14.3: Partial Waves

We can assume, without loss of generality, that the incident wavefunction is characterized by a wavevector $\mathbf{k}$ that is aligned parallel to the z-axis. The scattered wavefunction is characterized by a wavevector $\mathbf{k}'$ that has the same magnitude as $\mathbf{k}$, but, in general, points in a different direction. The direction of $\mathbf{k}'$ is specified by the polar angle θ (i.e., the angle subtended between the two wavevectors), and an azimuthal angle ϕ about the z-axis. Equations ([e17.38]) and ([e17.39]) strongly suggest that for a spherically symmetric scattering potential [i.e., $V(\mathbf{r}) = V(r)$] the scattering amplitude is a function of θ only: that is,

$$f(\theta,\phi) = f(\theta). \tag{14.3.1}$$

It follows that neither the incident wavefunction,

$$\psi_0(\mathbf{r}) = \sqrt{n}\,\exp(\,{\rm i}\,k\,z) = \sqrt{n}\,\exp(\,{\rm i}\,k\,r\cos\theta), \tag{14.3.2}$$

nor the large-r form of the total wavefunction,

$$\psi(\mathbf{r}) = \sqrt{n}\left[\exp(\,{\rm i}\,k\,r\cos\theta) + \frac{\exp(\,{\rm i}\,k\,r)\,f(\theta)}{r}\right], \tag{14.3.3}$$

depend on the azimuthal angle ϕ.

Outside the range of the scattering potential, both $\psi_0(\mathbf{r})$ and $\psi(\mathbf{r})$ satisfy the free-space Schrödinger equation,

$$(\nabla^{\,2}+k^{\,2})\,\psi = 0. \tag{14.3.4}$$

What is the most general solution to this equation in spherical polar coordinates that does not depend on the azimuthal angle ϕ? Separation of variables yields

$$\psi(r,\theta) = \sum_l R_l(r)\,P_l(\cos\theta), \tag{14.3.5}$$

because the Legendre functions, $P_l(\cos\theta)$, form a complete set in θ-space. The Legendre functions are related to the *spherical harmonics*, introduced in Chapter [sorb], via

$$P_l(\cos\theta) = \sqrt{\frac{4\pi}{2\,l+1}}\,Y_{l,0}(\theta,\varphi). \tag{14.3.6}$$

Equations ([e17.54]) and ([e17.55]) can be combined to give

$$r^{\,2}\,\frac{d^{\,2}R_l}{dr^{\,2}} + 2\,r\,\frac{dR_l}{dr} + [k^{\,2}\,r^{\,2} - l\,(l+1)]\,R_l = 0. \tag{14.3.7}$$

The two independent solutions to this equation are the spherical Bessel functions, $j_l(k\,r)$ and $y_l(k\,r)$, introduced in Section [rwell]. Recall that

$$j_l(z) = z^{\,l}\left(-\frac{1}{z}\frac{d}{dz}\right)^l\left(\frac{\sin z}{z}\right),$$

$$y_l(z) = -z^{\,l}\left(-\frac{1}{z}\frac{d}{dz}\right)^l\left(\frac{\cos z}{z}\right).$$

Note that the $j_l(z)$ are well behaved in the limit $z\rightarrow 0$, whereas the $y_l(z)$ become singular. The asymptotic behavior of these functions in the limit $z\rightarrow\infty$ is

$$j_l(z) \rightarrow \frac{\sin(z-l\,\pi/2)}{z},$$

$$y_l(z) \rightarrow -\frac{\cos(z-l\,\pi/2)}{z}.$$

We can write

$$\exp(\,{\rm i}\,k\,r\cos\theta) = \sum_l a_l\,j_l(k\,r)\,P_l(\cos\theta), \tag{14.3.8}$$

where the a_l are constants. Note there are no $y_l(k\,r)$ functions in this expression because they are not well-behaved as $r\rightarrow 0$. The Legendre functions are orthonormal ,

$$\int_{-1}^{1} P_n(\mu)\,P_m(\mu)\,d\mu = \frac{\delta_{nm}}{n+1/2}, \tag{14.3.9}$$

so we can invert the previous expansion to give

$$a_l\,j_l(k\,r) = (l+1/2)\int_{-1}^{1}\exp(\,\mathrm{i}\,k\,r\,\mu)\,P_l(\mu)\,d\mu. \tag{14.3.10}$$

It is well known that

$$j_l(y) = \frac{(-\mathrm{i})^{\,l}}{2}\int_{-1}^{1}\exp(\,\mathrm{i}\,y\,\mu)\,P_l(\mu)\,d\mu, \tag{14.3.11}$$

where $l=0,1,2,\cdots$. Thus,

$$a_l = \mathrm{i}^{\,l}\,(2\,l+1), \tag{14.3.12}$$

giving

$$\psi_0(\mathbf{r}) = \sqrt{n}\,\exp(\,\mathrm{i}\,k\,r\cos\theta) = \sqrt{n}\sum_l \mathrm{i}^{\,l}\,(2\,l+1)\,j_l(k\,r)\,P_l(\cos\theta). \tag{14.3.13}$$

The previous expression tells us how to decompose the incident plane-wave into a series of spherical waves. These waves are usually termed “partial waves”.

The most general expression for the total wavefunction outside the scattering region is

$$\psi(\mathbf{r}) = \sqrt{n}\sum_l\left[A_l\,j_l(k\,r)+B_l\,y_l(k\,r)\right]P_l(\cos\theta), \tag{14.3.14}$$

where the A_l and B_l are constants. Note that the $y_l(k\,r)$ functions are allowed to appear in this expansion because its region of validity does not include the origin. In the large-r limit, the total wavefunction reduces to

$$\psi(\mathbf{r}) \simeq \sqrt{n}\sum_l\left[A_l\,\frac{\sin(k\,r-l\,\pi/2)}{k\,r} - B_l\,\frac{\cos(k\,r-l\,\pi/2)}{k\,r}\right]P_l(\cos\theta), \tag{14.3.15}$$

where use has been made of Equations ([e17.59a]) and ([e17.59b]). The previous expression can also be written

$$\psi(\mathbf{r}) \simeq \sqrt{n}\sum_l C_l\,\frac{\sin(k\,r-l\,\pi/2+\delta_l)}{k\,r}\,P_l(\cos\theta), \tag{14.3.16}$$

where the sine and cosine functions have been combined to give a sine function which is phase-shifted by δ_l. Note that $A_l = C_l\,\cos\delta_l$ and $B_l = -C_l\,\sin\delta_l$.

Equation ([e17.68]) yields

$$\psi(\mathbf{r}) \simeq \sqrt{n}\sum_l C_l\left[\frac{\mathrm{e}^{\,\mathrm{i}\,(k\,r-l\,\pi/2+\delta_l)}-\mathrm{e}^{-\mathrm{i}\,(k\,r-l\,\pi/2+\delta_l)}}{2\,\mathrm{i}\,k\,r}\right]P_l(\cos\theta), \tag{14.3.17}$$

which contains both incoming and outgoing spherical waves. What is the source of the incoming waves? Obviously, they must be part of the large-r asymptotic expansion of the incident wavefunction. In fact, it is easily seen from Equations ([e17.59a]) and ([e15.49]) that

$$\psi_0(\mathbf{r}) \simeq \sqrt{n}\sum_l \mathrm{i}^{\,l}\,(2l+1)\left[\frac{\mathrm{e}^{\,\mathrm{i}\,(k\,r-l\,\pi/2)}-\mathrm{e}^{-\mathrm{i}\,(k\,r-l\,\pi/2)}}{2\,\mathrm{i}\,k\,r}\right]P_l(\cos\theta) \tag{14.3.18}$$

in the large-r limit. Now, Equations ([e17.52]) and ([e17.53]) give

$$\frac{\psi(\mathbf{r})-\psi_0(\mathbf{r})}{\sqrt{n}} = \frac{\exp(\,\mathrm{i}\,k\,r)}{r}\,f(\theta). \tag{14.3.19}$$

Note that the right-hand side consists of an outgoing spherical wave only. This implies that the coefficients of the incoming spherical waves in the large-r expansions of $\psi(\mathbf{r})$ and $\psi_0(\mathbf{r})$ must be the same. It follows from Equations ([e17.69]) and ([e17.70]) that

$$C_l = (2\,l+1)\,\exp[\,\mathrm{i}\,(\delta_l + l\,\pi/2)]. \tag{14.3.20}$$

Thus, Equations ([e17.69])–([e17.71]) yield

$$f(\theta) = \sum_{l=0,\infty}(2\,l+1)\,\frac{\exp(\,\mathrm{i}\,\delta_l)}{k}\,\sin\delta_l\,P_l(\cos\theta). \tag{14.3.21}$$

Clearly, determining the scattering amplitude, $f(\theta)$, via a decomposition into partial waves (i.e., spherical waves) is equivalent to determining the phase-shifts, δ_l.

Now, the differential scattering cross-section, $d\sigma/d\Omega$, is simply the modulus squared of the scattering amplitude, $f(\theta)$. [See Equation ([e15.17]).] The total cross-section is thus given by

$$\begin{aligned}\sigma_{\text{total}} &= \int |f(\theta)|^{\,2}\,d\Omega \\ &= \frac{1}{k^{\,2}}\oint d\phi\int_{-1}^{1}d\mu\sum_l\sum_{l'}(2\,l+1)\,(2\,l'+1)\exp[\,\mathrm{i}\,(\delta_l-\delta_{l'})]\,\sin\delta_l\,\sin\delta_{l'}\,P_l(\mu)\,P_{l'}(\mu),\end{aligned}$$

where $\mu = \cos\theta$. It follows that

$$\sigma_{\text{total}} = \frac{4\pi}{k^{\,2}}\sum_l(2\,l+1)\,\sin^2\delta_l, \tag{14.3.22}$$

where use has been made of Equation ([e17.61]).

Contributors and Attributions

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