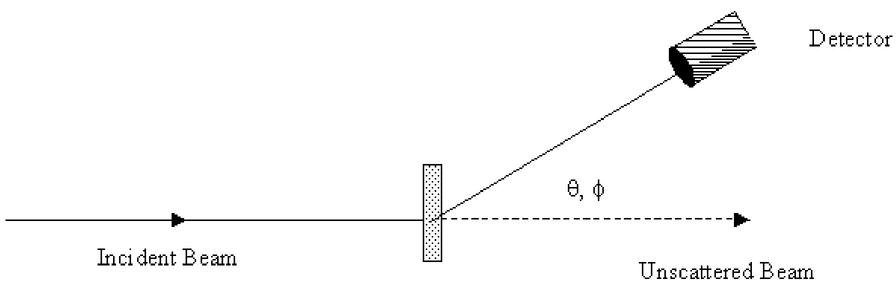
Chapter 9
SCATTERING THEORY

9.1 General Considerations

In this chapter we consider a situation of considerable experimental and theoretical interest, namely, the scattering of particles off of a medium containing some type of scattering centers, such as atoms, molecules, or nuclei. The basic experimental situation of interest is indicated in the figure below.



An incident beam of particles impinges upon a target, which maybe a cell containing atoms or molecules in a gas, a thin metallic foil, or a beam of particles moving at right angles to the incident beam. As a result of interactions between the particles in the initial beam and those in the target, some of the particles in the beam are deflected and emerge from the target traveling along a direction (θ, ϕ) with respect to the original beam direction, while some are left unscattered and emerge out the other side having undergone no deflection (or undergo "forward scattering"). The number of particles deflected along a given direction are then counted in a detector of some sort. The kinds of interactions and the analyis of general scattering situations of this type can be quite complicated. We will focus in the following discussion on the scattering of incident particles by scattering centers in the target uner the following conditions:

1. The incident beam is composed of idealized spinless, structureless, point particles.

2. The interaction of the particles with the scattering centers is assumed to be *elastic* so that the energy of the scattered particle is fixed, the internal structure of the scatterer (if any) and, thus, the potential seen by the scattered particle does not change during the scattering event.

3. There is no multiple scattering, so that each incident particle interacts with at most one scattering center, a condition that can be obtained with sufficiently thin or dilute targets.

4. The scattering potential $V(\vec{r}_1, \vec{r}_2) = V(|\vec{r}_1 - \vec{r}_2|)$ between the incident particle and the scattering center is a central potential, so we can work in the relative coordinate and reduced mass of the system.

Under these conditions, the picture of interest reduces to that depicted below, in with an incident particle characterized by a plane wave of wavevector $\vec{k} = k\hat{z}$ along a direction that we take parallel to the z-axis, and scattered particles emerging through a infinitesimal solid angle $d\Omega$ along some direction (θ, ϕ).

We may characterize the incident beam by its (assumed uniform) current density $\vec{J}_i$ along the z axis. Classically

$$\vec{J}_i = n\vec{v}_i$$

where $n = dN/dV$ is the particle number density characterizing the beam. The incident particle current through a specified surface S is then the surface integral

$$I = \frac{dN_S}{dt} = \int_S \vec{J}_i \cdot d\vec{S}.$$

The scattered particle current dI_S into a far away detector subtending solid angle $d\Omega$ along (θ, ϕ) is found to be proportional to (i) the magnitude of the incident flux density J_i, and (ii) the magnitude of the solid angle $d\Omega$ subtended by the detector. We write

$$dI_S = \frac{d\sigma(\theta, \phi)}{d\Omega} J_i d\Omega$$

where the constant of proportionality $d\sigma(\theta, \phi)/d\Omega$ is referred to as the differential cross section for elastic scattering in the direction (θ, ϕ). This quantity contains all information experimentally available regarding the interaction between scattered particles and the scattering center. We also define the *total cross section* $\sigma = \sigma_{\text{tot}}$ in terms of the total scattered current I_S through a detecting sphere centered on the scattering center:

$$I_S = \int dI_S = J_i \int \frac{d\sigma(\theta, \phi)}{d\Omega} d\Omega = J_i \sigma_{\text{tot}}$$

so that the total cross section is simply the integral over all solid angle

$$\sigma_{\text{tot}} = \int_{\text{sphere}} \frac{d\sigma(\theta, \phi)}{d\Omega} \delta\Omega.$$

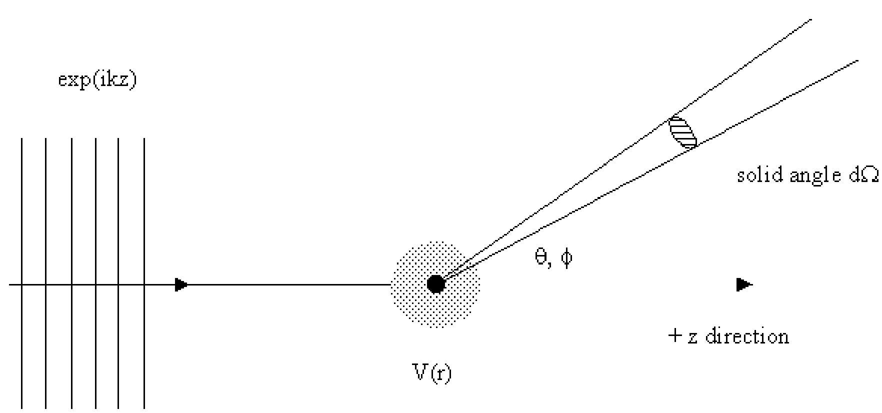


Figure 1

of the differential cross section. We note that $d\sigma/d\Omega$ and $\sigma_{\rm tot}$ both have units of area

$$\sigma_{\rm tot} = \frac{I_s}{J_i} \qquad\qquad \frac{d\sigma}{d\Omega} = \frac{1}{J_i}\frac{dI_S}{d\Omega}$$

and physically represent the effective cross sectional area of the target atom "seen" by the incident particle. As such it contains, in principle, information about the relative sizes of the particles involved in the collision as well as the effective range of the interaction potential $V(r)$ without which there would be no scattering. Cross sections are often measured in "barns", where by definition 1 barn = 10^{-24} cm^2 , which corresponds to the cross sectional area of an object with a linear extent on the order of 10^{-12} cm.

Thus, given that the cross section is the primary observable of a scattering experiment, the main theoretical task reduces to the following: given the scattering potential $V(r)$, calculate the differential and total scattering cross sections $d\sigma/d\Omega$ and $\sigma_{\rm tot}$ as a function of the energy or wavevector of the incident particle. This problem can be addressed in a number of different ways. Perhaps the simplest conceptual approach would be as follows:

1. Consider a particle in an initial state at $t = -\infty$ corresponding to a wave packet at $z = -\infty$ centered in momentum about $\vec{k} = k\hat{z}$.
2. Evolve the wavepacket accordiing to the full Schrödinger equation

   $$i\hbar\frac{d}{dt}|\psi(t)\rangle = H|\psi(t)\rangle$$

   to large positive times $t \to +\infty$.
3. Evaluate the probability current through $d\Omega$ along (θ, ϕ).

Such an approach leads to a study of the so-called S-matrix

$$S = \lim_{t\to\infty} U(t, -t) = U(-\infty, \infty).$$

Rather than proceed along this route, we make a few simplifying observations. First,we note that the essential scattering process is time-independent, and can yield steady-state scattering currents, with J_i and J_S independent of time. Secondly, for elastic scattering the particle energy is fixed and well defined, and it seems a shame to throw this away by forming a wavepacket of the type described. Finally, we note that the evolution of the system is completely governed by the positive energy solutions to the energy eigenvalue equation

$$(H - \varepsilon)|\psi\rangle = 0.$$

This last observation leads us to ask whether or not there generally exist stationary solutions to the energy eigenvalue equation that have asymptotic properties corresponding to the experimental situation of interest. The answer, in general, is yes and the solutions of interest are referred to as *stationary scattering states* of the associated potential $V(r)$. To understand these states it is useful to consider the $1D$ analogy of a free particle incident upon a potential barrier, as indicated in the diagram. For this situation, there exist solutions in which the wave function to the left of the barrier is a linear combination of a right-going (incident) and left-going (scattered) wave, while the wave function to the right of the barrier contains a part that corresponds to the transmitted or "forward scattered" part of the wave. We note that experimentally, the wave function in the barrier region is inaccessible, and the only information that we can obtain is by measuring the relative magnitudes of the forward and backward scattered waves.

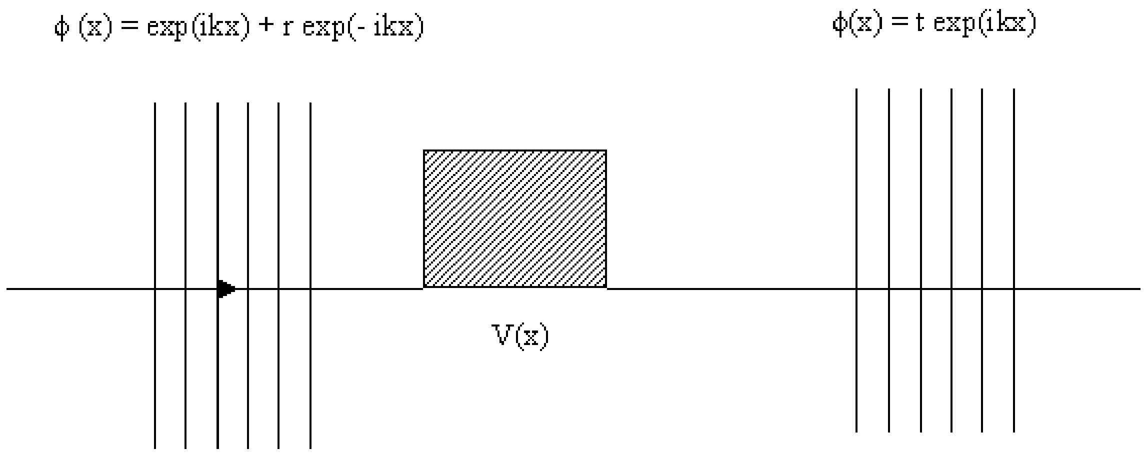


Figure 2

Similar arguments in 3-dimensions lead us to seek solutions to the eigenvalue equation of the form

$$\phi_\epsilon(\vec{r}) = e^{ikz} + \phi_S(\vec{r})$$

in which the first part on the right clearly corresponds to the incident part of the beam and the second term corresponds to the scattered part. The subscript ε indicates the energy of the incoming and outgoing particle, which is related to the wavevector of the incoming particle through the standard relation $\varepsilon = \hbar^2 k^2/2m$. We expect that at large distances from the scattering center, where the potential vanishes, the scattered part of the wave takes the form of an outward propagating wave. Hence, as $r \to \infty$, we anticipate that ϕ_S has the asymptotic behavior

$$\phi_S(\vec{r}) \sim \frac{f(\theta,\phi)e^{ikr}}{r} \qquad\qquad r \to \infty.$$

Note that this form satisfies the eigenvalue equation for large r beyond the range of the potential, where the Hamiltonian reduces simply to the kinetic energy $H \to H_0 = P^2/2m$.

Thus we seek solutions to the eigenvalue equation

$$(H_0 + V)\,|\phi_\epsilon\rangle = \varepsilon|\phi_\varepsilon\rangle$$

which have the asymptotic form

$$\phi_\varepsilon(\vec{r}) \sim e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}$$

where the quantity $f(\theta,\phi)$ which determines the angular distribution of the scattered part of the wave is referred to, appropriately as the *scattering amplitude* in the (θ,ϕ) direction or, alternatively, as the *scattering length* since it is readily determined by dimensional analysis that $f(\theta,\phi)$ has units of length. The obvious question that arises at this point is the following: what is the relation between the scattering length $f(\theta,\phi)$ and the scattering cross section $d\sigma(\theta,\phi)/d\Omega$? To anwer this question we note that, by definition, the current into the detector can be written

$$dI_S = \sigma(\theta,\phi)J_i d\Omega.$$

But we can also write this in terms of the scattered current density $\vec{J}_S = \vec{J}_S(r, \theta, \phi)$, i.e.,

$$dI_s = \vec{J}_S \cdot d\vec{S} = r^2 J_S d\Omega.$$

Thus, classically,

$$J_i \frac{d\sigma(\theta, \phi)}{d\Omega} = r^2 J_s(r, \theta, \phi).$$

Now for quantum systems these conditions will be obeyed by the corresponding mean values taken with respect to the stationary state of interest, so that

$$\frac{d\sigma(\theta, \phi)}{d\Omega} = r^2 \frac{\langle J_s(r, \theta, \phi)\rangle}{\langle J_i \rangle}.$$

Thus, we need operators corresponding to the current density. Classically, for a single particle at $\vec{r}$,

$$\vec{J}(\vec{r}_0) = n(\vec{r}_0)\vec{v} = \delta(\vec{r} - \vec{r}_0)\vec{v} = \delta(\vec{r} - \vec{r}_0)\frac{\vec{p}}{m}.$$

In going to quantum mechanics we replace $\vec{r}$ and $\vec{p}$ by operators and symmeterize to ensure Hermiticity. Thus,

$$J(\vec{r}_0) = \frac{1}{2m}[\delta(\vec{R} - r_0)\vec{P} + \vec{P}\delta(\vec{R} - \vec{r}_0)].$$

After a short calculation, the mean value of $\vec{J}(\vec{r}_0)$ in the state $|\phi\rangle$ is found to be

$$\langle \phi | \vec{J}(\vec{r}_0) | \phi \rangle = \frac{1}{m} \operatorname{Re}\left[\phi^*(\vec{r}_0)\frac{\hbar}{i}\vec{\nabla}\phi(\vec{r}_0)\right].$$

Using this, the incident flux, associated with the plane wave part of the eigenstate, can be written

$$\langle J_i \rangle = \left| \frac{1}{m} \operatorname{Re}\left[e^{-ikz}\frac{\hbar}{i}\vec{\nabla}e^{ikz}\right]\right| = \frac{\hbar k}{m}.$$

By contrast, the scattered flux is then given by the expression

$$\langle \vec{J}_S \rangle = \langle |\vec{J}(r, \theta, \phi)\rangle = \frac{1}{m} \operatorname{Re}\left[\phi_S^*(\vec{r})\frac{\hbar}{i}\vec{\nabla}\phi_S(\vec{r})\right]$$

which is most conveniently expressed in spherical coordinates, for which

$$\nabla_r = \frac{\partial}{\partial r} \qquad \nabla_\theta = \frac{1}{r}\frac{\partial}{\partial \theta} \qquad \nabla_\phi = \frac{1}{r \sin\theta}\frac{\partial}{\partial \phi}$$

Using these along with the assumed asymptotic form for ϕ_S we find that

$$\langle J_S \rangle_r = \frac{\hbar k}{m}\frac{1}{r^2}|f(\theta, \phi)|^2$$

$$\langle J_S \rangle_\theta = \frac{\hbar}{m}\frac{1}{r^3} \operatorname{Re}\left[\frac{1}{i}f^*\frac{\partial f}{\partial \theta}\right]$$

$$\langle J_S \rangle_\phi = \frac{\hbar}{m}\frac{1}{r^3 \sin\theta} \operatorname{Re}\left[\frac{1}{i}f^*\frac{\partial f}{\partial \phi}\right]$$

which shows that asymptotically the angular components of current density become negligible compared to the radial component. Thus, from the radial component of the current density we deduce that

$$\frac{d\sigma(\theta, \phi)}{d\Omega} = r^2 \frac{\langle J_s(r, \theta, \phi)\rangle_r}{\langle J_i \rangle} = |f(\theta, \phi)|^2.$$

Thus, there is a very simple relation

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

between the scattering length and the cross sections that are experimentally accessible. We now turn to the problem of actually solving the energy eigenvalue equation to find the stationary scattering solutions, and thereby to determine the scattering length $f(\theta,\phi)$ for a given potential $V(r)$.

9.2 An Integral Equation for the Scattering Eigenfunctions

We seek solutions to the eigenvalue equation

$$(H-\varepsilon)\,|\phi_\varepsilon\rangle = 0$$

$$H = H_0 + V$$

in which $H_0 = \hbar^2 K^2/2m$ and we assume that

$$V(r) \to 0 \qquad \text{as} \qquad r \to \infty \qquad (\text{at least as fast as } r^{-1})$$

Since we are describing a situation where we are sending in incident particles with well defined kinetic energy, we expect solutions for all positive energys $\varepsilon \geq 0$, so we need just find the corresponding eigenvectors $|\phi_\varepsilon\rangle$, which have the form

$$|\phi_\varepsilon\rangle = |\phi_0\rangle + |\phi_S\rangle$$

in which $|\phi_0\rangle = |\vec{k}_0\rangle$ is the incident part, which is an eigenstate of H_0 with energy $\varepsilon = \hbar^2 k^2/2m$

$$\phi_0(\vec{r}) = \langle \vec{r}|\phi_0\rangle = e^{i\vec{k}_0\cdot\vec{r}} = e^{ikz}$$

and $|\phi_S\rangle$ is the scattered part, which should dissapear as the potential $V(r)$ goes to zero. To proceed, we rewrite the eigenvalue equation

$$(H_0 + V - \varepsilon)\,|\phi_\varepsilon\rangle = 0$$

in the form

$$(\varepsilon - H_0)\,|\phi_\varepsilon\rangle = V|\phi_\varepsilon\rangle$$

and substitute in the assumed form of the solution to obtain

$$(\varepsilon - H_0)\,[|\phi_0\rangle + |\phi_S\rangle] = V|\phi_\varepsilon\rangle$$

or

$$(\varepsilon - H_0)|\phi_S\rangle = V|\phi_\varepsilon\rangle.$$

In this last form, only the scattered part of the state appears on the left hand side. We note at this point that if the operator $(\varepsilon - H_0)$ possessed an inverse, we could apply it to the left hand side to obtain a formal expression for $|\phi_S\rangle$. The problem with this idea is that for $\varepsilon > 0$ the operator $(\varepsilon - H_0)$ has a large degenerate subspace with eigenvalue 0, since H_0 generally has a degenerate subspace for any positive energy ε. Thus, strictly speaking, $\det(\varepsilon - H_0) = 0$ and the inverse is not defined.

To overcome this difficulty we employ a little analytic continuation, and define the resolvent operator $G(z)$, defined for all non-real z, as the operator inverse of $z - H_0$, i.e.,

$$G(z) = (z - H_0)^{-1}$$

since H_0 has no non-real eigenvalues, this operator exists for all non-real values of the complex parameter z. We then define the (causal) Green's function operator $G_+(\varepsilon)$ as the limit, if it exists, of $G(z)$ as $z \to \varepsilon + i\eta$, where $\eta = 0^+$ is a positive infinitesimal:

$$G_+(\varepsilon) = \lim_{\eta \to 0^+} (\varepsilon + i\eta - H_0)^{-1} \equiv (\varepsilon_+ - H_0)^{-1}.$$

where

$$\varepsilon_+ = \varepsilon + i\eta.$$

Thus, if the limit exists, then

$$\lim_{\eta \to 0^+} G(\varepsilon + i\eta)(\varepsilon - H_0) = G_+(\varepsilon)(\varepsilon - H_0) = 1$$

and we can write

$$G_+(\varepsilon)(\varepsilon - H_0)|\phi_S\rangle = G_+(\varepsilon)|\phi_\varepsilon\rangle$$

or, more simply,

$$|\phi_S\rangle = G_+(\varepsilon)|\phi_\varepsilon\rangle$$

Adding the incident part of the state $|\phi_0\rangle$ to both sides, we then obtain the so-called Lipmann-Schwinger equation

$$|\phi_\varepsilon\rangle = |\phi_0\rangle + G_+ V|\phi_\varepsilon\rangle$$

which is itself a representation independent form of what is often referred to as the integral scattering equation. The latter follows from the Lipmann-Schwinger equation by expressing it in the position representation. Multiplying on the left by the bra $\langle\vec{r}|$ we obtain

$$\langle\vec{r}|\phi_\varepsilon\rangle = \langle\vec{r}|\phi_0\rangle + \langle\vec{r}|G_+ V|\phi_\varepsilon\rangle$$

or, inserting a complete set of position states,

$$\phi_\varepsilon(\vec{r}) = e^{ikz} + \int d^3\vec{r}'\; G_+(\vec{r}, \vec{r}')V(\vec{r}')\phi_\varepsilon(\vec{r}').$$

Thus, we obtain an integral equation for the scattering eigenfunction $\phi_\varepsilon(\vec{r})$ which has, we hope, the correct asymptotic behavior. To make this useful,we need to (i) evaluate the matrix elements $G_+(\vec{r}, \vec{r}') = \langle\vec{r}|G_+(\varepsilon)|\vec{r}'\rangle$, and (ii) actually solve the integral equation, at least in the asymptotic regime.

9.2.1 Evaluation Of The Green's Function

To evaluate the matrix elements of the Green's function it is most convenient to begin the calculation in the wavevector representation in which the operator $(\varepsilon - H_0)$ is diagonal. Note that in k-space

$$\langle\vec{k}|(\varepsilon_+ - H_0)|\vec{k}'\rangle = (\varepsilon_+ - \varepsilon_k)\,\delta(\vec{k} - \vec{k}')$$

where

$$\varepsilon_k = \hbar^2 k^2/2m$$

so that

$$(\varepsilon_+ - H_0) = \int d^3q\; |\vec{q}\rangle\,(\varepsilon_+ - \varepsilon_q)\,\langle\vec{q}|$$

and hence, as is easily verified by direct multiplication,

$$(\varepsilon_+ - H_0)^{-1} = \int d^3q\; \frac{|\vec{q}\rangle\langle\vec{q}|}{(\varepsilon_+ - \varepsilon_q)}$$

If we set

$$k_+ = \sqrt{\frac{2m\varepsilon_+}{\hbar^2}} = k + i\eta \qquad\qquad (\eta = 0^+)$$

where the positivity of η in this last equation follows from the positive imaginary part of ε_+, then we can write

$$G_+(\varepsilon) = \frac{2m}{\hbar^2}\int d^3q \,\frac{|\vec{q}\rangle\langle\vec{q}|}{k_+^2 - q^2}$$

so that

$$\begin{aligned} G_+(\vec{r},\vec{r}') &= \frac{2m}{\hbar^2}\int d^3q \,\frac{\langle\vec{r}|\vec{q}\rangle\langle\vec{q}|\vec{r}'\rangle}{k_+^2 - q^2} \\ &= \frac{2m}{\hbar^2}\int \frac{d^3q}{(2\pi)^3}\,\frac{e^{i\vec{q}\cdot(\vec{r}-\vec{r}')}}{k_+^2 - q^2} \\ &= \frac{2m}{\hbar^2}\int_0^{2\pi} d\phi \int_0^{\pi} d\theta\, \sin\theta \int_0^{\infty} \frac{dq\, q^2}{(2\pi)^3}\,\frac{e^{i\vec{q}R\cos\theta}}{k_+^2 - q^2} \end{aligned}$$

where $\vec{R} = \vec{r} - \vec{r}'$ and $R = \left|\vec{R}\right|$. The angular integrations are readily evaluated and give

$$G_+(\vec{r},\vec{r}') = \frac{m}{\hbar^2\pi^2 R}\int_0^{\infty} dq\, \frac{q\sin(qR)}{k_+^2 - q^2} = \frac{m}{2\hbar^2\pi^2 R}\int_{-\infty}^{\infty} dq\, \frac{q\sin(qR)}{k_+^2 - q^2}$$

where we have used the fact that the integrand is an even function of q. Splitting $\sin(qR)$ into exponentials and setting $q' = -q$ in the second we find that

$$G_+(\vec{r},\vec{r}') = \frac{m}{\pi\hbar^2 R}\frac{1}{2\pi i}\int_{-\infty}^{\infty} dq\, \frac{qe^{iqR}}{k_{+2} - q^2}$$

This integral can be evaluated by contour integration in the complex q-plane using Cauchy's theorem,which states that for a function $f(z)$ that is analytic in and on a closed contour Γ in the complex z-plane enclosing the point $z = a$,

$$\frac{1}{2\pi i}\oint_{\Gamma} \frac{f(z)dz}{z - a} = f(a).$$

In our case we choose a closed path in which q runs from $-Q$to $+Q$ and then circles back around on a semicircle in the upper half plane, which is ultimately taken to occur at $|Q| = \infty$. Since the contribution from the integrand vanishes along this latter part, the integral over the closed contour coincides with the one of interest.

To proceed, we note that

$$k_+^2 - q^2 = (k_+ - q)\,(k_+ + q)$$

which generates simple poles at

$$q = k_+ = k + i\eta$$

and

$$q = -k_+ = -k - i\eta$$

only the first of which is enclosed by our contour. Setting

$$f(q) = \frac{qe^{iqR}}{k_+ + q}$$

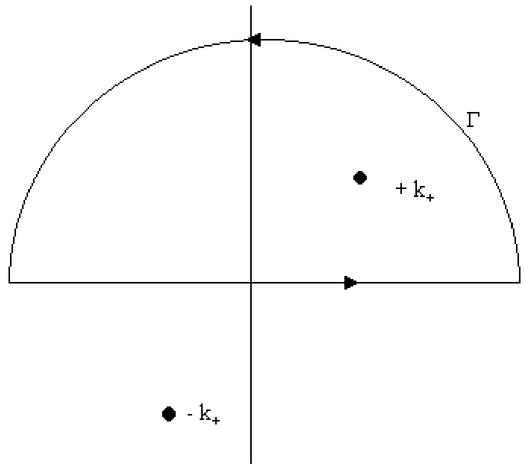


Figure 3

we find that

$$\frac{1}{2\pi i}\oint_{\Gamma}\frac{f(q)dq}{k_+ - q} = -\frac{1}{2\pi i}\oint_{\Gamma}\frac{f(q)dq}{q - k_+} = -f(k_+) = -\frac{e^{ik_+R}}{2}$$

Combing this with our previous formula, and taking the limit $k_+ \to k$ we obtain the Green's function of interest, i.e.,

$$G_+(\vec{r}, \vec{r}') = -\frac{me^{ik|\vec{r}-\vec{r}'|}}{2\pi\hbar^2\,|\vec{r}-\vec{r}'|} = G_+(\vec{r}-\vec{r}').$$

Putting this into our integral scattering equation gives the result

$$\phi_\varepsilon(\vec{r}) = e^{ikz} - \frac{m}{2\pi\hbar^2}\int d^3r'\;\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}V(\vec{r}')\phi_\varepsilon(\vec{r}').$$

Before proceeding to solve this integral equation we should, perhaps, check to see that it gives solutions with the correct asymptotic behavior. To this end, we note that the integrand has contributions primarily from those regions where r' is small, i.e., where the potential is significant. At the detector, however, the magnitude of r is very large, and $V(r)$ is negligible. Where the integrand is significant, therefore, we have $|\vec{r}| >> |\vec{r}'|$. In this limit we can write

$$\begin{aligned}
|\vec{r}-\vec{r}'| &= \sqrt{(\vec{r}-\vec{r}')\cdot(\vec{r}-\vec{r}')} = \sqrt{r^2 - 2\vec{r}\cdot\vec{r}' + r'^2} \\
&\simeq r\sqrt{1 - 2\vec{r}\cdot\vec{r}'/r^2} = r\left(1 - \vec{r}\cdot\vec{r}'/r^2\right) \\
&\simeq r - \hat{r}\cdot\vec{r}'
\end{aligned}$$

where $\hat{r} = \vec{r}/r$ is a unit vector along the direction (θ, ϕ) associated with the detector. Hence in this limit we can write

$$\frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} \simeq \frac{e^{ikr}}{r}e^{-ik\hat{r}\cdot\vec{r}'}$$

and so our integral equation provides a solution of the form

$$\begin{aligned}\phi_\varepsilon(\vec{r}) &\simeq e^{ikz} - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\int d^3r'\; e^{-ik\hat{r}\cdot\vec{r}'}V(\vec{r}')\phi_\varepsilon(\vec{r}') \\ &\simeq e^{ikz} + f(\theta,\phi)\frac{e^{ikr}}{r}\end{aligned}$$

where

$$f(\theta,\phi) = -\frac{m}{2\pi\hbar^2}\int d^3r'\; e^{-ik\hat{r}\cdot\vec{r}'}V(\vec{r}')\phi_\varepsilon(\vec{r}')$$

is independent of r, but depends only upon $\hat{r} = \hat{r}(\theta,\phi)$, as it should. Thus, a solution to this equation should indeed have the correct asymptotic properties associated with the stationary scattering states of interest.

9.3 The Born Expansion

Now that we have an explicit representation for the Green's function $G_+(\varepsilon)$ we can attempt a solution to the Lipmann-Schwinger equation

$$|\phi_\varepsilon\rangle = |\phi_0\rangle + G_+V|\phi_\varepsilon\rangle.$$

The traditional method of solving this kind of equation, or its integral equation equivalent is by iteration. Any approximation to $|\phi_\varepsilon\rangle$ can be substituted into the right-hand side of the equation to generate a new approximation . Moreover, we can formally write

$$\begin{aligned}|\phi_\varepsilon\rangle &= |\phi_0\rangle + G_+V\left[|\phi_0\rangle + G_+V|\phi_\varepsilon\rangle\right] \\ &= |\phi_0\rangle + G_+V|\phi_0\rangle + G_+VG_+V|\phi_\varepsilon\rangle\end{aligned}$$

Proceeding in this way generates the so-called Born expansion

$$\begin{aligned}|\phi_\varepsilon\rangle &= |\phi_0\rangle + G_+V|\phi_0\rangle + G_+VG_+V|\phi_0\rangle + \cdots \\ &= \sum_{k=0}^{\infty}(G_+V)^n\,|\phi_0\rangle.\end{aligned}$$

The Born expansion gives a an expansion in powers of the potential V, and obviously requires for its convergence that the effect of the perturbation V on the incident wave be small, hence $||\phi_S|| << ||\phi_0||, ||\phi_\varepsilon||$. The solution obtained by truncating the series at order n is referred to as the nth order Born approximation to the scattered state. We defer till later an exploration of the approximate solutions obtained in this fashion, and instead introduce additional ways of looking at the problem.

9.4 Scattering Amplitudes and T-Matrices

The form that we have developed for the scattering amplitude

$$f(\theta,\phi) = f(\hat{r}) = -\frac{m}{2\pi\hbar^2}\int d^3r'\; e^{-ik\hat{r}\cdot\vec{r}'}V(\vec{r}')\phi_\varepsilon(\vec{r}')$$

describes the amplitude for measuring a deflected particle along the direction $\hat{r}(\theta,\phi)$ with wavevector k. Thus, it measures a state of wavevector $\vec{k}_f = k\hat{r}$, so we can write $f(\theta,\phi) = f(\hat{r}) = f(\vec{k}_f,\vec{k}_0)$ in the form

$$f(\vec{k},\vec{k}_0) = -\frac{m}{2\pi\hbar^2}\int d^3r'\; e^{-ik_f\cdot\vec{r}'}V(\vec{r}')\phi_\varepsilon(\vec{r}')$$

which has the form of a projection of $V|\phi_\varepsilon\rangle$ onto the plane wave state $|\vec{k}_f\rangle$ associated with the wave function $\langle\vec{r}|\vec{k}_f\rangle = e^{i\vec{k}_f\cdot\vec{r}}$ (Note that the normalization of this plane wave state is a little different than usual, but is consistent with our choice of $|\phi_0\rangle$.) Thus, e.g.,

$$\langle\vec{k}_f|V|\phi_\varepsilon\rangle = \int d^3r'\ e^{-ik_f\cdot\vec{r}'}V(\vec{r}')\phi_\varepsilon(\vec{r}')$$

$$f(\vec{k}_f,\vec{k}_0) = -\frac{m}{2\pi\hbar^2}\langle\vec{k}_f|V|\phi_\varepsilon\rangle$$

which appears to be a matrix element of V, except that it is taken between states of different type. The state on the left is part of an ONB of free particle states, that on the right is an eigenstate of the same energy in the presence of the potential, which is "smoothly connected" to the plane wave state $|\phi_0\rangle = |k_0\rangle$ as $V \to 0$. It is useful to introduce an operator T, referred to as the T matrix, or transition operator which is defined so that

$$V|\phi_\varepsilon\rangle = T|\phi_0\rangle = T|\vec{k}_0\rangle.$$

This allows us to express the scattering amplitude

$$f(\theta,\phi) = f(\vec{k},\vec{k}_0) = -\frac{m}{2\pi\hbar^2}\langle\vec{k}_f|T|\vec{k}_0\rangle$$

as the matrix element of the transition operator between initial and final free particle states (which are the ones that we deal with in the laboratory, outside of the target region). Hence the T-matrix contains all information regarding the scattering transitions induced by the potential. How do we evaluate T? We generate an integral equation for it from the Lipmann-Schwinger equation, which gives

$$\begin{aligned}|\phi_\varepsilon\rangle &= |\phi_0\rangle + G_+V|\phi_\varepsilon\rangle.\\ &= |\phi_0\rangle + G_+T|\phi_0\rangle = (1+G_+T)|\phi_0\rangle\end{aligned}$$

We can compare this with the Born series to obtain

$$|\phi_\varepsilon\rangle = |\phi_0\rangle + G_+V|\phi_0\rangle + G_+VG_+V|\phi_0\rangle + \cdots$$

to obtain the operator relation

$$G_+T = |\phi_\varepsilon\rangle = G_+V + G_+VG_+V + \cdots$$

from which we deduce that

$$T = V + VG_+V + VG_+VG_+V + \cdots$$

which gives a Born expansion for T in powers of the potential V. Formally we can write

$$\begin{aligned}T &= V\left[1 + G_+V + G_+VG_+V + \cdots\right]\\ &= V + VG_+T\end{aligned}$$

which is the integral equation obeyed by the T-matrix that generates the Born series. The nth order Born approximation to the T-matrix is then obtained by truncating the series ath the nth order term. The first Born approximation to the T-matrix is just the scattering potential

$$T = T^{(1)} = V$$

and so we obtain to this order

$$f_B(\vec{k}_f,\vec{k}_i) = -\frac{m}{2\pi\hbar^2}\langle\vec{k}_f|V|\vec{k}_i\rangle.$$

To evaluate this, we work in the position representation

$$\begin{aligned} f_B(\vec{k}_f, \vec{k}_i) &= -\frac{m}{2\pi\hbar^2} \int d^3r \, \langle \vec{k}_f | \vec{r} \rangle V(\vec{r}) \langle \vec{r} | \vec{k}_i \rangle \\ &= -\frac{m}{2\pi\hbar^2} \int d^3r \, e^{-i(\vec{k}_f - \vec{k}_i)\cdot\vec{r}} V(\vec{r}). \end{aligned}$$

Clearly the vector

$$\vec{q} = \vec{k}_f - \vec{k}_i$$

is the momentum transferred in the collision, since $\vec{k}_f = \vec{k}_i + \vec{q}$. Moreover, since $|\vec{k}_f| = |\vec{k}_i| = k$ are the same, we can write

$$|\vec{q}| = 2k \sin\theta/2$$

where θ is the direction between the incoming beam and the deflected particle. Thus, we can write in the first Born approximation

$$f_B(\vec{k}_f, \vec{k}_i) = -\frac{m}{2\pi\hbar^2} \tilde{V}(\vec{q})$$

where

$$\tilde{V}(\vec{q}) = \int d^3r \, e^{-i\vec{q}\cdot\vec{r}} V(\vec{r})$$

is, up factors of 2π, simply the Fourier transform of the scattering potential. Thus, in the Born approximation the differential scattering cross section

$$\frac{d\sigma(\theta,\phi)}{d\Omega} = |f(\theta,\phi)|^2 = \frac{m^2}{4\pi^2\hbar^4} \left| \tilde{V}(\vec{q}) \right|^2$$

is, up to constant factors, simply the squared modulus of the Fourier transform of the scattering potential evaluated at the wavevector $\vec{q}$ corresponding to the momentum transferred in the scattering event.

As a special case of this formula, we can consider the case where the potential is spherically symmetric, so that $V(\vec{r}) = V(r)$, in which case

$$\tilde{V}(\vec{q}) = V(q) = \int_0^{2\pi} d\phi \int_{-\pi}^{\pi} d\theta \int_0^{\infty} dr \, r^2 \sin\theta \, e^{-iqr\cos\theta} V(r).$$

The angular integrals are readily evaluated to give

$$\int_0^{2\pi} d\phi \int_{-\pi}^{\pi} d\theta \, \sin\theta \, e^{-iqr\cos\theta} = \frac{4\pi}{qr} \sin(qr)$$

so the only remaining integral to perform is the radial one

$$\tilde{V}(q) = \frac{4\pi}{q} \int_0^{\infty} dr \, r \, \sin(qr) \, V(r)$$

which will depend upon the precise form of the scattering potential.

For example, if we take the so-called Yukawa (or screened-Coulomb) potential

$$V(r) = \frac{e^2}{r} e^{-\alpha r}$$

then

$$\tilde{V}(q) = \frac{4\pi e^2}{q}\int_0^\infty dr\ \sin(qr)\ e^{-\alpha r} = \frac{4\pi e^2}{\alpha^2+q^2}$$

Thus, in this case, $f(\theta,\phi) = f(\theta) = f(q)$, where $q = 2k\sin\theta/2$, and

$$f(\theta) = -\frac{2me^2}{\hbar^2}\frac{1}{\alpha^2+q^2} = -\frac{2me^2}{\hbar^2}\frac{1}{\alpha^2+4k^2\sin^2\theta/2}$$

and the cross section becomes

$$\frac{d\sigma}{d\Omega} = \frac{4m^2e^4}{\hbar^4\left(\alpha^2+4k^2\sin^2\theta/2\right)^2}.$$

By taking the limit that $\alpha \to 0$ we obtain the corresponding cross section, in the Born approximation, for the Coulomb potential

$$\frac{d\sigma}{d\Omega} = \frac{m^2e^4}{4\hbar^4k^4\sin^4\theta/2} = \frac{e^4}{16\varepsilon^2\sin^4\theta/2}.$$

As a second example, considering the elastic scattering of electrons by a neutral atom in its ground state with initial electron energies that are too small to excite the atom to any of its excited states. For an atom of atomic number Z, the charge density $\rho(\vec{r})$ can be written

$$\rho(\vec{r}) = e\left[Z\delta(\vec{r}) - n(\vec{r})\right]$$

where $n(\vec{r})$ is the number density of electrons in the atom at $\vec{r}$ and can be written

$$n(\vec{r}) = \langle\psi|\sum_i \delta(\vec{r}-\vec{r}_i)|\psi\rangle \simeq \sum_i \psi^*_{n_i}(\vec{r})\psi_{n_i}(\vec{r})$$

where the second form holds in an independent electron approximation. The electric potential $\varphi(\vec{r})$ at a point $\vec{r}$ due to the charge density of the bound electrons and the nucleus satisfies Poisson's equation

$$\nabla^2\varphi = -4\pi\rho(\vec{r}) = -4\pi e\left[Z\delta(\vec{r}) - n(\vec{r})\right]$$

where charge neutrality implies that $\int d^3r\ n(\vec{r}) = Z$. The corresponding potential energy seen by an incoming electron is given by

$$V(\vec{r}) = -e\varphi(\vec{r})$$

so that

$$\nabla^2 V(\vec{r}) = 4\pi e^2\left[Z - n(\vec{r})\right].$$

We now note that if

$$V(\vec{r}) = \int \frac{d^3q}{(2\pi)^3} e^{i\vec{q}\cdot\vec{r}}\tilde{V}(\vec{q}) \qquad \tilde{V}(\vec{q}) = \int d^3q\ e^{-i\vec{q}\cdot\vec{r}}\tilde{V}(\vec{r})$$

then

$$\nabla^2 V(\vec{r}) = \int \frac{d^3q}{(2\pi)^3} q^2 e^{-i\vec{q}\cdot\vec{r}}\tilde{V}(\vec{q})$$

has as its Fourier transform the function $-q^2\tilde{V}(q)$. We write, therefore, as the Fourier transform of Laplaces equation

$$-q^2\tilde{V}(q) = 4\pi e^2\left[Z - F(q)\right]$$

where the atomic form factor

$$F(\vec{q}) = \int d^3r\ e^{-i\vec{q}\cdot\vec{r}} n(\vec{r})$$

is the Fourier transform of the electronic charge density. Thus, we can solve for $\tilde{V}(\vec{q})$ to obtain

$$\tilde{V}(\vec{q}) = \frac{4\pi e^2\left[F(q) - Z\right]}{q^2},$$

which allows us to evaluate the scattering amplitude in the Born approximation

$$f(q) = -\frac{2e^2 m}{\hbar^2}\frac{\left[F(q) - Z\right]}{q^2}$$

and the corresponding cross section

$$\frac{d\sigma}{d\Omega} = \frac{4e^4m^2}{\hbar^4}\frac{\left|F(q) - Z\right|^2}{q^4}.$$

Thus, measurement of the cross section for all momentum transfer allows information to be inferred about the distribution of charge in the atom [as contained in the form factor $F(q)$]. For a spherically symmetric charge density it is possible, in principle, to invert this relation to determine the charge density $\rho(\vec{r})$ directly.

9.5 Partial Wave Expansions

In the last section we have not really used the fact that $V(r)$ is a spherically symmetric potential. In this section we explore some of the simplifications that occur as a result of this fact. Specifically, if $V = V(r)$, then H commutes with L^2 and L_z and we know that there exists a basis of eigenstates common to $\left\{H, L^2, L_z\right\}$. Let $|\varepsilon, \ell, m\rangle = |k, \ell, m\rangle$ denote such a basis for the positive energy subspace of the system of interest, where, as usual, $k = \sqrt{2m\varepsilon/\hbar^2}$.

We note, in particular, that the potential $V(r) = 0$ is spherically symmetric, so there must exist a basis of this sort for free particles. Let us denote by $|\varepsilon, \ell, m\rangle^{(0)} = |k, \ell, m\rangle^{(0)}$ the corresponding free particle eigenstates common to $\left\{H_0, L^2, L_z\right\}$. Both sets of states satisfy orthonormality relations

$$\langle k, \ell, m|k', \ell', m'\rangle = \delta(k - k')\delta_{\ell,\ell'}\delta_{m,m'} = {}^{(0)}\langle k, \ell, m|k', \ell', m'\rangle^{(0)}$$

and have functions of the following form

$$\psi_{k,\ell,m}(r, \theta, \phi) = F_{k,\ell}(r)Y_\ell^m(\theta, \phi) = \frac{\phi_{k,\ell}(r)}{r}Y_\ell^m(\theta, \phi)$$

$$\psi^{(0)}_{k,\ell,m}(r, \theta, \phi) = F^{(0)}_{k,\ell}(r)Y_\ell^m(\theta, \phi) = \frac{\phi^{(0)}_{k,\ell}(r)}{r}Y_\ell^m(\theta, \phi)$$

where the functions $\phi_{k,\ell}(r) = rF_{k,\ell}(r)$ obey the radial equation

$$\phi''_{k,\ell} - \left(\frac{\ell(\ell+1)}{r^2} + v(r) - k^2\right)\phi_{k,\ell} = 0$$

in which $v(r) = 2mV(r)/\hbar^2$ and $k^2 = 2m\varepsilon/\hbar^2 \geq 0$. Note that when $V = 0$ this reduces to

$$\phi_{k,\ell}^{(0)\prime\prime} - \left(\frac{\ell(\ell+1)}{r^2} - k^2\right)\phi_{k,\ell}^{(0)} = 0.$$

The solutions to this latter equation that are regular at the origin are well-known and related to the spherical Bessel functions $j_\ell(z)$ of order ℓ Specifically, it is found that

$$\phi_{k,\ell}^{(0)}(r) = \sqrt{\frac{2}{\pi}} kr\; j_\ell(kr),$$

so the free particle eigenstates of $\{H_0, L^2, L_z\}$ are

$$\psi_{k,\ell}^{(0)}(\vec{r}) = \sqrt{\frac{2}{\pi}} k\; j_\ell(kr)\; Y_\ell^m(\theta, \phi).$$

On the other hand, provided that $V(r) \to 0$ as $r \to \infty$ faster than $1/r$, then asymptotically both equations ($V \neq 0$ and $V = 0$)obey the equation

$$\phi'' + k^2\phi = 0 \qquad\qquad r \to \infty,$$

which has the general solution $\phi(r) \sim Ae^{ikr} + Be^{-ikr}$, so that the radial dependence of the $F(r) = \phi(r)/r$ has the form

$$F(r) \sim A\frac{e^{ikr}}{r} + B\frac{e^{-ikr}}{r}$$

of a superposition of incoming and outgoing spherical waves. To conserve probability, the flux into the origin has to balance the flux out of the origin, which imposes the requirement that $|A| = |B|$, in which case we can asymptotically write

$$\phi_{k,\ell}(r) \sim a_\ell \sin\left(kr - \varphi_\ell\right).$$

Indeed, it can be shown from the properties of the spherical Bessel functions that the free particle solutions have the asymptotic behavior

$$\phi_{k,\ell}^{(0)}(r) = \sqrt{\frac{2}{\pi}} kr\; j_\ell(kr) \sim a_\ell \sin\left(kr - \ell\pi/2\right)$$

so that

$$\varphi_\ell^{(0)} = \frac{\ell\pi}{2}$$

for a free particle ($V = 0$). When $V \neq 0$ it is convenient to write the phase of interest in the form

$$\varphi_\ell = \varphi_\ell^{(0)} - \delta_\ell = \frac{\ell\pi}{2} - \delta_\ell$$

$$\phi_{k,\ell}(r) = a_\ell \sin kr - \ell\pi/2 + \delta_\ell)$$

where $\delta_\ell is$ the *phase shift* that arises due to the potential ($\delta_\ell \to 0$ as $V \to 0$). and is uniquely determined by it (whereas a_ℓ scales with the normalization of the state).

Our goal is to obtain an expansion for the stationary scattering state $|\phi_\varepsilon\rangle$ in the complete set of states $|k, \ell, m\rangle$ and use it to obtain an expression for the scattering amplitude $f(\theta, \phi)$ expanded in spherical harmonics. In other words, we seek an expansion of the form

$$f(\theta, \phi) = \sum_{\ell,m} f_{\ell,m} Y_\ell^m(\theta, \phi).$$

As a preliminary simplification, we note that, because of the spherical symmetry of the potenital, there is azimuthal symmetry along the z-axis associated with the incident beam, thus, only $m = 0$ components exist in the expansion:

$$f(\theta, \phi) = f(\theta) = \sum_\ell f_\ell Y_\ell^0(\theta) \tag{9.1}$$

To proceed we express the stationary scattering states of interest as an expansion

$$\phi_\varepsilon(\vec{r}) \sim e^{ikz} + f(\theta)\frac{e^{ikr}}{r} = \sum_\ell A_\ell \; \psi_{k,\ell,0}(\vec{r})$$

in states of well-defined angular momentum. The ℓth term in this expansion is referred to as the ℓth partial wave. In terms of the spherical harmonics, this expansion takes the form

$$e^{ikz} + f(\theta)\frac{e^{ikr}}{r} = \sum_\ell A_\ell \frac{\phi_{k,\ell}}{r} Y_\ell^0(\theta).$$

To make this useful, we now use the known expansion of the function e^{ikz} in *free particle* spherical waves:

$$e^{ikz} = \sum_\ell c_\ell \; \psi^{(0)}_{k,\ell,0}(\vec{r}) = \sum_\ell B_\ell \; j_\ell(kr) \; Y_\ell^0(\theta).$$

The B_ℓ can be calculated exactly. The result is $B_\ell = i^\ell \sqrt{4\pi(2\ell+1)}$ so that

$$e^{ikz} = \sum_\ell i^\ell \sqrt{4\pi(2\ell+1)} \; j_\ell(kr) \; Y_\ell^0(\theta).$$

Thus we can write

$$\sum_\ell \left[B_\ell j_l(kr) + \frac{f_\ell e^{ikr}}{r} \right] Y_\ell^0(\theta) = \sum A_\ell \frac{\phi_{k,\ell}(r)}{r} Y_\ell^0(\theta).$$

Linear independence of the Y_ℓ^m's implies that

$$B_\ell r \; j_\ell(kr) + f_\ell e^{ikr} = A_\ell \phi_{k,\ell}(r).$$

Now asymptotically,

$$B_\ell r \; j_\ell(kr) \sim \frac{B_\ell}{k} \sin(kr - \ell\pi/2) = \frac{B_\ell}{2ik} \left[e^{ikr} e^{-i\ell\pi/2} - e^{-ikr} e^{i\ell\pi/2} \right]$$

and

$$\begin{aligned} A_\ell \phi_{k,\ell}(r) &\sim a_\ell \sin(kr - \ell\pi/2 + \delta_\ell) \\ &= \frac{a_\ell}{2i} \left[e^{ikr} e^{-i\ell\pi/2} e^{i\delta_\ell} - e^{-ikr} e^{i\ell\pi/2} e^{-i\delta_\ell} \right]. \end{aligned}$$

Substituting these last two equations into our previous expansion and equating coefficients of e^{ikr} and e^{-ikr} we find that

$$\frac{a_\ell}{2i} e^{-i\ell\pi/2} e^{i\delta_\ell} = \frac{B_\ell}{2ik} e^{-i\ell\pi/2} + f_\ell$$

and

$$\frac{a_\ell}{2i} e^{i\ell\pi/2} e^{-i\delta_\ell} = \frac{B_\ell}{2ik} e^{i\ell\pi/2}$$

which gives two equations in the two unknown quantities a_ℓ and f_ℓ. Solving for f_ℓ we find that

$$f_\ell = \frac{1}{k}\sqrt{4\pi(2\ell+1)}e^{i\delta_\ell}\sin\delta_\ell$$

so that

$$f(\theta) = \sum_\ell f_\ell Y_\ell^0(\theta) = \frac{1}{k}\sum_\ell \sqrt{4\pi(2\ell+1)}e^{i\delta_\ell}\sin\delta_\ell Y_\ell^0(\theta)$$

from which follows the expansion for the differential scattering cross section

$$\frac{d\sigma}{d\Omega}(\theta) = \frac{1}{k^2}\left|\sum_{\ell=0}^{\infty}\sqrt{4\pi(2\ell+1)}e^{i\delta_\ell}\sin\delta_\ell Y_\ell^0(\theta)\right|^2$$

The total cross section can then be written

$$\begin{aligned}\sigma_{\rm tot} &= \frac{1}{k^2}\int d\Omega\left|\sum_{\ell=0}^{\infty}\sqrt{4\pi(2\ell+1)}e^{i\delta_\ell}\sin\delta_\ell Y_\ell^0(\theta)\right|^2 \\ &= \frac{1}{k^2}\sum_{\ell=0}^{\infty}\sum_{\ell'=0}^{\infty}\sqrt{4\pi(2\ell+1)}\sqrt{4\pi(2\ell'+1)}e^{i(\delta_\ell-\delta_{\ell'})}\sin\delta_\ell\sin\delta_{\ell'}\int d\Omega Y_\ell^0(\theta)Y_{\ell'}^0(\theta)\end{aligned}$$

which reduces to

$$\begin{aligned}\sigma_{\rm tot} &= \frac{4\pi}{k^2}\sum_{\ell=0}^{\infty}(2\ell+1)\sin^2\delta_\ell \\ &= \sum_{\ell=0}^{\infty}\sigma_\ell\end{aligned}$$

where

$$\sigma_\ell = \frac{4\pi}{k^2}(2\ell+1)\sin^2\delta_\ell \le \frac{4\pi}{k^2}(2\ell+1)$$

is the scattering cross section to states with angular momentum ℓ. Note that for free particles $\delta_\ell \to 0$ and $\sigma_{\rm tot} \to 0$, as we would expect.