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

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

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

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 $R(r) = \frac{Z(kr)}{\sqrt{kr}} = \frac{Z(x)}{\sqrt{x}}$

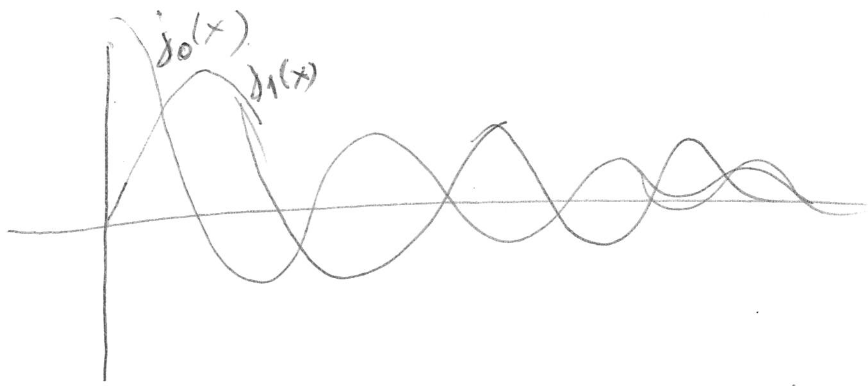
$$x^2 Z'' + x Z' + \left[x^2 - (\ell+\tfrac{1}{2})^2\right] Z = 0$$

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

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

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

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



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

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

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 polynomial

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 $e^{ikr} = e^{ikr\cos\theta}$ 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

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

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:

$$V(r) = \begin{cases} \infty & r \le b \\ 0 & r > b \end{cases} \qquad b \text{ – radius of the hard sphere}$$

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

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

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

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

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

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

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

With that we obtain:

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

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 $V(x>0) = \infty$)

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

If the potential is not zero

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

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

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

Meanwhile

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

when $r \to \infty$

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

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: $1 + 2ik\, a_\ell = e^{2i\delta_\ell}$

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

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

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