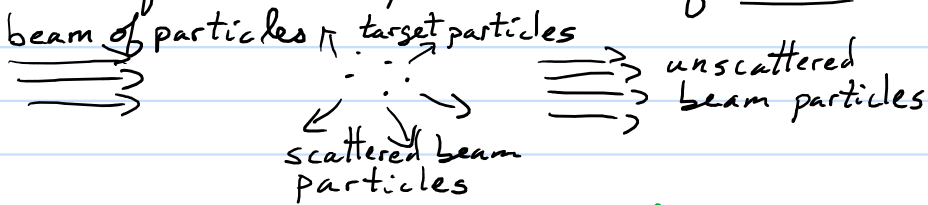
Chapter 10 – Scattering

Scattering is a difficult topic to describe because we don't typically think about it – even classical scattering. Very important to physics: Rutherford α – Au scattering ⇒ nuclei; Rutherford α – Al scatt ⇒ size of nucleus; scattering at CERN ⇒ W, Higgs, etc.

We'll first develop the idea of <u>total</u> cross section $\sigma(E)$



<u>Beer-Lambert Law</u> – Probability a beam particle is scattered during a short length dx is proportional to the density of target particles and the length dx. This means the change in the probability to <u>not</u> scatter is

$$dP = -\underbrace{\rho}_{\text{density of scatterers}} \cdot \sigma \cdot \overbrace{dx}^{\text{length traveled}} \cdot \underbrace{P}_{\text{probability to have not scattered}}$$

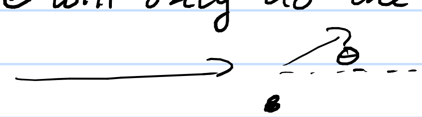
σ = proportionality constant
= cross section
unit = area

$$P = \underbrace{e^{-\rho \cdot \sigma \cdot L}}_{\text{for const. dens.}}$$

L = length traveled through target

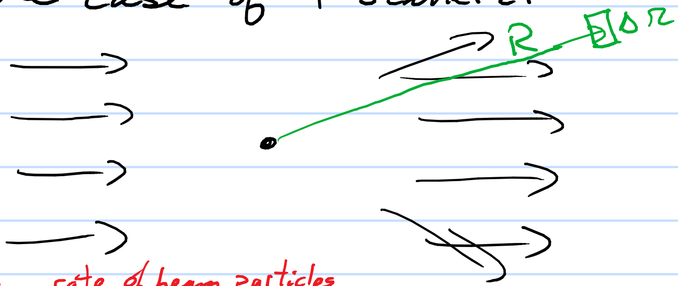
In general, σ depends on the energy, spin, ... of the beam particle.
Example of kid party game: pop the balloon throwing a dart blind folded $\sigma = \pi R^2$ R = radius of balloon

Can get more information if you can measure how much is scattered into each angle. For this first treatment of scattering we will only do the case where scattering is axisymmetric.



Probability to scatter will only depend on Θ; no φ dependence

Do the case of 1 scatterer



Rate through the small angular region is proportional to $\Delta\Omega$ and $\mathcal{L}$

$$\mathcal{L} = \frac{\text{rate of beam particles}}{\text{area}} = \frac{N}{A \cdot t}$$

$$Rate(\Omega, \Delta\Omega) = \mathcal{L}\, \frac{d\sigma}{d\Omega}\, \Delta\Omega$$

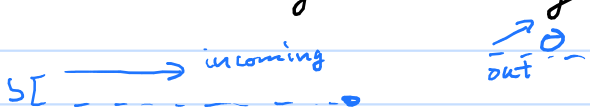
Book $D(\theta) = \frac{d\sigma}{d\Omega}$ ← differential cross section

Integrate Rate over whole sphere except exactly into the forward direction

$$\text{Total Scattering Rate} = \mathcal{L} \int_{4\pi} \frac{d\sigma}{d\Omega}\, d\Omega = \mathcal{L}\, \sigma$$

Does this match our definition from Beer-Lambert

Classically how to get $\frac{d\sigma}{d\Omega} = D(\theta)$??



The final scattering angle is a function of b. We'll look at how to calculate the general case for classical scattering below.

If the beam particles don't disappear the rate that the particles go through b and b+db is

$$Rate = \mathcal{L} \cdot 2\pi b\, db$$

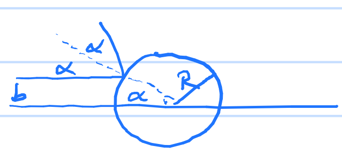
This is the same as the amount going out between $\theta(b)$ and $\theta(b+db)$

$$Rate = \mathcal{L}\, \frac{d\sigma}{d\Omega}\, 2\pi \sin\theta\, |\theta(b+db) - \theta(b)| = \mathcal{L}\, \frac{d\sigma}{d\Omega}\, 2\pi \sin\theta \left|\frac{d\theta}{db}\right| db$$

Combine the two expressions for the classical differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta} \left|\frac{db}{d\theta}\right| = \frac{1}{2} \left|\frac{d\, b^2}{d(\cos\theta)}\right|$$

Example of hard sphere



$$\theta = \pi - 2\alpha \Rightarrow \alpha = \frac{\pi}{2} - \frac{\theta}{2}$$

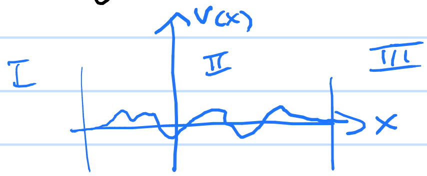
$$\sin(\alpha) = b/R = \sin\left(\frac{\pi}{2} - \frac{\theta}{2}\right) \Rightarrow \quad b = R\cos\left(\frac{\theta}{2}\right)$$

Plug into $\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| = \frac{R\cos(\frac{\theta}{2})\frac{1}{2}R\sin\theta/2}{\sin\theta} = \frac{R^2}{4}$

Calculate the total cross section $\sigma = \int_{4\pi} \frac{d\sigma}{d\Omega}d\Omega = \pi R^2$

Why must this be correct?

The big challenge is to figure out how to do the quantum version of the cross section. To get an idea, first look at 1D scattering



$\psi_I = A e^{ikx} + B e^{-ikx}$

$\psi_{II} =$ some complicated function

$\psi_{III} = C e^{ikx}$

why these forms

Let's do something simple $\psi(x) = Ae^{ikx} + \psi_{scat}(x) \equiv \psi^{(0)} + \psi_{scat}$

$\psi_{scat,I} = Be^{-ikx}$

$\psi_{scat,II} =$ some complicated function $- Ae^{ikx}$

$\psi_{scat,III} = (C-A)e^{ikx}$

The ψ_{scat} is not the solution of Schrodinger's Eq.

$H\psi(x) = E\psi(x) \Rightarrow \left(\frac{p^2}{2m} + V(x)\right)(\psi^{(0)} + \psi_{scat}) = E\psi^{(0)} + V\psi^{(0)} + H\psi_{scat}$

$= E\psi^{(0)} + E\psi_{scat}$

The equation for ψ_{scat}

$H\psi_{scat} = E\psi_{scat} - V(x)\psi^{(0)}$

This shows ψ_{scat} is the solution of an inhomogeneous differential equation

What about 3D? What does the solution have to look like??

$\psi(\vec{r}) = \psi^{(0)} + \psi_{scat} = Ae^{ikz} + \psi_{scat}$

The first term in general is $e^{i\vec{k}\cdot\vec{r}}$. Why do e^{ikz}?

We are doing situations where $V(\vec{r}) = V(r) \Rightarrow$ spherical symmetric

This means ψ_{scat} does not depend on φ. Why?? Also $V(r) = 0$ for $r > r_0$

The ψ_{scat} is the solution of $\frac{p^2}{2m}\psi_{scat} = E\psi_{scat}$ for $r > r_0$

In spherical coordinates, the solution is a superposition of Bessel fcts of r times spherical harmonics.

For $r > r_0$

$$\psi(\vec{r}) = A\left[e^{ikz} + \sum_{\ell m} C_{\ell,m}\, h_\ell^{(1)}(kr)\, Y_\ell^m(\theta,\phi)\right]$$

The $h_\ell^{(1)}(x)$ is a spherical Bessel function with the asymptotic form

$$h_\ell^{(1)}(x) \to \frac{1}{x}(-i)^{\ell+1} e^{ix} \qquad x\to\infty \qquad h_\ell^{(2)}(x) = h_\ell^{(1)}(x)^*$$

Why does ψ_{scat} only have $h^{(1)}$ and not $h^{(2)}$?? Go back to 1D case

For spherically symmetric potential, why $C_{\ell,m} = C_\ell\, \delta_{m,0}$??

Why do we need to sum over ℓ??

Now get the asymptotic form

$$\psi(\vec{r}) \to A\left\{ e^{ikz} + \left[\sum_\ell C_\ell \frac{(-i)^{\ell+1}}{k} Y_\ell^0(\theta,\phi)\right]\right\}\frac{e^{ikr}}{r} \qquad \text{as } r\to\infty$$

$$= A\left[e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right]$$

The scattering amplitude is $f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(-i)^{\ell+1} C_\ell Y_\ell^0(\theta,\varphi)$

A common way of writing this uses $Y_\ell^{(0)}(\theta,\varphi) = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta)$

$$f(\theta) = \sum_{\ell=0}^{\infty} \frac{1}{k}(-i)^{\ell+1}\sqrt{\frac{2\ell+1}{4\pi}}\, C_\ell P_\ell(\cos\theta) = \sum_{\ell=0}^{\infty}(2\ell+1)\, a_\ell P_\ell(\cos\theta) \Rightarrow C_\ell = i^{\ell+1} k\sqrt{4\pi(2\ell+1)}\, a_\ell$$

One of the tricky parts is to figure out how to use ψ to obtain the differential cross section. Just do it!

$$\text{Rate}(\Omega,\Delta\Omega) = \mathcal{L}\,\frac{d\sigma}{d\Omega}\,\Delta\Omega$$

Start with $\mathcal{L}$

$$\mathcal{L} = \hat{z}\cdot\vec{J} = \hat{z}\cdot\frac{\hbar}{2im}\left[\psi^{(0)*}\vec{\nabla}\psi^{(0)} - \psi^{(0)}\vec{\nabla}\psi^{(0)*}\right] = |A|^2\frac{\hbar k}{m}$$

Does this make sense?

Now do the scattered

Use $\vec{\nabla} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \varphi}$

$$\vec{J}_{scat} = \frac{\hbar}{2im}\left[\psi^*_{scat}\vec{\nabla}\psi_{scat} - \psi_{scat}\vec{\nabla}\psi^*_{scat}\right]$$

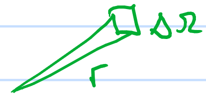
$$= \frac{\hbar|A|^2}{2im}\left[f^*(\theta)\frac{e^{-ikr}}{r}\left(\vec{\nabla} f(\theta)\frac{e^{ikr}}{r}\right) - f(\theta)\frac{e^{ikr}}{r}\vec{\nabla}\left(f^*(\theta)\frac{e^{-ikr}}{r}\right)\right] \quad \text{as } r \to \infty$$

Drop all terms proportional to $1/r^3$. Why?

$$= (\hbar/2im)|Af(\theta)|^2\left[\frac{e^{-ikr}}{r}\frac{\partial}{\partial r}\left(\frac{e^{ikr}}{r}\right) - \frac{e^{ikr}}{r}\frac{\partial}{\partial r}\left(\frac{e^{-ikr}}{r}\right)\right]\hat{r}$$

$$= \frac{\hbar k}{m}|A|^2|f(\theta)|^2\frac{1}{r^2}$$

Compute the rate through the area



Area $= r^2\Delta\Omega$

$$\text{Rate}(\Omega,\Delta\Omega) = \hat{r}\cdot\vec{J}_{scat}\, r^2\Delta\Omega = \frac{\hbar k}{m}|A^2|\,|f(\theta)|^2\cancel{\frac{1}{r^2}}\cancel{r^2}\Delta\Omega$$

Plug back into the definition

$$\text{Rate}(\Omega,\Delta\Omega) = \mathcal{L}\frac{d\sigma}{d\Omega}\Delta\Omega$$

$$\frac{\hbar k}{m}|A^2|\,|f(\theta)|^2\Delta\Omega = \frac{\hbar k}{m}|A|^2\frac{d\sigma}{d\Omega}\Delta\Omega$$

The differential cross section is $\frac{d\sigma}{d\Omega} = |f(\theta)|^2$ So simple!!!

Before going on, there is a simple formula for the <u>total</u> cross section.

$$\sigma = \int\frac{d\sigma}{d\Omega}d\Omega = 2\pi\int_{-1}^{1}|f(\theta)|^2\,d(\cos\theta)$$

$$= 2\pi\sum_{\ell=0}^{\infty}\sum_{\ell'=0}^{\infty}a^*_\ell a_{\ell'}(2\ell+1)(2\ell'+1)\int_{-1}^{1}P_\ell(\cos\theta)P_{\ell'}(\cos\theta)\,d(\cos\theta)$$

The integral is $\frac{2}{2\ell+1}\delta_{\ell\ell'}$

$$\sigma = 4\pi\sum_{\ell=0}^{\infty}(2\ell+1)|a_\ell|^2$$

The rest of the chapter is about how to compute the scattering amplitude: $f(\theta)$.

First, we're going to connect to the solution of the radial Schrodinger eq. Remember

$$-\frac{\hbar^2}{2m}\frac{d^2 u_{E,\ell}(r)}{dr^2} + \left(V(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2}\right) u_{E,\ell}(r) = E\, u_{E,\ell}(r)$$

The $u_{E,\ell}(r) \sim C\, r^{\ell+1}$ as $r \to 0$

$\sim D_{E,\ell} \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right)$ as $r \to \infty$ The $\frac{\ell\pi}{2}$ so $\delta_\ell = 0$ for $V=0$.

The ψ is made by superposing the different ℓ terms

$$\psi(\vec{r}) = \sum_\ell A_{E,\ell} \frac{u_{E,\ell}(r)}{r} Y_\ell^0(\cos\theta)$$ Note the $=$ and no restriction

Very tricky how to know what the $A_{E,\ell}$ should be.

Go back to the original equation for ψ on pg 4

$$\psi(\vec{r}) \underset{r>r_0}{=} A\left[e^{ikz} + \sum_{\ell=0}^{\infty} i^{\ell+1} k(2\ell+1) a_\ell\, h_\ell^{(1)}(kr) P_\ell(\cos\theta)\right]$$

Now use $e^{ikz} = \sum_{\ell=0}^{\infty} i^\ell (2\ell+1) j_\ell(kr) P_\ell(\cos\theta)$ Show how to get this?

$$\psi(\vec{r}) \underset{r>r_0}{=} A \sum_{\ell=0}^{\infty} i^\ell (2\ell+1)\left[j_\ell(kr) + ik a_\ell\, h_\ell^{(1)}(kr)\right] P_\ell(\cos\theta)$$

Compare the two forms at large r

$$\frac{\sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right)}{r} = k\left[j_\ell(kr)\cos(\delta_\ell) - n_\ell(kr)\sin(\delta_\ell)\right]$$ Show?

$$A\, i^\ell (2\ell+1)\left[j_\ell + ik a_\ell (j_\ell + i n_\ell)\right] = \overbrace{A_{E\ell} D_{E\ell}}^{\tilde{A}_{E\ell}} \left[j_\ell \cos\delta_\ell - n_\ell \sin\delta_\ell\right]$$

$$-\tan\delta_\ell = \frac{-k a_\ell}{1 + ik a_\ell} \Rightarrow (1 + ik a_\ell)\tan\delta_\ell = k a_\ell$$

$$\tan\delta_\ell = k(1 - i\tan\delta_\ell)\, a_\ell$$

$$a_\ell = \frac{1}{k}\frac{\tan\delta_\ell}{1 - i\tan\delta_\ell}$$

$$a_\ell = \frac{1}{k}\sin\delta_\ell\, e^{i\delta_\ell}$$

Plug this into the scattering cross sections

$$f(\theta) = \frac{1}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\sin\delta_\ell\, e^{i\delta_\ell} P_\ell(\cos\theta)$$ and $$\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell$$

Example: Hard sphere scattering $V(r) = \infty \quad r<a$
$ = 0 \quad r>a$

Calculate the phase shift

$$j_\ell(ka)\cos\delta_\ell - n_\ell(ka)\sin\delta_\ell = 0 \quad = \quad \tan\delta_\ell = \frac{j_\ell(ka)}{n_\ell(ka)}$$

$$\sin\delta_\ell e^{i\delta_\ell} = \frac{\tan\delta_\ell}{1-i\tan\delta_\ell} = \frac{j_\ell(ka)}{n_\ell(ka) - i j_\ell(ka)} = i\frac{j_\ell(ka)}{j_\ell(ka) + i n_\ell(ka)} = i\frac{j_\ell(ka)}{h_\ell^{(1)}(ka)}$$

Compute the scattering amplitude

$$f_E(\theta) = \frac{i}{k}\sum_{\ell=0}^{\infty}(2\ell+1)\left(j_\ell(ka)/h_\ell^{(1)}(ka)\right)P_\ell(\cos\theta)$$

and the total cross section

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

What happens as $E \to 0$ $\quad j_\ell(ka) \to \frac{2^\ell \ell!}{(2\ell+1)!}(ka)^\ell \qquad h_\ell^{(1)}(ka) \to -i\frac{(2\ell)!}{2^\ell \ell!}(ka)^{-(\ell+1)}$

$$f_E(\theta) \simeq \frac{i}{k}\sum_{\ell=0}^{\infty}(2\ell+1)(ka)^{2\ell+1}\frac{(2^\ell \ell!)^2}{(2\ell+1)((2\ell)!)^2}\frac{1}{-i}P_\ell(\cos\theta) \simeq -a \quad (\text{only } \ell=0)$$

$$\sigma(E) = \int_{4\pi}|-a|^2 d\Omega = 4\pi a^2$$ This is 4x the classical result. The whole surface area! Why?

Do an estimate when $ka \gg 1$.

$j_\ell(ka) \sim \sin(ka - \ell\pi/2)/(ka) \qquad h_\ell^{(1)}(ka) \sim -i\frac{e^{i(ka-\ell\pi/2)}}{ka}$

when $\ell \ll ka$ otherwise $j \to 0$

$$\sigma(E) \simeq \frac{4\pi}{k^2}\sum_{\ell=0}^{ka}(2\ell+1)\frac{\sin^2(ka - \frac{\ell\pi}{2})}{\cancel{k^2} a^2}\cancel{(k^2 a^2)} \simeq \frac{4\pi}{k^2}\sum_{\ell=0}^{ka}(2\ell+1)\frac{1}{2} \simeq \frac{2\pi}{k^2}\,\ell^2\Big|_0^{ka} = 2\pi a^2$$

This is 2X larger than classical.

Look at the plots. "Bright spot" in forward direction gives extra πa^2.

Green's function method: Now we'll develop a method that has similarity in style to the two methods for getting electrostatic potential

$$\nabla^2 V(\vec{r}) = -\rho(\vec{r})/\varepsilon_0 \quad \Longleftrightarrow \quad V(\vec{r}) = \int \frac{\rho(\vec{r}\,')}{4\pi\varepsilon_0|\vec{r}-\vec{r}\,'|}d^3\vec{r}\,'$$

This relationship uses $\nabla^2\frac{1}{|\vec{r}-\vec{r}\,'|} = -4\pi\,\delta(\vec{r}-\vec{r}\,')$

First show $\nabla^2 \frac{1}{r} = -4\pi\delta(\vec{r})$

$$\nabla^2 F(r) = \frac{1}{r}\frac{\partial^2}{\partial r^2}(rF) + \frac{1}{r^2}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \cancel{\frac{\partial F}{\partial\theta}}\right)^{\to 0} + \frac{1}{r^2\sin^2\theta}\cancel{\frac{\partial^2 F}{\partial\varphi^2}}^{\to 0}$$

For $F = 1/r$ $\quad \nabla^2 F = \frac{1}{r}\frac{\partial^2}{\partial r^2}\left(r\frac{1}{r}\right) = 0$ unless $r=0$ why?

To see how to handle the singularity do $1/(r+\varepsilon)$

$$\nabla^2 \frac{1}{r+\varepsilon} = \frac{1}{r}\frac{\partial^2}{\partial r^2}\left(\frac{r}{r+\varepsilon}\right) = \frac{1}{r}\frac{\partial^2}{\partial r^2}\left(1 - \frac{\varepsilon}{r+\varepsilon}\right) = -\frac{2\varepsilon}{r(r+\varepsilon)^3}$$

Clearly this is peaked at $r=0$, but is it a δ-function?

$$4\pi\int_0^\infty -\frac{2\varepsilon}{r(r+\varepsilon)^3}\, r^2 dr = -8\pi\varepsilon\int_0^\infty \frac{r+\varepsilon-\varepsilon}{(r+\varepsilon)^3}\, dr = -8\pi\varepsilon\int_0^\infty \frac{1}{(r+\varepsilon)^2} - \frac{\varepsilon}{(r+\varepsilon)^3}\, dr$$

$$= -8\pi\varepsilon\left[-\frac{1}{r+\varepsilon} + \frac{\varepsilon}{2(r+\varepsilon)^2}\right]\Big|_0^\infty = -8\pi\varepsilon\left[-\,-\frac{1}{\varepsilon} + -\frac{1}{2\varepsilon}\right] = -4\pi \quad \checkmark$$

Q.E.D.

How to use this kind of idea for the Schrodinger Eq.?

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi = \frac{\hbar^2 k^2}{2m}\psi \implies \nabla^2\psi + k^2\psi = \frac{2mV(\vec{r})}{\hbar^2}\psi \equiv Q(\vec{r})$$

We need a function that is the solution of

$$\nabla^2 G(\vec{r}) + k^2 G(\vec{r}) = \delta(\vec{r})$$

Green's function

If $k=0$ then $G(\vec{r}) = -\frac{1}{4\pi r}$

The solution of $\nabla^2 G + k^2 G = 0^{\,r\neq 0}$ is the $j_0(kr), n_0(kr), h_0^{(1)}(kr), h_0^{(2)}(kr)$

The $n_0, h_0^{(1)}, h_0^{(2)}$ diverge at small r and so could be the δ-function

$G_s(\vec{r}) = -\frac{\cos(kr)}{4\pi r}$ will work $\qquad G_\pm = -\frac{e^{\pm ikr}}{4\pi r}$ will work

Which one to use?? We will look at the new Schrodinger eq. to figure it out.

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \int G(\vec{r}-\vec{r}\,')\, Q(\vec{r}\,')\, d^3\vec{r}\,' \qquad \nabla^2\psi_0 + k^2\psi_0 = 0$$

Plug in to show this works

$$\nabla^2\psi + k^2\psi = \nabla^2\psi_0 + k^2\psi_0 + \int \left[\nabla^2 G(\vec{r}-\vec{r}\,') + k^2 G(\vec{r}-\vec{r}\,')\right] Q(\vec{r}\,')\, d^3\vec{r}\,'$$

$$= \quad 0 \quad + \int \delta(\vec{r}-\vec{r}\,')\, Q(\vec{r}\,')\, d^3\vec{r}\,'$$

$$= Q(\vec{r}) \qquad \text{QED.}$$

We can connect this to our previous notation

$$\psi(\vec{r}) = \psi_0(\vec{r}) + \psi_{scat}(\vec{r})$$

$$\psi_{scat}(\vec{r}) = \int G(\vec{r}-\vec{r}\,')\, Q(\vec{r}\,')\, d^3r' = \frac{2m}{\hbar^2}\int G(\vec{r}-\vec{r}\,')\, V(\vec{r}\,')\, \psi(\vec{r}\,')\, d^3r'$$

Since $\psi_{scat} \propto \frac{e^{ikr}}{r} \Rightarrow G = G_+$ why??

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

See book for alternative derivation

This equation is hard to use compared to the Poisson eq. because ψ is also under the integral. This is an integral eq.

It is especially hard to use because the large r behavior has to match the type of Green's function used as well as the $\psi_0(\vec{r})$.

An interesting equation for the scattering amplitude can be derived from the integral equation.

Remember $\psi(\vec{r}) = \psi_0(\vec{r}) + f(\theta)\frac{e^{ikr}}{r}$ as $r \to \infty$

$$|\vec{r}-\vec{r}\,'| = \sqrt{r^2 - 2\vec{r}\cdot\vec{r}\,' + r'^2} = r\sqrt{1 - \frac{2\vec{r}\cdot\vec{r}\,'}{r^2} + \frac{r'^2}{r^2}} \simeq r - \hat{r}\cdot\vec{r}\,' \quad \text{as } r \to \infty$$

Plug this into the integral equation

$$\psi(\vec{r}) = \psi_0(\vec{r}) - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int e^{-ik\hat{r}\cdot\vec{r}\,'}\, V(\vec{r}\,')\, \psi(\vec{r}\,')\, d^3r'$$

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

If you know ψ, you can get the scattering amplitude from this equation! But, if you know ψ, then you know f !!

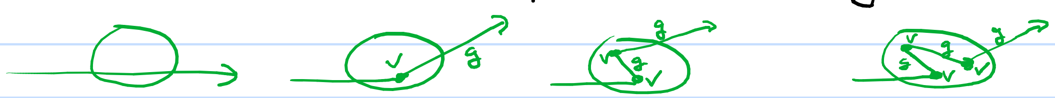
This equation is useful for developing a perturbative expansion of the wave function or scattering amplitude in powers of V

$$\psi(\vec r) = \psi_0(\vec r) - \frac{m}{2\pi\hbar^2}\int G(\vec r - \vec r\,')\, V(\vec r\,')\,\psi(\vec r\,')\, d^3r'$$

$$= \psi_0(\vec r) - \frac{m}{2\pi\hbar^2}\int G(\vec r - \vec r\,')\, V(\vec r\,')\,\psi_0(\vec r\,')\, d^3r' + \left(\frac{m}{2\pi\hbar^2}\right)^2 \iint G(\vec r - \vec r\,')\, V(\vec r\,')\, G(\vec r\,' - \vec r\,'')\, V(\vec r\,'')\,\psi(\vec r\,'')\, d^3r''\, d^3r'$$

etc.

This can be interpreted in a Feynman diagram-ish way



$$\psi = \psi_0 + \int g V \psi_0 + \iint g V g V \psi_0 + \iiint g V g V g V \psi_0 \;\ldots$$

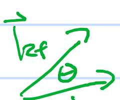
The first order Born approximation results when you stop at the first term

$$f_{\vec k_i}(\hat k_f) \equiv -\frac{m}{2\pi\hbar^2}\int e^{-i\vec k_f\cdot\vec r\,'}\, V(\vec r\,')\,\psi_0(\vec r\,')\, d^3\vec r\,' = -\frac{m}{2\pi\hbar^2}\int e^{i(\vec k_i - \vec k_f)\cdot\vec r\,'}\, V(\vec r\,')\, d^3\vec r\,'$$

$\hbar\vec k_i$ is the initial momentum; $\hbar\vec k_f$ is the final momentum

This works even when $V(\vec r)$ is not spherically symmetric. However, there is a further simplification when V is spherically symmetric

$\vec K \equiv \vec k_i - \vec k_f$



$K = k\sqrt{2 - 2\cos\theta} = 2k\sin\left(\frac{\theta}{2}\right)$

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int_0^\infty\int_{-1}^{1}\int_0^{2\pi} e^{iKr'\cos\theta'}\, V(r')\, r'^2\, d\phi'\, d(\cos\theta')\, dr'$$

$$= -\frac{m}{\hbar^2}\int_0^\infty\int_{-1}^{1} e^{iKr'\cos\theta'}\, V(r')\, r'^2\, d(\cos\theta')\, dr'$$

$$= -\frac{2m}{\hbar^2 K}\int_0^\infty \sin(Kr')\, V(r')\, r'\, dr'$$

In the limit of low energy $K \to 0$

$$f_{low}(\theta) = -\frac{2m}{\hbar^2}\int_0^\infty r'^2\left(1 - \frac{K^2 r'^2}{6}\right) V(r')\, dr'$$

1^{st} Born example: $V(\vec{r}) = \alpha\, \delta(\vec{r})$ units of α?

$$f_{\vec{k}_i}(\vec{k}_f) = -\frac{m}{2\pi\hbar^2}\int e^{i(\vec{k}_i-\vec{k}_f)\cdot\vec{r}\,'}\alpha\,\delta(\vec{r}\,')\,d^3\vec{r}\,' = -\frac{m\alpha}{2\pi\hbar^2} \quad \text{a constant}$$

$$\frac{d\sigma}{d\Omega} = |f|^2 = \frac{m^2\alpha^2}{4\pi^2\hbar^4} \implies \sigma = \frac{m^2\alpha^2}{\pi\hbar^4}$$

1^{st} Born example: $V(\vec{r}) = V_0 \quad r<r_0$ at low E
$\qquad = 0 \quad r>r_0$

$$f_{low} = -\frac{2m}{\hbar^2}\int_0^\infty r'^2\left(1-\frac{K^2r'^2}{6}\right)V(r')\,dr' = -\frac{2m}{\hbar^2}V_0\int_0^{r_0} r'^2 - \frac{K^2r'^4}{6}\,dr'$$

$$= -\frac{2mV_0}{\hbar^2}\frac{r_0^3}{3}\left(1-\frac{K^2r_0^2}{10}\right) \qquad K^2 = 2k^2(1-\cos\theta)$$

$$= \frac{-2mV_0}{\hbar^2}\frac{r_0^3}{3}\left(1-\frac{k^2r_0^2}{5}+\frac{k^2r_0^2}{5}\cos\theta\right) \quad \text{Note goes to constant as } k\to 0$$

$$\frac{d\sigma}{d\Omega} = \left(\frac{2mV_0r_0^3}{3\hbar^2}\right)^2\left(1-\frac{k^2r_0^2}{5}+\frac{k^2r_0^2}{5}\cos\theta\right)^2 \simeq \left(\frac{2mV_0r_0^3}{3\hbar^2}\right)^2\left(1-\frac{2k^2r_0^2}{5}+\frac{2k^2r_0^2}{5}\cos\theta\right)$$

$$\sigma \simeq 4\pi\left(\frac{2mV_0r_0^3}{3\hbar^2}\right)^2\left(1-\frac{2k^2r_0^2}{5}\right)$$

1^{st} Born example: Yukawa potential $V(\vec{r}) = \beta\frac{e^{-\mu r}}{r}$

$$f(\theta) = -\frac{2m\beta}{\hbar^2K}\int_0^\infty e^{-\mu r}\sin(Kr)\,dr = -\frac{2m\beta}{\hbar^2K}\,\mathrm{Im}\left[\int_0^\infty e^{-\mu r}e^{iKr}\,dr\right]$$

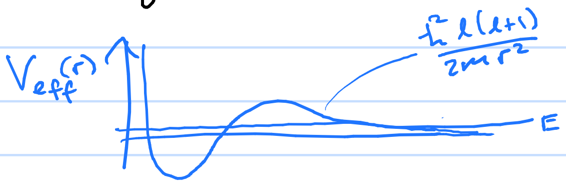
$$= -\frac{2m\beta}{\hbar^2(\mu^2+K^2)} = -\frac{2m\beta}{\hbar^2(\mu^2+2k^2-2k^2\cos\theta)}$$

Coulomb scattering when $\mu\to 0$. Should not be a good approximation but gives exact result

Scattering length example: We have seen a couple cases for low energy scattering going to a constant, isotropic cross section at low energy. Is there a way to see that this is a general feature?

We're dealing with a short range potential $V(\vec{r}) \simeq 0$ for $r > r_0$

First show that all phase shifts go to 0 very quickly as $E \to 0$ for $l > 0$.



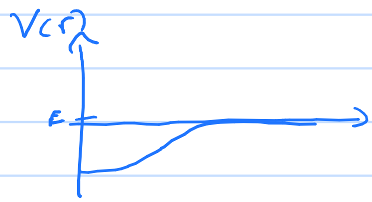
Turning point $\frac{\hbar^2 l(l+1)}{2mr^2} = \frac{\hbar^2 k^2}{2m}$

$r \sim (l + 1/2)/k$ goes to $r \to \infty$ as $k \to 0$

Have to tunnel large distance

This means $f(\theta) \simeq \frac{1}{k} e^{i\delta_0} \sin\delta_0$

Now do the $l=0$



The $u(r)$ hardly has energy dependence at r_0. Why?

Match to outer $l=0$ solution
$$u(r) = A\sin(kr + \delta_0)$$
$$u'(r) = A k\cos(kr + \delta_0)$$

$$\tan(kr_0 + \delta_0) = k\frac{u(r_0)}{u'(r_0)}$$

$$\delta_0 = \operatorname{atan}\left(k\frac{u(r_0)}{u'(r_0)}\right) - kr_0 \simeq k\left[\frac{u(r_0)}{u'(r_0)} - r_0\right] \quad \text{as} \quad k \to 0$$

$$f(\theta) \to \frac{\delta_0}{k} = -\left(r_0 - \frac{u(r_0)}{u'(r_0)}\right) \quad \text{as} \quad k \to 0$$

At low energy, all short range potentials have the same form for the scattering amplitude. The combination

$$r_0 - \frac{u(r_0)}{u'(r_0)} = a \quad \text{as } k \to 0 \qquad a \equiv \text{scattering length}$$

This concept is used extensively in cold scattering, BEC's...

There are many different kinds of variational principles that are useful in scattering calculations: Kohn var. princ., Schwinger var. princ., R-matrix method

Scattering by identical particles has a qualitatively new feature. This comes from having to correctly put in symmetry (Bosons) or antisymmetry (Fermions).

First go to center of mass coordinates. $X = \frac{x_1 + x_2}{2}$ $x = x_1 - x_2$

$$H = -\frac{\hbar^2}{2M}\nabla_{\vec{R}}^2 + -\frac{\hbar^2}{2\mu}\nabla_{\vec{r}}^2 + V(\vec{r})$$

For the total coordinate $1 \leftrightarrow 2$ unchanged $\vec{R} \to \vec{R}$
For the relative coordinate $1 \leftrightarrow 2$ reverse $\vec{r} \to -\vec{r}$
This means the wave function for $\vec{R}$ can have <u>any</u> form.
However, the $\psi_\pm(-\vec{r}) = \pm\psi(\vec{r})$

Cases

$s_1 = s_2 = 0 \Rightarrow$ Boson $\Rightarrow \psi(\vec{r}) = \psi(-\vec{r}) \Rightarrow \ell = 0, 2, 4, \ldots$

$s_1 = s_2 = 1/2 \Rightarrow$ Fermion $\Rightarrow$ $S=1$ $\psi(\vec{r}) = -\psi(-\vec{r}) \Rightarrow \ell = 1, 3, 5, \ldots$
$S=0$ $\psi(\vec{r}) = \psi(-\vec{r}) \Rightarrow \ell = 0, 2, 4, \ldots$

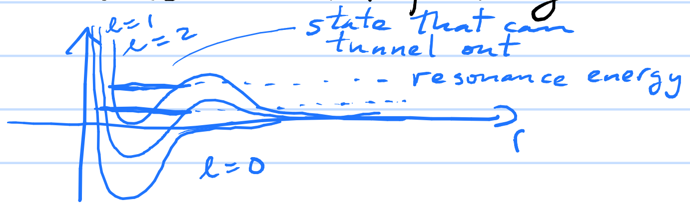
$s_1 = s_2 = 1 \Rightarrow$ Boson $\Rightarrow$ $S = 0$ or 2 $\psi(\vec{r}) = \psi(-\vec{r}) \Rightarrow \ell = 0, 2, 4, \ldots$
$S = 1$ $\psi(\vec{r}) = -\psi(-\vec{r}) \Rightarrow \ell = 1, 3, \ldots$

$s_1 = s_2 = 3/2 \Rightarrow$ Fermion $\Rightarrow$ $S = 1$ or 3 $\psi(\vec{r}) = -\psi(-\vec{r}) \Rightarrow \ell = 1, 3, 5, \ldots$
$S = 0$ or 2 $\psi(\vec{r}) = \psi(-\vec{r}) \Rightarrow \ell = 0, 2, 4, \ldots$

At low energy, Fermions with aligned spin have $S = 2s_1$ and must have $\ell = 1, 3, \ldots$ At low energy, $\ell = 1$ scattering goes to 0 as $E \to 0$. Scattering between Fermions can be suppressed at low temperature.

Atoms have internal structure which can give more complicated behavior, even at low energy. One of the important features is resonance because can enhance scattering.

Shape resonance: Combination of attractive short range potential and repelling $\hbar^2 l(l+1)/2mr^2$

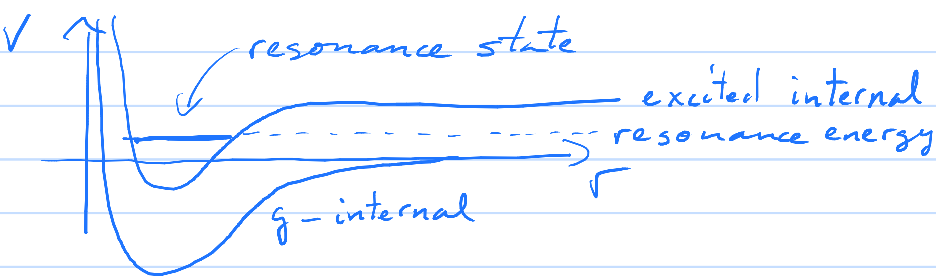


Example - low energy e^- + molecule → vibrational excitation

Show example $e^- + H_2, N_2, O_2$

Example e^- + DNA (!)

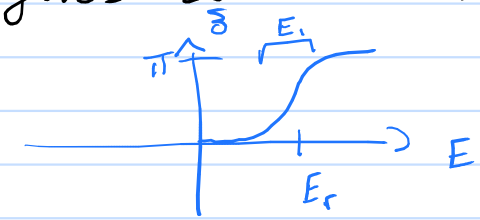
Another example is Feshbach resonance because put energy into internal state



Crude approx $\tan\delta_l(E) \approx -\frac{E_1}{E-E_R}$

cross section $\sim \sin^2\delta_l = \frac{\tan^2\delta_l}{1+\tan^2\delta_l} = \frac{E_1^2}{(E-E_R)^2+E_1^2}$

gives Lorentzian FWHM $= 2E_1$



R-matrix method is used to obtain the log derivative at an r_0. To see how it works, I'll do the case of a spherically symmetric potential. Want the log-derivative for $u_{E,\ell}(r)$ at r_0.

As with the energy variational principle assume

$u_t = u + \delta u$ where $-\frac{\hbar^2}{2m}u'' + V_{eff}\,u = E\,u$

Look at the following

$$\left[\int_0^{r_0} \frac{\hbar^2}{2m} u_t' u_t' + (V_{eff} - E)u_t u_t \, dr\right] / u_t^2(r_0)$$

$$= \left\{\frac{\hbar^2}{2m} u_t(r_0) u_t'(r_0) + \int_0^{r_0} u_t\left[-\frac{\hbar^2}{2m}u_t'' + V_{eff}u_t - Eu_t\right] dr\right\} / u_t^2(r_0)$$

$$= \left\{\frac{\hbar^2}{2m} u_t(r_0) u_t'(r_0) + \int_0^{r_0} \cancelto{u}{u_t}\left[-\frac{\hbar^2}{2m}\delta u'' + (V_{eff} - E)\delta u\right] dr\right\} / u_t^2(r_0) \quad + O(\delta u^2)$$

$$= \left\{\frac{\hbar^2}{2m} u_t(r_0) u_t'(r_0) + \int_0^{r_0} \frac{\hbar^2}{2m}\frac{d}{dr}\left(u'\delta u - u\,\delta u'\right) + \delta u\,\cancelto{0}{\left[-\frac{\hbar^2}{2m}u'' + (V_{eff} - E)u\right]} \; dr\right\} / u_t^2(r_0)$$

$$= \left\{\frac{\hbar^2}{2m} u_t(r_0) u_t'(r_0) + \frac{\hbar^2}{2m}\left(u'(r_0)\,\delta u(r_0) - u(r_0)\,\delta u'(r_0)\right)\right\} / u_t^2(r_0)$$

$$= \frac{\hbar^2}{2m}\left\{ u(r_0)u'(r_0) + \delta u(r_0)\,u'(r_0) + \cancel{u(r_0)\,\delta u'(r_0)} + u'(r_0)\,\delta u(r_0) - \cancel{u(r_0)\,\delta u'(r_0)}\right\} / u_t^2(r_0)$$

$$= \frac{\hbar^2}{2m}\, u'(r_0)\left(u(r_0) + 2\delta u(r_0)\right) / \left(u^2(r_0) + 2u(r_0)\,\delta u(r_0)\right)$$

$$= \frac{\hbar^2}{2m}\,\frac{u'(r_0)}{u(r_0)} \quad + \quad O(\delta u^2)$$

Cool!

$$\frac{u'(r_0)}{u(r_0)} = \left\{\frac{2m}{\hbar^2}\int_0^{r_0} \frac{\hbar^2}{2m} u_t' u_t' + (V_{eff} - E)u_t^2 \, dr\right\} / u_t^2(r_0) \quad + \quad O(\delta u^2)$$

Example: $V_{eff}(r) = 0$ $\quad u_t(r) = r \quad u(r) = A\sin(kr) \Rightarrow \frac{u'}{u} = k\cot(kr_0)$

$$\left(\frac{u'}{u}\right)_{var} = \left\{\frac{2m}{\hbar^2}\int_0^{r_0} \frac{\hbar^2}{2m} - E r^2 \, dr\right\} / r_0^2 = \frac{1}{r_0^2}\left(r_0 - \frac{k^2 r_0^3}{3}\right) = \frac{1}{r_0} - \frac{k^2 r_0}{3}$$

$$k/\tan(kr_0) = \frac{k}{kr_0 + \frac{k^3 r_0^3}{3}} = \frac{1}{r_0\left(1 + \frac{k^2 r_0^2}{3}\right)} \simeq \frac{1}{r_0} - \frac{k^2 r_0}{3} \quad \checkmark \text{ Cool}$$

In "real" calculations $u_t = c_1 y_1 + c_2 y_2 + c_3 y_3 + \ldots$

The equations are rewritten as

$$\underbrace{\left(\frac{u'}{u}\right)_{var} u_t^2}_{\text{matrix}} = \underbrace{\int_0^{r_0} \frac{\hbar^2}{2m} u_t' u_t' + \left(V_{eff} - E\right) u_t^2 \, dr}_{\text{matrix}}$$

Gives generalized matrix equation