Scattering Theory:

The Lippmann – Schwinger Equation:

Start with time-independent formulation of scattering process.

let $H = H_0 + V$

where $H_0 = \frac{p^2}{2m}$: kinetic energy operator.

If no scatterer, $V=0$, and we just have free particle.

let $|\phi\rangle$ be the eigenstate of kinetic energy

$$H_0|\phi\rangle = E|\phi\rangle$$

let $|\psi\rangle$ be the eigenstate of full Hamiltonian, $H = H_0 + V$ of the same eigenenergy E:

$$(H_0 + V)|\psi\rangle = E|\psi\rangle$$

look for solution such that $V \to 0$, $|\psi\rangle \to |\phi\rangle$

we argue:

$$\boxed{|\psi\rangle = \frac{V}{E - H_0}|\psi\rangle + |\phi\rangle}$$

ignore singularity of $\frac{1}{E-H_0}$

note by applying $(E - H_0)$

$$(E - H_0)|\psi\rangle = V|\psi\rangle + (E - H_0)|\phi\rangle$$

$$\hookrightarrow (H_0 + V)|\psi\rangle = E|\psi\rangle$$

To deal with singularity, make the solution slightly complex:

$$\boxed{|\psi^{(\pm)}\rangle = |\phi\rangle + \frac{1}{E-H_0 \pm i\varepsilon} V |\psi^{(\pm)}\rangle}$$

← Lippmann - Schwinger equation.

Physical meaning of $\pm$ is to be discussed by looking at $\langle x|\psi^{(\pm)}\rangle$ at large distances:

$$\langle \vec{x}|\psi^{(\pm)}\rangle = \langle \vec{x}|\phi\rangle + \int d^3x' \langle \vec{x}| \frac{1}{E-H_0 \pm i\varepsilon} |\vec{x}'\rangle \langle x'| V |\psi^{(\pm)}\rangle$$

if $|\phi\rangle$ is a plane-wave solution:

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

since free-particle wave function is not normalizable:

choose such that $\int d^3x \langle \vec{p}'|\vec{x}\rangle\langle \vec{x}|\vec{p}\rangle = \delta^{(3)}(\vec{p}-\vec{p}')$

In momentum space-representation, we have:

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

Returning to position basis:

let $$G_\pm(\vec{x},\vec{x}') = \frac{\hbar^2}{2m}\langle\vec{x}|\frac{1}{E-H_0\pm i\varepsilon}|\vec{x}'\rangle$$

claim

$$= -\frac{1}{4\pi}\frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{|\vec{x}-\vec{x}'|}$$

To prove the result above:

Using $E=\frac{\hbar^2k^2}{2m}$

then $$\frac{\hbar^2}{2m}\langle\vec{x}|\frac{1}{E-H_0\pm i\varepsilon}|\vec{x}'\rangle = \frac{\hbar^2}{2m}\int d^3p'\int d^3p''\,\langle x|p'\rangle$$

$$\times\langle p'|\frac{1}{E-\left(\frac{p'^2}{2m}\right)\pm i\varepsilon}|p''\rangle\langle p''|x\rangle$$

since H_0 acts on $\langle\vec{p}'|$, now use:

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

② $$\langle x|p'\rangle = \frac{e^{ip'\cdot x/\hbar}}{(2\pi\hbar)^{3/2}}$$

③ $$\langle p''|x'\rangle = \frac{e^{-ip'\cdot x'/\hbar}}{(2\pi\hbar)^{3/2}}$$

then the integral becomes:

$$\frac{\hbar^2}{2m}\int \frac{d^3p'}{(2\pi\hbar)^3} \frac{e^{ip'\cdot(x-x')/\hbar}}{E-\left(\frac{p'^2}{2m}\right)\pm i\varepsilon}$$

by using $E = \frac{\hbar^2 k^2}{2m}$ and $\vec{p}' = \hbar\vec{q}$

then

$$\frac{1}{(2\pi)^3}\int_0^\infty q^2 dq \int_0^{2\pi} d\phi \int_{-1}^{+1} d(\cos\theta)\, \frac{e^{i|\vec{q}||\vec{x}-\vec{x}'|\cos\theta}}{k^2-q^2\pm i\varepsilon}$$

$$= \frac{-1}{8\pi^2}\frac{1}{i|\vec{x}-\vec{x}'|}\int_{-\infty}^{\infty} dq\, \frac{q\left(e^{iq|\vec{x}-\vec{x}'|}-e^{-iq|\vec{x}-\vec{x}'|}\right)}{q^2-k^2\mp i\varepsilon}$$

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

note that $G_\pm(\vec{x},\vec{x}')$ is just the Green's function for Helmholtz equation:

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

$$\boxed{\text{Now the position representation of } |\psi^{(\pm)}\rangle \text{ is}}$$

Now the position representation of $|\psi^{(\pm)}\rangle$ is

$$\langle\vec{x}|\psi^{(\pm)}\rangle = \underbrace{\langle x|\phi\rangle}_{\text{sum of incident wave}} - \underbrace{\frac{2m}{\hbar^2}\int d^3x'\, \frac{e^{\pm ik|\vec{x}-\vec{x}'|}}{4\pi\,|\vec{x}-\vec{x}'|}\langle x'|V|\psi^{(\pm)}\rangle}_{\text{the effect of scattering}}$$

reduces to $\frac{e^{\pm ikr}}{r}$ at large distances let's consider V to be local, so there is only a potential diagonal, i.e.

$$\langle x' | V | x'' \rangle = V(x')\, \delta^{(3)}(x' - x'')$$

as a result:

$$\langle x' | V | \psi^{(\pm)} \rangle = \int d^3x'' \langle x' | V | x'' \rangle \langle x'' | \psi^{(\pm)} \rangle$$
$$\overset{!}{=} V(x') \langle x' | \psi^{(\pm)} \rangle$$

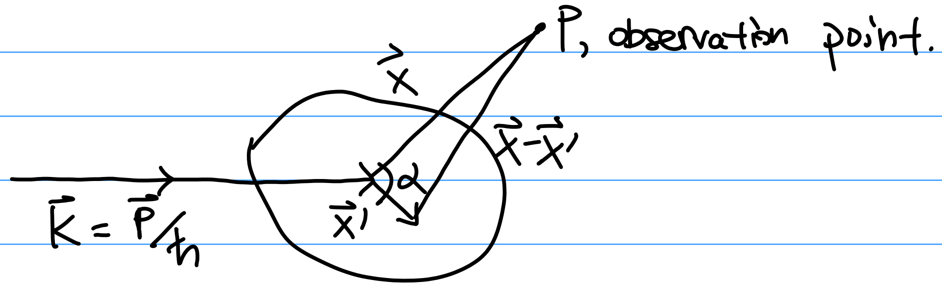
then the space representation becomes:

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

Since the detector is always much further away from scatterer, which is much further from the potential:

$$|\vec{x}| \gg |\vec{x}'|$$

then introduce $r = |\vec{x}|$ and $r' = |\vec{x}'|$



since $r \gg r'$

$$|\vec{x}-\vec{x}'| = \sqrt{r^2-2rr'\cos\alpha+r'^2}$$
$$= r\left(1-\frac{2r'}{r}\cos\alpha+\left(\frac{r'}{r}\right)^2\right)^{1/2}$$
$$\approx r-\hat{r}\cdot\vec{x}' \qquad \text{wher} \quad \hat{r}\equiv\frac{\vec{x}}{|\vec{x}|}$$

define $\vec{k}'\equiv k\hat{r}$, let $\vec{k}'$ represent the propagation vector for waves to reach point $\vec{x}$.

$$e^{\pm ik|\vec{x}-\vec{x}'|} \simeq e^{\pm ikr}\, e^{\mp i\vec{k}'\cdot\vec{x}'} \qquad \text{for large } r.$$

So we replace $\frac{1}{|\vec{x}-\vec{x}'|} = \frac{1}{r}$

and let $|\vec{k}\rangle \to |\vec{p}\rangle$ to get rid of $\hbar$ where $\vec{k}=\frac{\vec{p}}{\hbar}$

since $\langle\vec{k}|\vec{k}'\rangle = \delta^{(3)}(\vec{k}-\vec{k}')$

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

Finally:

$$\langle x|\psi^{(+)}\rangle \xrightarrow{r\text{ is large}} \langle x|\vec{k}\rangle - \frac{1}{4\pi}\frac{2m}{\hbar^2}\frac{e^{ikr}}{r}\int d^3x'\, e^{-i\vec{k}'\cdot x'}\, V(\vec{x}')\langle\vec{x}'|\psi^{(+)}\rangle$$

$$\boxed{\langle x|\psi^{(+)}\rangle \doteq \frac{1}{(2\pi)^{3/2}}\left[e^{i\vec{k}\cdot\vec{x}} + \frac{e^{ikr}}{r} f(\vec{k}',\vec{k})\right]}$$

At large distance.

$$\boxed{\begin{aligned}&\underline{\text{given}}: \\ &f(\vec{k}', \vec{k}) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}(2\pi)^3\int d^3x' \frac{e^{-i\vec{k}'\cdot\vec{x}'}}{(2\pi)^{3/2}} V(\vec{x}')\langle\vec{x}'|\psi^{(+)}\rangle \\ &\qquad = -\frac{1}{4\pi}(2\pi)^3\frac{2m}{\hbar^2}\langle\vec{k}'|V|\psi^{(+)}\rangle\end{aligned}}$$

Differential cross-section : $d\sigma/d\Omega$

$$\frac{d\sigma}{d\Omega}d\Omega = \frac{\text{number of particles scattered into } d\Omega \text{ per unit time}}{\text{number of incident particles crossing unit area per unit time}}$$

$$= \frac{r^2|\vec{J}_{scatter}|\,d\Omega}{|\vec{J}_{incident}|}$$

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

so $\boxed{\dfrac{d\sigma}{d\Omega} = |f(\vec{k}, \vec{k}')|^2}$

Born - Approximation

→ To determine $\langle x|\psi^+\rangle$, we mainly just need to evaluate $f(\vec{k},\vec{k}')$:

→ The original expression can be simplified if the effect of scattering is not strong.

First - Order Born - Approximation: $\langle x'|\psi^+\rangle \to \langle x'|\phi\rangle = \frac{e^{i\vec{k}\cdot\vec{x}'}}{(2\pi)^{3/2}}$

Treating V to first order:

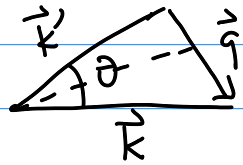
First-order Born-Approximation in general potential

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

let $\vec{q} = \vec{k}-\vec{k}'$ $\quad\to\quad q = |\vec{k}-\vec{k}'| = \sqrt{(\vec{k}-\vec{k}')\cdot(\vec{k}-\vec{k}')}$

$$= (k^2+k'^2-2\vec{k}\cdot\vec{k}')^{1/2}$$

$$= 2k\sin\frac{\theta}{2}$$



and if spherical-symmetric potential, then $V(|\vec{k}-\vec{k}'|) = V(q)$

$$\hookrightarrow f^{(1)}(\theta) = -\frac{1}{2}\frac{2m}{\hbar^2}\frac{1}{iq}\int_0^\infty \frac{r^2}{r}V(r)\left(e^{iqr}-e^{-iqr}\right)dr$$

*
$$\boxed{f^{(1)}(\theta) = -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^\infty r V(r)\sin qr\, dr}$$

First order Born-Approximation with spherical-symmetric potential

$$\boxed{\begin{aligned}&\text{Note } q = |\vec{k}-\vec{k}'| = 2k\sin\frac{\theta}{2}\\ &q^2 = 4k^2\sin^2\frac{\theta}{2} = 2k^2(1-\cos\theta)\end{aligned}}$$

Ex: $V(r) = \frac{V_0 e^{-ur}}{ur}$ $\Rightarrow$ Notice $V \to 0$ as $r \gg \frac{1}{u}$

Using Born-Approximation

$$f^{(1)}(\theta) = -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^\infty r\, V(r) \sin qr\, dr$$

$$= -\frac{2m}{\hbar^2}\frac{1}{q}\underbrace{\int_0^\infty \cancel{r}\, \frac{V_0 e^{-ur}}{u\cancel{r}} \sin qr\, dr}_{= \frac{V_0}{qu}\frac{q}{q^2+u^2}}$$

$$= -\left(\frac{2mV_0}{u\hbar^2}\right)\frac{1}{q^2+u^2}$$

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

since $\frac{d\sigma}{d\Omega} = |f^{(1)}(q)|^2 = \left(\frac{2mV_0}{u\hbar^2}\right)^2 \frac{1}{[2k^2(1-\cos\theta)+u^2]^2}$

at the limit $u \to 0$, it reduces to, by letting $\hbar k \equiv |p|$

$$\frac{d\sigma}{d\Omega} \simeq \frac{1}{16}\left(\frac{ZZ'e^2}{E_{KE}}\right)^2 \frac{1}{\sin^4(\theta/2)}$$ $\leftarrow$ classical Rutherford scattering cross-section

General Remarks of spherical symmetric potential using first-Born:

1) $d\sigma/d\Omega$ or $f(\theta)$ is a function of q only, that is, it depends on energy $\hbar^2 k^2/2m$ and θ through $q^2 = 2k^2(1-\cos\theta)$
2) $f(\theta)$ is always real
3) $d\sigma/d\Omega$ is independent of the sign of V
4) For small k (small q): $f^{(1)}(\theta) = -\frac{1}{4\pi}\frac{2m}{\hbar^2}\int V(r)\, d^3x$
   $\uparrow$ volume integral independent of θ
5) $f(\theta)$ is small for large q due to rapid oscillation.

Validity of the first-order Born-Approximation:

In first-order Born Approximation, we replaced $\langle x|\psi^+\rangle$ and $\langle x|\phi\rangle$, so $\langle x|\psi^+\rangle$ and $\langle x|\phi\rangle$ should not be very different.

So the distortion in the incident wave $|\phi\rangle$ must be small.

If $\langle x|\psi^+\rangle$ is similar to $\langle x|\phi\rangle$, then it means at $\vec{x}=0$

we previously know the exact solution of $\langle x|\psi^+\rangle$ is

$$\langle x|\psi^{\pm}\rangle = \langle x|\phi\rangle \underbrace{- \frac{2m}{\hbar^2}\int d^3x' \frac{e^{\pm ik|x-x'|}}{4\pi|x-x'|} V(x')\langle x'|\psi^{\pm}\rangle}_{\text{so this part must be } \ll 1}$$

setting $\vec{x}=0$:

Condition for applicability $\Rightarrow$

$$\boxed{\left| \frac{-2m}{\hbar^2}\frac{1}{4\pi}\int d^3x' \frac{e^{ikr'}}{r'} V(x')e^{ikx'} \right| \ll 1}$$

Using ↗, we can check for the case of Yukawa potential. $V(r) = \frac{V_0 e^{-\mu r}}{\mu r}$

↳ $\frac{-2m}{\hbar^2} \frac{1}{4\pi} \int d^3x' \frac{V_0 e^{-\mu x}}{\mu x} \frac{e^{ikr'}}{r'} e^{ikx'} \ll 1$

⇒ For low energy limit, i.e. $ka \ll 1$, the $e^{ikr} \sim 1$

we have condition: $\frac{2m}{\hbar^2} |V_0| a^2 \ll 1$

⇒ For high energy limit. i.e. $k \gg \mu$,

we have condition: $\frac{2m}{\hbar^2} \frac{|V_0| a}{k} \ln(ka) \ll 1$

a is the length scale and $a = \frac{1}{\mu}$ for Yukawa potential

as k increase, this condition is easier satisfied, so first-order Born approximation works better with high energy.

⇒ For Yukawa potential to develop bound state, require

$$\frac{2m}{\hbar^2 \mu^2} |V_0| \geq 2.7$$

so if potential, V_0, is strong enough to create bound state, thee first born approximation is not accurate.

Ex 2: $U(r) = \alpha\,\delta(r-R)$

$$f^{(1)}(\theta) = -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^\infty r\,U(r)\sin qr\,dr$$

$$= -\frac{2m}{\hbar^2}\frac{1}{q}\alpha\,R\,\sin qR$$

$$= -\frac{2m\alpha R^2}{\hbar^2}\frac{\sin qR}{qR} \qquad \text{where } q = 2k\sin\frac{\theta}{2}$$

since $\frac{d\sigma}{d\Omega} = |f^{(1)}(\theta)|^2$

$$\sigma = \left[\frac{2m\alpha R^2}{\hbar^2}\right]^2 \int_0^\pi \frac{\sin^2 qR}{(qR)^2}\,2\pi\,d\theta\sin\theta$$

let

$x = qR = 2k\sin\frac{\theta}{2}R$

$dx = \frac{2kR}{2}\cos\frac{\theta}{2}d\theta$

$= kR\cos\frac{\theta}{2}\,d\theta$

$$= \left[\frac{2m\alpha R^2}{\hbar^2}\right]^2 \int_0^\pi \frac{\sin^2 x}{x^2}\,2\pi\,\frac{dx}{kR\cancel{\cos\frac{\theta}{2}}}\underbrace{\sin\theta}_{=2\sin\frac{\theta}{2}\cancel{\cos\frac{\theta}{2}}}$$

$$= \left[\frac{2m\alpha R^2}{\hbar^2}\right]^2 \int_0^{2kR} \frac{\sin^2 x}{x^2}\,2\pi\,dx\,\underbrace{\frac{2}{kR}\sin\frac{\theta}{2}}_{=\frac{x}{(kR)^2}}$$

$$\sigma = \left[\frac{2m\alpha R^2}{\hbar^2}\right]^2 \frac{2\pi}{(kR)^2}\int_0^{2kR}\frac{\sin^2 x}{x}\,dx$$

If large energy $kR \gg 1$, then $\sin^2 x$ oscillates quickly, so take average, $\sin^2 x \sim 1/2$

then $$\sigma = \left[\frac{2m\alpha R^2}{\hbar^2}\right]^2 \frac{2\pi}{(kR)^2} \int_0^{2kR} \frac{1}{2x}\, dx$$

$$= \left[\frac{2m\alpha R^2}{\hbar^2}\right]^2 \frac{\pi}{(kR)^2} \ln(2kR)$$

with $E = \frac{\hbar^2 k^2}{2m}$ $$= \frac{2\pi m \alpha^2 R^2}{\hbar^2 E} \ln 2kR$$

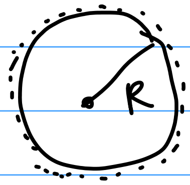
If small energy limit $kR \ll 1$: $\frac{\sin^2 x}{x} \approx x$

so $$\sigma = \left[\frac{2m\alpha R^2}{\hbar^2}\right]^2 \frac{\pi}{(kR)^2} \int_0^{2kR} x\, dx$$

$$= \left[\frac{2m\alpha R^2}{\hbar^2}\right]^2 \frac{\pi}{(kR)^2} \left.\frac{x^2}{2}\right|_0^{2kR}$$

$$\sigma = \frac{8\pi m^2 \alpha^2 R^4}{\hbar^4} \quad \text{for } kR \ll 1$$

To find the applicability: find typical energy V_0



$$\int_0^{R+\varepsilon} U(r)\, 4\pi r^2 dr = \alpha 4\pi R^2$$

$$V_0 \approx \frac{\alpha 4\pi R^2}{\frac{4}{3}\pi R^3} = \frac{3\alpha}{R}$$

the applicability of large energy $(ka \gg 1)$ is when:

$$\frac{2m}{\hbar^2} \frac{|V_0| a}{k} \ln(ka) \ll 1$$

so $$\frac{2m}{\hbar^2} \frac{3\alpha}{\cancel{R}} \frac{\cancel{R}}{k} \ln(kR) \cong \frac{m}{\hbar^2} \frac{\alpha}{k} \ln(kR) \ll 1$$

the applicability of small energy $(kR \ll 1)$ is when:

$$\frac{2ma^2}{\hbar^2} |V_0| \ll 1$$

or $$\frac{2mR^{\cancel{2}}}{\hbar^2} \frac{\alpha}{\cancel{R}} \cong \frac{\alpha m R}{\hbar^2} \ll 1$$

Ex 3: $V(r) = \begin{cases} V_0 & r \le a \\ 0 & r \ge a \end{cases}$

then $f^{(1)}(\theta) = -\frac{2m}{\hbar^2}\frac{1}{q}\int_0^a r V_0 \sin qr \, dr$

since $\frac{d}{dr}\left(\frac{r}{q}\cos qr\right) = \frac{1}{q}\cos qr - r\sin qr$

$\hookrightarrow \quad r\sin qr = \frac{1}{q}\cos qr - \frac{d}{dr}\left(\frac{r}{q}\cos qr\right)$

$$= -\frac{2m}{\hbar^2}\frac{V_0}{q}\left[-\frac{r}{q}\cos qr\Big|_0^a + \frac{1}{q}\underbrace{\int_0^a \cos qr \, dr}_{\frac{1}{q}\sin qr\big|_0^a}\right]$$

$$= -\frac{2m}{\hbar^2}\frac{V_0}{q}\left[-\frac{a}{q}\cos qa + \frac{1}{q^2}\sin qa\right]$$

$$f^{(1)}(\theta) = -\frac{2m}{\hbar^2}\frac{V_0 a^3}{(qa)^2}\left[\frac{\sin qa}{qa} - \cos qa\right]$$

then $\frac{d\sigma}{d\Omega} = \left|f^{(1)}(\theta)\right|^2 \simeq \left[\frac{2m}{\hbar^2}\frac{V_0 a^3}{(qa)^2}\right]^2\left[\frac{\sin qa}{qa} - \cos qa\right]^2$