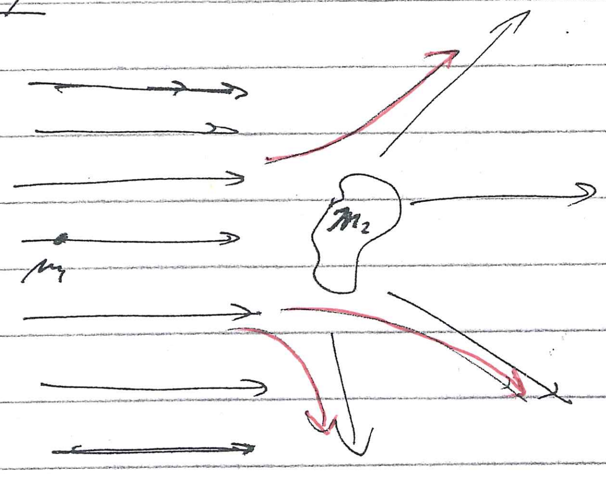
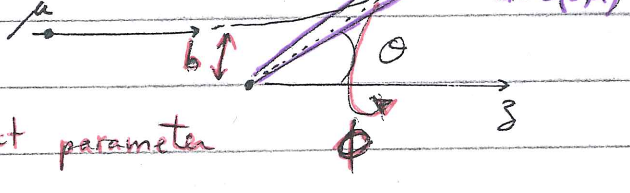
Quantum Scattering Theory

Thursday, April 18, 2013

Classical scattering:



In the center-of-mass frame, we consider a particle of ~~mass μ~~ reduced mass μ: $\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$



b = impact parameter

definitions:

alternate notation

$$\sigma(\theta,\phi) = \frac{d\sigma(\theta,\phi)}{d\Omega} = \text{differential scattering cross-section}$$

$$= \frac{\text{Number particles scattered in the } (\theta,\phi) \text{ direction}}{\text{Total number of incident particles/unit area}}$$

$$= \frac{N(\theta,\phi)}{\text{Flux}}$$

= units of area

$$\text{Flux} = \frac{N_{Total}}{\text{Area}}$$

$d\Omega$ = differential solid angle

$= \sin\theta \, d\theta \, d\phi$

$$\sigma_{total} = \text{total scattering cross-section}$$

~ effective area of colliding particles

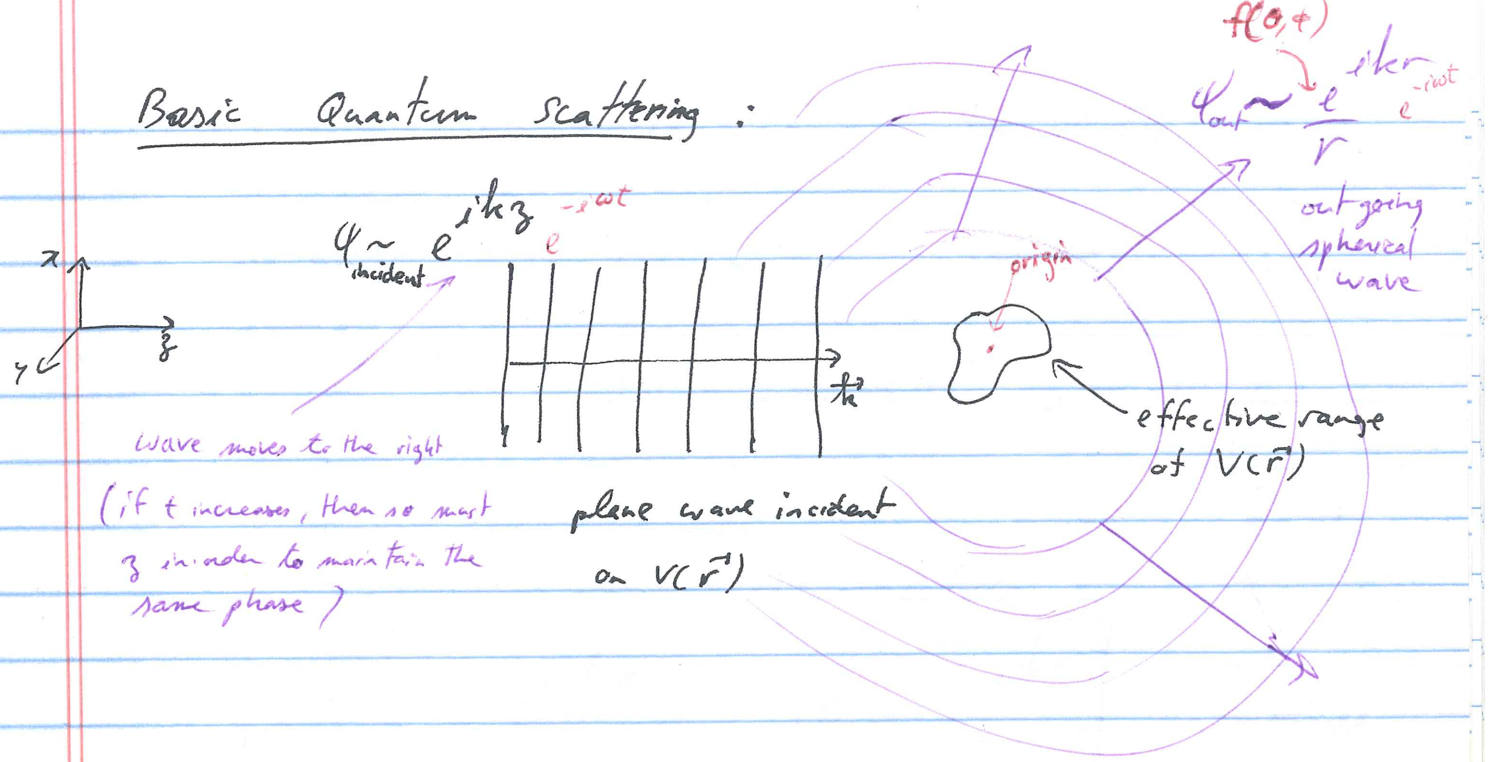
$$= \int_{\Omega} \sigma(\theta,\phi) \, d\Omega$$

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

$$= \text{units of area} = \frac{\text{total number of particles scattered}}{\frac{\text{Total number of incident particles}}{\text{area}}}$$

For quantum scattering, we are ultimately interested in $\frac{d\sigma(\theta,\phi)}{d\Omega}$ and σ_{Total} | The same (experimental) definitions apply.

Basic Quantum scattering:



For elastic scattering (no energy loss or gain), we have $E_{in} = E_{out} = E_0$

so
$$\left\{\begin{array}{l} \psi_{in}(\vec r, t) = \psi_{in}(\vec r)\, e^{-i\frac{E_0}{\hbar}t} \\ \psi_{out}(\vec r, t) = \psi_{out}(\vec r)\, e^{-i\frac{E_0}{\hbar}t} \end{array}\right\}$$
and the time dependence

is trivial (~~at~~ i.e. adds ~~nothing~~ no extra ~~insight~~ information).

the Schrodinger equation (time independent) for the scattering problem is

$$H = \frac{P^2}{2\mu} + V(\vec r) \Rightarrow \left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(\vec r)\right)\psi(\vec r) = E\,\psi(\vec r)$$

we will assume that for $|\vec r| \gg$ effective range (i.e. $V(r)=0$ for $r>r_0$) of $V(\vec r)$

can write $\psi(\vec r) \approx \alpha\, \psi_{in}(\vec r) + \beta\, \psi_{out}(\vec r)$

We are not interested in $\psi(\vec r)$ in the vicinity of $V(\vec r)$.

In the region where $V(\vec r) \simeq 0$, we can write

$$-\frac{\hbar^2}{2\mu}\nabla^2\psi(\vec r) = E\,\psi(\vec r), \text{ and } H = \frac{P^2}{2\mu}$$

$|\vec k_{in}| = |\vec k_{out}|$

We will look for solutions of the form

$$\boxed{\psi(\vec r) = e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}}$$

un-normalized

incident plane wave ~~plane~~

outgoing pseudo-spherical wave such that $\lim_{V\to 0} f(\theta,\phi) \to 0$

Angular momentum states of the collision

If we consider a spherically symmetric $V(\vec r) = V(r)$, then angular momentum must be conserved during the course of the collision.

$$[L^2, H] = 0 \quad \text{and} \quad [L_z, H] = 0$$

what are the common eigenstates of H, L^2, L_z for $r \to +\infty$ (i.e. far from $V(r)$)?

Quantum numbers $E \to k$ (i.e. $E = \frac{(\hbar k)^2}{2\mu}$) far from $V(r)$, l, and m_l

consider only $m=0$ for $V(|\vec r|)$

$$\langle x | k, l, \cancel{m}\rangle = R_{k,l}(r)\,Y_l^m(\theta,\phi) = \frac{1}{r}u_{k,l}(r)\,Y_l^0(\theta)$$

set $m_l = 0$ to remove ~~dependen~~ ϕ-dependence

with $u_{k,l}(r=0) = 0$ same as for hydrogen

Schrodinger equation for the radial term becomes

$$\left[-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \underbrace{\frac{l(l+1)\hbar^2}{2\mu}\frac{1}{r^2}}_{V_{eff}} + V(r)\right] u_{k,l}(r) = \underset{\uparrow}{\epsilon}\, u_{k,l}(r)$$

define as $\epsilon = \frac{\hbar^2 k^2}{2\mu}$

for $r \to \infty$, $V_{eff} = \frac{l(l+1)\hbar^2}{2\mu}\frac{1}{r^2} + V(r) \longrightarrow 0$

thus the Schrodinger equation becomes

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}u_{k,l} \underset{r\to\infty}{\simeq} \frac{\hbar^2 k^2}{2\mu} \iff \left[\frac{d^2}{dr^2} + k^2\right] u_{k,l}(r) \underset{r\to\infty}{\simeq} 0$$

(Since this is a standard wave equation, we get)

$$\Rightarrow u_{k,l}(r) \underset{r\to\infty}{\simeq} \underset{\uparrow}{A} e^{ikr} + \underset{\uparrow}{B} e^{-ikr} = |A|\left(e^{ikr}e^{i\varphi_A} + e^{-ikr}e^{-i\varphi_B}\right)$$

outgoing wave

in going wave

we require $|A|^2 = |B|^2$ to ensure ingoing particle # = outgoing particle #

thus $R_{k,l}(r) \underset{r\to\infty}{=} \frac{u_{k,l}(r)}{r} = |A|\left(\frac{e^{ikr}e^{i\varphi_A}}{r} + \frac{e^{-ikr}e^{i\varphi_B}}{r}\right)$

if $V(r) = 0$, then $R_{k,l}(r) = \sqrt{\frac{2k^2}{\pi}}\, j_l(kr)$ + cst $n_l(kr)$

where n_l is a spherical Neumann function (diverges at origin → omit)

$j_l(x)$ is a spherical Bessel function of order l.

Asymptotically, we have

$$j_l(kr) \underset{r\to\infty}{\simeq} \frac{1}{kr}\sin\left(kr - l\frac{\pi}{2}\right)$$

Thus for $V(r) = 0$, including $r \sim 0$ then $R_{k,l} \underset{r\to\infty}{=} \sqrt{\frac{2}{\pi}}\frac{1}{2i}\left[\frac{e^{i(kr - l\frac{\pi}{2})}}{r} - \frac{e^{-i(kr - l\frac{\pi}{2})}}{r}\right]$

Thus for $V(r) \neq 0$, we can adjust φ_A & φ_B to match the free particle case

omitting overall phase and amplitude

$$R_{k,l}(r) \underset{r\to+\infty}{\sim} \frac{e^{i(kr - l\pi/2 + \delta_l)}}{r} - \frac{e^{-i(kr - l\frac{\pi}{2} + \delta_l)}}{r}$$

$$\sim \frac{1}{r}\sin(kr - l\pi/2 + \delta_l)$$

<u>Important:</u> At large distances, the only effect of the scattering potential is to modify the phase $\underset{\substack{\uparrow \\ \delta_l(V)}}{\delta_l}$ ingoing and outgoing wave.

<u>note:</u> we can remove the phase on the ingoing wave (multiply by $-e^{i\delta_l}$) to obtain

$$R_{kl}(r) \underset{r\to+\infty}{\sim} \underset{\substack{\uparrow \\ \text{in going} \\ \text{spherical wave}}}{\frac{e^{-i(kr - l\pi/2)}}{r}} - \underset{\substack{\uparrow \\ \text{out going} \\ \text{spherical wave}}}{\frac{e^{i(kr - l\pi/2 + 2\delta_l)}}{r}}$$

Thus we consider scattering eigenstates of the form

$$\langle x|k,l,m=0\rangle \underset{r\to+\infty}{\simeq} \left[\frac{e^{-i(kr - l\pi/2)}}{r} - \frac{e^{i(kr - l\pi/2 + 2\delta_l)}}{r}\right] \underbrace{Y_l^0(\theta)}_{\sqrt{\frac{2l+1}{4\pi}}\,P_l(\cos\theta)}$$

↳ we can take any linear combination of these states

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We want to construct scattering wavefunctions of the form

$$\Psi(\vec{r}) \underset{r\to+\infty}{=} \underset{\substack{\uparrow \\ \text{incident plane} \\ \text{wave}}}{e^{ikz}} + \underset{\substack{\uparrow \\ \text{outgoing spherical wave}}}{f(\theta;k)\frac{e^{ikr}}{r}}$$

$$\underset{r\to+\infty}{=} \frac{i}{2k}\sum_{l=0}^{\infty} i^{l}(2l+1)\left[\frac{e^{-i(kr-l\pi/2)}}{r} - \frac{e^{i(kr-l\pi/2)}}{r}\right]P_l(\cos\theta)$$

$$1 = (1)^l = (i(-i))^l = i^l e^{-i\pi/2\, l}$$

$$+ \underbrace{\left(\frac{-i}{2k}\sum_{l=0}^{\infty}(2l+1)f_l(k)P_l(\cos\theta)\right)}_{\substack{\text{expansion of } f(\theta;k) \\ \text{in terms of } P_l(\cos\theta)}}\frac{e^{ikr}}{r}$$

$$= \frac{i}{2k}\sum_{l=0}^{\infty} i^{l}(2l+1)\left[\frac{e^{-i(kr-l\pi/2)}}{r} - \underbrace{\left(1+f_l(k)\right)}_{e^{i2\delta_l}}\frac{e^{i(kr-l\pi/2)}}{r}\right]P_l(\cos\theta)$$