# QUANTUM SCATTERING: PARTIAL WAVE ANALYSIS

Link to: physicspages home page.

To leave a comment or report an error, please use the auxiliary blog.

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problems 11.3-11.4.

Post date: 9 Jun 2015.

For spherically symmetric potentials, the general solution to the Schrödinger equation for the scattering problem has the form

$$\psi(r,\theta)=A\left(e^{ikz}+f(\theta)\frac{e^{ikr}}{r}\right) \tag{1}$$

where $f$ is the scattering amplitude. The first term on the RHS represents the incident plane wave, and the second term on the RHS represents the scattered wave. One way of finding $f$ is *partial wave analysis*, which Griffiths describes in detail in his section 11.2, so I won't repeat the whole derivation here. It is worth, however, giving an overview of the technique to highlight the main concepts.

The main idea is to use the solution of the three-dimensional Schrödinger equation for a spherically symmetric potential that we considered earlier. The solution splits into two factors: a spherical harmonic $Y_l^m(\theta,\phi)$ that depends only on the angular coordinates and is independent of the potential, and a radial function $R(r)$ that depends only on the radial coordinate and *does* depend on the potential. The function $u(r)\equiv rR(r)$ satisfies the radial equation

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

In the region far from the target, where $V$ is very small, we can neglect the potential term and get the equation

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}u=Eu \tag{3}$$

This ODE can be solved in general using Hankel functions, and if we restrict our attention only to outgoing waves (since we're considering only particles scattering outwards from the target), we end up with an overall wave function of

$$\psi(r,\theta) = A\left\{e^{ikz} + k\sum_{l=0}^{\infty} i^{l+1}(2l+1)\,a_l h_l^{(1)}(kr)\,P_l(\cos\theta)\right\} \tag{4}$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \tag{5}$$

the Hankel function of the first kind is defined by

$$h_l^{(1)}(x) \equiv j_l(x) + i n_l(x) \tag{6}$$

(with $j_l$ and $n_l$ being spherical Bessel functions), and the $P_l$ being Legendre polynomials. The coefficients $a_l$ are what must be calculated for the particular potential being used.

For large $r$ (far from the target), we can use the asymptotic forms of the $h_l^{(1)}(kr)$ which are

$$h_l^{(1)}(kr) \sim (-i)^{l+1}\frac{e^{ikr}}{kr} \tag{7}$$

so in this region the wave function becomes

$$\psi(r,\theta) \approx A\left\{e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right\} \tag{8}$$

$$f(\theta) \equiv \sum_{l=0}^{\infty}(2l+1)\,a_l P_l(\cos\theta) \tag{9}$$

so we get an explicit formula for the scattering amplitude $f$.

The differential cross-section is given by a rather ugly formula:

$$D(\theta) = \frac{d\sigma}{d\Omega} = |f(\theta)|^2 \tag{10}$$

$$= \sum_{l=0}^{\infty}\sum_{l'=0}^{\infty}(2l+1)\left(2l'+1\right)a_l a_{l'} P_l(\cos\theta)\,P_{l'}(\cos\theta) \tag{11}$$

Integrating this over solid angle and using the orthonormality of the $P_l$, we get the total cross-section

$$\sigma = 4\pi\sum_{l=0}^{\infty}(2l+1)\,|a_l|^2 \tag{12}$$

Finally, to get a consistent formula where everything is in spherical coordinates, we need to convert the plane wave $e^{ikz}$ to spherical coordinates which gives the final result for the wave function:

$$\psi(r,\theta) = A\sum_{l=0}^{\infty} i^l (2l+1)\left[j_l(kr) + ika_l h_l^{(1)}(kr)\right] P_l(\cos\theta) \tag{13}$$

To find the $a_l$s, we need to solve the Schrödinger equation for the region near the target, where $V \neq 0$, and then match this solution up to the exterior solution 13 at the boundary between the two regions. Doing this requires a well-defined boundary, so it would seem that this method doesn't work for potentials that fall off continuously out to infinity.

**Example 1.** As a simple example of how this boundary matching process works, we consider the case of hard-sphere scattering. We have a sphere that is impenetrable so that

$$V = \begin{cases} \infty & r \le a \\ 0 & r > a \end{cases} \tag{14}$$

An infinite potential means that $\psi(r,\theta) = 0$ for $r \le a$, so the boundary condition occurs over the sphere $r = a$. Matching this to 13, we get

$$\sum_{l=0}^{\infty} i^l (2l+1)\left[j_l(ka) + ika_l h_l^{(1)}(ka)\right] P_l(\cos\theta) = 0 \tag{15}$$

We can work out $a_l$ by multiplying this equation by $P_{l'}(\cos\theta)$ and integrating over $\theta$, using the orthonormality of the $P_l$:

$$\sum_{l=0}^{\infty} i^l (2l+1)\left[j_l(ka) + ika_l h_l^{(1)}(ka)\right] \int_0^{\pi} P_l(\cos\theta) P_{l'}(\cos\theta) = 0 \tag{16}$$

$$\sum_{l=0}^{\infty} i^l (2l+1)\left[j_l(ka) + ika_l h_l^{(1)}(ka)\right] \delta_{ll'} = 0 \tag{17}$$

$$i^{l'}\left(2l'+1\right)\left[j_{l'}(ka) + ika_{l'} h_{l'}^{(1)}(ka)\right] = 0 \tag{18}$$

Therefore, the coefficients are

$$a_l = i\frac{j_l(ka)}{kh_l^{(1)}(ka)} \tag{19}$$

[Note that Griffiths's eqn 11.33 is wrong: there shouldn't be a minus sign on the RHS.]

**Example 2.** The delta-function spherical shell. Given the potential

$$V(r) = \alpha\delta(r-a) \tag{20}$$

we want to find $f(\theta)$. We'll take the incident particle to have very low energy, so that $ka \ll 1$. Since $k = 2\pi/\lambda$ this amounts to saying that $\lambda \gg a$ so that the wavelength of the particle is much greater than the size of the target. From Planck's formula $E = h\nu = h/\lambda$, this is equivalent to the particle having a low energy. In the text, Griffiths shows that the cross section can be expanded in powers of $(ka)^l$, so for low energy, only the $l = 0$ term is significant, so we'll restrict our analysis to that case.

The exterior solution is given by the $l = 0$ term from 13:

$$\psi_{ext} = A\left[j_0(kr) + ika_0 h_0^{(1)}(kr)\, P_0(\cos\theta)\right] \tag{21}$$

The Bessel and Hankel functions can be written in their exact forms in this case:

$$\begin{aligned} j_0(kr) &= \frac{\sin kr}{kr} &\quad (22)\\ h_0^{(1)}(kr) &= -i\frac{e^{ikr}}{kr} &\quad (23)\end{aligned}$$

Also, $P_0 = 1$ so we get, for $r \geq a$:

$$\psi_{ext} = \frac{A}{kr}\left[\sin kr + ka_0 e^{ikr}\right] \tag{24}$$

For the internal function for $r < a$, the potential is $V = 0$, so the general solution of the radial equation 2 is

$$\begin{aligned} u(r) &= B\sin kr + D\cos kr &\quad (25)\\ R(r) &= \frac{u(r)}{r} &\quad (26)\\ &= B\frac{\sin kr}{r} + D\frac{\cos kr}{r} &\quad (27)\end{aligned}$$

This solution must be valid at $r = 0$, so only the $\frac{\sin kr}{r}$ term is finite there, so we must have $D = 0$, giving

$$\psi_{in}(r) = B\frac{\sin kr}{r} \tag{28}$$

The wave function must be continuous at the boundary $r = a$, so

$$\frac{A}{ka}\left[\sin ka + ka_0 e^{ika}\right] = B\frac{\sin ka}{a} \tag{29}$$

Since the delta function is infinite at $r = a$, we can't assume that the derivative of the wave function is continuous there, but we can use the same method that we used in analyzing the delta function well to get another boundary condition. The radial equation 2 for $u$ is the same as the one dimensional Schrödinger equation that we solved for the delta function well, except that the delta function here is a barrier rather than a well, so we replace $-\alpha$ by $+\alpha$ to get the condition on the derivative. The radial equation for $l = 0$ is

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + \alpha\delta(x)u = Eu \tag{30}$$

Now if we integrate this equation term by term across the boundary, we get, for some value of $\epsilon$:

$$-\frac{\hbar^2}{2m}\int_{-\epsilon}^{\epsilon}\frac{d^2u}{dr^2}dr + \alpha\int_{a-\epsilon}^{a+\epsilon}\delta(r-a)u\,dr = E\int_{a-\epsilon}^{a+\epsilon}u\,dr \tag{31}$$

$$-\frac{\hbar^2}{2m}\frac{du}{dr}\bigg|_{a-\epsilon}^{a+\epsilon} + \alpha u(a) = E\int_{a-\epsilon}^{a+\epsilon}u\,dr \tag{32}$$

If we take the limit as $\epsilon \to 0$, the integral on the right tends to zero, since it is the integral of a continuous function over an infinitesimally small interval. The first term on the left, however, will *not* be zero, since derivative of the wave function is not continuous when the potential is infinite. Thus we get

$$\lim_{\epsilon\to 0}\frac{du}{dr}\bigg|_{a-\epsilon}^{a+\epsilon} = \frac{2m\alpha}{\hbar^2}u(a) \tag{33}$$

To simplify the notation in what follows I'll use the following shorthand:

$$s \equiv \sin ka \tag{34}$$

$$c \equiv \cos ka \tag{35}$$

$$e \equiv e^{ika} \tag{36}$$

From 24 and 28

$$\begin{aligned}
u_{ext}(r) &= r\psi_{ext}(r) && (37)\\
&= \frac{A}{k}(s+ka_0e) && (38)\\
\left.\frac{du_{ext}}{dr}\right|_{r=a} &= A(c+ika_0e) && (39)\\
u_{in}(r) &= r\psi_{in}(r) && (40)\\
&= Bs && (41)\\
\left.\frac{du_{in}}{dr}\right|_{r=a} &= Bkc && (42)
\end{aligned}$$

From 33 we get

$$\begin{aligned}
\lim_{\epsilon\to 0}\left.\frac{du}{dr}\right|_{a-\epsilon}^{a+\epsilon} &= \left.\frac{du_{ext}}{dr}\right|_{r=a} - \left.\frac{du_{in}}{dr}\right|_{r=a} && (43)\\
&= (A-Bk)c + Aika_0e && (44)\\
&= \frac{2m\alpha}{\hbar^2}u(a) && (45)\\
&= \frac{2m\alpha}{\hbar^2}Bs && (46)
\end{aligned}$$

To get rid of the constants $A$ and $B$ we use 29:

$$B = \frac{s+ka_0e}{ks}A \tag{47}$$

so we get from 44 and 46

$$\left(1-\frac{s+ka_0e}{s}\right)c + ika_0e = \frac{s^2+ka_0es}{sk}\frac{\beta}{a} \tag{48}$$

where

$$\beta \equiv \frac{2m\alpha a}{\hbar^2} \tag{49}$$

Solving for $a_0$ gives (restoring the full notation):

$$a_0 = -\frac{\beta e^{-ika}\sin^2 ka}{(\beta\sin ka + ka\cos ka - iak\sin ka)k} \tag{50}$$

For $ka \ll 1$ we can approximate $\sin ka \approx ka$, $\cos ka \approx 1$ and $e^{-ika} \approx 1$, so

$$a_0 \approx -\frac{\beta (ka)^2}{\left(\beta ka + ka - i(ak)^2\right)k} \tag{51}$$

$$\approx -\frac{\beta a}{1+\beta} \tag{52}$$

where we dropped the imaginary term in the denominator since it is of second order in $ak$.

The scattering amplitude, differential cross section and total cross section are, from 9, 11 and 12:

$$f(\theta) = a_0 = -\frac{\beta a}{1+\beta} \tag{53}$$

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \frac{\beta^2 a^2}{(1+\beta)^2} \tag{54}$$

$$\sigma = 4\pi |a_0|^2 = 4\pi \frac{\beta^2 a^2}{(1+\beta)^2} \tag{55}$$

As the strength $\alpha$ of the delta function gets higher, $\beta \to \infty$ and the cross section tends to $4\pi a^2$, which is the cross section for a hard sphere. Thus even though the delta function presents an infinite barrier, if it is of finite strength, the total cross section is less than that of a hard sphere.

## PINGBACKS

Pingback: Partial waves in three dimensions: hard sphere scattering
Pingback: Phase shift in the spherical delta function shell
Pingback: Born approximation for a spherical delta function shell