^2 (l+\frac{1}{2})} \left(\frac{k}{l+\frac{1}{2}}\right)^{n-2} \int_1^{\infty} \frac{dx}{x^{n-1}\sqrt{x^2-1}} \qquad \left(\begin{array}{l}\text{we have}\\ \text{set } x = \frac{r}{r_0}\end{array}\right)$$

The integral is of order 1 and we see that $\delta_l \sim \frac{1}{(l+\frac{1}{2})^{n-1}}$ so for any potential with $n>1$, ~~then~~ $\delta_l \ll 1$ for large l.

We can check finiteness of the total cross-section:

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

$$\simeq \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1)\, \delta_l^2$$

$$\simeq \frac{4\pi}{k^2} \sum_{l=0}^{\infty} \frac{1}{l^{2n-3}}$$

which converges for $2n-3 > 1$, ie $n > 2$.

Another convergence question concerns the forward scattering amplitude, $f_k(\theta = 0)$.

We have:

$$f_k(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(e^{2i\delta_l} - 1) P_l(\cos\theta)$$

from which we get (using $P_l(1) = 1$):

$$f_k(\theta = 0) \simeq \frac{2i}{2ik} \sum_{l=0}^{\infty} (2l+1).\delta_l$$

$$\simeq \frac{1}{k} \sum_{l=0}^{\infty} \frac{1}{l^{n-2}}$$

which converges only if $n > 3$.

Finally let us consider non-forward scattering.

For this we use the identity:

$$\sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta) = 4\,\delta(1 - \cos\theta)$$

$$= 0 \quad \text{for } \theta \neq 0.$$

Hence at $\theta \neq 0$ we can drop the -1 in $(e^{2i\delta_l} - 1)$ and get:

$$f_k(\theta \neq 0) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)\, e^{2i\delta_l}\, P_l(\cos\theta)$$

Now if $n \leq 1$ then the δ_l are formally infinite so it seems we cannot obtain any finite scattering amplitude or cross-section.

However there is a useful trick. Let us consider the non-forward scattering amplitude $f_k(\theta \neq 0)$ and multiply it by a fixed phase $e^{-2i\delta_0}$ (the inverse of the phase-shift for $l=0$). Thus, define:

$$\tilde{f}_k(\theta \neq 0) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) e^{2i(\delta_l - \delta_0)} P_l(\cos\theta)$$

$$= e^{-2i\delta_0} f_k(\theta \neq 0).$$

Now $\frac{d\sigma}{d\Omega} = |f_k(\theta)|^2 = |\tilde{f}_k(\theta)|^2$ as long as $\theta \neq 0$, because the overall phase drops out.

Now it is easy to see that the "shifted phase-shifts" $\tilde{\delta}_l = \delta_l - \delta_0$ are <u>finite</u> and this allows us to obtain a finite cross-section:

$$\tilde{\delta}_l = \delta_l - \delta_0 \simeq \frac{-m}{\hbar^2} \int_{r_0}^{\infty} V(r)\, dr \left(\frac{1}{\sqrt{k^2 - \frac{(l+\frac{1}{2})^2}{r^2}}} - \frac{1}{k} \right)$$

For large r, if $V(r) \sim \frac{1}{r^n}$ as before then the integrand goes like $\frac{1}{r^{n+2}}$.

So this time the integral converges for all $n > 0$! This enables us to deal with Coulomb's law, $n=1$.

Optical theorem

We have seen that:

$$f_k(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(e^{2i\delta_l} - 1) P_l(\cos\theta)$$

Now consider $\theta = 0$, then $P_l(\cos\theta) = 1$ and:

$$f_k(0) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(e^{2i\delta_l} - 1)$$

$$= \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)\left(\cos 2\delta_l - 1 + i \sin 2\delta_l \right)$$

Thus the imaginary part of $f_k(0)$ is:

$$\mathrm{Im}\, f_k(0) = \frac{1}{2k} \sum_{l=0}^{\infty} (2l+1) \cdot 2\sin^2\delta_l$$

$$= \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \sin^2\delta_l$$

Comparing this with:

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

we see that

$$\boxed{\sigma = \frac{4\pi}{k} \mathrm{Im} f(0)}$$

→ "optical theorem"

This result holds more generally, even if the force is not central.

Calculation of δ_ℓ for a simple problem: the hard sphere.

This problem, being much simpler than the physically relevant Coulomb or Yukawa potential, ~~illustrates~~ ~~the~~ ~~easy~~ permits exact computation of the phase shifts.

We choose a potential: $V(r) = 0, \quad r > r_0$
$= \infty, \quad r < r_0.$

This amounts to an infinite potential barrier in the radial direction. By analogy with the 1d case, we start with a general radial wave function for a free particle.

For fixed ℓ there are (as usual) two solutions, spherical Bessel functions. One is $j_\ell(kr)$ as we already saw, while the other is called $n_\ell(kr)$. The definitions are:

$$j_\ell(\rho) = (-1)^\ell \rho^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \left(\frac{\sin\rho}{\rho}\right)$$

$$n_\ell(\rho) = (-1)^\ell \rho^\ell \left(\frac{1}{\rho}\frac{d}{d\rho}\right)^\ell \left(-\frac{\cos\rho}{\rho}\right)$$

Thus, $R_\ell(r) = A_\ell j_\ell(kr) + B_\ell n_\ell(kr)$

Note that n_ℓ diverges at $r=0$, but now $r=0$ is excluded from the problem so n_ℓ is allowed. The boundary condition is

$$R_\ell(r_0) = 0.$$

It follows that $\dfrac{B_\ell}{A_\ell} = -\dfrac{j_\ell(kr_0)}{n_\ell(kr_0)}$

We have already once used the fact that for large ρ, $j_\ell(\rho) \to \dfrac{\sin(\rho - \frac{\ell\pi}{2})}{\rho}$.

Similarly it can be shown that

$$n_\ell(\rho) \to - \frac{\cos(\rho - \frac{\ell\pi}{2})}{\rho}$$

Hence $R_\ell(r) \xrightarrow{r\to\infty} \dfrac{1}{kr}\left(A_\ell \sin(kr - \frac{\ell\pi}{2}) - B_\ell \cos(kr - \frac{\ell\pi}{2})\right)$

We want to put this in the form of a term $\frac{1}{i} e^{i(kr - \frac{\ell\pi}{2} + \delta_\ell)}$ and another term $\frac{1}{i} e^{-i(kr - \frac{\ell\pi}{2} + \delta_\ell)}$. This is done by expanding the sin and cos as exponentials:

$$R_\ell(r) \xrightarrow{r\to\infty} \frac{1}{2ikr}\left[(A_\ell - iB_\ell) e^{i(kr - \frac{\ell\pi}{2})} - (A_\ell + iB_\ell) e^{-i(kr - \frac{\ell\pi}{2})}\right]$$

Now $A_\ell - iB_\ell = |A_\ell - iB_\ell|\, e^{i\delta_\ell}$

$= \sqrt{A_\ell^2 + B_\ell^2}\, e^{i\delta_\ell}$

where $\tan\delta_\ell = -\dfrac{B_\ell}{A_\ell} = \dfrac{j_\ell(kr_0)}{n_\ell(kr_0)}$

Thus we have:

$$\boxed{\delta_\ell = \tan^{-1} \frac{j_\ell(kr_0)}{n_\ell(kr_0)}}$$

→ a completely explicit result!

For $l_0 = 0$ we have:

$$j_0(\rho) = \frac{\sin\rho}{\rho}, \quad n_0(\rho) = -\frac{\cos\rho}{\rho}$$

So $$\frac{j_0(kr_0)}{n_0(kr_0)} = -\tan kr_0$$

Hence $$\delta_0 = \tan^{-1}(-\tan kr_0) = -kr_0 .$$

The negative value is common to a repulsive potentials. Of course δ_l is defined only mod 2π. Notice that if $kr_0 = 2\pi$ then $\delta_0 = 0$, then $f_k(\theta)$ and σ do not receive any contribution with $l = 0$!

Also note that for $\rho \ll l$,

$$j_l(\rho) \sim \frac{2^l\, l!}{(2l+1)!}\rho^l = \frac{\rho^l}{(2l+1)!!}$$

$$n_l(\rho) \sim \frac{-(2l)!}{2^l\, l!}\rho^{-l-1} = -\rho^{-l-1}(2l-1)!!$$

So $$\frac{j_l(kr_0)}{n_l(kr_0)} \sim -\frac{2^{2l}(l!)^2}{(2l)!\,(2l+1)!}(kr_0)^{2l+1}$$

$$= -\frac{1}{(2l+1)!!}\,\frac{1}{(2l-1)!!}(kr_0)^{2l+1}$$

which shows a very rapid fall off for large l.

Since $\delta_l = \tan^{-1}\left(\frac{j_l(kr_0)}{n_l(kr_0)}\right)$ and $\tan^{-1}\epsilon \simeq \epsilon$ for $\epsilon \ll 1$, we have in this limit

$$\delta_l \simeq \frac{-1}{(2l+1)!!\,(2l-1)!!}(kr_0)^{2l+1}$$