Potential scattering and The Born approximation

let us consider a finite Potential $V(\vec{r})$; $V \to 0$ as $r \to \infty$, then the schrodinger equation reads

$$H\psi = E\psi \Rightarrow \left[\frac{p^2}{2m} + V(\vec{r})\right]\psi(\vec{r}) = E\,\psi(\vec{r}) \quad ; \quad \vec{p} = -i\hbar\vec{\nabla}$$

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

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

inhomogeneous 2^{nd} order diff equation with $k^2 = \frac{2mE}{\hbar^2}$

here we are concerned with elastic scattering, where energy is conserved.

so we need to solve the above eq^n for $E > 0$ (scattering solution). the solution can be written as

$$\psi(\vec{r}) = \underbrace{e^{i\vec{k}\cdot\vec{r}}}_{\text{incident wave}} + \underbrace{\tilde{\psi}(\vec{r})}_{\text{scattered wave}}$$

, where $\tilde{\psi}(\vec{r}) \approx f(\vec{k},\vec{k}')\,\frac{e^{ikr}}{r}$ as $r \to \infty$

substitute the last solution into the schrodinger eq^n yields

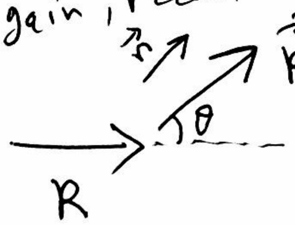
$$(\nabla^2 + k^2)\,\tilde{\psi}(\vec{r}) = \frac{2m}{\hbar^2}V(\vec{r})\,\psi(\vec{r}) \quad \text{---}(*)$$

; where $(\nabla^2 + k^2)\,e^{i\vec{k}\cdot\vec{r}} = 0$

the last eq^n has the form of Helmholtz equation, it can be solved with the help of Green's functions.

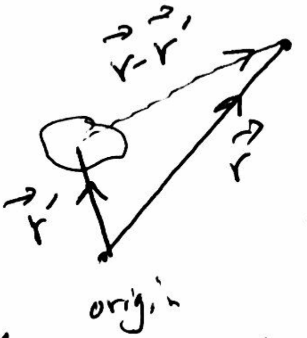
Again, recall that for elastic scattering

$\vec{k}' = \vec{k}\cdot\vec{n} = \vec{k}\cdot\frac{\vec{r}}{r}$; with $|\vec{k}'| = |\vec{k}|$



let us assume that our source (target) is localized at $\vec{r}'$ and we need to find $\tilde{\psi}$ at point $\vec{r}$

when $r \gg r'$



Claim $\tilde{\psi}(\vec{r}) = \frac{-m}{2\pi\hbar^2}\int d^3\vec{r}'\, G(\vec{r},\vec{r}')\, V(\vec{r}')\, \psi(\vec{r}')$

where the Green's function $G(\vec{r},\vec{r}')$ satisfy the point-source equation $(\nabla^2+k^2)\, G(\vec{r},\vec{r}') = -4\pi\, \delta(\vec{r}-\vec{r}')$

free motion everywhere except at $\vec{r}=\vec{r}'$

let us check that $\tilde{\psi}(\vec{r})$ satisfy the schrodinger eq^n (*).

$$(\nabla_r^2+k^2)\,\tilde{\psi}(\vec{r}) = \frac{-m}{2\pi\hbar^2}\int d^3\vec{r}'\, (\nabla_r^2+k^2)\, G(\vec{r},\vec{r}')\, V(\vec{r}')\, \psi(\vec{r}')$$

$$= \frac{-m}{2\pi\hbar^2}\int d^3\vec{r}'\, (-4\pi\, \delta(\vec{r}-\vec{r}'))\, V(\vec{r}')\, \psi(\vec{r}')$$

$$= \frac{2m}{\hbar^2}\, V(\vec{r})\, \psi(\vec{r}) \quad \text{as expected.}$$

$\Rightarrow$ the total wave function $\psi(\vec{r})$ is given by

$$\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} + \tilde{\psi}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{m}{2\pi\hbar^2}\int d^3\vec{r}'\, G(\vec{r},\vec{r}')\, V(\vec{r}')\, \psi(\vec{r}')$$

This an integral eq^n equivalent to schrodinger eq^n

now what is $G(\vec{r},\vec{r}')$??

let us put the source at the origin for a moment $(\vec{r}'=0)$

$\Rightarrow (\nabla^2+k^2)\, G(r,0) = -4\pi\, \delta(r)$

if $r \neq 0 \Rightarrow G_{\pm}(r,0) = \frac{e^{\pm ikr}}{r}$ + outgoing spher. wave

− incoming " "

let us focus on the outgoing spherical wave solution G_+

$$G_+ = \text{shortly} = G(r,0) = \frac{e^{ikr}}{r}$$

let us check to see that it satisfies $(\nabla^2+k^2)G = 0$; for $r \neq 0$

$$\nabla_r^2 = \frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} \quad \text{in spherical}$$

$$\frac{d}{dr} G(r,0) = \frac{ik}{r} e^{ikr} - \frac{1}{r^2} e^{ikr}$$

$$\frac{d^2}{dr^2} G(r,0) = \frac{(ik)^2}{r} e^{ikr} - \frac{2ik}{r^2} e^{ikr} + \frac{2}{r^3} e^{ikr}$$

$$\Rightarrow \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) G(r,0) = \frac{(ik)^2}{r} e^{ikr} \cancel{- \frac{2ik}{r^2} e^{ikr}} \cancel{+ \frac{2}{r^3} e^{ikr}} \cancel{+ \frac{2ik}{r} e^{ikr}} \cancel{- \frac{2}{r^3} e^{ikr}}$$

$$= -\frac{k^2}{r} e^{ikr}$$

$$\Rightarrow (\nabla^2 + k^2) G = -\frac{k^2}{r} e^{ikr} + k^2 \frac{e^{ikr}}{r} = 0 \quad \checkmark$$

in textbook, it is written as $G(\vec{r}-\vec{r}')$

$$\text{so} \quad G(r,0) = \frac{e^{ikr}}{r}$$

$$\text{so by induction} \quad G(\vec{r},\vec{r}') = \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \quad \text{outgoing}$$

$$\therefore \psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} - \frac{m}{2\pi\hbar^2} \int d^3\vec{r}'\, G(\vec{r},\vec{r}')\, V(\vec{r}')\, \psi(\vec{r}') \quad \text{---} \ (**)$$

Notice that ψ appears on both sides of the equation. this equation can be solved approximately by iterative approximations, known as Born approximation

- the zeroth solution is $\psi_0(\vec{r}) = e^{i\vec{k}.\vec{r}}$
- the first order solution $\psi_1(\vec{r})$ is obtained by inserting $\psi_0(\vec{r}) = e^{i\vec{k}.\vec{r}}$ into the integrand (i.e $\psi(\vec{r}') = e^{i\vec{k}.\vec{r}'}$)

$$\Rightarrow \psi_1(\vec{r}) = e^{i\vec{k}.\vec{r}} - \frac{m}{2\pi\hbar^2}\int d^3\vec{r}' \, \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') e^{i\vec{k}.\vec{r}'}$$

- the second order solution is obtained by inserting $\psi_1(\vec{r})$ into the integrand

$$\psi_2(\vec{r}) = e^{i\vec{k}.\vec{r}} - \frac{m}{2\pi\hbar^2}\int d^3\vec{r}'' \, \frac{e^{ik|\vec{r}-\vec{r}''|}}{|\vec{r}-\vec{r}''|} V(\vec{r}'')\, \psi_1(\vec{r}'')$$

$$= e^{i\vec{k}.\vec{r}} - \frac{m}{2\pi\hbar^2}\int d^3\vec{r}'' \, \frac{e^{ik|\vec{r}-\vec{r}''|}}{|\vec{r}-\vec{r}''|} V(\vec{r}'') \left[e^{i\vec{k}.\vec{r}''} - \frac{m}{2\pi\hbar^2}\int d^3 r' \, \frac{e^{ik|\vec{r}''-\vec{r}'|}}{|\vec{r}''-\vec{r}'|} V(\vec{r}') \underbrace{e^{i\vec{k}.\vec{r}}}_{e^{i\vec{k}.\vec{r}'}} \right]$$

$$= e^{i\vec{k}.\vec{r}} - \frac{m}{2\pi\hbar^2}\int d^3 r'' \, \frac{e^{ik|\vec{r}-\vec{r}''|}}{|\vec{r}-\vec{r}''|} V(\vec{r}'') e^{i\vec{k}.\vec{r}''}$$

$$+ \left(\frac{m}{2\pi\hbar^2}\right)^2 \int d^3 r'' \, \frac{e^{ik|\vec{r}-\vec{r}''|}}{|\vec{r}-\vec{r}''|} V(\vec{r}'') \int d^3 r' \, \frac{e^{ik|r''-r'|}}{|r''-r'|} V(\vec{r}') e^{i\vec{k}.\vec{r}'}$$

and so on.

let us now check that our solution (eq^n ★★) reduces to $\psi(\vec{r}) = e^{i\vec{k}.\vec{r}} + f(\theta,\phi)\frac{e^{ikr}}{r}$ for large values of r. in a typical scattering experiment, the detector is located at a distance r from the target that is much larger than the size of the target (r') i.e $r \gg r'$, then we may approximate $|\vec{r}-\vec{r}'|$ as follows

$$(\vec{r}-\vec{r}')^2 = (\vec{r}-\vec{r}')\cdot(\vec{r}-\vec{r}') = r^2 - 2\vec{r}\cdot\vec{r}' + r'^2$$

$$\Rightarrow |\vec{r}-\vec{r}'| = \sqrt{r^2 - 2\vec{r}\cdot\vec{r}' + r'^2} \approx \sqrt{r^2 - 2\vec{r}\cdot\vec{r}'} \quad ; \text{ as } r \gg r'$$

$$\approx r\sqrt{1 - \frac{2\vec{r}\cdot\vec{r}'}{r}} = r\left(1 - \frac{2\vec{r}\cdot\vec{r}'}{r}\right)^{1/2} \approx r\left(1 - \frac{\vec{r}\cdot\vec{r}'}{r^2}\right)$$

$$= r - \frac{\vec{r}}{r}\cdot\vec{r}' = r - \vec{n}\cdot\vec{r}' \quad ; \vec{n} \text{ is a unit vector along}$$

the observation point (detector)

$$\Rightarrow G(\vec{r},\vec{r}') = \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \approx \frac{1}{r} e^{ik(r - \vec{n}\cdot\vec{r}')} = \frac{e^{ikr}}{r} e^{-ik\vec{n}\cdot\vec{r}'}$$

$$= \frac{e^{ikr}}{r} e^{-i\vec{k}'\cdot\vec{r}'} \quad ; \text{ when } \vec{k}' = k\vec{n} = k\cdot\vec{n}$$

to check take $r' = 0 \Rightarrow G(r,0) = \frac{e^{ikr}}{r}$

so for $r \gg R$, we have

$$\Psi(\vec{r}) \approx e^{i\vec{k}\cdot\vec{r}} - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3r'\, e^{-i\vec{k}'\cdot\vec{r}'} V(\vec{r}')\Psi(\vec{r}')$$

comparing this result with $\Psi(\vec{r}) \approx e^{i\vec{k}\cdot\vec{r}} + f(\vec{k},\vec{k}')\frac{e^{ikr}}{r}$

we found for $f(\vec{k},\vec{k}') = f(\theta,\phi)$

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

for 1st Born approximation (single scattering) $\Psi(\vec{r}') = e^{i\vec{k}\cdot\vec{r}'}$

$$f(\vec{k}',\vec{k}) = \frac{-m}{2\pi\hbar^2}\int d^3r'\, e^{i(\vec{k}-\vec{k}')\cdot\vec{r}'} V(\vec{r}') \quad , \text{ rename } \vec{r}' \to \vec{r}$$

r' is dummy

$$= -\frac{m}{2\pi\hbar^2}\underbrace{\int d^3r\, e^{i\vec{q}\cdot\vec{r}} V(\vec{r})}_{V_q} \quad ; \quad \vec{q} = \vec{k} - \vec{k}'$$

$\hookrightarrow$ transfer momentum

$$= \frac{-m}{2\pi\hbar^2} V_q$$

Now $\frac{d\sigma}{d\Omega} = |f(\vec{k},\vec{k}')|^2 = \left(\frac{m}{2\pi\hbar^2}\right)^2 |V_q|^2$

when $V_q = \int d^3r \, e^{i\vec{q}\cdot\vec{r}} V(\vec{r})$

for elastic scattering, what is $|q|$; $|k'| = |k|$

$\vec{q} = \vec{k} - \vec{k}' \Rightarrow q^2 = k^2 + k'^2 - 2\vec{k}\cdot\vec{k}' = 2k^2 - 2k^2\cos\theta$

$= 2k^2(1-\cos\theta) = 4k^2\sin^2\frac{\theta}{2}$

$$\Rightarrow \boxed{q = 2k\sin\frac{\theta}{2}}$$

- now for spherically symmetric potential $V(\vec{r}) = V(r)$

$V_q = \cancel{\int d\Omega\, e^{i}} = \int d^3r \, e^{i\vec{q}\cdot\vec{r}} V(\vec{r}) = \int d\Omega\, r^2 dr \, e^{iqr\cos\alpha} V(r)$

; when $d\Omega = \sin\alpha \, d\alpha \, d\phi$

$= 2\pi \int \sin\alpha \, d\alpha \, e^{iqr\cos\alpha} r^2 dr \, V(r)$

we use α as θ was preserved for the scattering angle

$= 2\pi \int_0^\infty r^2 dr \, V(r) \underbrace{\int_0^\pi d\alpha \sin\alpha \, e^{iqr\cos\alpha}}$

Now let $t = \cos\alpha \Rightarrow dt = -\sin\alpha \, d\alpha$

$\int_0^\pi d\alpha \sin\alpha \, e^{iqr\cos\alpha} = -\int_1^{-1} dt \, e^{iqrt} = \int_{-1}^{1} dt \, e^{iqrt} = \frac{1}{iqr}\left(e^{iqr} - e^{-iqr}\right)$

$= \frac{2i\sin qr}{iqr}$

$= \frac{2}{qr}\sin qr$

$\Rightarrow V_q = \frac{4\pi}{q}\int_0^\infty dr \, r\, V(r) \sin(qr)$

$\Rightarrow \frac{d\sigma}{d\Omega} = \left(\frac{m}{2\pi\hbar^2}\right)^2 |V_q|^2 = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left|\frac{4\pi}{q}\int_0^\infty dr \, r\, V(r)\sin qr\right|^2$

$\equiv |f(q)|^2$

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

let $w = q^2 = 4k^2 \sin^2\frac{\theta}{2} \Rightarrow dw = 8k^2 \sin\frac{\theta}{2}\cos\frac{\theta}{2} \cdot \frac{1}{2}\, d\theta$

$$= 4k^2\left(\sin\tfrac{\theta}{2}\cos\tfrac{\theta}{2}\right) d\theta$$

$$\Rightarrow \sigma = \frac{\pi}{k^2}\int_0^{4k^2} dw \, |f(q)|^2 \qquad = 4k^2\left(\tfrac{1}{2}\sin\theta\right) d\theta$$

$$= 2k^2 \sin\theta \, d\theta$$

– Validity of the first Born approximation!

the first Born approximation is valid whenever $\psi(\vec r)$ is only slightly different from the incident plane wave i.e

$$\left| \frac{m}{2\pi\hbar^2}\int d^3\vec r' \, V(\vec r') \, \frac{e^{ik|\vec r - \vec r'|}}{|\vec r - \vec r'|} \, e^{i\vec k\cdot\vec r'} \right| \ll \left| e^{i\vec k\cdot\vec r} \right| = 1$$

for simplicity, let us take $r = 0$

$$\Rightarrow \frac{m}{2\pi\hbar^2}\left| \int d^3\vec r' \, V(\vec r') \, \frac{e^{ikr' + i\vec k\cdot\vec r'}}{|r'|} \right| \ll 1$$

let $\vec r' \to \vec r$

$$\frac{m}{2\pi\hbar^2}\left| \int d^3\vec r \, V(\vec r) \, \frac{e^{ikr + i\vec k\cdot\vec r}}{|\vec r|} \right| \ll 1$$

$\hookrightarrow$ over the size of potential typically $\int_0^R$

let us look at the Born approximation at both low and high energy limits for a finite potential of size $\underline{\underline{R}}$

for central potential $\frac{2m}{\hbar^2}\left| \int r^2 dr \, V(r) \, \frac{e^{ikr + i\vec k\cdot\vec r}}{r} \right| \ll 1$

when $d^3\vec r = r^2 dr \, d\Omega$

$$\Rightarrow \frac{2m}{\hbar^2}\left|\int r\,dr\, V(r)\, e^{ikr + i\vec{k}\cdot\vec{r}}\right| \ll 1$$

c) low energy limit (long wavelength limit); $kR \ll 1$

$R \ll \frac{1}{k} \sim \lambda$

$e^{ikr + i\vec{k}\cdot\vec{r}} \longrightarrow 1$

$R \ll \lambda$

$$\Rightarrow \frac{2m}{\hbar^2}\left|\int dr\; r\, V(r)\right| \ll 1$$

and smoothly

if $V(r)$ varies slowly over the potential range, we can average i.e as $\bar{V}$

$$\Rightarrow \frac{2m}{\hbar^2}\bar{V}\int_0^R r\,dr \ll 1 \Rightarrow \frac{2m}{\hbar^2}\bar{V}\frac{R^2}{2} \ll 1$$

$$\frac{\bar{V}}{\left(\hbar^2/mR^2\right)} \ll 1 \Rightarrow \frac{\bar{V}}{\bar{K}} \ll 1 \;;\; \bar{K}: \text{average kinetic energy.}$$

$\downarrow$

Recall Particle in a box

$\Delta r = R$

$\Delta p = \frac{\hbar}{R}$

$\Rightarrow \bar{K} = \frac{(\Delta p)^2}{2m} = \frac{\hbar^2}{2mR^2}$

$\therefore \frac{\bar{V}}{\bar{K}} \equiv \beta \ll 1$

the potential is weak relative to the particles' kinetic energy:

cc) high energy limit (short wavelength limit)

$kR \gg 1 \Rightarrow R \gg \frac{1}{k} \Rightarrow R \gg \lambda$

$$\frac{m}{2\pi\hbar^2}\left|\int_0^R d^3\vec{r}\; V(\vec{r})\,\frac{e^{ikr + i\vec{k}\cdot\vec{r}}}{|\vec{r}|}\right| \ll 1$$

$$\frac{m}{2\pi\hbar^2}\left|\int r^2 dr\,\frac{V(r)}{r}\; e^{ikr}\int d\Omega\, e^{i\vec{k}\cdot\vec{r}}\right| \ll 1$$

Now $\int d\Omega\, e^{i\vec{k}\cdot\vec{r}} = \int d\Omega\, e^{ikr\cos\alpha} = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\alpha\, d\alpha\, e^{ikr\cos\alpha} = \frac{2\pi}{ikr}\left(e^{ikr} - e^{-ikr}\right)$

$$\Rightarrow \frac{m}{\hbar^2 k}\left|\int_0^R dr\, V(r)\,\left(e^{2ikr}-1\right)\right| \ll 1$$

Very fast oscillating term $\ll 1$ can be neglected by stationary phase method

$$\Rightarrow \frac{m}{\hbar^2 k}\left|\int_0^R dr\, V(r)\right| \ll 1$$

$$\therefore \boxed{\frac{m}{\hbar^2 k}\left|\int_0^R dr\, V(r)\right| \ll 1}$$

if $V(r)$ varies slowly $\Rightarrow$ $V(r) \to \bar{V}$

$$\frac{m R \bar{V}}{k\hbar^2} \ll 1 \Rightarrow \frac{m \bar{V} R^2}{kR\hbar^2} \ll 1 \Rightarrow \frac{\bar{V}}{kR\left(\hbar^2/mR^2\right)} \ll 1$$

$$\Rightarrow \frac{\bar{V}}{kR\bar{T}} \ll 1 \Rightarrow \frac{\bar{V}}{\bar{T}} \ll \underbrace{kR}_{\eta} \Rightarrow \frac{\bar{V}}{\bar{T}} \ll \eta$$

$$\beta \ll \eta$$

$\therefore$ $\underline{\eta = kR}$

$\eta \ll 1$ $\longrightarrow$ $\eta \gg 1$

β low energy limit $\beta \ll 1$

high energy limit $1 \ll \beta \ll \eta$