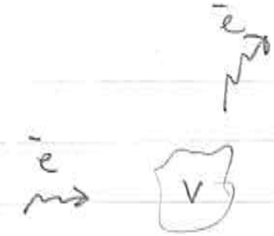
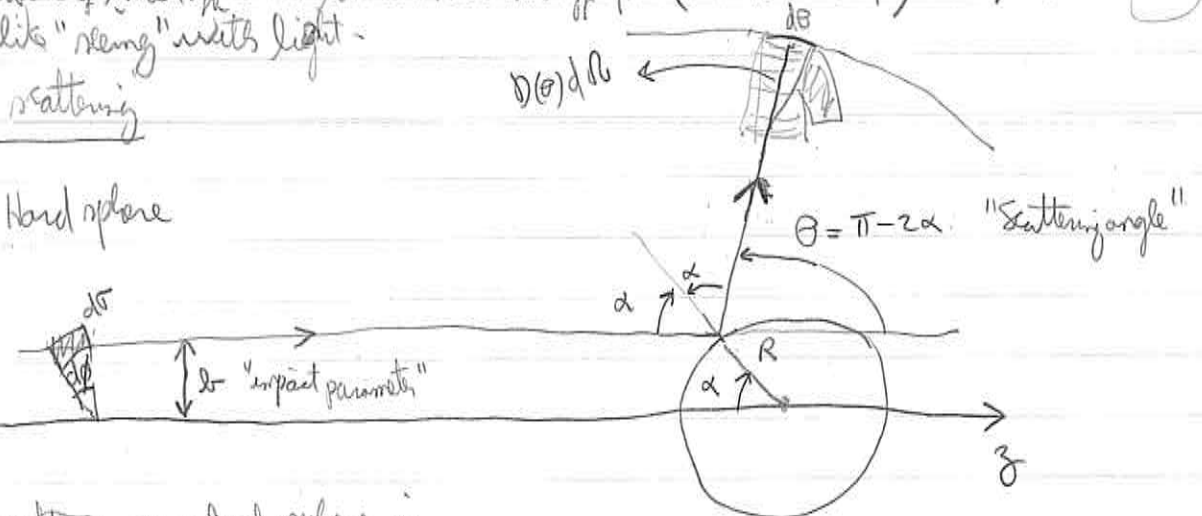


P423 - Lecture 20: Scattering

- Main probe of small effects is to scatter electrons off of it (electron microscope). Just like "seeing" with light.

Classical scattering

Example: Hard sphere



Elastic scattering off a hard sphere is specular (why? Cons. of momentum ⊥ radial vector, which gives direction for the force).

$$b = R\sin(\alpha) = R\sin\left[\frac{\pi}{2} - \frac{\theta}{2}\right] = R\cos\left(\frac{\theta}{2}\right)$$

$$\Rightarrow \quad \theta = \begin{cases} 2\arccos\left(\frac{b}{R}\right) & \text{if } b \le R \\ 0 & \text{if } b > R \end{cases}$$

Differential scattering cross section relates to $b(\theta)$:

$$D(\theta) = \frac{d\sigma}{d\Omega} \Rightarrow d\sigma = D(\theta)\, d\Omega$$ [Particles entering area $d\sigma$ get scattered into area $D(\theta)\, d\Omega$]

But $d\sigma = (b\, d\phi)|db|$ and $d\Omega = \dfrac{(r\sin(\theta)\, d\phi)\, r|d\theta|}{r^2} = \sin(\theta)\, d\phi |d\theta|$

$$\Rightarrow D(\theta) = \frac{d\sigma}{d\Omega} = \frac{b\, \cancel{d\phi} |db|}{\sin(\theta) \cancel{d\phi} |d\theta|} = \frac{b}{\sin(\theta)}\left|\frac{db}{d\theta}\right|$$ (need modulus because when b increases, θ decreases, so $\frac{db}{d\theta} < 0$)

$$\boxed{D(\theta) = \frac{b}{\sin(\theta)}\left|\frac{db}{d\theta}\right|}$$, for hard sphere: $D(\theta) = \dfrac{R\cos(\frac{\theta}{2})}{\sin(\theta)} \dfrac{R}{2}\sin\left(\frac{\theta}{2}\right) = \dfrac{R^2}{2} \dfrac{\cos(\frac{\theta}{2})\sin(\frac{\theta}{2})}{2\sin(\frac{\theta}{2})\cos(\frac{\theta}{2})} = \dfrac{R^2}{4}$ //

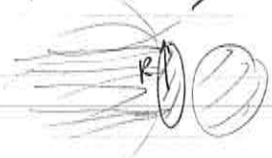
2

The total cross section is:

$$\sigma = \int d\sigma = \int D(\theta)\, d\Omega = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin(\theta)\, D(\theta)$$

Since $D(\theta) = \frac{R^2}{4} = \text{const}$: $\quad \sigma = \frac{4\pi R^2}{4} = \pi R^2$

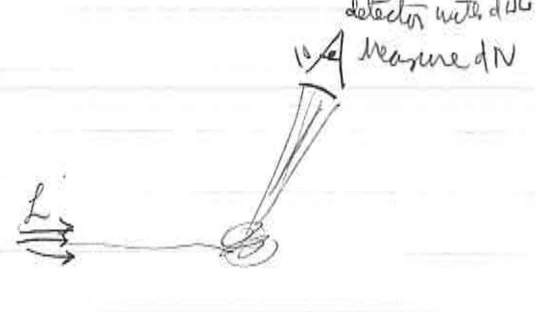
This is just the cross sectional area of the sphere.



Experimental definition of $D(\theta)$:

Flux or luminosity: # of incident particles per unit area, per unit time

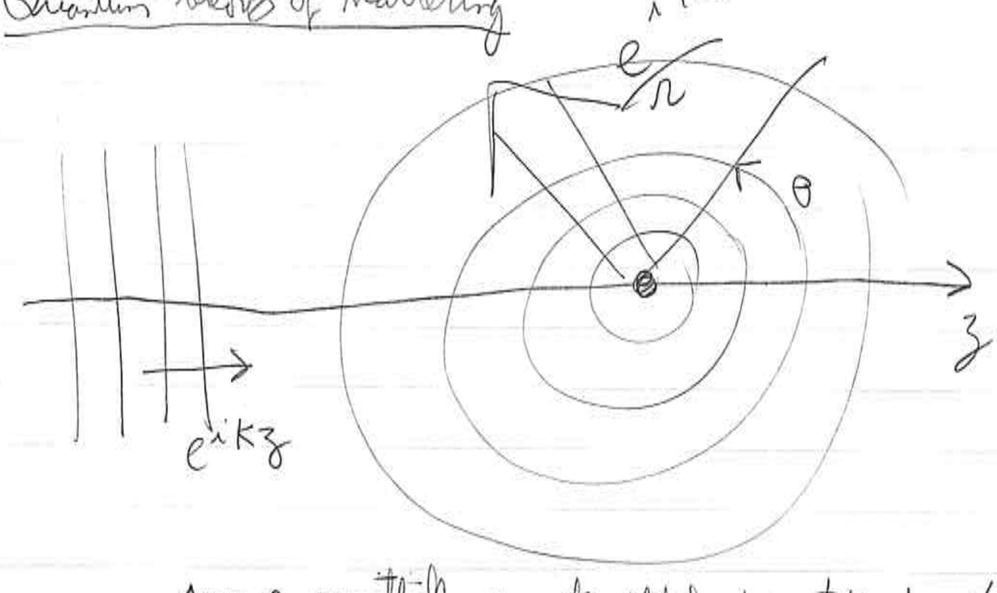
$$\underbrace{\mathcal{L}\, d\sigma}_{= dN} = \mathcal{L}\, D(\theta)\, d\Omega \Rightarrow \boxed{D(\theta) = \frac{1}{\mathcal{L}} \frac{dN}{d\Omega}}$$



$= dN$: # of scattered particles per unit time

Particles entered at $d\sigma$ and scattered at $d\Omega$

<u>Quantum theory of scattering</u>



Assume azimuthally symmetric potential, does not depend on ϕ.

For large r we must have

$$\psi(r,\theta) \approx A\left\{ \underset{\substack{\uparrow \\ \text{incident}}}{e^{ikz}} + \underset{\substack{\uparrow \\ \text{scattered}}}{f(\theta)}\frac{e^{ikr}}{r} \right\} \qquad (\text{large } r)$$

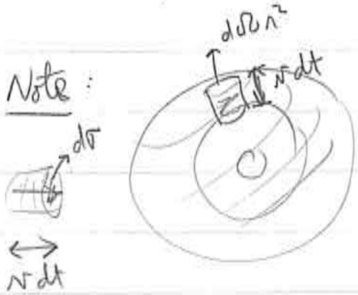
Here $k = \frac{\sqrt{2mE}}{\hbar}$. Spherical wave has to be this way to preserve probability

$dP = |\psi|^2 4\pi r^2$ Can not depend on r.

Later we will prove that this is indeed an asymptotic solution of Schrödinger eqn.

How to compute $D(\theta)$?

Note:



Probability of having particle scattered in dV is:

$$dP = |\psi_{\text{scattered}}|^2 \underbrace{(v\,dt)(d\Omega\, r^2)}_{dV} = |A|^2 \frac{|f(\theta)|^2}{\cancel{r^2}}(v\,dt)\,d\Omega\,\cancel{r^2}$$

Should be the same as probability of having incident particle at $d\sigma$:

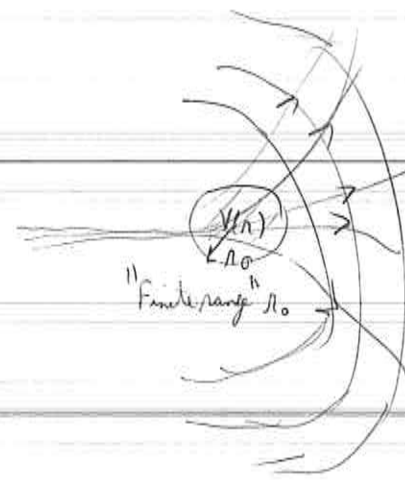
$$dP = |\psi_{\text{incident}}|^2 (v\,dt)\,d\sigma = |A|^2 (v\,dt)\,d\sigma$$

Equate $\Rightarrow$ $\cancel{|A|^2}\cancel{(v\,dt)}\,d\sigma = \cancel{|A|^2}|f(\theta)|^2 \cancel{(v\,dt)}\,d\Omega \Rightarrow |f(\theta)|^2 = \frac{d\sigma}{d\Omega} = D(\theta)$

$$\boxed{D(\theta) = |f(\theta)|^2}.$$

Two techniques to find $f(\theta)$: Partial wave analysis and Born approximation.

Partial wave analysis (Takes advantage of spherical symmetry)



Assume scattering potential is $V = V(r)$ ("spherically symmetric").

Schrödinger eqn: $-\frac{\hbar^2}{2m}\nabla^2\psi + V(r)\psi = \underbrace{\left(\frac{\hbar^2 k^2}{2m}\right)}_{=E \text{ because far away } V(r)=0!}\psi$

$$\psi(r,\theta,\phi) = R(r)\, Y_\ell^m(\theta,\phi)$$

where we write $R(r) = \frac{u(r)}{r}$ for radial eqn, and u satisfies:

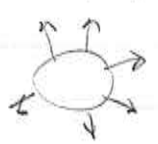
$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \Big[V(r) + \underbrace{\frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}}_{\text{Centrifugal potential}}\Big]u = E\,u$$

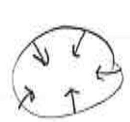
▷ At $r \gg r_0$ we can drop $V(r)$

~~▷ At even larger r we can drop centrifugal ($kr \gg 1$)~~

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} \approx E u \Rightarrow \frac{d^2u}{dr^2} \approx -k^2 u \Rightarrow u(r) \approx C e^{ikr} + D e^{-ikr}$$

$$\Rightarrow R(r) \simeq \underbrace{C\frac{e^{ikr}}{r}}_{\text{"outgoing"}} + \underbrace{D\frac{e^{-ikr}}{r}}_{\text{"Incoming"}}$$





(why? recall $R(r,t) = e^{\pm i(kr - \frac{E}{\hbar}t)}$)
So as time increases, e^{ikr} goes outward, e^{-ikr} goes inward.

For $r_0 < r < \frac{1}{k}$ "intermediate region" we must solve with centrifugal term:

$$\frac{d^2u}{dr^2} - \frac{l(l+1)}{r^2}u = -k^2 u \qquad (r > r_0)$$

General solution is linear comb. of spherical Bessel fncs:

$$u(r) = A\, r\, \underbrace{j_l(kr)}_{\text{like } \frac{\sin(kr)}{r}} + B\, r\, \underbrace{n_l(kr)}_{\text{like } \frac{\cos(kr)}{r}}$$

"Neumann", blows up at $r \to 0$

But what we need are spherical Hankel fncs:

$$h_l^{(1)}(x) = j_l(x) + i\, n_l(x) \qquad h_l^{(2)}(x) = j_l(x) - i\, n_l(x)$$

like $\frac{e^{ikr}}{r}$ "outgoing" like $\frac{e^{-ikr}}{r}$, "incoming".

Thus the exact wave fnc for $r > r_0$ (when $V=0$) is:

$$\psi(r,\theta,\phi) = A\left\{e^{ikz} + \sum_{l,m} C_{lm}\, h_l^{(1)}(kr)\, Y_l^m(\theta,\phi)\right\}$$

Since $Y_l^m(\theta,\phi) \propto e^{im\phi}$ and the outgoing scattered wave can not depend on ϕ, we only have $m=0$: $\quad Y_l^{m=0}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta)$.

For convenience, $C_{l,0} = i^{l+1} k \sqrt{4\pi(2l+1)}\, a_l$:

6

$$\psi(r,\theta) = A\left\{e^{ikz} + k\sum_{l=0}^{\infty} i^{l+1}(2l+1)\underset{\substack{\uparrow \\ l^{\text{th}}\text{ partial wave amplitude.}}}{a_l}\, h_l^{(1)}(kr)\,P_l(\cos\theta)\right\}$$

For very large l, $h_l^{(1)}(kr) \simeq (-i)^{l+1}\dfrac{e^{ikr}}{kr}$ so

$$\psi(r,\theta) \simeq A\left\{e^{ikz} + \underbrace{\left[\sum_{l=0}^{\infty}(2l+1)a_l\,P_l(\cos\theta)\right]}_{f(\theta)}\frac{e^{ikr}}{r}\right\}$$

And

$$D(\theta) = |f(\theta)|^2 = \sum_{l,l'=0}^{\infty}(2l+1)(2l'+1)\,a_l a_{l'}^*\,P_l(\cos\theta)\,P_{l'}(\cos\theta)$$

And

$$\sigma = \int d\Omega\, D(\theta) = 2\pi\int_{-1}^{1} d(\cos\theta)\sum_{l,l'}(2l+1)(2l'+1)\,a_l a_{l'}^*\,P_l(\cos\theta)\,P_{l'}(\cos\theta)$$

Use: $\displaystyle\int_{-1}^{1} d(\cos\theta)\,P_l(\cos\theta)\,P_{l'}(\cos\theta) = \frac{2}{2l+1}\,\delta_{l,l'}$

$$\boxed{\sigma = 4\pi\sum_{l=0}^{\infty}(2l+1)|a_l|^2}$$

<u>How to determine partial wave amplitudes a_l</u>:

Use Rayleigh's formula: $\displaystyle e^{ikz} = \sum_{l=0}^{\infty} i^l(2l+1)\,j_l(kr)\,P_l(\cos\theta)$ into $\psi(r,\theta)$:

$$\psi(r,\theta) = A\sum_{l=0}^{\infty} i^l(2l+1)\left[j_l(kr) + ik\,a_l\,h_l^{(1)}(kr)\right]P_l(\cos\theta)$$

<u>Exact for $r > r_0$</u>

find $u_{k\ell}(r)$ — $r \geq r_0$

Now, we find the solution for $\psi(r,\theta)$ inside the potential region and match to this to get the a_ℓ's.

Example: Quantum hard sphere scattering

$$V(r) = \begin{cases} \infty & \text{for } r \leq R \\ 0 & \text{for } r > R \end{cases}$$

Boundary condition $\psi(R,\theta) = 0$, so

$$\sum_{\ell=0}^{\infty} i^\ell (2\ell+1)\left[j_\ell(kR) + ik a_\ell h_\ell^{(1)}(kR)\right] P_\ell(\cos\theta) = 0$$

Since the $P_\ell(\cos\theta)$ are orthogonal, we must have

$$ik a_\ell h_\ell^{(1)}(kR) = -j_\ell(kR) \Rightarrow \boxed{a_\ell = \frac{i j_\ell(kR)}{k\, h_\ell^{(1)}(kR)}}$$

Total cross section:

$$\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\left|\frac{j_\ell(kR)}{h_\ell^{(1)}(kR)}\right|^2$$

Low energy limit. $kR \ll 1$:

$$j_\ell(kR) \approx 2^\ell \ell!\,(kR)^\ell \frac{1}{(2\ell+1)!}$$

$$h_\ell^{(1)}(kR) = i n_\ell(kR) \approx -(2\ell)!\frac{1}{(kR)^{\ell+1}}\frac{1}{2^\ell \ell!}$$

$$\Rightarrow \sigma \approx \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\left|\frac{2^\ell \ell!(kR)^\ell \frac{1}{(2\ell+1)!}}{\underbrace{(2\ell)!\frac{1}{(kR)^{\ell+1}}\frac{1}{2^\ell \ell!}}}\right|^2 = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}\frac{1}{(2\ell+1)}\left(\frac{2^\ell \ell!}{(2\ell)!}\right)^4 (kR)^{4\ell+2}$$

$$\to \frac{1}{(2\ell+1)}\frac{2^{2\ell}(\ell!)^2 (kR)^{2\ell+1}}{[(2\ell)!]^2}$$

When $kR \ll 1$, only $l=0$ term survives:

$$\sigma \approx \sigma_{l=0} = \frac{4\pi}{k^2}(kR)^2 = 4\pi R^2$$

4 X larger than Classical! As if electron "sensed" the whole sphere surface.

Typical for wave scattering (also happens in optics - You "see" more than what you would expect).

Note that $\hbar \to 0$ limit does not agree with classical mechanics result here.
But it does agree with classical Electrodynamics!