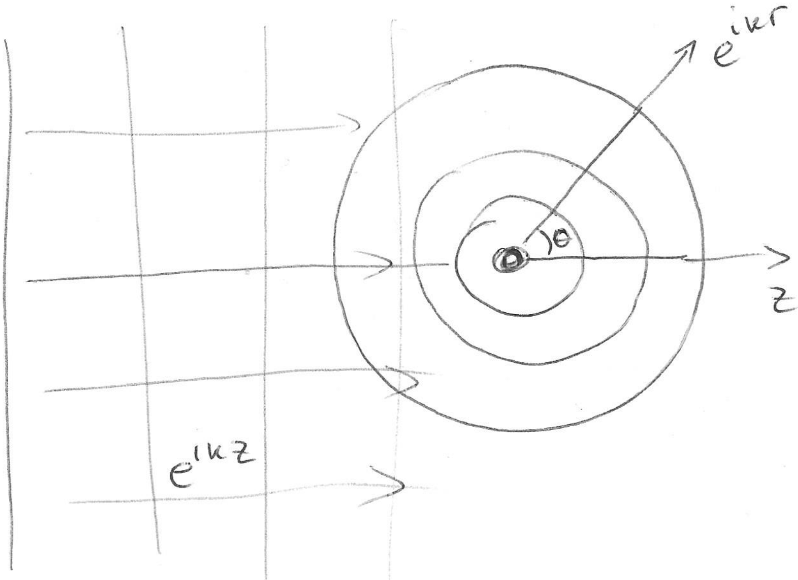
Scattering of waves (quantum scattering)

The general scattering problem in quantum mechanics is the calculation of $\frac{d\sigma}{d\Omega}$ for a particle incident on an arbitrary potential V. In principle, the Schrödinger (or equivalent) equation should be solved and the resulting wave function used to find the cross section. In practice, the SE for scattering problems is usually difficult to solve, so approximation methods must be used. There are two cases for which the problem becomes simpler. In the limit when $E \ll V$ the method of partial waves can be utilized. In the opposite limit, when $E \gg V$ it is possible to use a variant of perturbation theory called the Born approximation. We will first consider the $E \ll V$ case. But before that let us consider some general properties of the scattering wave function.

Suppose we have an incident wave of particles traveling in the z-direction, Ae^{ikz}. When it encounters a scattering potential it produces an outgoing spherical wave. Hence we will look for solutions of the SE in the form

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



In the case of spherically symmetric potentials $V = V(|\vec{r}|)$ there will be no dependence on ϕ angle. Thus $f = f(\theta)$. Here $k = \frac{\sqrt{2mE}}{\hbar}$

The spherical wave contains $1/r$ factor because the total probability (which goes as $\underbrace{1/r^2}_{|f(\theta)|^2} \cdot \underbrace{r^2}_{\text{area of sphere}}$) must be conserved.

The goal of the scattering theory is to determine $f(\theta)$ — the scattering amplitude as it tells us the probability of scattering in a given direction θ.

Indeed the number of particles scattered into angle $d\Omega$ (which is in the direction of $\vec{e}_r$) is

$$\vec{J}_{incident} \cdot \vec{d\sigma} = r^2 J_{scattered,r}\, d\Omega$$

$$J_{scattered,r} = \frac{\hbar}{2mi}\left(\psi_{sc}^* \frac{\partial \psi_{sc}}{\partial r} - \psi_{sc}\frac{\partial \psi_{sc}^*}{\partial r}\right)$$

[recall $\vec{J} = \frac{\hbar}{2mi}(\psi^* \nabla\psi - \psi\nabla\psi^*)$ for Cartesian coordinates]

$$\psi_{incident} = Ae^{ikz} \Rightarrow J_{incident} = \frac{\hbar k}{m}$$

$$J_{scattered,r} = \frac{\hbar k}{mr^2}|f(\theta)|^2$$

Therefore

$$r^2 \frac{\hbar k}{mr^2}|f(\theta)|^2 d\Omega = \frac{\hbar k}{m} d\sigma$$

and

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

The problem of determining $\frac{d\sigma}{d\Omega}$ (differential cross section) is equivalent to finding the scattering amplitude $f(\theta)$.

Partial wave analysis

For a spherically symmetric potential $V(r)$ we can use the separation of variables $\psi(r,\theta,\phi) = R(r) Y_\ell^m(\theta,\phi)$ and the radial equation for $R(r) = \frac{u(r)}{r}$ looks as follows

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

At $r \to \infty$ $V(\vec{r}) \to 0$ and we get

$$\frac{d^2u}{dr^2} = -k^2 u$$

with the general solution $u(r) = Ce^{ikr} + De^{-ikr}$. For the scattered wave the incoming term De^{-ikr} must vanish. Thus, $D=0$. Then

at $r \to \infty$ $\quad R(r) \to \frac{e^{ikr}}{r}$

If we assume that $V(r)$ is a short-range potential (i.e. $V(r)$ decays faster than $\frac{1}{r^3}$ at $r \to \infty$), where we can build up the next approximation, where we neglect $V(r)$ at $r \to \infty$ but keep $\frac{\ell(\ell+1)}{r^2}$ term:

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

or

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

The solutions of this equation are called spherical Bessel and spherical Neuman functions. The above equation can be reduced to the standard Bessel equation by a substitution $R(r) = \frac{Z(kr)}{\sqrt{kr}} = \frac{Z(x)}{\sqrt{x}}$

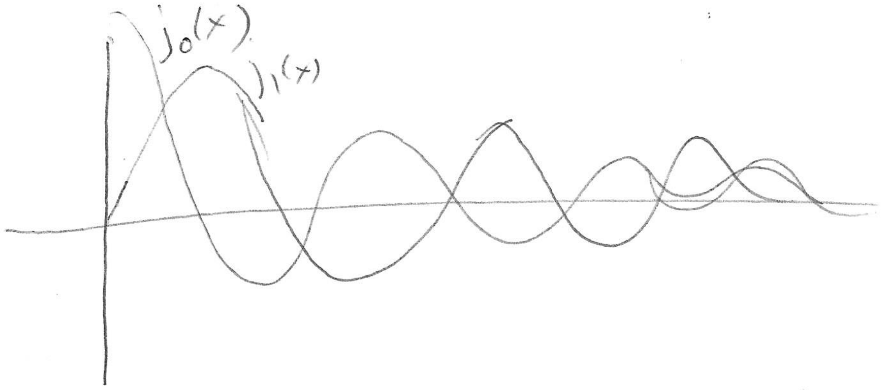
$$x^2 Z'' + x Z' + \left[x^2 - (\ell+\tfrac{1}{2})^2\right] Z = 0$$

$$R(r) = A \frac{J_{\ell+\frac{1}{2}}(kr)}{\sqrt{kr}} + B \frac{N_{\ell+\frac{1}{2}}(kr)}{\sqrt{kr}} = \underbrace{A' j_\ell(kr) + B' n_\ell(kr)}_{\text{general solution}}$$

$$j_0(x) = \frac{\sin x}{x} \qquad n_0(x) = -\frac{\cos x}{x}$$

$$j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x} \qquad n_1 = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

$$j_2(x) = \left(\frac{3}{x^3} - \frac{1}{x}\right)\sin x - \frac{3}{x^2}\cos x \quad \ldots$$



Neither j_ℓ nor n_ℓ represent an outgoing or incoming wave. Similarly to the familiar transformation

$$A\cos x + B\sin x \longrightarrow A' e^{ix} + B' e^{-ix}$$

we can introduce new linear combinations called spherical Hankel functions of the first and second kind

$$h_\ell^{(1,2)}(x) \equiv j_\ell(x) \pm i\, n_\ell(x)$$

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

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

At large r $h_\ell^{(1)}(kr)$ goes like $\frac{e^{ikr}}{r}$ whereas

$$h^{(2)}(kr) \rightarrow \frac{e^{-ikr}}{r}$$

With that the wave function outside the scattering region $(V(r)=0)$ can be expanded as

$$\psi(r,\theta,\phi) = A\Big\{\underbrace{e^{ikz}}_{\text{incident wave}} + \underbrace{\sum_{\ell m} C_{\ell m} h_\ell^{(1)}(kr)\, Y_\ell^m(\theta,\phi)}_{\text{scattered wave}}\Big\}$$

In our case there is no dependence on ϕ due to the spherical symmetry of $V(r)$ so only terms with $m=0$ survive (recall $Y_\ell^m \sim e^{im\phi}$). Given that $Y_\ell^0(\theta,\phi) = \sqrt{\frac{2\ell+1}{4\pi}}\, P_\ell(\cos\theta)$ where P_ℓ are Legendre polynomials we obtain

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

where we defined the coefficients a_ℓ in such a way that $C_{\ell 0} = i^{\ell+1} k \sqrt{4\pi(2\ell+1)}\, a_\ell$

For very large r $\quad h_\ell^{(1)}(kr) \to (-i)^{\ell+1}\frac{e^{ikr}}{kr}$, so

$$\psi(r,\theta) \to A\Big\{e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\Big\}$$

with

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

The differential cross section is then

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

while the total cross section becomes (if we use the orthogonality of P_ℓ: $\int_0^\pi P_\ell(\cos\theta)P_{\ell'}(\cos\theta)\sin\theta\, d\theta = \frac{2}{2\ell+1}\delta_{\ell\ell'}$)

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

The question that remains now is how to determine coefficients a_ℓ called partial wave amplitudes. This is done by solving the SE in the interior region (where $V \neq 0$) and matching it to the exterior solution $\psi = A\left\{ e^{ikz} + k \sum_{\ell=0}^{\infty} i^{\ell+1} (2\ell+1)\, a_\ell\, h_\ell^{(1)}(kr)\, P_\ell(\cos\theta) \right\}$ using the appropriate boundary conditions. To make things easier we expand $e^{ikz} = e^{ikr\cos\theta}$ in terms of spherical Bessel functions (any nonsingular function $g(x)$ can be expanded in terms of $j_\ell(x)$ as the latter form a complete set). It is known that

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

– Rayleigh formula

with that we can write the exterior solution as

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

To illustrate the above approach let us consider quantum scattering from a hard sphere:

$$V(r) = \begin{cases} \infty & r \le b \\ 0 & r > b \end{cases}$$

b - radius of the hard sphere

Boundary condition $\psi(b,\theta) = 0$, so

$$\sum_{\ell=0}^{\infty} i^\ell (2\ell+1) \left[j_\ell(ka) + ik a_\ell h_\ell^{(1)}(kb) \right] P_\ell(\cos\theta) = 0 \quad \forall\, \theta$$

Multiplying by $P_{\ell'}(\cos\theta)\sin\theta\, d\theta$ and integrating from 0 to π we get

$$2i^l\left[j_l(kb) + ik a_l h_l^{(1)}(kb)\right] = 0$$

and hence

$$a_l = -\frac{j_l(kb)}{ik\, h_l^{(1)}(kb)}$$

The total cross section is

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\left|\frac{j_l(kb)}{h_l^{(1)}(kb)}\right|^2$$

For low energy scattering $kb \ll 1$ ($k = \frac{2\pi}{\lambda}$ - the wavelength is much greater than b). For small value of the argument

$$\frac{j_l(x)}{h_l^{(1)}(x)} = \frac{j_l(x)}{j_l(x)+i n_l(x)} \simeq -i\frac{j_l(x)}{n_l(z)} \simeq \frac{i}{2l+1}\left[\frac{2^l l!}{(2l)!}\right]^2 z^{2l+1}$$

(we used $j_l(x) \xrightarrow[x\to 0]{} \frac{2^l l!}{(2l+1)!}x^l$ $\quad n_l(x) \xrightarrow[x\to 0]{} \frac{(2l)!}{2^l l!}\frac{1}{x^{l+1}}$)

With that we obtain:

$$\sigma \simeq \frac{4\pi}{k^2}\sum_{l=0}^{\infty}\frac{1}{2l+1}\left[\frac{2^l l!}{(2l)!}\right]^4 (kb)^{4l+2} \simeq 4\pi b^2$$

Phase shifts

The notion of phase shifts can be nicely illustrated in 1D case, when we have an impenetrable wall at $x=0$ and some localized potential near it. The incident wave $\psi_i = Ae^{ikx}$ $(x<-a)$ and the reflected wave $\psi_r = Be^{-ikx}$ $(x<-a)$ [here we assume V is nonzero at $-a<x<0$, and then $V=\infty$ at $x>0$]

No matter what happens in the interaction region

$(-a < x < 0)$ the amplitude of the reflected wave must be the same as that of the incident wave by conservation of probability. The only thing that can change is the phase. If $V=0$ everywhere than $B=-A$ since $\psi_{total} = \psi_i + \psi_r$ must vanish at $x=0$ (as $V(x>0)=\infty$)

$$\psi_{total} = A(e^{ikx} - e^{-ikx})$$

If the potential is not zero

$$\psi_{total} = A(e^{ikx} - e^{i(2\delta - kx)})$$

δ's are called phase shifts

The whole theory of elastic scattering reduces to calculating the phase shifts δ as a function of k.

In 3D case the incident wave carries no angular momentum in z-direction. Because the angular momentum is conserved (V is spherically symmetric) each partial wave scatters independently with no change in amplitude. If $V \equiv 0$ then the l-th partial wave is $\psi_{total} = Ae^{ikz}$ or

$$\psi^{(l)}_{total} = A i^l (2l+1) j_l(kr) P_l(\cos\theta)$$

Meanwhile

$$j_l(x) = \frac{1}{2}\left[h_l^{(1)}(x) + h_l^{(2)}(x)\right] \approx \frac{1}{2x}\left[(-i)^{l+1}e^{ix} + i^{l+1}e^{-ix}\right] \quad x \gg 1$$

when $r \to \infty$

$$\psi^{(l)}_{total} \approx A\frac{(2l+1)}{2ikr}\left[e^{ikr} - (-1)^l e^{-ikr}\right] P_l(\cos\theta)$$

The second term in the square brackets represents an incoming spherical wave. The first term is the outgoing wave. It picks up a phase shift δ_ℓ

$$\psi^{(\ell)} \approx A \frac{(2\ell+1)}{2ikr}\left[e^{i(kr+2\delta_\ell)} - (-1)^\ell e^{-ikr}\right] P_\ell(\cos\theta)$$

Previously we had expressed everything in terms of partial wave amplitudes a_ℓ. Now we have expressed everything in terms of δ_ℓ. The connection between the two is established when we consider the asymptotic form of $\psi(r,\theta) = A\left\{e^{ikz} + k\sum_{\ell=0}^{\infty} i^{\ell+1}(2\ell+1)a_\ell h_\ell^{(1)}(kr) P_\ell(\cos\theta)\right\}$

$$\psi^{(\ell)} \approx A\left\{\frac{2\ell+1}{2ikr}\left[e^{ikr} - (-1)^\ell e^{-ikr}\right] + \frac{2\ell+1}{r} a_\ell e^{ikr}\right\} P_\ell(\cos\theta)$$

By comparing this with the above formula we find

$$a_\ell = \frac{1}{2ik}\left(e^{2i\delta_\ell} - 1\right) = \frac{1}{k} e^{i\delta_\ell} \sin\delta_\ell$$

I follows that

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

and

$$\sigma = \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell$$