9. Scattering theory: Generalities

SS 2024

AQM

[illegible]

[illegible]

Scattering theory is the second MAIN TOPIC of this course.

Till now we have considered time-dependent processes as emission / absorbtion of light by atoms

$\Rightarrow$ SPECTROSCOPY important to understand Atoms & molecules

we concluded last lecture with the decay of $2p \to 1s$ of a Hydrogen Atom, and estimated a LIFETIME $\tau \sim 1.6 \cdot 10^{-9}\,s$

We could see this as some sort of SCATTERING, some projectile hits Atom, excites it, till it decays

$\Rightarrow$ IMPORTANT POINT interaction time-scale MUCH SHORTER than "life-time" of Atom

$$T_{characteristic} \sim \frac{a_0}{\alpha c} \sim 2 \cdot 10^{-17}\,s$$

time for e^- to revolve around nucleus

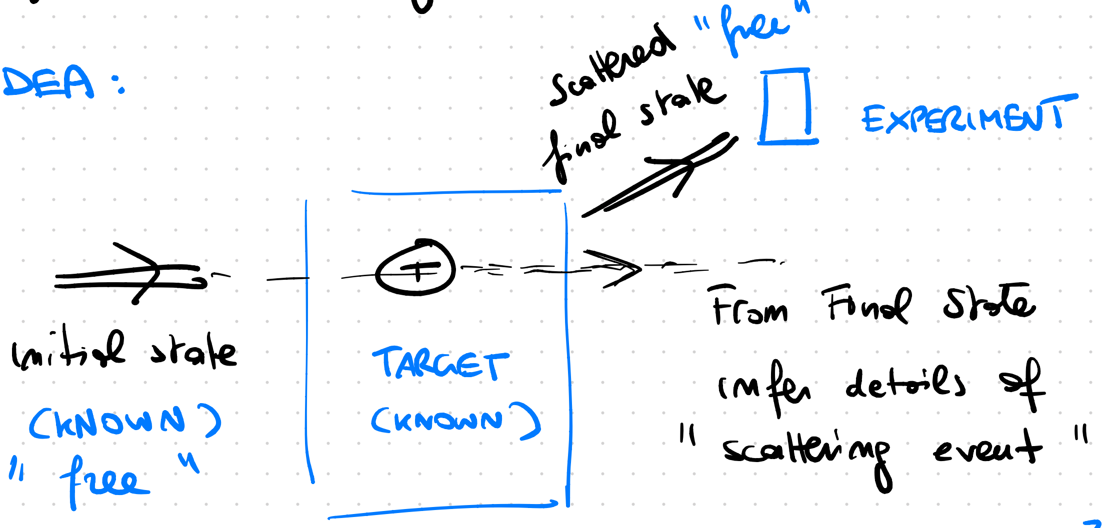
So we can imagine to "separate" DECAY from EXCITATION such that details of how state decays are independent from the actual process that generated excited state

In SCATTERING [COLLISION] THEORY we don't make this assumption anymore

⇒ We discuss the PROCESS at ONCE as a WHOLE

Crucial to understand NUCLEAR STRUCTURE, high-energy scattering (CERN LHC etc)

IDEA:



In back of our minds, we imagine to work with WAVE PACKETS $\Rightarrow$ $\begin{cases} \text{Longer than target} \\ \text{Smaller than Laboratory} \end{cases}$

In practice, we simplify our treatment working with PLANE WAVES $\Rightarrow$ solutions of FREE SCHRÖDINGER EQUATION

Let us recap some details

$$i\hbar \frac{\partial \psi(\vec{x},t)}{\partial t} = H \psi(\vec{x},t) \qquad \text{3 Dim Schröd. Eq.}$$

$$H = \frac{\vec{P}^2}{2m} + V(\vec{x}) \qquad V(\vec{x}) \in \mathbb{R}$$

Remember that PROBABILITY DENSITY $\rho = \psi^* \psi$:

$$\frac{\partial}{\partial t}(\psi^*\psi) = \psi^* \frac{1}{i\hbar}\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + V\psi\right]$$

$$- \frac{1}{i\hbar}\left[-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi^* + V\psi^*\right]\psi \quad =$$

$$= \frac{i\hbar}{2m}\left[\psi^* \vec{\nabla}^2\psi - \vec{\nabla}^2(\psi^*)\psi\right]$$

$$= \vec{\nabla}\cdot\left[\frac{i\hbar}{2m}\left(\psi^* \vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi\right)\right]$$

$$\underbrace{\vec{j} = -\frac{i\hbar}{2m}\left(\psi^* \vec{\nabla}\psi - \psi\vec{\nabla}\psi^*\right)}_{\text{CURRENT}} \Rightarrow \underbrace{\frac{\partial\rho}{\partial t} = -\vec{\nabla}\cdot\vec{j}}_{\text{CURRENT CONSERVATION}}$$

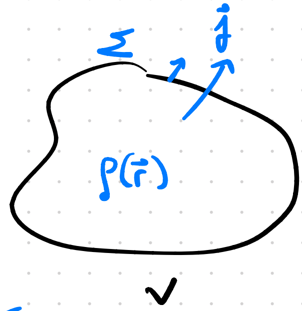
if PLANE WAVE $\psi = A e^{-i(Et - \vec{p}\cdot\vec{x})/\hbar}$

$$\vec{j} = |A|^2 \frac{\vec{p}}{m} \propto \text{velocity of wave!}$$

$$= |A|^2 \frac{\hbar\vec{k}}{m}$$

$\vec{j}$ current also called FLUX $\Rightarrow$ # of particles per unit time crossing a unit area normal to incident direction

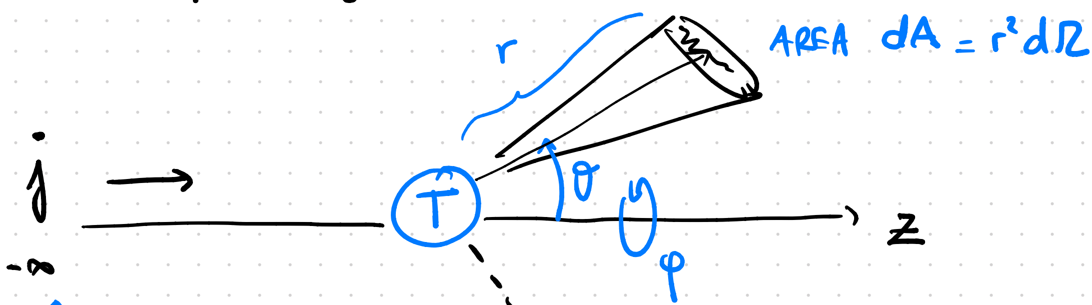
$$\Rightarrow \int_V \frac{\partial \rho}{\partial t}\, d^3\vec{r} = -\int \vec{\nabla}\cdot\vec{j}\, d^3\vec{r}$$



$$\frac{\partial}{\partial t}[P] = -\int_\Sigma \vec{j}\cdot d\vec{\sigma}$$

Probability to cross Σ in unit time

Consider following set-up



initial flux "$\vec{j}$" in z direction

Target could recoil in general

$\Rightarrow$ IGNORE RECOIL

(use REDUCED mass μ see lecture 2!)

θ POLAR ANGLE
φ AZIMUTHAL ANGLE
$\Big\}$ determine direction of scattered particle

If the dector measures δn particles / second, then

$$\delta n = j \left[\frac{d\sigma(\vartheta,\varphi)}{d\Omega}\right] d\Omega$$

RATE

INCOMING FLUX

DIFFERENTIAL CROSS-SECTION (per solid angle $d\Omega$)

AREA IS $r^2 d\Omega = dA$

(notice no dA here!)

$$\left.\frac{\delta n}{j\, dA}\right\} \text{measurable quantities} \Rightarrow \frac{d\sigma}{d\Omega}$$

can be computed in Q.M.

DEPENDS ON POTENTIAL V

We can then turn problem around and use measured $d\sigma$ to INFER POTENTIAL V !

Start from Schrödinger Equation

$$\left[-\frac{\hbar^2}{2\mu}\nabla^2_{\vec{x}} + V(\vec{x})\right]\psi = E\psi$$

• if $E<0$ bound state in $V(x)$

$\Rightarrow$ Hydrogen Atom, no Scattering!

• if $E>0$ continuum of solutions for E

Define $E = \frac{\hbar^2}{2\mu} k^2$; $V(x) = \frac{\hbar^2}{2\mu} U(x)$

so Schrödinger Equation becomes

$$\Rightarrow \quad (\vec{\nabla}^2 + k^2)\psi - U(x)\psi = 0$$

SCATTERING EQUATION

Now assuming interaction happens in SMALL REGION where $V \neq 0$, we start looking of form of solution ASYMPTOTICALLY FAR AWAY where $V = 0$!

Start with INCIDENT PLANE WAVE along z

$$E = \frac{\hbar^2}{2\mu} k^2 \qquad \psi_{inc} = \underset{\substack{\uparrow \\ \text{normalization}}}{1}\, e^{ikz}$$

$$\Rightarrow \left(\vec{\nabla}^2 + k^2\right)\psi_{inc} = 0 \quad \text{of course}$$

[some of this ψ_{inc} continues unscattered !]

After interaction ψ_{SCAT} $\Rightarrow$ particles come out "in any direction", solution should somehow still solve FREE SCATTERING EQUATION

Let's write it in SPHERICAL COORDINATES

$$\left(\vec{\nabla}^2 + k^2\right)\psi = \left[\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi) + k^2\psi\right]$$

$$+ \frac{1}{r^2}\underbrace{\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\,\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}\right]}_{-\frac{L^2}{\hbar^2}}$$

$$= 0$$

as we are interested in asymptotic solution ($r \to \infty$) we try the following Ansatz

$$\psi_{scat} = e^{ikr}\left[\sum_{i=1}^{\infty} f_k^{(i)}(\vartheta,\varphi)\left(\frac{1}{r}\right)^i\right] \Rightarrow \left(kr \overset{!}{=} |\vec{k}||\vec{r}|\right)$$

$$= \frac{e^{ikr}}{r}\left[f_k(\vartheta,\varphi) + \mathcal{O}\left(\frac{1}{r}\right)\right]$$

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}\left[r\,\frac{e^{ikr}}{r} f_k(\vartheta,\varphi)\right] = -k^2\frac{e^{ikr}}{r} f_k(\vartheta,\varphi)$$

$$\frac{1}{r}\frac{\partial^2}{\partial r^2}\left[\frac{e^{ikr}}{r}\frac{g(\vartheta,\varphi)}{r}\right] \propto -k^2\frac{e^{ikr}}{r}\frac{g(\vartheta,\varphi)}{r} + \mathcal{O}\left(\frac{1}{r^3}\right)$$

higher order corrections

$$\frac{1}{r^2}\left[-\frac{L^2(\vartheta,\varphi)}{\hbar^2}\right]\left(\frac{e^{ikr}}{r} f_k(\vartheta,\varphi) + \mathcal{O}\left(\frac{1}{r}\right)\right) \propto \mathcal{O}\left(\frac{1}{r^2}\right)$$

$\Rightarrow$ ψ_{scat} solves scattering equation asymptotically!

$f_k(\theta,\varphi)$ is a function of the angles only and at the moment is unconstrained

$f_k(\theta,\varphi)$ called <u>SCATTERING AMPLITUDE</u>

A full solution asymptotically $[\, V(\vec{x})=0 \,]$ is

$$\psi = e^{ikz} + \frac{e^{ikr}}{r} f_k(\theta,\varphi)\left[1 + O\left(\frac{1}{r}\right)\right]$$

Now let's compute the current $\vec{j}$ $\left(e^{ikz} = e^{i\vec{k}\cdot\vec{r}}\right)$

$$\vec{j} = -\frac{i\hbar}{2\mu}\left(\psi^* \vec{\nabla}\psi - \psi \vec{\nabla}\psi^*\right)$$

$$= \frac{\hbar}{2i\mu}\left\{\left[e^{-ikz} + f_k^*(\theta,\varphi)\frac{e^{-ikr}}{r}\right] \times\right.$$

$$\times\left[ike^{ikz}\hat{z} + \left(ik\frac{e^{ikr}}{r} - \frac{e^{ikr}}{r^2}\right)f_k(\theta,\varphi)\hat{r} + \frac{1}{r}\frac{\partial f_k}{\partial\theta}\frac{e^{ikr}}{r}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial f_k}{\partial\varphi}\hat{\varphi}\right]$$

$$\left. - \text{complex conjugated} \right\}$$

evaluating the products we get

$$\vec{j} = \frac{\hbar k}{\mu}\hat{z} + \frac{\hbar k}{\mu}\frac{\hat{r}}{r^2}|f_k(\vartheta,\varphi)|^2 + O\left(\frac{1}{r^3}\right)$$

+ interference terms with e^{ikr} & e^{ikz} !

- $O\left(\frac{1}{r^3}\right)$ clearly suppressed at large distance !

- What about INTERFERENCE TERMS ?

they contain both types of exponentials

$$\vec{j}_{INT} \propto A\, e^{ikr} e^{-ikz} + c.c.$$

$$\sim A\, e^{ikr(1-\cos\vartheta)} + c.c. \quad \left(\text{using } \underline{z = r\cos\vartheta}\right)$$

NOTICE : we always care about $\vartheta \neq 0$ (there is no way to distinguish scattered from unscattered particles in FORWARD DIRECTION !)

Now in a REALISTIC EXPERIMENT we must integrate $\vec{j}$ over some SMALL $d\Omega$

$$\sim \int d\cos\vartheta \, d\varphi \; g(\vartheta,\varphi) \, e^{ikr(1-\cos\vartheta)} \; A$$

unspecified smooth "acceptance" function for the DETECTOR

when $r \to \infty$, integral of some smooth function times a RAPIDLY OSCILLATING ONE $e^{ikr(1-\cos\vartheta)}$

Riemann - Lebesgue lemma says this integral VANISHES FASTER THAN ANY $\frac{1}{r^n}$!

(SEE EXERCISES !)

so we can neglect all interference terms and

$$\boxed{\vec{j} = \frac{\hbar k}{\mu} \hat{z} + \frac{\hbar k}{\mu} \frac{\hat{r}}{r^2} |f_k(\vartheta,\varphi)|^2}$$

TOTAL FLUX FAR AWAY !

Using this current in our formula for the cross-section gives

$$d\sigma(\vartheta,\varphi) = j_I^{-1} \cdot j_{SCATT} \cdot dA = \cancel{\frac{\mu}{\hbar k}} \left[\frac{1}{\cancel{r^2}} \cancel{\frac{\hbar k}{\mu}} |f_k(\vartheta,\varphi)|^2 \right] \cancel{r^2} d\Omega$$

INCIDENT

j_I FLUX $\sim \hat{z} \frac{\hbar k}{\mu}$

AREA SUBTENDS SOLID ANGLE $d\Omega$

SCATTERING RATE $\Rightarrow$ FLUX SCATTERED!

$\sim \frac{\hat{r}}{r^2} \frac{\hbar k}{\mu} |f_k(\vartheta,\varphi)|^2$

$$\Rightarrow \boxed{d\sigma(\vartheta,\varphi) = |f_k(\vartheta,\varphi)|^2 \, d\Omega}$$

CROSS SECTION

Notice that terms $\propto O(\frac{1}{r^3})$ in $\vec{j}$ would contribute to cross-section with $\propto O(\frac{1}{r})$ due to the r^2 at the numerator of integration measures $\Rightarrow$ confirms it is ok to neglect them! B more explicitly: our starting formula was

$$\delta n = j_I \left(\frac{d\sigma(\vartheta, \varphi)}{d\Omega} \right) d\Omega$$

which implies

$$\frac{d\sigma}{d\Omega} = j_I^{-1} \frac{\delta n}{d\Omega}$$

now δn is rate measured by detector

$$\Rightarrow \delta n = j_{scatt} \times dA$$

$dA = r^2 d\Omega$
area subtended by $d\Omega$ at detector!

$$\Rightarrow \frac{d\sigma}{d\Omega} = j_I^{-1} \frac{j_{SCATT} \cdot r^2 \cdot d\Omega}{d\Omega}$$

$$= \frac{\cancel{\mu}}{\cancel{\hbar} k} \frac{1}{\cancel{r^2}} \frac{\hbar \cancel{k}}{\cancel{\mu}} |f_k(\vartheta, \varphi)|^2 \frac{\cancel{r^2} \cancel{d\Omega}}{\cancel{d\Omega}}$$

$$= |f_k(\vartheta, \varphi)|^2$$

$\Rightarrow$ in order to compute cross-section, we need the scattering amplitude

To compute it, we need to solve Schrödinger Eq. and see what information is brought in by the potential $V(x)$. To do that, we use the GREEN'S FUNCTION method, that you should know from Electrodynamics.

Start from $\underbrace{(\vec{\nabla}^2 + k^2)}_{\text{Free Schrödinger Operator}} \psi = 0$

Green's function $G(x)$ is defined as

$$(\vec{\nabla}^2 + k^2)\, G(\vec{x}) = \delta^{(3)}(\vec{x}) \leftarrow$$ DIRAC δ function in 3-dim

$$\delta^{(3)}(\vec{x}) = \delta(x_1)\,\delta(x_2)\,\delta(x_3)$$ $\vec{x} = (x_1, x_2, x_3) \sim (x, y, z)$

indeed, if we have $G(\vec{x})$, then we can write

$$\boxed{\psi(\vec{x}) = \psi_0(\vec{x}) + \int d^3\vec{y}\; G(\vec{x}-\vec{y})\, U(\vec{y})\, \psi(\vec{y})}$$

with $(\vec{\nabla}^2 + k^2)\,\psi_0(\vec{x}) = 0$

then acting on $\psi(\vec{x})$ with $\vec{\nabla}^2 + k^2$ we get

$$(\vec{\nabla}_{\vec{x}}^2 + k^2)\psi = 0 + \int d^3\vec{y}\; (\vec{\nabla}_{\vec{x}}^2 + k^2) G(\vec{x}-\vec{y})\, U(\vec{y})\, \psi(\vec{y})$$

$$= \int d^3\vec{y}\; \delta^{(3)}(\vec{x}-\vec{y})\, U(\vec{y})\, \psi(\vec{y})$$

$$= U(\vec{x})\, \psi(\vec{x})$$

So boxed equation above is a solution of the Schrödinger Equation $\Rightarrow$ we still need to make sure we fix BOUNDARY CONDITION to get physical solution!

$\psi_0(x)$ & $G(\vec{x}-\vec{x}')$

Before thinking about how to compute $G(\vec{x})$, Notice that this equation is again an integral Equation, very similar to the one we wrote when studying time-dependent perturbation theory.

It becomes USEFUL if we assume that $U(\vec{y})$ is "small" and we can then ITERATE the equation to get a Series Expansion in U

$\Rightarrow$ "BORN" EXPANSION (SERIES)

$$\psi(x) = \psi_0(x) + \int d^3\vec{y}\, G(\vec{x}-\vec{y})\, U(\vec{y})\, \psi_0(\vec{y})$$

$$+ \int d^3\vec{y}\, G(\vec{x}-\vec{y})\, U(\vec{y}) \int d^3\vec{z}\, G(\vec{y}-\vec{z})\, U(\vec{z})\, \psi_0(\vec{z})$$

$$+ O(U(x)^3) \quad \text{etc}$$

$\Rightarrow$ useful because $\psi_0(\vec{x})$ is known!

$\psi_0(x) = e^{ikz}$ incoming (unscattered) wave the first order is called

(first) <u>BORN APPROXIMATION</u>

$$\psi^{(1)}_{scatt}(\vec{x}) = \frac{2\mu}{\hbar^2}\int d^3\vec{y}\; G(\vec{x}-\vec{y})\; V(\vec{y})\; e^{iky_3}$$

back to STANDARD POTENTIAL

incoming wave

$$\left\{ \vec{k} = (0,0,k) \;;\; \vec{y} = (y_1, y_2, y_3) \right\}$$

To make use of this formula, we need $G(\vec{x}-\vec{y})$!

We will prove more properly in next lecture that

$$G(\vec{x}) = G(|\vec{x}|) = -\frac{e^{+ik|\vec{x}|}}{4\pi|\vec{x}|}$$

is right solution for OUTGOING SPHERICAL WAVE

To prove it, we should see that:

$$(\vec{\nabla}^2 + k^2)\, G(|\vec{x}|) = (\vec{\nabla} + k^2)\, G(r) \overset{?}{=} \delta^{(3)}(\vec{x})$$

spherical coordinates

as long as $r \neq 0$ we can just differentiate:

$$= \frac{1}{r}\frac{\partial^2}{\partial r^2}\left(r G(r)\right) + k^2 G(k)$$

$$= -\frac{1}{r}\frac{\partial^2}{\partial r^2}\left[\cancel{r}\, \frac{e^{+ikr}}{4\pi \cancel{r}}\right] - k^2 \frac{e^{+ikr}}{4\pi r}$$

$$= +\frac{k^2}{r 4\pi} e^{+ikr} - k^2 \frac{e^{+ikr}}{4\pi r} = 0 \qquad \checkmark$$

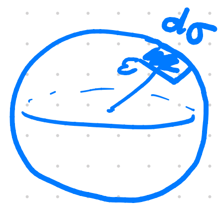
$\Rightarrow$ @ $r = 0$ $\quad \frac{\partial}{\partial r}$ etc all ill defined

We should find $\delta^{(3)}(\vec{x}) \Rightarrow$ DISTRIBUTION, makes sense only upon integration on some region of space $\Rightarrow$ SOME SPHERE CENTRED @ $\vec{x} = 0$

$$\int_{S_\varepsilon} dV \, \vec{\nabla}^2 G(r) =$$

S_ε sphere of radius ε

$$= \text{DIVERGENCE THEOREM} = \int_{\Sigma_\varepsilon} \left(\vec{\nabla} \cdot G\right) \cdot \hat{r} \, d\sigma$$



now $\vec{\nabla} \cdot G(r) = \hat{r} \dfrac{\partial G}{\partial r}$

$$= \frac{\hat{r}}{4\pi} \left[\frac{1}{r^2} - \frac{ik}{r} \right] e^{ikr}$$

$$= \int_{\Sigma_\varepsilon} \frac{1}{4\pi} \left[\frac{1}{r^2} - \frac{ik}{r} \right] e^{ikr} \, d\sigma = \cancel{4\pi} \varepsilon^2 \frac{1}{\cancel{4\pi}} \left[\frac{1}{\varepsilon^2} - \frac{ik}{\varepsilon} \right] e^{ik\varepsilon}$$

surface is @ r fixed $\equiv \varepsilon$

$$= \underline{1} + O(\varepsilon^2)$$

so we find that as $\varepsilon \to 0$, $\int_{S_\varepsilon} \nabla^2 G \, dV = 1$

which is exactly what we expect from $\delta^{(3)}(\vec{x})$

$\Longrightarrow$ for other smooth function integral would go to zero when volume shrinks

Now, using $G(\vec{x}) = -\dfrac{e^{+i|k||\vec{x}|}}{4\pi|\vec{x}|}$ in formula for

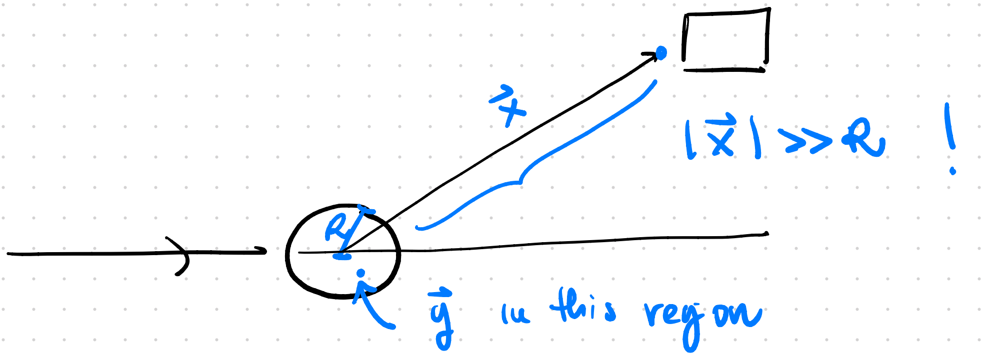
FIRST ORDER Born Approximation

$$\psi^{(1)}_{scatt}(\vec{x}) = \frac{2\mu}{\hbar^2} \int d^3\vec{y} \; G(\vec{x}-\vec{y}) \, V(\vec{y}) \, e^{iky_3}$$

$$= -\frac{\mu}{2\pi\hbar^2} \int d^3\vec{y} \; \frac{e^{+ik|\vec{x}-\vec{y}|}}{|\vec{x}-\vec{y}|} \, V(\vec{y}) \, e^{iky_3}$$

(remember $y_3 = \hat{z}\cdot\vec{y}$; etc)

Typically $V(\vec{x}) \neq 0$ in some bounded region $|\vec{x}| < R \Rightarrow$ FINITE RANGE POTENTIAL



then we can simplify the integral using

$$|\vec{x}-\vec{y}| = \sqrt{\vec{x}^2+\vec{y}^2-2\vec{x}\cdot\vec{y}} = |\vec{x}|\sqrt{1-2\frac{\vec{x}\cdot\vec{y}}{|\vec{x}|}+\frac{|\vec{y}|^2}{|\vec{x}|^2}}$$

$$\simeq |\vec{x}| - \hat{x}\cdot\vec{y} + O\left(\frac{|\vec{y}|}{|\vec{x}|^2}\right)$$ and

$$\psi^{(1)}_{SCAT}(\vec{x}) \simeq -\frac{\mu e^{ik|\vec{x}|}}{2\pi\hbar^2|\vec{x}|}\int d^3\vec{y}\, e^{-ik\hat{x}\cdot\vec{y}}\, e^{ik\hat{z}\cdot\vec{y}}\, V(\vec{y})$$

$$= -\frac{\mu}{2\pi\hbar^2}\frac{e^{ik|\vec{x}|}}{|\vec{x}|}\int d^3\vec{y}\, e^{i(\vec{k}_i-\vec{k}_f)\cdot\vec{y}}\, V(\vec{y})$$

where $\begin{cases} \vec{k}_i = (0,0,k) & \text{wave vector of incident particle} \\ \vec{k}_f = k\,\hat{x} & \text{wave vector of scattered particle} \end{cases}$

notice that this is exactly in form

$$\psi = e^{ikz} + \frac{e^{ikr}}{r} f_k(\theta,\varphi)\left[1 + O\left(\frac{1}{r}\right)\right]$$

with

$$f_k(\theta,\varphi) = -\frac{\mu}{2\pi\hbar^2}\int d^3\vec{y}\, e^{i(\vec{k}_i-\vec{k}_f)\cdot\vec{y}}\, V(\vec{y})$$

$\Rightarrow$ the SCATTERING AMPLITUDE in BORN APPROX is given by the FOURIER TRANSFORM of the SCATTERING POTENTIAL

!