Quantum cross-sections and scattering in 3D: So far we have used the flux (i.e. plane-waves)

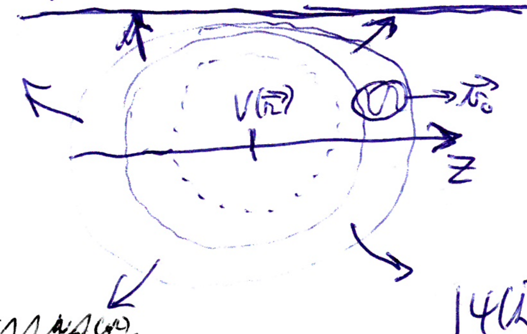
- consider scattering of a single spinless particle in a (short-range) central field $V(\vec{r})$, e.g. $e^- + A \rightarrow e^- + A$, where we approximate the interaction by a potential
- as in the classical case we do the experiment ~~…~~ by sending particles with a well-defined velocity towards the target:

at $t \ll 0$:

$|\psi(t)\rangle = |\psi_{in}\rangle =$

$$= \int d^3p \, \phi(\vec{p}) \, |\vec{p}\rangle$$

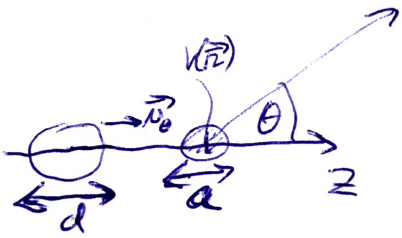
WE EXPECT at $t \gg 0$:



- unscattered wavepacket
- scattered part moving radially outward

$$|\psi(t)\rangle = |\psi_{in}(t)\rangle + |\psi_{sc}(t)\rangle$$

- We measure as before the number of particles going into a given direction (θ, φ):



- what is the probability of finding the particle in the direction (θ, φ)?

$$w(\psi_{in}(\vec{r}) \rightarrow d\Omega(\theta,\varphi)) = d\Omega \int_0^\infty dr \, r^2 \, |\psi(r \cdot \vec{r}, t)|^2, \; t \gg 0$$

$\vec{r}$ points in the direction (θ, φ)

- We repeat the experiment many times with different displacements (impact parameters) b:

$$N_{sc}(d\Omega) = \int \underbrace{d^2b}_{\text{area perp. to } \vec{v}_0} \; \underbrace{n_{inc}}_{\#\text{ particles per area (we assume this uniform)}} \, w(\psi_{in}^{(\vec{b})} \rightarrow d\Omega) = n_{inc} \int d^2b \, w(\psi_{in}(\vec{b}) \rightarrow d\Omega)$$

$\rightarrow \int d^2b \, w(\psi_{in} \rightarrow d\Omega)$ has dimensions of area $\Rightarrow \boxed{\sigma(\psi_{in} \rightarrow d\Omega) = \int d^2b \, w(\psi_{in}(\vec{b}) \rightarrow d\Omega)}$

$\rightarrow$ we can interpret it as an area integral where each element is weighted by w! I.E. IT IS AN EFFECTIVE AREA AND WE LOOSE THE SIMPLE CLASSICAL INTERPRETATION!

- Similarly to the class. case $\sigma \sim d\Omega \Rightarrow \sigma(\psi_{in} \rightarrow d\Omega) = \underbrace{\left(\frac{d\sigma}{d\Omega}\right)}_{\text{Differential cross section for scattering into } (\theta,\varphi)} d\Omega$

Calculation of the scattering probability: $\boxed{\text{USING ATOMIC UNITS FROM NOW ON}}$

$$w\left(\psi_{in}(\vec{r}) \to d\Omega(\theta,\varphi)\right) = d\Omega \int_0^\infty dr\, r^2 \left|\psi(r\cdot\underbrace{\hat{r}}_{(\theta,\varphi)},t)\right|^2, \quad t \gg 0$$

- How do we find $\psi(\vec{r},t)$?
- We have solve Schr. eq. $i\,\cancel{\hbar}\dfrac{\partial\psi(\vec{r},t)}{\partial t} = H\psi(\vec{r},t)$

$$\psi(\vec{r},t_0) = \psi_{in}(\vec{r}), \quad t_0 \ll 0$$

- We have H indep. of time so we can ~~also~~ write the solution as a superposition of stationary solutions:

$$\psi(\vec{r},t) = (2\pi)^{-3/2}\int d^3p\, \underbrace{\phi(\vec{p})}_{\text{sharply peaked around } \vec{p}_0 = m\vec{v}_0} \cdot \psi^{(+)}_{\vec{p}}(\vec{r})\cdot e^{-iE_p\cdot t}$$

$$H\psi^{(+)}_{\vec{p}} = E_p\cdot\psi^{(+)}_{\vec{p}}$$

→ BCs on $\psi^{(+)}_{\vec{p}}$ must ensure that the solution of the TD equation is the one intended

→ Our intuition from 1D tells us that:

$$\psi^{(+)}_{\vec{p}}(\vec{r}) \xrightarrow[r\to\infty]{} (2\pi)^{-3/2}\left[\underbrace{e^{i\vec{p}\cdot\vec{r}}}_{\text{incoming wave}} + \underbrace{f(\vec{p}\to p\cdot\hat{r})}_{\text{amplitude describing angular dependence}}\cdot\underbrace{\frac{e^{ipr}}{r}}_{\text{spherical outgoing wave}}\right]$$

→ We will now show that this choice of BCs indeed gives at $t \gg 0$:

1) outgoing unscattered wave with the same momentum
2) scattered outgoing wave

→ For $\phi(p)$ we choose a Gaussian wavepacket:

$$\phi(p) = \left(\frac{d^2}{2\pi^3}\right)^{3/4}\cdot\exp\left[-(\vec{p}-\vec{p}_0)^2\cdot d^2\right] \Rightarrow \Delta p = \frac{1}{2d} \text{ while}$$

$$\Delta x = d$$

⇒ consistent with the uncertainty principle $\Delta p\Delta x \geq \frac{1}{2}$

- detailed shape of $\phi(p)$ is not important as long as it is sharply peaked around $\vec{p}_0$ ⇒ we will make expansions around ~~the~~ $\vec{p}_0$ of the integrand.

→ ~~[illegible]~~

– We need to consider $\psi(\vec{r},t)$ at $t \ll 0$ and $t \gg 0$ and $|\vec{r}| \to +\infty$

$$\psi(\vec{r},t) = (2\pi)^{-3/2}\int d^3p\,\phi(\vec{p})\,\psi^{(+)}_{\vec{p}}(\vec{r})\cdot e^{-iE_p t} \xrightarrow{r\to+\infty}$$

$$\longrightarrow (2\pi)^{-3/2}\int d^3p\,\phi(p)\left[e^{i\vec{p}\vec{r}} + f(\vec{p}\to p\hat{\vec{r}})\cdot\frac{e^{ipr}}{r}\right]e^{-iE_p t}$$

– We expand E_p about the mean momentum: $\frac{\partial E_p}{\partial \vec{p}} = \frac{\partial}{\partial \vec{p}}\left(\frac{(\vec{p}\cdot\vec{p})}{2m}\right) = \frac{\vec{p}}{m} = \vec{v}$

$$E_p = E_0 + \vec{v}_0(\vec{p}-\vec{p}_0) + \mathcal{O}\left(\frac{\Delta p^2}{m}\right)$$

2nd Taylor order

$e^{i\mathcal{O}\left(\frac{\Delta p^2}{m}\right)t} \sim 1 + i\mathcal{O}\left(\frac{\Delta p^2}{m}\right)$

for time evolution

$(E_p = E_0 + \vec{v}_0(\vec{p}-\vec{p}_0))$

→ ~~[illegible]~~ incoming-wave term we see

$$\psi_{in}(\vec{r},t) = (2\pi)^{-3/2} e^{iE_0 t}\int d^3p\,\phi(\vec{p})\cdot e^{i\vec{p}(\vec{r}-\vec{v}_0 t)}\left[1+\mathcal{O}\left(\frac{\Delta p^2 t}{m}\right)\right] =$$

$$= e^{-iE_0 t}\cdot\overbrace{\psi_{in}(\vec{r}-\vec{v}_0 t, 0)}^{=\text{FT of }\phi(\vec{p})}\left[1+\mathcal{O}\left(\frac{t}{m b^2}\right)\right]$$

$\frac{1}{b^2} \sim \Delta p^2$ ($\Delta x\,\Delta p \sim 1$, minimal wave packet)

from uncertainty relations for FT

⇒ $\boxed{\text{as long as } \frac{t}{mb^2} \ll 1}$ we can consider the initial wavepacket as rigidly translating through space.

⇒ ~~[illegible]~~ outgoing-wave term.

(microscopic vs macroscopic scales)

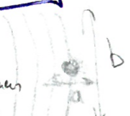
$d \gg a$ (the sc part is small compared to the size of the exp. setup)

$$\psi_{sc}(\vec{r},t) = (2\pi)^{-3/2}\int d^3p\,\phi(\vec{p})\,f(\vec{p}\to p\cdot\hat{\vec{r}})\frac{e^{ipr}}{r}e^{-iE_p t}$$

$$\sim (2\pi)^{-3/2}\frac{f(\vec{p}_0\to p_0\cdot\hat{\vec{r}})}{r}\int d^3p\,\phi(\vec{p})\cdot e^{i(p\cdot r - E_p t)}$$

Born $f \sim \langle p'|V|p\rangle$ = FT of potential
we want f to be broad so V must be small
$\sim$
~~the amplitude is small compared~~ $\phi(\vec{p})$

⇒ $\boxed{b \gg a}$



the wavepacket must not change over dimensions of a

⇒ expand the phase $i(p\cdot r - E_p t)$ around mean momentum:

$$ipr - i\frac{(\vec{p}\cdot\vec{p})}{2m}t = i p_0\cdot r - i\cdot\frac{p_0^2}{2m}t + i\left(r - \frac{p_0}{m}t\right)\frac{\vec{p}_0}{p_0}\cdot(\vec{p}-\vec{p}_0) +$$
$$+\,\mathcal{O}(p-p_0)$$

⇒ this phase appears under the integral so it is stationary only if: $\nabla_{\vec{p}}\phi(\vec{p}) = 0 \Leftrightarrow \nabla\left(r-\frac{p_0}{m}t\right)\frac{\vec{p}_0}{p_0}(\vec{p}-\vec{p}_0) = 0$

$$\Rightarrow \boxed{r - v_0 t = 0}$$

⇒ this is only stationary for $t > 0$

⇒ indeed the scattered part doesn't contribute at $t \ll 0$.

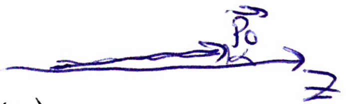
⇒ it describes a spherical shell of radius $r = v_0 t$
an expanding

Let's work with the phase $i(pr - E_p t)$ further:

$$\Rightarrow pr = \underbrace{\vec{p}\cdot\hat{\vec{z}}}_{} + \mathcal{O}\left(\frac{\Delta p^2 r}{p}\right)$$

$\sin\alpha \sim \frac{\Delta p}{p_0} \Rightarrow \cos\alpha = 1 - \frac{\Delta p^2}{p_0^2}$

$\hookrightarrow$ $\vec{p}_0$ $\phi(\vec{p})$ is well localized around $\vec{p}_0$ which is parallel to $\hat{\vec{z}}$:



$$\vec{p}_0\cdot\hat{\vec{z}} = p_0\cdot z \underbrace{\cos\alpha}_{\sim 1 - \frac{\Delta p^2}{p_0^2}}$$

$$\Rightarrow p_0 z \sim \vec{p}_0\cdot\hat{\vec{z}} + \underbrace{\mathcal{O}\left(p_0 z\cdot\frac{\Delta p^2}{p_0^2}\right)}_{=\,\mathcal{O}\left(\frac{r\Delta p^2}{p_0}\right)}$$

(i.e. the short-range part is small compared to the experimental setup) $d \gg a$

$$\Rightarrow \psi_{sc}(\vec{r},t) \sim (2\pi)^{-3/2}\,\frac{f(\vec{p}_0 \to p_0\hat{\vec{r}})}{r}\int d^3p\,\phi(\vec{p})\cdot e^{i(\vec{p}\cdot\hat{\vec{z}} - E_p t)} =$$

$$= \frac{f(\vec{p}_0 \to p_0\hat{\vec{r}})}{r}\,\psi_{in}(\hat{\vec{z}},t)\left[1 + \mathcal{O}\left(\frac{r}{p_0 b^2}\right)\right]$$

$\mathcal{O}\left(\frac{\Delta p^2 r}{p}\right) \quad \Delta p \sim \frac{1}{b}$

spherical shell of radius $v_0 t$.

$t \gg 0$

$\Rightarrow$ scattered wave $\sim$ unscattered on the z-axis times $\frac{f}{r}$

$\Rightarrow$ therefore there is no scattered wave at $t \ll 0$ until ψ_{in} has hit the target

$\Rightarrow$ if ψ_{in} misses the target then there is no scattering

$$\boxed{\text{provided: } \frac{r}{p_0 b^2} \ll 1}$$

$\Rightarrow$ Now we can calculate the scattering prob. for detector not in the path of the unscattered packet $(d\cdot\sin\theta \gg b)$

$$w(\psi_{in} \to d\Omega) = d\Omega\int_0^\infty r^2 dr\,|\psi_{sc}(\vec{r},t)|^2 =$$

$$= d\Omega\,|f(\vec{p}_0 \to p_0\hat{\vec{r}})|^2\int_{-\infty}^{\infty} dz\,|\psi_{in}(\hat{\vec{z}},t)|^2$$

$\hookrightarrow$ ψ_{in} is zero on the neg. axis for $t \gg 0$

Sum over all impact parameters:

$$\Rightarrow \sigma(\psi_{in} \to d\Omega) = \int d^2b\; w(\psi_{in}(b) \to d\Omega) =$$

$$= d\Omega\,|f|^2\cdot\int d^2b\int_{-\infty}^{\infty} dz\,|\psi_{in}(\vec{z} - \vec{b},t)|^2 =$$

wp. shift in plane perp. to $\vec{p}_0$ (and $\vec{z}$)

$$= d\Omega\,|f|^2\cdot\underbrace{\int d^3r\,|\psi_{in}(\vec{r},t)|^2}_{=1 \text{ it is normalized}} = d\Omega\,|f|^2$$

$$\Rightarrow \boxed{\left(\frac{d\sigma}{d\Omega}\right) = |f(\vec{p}_0 \to p_0\cdot\vec{p})|^2}$$

Assumptions on the validity of:

$$\frac{d\sigma}{d\Omega} = |f|^2$$

1) No distortion of the incoming wavepacket: $\frac{t}{mb^2} \ll 1$

$\Longleftrightarrow t = \frac{d}{v_0}$, $\boxed{\frac{d}{p_0 b^2} \ll 1}$

2) Use of the asymptotic form for $\psi^{(+)}_{\vec{p}}(\vec{r})$

$\boxed{a \ll d}$

3) Removal of f outside integral $\boxed{a \ll b}$

4) $p \cdot r \sim \vec{p} \cdot \vec{z}$ $\Leftrightarrow$ $\boxed{d \ll p_0 b^2}$.

5) Unscattered wave not measured $b \ll d \cdot \sin\theta \rightarrow \boxed{b \ll d}$

Together we have:

$$a \ll b \ll d \ll p_0 b^2$$

ALMOST ALWAYS MET

For 10 eV electron ($p \sim 10^{10}\,m^{-1}$) collimated through 1-mm slits ($b \sim 10^{-3} m$), scattering from atom ($a \sim 10^{-10} m$) and detected 1 m away from the target ($d \sim 1 m$)

$$10^{-10} \ll 10^{-3} \ll 1 \ll 10^{4}$$

~~The~~ Orientational averaging for molecules

- the summation over impact pars. is ~~good~~ sufficient only for spherically symmetric targets, i.e. not for molecules
- the molecular amplitude $f^M(\theta, \varphi; R)$ depends on the rotation of the molecular frame with lab frame.
- we need additional averaging ~~over the~~ (summation) over all orientations:

$$\left(\frac{d\sigma}{d\Omega}\right)_{molecular} = \frac{1}{8\pi^2} \int dR\, |f(\theta, \varphi; R)|^2$$

Comment on $\psi^{(-)}(\vec{r})$: this solution has the scattered part only for ~~t~~ $t<0$, for $t>0$ it represents a ~~plane~~ free wavepacket with a well defined outgoing momentum (direction)

$\varphi_{in} \rightarrow \vec{k}$ start to $+$ $\rightarrow \vec{k}$

JD