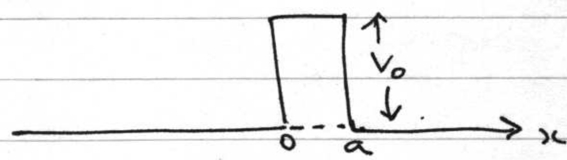
Scattering theory.

We now turn to the problem of studying particle interactions with a scattering centre. Thus we are interested in continuum states of the Schrodinger eqn with given asymptotic behaviours.

The simplest example is the 1d potential barrier:



We consider $\psi(x) = Ae^{ikx} + Be^{-ikx} \quad x \leq 0$
$\psi(x) = Ce^{ikx} \quad x \geq a$

So A is the coefficient of the incoming wave, B of the reflected wave and C of the transmitted wave. This is an easy problem to solve because V is piecewise constant and 1d. Still, one finds interesting behaviours of B and C depending on the barrier height and thickness, including resonant transmission when

$$\sqrt{2m(E-V_0)}\,\frac{a}{\hbar} = \pi, \; 2\pi, \; \ldots \qquad (E > V_0),$$

and tunneling when $E < V_0$.

In 3d the situation is much more complicated because of the nature of the Schrodinger eq in 3d. As for the bound state case, we restrict to spherically symmetric potentials $V = V(r)$ and use spherical polar coordinates. We work in the CM frame, with elastic scattering. Assume the incoming wave is along the z-axis:

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

while the outgoing or scattered wave is radially outward but with an angle-dependent coefficient:

$$\psi \sim f(\theta)\,\frac{e^{ikr}}{r}.$$

$f(\theta)$ is called the scattering amplitude.

We get $\frac{e^{ikr}}{r}$ because the radial wave fn. $R(r)$ is written $R(r) = \frac{u(r)}{r}$ where $u(r)$ satisfies:

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

As $r \to \infty$ if $V(r) \to 0$ then u is a plane wave:

$$u(r) = e^{ikr}$$

and $R(r) = \frac{u(r)}{r} = \frac{e^{ikr}}{r}$.

This must be multiplied by an angular wave fn which we call $f(\theta)$, where θ is the scattering angle.

thus, far from the scattering centre we have:

$$\psi \sim A\left[e^{ikz} + f(\theta)\,\frac{e^{ikr}}{r}\right] \qquad A \sim \frac{1}{L^{3/2}}$$

We cannot apply any requirements on this at $r \to 0$ such as boundary conditions, since this eqn is invalid as $r \to 0$.

Let us define a surface element dS through which the outgoing particle passes:

then $dS = r^2\, d\Omega$. Then the probability per unit time that the scattered particle will pass through the element dS is:

$$v\,|\psi|^2\, dS \qquad \left(\text{dimensions} = \frac{1}{\text{time}}\right)$$

$$= |A|^2 v \,.\, \frac{|f(\theta)|^2}{r^2} \,.\, r^2\, d\Omega$$

$$= |A|^2\, v\, |f(\theta)|^2\, d\Omega$$

For the incoming particle, the incident current density ~~probability per unit time of being incident on the scattering centre~~ is proportional to

$$|\psi|^2 v \quad = \quad |A|^2 v. \qquad \left(\text{dimensions} = \frac{1}{L^2 T}\right)$$

Thus the ratio is

$$\frac{|A|^2 \, v \, |f(\theta)|^2 \, d\Omega}{|A|^2 \, v} = |f(\theta)|^2 \, d\Omega.$$
$$= |f(\theta)|^2 \cdot 2\pi \sin\theta \, d\theta$$

This is called the scattering cross-section. It has dimensions of area.

Because of way we have chosen the z-axis (along the incident beam) the problem is independent of the azimuthal angle φ. Thus the only angular wave functions which can appear are $Y_{l0} = P_l(\cos\theta)$.

Hence the required wave fn in a spherically symmetric potential is

$$\psi = \sum_{l=0}^{\infty} A_l \, P_l(\cos\theta) \, R_{kl}(r)$$

where R_{kl} are the radial wave fns, satisfying

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{dR_{kl}}{dr}\right) + \left(k^2 - \frac{l(l+1)}{r^2} - \frac{2m}{\hbar^2} V(r)\right) R_{kl}(r) = 0$$

Now we can choose the coefficients A_l so that

$$\psi \xrightarrow{r\to\infty} e^{ikz} + f(\theta)\frac{e^{ikr}}{r}.$$

For large r, the radial eqn is solved by:

$$\cancel{\frac{k}{r}} \quad R_{kl}(r) \xrightarrow{r\to\infty} A\,\frac{e^{ikr}}{r} + B\,\frac{e^{-ikr}}{r}$$

$$\sim 2\,\frac{\sin(kr+\alpha_l)}{r} \qquad \text{(choose the norm)}$$

where α_l is an angle which in general can be l-dependent.

So $$R_{kl}(r) \xrightarrow{r\to\infty} \frac{e^{i(kr+\alpha_l)} - e^{-i(kr+\alpha_l)}}{ir}$$

Now $$\Psi(r,\theta) = \sum_{l=0}^{\infty} A_l\, P_l(\cos\theta)\, R_{kl}(r)$$

$$\xrightarrow{r\to\infty} \sum_{l=0}^{\infty} A_l\, P_l(\cos\theta)\left(\frac{e^{i(kr+\alpha_l)} - e^{-i(kr+\alpha_l)}}{ir}\right)$$

$$= \left(\sum_{l=0}^{\infty} A_l\, P_l(\cos\theta)\, e^{i\alpha_l}\right)\frac{e^{ikr}}{ir}$$

$$- \left(\sum_{l=0}^{\infty} A_l\, P_l(\cos\theta)\, e^{-i\alpha_l}\right)\frac{e^{-ikr}}{ir}$$

Now we need to know the expansion of the plane wave e^{ikz} in terms of $e^{\pm ikr}$

$$e^{ikz} = \sum_{l=0}^{\infty} (-i)^l (2l+1)\, P_l(\cos\theta)\left(\frac{r}{k}\right)^l \left(\frac{1}{r}\frac{d}{dr}\right)^l \frac{\sin kr}{kr}$$

$$\overset{r\to\infty}{\simeq} \frac{1}{kr}\sum_{l=0}^{\infty} i^l\,(2l+1)\, P_l(\cos\theta)\,\sin\left(kr - \tfrac{1}{2}l\pi\right)$$

$$= \frac{1}{2ikr}\sum_{l=0}^{\infty} i^l\,(2l+1)\,P_l(\cos\theta)\left[e^{ikr}e^{-\frac{il\pi}{2}} - e^{-ikr}e^{\frac{il\pi}{2}}\right]$$

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

$$= \frac{1}{2ikr} \sum_{l=0}^{\infty} (2l+1) P_l(\cos\theta) \left[e^{ikr} + (-1)^{l+1} e^{-ikr} \right]$$

Thus it follows that

$$-\frac{A_l}{i} e^{-i\alpha_l} = \frac{1}{2ik} \cdot (2l+1) \cdot (-1)^{l+1}$$

So $A_l = \frac{1}{2k} (-1)^l (2l+1)\, e^{i\alpha_l}$

Historically it is common to define

$$\alpha_l = \delta_l - \tfrac{1}{2} l\pi$$

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

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

Now we also must have:

$$\sum_l P_l(\cos\theta) \frac{A_l}{i} e^{i\alpha_l} = \sum_l \frac{1}{2ik} (2l+1) P_l(\cos\theta) + f(\theta)$$

So $f(\theta) = \sum_l \left\{ \frac{1}{2ik} \left(2k A_l e^{i\delta_l} (-i)^l - (2l+1) \right) P_l(\cos\theta) \right\}$

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

We see that the scattering ~~amplitude~~ $|f(\theta)|^2$ ~~cross-section, which is completely determined by $f(\theta)$~~, is entirely determined if we know the δ_ℓ. The δ_ℓ are angle-valued numbers called the phase shifts.

We can also define the total cross-section σ as

$$\sigma = 2\pi \int_0^{\pi} \sin\theta \, |f(\theta)|^2 \, d\theta$$

$$= \sum_{\ell,\ell'} \left[\frac{2\pi}{(2k)^2} \left(e^{2i\delta_\ell} - 1\right)\left(e^{2i\delta_{\ell'}} - 1\right) (2\ell+1)(2\ell'+1) \int_0^{\pi} \underbrace{P_\ell(\cos\theta) P_{\ell'}(\cos\theta) \sin\theta \, d\theta}_{\frac{2\delta_{\ell\ell'}}{2\ell+1}} \right]$$

$$= \frac{2\pi}{(2k)^2} \sum_{\ell=0}^{\infty} \left| e^{2i\delta_\ell} - 1 \right|^2 2(2\ell+1)$$

$$= \frac{\pi}{k^2} \sum_{\ell=0}^{\infty} 4 \sin^2\delta_\ell \, (2\ell+1)$$

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

Clearly if all $\delta_\ell = 0$ then $\sigma = 0$. Moreover each term is the "partial cross-section" for the scattering of particles with orbital angular momentum ℓ.

The partial "scattering amplitudes" f_l defined from

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

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

are $f_l = \dfrac{e^{2i\delta_l}-1}{2ik}$

and we have

$$\sigma_l = 4\pi(2l+1)|f_l|^2 .$$

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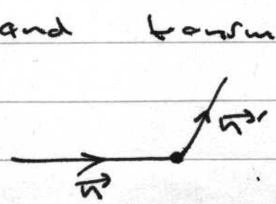
<u>Unitarity & S-Matrix</u>

Suppose the potential V is not central, $V = V(r,\theta,\varphi)$. We can define the scattering process by two unit vectors $\vec{n}, \vec{n}'$ along the direction of incidence and transmission:



Far from the scattering centre,

$$\psi \sim e^{ikr\vec{n}\cdot\vec{n}'} + f(\vec{n},\vec{n}')\frac{e^{ikr}}{r}$$

Any linear combination of these functions with a weight factor $F(\vec{n}')$ also represents a possible scattering process.

Thus we have

$$\int F(\vec{n})\, e^{ikr\vec{n}\cdot\vec{n}'} d\Omega + \frac{e^{ikr}}{r}\int F(\vec{n}) f(\vec{n},\vec{n}')\, d\Omega$$

For large r, the first term is a rapidly oscillating fn. of $\vec{n}$. The largest contribution comes from the values $\vec{n}\cdot\vec{n}' = \pm 1$, ie $\vec{n} = \pm\vec{n}'$. In each of these regions, $F(\vec{n}) \simeq F(\pm\vec{n}')$. ~~and we have~~

$$F(\vec{n}')\int e^{ikr\cos\theta} d\Omega + F(-\vec{n}')\int e^{-ikr\cos\theta} d\Omega$$

$$+ \frac{e^{ikr}}{r}\int F(\vec{n}) f(\vec{n},\vec{n}')\, d\Omega$$

Now
$$\int e^{ikr\cos\theta} d\Omega = -2\pi\int_0^{\pi} e^{ikr\cos\theta} d(\cos\theta)$$

$$= -2\pi\left[\frac{e^{ikr\cos\theta}}{ikr}\right]_{\cos\theta = 1}^{\cos\theta = -1}$$

$$= \frac{-2\pi}{ikr}\left(e^{-ikr} - e^{ikr}\right)$$

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

At these two end-points, $F(\vec{n})$ is $F(-\vec{n}')$ and $F(\vec{n}')$ respectively. Thus,

$$\int F(\vec{n})\, e^{ikr\vec{n}\cdot\vec{n}'} d\Omega \simeq \frac{2\pi i}{kr}\left(F(-\vec{n}')e^{-ikr} - F(\vec{n}')e^{ikr}\right)$$

Thus the asymptote wave fn. is:

$$\frac{2\pi i}{k}\left\{ \frac{e^{-ikr}}{r} F(-\vec{n}') - \frac{e^{ikr}}{r} F(\vec{n}') - \frac{ik}{2\pi}\frac{e^{ikr}}{r}\int F(\vec{n}) f(\vec{n},\vec{n}')\, d\Omega \right.$$

Dropping the factor $\frac{2\pi i}{k}$, we have:

$$\psi \sim \frac{e^{-ikr}}{r} F(-\vec{n}') - \frac{e^{ikr}}{r}\left(1 + 2ik\hat{f}\right) F(\vec{n}')$$

where
$$\hat{f}\, F(\vec{n}') = \frac{1}{4\pi}\int f(\vec{n},\vec{n}')\, F(\vec{n})\, d\Omega$$

Define $1 + 2ik\hat{f} = \hat{S}$, then

$$\psi \sim \frac{e^{-ikr}}{r} F(-\vec{n}') - \frac{e^{ikr}}{r} \hat{S}\, F(\vec{n}')$$

The operator $\hat{S}$ is called the scattering matrix or S-matrix. It expresses the proportion of ingoing to outgoing wave at the scattering centre. Conservation of probability requires that

$$\hat{S}\hat{S}^{+} = 1 \quad \text{viz}$$

Equivalently,
$$(1 + 2ik\hat{f})(1 - 2ik\hat{f}^{+}) = 1$$

$$\rightarrow \quad 2ik(\hat{f} - \hat{f}^{+}) = -4k^2 \hat{f}\hat{f}^{+}$$

or
$$\hat{f} - \hat{f}^{+} = 2ik\, \hat{f}\hat{f}^{+}$$

From the definition, this is:

$$f(\vec{n},\vec{n}') - f^{*}(\vec{n}',\vec{n}) = \frac{ik}{2\pi}\int f(\vec{n},\vec{n}'')\, f^{*}(\vec{n}',\vec{n}'')\, d\Omega''$$

For the special case $\vec{n} = \vec{n}'$, the RHS is

$$\int |f(\vec{n}, \vec{n}'')|^2 \, d\Omega'' = \sigma$$

the total scattering cross-section. The LHS is

$$f(\vec{n}, \vec{n}) - f^*(\vec{n}, \vec{n}) = 2i \, \mathrm{Im} \, f(\vec{n}, \vec{n})$$

Thus

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

This is called the <u>optical theorem</u>, and says that the imaginary part of the for<u>ward</u> scattering amplitude is proportional to the total cross-section.