Lecture 6

Quantum scattering in 3d

Consider two quantum particles whose interaction in 3d is described by the potential $U(\vec{r}_1, \vec{r}_2) = U(|\vec{r}_2 - \vec{r}_1|)$.

Remark: more general potentials are considered in the specialized literature.

$$i\hbar \frac{\partial \psi_{tot}}{\partial t} = \hat{H} \psi_{tot} = \left(-\frac{\hbar^2}{2m_1} \Delta_1 - \frac{\hbar^2}{2m_2} \Delta_2 + U(\vec{r}_2 - \vec{r}_1) \right) \psi_{tot}$$

$\vec{r}_1, \vec{r}_2 \to \vec{r}, \vec{R}$, where

$$\begin{cases} \vec{r} = \vec{r}_2 - \vec{r}_1 = (x, y, z) \\ \vec{R} = \dfrac{m_1 \vec{r}_1 + m_2 \vec{r}_2}{m_1 + m_2} = (X, Y, Z) \end{cases}$$

$$i\hbar \frac{\partial \psi_{tot}}{\partial t} = \left(-\frac{\hbar^2}{2m} \Delta_{\vec{r}} - \frac{\hbar^2}{2M} \Delta_{\vec{R}} + U(|\vec{r}|) \right) \psi_{tot},$$

where $\Delta_{\vec{r}} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$,

$$\Delta_{\vec{R}} = \frac{\partial^2}{\partial X^2} + \frac{\partial^2}{\partial Y^2} + \frac{\partial^2}{\partial Z^2}, \quad M = m_1 + m_2,$$

$m = \frac{m_1 m_2}{m_1 + m_2}$ is the reduced mass.

With $\Psi_{tot} = \psi(\vec{r}, t)\,\Psi_{CMF}(\vec{R}, t)$ and further considering stationary states with

$\psi \sim e^{-iEt/\hbar}$ and $\Psi_{CMF} \sim e^{-iE_{CMF}t/\hbar}$

we find (check this!)

$$-\frac{\hbar^2}{2M}\Delta_{\vec{R}}\,\Psi_{CMF}(\vec{R}) = E_{CMF}\,\Psi_{CMF}(\vec{R})$$

$$\left(-\frac{\hbar^2}{2m}\Delta_{\vec{r}} + V(|\vec{r}|)\right)\psi(\vec{r}) = E\,\psi(\vec{r}).$$

$\Rightarrow$ the two-body problem is reduced to scattering of ~~a~~ particle with mass m by a central potential $V(r)$, $r = |\vec{r}|$.

$$\Delta\psi = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\psi = \frac{1}{r}\frac{\partial^2}{\partial r^2}(r\psi) +$$

$$+ \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2\psi}{\partial\varphi^2}$$

Assume $U(r) \to 0$ for $r \to \infty$.

Rotational symmetry $\Rightarrow \hat{H}, \hat{L}^2, \hat{L}_z$ commute

$\Rightarrow \psi(r,\theta,\varphi) = R(r)\,Y_{lm}(\theta,\varphi)$ are common eigenfunctions obeying

$$\frac{\hbar^2}{2m}\left[-\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{\hat{L}^2}{r^2}\psi\right] + U(r)\psi = E\psi$$

$$\hat{L}^2 Y_{lm} = l(l+1)\,Y_{lm}$$

$$\hat{L}_z Y_{lm} = m\,Y_{lm}$$

$$Y_{lm} = \frac{1}{\sqrt{2\pi}} e^{im\varphi}(-1)^m i^l \sqrt{\frac{(2l+1)(l-m)!}{2(l+m)!}}\, P_l^m(\cos\theta)$$

$$P_\ell^m(\cos\theta) = \frac{1}{2^\ell \ell!} \sin^m\theta \frac{d^{m+\ell}}{(d\cos\theta)^{m+\ell}} \left(\cos^2\theta - 1\right)^\ell$$

are associated Legendre polynomials, solutions of the Legendre eq for $y(x)$:

$$(1-x^2)y'' - 2xy' + \left(\ell(\ell+1) - \frac{m^2}{1-x^2}\right)y = 0 .$$

The free radial eq.

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{\ell(\ell+1)}{r^2}R + k^2R = 0,$$

where $k^2 = 2mE/\hbar^2$, with $x = kr$ and $R = r^{-1/2}Z$ reduces to Bessel eq

$$x^2Z'' + xZ' + \left(x^2 - \ell(\ell+1) - \frac{1}{4}\right)Z = 0,$$

so $R(r) = A\, j_\ell(kr) + B\, n_\ell(kr)$, where

$$j_\ell(z) = \sqrt{\frac{\pi}{2z}}\, J_{\ell+1/2}(z), \quad n_\ell(z) = \sqrt{\frac{\pi}{2z}}\, N_{\ell+1/2}(z)$$

are spherical Bessel functions:

$$j_0(z) = \frac{\sin z}{z}$$

$$j_1(z) = \frac{\sin z}{z^2} - \frac{\cos z}{z} \quad \text{etc}$$

and Neumann functions

$$n_0(z) = -\frac{\cos z}{z}$$

$$n_1(z) = -\frac{\sin z}{z} - \frac{\cos z}{z^2} \quad \text{etc.}$$

<u>Note</u>: $$j_\ell(z) \sim \frac{\sin(z - \ell\pi/2)}{z}$$

$$n_\ell(z) \sim -\frac{\cos(z - \ell\pi/2)}{z}$$

for $z \to \infty$, $z > \ell$.

<u>Note</u>: spherical Hankel functions:

$$h_\ell^\pm(z) = j_\ell(z) \pm i\, n_\ell(z).$$

Solutions $\psi = R(r)\, Y_{lm}(\theta, \varphi)$ form a complete set $\Rightarrow$ any (reasonable) $F(r, \theta, \varphi)$ can be expanded using them as basis, e.g.

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} \sqrt{4\pi(2l+1)}\, i^l j_l(kr)\, Y_{l0}(\theta) =$$

$$= \sum_{l=0}^{\infty} (2l+1)\, i^l j_l(kr)\, P_l(\cos\theta) .$$

<u>Exercise</u>: derive this expansion.

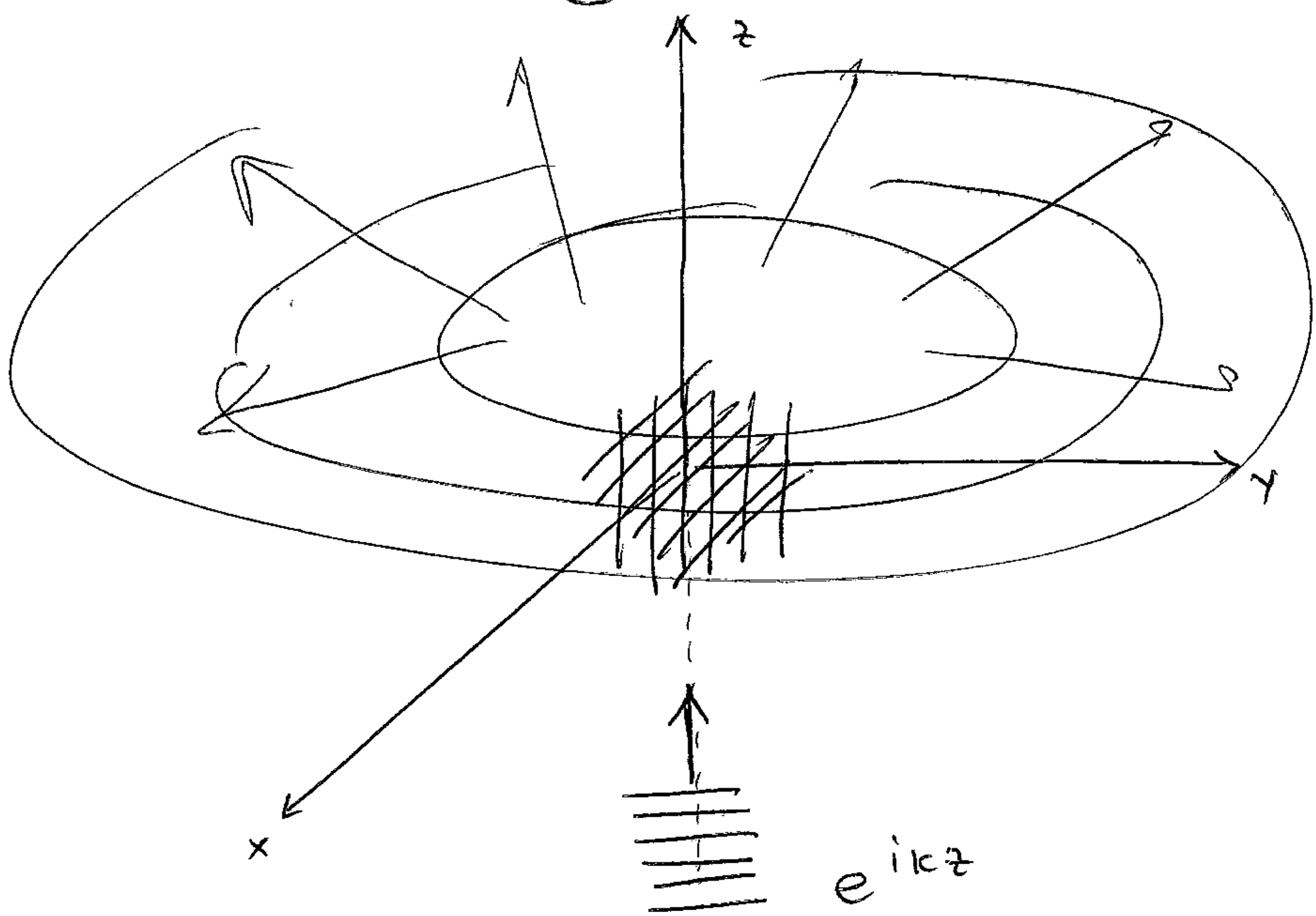
Now consider free particle with momentum $\vec{p} = \hbar \vec{k}$ at $r \to \infty$ $\left(U(r) \to 0 \text{ for } r \to \infty \right)$.

The solution of $-\frac{\hbar^2}{2m} \Delta_{\vec{r}}\, \psi = E \psi$,

$E = \hbar^2 k^2 / 2m$ is a plane wave

$$\psi(x, y, z) = e^{\pm i \vec{k} \cdot \vec{r}}$$

Orient coord. system with positive z along $\vec{k}$, $\psi = e^{ikz} = e^{ikr\cos\theta}$ at $r \to \infty$ (incoming wave):



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

$$j_{\ell}(kr) \approx \frac{1}{2ikr}\left(e^{i(kr-\ell\pi/2)} - e^{-i(kr-\ell\pi/2)} \right)$$

outgoing spherical wave for $r \to \infty$ incoming spherical wave

Recall: $e^{-i\omega t \pm ikr}$

Const. phase: $-\omega t \pm kr = \text{const}$

$\Rightarrow -\omega\, dt \pm k\, dr = 0 \Rightarrow \frac{dr}{dt} = \pm \frac{\omega}{k}$

$\Rightarrow e^{ikr}$: outgoing

e^{-ikr} : incoming

When $U(r) = 0$, e^{ikz} is an exact solution.

With $U(r) \neq 0$, the radial wave f. at $r \to \infty$ is:

$$R(r) \sim \frac{1}{2ikr}\left(\underbrace{S_\ell(k)\, e^{i(kr - \ell\pi/2)}}_{\substack{\text{outgoing}\\ \text{spher. wave}\\ \text{modified by } U(r)}} - \underbrace{e^{-i(kr-\ell\pi/2)}}_{\substack{\text{inc. spher. wave}\\ \text{unchanged}}} \right)$$

The solution to the full Schrödinger eq is

$$\psi(\vec{r}) = e^{ikz} + \psi_{\text{scatter}}(\vec{r}),$$ where

for $r \to \infty$

$$\psi_{scatter}(\vec{r}) \sim \frac{1}{2ik} \frac{e^{ikr}}{r} \sum_{l=0}^{\infty} (2l+1)(S_l - 1) P_l(\cos\theta)$$

Or else: for $r \to \infty$

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

where the <u>scattering amplitude $f(\theta)$</u> is

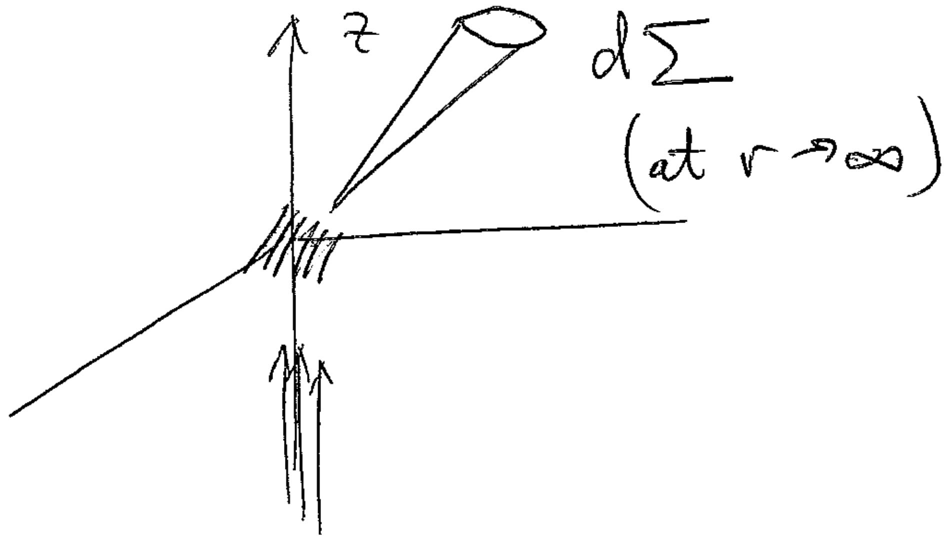
$$f(\theta) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(S_l - 1) P_l(\cos\theta).$$

H. Faxen, J. Holtsmark, 1927.

<u>Note</u>: $[f(\theta)] = L$ (length).

The incident particle has probability density flux $j = P/m = v$: for e^{ikz}

$$j_{inc} = \frac{i\hbar}{2m}\left(\psi \partial_z \psi^* - \psi^* \partial_z \psi\right) = \frac{\hbar k}{m} = v.$$



Probability for scattered particle to pass through $d\Sigma = r^2 d\Omega$ per unit time is

$$v \frac{|f|^2}{r^2} d\Sigma = v|f|^2 d\Omega = j_{scatt}$$

$$d\sigma = \frac{j_{scatt}}{j_{inc}} = |f(\theta)|^2 d\Omega$$ is called the differential cross-section:

$$d\sigma = 2\pi \sin\theta \, |f(\theta)|^2 d\theta .$$

<u>Note</u>: $[\sigma] = L^2$.

<u>Note</u>: Tacitly assumed no interference

between e^{ikz} and $\frac{e^{ikr}}{r} f(\theta)$ at large r. This is true for $\theta \neq 0$.

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

$$|f|^2 = \frac{1}{4k^2} \sum_{l_1 l_2} (2l_1+1)(2l_2+1) P_{l_1}(\cos\theta) P_{l_2}(\cos\theta) \, |S_{l_1}-1| \, |S_{l_2}-1|$$

Note: $\int_0^{\pi} \sin\theta \, P_k(\cos\theta) P_l(\cos\theta) \, d\theta = \frac{2\delta_{kl}}{2l+1}$

For elastic scattering $|S_l| = 1$.

Parametrize $S_l = e^{i2\delta_l}$ (phase shift)

$$\Rightarrow \quad \sigma = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l+1) \sin^2\delta_l = \sum_{l=0}^{\infty} \sigma_l .$$

It will be useful to introduce partial

amplitudes f_ℓ by

$$f(\theta) = \sum_{\ell=0}^{\infty} (2\ell+1)\, f_\ell(k)\, P_\ell(\cos\theta),$$

where $f_\ell = \frac{1}{2ik}\left(S_\ell - 1\right) = \frac{1}{2ik}\left(e^{2i\delta_\ell} - 1\right)$.

Note:

$$\text{Im}\, f(\theta) = \frac{1}{k} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2\delta_\ell\, P_\ell(\cos\theta)$$

Comparing with σ we get

$$\boxed{\text{Im}\, f(0) = \frac{k}{4\pi}\sigma}$$

(the optical theorem).