14.1: Fundamentals of Scattering Theory

Consider time-independent, energy conserving scattering in which the Hamiltonian of the system is written

$$H = H_0 + V(\mathbf{r}), \tag{14.1.1}$$

where

$$H_0 = \frac{p^2}{2\,m} \equiv -\frac{\hbar^2}{2\,m}\,\nabla^2 \tag{14.1.2}$$

is the Hamiltonian of a free particle of mass m, and $V(\mathbf{r})$ the scattering potential. This potential is assumed to only be non-zero in a fairly localized region close to the origin. Let

$$\psi_0(\mathbf{r}) = \sqrt{n}\,\mathrm{e}^{\,\mathrm{i}\,\mathbf{k}\cdot\mathbf{r}} \tag{14.1.3}$$

represent an incident beam of particles, of number density n, and velocity $\mathbf{v} = \hbar\,\mathbf{k}/m$. [See Equation ([e14.14gg]).] Of course,

$$H_0\,\psi_0 = E\,\psi_0, \tag{14.1.4}$$

where $E = \hbar^2\,k^2/(2\,m)$ is the particle energy. Schrödinger's equation for the scattering problem is

$$(H_0 + V)\,\psi = E\,\psi, \tag{14.1.5}$$

subject to the boundary condition $\psi \rightarrow \psi_0$ as $V \rightarrow 0$.

The previous equation can be rearranged to give

$$(\nabla^2 + k^2)\,\psi = \frac{2\,m}{\hbar^2}\,V\,\psi. \tag{14.1.6}$$

Now,

$$(\nabla^2 + k^2)\,u(\mathbf{r}) = \rho(\mathbf{r}) \tag{14.1.7}$$

is known as the *Helmholtz equation*. The solution to this equation is well known

$$u(\mathbf{r}) = u_0(\mathbf{r}) - \int \frac{\mathrm{e}^{\,\mathrm{i}\,k\,|\mathbf{r}-\mathbf{r}'|}}{4\pi\,|\mathbf{r}-\mathbf{r}'|}\,\rho(\mathbf{r}')\,d^3\mathbf{r}'. \tag{14.1.8}$$

Here, $u_0(\mathbf{r})$ is any solution of $(\nabla^2 + k^2)\,u_0 = 0$. Hence, Equation ([e15.6]) can be inverted, subject to the boundary condition $\psi \rightarrow \psi_0$ as $V \rightarrow 0$, to give

$$\psi(\mathbf{r}) = \psi_0(\mathbf{r}) - \frac{2m}{\hbar^2}\int \frac{\mathbf{e}^{ik|\mathbf{r}-\mathbf{r}'|}}{4\pi\,|\mathbf{r}-\mathbf{r}'|} V\left(\mathbf{r}'\right)\psi\left(\mathbf{r}'\right)d^3\mathbf{r}' \tag{14.1.9}$$

Let us calculate the value of the wavefunction $\psi(\mathbf{r})$ well outside the scattering region. Now, if $r \gg r'$ then

$$|\mathbf{r}-\mathbf{r}'| \simeq r - \hat{\mathbf{r}}\cdot\mathbf{r}' \tag{14.1.10}$$

to first-order in r'/r, where $\hat{\mathbf{r}}/r$ is a unit vector that points from the scattering region to the observation point. It is helpful to define $\mathbf{k}' = k\,\hat{\mathbf{r}}$. This is the wavevector for particles with the same energy as the incoming particles (i.e., $k' = k$) that propagate from the scattering region to the observation point. Equation ([e15.9]) reduces to

$$\psi(\mathbf{r}) \simeq \sqrt{n}\left[\mathrm{e}^{\,\mathrm{i}\,\mathbf{k}\cdot\mathbf{r}} + \frac{e^{\,\mathrm{i}\,k\,r}}{r}\,f(\mathbf{k},\mathbf{k}')\right], \tag{14.1.11}$$

where

$$f(\mathbf{k},\mathbf{k}') = -\frac{m}{2\pi\sqrt{n}\,\hbar^2}\int \mathrm{e}^{-\mathrm{i}\,\mathbf{k}'\cdot\mathbf{r}'}\,V(\mathbf{r}')\,\psi(\mathbf{r}')\,d^3\mathbf{r}'. \tag{14.1.12}$$

The first term on the right-hand side of Equation ([e15.11]) represents the incident particle beam, whereas the second term represents an outgoing spherical wave of scattered particles.

The *differential scattering cross-section*, $d\sigma/d\Omega$, is defined as the number of particles per unit time scattered into an element of solid angle $d\Omega$, divided by the incident particle flux. From Section [s7.2], the probability flux (i.e., the particle flux) associated with a wavefunction ψ is

$$\mathbf{j} = \frac{\hbar}{m}\,\mathrm{Im}(\psi^\ast\,\nabla\psi). \tag{14.1.13}$$

Thus, the particle flux associated with the incident wavefunction ψ_0 is

$$\mathbf{j} = n\,\mathbf{v}, \tag{14.1.14}$$

where $\mathbf{v} = \hbar\,\mathbf{k}/m$ is the velocity of the incident particles. Likewise, the particle flux associated with the scattered wavefunction $\psi-\psi_0$ is

$$\mathbf{j}' = n\,\frac{|f(\mathbf{k},\mathbf{k}')|^{\,2}}{r^{\,2}}\,\mathbf{v}', \tag{14.1.15}$$

where $\mathbf{v}' = \hbar\,\mathbf{k}'/m$ is the velocity of the scattered particles. Now,

$$\frac{d\sigma}{d\Omega}\,d\Omega = \frac{r^{\,2}\,d\Omega\,|\mathbf{j}'|}{|\mathbf{j}|}, \tag{14.1.16}$$

which yields

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{k},\mathbf{k}')|^{\,2}. \tag{14.1.17}$$

Thus, $|f(\mathbf{k},\mathbf{k}')|^{\,2}$ gives the differential cross-section for particles with incident velocity $\mathbf{v} = \hbar\,\mathbf{k}/m$ to be scattered such that their final velocities are directed into a range of solid angles $d\Omega$ about $\mathbf{v}' = \hbar\,\mathbf{k}'/m$. Note that the scattering conserves energy, so that $|\mathbf{v}'| = |\mathbf{v}|$ and $|\mathbf{k}'| = |\mathbf{k}|$.

Contributors and Attributions

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