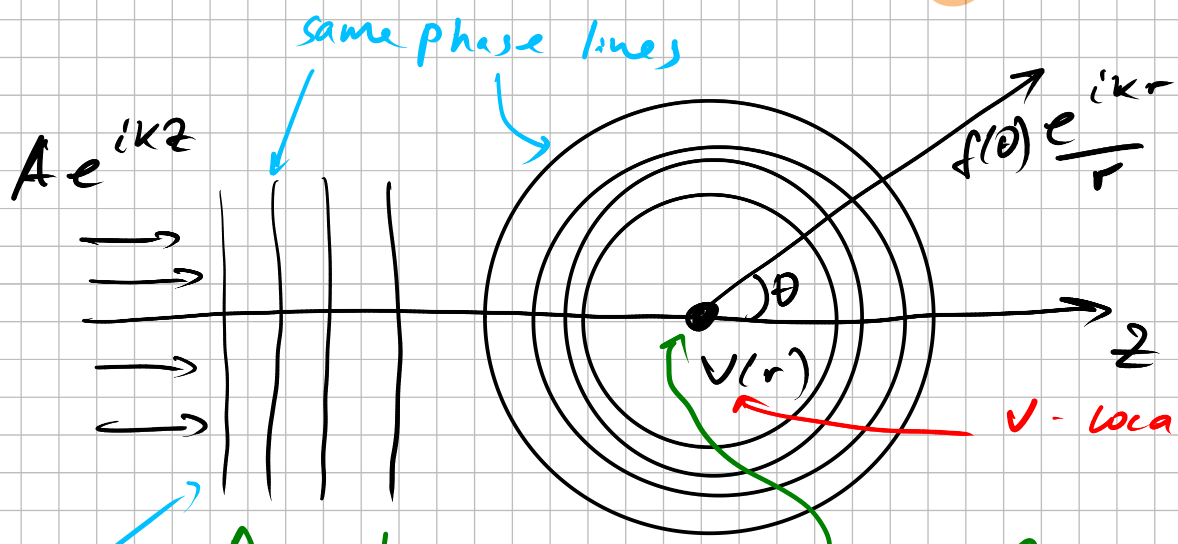
Quantum scattering

$k = \frac{2\pi}{\lambda}$ wave number

λ ← wave length



V - localized

Axial symmetry (no φ dependense)

incoming plane wave traveling

for large r ($r \to \infty$)

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

incoming wave

scattering wave

spherical $\frac{e^{ikr}}{r}$

similar to light from point source

total probability on a spherical surface preserves

$\langle\psi|\psi\rangle$ cannot be normilized

so A is treated as Amplitude

I find the easiest to apply my intuition of the light scattering to see similarity (when $V=0$ eq. of motions are the same: $(\nabla^2+k^2)\psi_E = 0$

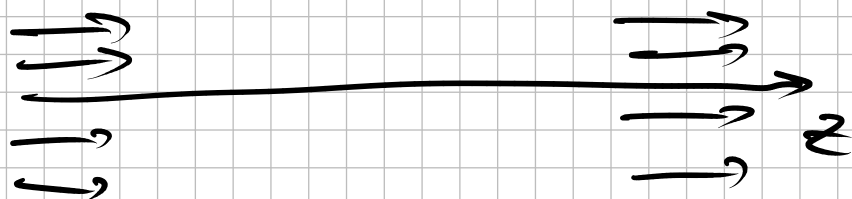
Think about laser pointer ⇛ it goes to infinity and has ∞ number of photons ⇒ ∞ Energy. This is unphysical so we talk about local Amplitude and not normalization.

Why this paradox? We assumed infinite time of observation

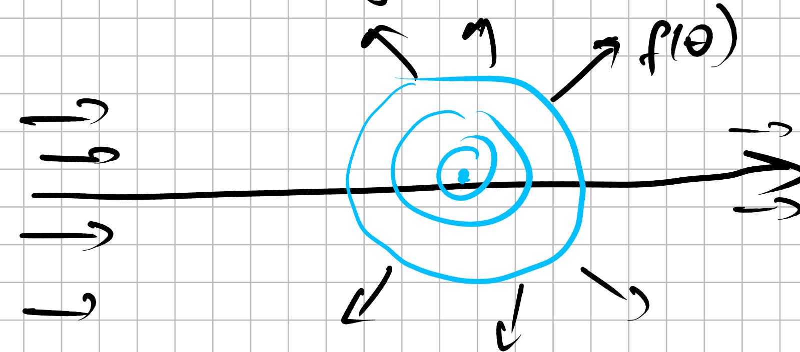
Compare two cases:

no scattering potential

nothing scatters



scattering potential



so $f(\theta)$ proportional to probability to find a scattered particle at angle (θ) or (Ω)

Differential cross section

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

In QM we are concerned with finding $f(\theta) \Rightarrow \sigma$

$$\sigma = \int |f(\theta)|^2 \, d\Omega$$

in experiment we can access $|f(\theta)|$ and we want to know σ and $V(r)$

What is our justification for

$$\psi = A\left(e^{ikz} + f(\theta)e^{ikr}\right)$$

this force particular shape (plane wave) of incoming way. i.e. we assume we know it.

$$H\psi = E\psi$$

$$\frac{\vec{p}^{\,2}}{2m} + V(r) = E\psi$$

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right)\psi = E\psi(r,\theta,\varphi)$$

we assume symmetry so φ is irrelevant $\Rightarrow m=0$

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

$$u = r\cdot R(r)$$

$r\to\infty \Rightarrow V(r)\to 0$

θ part

$$\simeq -\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\cancelto{0}{V(r)} + \frac{\hbar^2}{2m}\cancelto{0}{\frac{\ell(\ell+1)}{r^2}}\right] = Eu \qquad (*)$$

$r\to\infty$

this follow from

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left[V(r)-E\right]R = \ell(\ell+1)R$$

$$r \to \infty \Rightarrow \quad -\frac{\hbar^2}{2m}\frac{d^2u(r)}{dr^2} = E\,u(r)$$

$$u(r) = Ce^{ikr} + \cancel{De^{-ikr}}$$

outgoing wave

ingoing wave

we force discussion to outgoing wave only (scattering)

Combining all together

$$\psi(r,\theta) = A\left(e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right) \qquad \sim \frac{u}{r} = R(r)$$

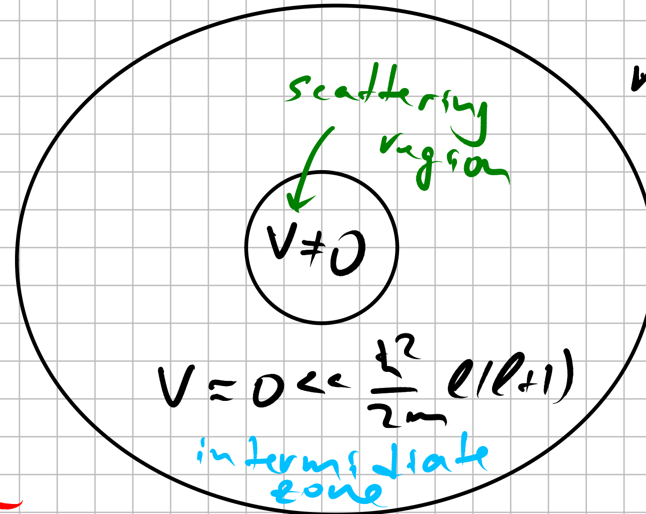
Partial wave analysis

Intermidiate zone

$$V(r) \ll \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}$$

we can neglect it in intermidiate zone

Note electrostatic potential $\sim 1/r$ does not satisfy this condition!



$kr \gg 1$

Radiation zone

in optical sense

from $(*)$ $$\frac{d^2u}{dr^2} - \frac{l(l+1)}{r^2}u = -\frac{2mE}{\hbar^2}u = -k^2 u$$

solution

$$u(r) = A r j_l(kr) + B r n_l(kr)$$

sometimes called spherical Neumann function

spherical Bessel function

analogous to 1D

sin, cos in 1D

similar to $e^{i\varphi} = \cos\varphi + i\sin\varphi$

we can write

$h_\ell^{(1)} = j_\ell(x) + i n_\ell(x)$; $h_\ell^{(2)}(x) = j_\ell(x) - i n_\ell(x)$

spherical Hankel functions of

the first and second kind

$$h_0^{(1)} = -i\frac{e^{ix}}{x} \qquad h_0^{(2)} = i\frac{e^{-ix}}{x}$$

$$h_1^{(1)} = \left(-\frac{i}{x^2} - \frac{1}{x}\right)e^{ix} \qquad h_1^{(2)} = \left(\frac{i}{x^2} - \frac{1}{x}\right)e^{-ix}$$

$$h_2^{(1)} = \left(-\frac{3i}{x^3} - \frac{3}{x^2} + \frac{i}{x}\right)e^{ix} \qquad h_2^{(2)} = \left(\frac{3i}{x^3} - \frac{3}{x^2} - \frac{i}{x}\right)e^{ix}$$

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

So $\psi(r,\theta)$ can be thought as $A' h_\ell^{(1)}(\kappa r) + B' h_\ell^{(2)}(\kappa r)$

but $h_\ell^{(2)} \sim e^{-i\kappa r}$ and thus $B' = 0$

ingoing wave

Extra note on Math Physics

$$j_\ell(x) = (-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\sin x}{x} \Rightarrow j_0(x) = \frac{\sin x}{x}$$

$$n_\ell(x) = -(-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\cos x}{x} \Rightarrow n_\ell(x) = -\frac{\cos x}{x}$$

for $x \to 0$

$$j_\ell(x \approx 0) \approx \frac{2^\ell \ell!}{(2\ell+1)} x^\ell \qquad n_\ell(x \approx 0) \approx \frac{(2\ell)!}{2^\ell \ell!} \frac{1}{x^{\ell+1}}$$

So most general solution $R(r) \sim \sum A_\ell' h_\ell^{(1)}(r)$

$m=0$ no φ dependence

$$\psi(r,\theta) = A\left(e^{ikz} + \sum_\ell A_\ell' h_\ell^{(1)}(kr)\, Y_\ell^0(\theta,\varphi) \right)$$

Recall $Y_\ell^0(\theta,\varphi) = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta)$

$\uparrow$ Legendre polynomial

$$\Rightarrow \boxed{\psi(r,\theta) = A\left\{ e^{ikz} + k\sum_{\ell=0}^{\infty} i^{\ell+1}(2\ell+1)\, a_\ell\, h_\ell^{(1)}(kr)\, P_\ell(\cos\theta)\right\}} \quad (\ast\ast)$$

note we redifined $A_\ell' = i^{\ell+1} k \sqrt{4\pi(2\ell+1)}\, a_\ell$

a_ℓ - called partial wave amplitude

You may have heard s-wave ($\ell=0$) p-wave ($\ell=1$) etc.

why such complicated form?

for $r \to \infty$: $h_\ell(kr) = (-1)^{\ell+1} e^{ikr}/kr$

$$\boxed{\psi(r,\theta) = A\left\{ e^{ikz} + \frac{e^{ikr}}{r}\sum_{\ell=0}^{\infty}(2\ell+1)\, a_\ell\, P_\ell(\cos\theta)\right\} = A\left\{ e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right\}}$$

One more simplification

$$\sigma = D(\theta)\,d\Omega = \int |f(\theta)|^2\,d\Omega = \frac{1}{r^2}\int \sum_{\ell}\sum_{\ell'} (2\ell+1)(2\ell'+1)\, a_\ell^* a_{\ell'} \underbrace{P_\ell(\cos\theta) P_{\ell'}(\cos\theta)\, d\Omega}_{\substack{\text{orthonormal} \\ \delta_{\ell\ell'}}}$$

$d\Omega \to r^2 \sin\theta\, d\varphi\, d\theta$

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

$$\boxed{\int_{-1}^{1} P_{\ell'}(x) P_\ell(x)\, dx = \frac{2}{2\ell+1}\delta_{\ell\ell'}}$$

We may wonder why we keep $(2\ell+1)$ in front of a_ℓ (we could have absorbed it into a_ℓ)?

It helps to simplify the following:

note that we use z and r, θ which seems not needed since $z = r\cos(0)$ or $r\cos(\pi)$

There is Rayleigh's formula:

$$\boxed{e^{ikz} = \sum_{\ell=0}^{\infty} i^\ell (2\ell+1)\, j_\ell(kr)\, P_\ell(\cos\theta)}$$

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

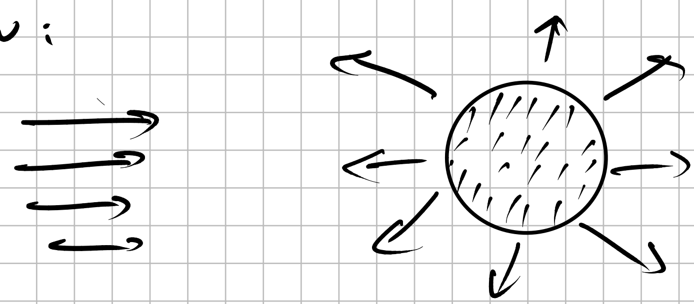
In region where we neglect $V(r)$

see $(**)$ for start point

Example: hard-sphere scattering

$$V(r) = \begin{cases} \infty, & r < a \\ 0, & r \geq a \end{cases}$$

2D view:



Boundary condition

$$\psi(a,\theta) = 0$$

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

at first it seems hard since $\sum_\ell$ is involved

Observe $\int P_{\ell'}(\cos\theta)\, \psi(a,\theta)\, d\Omega = 0$

ℓ prime $= \text{Const.} \cdot \{\cdots\} \delta_{\ell\ell'} = 0 \Rightarrow \{\cdots\} = 0$

$$\Rightarrow j_\ell(ka) + ik \cdot a_\ell h_\ell^{(1)}(ka) = 0$$

$$\Rightarrow \boxed{a_\ell = \frac{i}{k} \frac{j_\ell(ka)}{h_\ell^{(1)}(ka)}}$$

Scattering amplitude depends on $k = \frac{2\pi}{\lambda}$ and thus Energy

Classically this was not the case!

let's consider the case of long-wave / low-energy scattering

$\lambda \gg a \iff ka \ll 1$

$$a_\ell = \frac{i}{k}\frac{j_\ell(ka)}{h_\ell^{(1)}(ka)} = \frac{i}{k}\frac{j_\ell(ka)}{\cancel{j_\ell(ka)} + i n_\ell(ka)}$$

small compare to n_ℓ for $ka \ll 1$

for $x \to 0$

$$j_\ell(x \approx 0) = \frac{2^\ell \ell!}{(2\ell+1)!} x^\ell \qquad n_\ell(x \approx 0) = \frac{(2\ell)!}{2^\ell \ell!}\frac{1}{x^{\ell+1}}$$

$$\boxed{a_\ell = \frac{1}{k}\frac{i}{2\ell+1}\frac{(2^\ell \ell!)^2}{(2\ell)!}(ka)^{2\ell+1}}$$

for $ka \ll 1$

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

drops like a rock as ℓ goes up

so we keep only $\ell = 0$

$$\boxed{\sigma \approx 4\pi a^2}$$

wow! 4 larger than classical case! Full area of sphere $\iff \psi$ "feels" it