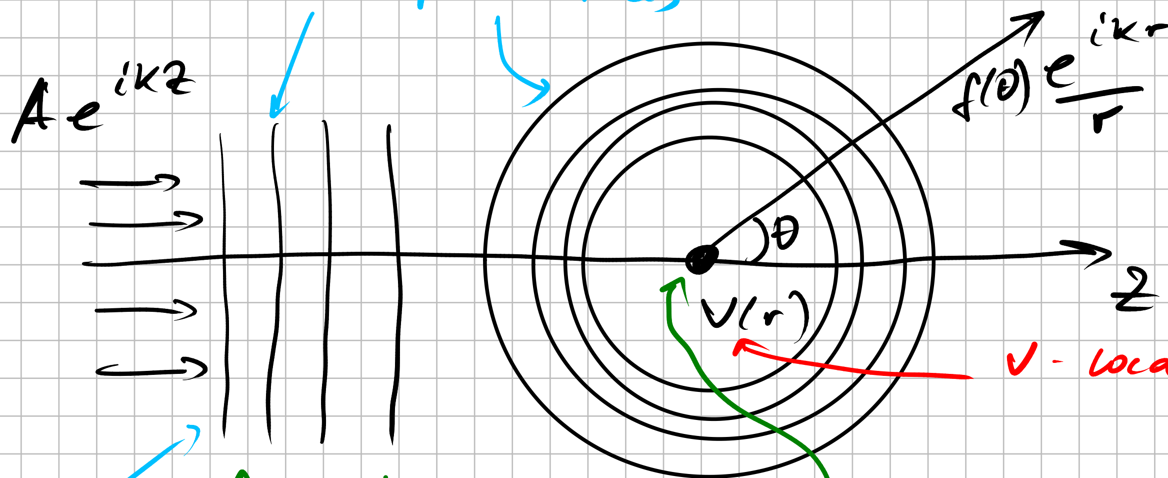
Quantum scattering

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

$\lambda \leftarrow$ wave length

same phase lines



V - localized

Axial symmetry (no φ dependense)

incoming traveling plane wave

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

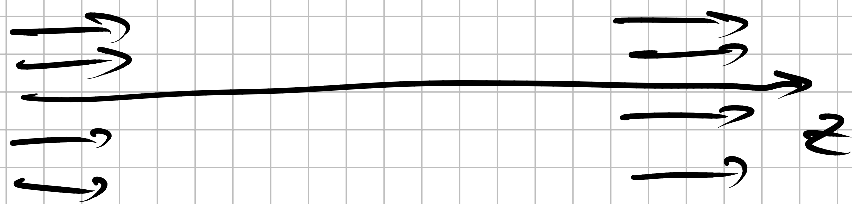
I find the easiest to apply my intuition of the light scattering to see similarity (when $V=0$ eq. of motions are the same: $(\nabla^2 + k^2)\psi_E = 0$

Think about laser pointer $\Longrightarrow$ it goes to infinity and has ∞ number of photons $\Rightarrow$ ∞ Energy. This is unphysical so we talk about local Amplitude and not normalization. Why this paradox? We assumed infinite time of observation.

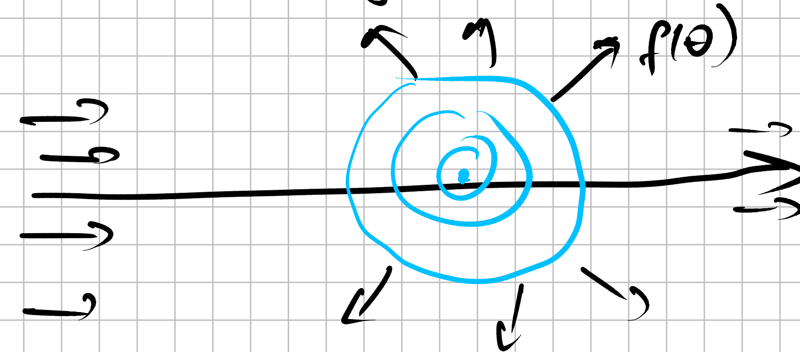
Compare two cases:

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 $\Rightarrow m=0$

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

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

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

θ part

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

$\to 0 \qquad \to 0 \quad r\to\infty$

this follow from

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

$r \to \infty$

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

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

outgoing wave

ingoing wave

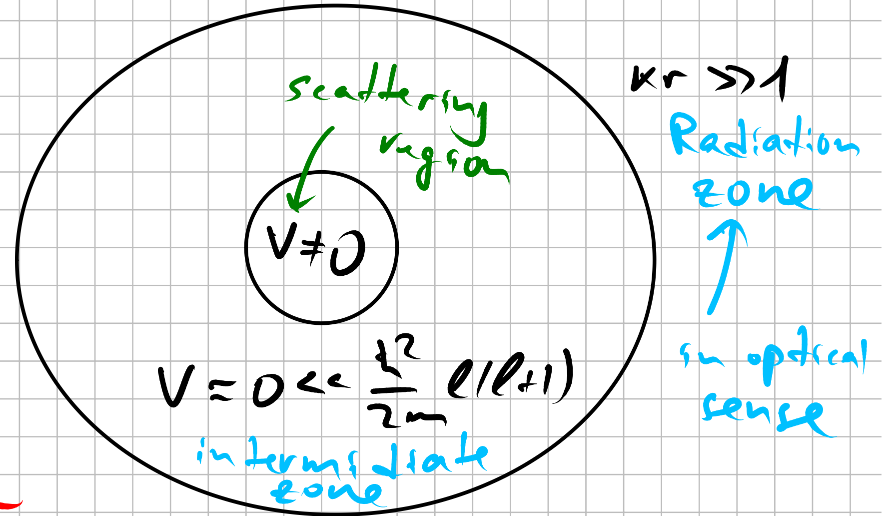
we force discussion to outgoing wave only (scattering)

Combining all together

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

$\sim \frac{u}{r} = R(r)$

Partial wave analysis



Intermidiate zone

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

we can neglect it
in intermidiate zone

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

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

solution
$$u(r) = A r j_\ell(kr) + B r n_\ell(kr)$$

some times called **spherical Neumann** function

spherical Bessel function
analogous to 1D
sin, cos in 1D

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

we can write

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

spherical Hankel functions of the first and second kind

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

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

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

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

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

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

ingoing wave

Extra note on Math Physics

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

$$n_\ell(x) = -(-x)^\ell \left(\frac{1}{x}\frac{d}{dx}\right)^\ell \frac{\cos x}{x} \Rightarrow n_0(x) = -\frac{\cos x}{x}$$

for $x \to 0$

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

So most general solution $R(r) \sim \sum A_l' h_l^{(1)}(r)$

$m=0$ no φ dependence

$$\psi(r,\theta) = A\left(e^{ikz} + \sum_l A_l' h_l^{(1)}(kr)\, Y_l^0(\theta,\varphi)\right)$$

Recall $Y_l^0(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}}\, P_l(\cos\theta)$

Legendre polynomial

$$\Rightarrow \boxed{\psi(r,\theta) = A\left\{e^{ikz} + k\sum_{l=0}^{\infty} i^{l+1}(2l+1)\, a_l\, h_l^{(1)}(kr)\, P_l(\cos\theta)\right\}} \quad (\ast\ast)$$

note we redefined $A_l' = i^{l+1} k \sqrt{4\pi(2l+1)}\, a_l$

a_l - called partial wave amplitude

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

why such complicated form?

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

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

orthonormal

One more simplification

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

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

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

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

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:

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

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

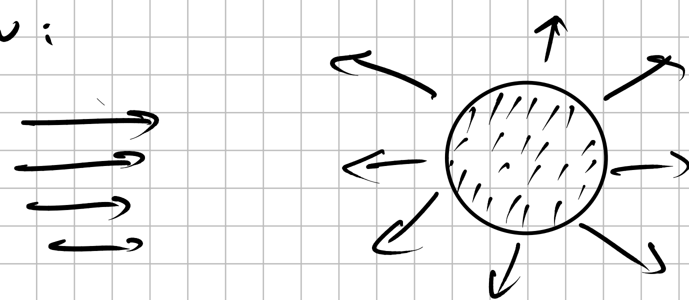
In region where we neglect $V(r)$

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

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

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

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

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

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

$$\Rightarrow j_\ell(\kappa a) + i\kappa \cdot a_\ell h_\ell^{(1)}(\kappa a) = 0$$

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

Scattering amplitude depends on $\kappa = \frac{2\pi}{\lambda}$ 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! 4π larger than classical case!

Full area of sphere $\iff \psi$ "feels" it