

Scattering Theory

This last chapter of the book is devoted to the theory of scattering and, more generally, collision processes. It is impossible to overemphasize the importance of this subject.

7.1. THE LIPPMANN-SCHWINGER EQUATION

We begin with a time-independent formulation of scattering processes. We assume that the Hamiltonian can be written as

$$H = H_0 + V \quad (7.1.1)$$

where H_0 stands for the kinetic-energy operator

$$H_0 = \frac{\mathbf{p}^2}{2m}. \quad (7.1.2)$$

In the absence of a scatterer, V would be zero, and an energy eigenstate would be just a free particle state $|\mathbf{p}\rangle$. The presence of V causes the energy eigenstate to be different from a free-particle state. However, if the scattering process is to be elastic—that is, no change in energy—we are interested in obtaining a solution to the full-Hamiltonian Schrödinger equation with the same energy eigenvalue. More specifically, let $|\phi\rangle$ be the energy eigenket

of H_0 :

$$H_0|\phi\rangle = E|\phi\rangle. \quad (7.1.3)$$

(We use $|\phi\rangle$ here rather than $|\mathbf{p}\rangle$ because we may later be interested in free-spherical wave rather than plane-wave states; $|\phi\rangle$ may stand for either.) The basic Schrödinger equation we wish to solve is

$$(H_0 + V)|\psi\rangle = E|\psi\rangle. \quad (7.1.4)$$

Both H_0 and $H_0 + V$ exhibit *continuous* energy spectra. We look for a solution to (7.1.4) such that, as $V \rightarrow 0$, we have $|\psi\rangle \rightarrow |\phi\rangle$, where $|\phi\rangle$ is the solution to the free-particle Schrödinger equation [(7.1.3)] with the *same* energy eigenvalue.

It may be argued that the desired solution is

$$|\psi\rangle = \frac{1}{E - H_0} V|\psi\rangle + |\phi\rangle, \quad (7.1.5)$$

apart from complications arising from the singular nature of the operator $1/(E - H_0)$. We can see this by noting that $E - H_0$ applied to (7.1.5) immediately gives the correct equation, (7.1.4). The presence of $|\phi\rangle$ is reasonable because $|\psi\rangle$ must reduce to $|\phi\rangle$ as V vanishes. However, without prescriptions for dealing with a singular operator, an equation of type (7.1.5) has no meaning. The trick we used in time-independent perturbation theory—inserting the complimentary projection operator, and so on (see Section 5.1)—does not work well here because both $|\phi\rangle$ and $|\psi\rangle$ exhibit continuous eigenvalues. Instead, this time the solution is specified by making E slightly complex:

$$|\psi^{(\pm)}\rangle = |\phi\rangle + \frac{1}{E - H_0 \pm i\epsilon} V|\psi^{(\pm)}\rangle. \quad (7.1.6)$$

This is known as the **Lippmann-Schwinger equation**. The physical meaning of \pm is to be discussed in a moment by looking at $\langle \mathbf{x} | \psi^{(\pm)} \rangle$ at large distances.

The Lippmann-Schwinger equation is a *ket equation* independent of particular representations. We now confine ourselves to the position basis by multiplying $\langle \mathbf{x} |$ from the left. Thus

$$\langle \mathbf{x} | \psi^{(\pm)} \rangle = \langle \mathbf{x} | \phi \rangle + \int d^3x' \left\langle \mathbf{x} \left| \frac{1}{E - H_0 \pm i\epsilon} \right| \mathbf{x}' \right\rangle \langle \mathbf{x}' | V | \psi^{(\pm)} \rangle. \quad (7.1.7)$$

This is an **integral equation** for scattering because the unknown ket $|\psi^{(\pm)}\rangle$ appears under an integral sign. If $|\phi\rangle$ stands for a plane-wave state with momentum \mathbf{p} , we can write

$$\langle \mathbf{x} | \phi \rangle = \frac{e^{i\mathbf{p} \cdot \mathbf{x}/\hbar}}{(2\pi\hbar)^{3/2}} \quad (7.1.8)$$

[Editor's Note: In contrast to bound states, the plane-wave state (7.1.8) is, of course, not normalizable and not really a vector in Hilbert space. Dealing with such states is one of the inconveniences of time-independent scattering theory. The "normalization" in (7.1.8) is such that

$$\int d^3x \langle \mathbf{p}' | \mathbf{x} \rangle \langle \mathbf{x} | \mathbf{p} \rangle = \delta^{(3)}(\mathbf{p} - \mathbf{p}'). \quad (7.1.9)]$$

If, on the other hand, the Lippman-Schwinger equation is written using the momentum basis, we obtain

$$\langle \mathbf{p} | \psi^{(\pm)} \rangle = \langle \mathbf{p} | \phi \rangle + \frac{1}{E - (p'^2/2m) \pm i\epsilon} \langle \mathbf{p} | V | \psi^{(\pm)} \rangle. \quad (7.1.10)$$

We shall come back to this equation in Section 7.2.

Let us consider specifically the position basis and work with (7.1.7). To make any progress we must first evaluate the kernel of the integral equation defined by

$$G_{\pm}(\mathbf{x}, \mathbf{x}') \equiv \frac{\hbar^2}{2m} \left\langle \mathbf{x} \left| \frac{1}{E - H_0 \pm i\epsilon} \right| \mathbf{x}' \right\rangle. \quad (7.1.11)$$

We claim that $G_{\pm}(\mathbf{x}, \mathbf{x}')$ is given by

$$G_{\pm}(\mathbf{x}, \mathbf{x}') = -\frac{1}{4\pi} \frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x} - \mathbf{x}'|} \quad (7.1.12)$$

where $E \equiv \hbar^2 k^2 / 2m$. To show this, we evaluate (7.1.11) as follows:

$$\begin{aligned} \frac{\hbar^2}{2m} \left\langle \mathbf{x} \left| \frac{1}{E - H_0 \pm i\epsilon} \right| \mathbf{x}' \right\rangle &= \frac{\hbar^2}{2m} \int d^3p' \int d^3p'' \langle \mathbf{x} | \mathbf{p}' \rangle \\ &\times \left\langle \mathbf{p}' \left| \frac{1}{E - (\mathbf{p}'^2/2m) \pm i\epsilon} \right| \mathbf{p}'' \right\rangle \langle \mathbf{p}'' | \mathbf{x}' \rangle, \end{aligned} \quad (7.1.13)$$

where H_0 acts on $\langle \mathbf{p}' |$. Now use

$$\begin{aligned} \left\langle \mathbf{p}' \left| \frac{1}{E - (\mathbf{p}'^2/2m) \pm i\epsilon} \right| \mathbf{p}'' \right\rangle &= \frac{\delta^{(3)}(\mathbf{p}' - \mathbf{p}'')}{E - (\mathbf{p}'^2/2m) \pm i\epsilon} \\ \langle \mathbf{x} | \mathbf{p}' \rangle &= \frac{e^{i\mathbf{p}' \cdot \mathbf{x}/\hbar}}{(2\pi\hbar)^{3/2}}, \quad \langle \mathbf{p}'' | \mathbf{x}' \rangle = \frac{e^{-i\mathbf{p}'' \cdot \mathbf{x}'/\hbar}}{(2\pi\hbar)^{3/2}}. \end{aligned} \quad (7.1.14)$$

The right-hand side of (7.1.13) becomes

$$\frac{\hbar^2}{2m} \int \frac{d^3p'}{(2\pi\hbar)^3} \frac{e^{i\mathbf{p}' \cdot (\mathbf{x} - \mathbf{x}')/\hbar}}{[E - (\mathbf{p}'^2/2m) \pm i\epsilon]}. \quad (7.1.15)$$

Now write $E = \hbar^2 k^2 / 2m$ and set $\mathbf{p}' \equiv \hbar \mathbf{q}$. Equation (7.1.15) becomes

$$\begin{aligned} & \frac{1}{(2\pi)^3} \int_0^\infty q^2 dq \int_0^{2\pi} d\phi \int_{-1}^{+1} \frac{d(\cos\theta) e^{\imath|\mathbf{q}||\mathbf{x}-\mathbf{x}'|\cos\theta}}{k^2 - q^2 \pm i\epsilon} \\ &= \frac{-1}{8\pi^2} \frac{1}{i|\mathbf{x}-\mathbf{x}'|} \int_{-\infty}^{+\infty} \frac{dq q (e^{\imath q|\mathbf{x}-\mathbf{x}'|} - e^{-\imath q|\mathbf{x}-\mathbf{x}'|})}{q^2 - k^2 \mp i\epsilon} \\ &= -\frac{1}{4\pi} \frac{e^{\pm \imath k|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}. \end{aligned} \quad (7.1.16)$$

In the last step we used the method of residues, noting that the integrand has poles in the complex q -plane at

$$q = \pm k \sqrt{1 \pm \left(\frac{i\epsilon}{k^2} \right)} \simeq \pm k \pm i\epsilon'. \quad (7.1.17)$$

The reader may recognize that G_\pm is nothing more than Green's function for the Helmholtz equation,

$$(\nabla^2 + k^2)G_\pm(\mathbf{x}, \mathbf{x}') = \delta^{(3)}(\mathbf{x} - \mathbf{x}'). \quad (7.1.18)$$

Armed with the explicit form of G_\pm as in Equation (7.1.12), we can use (7.1.11) to write Equation (7.1.7) as

$$\langle \mathbf{x} | \psi^{(\pm)} \rangle = \langle \mathbf{x} | \phi \rangle - \frac{2m}{\hbar^2} \int d^3x' \frac{e^{\pm \imath k|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} \langle \mathbf{x}' | V | \psi^{(\pm)} \rangle. \quad (7.1.19)$$

Notice that the wave function $\langle \mathbf{x} | \psi^{(\pm)} \rangle$ in the presence of the scatterer is written as the sum of the wave function for the incident wave $\langle \mathbf{x} | \phi \rangle$ and a term that represents the effect of scattering. As we will see explicitly later, at sufficiently large distances the spatial dependence of the second term is $e^{\pm \imath kr}/r$ provided that the potential is of finite range. This means that the positive solution (negative solution) corresponds to the plane wave plus an outgoing (incoming) spherical wave. In most physical problems we are interested in the positive solution because it is difficult to prepare a system satisfying the boundary condition appropriate for the negative solution.

To see the behavior of $\langle \mathbf{x} | \psi^{(\pm)} \rangle$ more explicitly, let us consider the specific case where V is a local potential—that is, a potential diagonal in the \mathbf{x} -representation. Potentials that are functions only of the position operator \mathbf{x} belong to this category. In precise terms V is said to be **local** if it can be written as

$$\langle \mathbf{x}' | V | \mathbf{x}'' \rangle = V(\mathbf{x}') \delta^{(3)}(\mathbf{x}' - \mathbf{x}''). \quad (7.1.20)$$

As a result, we obtain

$$\begin{aligned}\langle \mathbf{x}' | V | \psi^{(\pm)} \rangle &= \int d^3x'' \langle \mathbf{x}' | V | \mathbf{x}'' \rangle \langle \mathbf{x}'' | \psi^{(\pm)} \rangle \\ &= V(\mathbf{x}') \langle \mathbf{x}' | \psi^{(\pm)} \rangle.\end{aligned}\quad (7.1.21)$$

The integral equation (7.1.19) now simplifies as

$$\langle \mathbf{x} | \psi^{(\pm)} \rangle = \langle \mathbf{x} | \phi \rangle - \frac{2m}{\hbar^2} \int d^3x' \frac{e^{\pm ik|\mathbf{x}-\mathbf{x}'|}}{4\pi|\mathbf{x}-\mathbf{x}'|} V(\vec{\mathbf{x}}') \langle \mathbf{x}' | \psi^{(\pm)} \rangle. \quad (7.1.22)$$

Let us attempt to understand the physics contained in this equation. The vector \mathbf{x} is understood to be directed towards the observation point at which the wave function is evaluated. For a finite range potential, the region that gives rise to a nonvanishing contribution is limited in space. In scattering processes we are interested in studying the effect of the scatterer (that is, the finite range potential) at a point far outside the range of the potential. This is quite relevant from a practical point of view because we cannot put a detector at short distance near the scattering center. Observation is always made by a detector placed very far away from the scatterer at r greatly larger than the range of the potential. In other words, we can safely set

$$|\mathbf{x}| \gg |\mathbf{x}'|, \quad (7.1.23)$$

as depicted in Figure 7.1.

Introducing

$$\begin{aligned}r &= |\mathbf{x}| \\ r' &= |\mathbf{x}'|\end{aligned}\quad (7.1.24)$$

and

$$\alpha = \angle(\mathbf{x}, \mathbf{x}'), \quad (7.1.25)$$

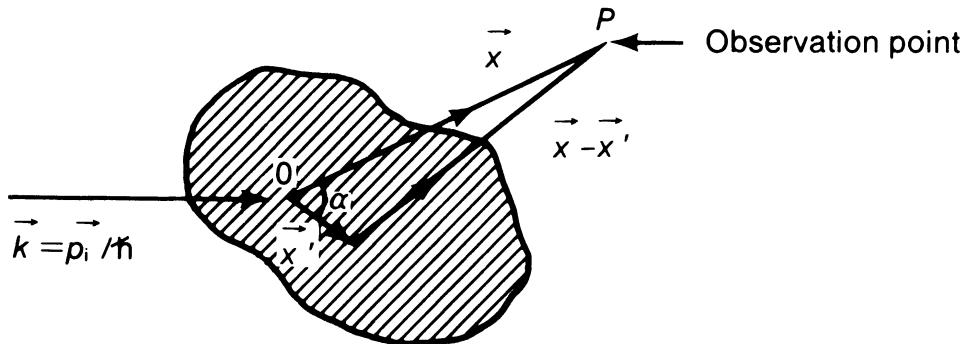


FIGURE 7.1. Finite-range scattering potential. The *observation point* P is where the wave function $\langle \mathbf{x} | \psi^{(\pm)} \rangle$ is to be evaluated, while the contribution to the integral in Equation (7.1.22) is for $|\mathbf{x}'|$ less than the range of the potential, as depicted by the shaded region of the figure.

we have for $r \gg r'$,

$$\begin{aligned} |\mathbf{x} - \mathbf{x}'| &= \sqrt{r^2 - 2rr' \cos \alpha + r'^2} \\ &= r \left(1 - \frac{2r'}{r} \cos \alpha + \frac{r'^2}{r^2} \right)^{1/2} \\ &\approx r - \hat{\mathbf{r}} \cdot \mathbf{x}' \end{aligned} \quad (7.1.26)$$

where

$$\hat{\mathbf{r}} \equiv \frac{\mathbf{x}}{|\mathbf{x}|}. \quad (7.1.27)$$

Also define

$$\mathbf{k}' \equiv k \hat{\mathbf{r}}. \quad (7.1.28)$$

The motivation for this definition is that \mathbf{k}' represents the propagation vector for waves reaching observation point \mathbf{x} . We then obtain

$$e^{\pm i\mathbf{k}|\mathbf{x}-\mathbf{x}'|} \approx e^{\pm ikr} e^{\mp i\mathbf{k}' \cdot \mathbf{x}'} \quad (7.1.29)$$

for large r . It is legitimate to replace $1/|\mathbf{x} - \mathbf{x}'|$ by just $1/r$. Furthermore, to get rid of the \hbar 's in expressions such as $1/(2\pi\hbar)^{3/2}$, it is convenient to use $|\mathbf{k}\rangle$ rather than $|\mathbf{p}_t\rangle$, where

$$\mathbf{k} \equiv \frac{\mathbf{p}_t}{\hbar}. \quad (7.1.30)$$

Because $|\mathbf{k}\rangle$ is normalized as

$$\langle \mathbf{k} | \mathbf{k}' \rangle = \delta^{(3)}(\mathbf{k} - \mathbf{k}') \quad (7.1.31)$$

we have

$$\langle \mathbf{x} | \mathbf{k} \rangle = \frac{e^{i\mathbf{k} \cdot \mathbf{x}}}{(2\pi)^{3/2}}. \quad (7.1.32)$$

So, finally,

$$\begin{aligned} \langle \mathbf{x} | \psi^{(+)} \rangle &\xrightarrow{r \text{ large}} \langle \mathbf{x} | \mathbf{k} \rangle - \frac{1}{4\pi} \frac{2m}{\hbar^2} \frac{e^{ikr}}{r} \int d^3x' e^{-i\mathbf{k}' \cdot \mathbf{x}'} V(\mathbf{x}') \langle \mathbf{x}' | \psi^{(+)} \rangle \\ &= \frac{1}{(2\pi)^{3/2}} \left[e^{i\mathbf{k} \cdot \mathbf{x}} + \frac{e^{ikr}}{r} f(\mathbf{k}', \mathbf{k}) \right]. \end{aligned} \quad (7.1.33)$$

This form makes it very clear that we have the original plane wave in propagation direction \mathbf{k} plus an outgoing spherical wave with amplitude $f(\mathbf{k}', \mathbf{k})$ given by

$$\begin{aligned} f(\mathbf{k}', \mathbf{k}) &\equiv - \frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \int d^3x' \frac{e^{-i\mathbf{k}' \cdot \mathbf{x}'}}{(2\pi)^{3/2}} V(\mathbf{x}') \langle \mathbf{x}' | \psi^{(+)} \rangle \\ &= - \frac{1}{4\pi} (2\pi)^3 \frac{2m}{\hbar^2} \langle \mathbf{k}' | V | \psi^{(+)} \rangle. \end{aligned} \quad (7.1.34)$$

Similarly, we can readily show from (7.1.22) and (7.1.29) that $\langle \mathbf{x} | \psi^{(-)} \rangle$ corresponds to the original plane wave in propagation direction \mathbf{k} plus an incoming spherical wave with spatial dependence e^{-ikr}/r and amplitude $-(1/4\pi)(2\pi)^3(2m/\hbar^2)\langle -\mathbf{k}' | V | \psi^{(-)} \rangle$.

To obtain the **differential cross section** $d\sigma/d\Omega$, we may consider a large number of identically prepared particles all characterized by the wave function (7.1.32). We can then ask, what is the number of incident particles crossing a plane perpendicular to the incident direction per unit area per unit time? This is just proportional to the probability flux due to the first term on the right-hand side in (7.1.33). Likewise we may ask, what is the number of scattered particles going into a small area $d\sigma$ subtending a differential solid-angle element $d\Omega$? Clearly,

$$\begin{aligned} \frac{d\sigma}{d\Omega} d\Omega &= \frac{\text{number of particles scattered into } d\Omega \text{ per unit time}}{\text{number of incident particles crossing unit area per unit time}} \\ &= \frac{r^2 |\mathbf{j}_{\text{scatt}}| d\Omega}{|\mathbf{j}_{\text{incid}}|} = |f(\mathbf{k}', \mathbf{k})|^2 d\Omega. \end{aligned} \quad (7.1.35)$$

Hence the differential cross section is

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{k}', \mathbf{k})|^2. \quad (7.1.36)$$

Wave-Packet Description

The reader may wonder here whether our time-independent formulation of scattering has anything to do with the motion of a particle being

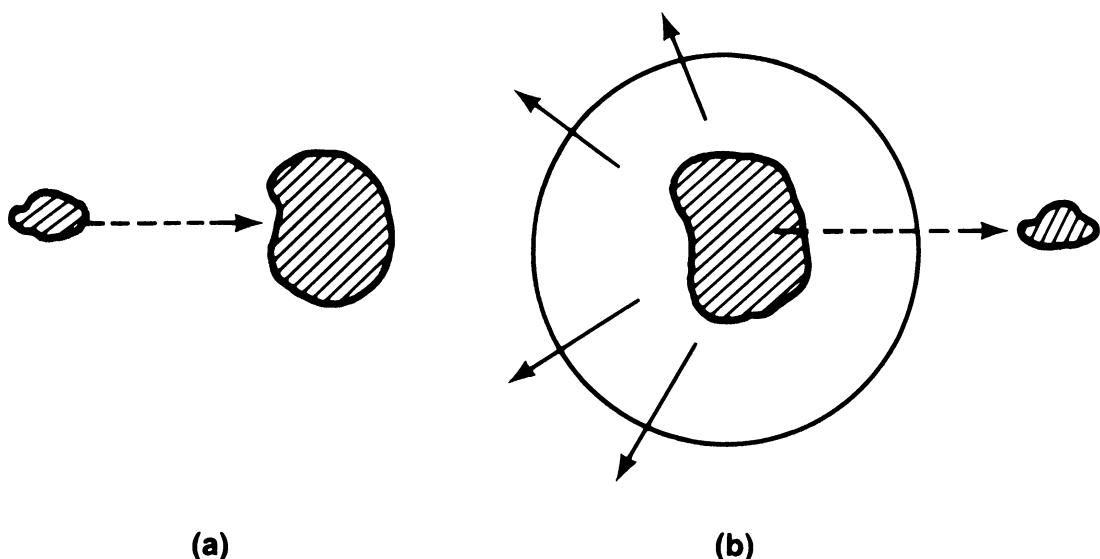


FIGURE 7.2. (a) Incident wave packet approaching scattering center initially. (b) Incident wave packet continuing to move in the original direction plus spherical outgoing wave front (after a long time duration).

bounced by a scattering center. The incident plane wave we have used is infinite in extent in both space and time. In a more realistic situation, we consider a wave packet (a difficult subject!) that approaches the scattering center.* After a long time we have both the original wave packet moving in the original direction plus a spherical wave front that moves outward, as in Figure 7.2. Actually the use of a plane wave is satisfactory as long as the dimension of the wave packet is much larger than the size of the scatterer (or range of V).

7.2. THE BORN APPROXIMATION

Equation (7.1.34) is still not directly useful in computing the differential cross section because in the expression for $f(\mathbf{k}', \mathbf{k})$ the unknown ket $|\psi^{(+)}\rangle$ appears. If the effect of the scatterer is not very strong, we may infer that it is not such a bad approximation to replace $\langle \mathbf{x}' | \psi^{(+)} \rangle$ (which appears under the integral sign) by $\langle \mathbf{x}' | \phi \rangle$ —that is,

$$\langle \mathbf{x}' | \psi^{(+)} \rangle \rightarrow \langle \mathbf{x}' | \phi \rangle = \frac{e^{i\mathbf{k} \cdot \mathbf{x}'}}{(2\pi)^{3/2}}. \quad (7.2.1)$$

We then obtain an approximate expression for $f(\mathbf{k}', \mathbf{k})$. Because we treat the potential V to first order, the approximate amplitude so obtained is known as the **first-order Born amplitude** and is denoted by $f^{(1)}$:

$$f^{(1)}(\mathbf{k}', \mathbf{k}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3x' e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{x}'} V(\mathbf{x}'). \quad (7.2.2)$$

In other words, apart from $-(2m/4\pi\hbar^2)$, the first-order amplitude is just the three-dimensional Fourier transform of the potential V with respect to $\mathbf{q} \equiv \mathbf{k} - \mathbf{k}'$.

For a spherically symmetric potential, $f^{(1)}(\mathbf{k}', \mathbf{k})$ is a function of $|\mathbf{k} - \mathbf{k}'|$, given by (remember $|\mathbf{k}'| = k$ by energy conservation)

$$|\mathbf{k} - \mathbf{k}'| \equiv q = 2k \sin \frac{\theta}{2}; \quad (7.2.3)$$

see Figure 7.3. We can perform the angular integration explicitly to obtain

$$\begin{aligned} f^{(1)}(\theta) &= -\frac{1}{2} \frac{2m}{\hbar^2} \frac{1}{iq} \int_0^\infty \frac{r^2}{r} V(r) (e^{iqr} - e^{-iqr}) dr \\ &= -\frac{2m}{\hbar^2} \frac{1}{q} \int_0^\infty r V(r) \sin qr dr. \end{aligned} \quad (7.2.4)$$

*For a fuller account of the wave-packet approach, see M. L. Goldberger and K. M. Watson, *Collision Theory*, Chapter 3 (New York: John Wiley, 1964); R. G. Newton, *Scattering Theory of Waves and Particles*, Chapter 6 (New York: McGraw-Hill, 1966).

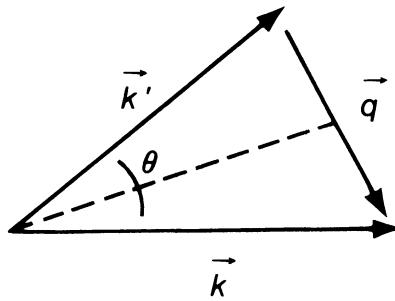


FIGURE 7.3. Scattering through angle θ , where $\mathbf{q} = \mathbf{k} - \mathbf{k}'$.

An example is now in order. Consider scattering by a Yukawa potential

$$V(r) = \frac{V_0 e^{-\mu r}}{\mu r}, \quad (7.2.5)$$

where V_0 is independent of r and $1/\mu$ corresponds, in a certain sense, to the range of the potential. Notice that V goes to zero very rapidly for $r \gg 1/\mu$. For this potential we obtain [from (7.2.4)]

$$f^{(1)}(\theta) = - \left(\frac{2mV_0}{\mu \hbar^2} \right) \frac{1}{q^2 + \mu^2}, \quad (7.2.6)$$

where we have used

$$\begin{aligned} \text{Im} \left[\int_0^\infty e^{-\mu r} e^{iqr} dr \right] &= - \text{Im} \left(\frac{1}{-\mu + iq} \right) \\ &= \frac{q}{\mu^2 + q^2}. \end{aligned} \quad (7.2.7)$$

Notice also that

$$q^2 = 4k^2 \sin^2 \frac{\theta}{2} = 2k^2(1 - \cos \theta). \quad (7.2.8)$$

So, in the first Born approximation, the differential cross section for scattering by a Yukawa potential is given by

$$\left(\frac{d\sigma}{d\Omega} \right) \simeq \left(\frac{2mV_0}{\mu \hbar^2} \right)^2 \frac{1}{[2k^2(1 - \cos \theta) + \mu^2]^2}. \quad (7.2.9)$$

It is amusing to observe here that as $\mu \rightarrow 0$, the Yukawa potential is reduced to the Coulomb potential, provided the ratio V_0/μ is fixed—for example, to be $ZZ'e^2$ —in the limiting process. We see that the first Born differential cross section obtained in this manner becomes

$$\left(\frac{d\sigma}{d\Omega} \right) \simeq \frac{(2m)^2 (ZZ'e^2)^2}{\hbar^4} \frac{1}{16k^4 \sin^4(\theta/2)}. \quad (7.2.10)$$

Even the \hbar disappears if $\hbar k$ is identified as $|\mathbf{p}|$, so

$$\left(\frac{d\sigma}{d\Omega} \right) = \frac{1}{16} \left(\frac{ZZ'e^2}{E_{KE}} \right)^2 \frac{1}{\sin^4(\theta/2)}, \quad (7.2.11)$$

where $E_{KE} = |\mathbf{p}|^2/2m$; this is precisely the Rutherford scattering cross section that can be obtained *classically*.

Coming back to (7.2.4), the Born amplitude with a spherically symmetric potential, there are several general remarks we can make if $f(\mathbf{k}', \mathbf{k})$ can be approximated by the corresponding first Born amplitude, $f^{(1)}$.

1. $d\sigma/d\Omega$, or $f(\theta)$, is a function of q only; that is, $f(\theta)$ depends on the energy ($\hbar^2 k^2/2m$) and θ only through the combination $2k^2(1 - \cos \theta)$.
2. $f(\theta)$ is always real.
3. $d\sigma/d\Omega$ is independent of the sign of V .
4. For small k (q necessarily small),

$$f^{(1)}(\theta) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int V(r) d^3x$$

involving a volume integral independent of θ .

5. $f(\theta)$ is small for large q due to rapid oscillation of the integrand.

Let us now discuss the validity of the first-order Born approximation. It is clear from the derivation that if the Born approximation is to be applicable, $\langle \mathbf{x} | \psi^{(+)} \rangle$ should not be too different from $\langle \mathbf{x} | \phi \rangle$ inside the range of potential—that is, in the region where $V(\mathbf{x})$ is appreciable. Otherwise, it is not legitimate to replace $|\psi^{(+)}\rangle$ by $|\phi\rangle$. In other words, the distortion of the incident wave must be small. Going back to the exact expression (7.1.22), we note that the condition that $\langle \mathbf{x} | \psi^{(+)} \rangle$ be not too different from $\langle \mathbf{x} | \phi \rangle$ at the center of the scattering potential $\mathbf{x} \approx 0$ is seen to be

$$\left| \frac{2m}{\hbar^2} \frac{1}{4\pi} \int d^3x' \frac{e^{ikr'}}{r'} V(\mathbf{x}') e^{i\mathbf{k} \cdot \mathbf{x}'} \right| \ll 1. \quad (7.2.12)$$

We now consider what the special case of the Yukawa potential in (7.2.5) may imply. At low energies—that is, for small k ($k \ll \mu$)—it is legitimate to replace $e^{ikr'}$ by 1. So we must have

$$\frac{2m}{\hbar^2} \frac{|V_0|}{\mu^2} \ll 1. \quad (7.2.13)$$

This requirement may be compared with the condition for the Yukawa potential to develop a bound state, which we can show to be

$$\frac{2m}{\hbar^2 \mu^2} |V_0| \geq 2.7 \quad (7.2.14)$$

with V_0 negative. In other words, if the potential is strong enough to develop a bound state, the Born approximation will probably give a misleading result. In the opposite high k -limit, the condition that the second term in (7.1.22) is small can be shown to imply

$$\frac{2m}{\hbar^2} \frac{|V_0|}{\mu k} \ln\left(\frac{k}{\mu}\right) \ll 1. \quad (7.2.15)$$

As k becomes larger, this inequality is more easily satisfied. Quite generally, the Born approximation tends to get better at higher energies.

The Higher-Order Born Approximation

Let us now consider the higher-order Born approximation. Here, it is more compact to use the symbolic approach. For the transition operator T , we define T such that

$$V|\psi^{(+)}\rangle = T|\phi\rangle. \quad (7.2.16)$$

Multiplying the Lippmann-Schwinger equation (7.1.6) by V , we obtain

$$T|\phi\rangle = V|\phi\rangle + V \frac{1}{E - H_0 + i\epsilon} T|\phi\rangle. \quad (7.2.17)$$

This is supposed to hold for $|\phi\rangle$ taken to be any plane-wave state; furthermore, we know that these momentum eigenkets are complete. Therefore, we must have the following operator equation satisfied:

$$T = V + V \frac{1}{E - H_0 + i\epsilon} T. \quad (7.2.18)$$

The scattering amplitude of (7.1.34) can now be written as [using (7.2.16) with the $|\phi\rangle$ as momentum eigenkets]

$$f(\mathbf{k}', \mathbf{k}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \mathbf{k}' | T | \mathbf{k} \rangle. \quad (7.2.19)$$

Thus to determine $f(\mathbf{k}', \mathbf{k})$, it is sufficient to know the transition operator T .

We can obtain an iterative solution for T as follows:

$$T = V + V \frac{1}{E - H_0 + i\epsilon} V + V \frac{1}{E - H_0 + i\epsilon} V \frac{1}{E - H_0 + i\epsilon} V + \dots \quad (7.2.20)$$

Correspondingly, we can expand f as follows:

$$f(\mathbf{k}', \mathbf{k}) = \sum_{n=1}^{\infty} f^{(n)}(\mathbf{k}', \mathbf{k}), \quad (7.2.21)$$

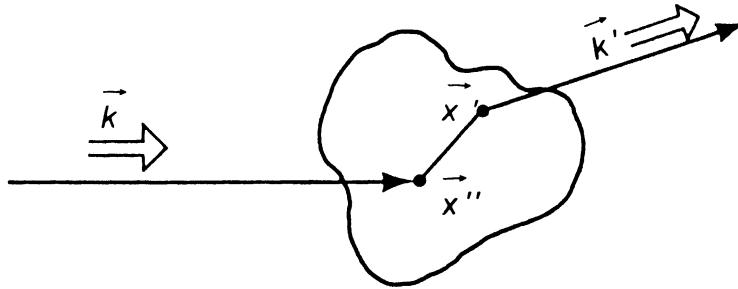


FIGURE 7.4. Physical interpretation of the higher-order Born term $f^{(2)}(\mathbf{k}', \mathbf{k})$.

where n is the number of times the V operator enters. We have

$$\begin{aligned} f^{(1)}(\mathbf{k}', \mathbf{k}) &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \mathbf{k}' | V | \mathbf{k} \rangle \\ f^{(2)}(\mathbf{k}', \mathbf{k}) &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \mathbf{k}' | V \frac{1}{E - H_0 + i\epsilon} V | \mathbf{k} \rangle \\ &\vdots \end{aligned} \quad (7.2.22)$$

If an explicit form is required for $f^{(2)}$, we can write it as

$$\begin{aligned} f^{(2)} &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \int d^3x' \int d^3x'' \langle \mathbf{k}' | \mathbf{x}' \rangle V(\mathbf{x}') \\ &\quad \times \left\langle \mathbf{x}' \left| \frac{1}{E - H_0 + i\epsilon} \right| \mathbf{x}'' \right\rangle V(\mathbf{x}'') \langle \mathbf{x}'' | \mathbf{k} \rangle \\ &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3x' \int d^3x'' e^{-i\mathbf{k}' \cdot \mathbf{x}'} V(\mathbf{x}') \\ &\quad \times \left[\frac{2m}{\hbar^2} G_+(\mathbf{x}', \mathbf{x}'') \right] V(\mathbf{x}'') e^{i\mathbf{k}' \cdot \mathbf{x}''}. \end{aligned} \quad (7.2.23)$$

A physical interpretation of (7.2.23) is given in Figure 7.4, where the incident wave interacts at \mathbf{x}'' —which explains the appearance of $V(\mathbf{x}'')$ —and then propagates from \mathbf{x}'' to \mathbf{x}' via Green's function for the Helmholtz equation (7.1.18); subsequently, a second interaction occurs at \mathbf{x}' —thus the appearance of $V(\mathbf{x}')$ —and, finally, the wave is scattered into the direction \mathbf{k}' . In other words, $f^{(2)}$ corresponds to scattering viewed as a two-step process; likewise, $f^{(3)}$ is viewed as a three-step process, and so on.

7.3 OPTICAL THEOREM

There is a very famous relationship popularly attributed to Bohr, Peierls, and Placzek [Editor's Note: This relationship is in fact due to Eugene Feenberg* (*Phys. Rev.* **40**, 1932); see R. G. Newton (*Am. J. Phys.* **44**,

* As pointed out by Newton in his Review (c.f. Ref. 8 therein), Feenberg's paper is also remarkable for the fact that it was published on 1 April 1932, with a receipt date stated as 8 September 1932—thus violating causality!

639, 1976) for the historical background.] called the **optical theorem**, which relates the imaginary part of the forward scattering amplitude $f(\theta = 0)$ to the total cross section σ_{tot} , as follows:

Optical Theorem

$$\text{Im } f(\theta = 0) = \frac{k\sigma_{\text{tot}}}{4\pi} \quad (7.3.1)$$

where

$$f(\theta = 0) \equiv f(\mathbf{k}, \mathbf{k}), \quad (7.3.2)$$

the setting of $\mathbf{k}' \equiv \mathbf{k}$ imposes scattering in the forward direction, and

$$\sigma_{\text{tot}} \equiv \int \frac{d\sigma}{d\Omega} d\Omega. \quad (7.3.3)$$

Proof. From (7.2.19) we have

$$f(\theta = 0) = f(\mathbf{k}, \mathbf{k}) = -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \mathbf{k} | T | \mathbf{k} \rangle. \quad (7.3.4)$$

We next evaluate $\text{Im} \langle \mathbf{k} | T | \mathbf{k} \rangle$ using (7.2.16), (7.1.6), and the hermiticity of V :

$$\begin{aligned} \text{Im} \langle \mathbf{k} | T | \mathbf{k} \rangle &= \text{Im} \langle \mathbf{k} | V | \psi^{(+)} \rangle \\ &= \text{Im} \left[\left(\langle \psi^{(+)} | - \langle \psi^{(+)} | V \frac{1}{E - H_0 - i\epsilon} \right) V | \psi^{(+)} \rangle \right]. \end{aligned} \quad (7.3.5)$$

Now we use the well-known relation

$$\frac{1}{E - H_0 - i\epsilon} = \text{Pr.} \left(\frac{1}{E - H_0} \right) + i\pi\delta(E - H_0)$$

to reduce the right-hand side of (7.3.5) to the form

$$\begin{aligned} \text{Im} (\langle \psi^{(+)} | V | \psi^{(+)} \rangle) - \text{Im} \langle \psi^{(+)} | V \text{Pr.} \frac{1}{E - H_0} V | \psi^{(+)} \rangle \\ - \text{Im} \langle \psi^{(+)} | V i\pi\delta(E - H_0) V | \psi^{(+)} \rangle. \end{aligned} \quad (7.3.6)$$

The first two terms of (7.3.6) vanish because of the hermiticity of V and $V \text{Pr.}[1/(E - H_0)]V$; hence (7.3.6) reduces to

$$-\pi \langle \psi^{(+)} | V \delta(E - H_0) V | \psi^{(+)} \rangle. \quad (7.3.7)$$

Again, we can recast (7.3.7) using (7.2.16) and $|\phi\rangle = |\mathbf{k}\rangle$ as

$$\begin{aligned} \text{Im} \langle \mathbf{k} | T | \mathbf{k} \rangle &= -\pi \langle \mathbf{k} | T^\dagger \delta(E - H_0) T | \mathbf{k} \rangle \\ &= -\pi \int d^3 k' \langle \mathbf{k} | T^\dagger | \mathbf{k}' \rangle \langle \mathbf{k}' | T | \mathbf{k} \rangle \delta \left(E - \frac{\hbar^2 k'^2}{2m} \right) \\ &= -\pi \int d\Omega' \frac{mk}{\hbar^2} |\langle \mathbf{k}' | T | \mathbf{k} \rangle|^2, \end{aligned} \quad (7.3.8)$$

where we have used $d^3k' = k'^2 dE (dk'/dE) d\Omega'$, the δ -function constraint $E = \hbar^2 k'^2 / 2m$ [hence $dE = (\hbar^2 k'/m) dk'$], and—finally— $k' = k$. From (7.3.4) and (7.3.8), we have

$$\begin{aligned} \text{Im } f(0) &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \left(-\frac{\pi mk}{\hbar^2} \int d\Omega' |\langle \mathbf{k}' | T | \mathbf{k} \rangle|^2 \right) \\ &= \frac{k\sigma_{\text{tot}}}{4\pi}, \end{aligned} \quad (7.3.9)$$

where in the last step we have used (7.1.36), (7.2.19), and (7.3.3). \square

We can appreciate the physical significance of the optical theorem after we discuss shadow scattering.

7.4. EIKONAL APPROXIMATION

This approximation covers a situation in which $V(\mathbf{x})$ varies very little over a distance of order of wavelength λ (which can be regarded as “small”). Note that V itself need not be weak as long as $E \gg |V|$; hence the domain of validity here is different from the Born approximation. Under these conditions, the semiclassical path concept becomes applicable, and we replace the exact wave function $\psi^{(+)}$ by the semiclassical wave function [see (2.4.18) and (2.4.22)], namely,

$$\psi^{(+)} \sim e^{iS(\mathbf{x})/\hbar}. \quad (7.4.1)$$

This leads to the Hamilton-Jacobi equation for S ,

$$\frac{(\nabla S)^2}{2m} + V = E = \frac{\hbar^2 k^2}{2m}, \quad (7.4.2)$$

as discussed in Section 2.4. We propose to compute S from (7.4.2) by making the further approximation that the classical trajectory is a straight-line path, which should be satisfactory for small deflection at high energy.* Consider the situation depicted in Figure 7.5, where the straight-line trajectory is along the z -direction. Integrating (7.4.2) we have

$$\frac{S}{\hbar} = \int_{-\infty}^z \left[k^2 - \frac{2m}{\hbar^2} V(\sqrt{b^2 + z'^2}) \right]^{1/2} dz' + \text{constant}. \quad (7.4.3)$$

The additive constant is to be chosen in such a way that

$$\frac{S}{\hbar} \rightarrow kz \quad \text{as} \quad V \rightarrow 0 \quad (7.4.4)$$

so that the plane-wave form for (7.4.1) is reproduced in this zero-potential

*Needless to say, solution of (7.4.2) to determine the classical trajectory would be a forbidding task in general.

limit. We can then write Equation (7.4.3) as

$$\begin{aligned} \frac{S}{\hbar} &= kz + \int_{-\infty}^z \left[\sqrt{k^2 - \frac{2m}{\hbar^2} V(\sqrt{b^2 + z'^2})} - k \right] dz' \\ &\cong kz - \frac{m}{\hbar^2 k} \int_{-\infty}^z V(\sqrt{b^2 + z'^2}) dz' \end{aligned} \quad (7.4.5)$$

where for $E \gg V$, we have used

$$\sqrt{k^2 - \frac{2m}{\hbar^2} V(\sqrt{b^2 + z'^2})} \sim k - \frac{mV}{\hbar^2 k}$$

at high $E = \hbar^2 k^2 / 2m$. So

$$\psi^{(+)}(\mathbf{x}) = \psi^{(+)}(\mathbf{b} + z\hat{\mathbf{z}}) \approx \frac{1}{(2\pi)^{3/2}} e^{ikz} \exp \left[-\frac{im}{\hbar^2 k} \int_{-\infty}^z V(\sqrt{b^2 + z'^2}) dz' \right]. \quad (7.4.6)$$

Though (7.4.6) does not have the correct asymptotic form appropriate for an incident plus spherical outgoing wave (that is, it is not of form $e^{i\vec{\mathbf{k}} \cdot \vec{\mathbf{x}}} + f(\theta)(e^{ikr}/r)$ and indeed refers only to motion along the original direction), it can nevertheless still be used in (7.1.34) to obtain an approximate expression for $f(\mathbf{k}', \mathbf{k})$, to wit,

$$\begin{aligned} f(\mathbf{k}', \mathbf{k}) &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3x' e^{-i\mathbf{k}' \cdot \mathbf{x}'} V(\sqrt{b^2 + z'^2}) e^{i\mathbf{k} \cdot \mathbf{x}'} \\ &\times \exp \left[-\frac{im}{\hbar^2 k} \int_{-\infty}^{z'} V(\sqrt{b^2 + z''^2}) dz'' \right]. \end{aligned} \quad (7.4.7)$$

Note that without the last factor, $\exp [\dots]$, (7.4.7) is just like the first-order Born amplitude in (7.2.2). We perform the three-dimensional (d^3x') integration in (7.4.7) by introducing cylindrical coordinates $d^3x' = b db d\phi_b dz'$ (see

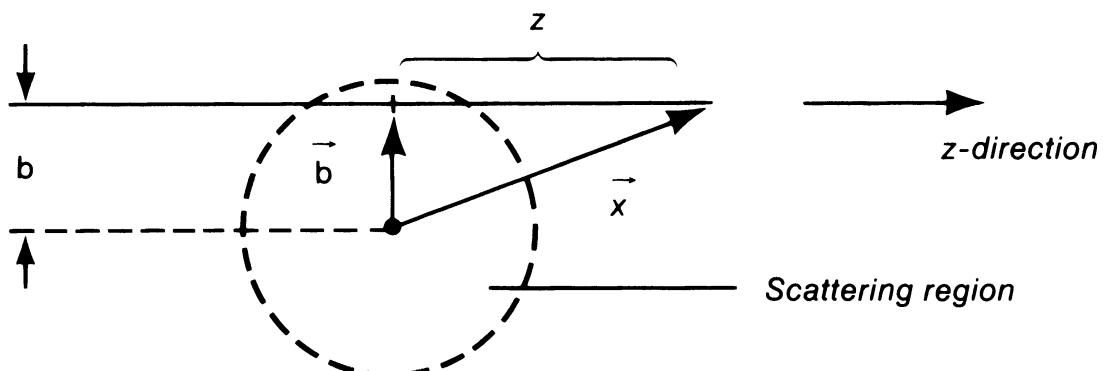


FIGURE 7.5. Schematic diagram of eikonal approximation scattering where the classical straight line trajectory is along the z -direction, $|\mathbf{x}| = r$, and $b = |\mathbf{b}|$ is the impact parameter.

Figure 7.5) and noting that

$$(\mathbf{k} - \mathbf{k}') \cdot \mathbf{x}' = (\mathbf{k} - \mathbf{k}') \cdot (\mathbf{b} + z' \hat{\mathbf{z}}) \simeq -\mathbf{k}' \cdot \mathbf{b}, \quad (7.4.8)$$

where we have used $\mathbf{k} \perp \mathbf{b}$ and $(\mathbf{k} - \mathbf{k}') \cdot \hat{\mathbf{z}} \sim 0(\theta^2)$, which can be ignored for small deflection θ . Without loss of generality we choose scattering to be in the xz -plane and write

$$\mathbf{k}' \cdot \mathbf{b} = (k \sin \theta \hat{\mathbf{x}} + k \cos \theta \hat{\mathbf{z}}) \cdot (b \cos \phi_b \hat{\mathbf{x}} + b \sin \phi_b \hat{\mathbf{y}}) \simeq kb\theta \cos \phi_b. \quad (7.4.9)$$

The expression for $f(\mathbf{k}', \mathbf{k})$ becomes

$$\begin{aligned} f(\mathbf{k}', \mathbf{k}) = & -\frac{1}{4\pi} \frac{2m}{\hbar^2} \int_0^\infty b db \int_0^{2\pi} d\phi_b e^{-ikb\theta \cos \phi_b} \\ & \times \int_{-\infty}^{+\infty} dz V \exp \left[\frac{-im}{\hbar^2 k} \int_{-\infty}^z V dz' \right]. \end{aligned} \quad (7.4.10)$$

We next use the following identities:

$$\int_0^{2\pi} d\phi_b e^{-ikb\theta \cos \phi_b} = 2\pi J_0(kb\theta) \quad (7.4.11)$$

and

$$\int_{-\infty}^{+\infty} dz V \exp \left[\frac{-im}{\hbar^2 k} \int_{-\infty}^z V dz' \right] = \frac{i\hbar^2 k}{m} \exp \left[\frac{-im}{\hbar^2 k} \int_{-\infty}^z V dz' \right] \Big|_{z=-\infty}^{z=+\infty}, \quad (7.4.12)$$

where, of course, the contribution from $z = -\infty$ on the right-hand side of (7.4.12) vanishes in the exponent. So, finally

$$f(\mathbf{k}', \mathbf{k}) = -ik \int_0^\infty db b J_0(kb\theta) [e^{2i\Delta(b)} - 1], \quad (7.4.13)$$

where

$$\Delta(b) \equiv \frac{-m}{2k\hbar^2} \int_{-\infty}^{+\infty} V(\sqrt{b^2 + z^2}) dz. \quad (7.4.14)$$

In (7.4.14) we fix the impact parameter b and integrate along the straight-line path z , shown in Figure 7.5. There is no contribution from $[e^{2i\Delta(b)} - 1]$ in (7.4.13) if b is greater than the range of V .

It can be shown in a straightforward manner that the eikonal approximation satisfies the optical theorem (7.3.1). This proof plus some interesting applications—for example, when V is a Gaussian potential $\Delta(b)$ becomes Gaussian in b -space—are discussed in the literature (Gottfried 1966). For the case where V is a Yukawa potential, see Problem 7 in this chapter.

7.5. FREE-PARTICLE STATES: PLANE WAVES VERSUS SPHERICAL WAVES

In considering scattering by a spherically symmetric potential, we often examine how states with definite angular momenta are affected by the scatterer. Such considerations lead to the method of partial waves, to be discussed in detail in Section 7.6. However, before discussing the angular momentum decomposition of scattering states, let us first talk about free-particle states, which are also eigenstates of angular momentum.

For a free particle the Hamiltonian is just the kinetic-energy operator, which obviously commutes with the momentum operator. It is for this reason that in Section 7.1 we also took $|\phi\rangle$, an eigenket of the free-particle Hamiltonian, to be a momentum eigenket or a plane-wave state $|\mathbf{k}\rangle$, where the eigenvalue of the momentum operator is $\hbar\mathbf{k}$. We note, however, that the free-particle Hamiltonian also commutes with \mathbf{L}^2 and L_z . Thus it is possible to consider a simultaneous eigenket of H_0 , \mathbf{L}^2 , and L_z . Ignoring spin, such a state is denoted by $|E, l, m\rangle$, often called a **spherical-wave state**.

More generally, the most general free-particle state can be regarded as a superposition of $|E, l, m\rangle$ with various E , l , and m in much the same way as the most general free-particle state can be regarded as a superposition of $|\mathbf{k}\rangle$ with different \mathbf{k} , different in both magnitude and direction. Put in another way, a free-particle state can be analysed using either the plane-wave basis $\{|\mathbf{k}\rangle\}$ or the spherical-wave basis $\{|E, l, m\rangle\}$.

We now derive the transformation function $\langle \mathbf{k}|E, l, m\rangle$ that connects the plane-wave basis with the spherical-wave basis. We can also regard this quantity as the momentum-space wave function for the spherical wave characterized by E , l , and m . We adopt the normalization convention for the spherical-wave eigenket as follows:

$$\langle E', l', m'|E, l, m\rangle = \delta_{ll'}\delta_{mm'}\delta(E - E'). \quad (7.5.1)$$

In analogy with the position-space wave function, we may guess the angular dependence:

$$\langle \mathbf{k}|E, l, m\rangle = g_{lE}(k)Y_l^m(\hat{\mathbf{k}}). \quad (7.5.2)$$

To prove this rigorously, we proceed as follows. First, consider the momentum eigenket $|k\hat{\mathbf{z}}\rangle$ —that is, a plane-wave state whose propagation direction is along the positive z -axis. An important property of this state is that it has no orbital angular-momentum component in the z -direction:

$$L_z|k\hat{\mathbf{z}}\rangle = (xp_y - yp_x)|k_x = 0, k_y = 0, k_z = k\rangle = 0. \quad (7.5.3)$$

Actually this is plausible from classical considerations: The angular-momentum component must vanish in the direction of propagation because $\mathbf{L} \cdot \mathbf{p} = (\mathbf{x} \times \mathbf{p}) \cdot \mathbf{p} = 0$. Because of (7.5.3)—and since $\langle E', l', m'|k\hat{\mathbf{z}}\rangle = 0$ for

$m' \neq 0$ —we must be able to expand $|k\hat{\mathbf{z}}\rangle$ as follows:

$$|k\hat{\mathbf{z}}\rangle = \sum_{l'} \int dE' |E', l', m' = 0\rangle \langle E', l', m' = 0| k\hat{\mathbf{z}}\rangle. \quad (7.5.4)$$

Notice that there is no m' sum; m' is always zero. We can obtain the most general momentum eigenket, with the direction of \mathbf{k} specified by θ and ϕ , from $|k\hat{\mathbf{z}}\rangle$ by just applying the appropriate rotation operator as follows [see Figure 3.3 and (3.6.47)]:

$$|\mathbf{k}\rangle = \mathcal{D}(\alpha = \phi, \beta = \theta, \gamma = 0)|k\hat{\mathbf{z}}\rangle. \quad (7.5.5)$$

Multiplying (7.5.5) by $\langle E, l, m|$ on the left, we obtain

$$\begin{aligned} \langle E, l, m | \mathbf{k} \rangle &= \sum_{l'} \int dE' \langle E, l, m | \mathcal{D}(\alpha = \phi, \beta = \theta, \gamma = 0) | E', l', m' = 0 \rangle \\ &\quad \times \langle E', l', m' = 0 | k\hat{\mathbf{z}} \rangle \\ &= \sum_{l'} \int dE' \mathcal{D}_{m0}^{(l')}(\alpha = \phi, \beta = \theta, \gamma = 0) \\ &\quad \times \delta_{ll'} \delta(E - E') \langle E', l', m' = 0 | k\hat{\mathbf{z}} \rangle \\ &= \mathcal{D}_{m0}^{(l)}(\alpha = \phi, \beta = \theta, \gamma = 0) \langle E, l, m = 0 | k\hat{\mathbf{z}} \rangle. \end{aligned} \quad (7.5.6)$$

Now $\langle E, l, m = 0 | k\hat{\mathbf{z}} \rangle$ is independent of the orientation of \mathbf{k} —that is, independent of θ and ϕ —and we may as well call it $\sqrt{\frac{2l+1}{4\pi}} g_{lE}^*(k)$. So we can write, using (3.6.51),

$$\langle \mathbf{k} | E, l, m \rangle = g_{lE}(k) Y_l^m(\hat{\mathbf{k}}). \quad (7.5.7)$$

Let us determine $g_{lE}(k)$. First, we note that

$$(H_0 - E) |E, l, m\rangle = 0. \quad (7.5.8)$$

But we also let $H_0 - E$ operate on a momentum eigenbra $\langle \mathbf{k}|$ as follows:

$$\langle \mathbf{k} | (H_0 - E) = \left(\frac{\hbar^2 k^2}{2m} - E \right) \langle \mathbf{k} |. \quad (7.5.9)$$

Multiplying (7.5.9) with $|E, l, m\rangle$ on the right, we obtain

$$\left(\frac{\hbar^2 k^2}{2m} - E \right) \langle \mathbf{k} | E, l, m \rangle = 0. \quad (7.5.10)$$

This means that $\langle \mathbf{k} | E, l, m \rangle$ can be nonvanishing only if $E = \hbar^2 k^2 / 2m$; so we must be able to write $g_{lE}(k)$ as

$$g_{lE}(k) = N \delta \left(\frac{\hbar^2 k^2}{2m} - E \right). \quad (7.5.11)$$

To determine N we go back to our normalization convention (7.5.1). We obtain

$$\begin{aligned}
 \langle E', l', m' | E, l, m \rangle &= \int d^3 k'' \langle E', l', m' | \mathbf{k}'' \rangle \langle \mathbf{k}'' | E, l, m \rangle \\
 &= \int k''^2 dk'' \int d\Omega_{\mathbf{k}''} |N|^2 \delta\left(\frac{\hbar^2 k''^2}{2m} - E'\right) \\
 &\quad \times \delta\left(\frac{\hbar^2 k''^2}{2m} - E\right) Y_{l'}^{m'*}(\hat{\mathbf{k}}'') Y_l^m(\hat{\mathbf{k}}'') \\
 &= \int \frac{k''^2 dE''}{dE''/dk''} \int d\Omega_{\mathbf{k}''} |N|^2 \delta\left(\frac{\hbar^2 k''^2}{2m} - E'\right) \delta\left(\frac{\hbar^2 k''^2}{2m} - E\right) \\
 &\quad \times Y_{l'}^{m'*}(\hat{\mathbf{k}}'') Y_l^m(\hat{\mathbf{k}}'') \\
 &= |N|^2 \frac{mk'}{\hbar^2} \delta(E - E') \delta_{ll'} \delta_{mm'}, \tag{7.5.12}
 \end{aligned}$$

where we have defined $E'' = \hbar^2 k''^2 / 2m$ to change k'' -integration into E'' -integration. Comparing this with (7.5.1), we see that $N = \hbar / \sqrt{mk}$ will suffice. Therefore, we can finally write

$$g_{lE}(k) = \frac{\hbar}{\sqrt{mk}} \delta\left(\frac{\hbar^2 k^2}{2m} - E\right); \tag{7.5.13}$$

hence

$$\langle \mathbf{k} | E, l, m \rangle = \frac{\hbar}{\sqrt{mk}} \delta\left(\frac{\hbar^2 k^2}{2m} - E\right) Y_l^m(\hat{\mathbf{k}}). \tag{7.5.14}$$

From (7.5.14) we infer that the plane-wave state $|\mathbf{k}\rangle$ can be expressed as a superposition of free spherical-wave states with all possible l -values; in particular,

$$\begin{aligned}
 |\mathbf{k}\rangle &= \sum_l \sum_m \int dE |E, l, m\rangle \langle E, l, m | \mathbf{k}\rangle \\
 &= \sum_{l=0}^{\infty} \sum_{m=-l}^l |E, l, m\rangle \Big|_{E = \hbar^2 k^2 / 2m} \left(\frac{\hbar}{\sqrt{mk}} Y_l^{m*}(\hat{\mathbf{k}}) \right). \tag{7.5.15}
 \end{aligned}$$

Because the transverse dimension of the plane wave is infinite, we expect that the plane wave must contain all possible values of impact parameter b (semiclassically, the impact parameter $b \approx \hbar/p$). From this point of view it is no surprise that the momentum eigenstates $|\mathbf{k}\rangle$, when analyzed in terms of spherical-wave states, contain all possible values of l .

We have derived the wave function for $|E, l, m\rangle$ in momentum space. Next, we consider the corresponding wave function in position space.

From wave mechanics, the reader should be familiar with the fact that the wave function for a free spherical wave is $j_l(kr)Y_l^m(\hat{\mathbf{r}})$, where $j_l(kr)$ is the spherical Bessel function of order l (see Appendix A). The second solution $n_l(kr)$, although it satisfies the appropriate differential equation, is inadmissible because it is singular at the origin. So we can write

$$\langle \mathbf{x}|E, l, m\rangle = c_l j_l(kr) Y_l^m(\hat{\mathbf{r}}). \quad (7.5.16)$$

To determine c_l , all we have to do is compare

$$\begin{aligned} \langle \mathbf{x}|\mathbf{k}\rangle &= \frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} = \sum_l \sum_m \int dE \langle \mathbf{x}|E, l, m\rangle \langle E, l, m|\mathbf{k}\rangle \\ &= \sum_l \sum_m \int dE c_l j_l(kr) Y_l^m(\hat{\mathbf{r}}) \frac{\hbar}{\sqrt{mk}} \delta\left(E - \frac{\hbar^2 k^2}{2m}\right) Y_l^{m*}(\hat{\mathbf{k}}) \\ &= \sum_l \frac{(2l+1)}{4\pi} P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}) \frac{\hbar}{\sqrt{mk}} c_l j_l(kr), \end{aligned} \quad (7.5.17)$$

where we have used the addition theorem

$$\sum_m Y_l^m(\hat{\mathbf{r}}) Y_l^{m*}(\hat{\mathbf{k}}) = [(2l+1)/4\pi] P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}})$$

in the last step. Now $\langle \mathbf{x}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{x}}/(2\pi)^{3/2}$ can also be written as

$$\frac{e^{i\mathbf{k}\cdot\mathbf{x}}}{(2\pi)^{3/2}} = \frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) i^l j_l(kr) P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}), \quad (7.5.18)$$

which can be proved by using the following integral representation for $j_l(kr)$:

$$j_l(kr) = \frac{1}{2i^l} \int_{-1}^{+1} e^{ikr \cos \theta} P_l(\cos \theta) d(\cos \theta). \quad (7.5.19)$$

Comparing (7.5.17) with (7.5.18), we have

$$c_l = \frac{i^l}{\hbar} \sqrt{\frac{2mk}{\pi}}. \quad (7.5.20)$$

To summarize, we have

$$\langle \mathbf{k}|E, l, m\rangle = \frac{\hbar}{\sqrt{mk}} \delta\left(E - \frac{\hbar^2 k^2}{2m}\right) Y_l^m(\hat{\mathbf{k}}) \quad (7.5.21a)$$

$$\langle \mathbf{x}|E, l, m\rangle = \frac{i^l}{\hbar} \sqrt{\frac{2mk}{\pi}} j_l(kr) Y_l^m(\hat{\mathbf{r}}). \quad (7.5.21b)$$

These expressions are extremely useful in developing the partial-wave expansion discussed in the next section.

We conclude this section by applying (7.5.21a) to a decay process. Suppose a parent particle of spin j disintegrates into two spin-zero particles A (spin j) $\rightarrow B$ (spin 0) + C (spin 0). The basic Hamiltonian responsible for

such a decay process is, in general, very complicated. However, we do know that angular momentum is conserved because the basic Hamiltonian must be rotationally invariant. So the momentum-space wave function for the final state must be of the form (7.5.21a), with l identified with the spin of the parent particle. This immediately enables us to compute the angular distribution of the decay product because the momentum-space wave function is nothing more than the probability amplitude for finding the decay product with relative momentum direction \mathbf{k} .

As a concrete example from nuclear physics, let us consider the decay of an excited nucleus, Ne^{20^*} :



Both O^{16} and He^4 are known to be spinless particles. Suppose the magnetic quantum number of the parent nucleus is ± 1 , relative to some direction z . Then the angular distribution of the decay product is proportional to $|Y_1^{\pm 1}(\theta, \phi)|^2 = (3/8\pi)\sin^2\theta$, where (θ, ϕ) are the polar angles defining the relative direction \mathbf{k} of the decay product. On the other hand, if the magnetic quantum number is 0 for a parent nucleus with spin 1, the decay angular distribution varies as $|Y_1^0(\theta, \phi)|^2 = (3/4\pi)\cos^2\theta$.

For a general spin orientation we obtain

$$\sum_{m=-1}^1 w(m) |Y_{l=1}^m|^2. \quad (7.5.23)$$

For an unpolarized nucleus the various $w(m)$ are all equal, and we obtain an isotropic distribution; this is not surprising because there is no preferred direction if the parent particle is unpolarized.

For a higher spin object, the angular distribution of the decay is more involved; the higher the spin of the parent decaying system, the greater the complexity of the angular distribution of the decay products. Quite generally, through a study of the angular distribution of the decay products, it is possible to determine the spin of the parent nucleus.

7.6. METHOD OF PARTIAL WAVES

Partial-Wave Expansion

Let us now come back to the case $V \neq 0$. We assume that the potential is spherically symmetric, that is, invariant under rotations in three dimensions. It then follows that the transition operator T , which is given by (7.2.20), commutes with \mathbf{L}^2 and \mathbf{L} . In other words, T is a scalar operator.

It is now useful to use the spherical-wave basis because the Wigner-Eckart theorem [see (3.10.38)], applied to a scalar operator, immediately

gives

$$\langle E', l', m' | T | E, l, m \rangle = T_l(E) \delta_{ll'} \delta_{mm'}. \quad (7.6.1)$$

In other words, T is diagonal both in l and in m ; furthermore, the (nonvanishing) diagonal element depends on E and l but not on m . This leads to an enormous simplification, as we will see shortly.

Let us now look at the scattering amplitude (7.2.19):

$$\begin{aligned} f(\mathbf{k}', \mathbf{k}) &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \langle \mathbf{k}' | T | \mathbf{k} \rangle \\ &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \sum_l \sum_m \sum_{l'} \sum_{m'} \int dE \int dE' \langle \mathbf{k}' | E' l' m' \rangle \\ &\quad \times \langle E' l' m' | T | E l m \rangle \langle E l m | \mathbf{k} \rangle \\ &= -\frac{1}{4\pi} \frac{2m}{\hbar^2} (2\pi)^3 \frac{\hbar^2}{mk} \sum_l \sum_m T_l(E) \Big|_{E=\hbar^2 k^2 / 2m} Y_l^m(\hat{\mathbf{k}}') Y_l^{m*}(\hat{\mathbf{k}}) \\ &= -\frac{4\pi^2}{k} \sum_l \sum_m T_l(E) \Big|_{E=\hbar^2 k^2 / 2m} Y_l^m(\hat{\mathbf{k}}') Y_l^{m*}(\hat{\mathbf{k}}). \end{aligned} \quad (7.6.2)$$

To obtain the angular dependence of the scattering amplitude, let us choose the coordinate system in such a way that \mathbf{k} , as usual, is in the positive z -direction. We then have [see (3.6.50)]

$$Y_l^m(\hat{\mathbf{k}}) = \sqrt{\frac{2l+1}{4\pi}} \delta_{m0}, \quad (7.6.3)$$

where we have used $P_l(1)=1$; hence only the terms $m=0$ contribute. Taking θ to be the angle between \mathbf{k}' and \mathbf{k} , we can write

$$Y_l^0(\hat{\mathbf{k}}') = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos \theta). \quad (7.6.4)$$

It is customary here to define the **partial-wave amplitude** $f_l(k)$ as follows:

$$f_l(k) \equiv -\frac{\pi T_l(E)}{k}. \quad (7.6.5)$$

For (7.6.2) we then have

$$f(\mathbf{k}', \mathbf{k}) = f(\theta) = \sum_{l=0}^{\infty} (2l+1) f_l(k) P_l(\cos \theta), \quad (7.6.6)$$

where $f(\theta)$ still depends on k (or the incident energy) even though k is suppressed.

To appreciate the physical significance of $f_l(k)$, let us study the large-distance behavior of the wave function $\langle \mathbf{x} | \psi^{(+)} \rangle$ given by (7.1.33). Using the expansion of a plane wave in terms of spherical waves [(7.5.18)]

and noting that (Appendix A)

$$j_l(kr) \xrightarrow{\text{large } r} \frac{e^{i(kr - l\pi/2)} - e^{-i(kr - l\pi/2)}}{2ikr}, \quad (i^l = e^{i(\pi/2)l}) \quad (7.6.7)$$

and that $f(\theta)$ is given by (7.6.6), we have

$$\begin{aligned} \langle \mathbf{x} | \psi^{(+)} \rangle &\xrightarrow{\text{large } r} \frac{1}{(2\pi)^{3/2}} \left[e^{ikz} + f(\theta) \frac{e^{ikr}}{r} \right] \\ &= \frac{1}{(2\pi)^{3/2}} \left[\sum_l (2l+1) P_l(\cos \theta) \left(\frac{e^{ikr} - e^{-i(kr - l\pi)}}{2ikr} \right) \right. \\ &\quad \left. + \sum_l (2l+1) f_l(k) P_l(\cos \theta) \frac{e^{ikr}}{r} \right] \\ &= \frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) \frac{P_l}{2ik} \left[[1 + 2ikf_l(k)] \frac{e^{ikr}}{r} - \frac{e^{-i(kr - l\pi)}}{r} \right]. \end{aligned} \quad (7.6.8)$$

The physics of scattering is now clear. When the scatterer is absent, we can analyze the plane wave as the sum of a spherically outgoing wave behaving like e^{ikr}/r and a spherically incoming wave behaving like $-e^{-i(kr - l\pi)}/r$ for each l . The presence of the scatterer changes only the coefficient of the outgoing wave, as follows:

$$1 \rightarrow 1 + 2ikf_l(k). \quad (7.6.9)$$

The incoming wave is completely unaffected.

Unitarity and Phase Shifts

We now examine the consequences of probability conservation, or unitarity. In a time-independent formulation, the flux current density \mathbf{j} must satisfy

$$\nabla \cdot \mathbf{j} = - \frac{\partial |\psi|^2}{\partial t} = 0. \quad (7.6.10)$$

Let us now consider a spherical surface of very large radius. By Gauss's theorem, we must have

$$\int_{\text{spherical surface}} \mathbf{j} \cdot d\mathbf{S} = 0. \quad (7.6.11)$$

Physically (7.6.10) and (7.6.11) mean that there is no source or sink of particles. The outgoing flux must equal the incoming flux. Furthermore, because of angular-momentum conservation, this must hold for each partial

wave separately. In other words, the coefficient of e^{ikr}/r must be the same in magnitude as the coefficient of e^{-ikr}/r . Defining $S_l(k)$ to be

$$S_l(k) \equiv 1 + 2ikf_l(k), \quad (7.6.12)$$

this means [from (7.6.9)] that

$$|S_l(k)| = 1, \quad (7.6.13)$$

that is, the most that can happen is a change in the phase of the outgoing wave. Equation (7.6.13) is known as the **unitarity relation** for the l th partial wave. In a more advanced treatment of scattering, $S_l(k)$ can be regarded as the l th diagonal element of the S operator, which is required to be unitary as a consequence of probability conservation.

We thus see that the only change in the wave function at a large distance as a result of scattering is to change the *phase* of the outgoing wave. Calling this phase $2\delta_l$ (the factor of 2 here is conventional), we can write

$$S_l = e^{2i\delta_l}, \quad (7.6.14)$$

with δ_l real. It is understood here that δ_l is a function of k even though we do not explicitly write δ_l as $\delta_l(k)$. Returning to f_l , we can write [from (7.6.12)]

$$f_l = \frac{(S_l - 1)}{2ik} \quad (7.6.15)$$

or, explicitly in terms of δ_l ,

$$f_l = \frac{e^{2i\delta_l} - 1}{2ik} = \frac{e^{i\delta_l} \sin \delta_l}{k} = \frac{1}{k \cot \delta_l - ik}, \quad (7.6.16)$$

whichever is convenient. For the full scattering amplitude we have

$$\begin{aligned} f(\theta) &= \sum_{l=0}^{\infty} (2l+1) \left(\frac{e^{2i\delta_l} - 1}{2ik} \right) P_l(\cos \theta) \\ &= \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) e^{i\delta_l} \sin \delta_l P_l(\cos \theta) \end{aligned} \quad (7.6.17)$$

with δ_l real. This expression for $f(\theta)$ rests on the twin principles of **rotational invariance** and **probability conservation**. In many books on wave mechanics, (7.6.17) is obtained by explicitly solving the Schrödinger equation with a real, spherically symmetric potential; our derivation of (7.6.17) may be of interest because it can be generalized to situations when the potential described in the context of nonrelativistic quantum mechanics may fail.

The differential cross section $d\sigma/d\Omega$ can be obtained [see (7.1.36)] by just taking the modulus squared of (7.6.17). To obtain the total cross

section we have

$$\begin{aligned}
 \sigma_{\text{tot}} &= \int |f(\theta)|^2 d\Omega \\
 &= \frac{1}{k^2} \int_0^{2\pi} d\phi \int_{-1}^{+1} d(\cos \theta) \sum_l \sum_{l'} (2l+1)(2l'+1) \\
 &\quad \times e^{i\delta_l} \sin \delta_l e^{-i\delta_{l'}} \sin \delta_{l'} P_l P_{l'} \\
 &= \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l. \tag{7.6.18}
 \end{aligned}$$

We can check the optical theorem (7.3.1), which we obtained earlier using a more general argument. All we need to do is note from (7.6.17) that

$$\begin{aligned}
 \text{Im } f(\theta = 0) &= \sum_l \left. \frac{(2l+1)\text{Im}[e^{i\delta_l} \sin \delta_l]}{k} P_l(\cos \theta) \right|_{\theta=0} \\
 &= \sum_l \frac{(2l+1)}{k} \sin^2 \delta_l, \tag{7.6.19}
 \end{aligned}$$

which is the same as (7.6.18) except for $4\pi/k$.

As a function of energy, δ_l changes; hence $f_l(k)$ changes also. The unitarity relation of (7.6.13) is a restriction on the manner in which f_l can vary. This can be most conveniently seen by drawing an Argand diagram for kf_l . We plot kf_l in a complex plane, as shown in Figure 7.6, which is

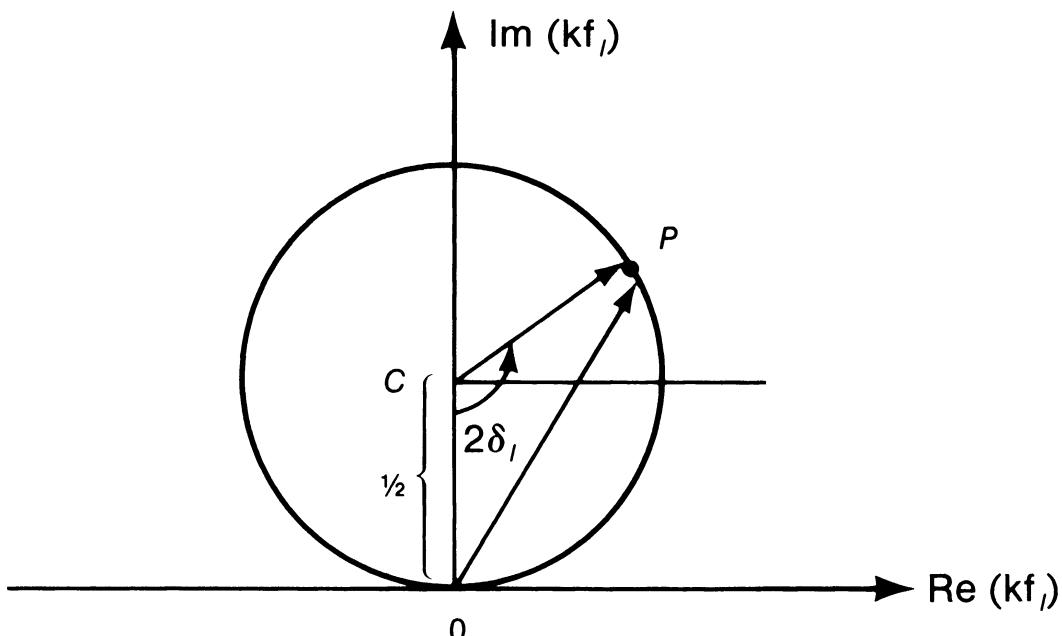


FIGURE 7.6. Argand diagram for kf_l . OP is the magnitude of kf_l , while CO and CP are each radii of length $\frac{1}{2}$ on the unitary circle; angle $OCP = 2\delta_l$.

self-explanatory if we note from (7.6.16) that

$$kf_l = \frac{i}{2} + \frac{1}{2} e^{-(i\pi/2) + 2i\delta_l}. \quad (7.6.20)$$

Notice that there is a circle of radius $\frac{1}{2}$, known as the **unitary circle**, on which kf_l must lie.

We can see many important features from Figure 7.6. Suppose δ_l is small. Then f_l must stay near the bottom of the circle. It may be positive or negative, but f_l is almost purely real:

$$f_l = \frac{e^{i\delta_l} \sin \delta_l}{k} \approx \frac{(1 + i\delta_l)\delta_l}{k} \approx \frac{\delta_l}{k}. \quad (7.6.21)$$

On the other hand, if δ_l is near $\pi/2$, kf_l is almost purely imaginary, and the magnitude of kf_l is maximal. Under such a condition the l th partial wave may be in resonance, a concept to be discussed in some detail in Section 7.8. Note that the maximum partial cross section

$$\sigma_{\max}^{(l)} = 4\pi\lambda^2(2l+1) \quad (7.6.22)$$

is achieved [see (7.6.18)] when $\sin^2\delta_l = 1$.

Connection with the Eikonal Approximation

The eikonal approximation discussed in 7.4 is valid at high energies ($\lambda \ll$ range R); hence many partial waves contribute. We may regard l as a continuous variable. As an aside we note the semiclassical argument that $l = bk$ (because angular momentum $l\hbar = bp$, where b is the impact parameter and momentum $p = \hbar k$). We take

$$l_{\max} = kR; \quad (7.6.23)$$

then we make the following substitutions in expression (7.6.17):

$$\begin{aligned} l_{\max} &= kR \\ \sum_l &\rightarrow k \int db, \quad P_l(\cos \theta) \underset{\substack{\text{large } l, \\ \text{small } \theta}}{\approx} J_0(l\theta) = J_0(kb\theta), \\ \delta_l &\rightarrow \Delta(b)|_{b=l/k}, \end{aligned} \quad (7.6.24)$$

where $l_{\max} = kR$ implies that

$$e^{2i\delta_l} - 1 = e^{2i\Delta(b)} - 1 = 0 \quad \text{for } l > l_{\max}. \quad (7.6.25)$$

We have

$$\begin{aligned} f(\theta) &\rightarrow k \int db \frac{2kb}{2ik} (e^{2i\Delta(b)} - 1) J_0(kb\theta) \\ &= -ik \int db b J_0(kb\theta) [e^{2i\Delta(b)} - 1]. \end{aligned} \quad (7.6.26)$$

The computation of δ_l can be done by using the explicit form for $\Delta(b)$ given by (7.4.14) (see Problem 7 in this chapter).

Determination of Phase Shifts

Let us now consider how we may actually determine the phase shifts given a potential V . We assume that V vanishes for $r > R$, R being the range of the potential. Outside (that is, for $r > R$) the wave function must be that of a free spherical wave. This time, however, there is no reason to exclude $n_l(r)$ because the origin is excluded from our consideration. The wave function is therefore a linear combination of $j_l(kr)P_l(\cos\theta)$ and $n_l(kr)P_l(\cos\theta)$ or, equivalently, $h_l^{(1)}P_l$ and $h_l^{(2)}P_l$, where $h_l^{(1)}$ and $h_l^{(2)}$ are the spherical Hankel functions defined by

$$h_l^{(1)} = j_l + in_l, \quad h_l^{(2)} = j_l - in_l; \quad (7.6.27)$$

these have the asymptotic behavior (see Appendix A)

$$h_l^{(1)} \xrightarrow{r \text{ large}} \frac{e^{i(kr - l\pi/2)}}{ikr}, \quad h_l^{(2)} \xrightarrow{r \text{ large}} -\frac{e^{-i(kr - l\pi/2)}}{ikr}. \quad (7.6.28)$$

The full-wave function at any r can then be written as:

$$\langle \mathbf{x} | \psi^{(+)} \rangle = \frac{1}{(2\pi)^{3/2}} \sum_l i^l (2l+1) A_l(r) P_l(\cos\theta) \quad (r > R). \quad (7.6.29)$$

For $r > R$ we have (for the radial-wave function)

$$A_l = c_l^{(1)} h_l^{(1)}(kr) + c_l^{(2)} h_l^{(2)}(kr), \quad (7.6.30)$$

where the coefficient that multiplies A_l in (7.6.29) is chosen so that, for $V=0$, $A_l(r)$ coincides with $j_l(kr)$ everywhere. Using (7.6.28), we can compare the behavior of the wave function for large r given by (7.6.29) and (7.6.30) with

$$\frac{1}{(2\pi)^{3/2}} \sum_l (2l+1) P_l \left[\frac{e^{2i\delta_l} e^{ikr}}{2ikr} - \frac{e^{-i(kr - l\pi)}}{2ikr} \right]. \quad (7.6.31)$$

Clearly, we must have

$$c_l^{(1)} = \frac{1}{2} e^{2i\delta_l}, \quad c_l^{(2)} = \frac{1}{2}. \quad (7.6.32)$$

So the radial-wave function for $r > R$ is now written as

$$A_l(r) = e^{i\delta_l} [\cos\delta_l j_l(kr) - \sin\delta_l n_l(kr)]. \quad (7.6.33)$$

Using this, we can evaluate the logarithmic derivative at $r = R$ —that is, just outside the range of the potential—as follows:

$$\begin{aligned} \beta_l &\equiv \left(\frac{r}{A_l} \frac{dA_l}{dr} \right)_{r=R} \\ &= kR \left[\frac{j_l'(kR)\cos\delta_l - n_l'(kR)\sin\delta_l}{j_l(kR)\cos\delta_l - n_l(kR)\sin\delta_l} \right], \end{aligned} \quad (7.6.34)$$

where $j_l'(kR)$ stands for the derivative of j_l with respect to kr evaluated at

$kr = kR$. Conversely, knowing the logarithmic derivative at R , we can obtain the phase shift as follows:

$$\tan \delta_l = \frac{kRj'_l(kR) - \beta_l j_l(kR)}{kRn'_l(kR) - \beta_l n_l(kR)}. \quad (7.6.35)$$

The problem of determining the phase shift is thus reduced to that of obtaining β_l .

We now look at the solution to the Schrödinger equation for $r < R$ —that is, inside the range of the potential. For a spherically symmetric potential, we can solve the Schrödinger equation in three dimensions by looking at the equivalent one-dimensional equation

$$\frac{d^2 u_l}{dr^2} + \left(k^2 - \frac{2m}{\hbar^2} V - \frac{l(l+1)}{r^2} \right) u_l = 0, \quad (7.6.36)$$

where

$$u_l = rA_l(r) \quad (7.6.37)$$

subject to the boundary condition

$$u_l|_{r=0} = 0. \quad (7.6.38)$$

We integrate this one-dimensional Schrödinger equation—if necessary, numerically—up to $r = R$, starting at $r = 0$. In this way we obtain the logarithmic derivative at R . By continuity we must be able to match the logarithmic derivative for the inside and outside solutions at $r = R$:

$$\beta_l|_{\text{inside solution}} = \beta_l|_{\text{outside solution}}, \quad (7.6.39)$$

where the left-hand side is obtained by integrating the Schrödinger equation up to $r = R$, while the right-hand side is expressible in terms of the phase shifts that characterize the large-distance behavior of the wave function. This means that the phase shifts are obtained simply by substituting β_l for the inside solution into $\tan \delta_l$ [(7.6.35)]. For an alternative approach it is possible to derive an integral equation for $A_l(r)$, from which we can obtain phase shifts (see Problem 8 of this chapter).

Hard-Sphere Scattering

Let us work out a specific example. We consider scattering by a hard, or rigid, sphere

$$V = \begin{cases} \infty & \text{for } r < R \\ 0 & \text{for } r > R. \end{cases} \quad (7.6.40)$$

In this problem we need not even evaluate β_l (which is actually ∞). All we need to know is that the wave function must vanish at $r = R$ because the

sphere is impenetrable. Therefore,

$$A_l(r)|_{r=R} = 0 \quad (7.6.41)$$

or, from (7.6.33),

$$j_l(kR)\cos\delta_l - n_l(kR)\sin\delta_l = 0 \quad (7.6.42)$$

or

$$\tan\delta_l = \frac{j_l(kR)}{n_l(kR)}. \quad (7.6.43)$$

Thus the phase shifts are now known for any l . Notice that no approximations have been made so far.

To appreciate the physical significance of the phase shifts, let us consider the $l=0$ case (*S*-wave scattering) specifically. Equation (7.6.43) becomes, for $l=0$,

$$\tan\delta_0 = \frac{\sin kR/kR}{-\cos kR/kR} = -\tan kR, \quad (7.6.44)$$

or $\delta_0 = -kR$. The radial-wave function (7.6.33) with $e^{i\delta_0}$ omitted varies as

$$A_{l=0}(r) \propto \frac{\sin kr}{kr} \cos\delta_0 + \frac{\cos kr}{kr} \sin\delta_0 = \frac{1}{kr} \sin(kr + \delta_0). \quad (7.6.45)$$

Therefore, if we plot $rA_{l=0}(r)$ as a function of distance r , we obtain a sinusoidal wave, which is shifted when compared to the free sinusoidal wave by amount R ; see Figure 7.7.

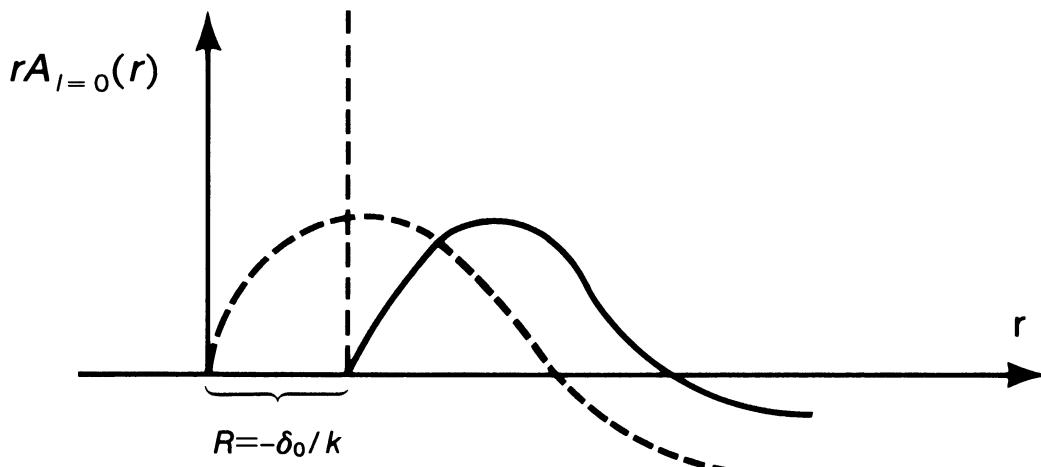


FIGURE 7.7. Plot of $rA_{l=0}(r)$ versus r (with the $e^{i\delta_0}$ factor removed). The dashed curve for $V = 0$ behaves like $\sin kr$, while the solid curve is for *S*-wave hard-sphere scattering, shifted by $R = -\delta_0/k$ from the case $V = 0$.

Let us now study the low and high energy limits of $\tan \delta_l$. Low energy means kR small, $kR \ll 1$. We can then use (see Appendix A)

$$\begin{aligned} j_l(kr) &\simeq \frac{(kr)^l}{(2l+1)!!} \\ n_l(kr) &\simeq -\frac{(2l-1)!!}{(kr)^{l+1}} \end{aligned} \quad (7.6.46)$$

to obtain

$$\tan \delta_l = \frac{-(kR)^{2l+1}}{\{(2l+1)[(2l-1)!!]\}^2}. \quad (7.6.47)$$

It is therefore all right to ignore δ_l with $l \neq 0$. In other words, we have S-wave scattering only, which is actually expected for almost any finite-range potential at low energy. Because $\delta_0 = -kR$ regardless of whether k is large or small, we obtain

$$\frac{d\sigma}{d\Omega} = \frac{\sin^2 \delta_0}{k^2} \simeq R^2 \quad \text{for } kR \ll 1. \quad (7.6.48)$$

It is interesting that the total cross section, given by

$$\sigma_{\text{tot}} = \int \frac{d\sigma}{d\Omega} d\Omega = 4\pi R^2, \quad (7.6.49)$$

is *four* times the *geometric cross section* πR^2 . By geometric cross section we mean the area of the disc of radius R that blocks the propagation of the plane wave (and has the same cross section area as that of a hard sphere). Low-energy scattering, of course, means a very large wavelength scattering, and we do not necessarily expect a classically reasonable result.

One might conjecture that the geometric cross section is reasonable to expect for high-energy scattering because at high energies the situation might look similar to the semiclassical situation. At high energies many l -values contribute, up to $l_{\text{max}} \simeq kR$, a reasonable assumption. The total cross section is therefore given by

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2} \sum_{l=0}^{l \approx kR} (2l+1)\sin^2 \delta_l. \quad (7.6.50)$$

But using (7.6.43), we have

$$\begin{aligned} \sin^2 \delta_l &= \frac{\tan^2 \delta_l}{1 + \tan^2 \delta_l} = \frac{[j_l(kR)]^2}{[j_l(kR)]^2 + [n_l(kR)]^2} \simeq \sin^2 \left(kR - \frac{\pi l}{2} \right), \\ \end{aligned} \quad (7.6.51)$$

where we have used

$$\begin{aligned} j_l(kr) &\sim \frac{1}{kr} \sin\left(kr - \frac{l\pi}{2}\right) \\ n_l(kr) &\sim -\frac{1}{kr} \cos\left(kr - \frac{l\pi}{2}\right). \end{aligned} \quad (7.6.52)$$

We see that δ_l decreases by 90° each time l increases by one unit. Thus, for an adjacent pair of partial waves, $\sin^2\delta_l + \sin^2\delta_{l+1} = \sin^2\delta_l + \sin^2(\delta_l - \pi/2) = \sin^2\delta_l + \cos^2\delta_l = 1$, and with so many l -values contributing to (7.6.50), it is legitimate to replace $\sin^2\delta_l$ by its average value, $\frac{1}{2}$. The number of terms in the l -sum is roughly kR , as is the average of $2l+1$. Putting all the ingredients together, (7.6.50) becomes

$$\sigma_{\text{tot}} = \frac{4\pi}{k^2} (kR)^2 \frac{1}{2} = 2\pi R^2, \quad (7.6.53)$$

which is not the geometric cross section πR^2 either! To see the origin of the factor of 2, we may split (7.6.17) into two parts:

$$\begin{aligned} f(\theta) &= \frac{1}{2ik} \sum_{l=0}^{kR} (2l+1) e^{2il\delta_l} P_l(\cos \theta) + \frac{i}{2k} \sum_{l=0}^{kR} (2l+1) P_l(\cos \theta) \\ &= f_{\text{reflection}} + f_{\text{shadow}}. \end{aligned} \quad (7.6.54)$$

In evaluating $\int |f_{\text{refl}}|^2 d\Omega$, the orthogonality of the $P_l(\cos \theta)$'s ensures that there is no interference amongst contributions from different l , and we obtain the sum of the square of partial-wave contributions:

$$\begin{aligned} \int |f_{\text{refl}}|^2 d\Omega &= \frac{2\pi}{4k^2} \sum_{l=0}^{l_{\max}} \int_{-1}^{+1} (2l+1)^2 [P_l(\cos \theta)]^2 d(\cos \theta) \\ &= \frac{\pi l_{\max}^2}{k^2} = \pi R^2. \end{aligned} \quad (7.6.55)$$

Turning our attention to f_{shad} , we note that it is pure imaginary. It is particularly strong in the forward direction because $P_l(\cos \theta) = 1$ for $\theta = 0$, and the contributions from various l -values all add up coherently—that is, with the same phase, pure imaginary and positive in our case. We can use the small-angle approximation for P_l [see (7.6.24)] to obtain

$$\begin{aligned} f_{\text{shad}} &\simeq \frac{i}{2k} \sum (2l+1) J_0(l\theta) \\ &\simeq ik \int_0^R bdb J_0(kb\theta) \\ &= \frac{iR J_1(kR\theta)}{\theta}. \end{aligned} \quad (7.6.56)$$

But this is just the formula for Fraunhofer diffraction in optics with a strong

peaking near $\theta \approx 0$. Letting $\xi = kR\theta$ and $d\xi/\xi = d\theta/\theta$, we can evaluate

$$\begin{aligned} \int |f_{\text{shad}}|^2 d\Omega &= 2\pi \int_{-1}^{+1} \frac{R^2 [J_1(kR\theta)]^2}{\theta^2} d(\cos\theta) \\ &\simeq 2\pi R^2 \int_0^\infty \frac{[J_1(\xi)]^2}{\xi} d\xi \\ &\simeq \pi R^2. \end{aligned} \quad (7.6.57)$$

Finally, the interference between f_{shad} and f_{refl} vanishes:

$$\text{Re}(f_{\text{shad}}^* f_{\text{refl}}) \simeq 0 \quad (7.6.58)$$

because the phase of f_{refl} oscillates ($2\delta_{l+1} = 2\delta_l - \pi$), approximately averaging to zero, while f_{shad} is pure imaginary. Thus

$$\sigma_{\text{tot}} = \pi R^2 + \pi R^2. \quad (7.6.59)$$

$\uparrow \quad \uparrow$
 $\sigma_{\text{refl}} \quad \sigma_{\text{shad}}$

The second term (coherent contribution in the forward direction) is called a *shadow* because for hard-sphere scattering at high energies, waves with impact parameter less than R must be deflected. So, just *behind* the scatterer there must be zero probability for finding the particle and a shadow must be created. In terms of wave mechanics, this shadow is due to destructive interference between the original wave (which would be there even if the scatterer were absent) and the newly scattered wave. Thus we need scattering in order to create a shadow. That this shadow amplitude must be pure imaginary may be seen by recalling from (7.6.8) that the coefficient of $e^{ikr}/2ikr$ for the l th partial wave behaves like $1 + 2ikf_l(k)$, where the 1 would be present even without the scatterer; hence there must be a positive imaginary term in f_l to get cancellation. In fact, this gives a physical interpretation of the optical theorem, which can be checked explicitly. First note that

$$\frac{4\pi}{k} \text{Im } f(0) \simeq \frac{4\pi}{k} \text{Im}[f_{\text{shad}}(0)] \quad (7.6.60)$$

because $\text{Im}[f_{\text{refl}}(0)]$ averages to zero due to oscillating phase. Using (7.6.54), we obtain

$$\frac{4\pi}{k} \text{Im } f_{\text{shad}}(0) = \frac{4\pi}{k} \text{Im} \left[\frac{i}{2k} \sum_{l=0}^{kR} (2l+1) P_l(1) \right] = 2\pi R^2 \quad (7.6.61)$$

which is indeed equal to σ_{tot} .

7.7. LOW-ENERGY SCATTERING AND BOUND STATES

At low energies—or, more precisely, when $\lambda = 1/k$ is comparable to or larger than the range R —partial waves for higher l are, in general, unimportant. This point may be obvious classically because the particle cannot

penetrate the centrifugal barrier; as a result the potential inside has no effect. In terms of quantum mechanics, the effective potential for the l th partial wave is given by

$$V_{\text{eff}} = V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}; \quad (7.7.1)$$

unless the potential is strong enough to accommodate $l \neq 0$ bound states near $E \approx 0$, the behavior of the radial-wave function is largely determined by the centrifugal barrier term, which means that it must resemble $j_l(kr)$. More quantitatively, it is possible to estimate the behavior of the phase shift using the integral equation for the partial wave (see Problem 8 of this chapter):

$$\frac{e^{i\delta_l} \sin \delta_l}{k} = -\frac{2m}{\hbar^2} \int_0^\infty j_l(kr) V(r) A_l(r) r^2 dr. \quad (7.7.2)$$

If $A_l(r)$ is not too different from $j_l(kr)$ and $1/k$ is much larger than the range of the potential, the right-hand side would vary as k^{2l} ; for small δ_l , the left-hand side must vary as δ_l/k . Hence, the phase shift k goes to zero as

$$\delta_l \sim k^{2l+1} \quad (7.7.3)$$

for small k . This is known as **threshold behavior**.

It is therefore clear that at low energies with a finite range potential, S-wave scattering is important.

Rectangular Well or Barrier

To be specific let us consider S-wave scattering by

$$V = \begin{cases} V_0 = \text{constant} & \text{for } r < R \\ 0 & \text{otherwise} \end{cases} \quad \begin{cases} V_0 > 0 & \text{repulsive} \\ V_0 < 0 & \text{attractive} \end{cases} \quad (7.7.4)$$

Many of the features we obtain here are common to more-complicated finite range potentials.

We have already seen that the outside-wave function [see (7.6.33) and (7.6.45)] must behave like

$$e^{i\delta_0} [j_0(kr) \cos \delta_0 - n_0(kr) \sin \delta_0] \simeq \frac{e^{i\delta_0} \sin(kr + \delta_0)}{kr}. \quad (7.7.5)$$

The inside solution can also easily be obtained for V_0 a constant:

$$u \equiv r A_{l=0}(r) \propto \sin k'r, \quad (7.7.6)$$

with k' determined by

$$E - V_0 = \frac{\hbar^2 k'^2}{2m}, \quad (7.7.7)$$

where we have used the boundary condition $u = 0$ at $r = 0$. In other words,

the inside wave function is also sinusoidal as long as $E > V_0$. The curvature of the sinusoidal wave is different than in the free-particle case; as a result the wave function can be pushed in ($\delta_0 > 0$) or pulled out ($\delta_0 < 0$) depending on whether $V_0 < 0$ (attractive) or $V_0 > 0$ (repulsive), as shown in Figure 7.8. Notice also that (7.7.6) and (7.7.7) hold even if $V_0 > E$, provided we understand sin to mean sinh—that is, the wave function behaves like

$$u(r) \propto \sinh[\kappa r], \quad (7.7.6')$$

where

$$\frac{\hbar^2 \kappa^2}{2m} = (V_0 - E). \quad (7.7.7')$$

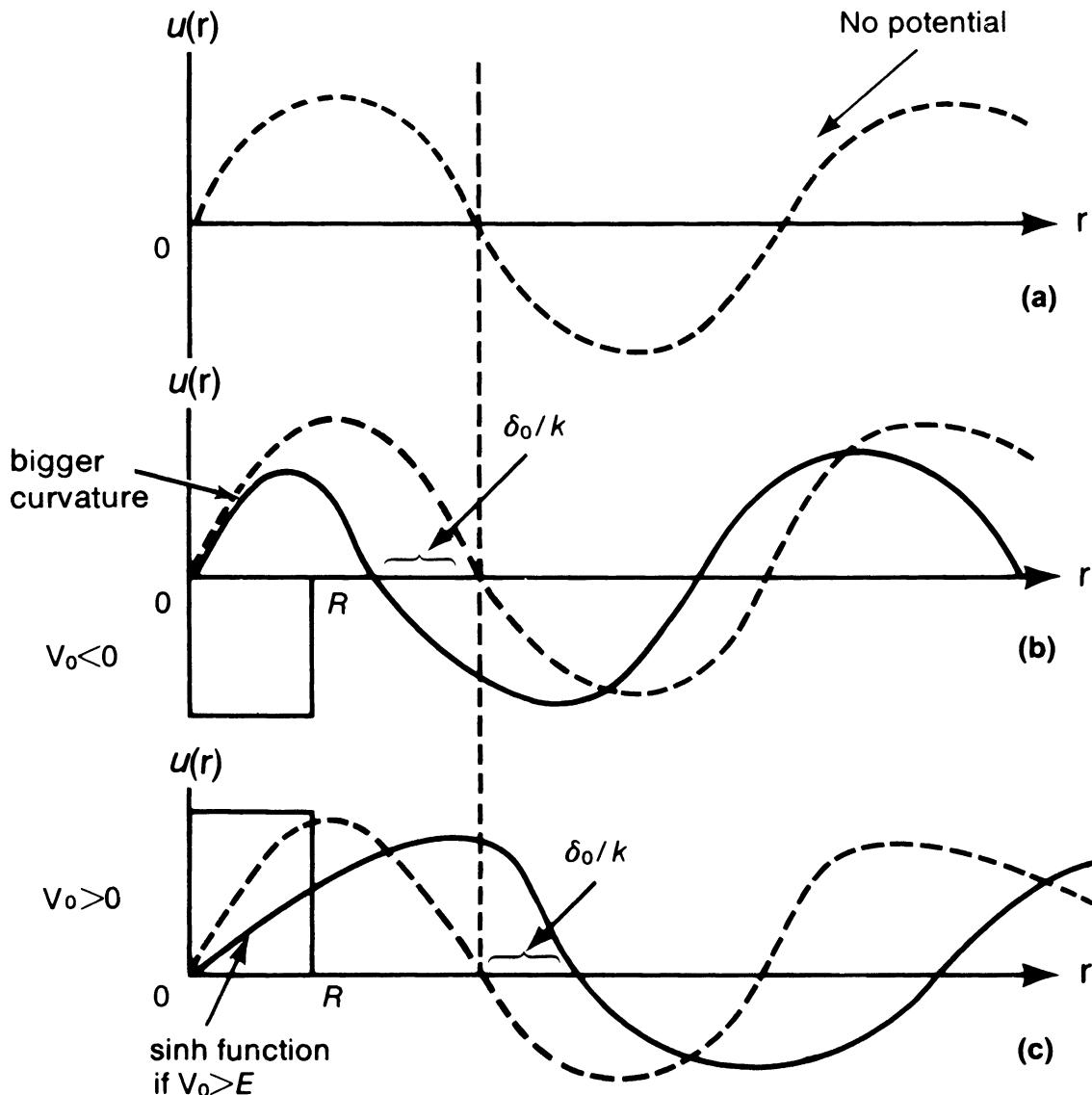


FIGURE 7.8 Plot of $u(r)$ versus r . (a) For $V = 0$ (dashed line). (b) For $V_0 < 0$, $\delta_0 > 0$ with the wave function (solid line) pushed in. (c) For $V_0 > 0$, $\delta_0 < 0$ with the wave function (solid line) pulled out.

We now concentrate on the attractive case and imagine that the magnitude of V_0 is increased. Increased attraction will result in a wave function with a larger curvature. Suppose the attraction is such that the interval $[0, R]$ just accommodates one-fourth cycle of the sinusoidal wave. Working in the low energy $kR \ll 1$ limit, the phase shift is now $\delta_0 = \pi/2$, and this results in a maximal S-wave cross section for a given k because $\sin^2 \delta_0$ is unity. Now increase the well depth V_0 even further. Eventually the attraction is so strong that one-half cycle of the sinusoidal wave can be fitted within the range of the potential. The phase shift δ_0 is now π ; in other words, the wave function outside R is 180° out of phase compared to the free-particle-wave function. What is remarkable is that the partial cross section vanishes ($\sin^2 \delta_0 = 0$),

$$\sigma_{l=0} = 0, \quad (7.7.8)$$

despite the very strong attraction of the potential. In addition, if the energy is low enough for $l \neq 0$ waves still to be unimportant, we then have an almost-perfect transmission of the incident wave. This kind of situation, known as the **Ramsauer-Townsend effect**, is actually observed experimentally for scattering of electrons by such rare gases as argon, krypton, and xenon. This effect was first observed in 1923 prior to the birth of wave mechanics and was considered to be a great mystery. Note the typical parameters here are $R \sim 2 \times 10^{-8}$ cm for electron kinetic energy of order 0.1 eV, leading to $kR \sim 0.324$.

Zero-Energy Scattering and Bound States

Let us consider scattering at extremely low energies ($k \approx 0$). For $r > R$ and for $l = 0$, the outside radial-wave function satisfies

$$\frac{d^2 u}{dr^2} = 0. \quad (7.7.9)$$

The obvious solution to (7.7.9) is

$$u(r) = \text{constant}(r - a), \quad (7.7.10)$$

just a straight line! This can be understood as an infinitely long wavelength limit of the usual expression for the outside-wave function [see (7.6.37) and (7.6.45)],

$$\lim_{k \rightarrow 0} \sin(kr + \delta_0) = \lim_{k \rightarrow 0} \sin\left[k\left(r + \frac{\delta_0}{k}\right)\right], \quad (7.7.11)$$

which looks like (7.7.10). We have

$$\frac{u'}{u} = k \cot\left[k\left(r + \frac{\delta_0}{k}\right)\right] \xrightarrow{k \rightarrow 0} \frac{1}{r - a}. \quad (7.7.12)$$

Setting $r = 0$ [even though at $r = 0$, (7.7.10) is not the true wave function], we obtain

$$\lim_{k \rightarrow 0} k \cot \delta_0 \xrightarrow{k \rightarrow 0} -\frac{1}{a}. \quad (7.7.13)$$

The quantity a is known as the **scattering length**. The limit of the total cross section as $k \rightarrow 0$ is given by [see (7.6.16)]

$$\sigma_{\text{tot}} = \sigma_{l=0} = 4\pi \lim_{k \rightarrow 0} \left| \frac{1}{k \cot \delta_0 - ik} \right|^2 = 4\pi a^2. \quad (7.7.14)$$

Even though a has the same dimension as the range of the potential R , a and R can differ by orders of magnitude. In particular, for an attractive potential, it is possible for the magnitude of the scattering length to be far greater than the range of the potential. To see the physical meaning of a , we note that a is nothing more than the intercept of the outside-wave function. For a repulsive potential, $a > 0$ and is roughly of order of R , as seen in Figure 7.9a. However, for an attractive potential, the intercept is on the negative side (Figure 7.9b). If we *increase* the attraction, the outside-wave function can again cross the r -axis on the positive side (Figure 7.9c).

The sign change resulting from increased attraction is related to the development of a bound state. To see this point quantitatively, we note from Figure 7.9c that for a very large and positive, the wave function is essentially flat for $r > R$. But (7.7.10) with a very large is not too different from $e^{-\kappa r}$ with κ essentially zero. Now $e^{-\kappa r}$ with $\kappa \approx 0$ is just a bound-state-wave function for $r > R$ with energy E infinitesimally negative. The inside-wave function ($r < R$) for the $E = 0+$ case (scattering with zero kinetic energy) and the $E = 0-$ case (bound state with infinitesimally small binding energy) are essentially the same because in both cases k' in $\sin k'r$ [(7.7.6)] is determined by

$$\frac{\hbar^2 k'^2}{2m} = E - V_0 \approx |V_0| \quad (7.7.15)$$

with E infinitesimal (positive or negative).

Because the inside-wave functions are the same for the two physical situations ($E = 0+$ and $E = 0-$), we can equate the logarithmic derivative of the bound-state-wave function with that of the solution involving zero kinetic-energy scattering,

$$-\frac{\kappa e^{-\kappa r}}{e^{-\kappa r}} \Big|_{r=R} = \left(\frac{1}{r-a} \right) \Big|_{r=R}, \quad (7.7.16)$$

or, if $R \ll a$,

$$\kappa \approx \frac{1}{a}. \quad (7.7.17)$$

The binding energy satisfies

$$E_{\text{BE}} = -E_{\text{bound state}} = \frac{\hbar^2 \kappa^2}{2m} \approx \frac{\hbar^2}{2ma^2}, \quad (7.7.18)$$

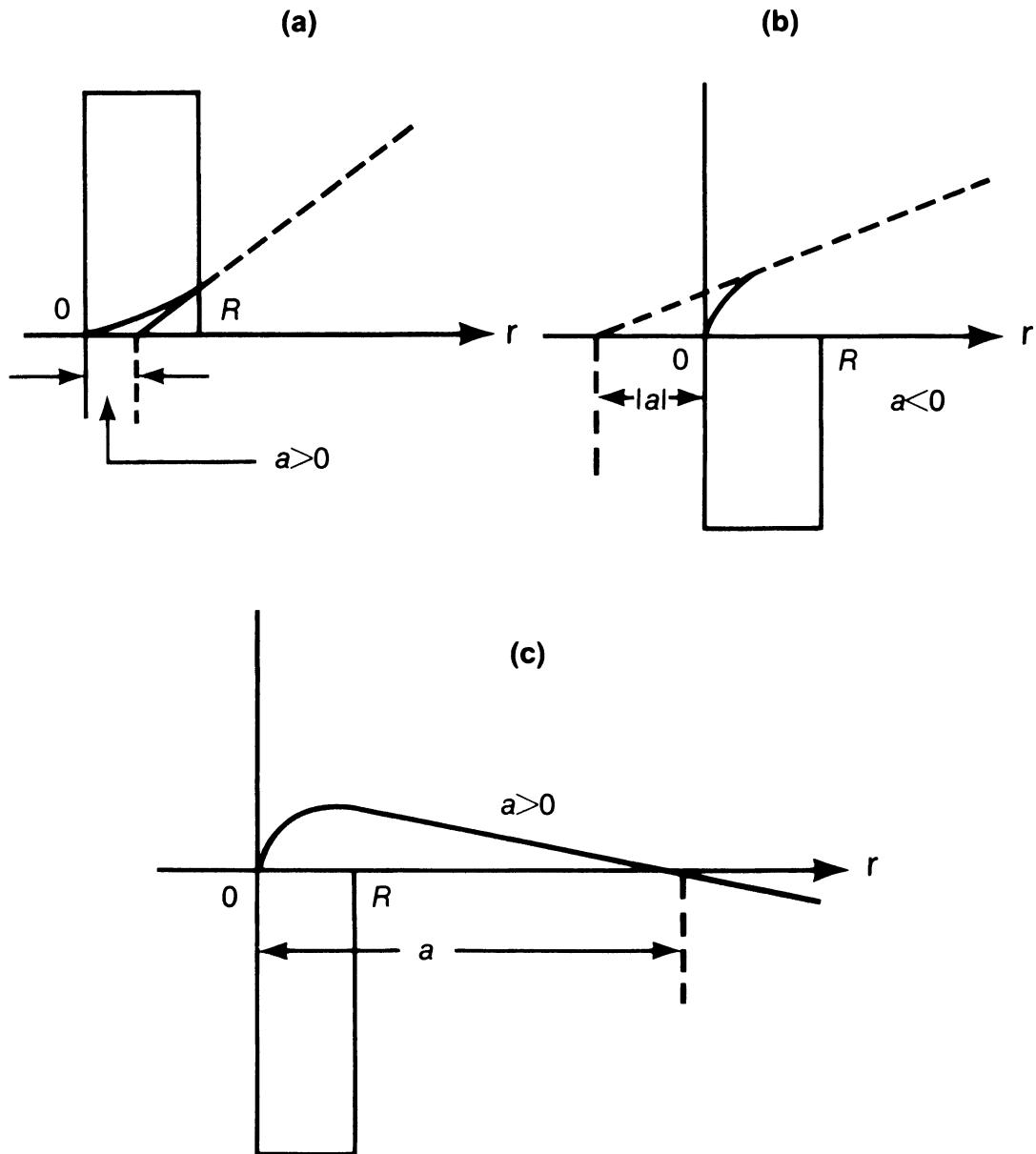


FIGURE 7.9. Plot of $u(r)$ versus r for (a) repulsive potential, (b) attractive potential, and (c) deeper attraction. The intercept a of the zero-energy outside-wave function with the r -axis is shown for each of three cases.

and we have a relation between scattering length and bound-state energy. This is a remarkable result. To wit, if there is a loosely bound state, we can infer its binding energy by performing scattering experiments near zero kinetic energy, provided a is measured to be large compared with the range R of the potential. This connection between the scattering length and the bound-state energy was first pointed out by Wigner, who attempted to apply (7.7.18) to np -scattering.

Experimentally, the 3S_1 -state of the np -system has a bound state, that is, the deuteron with

$$E_{\text{BE}} = 2.22 \text{ MeV}. \quad (7.7.19)$$

The scattering length is measured to be

$$a_{\text{triplet}} = 5.4 \times 10^{-13} \text{ cm}, \quad (7.7.20)$$

leading to the binding-energy prediction

$$\begin{aligned} \frac{\hbar^2}{2\mu a^2} &= \frac{\hbar^2}{m_N a^2} = m_N c^2 \left(\frac{\hbar}{m_N c a} \right)^2 \\ &= (938 \text{ MeV}) \left(\frac{2.1 \times 10^{-14} \text{ cm}}{5.4 \times 10^{-13} \text{ cm}} \right)^2 = 1.4 \text{ MeV} \end{aligned} \quad (7.7.21)$$

where μ is the reduced mass approximated by $m_{n,p}/2$. The agreement between (7.7.19) and (7.7.21) is not too satisfactory. The discrepancy is due to the fact that the inside-wave functions are not exactly the same and that $a_{\text{triplet}} \gg R$ is not really such a good approximation for the deuteron. A better result can be obtained by keeping the next term in the expansion of $k \cot \delta$ as a function of k ,

$$k \cot \delta_0 = -\frac{1}{a} + \frac{1}{2} r_0 k^2, \quad (7.7.22)$$

where r_0 is known as the effective range (see, for example, Preston 1962, 23).

Bound States as Poles of $S_l(k)$

We conclude this section by studying the analytic properties of the amplitude $S_l(k)$ for $l = 0$. Let us go back to (7.6.8) and (7.6.12), where the radial wave function for $l = 0$ at large distance was found to be proportional to

$$S_{l=0}(k) \frac{e^{ikr}}{r} - \frac{e^{-ikr}}{r}. \quad (7.7.23)$$

Compare this with the wave function for a bound state at large distance,

$$\frac{e^{-\kappa r}}{r}. \quad (7.7.24)$$

The existence of a bound state implies that a nontrivial solution to the Schrödinger equation with $E < 0$ exists only for a particular (discrete) value of κ . We may argue that $e^{-\kappa r}/r$ is like e^{ikr}/r , except that k is now purely imaginary. Apart from k being imaginary, the important difference between (7.7.23) and (7.7.24) is that in the bound-state case, $e^{-\kappa r}/r$ is present even without the analogue of the incident wave. Quite generally only the ratio of the coefficient of e^{ikr}/r to that of e^{-ikr}/r is of physical interest, and this is given by $S_l(k)$. In the bound-state case we can sustain the outgoing wave (with imaginary k) even without an incident wave. So the ratio is ∞ , which means that $S_{l=0}(k)$, regarded as a function of a complex variable k , has a

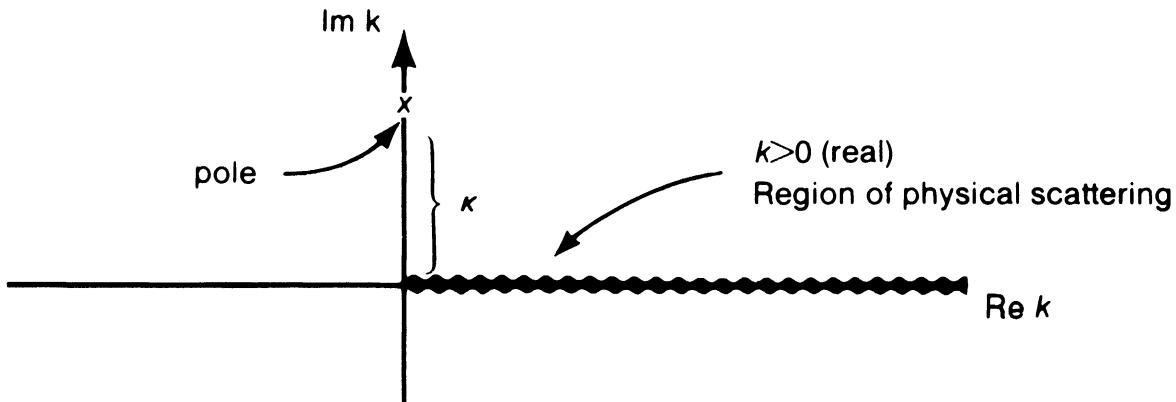


FIGURE 7.10. The complex k -plane with bound-state pole at $k = +i\kappa$.

pole at $k = i\kappa$. Thus a bound state implies a pole (which can be shown to be a simple pole) on the positive imaginary axis of the complex k -plane; see Figure 7.10. For k real and positive, we have the region of physical scattering. Here we must require [compare with (7.6.14)]

$$S_{l=0} = e^{2i\delta_0} \quad (7.7.25)$$

with δ_0 real. Furthermore, as $k \rightarrow 0$, $k \cot \delta_0$ has a limiting value $-1/a$ [(7.7.13)], which is finite, so δ_0 must behave as follows:

$$\delta_0 \rightarrow 0, \pm \pi, \dots. \quad (7.7.26)$$

Hence $S_{l=0} = e^{2i\delta_0} \rightarrow 1$ as $k \rightarrow 0$.

Now let us attempt to construct a simple function satisfying:

1. Pole at $k = i\kappa$ (existence of bound state).
2. $|S_{l=0}| = 1$ for $k > 0$ real (unitarity). (7.7.27)
3. $S_{l=0} = 1$ at $k = 0$ (threshold behavior).

The simplest function that satisfies all three conditions of (7.7.27) is

$$S_{l=0}(k) = \frac{-k - i\kappa}{k - i\kappa}. \quad (7.7.28)$$

[Editor's Note: Equation (7.7.28) is chosen for simplicity rather than as a physically realistic example. For reasonable potentials (not hard spheres!) the phase shift vanishes as $k \rightarrow \infty$.]

An assumption implicit in choosing this form is that there is no other singularity that is important apart from the bound-state pole. We can then use (7.6.15) to obtain, for $f_{l=0}(k)$,

$$f_{l=0} = \frac{S_{l=0} - 1}{2ik} = \frac{1}{-\kappa - ik}. \quad (7.7.29)$$

Comparing this with (7.6.16),

$$f_{l=0} = \frac{1}{k \cot \delta_0 - ik}, \quad (7.7.30)$$

we see that

$$\lim_{k \rightarrow 0} k \cot \delta_0 = -\frac{1}{a} = -\kappa, \quad (7.7.31)$$

precisely the relation between bound state and scattering length [(7.7.17)].

It thus appears that by exploiting unitarity and analyticity of $S_l(k)$ in the k -plane, we may obtain the kind of information that can be secured by solving the Schrödinger equation explicitly. This kind of technique can be very useful in problems where the details of the potential are not known.

7.8. RESONANCE SCATTERING

In atomic, nuclear, and particle physics, we often encounter a situation where the scattering cross section for a given partial wave exhibits a pronounced peak. This section is concerned with the dynamics of such a **resonance**.

We continue to consider a finite-ranged potential $V(r)$. The *effective* potential appropriate for the radial wave function of the l th partial wave is $V(r) + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}$ plus the centrifugal barrier term as given by (7.7.1). Suppose $V(r)$ itself is attractive. Because the second term,

$$\frac{\hbar^2}{2m} \frac{l(l+1)}{r^2}$$

is repulsive, we have a situation where the effective potential has an attractive well followed by a repulsive barrier at larger distances, as shown in Figure 7.11.

Suppose the barrier were infinitely high. It would then be possible for particles to be trapped inside, which is another way of saying that we expect bound states, with energy $E > 0$. They are *genuine* bound states in the sense that they are eigenstates of the Hamiltonian with definite values of E . In other words, they are *stationary* states with infinite lifetime.

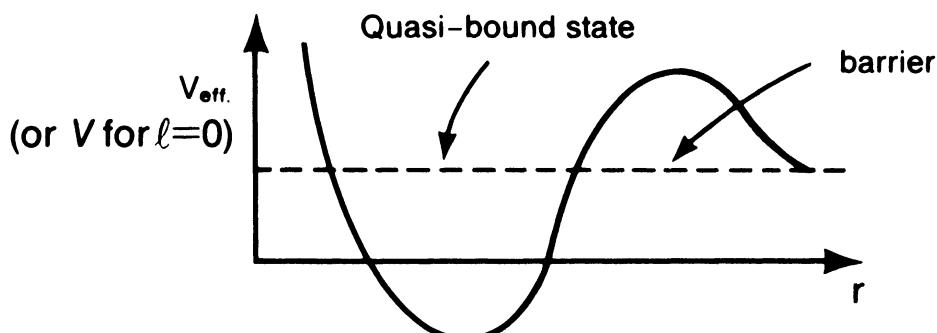


FIGURE 7.11. $V_{\text{eff}} = V(r) + (\hbar^2/2m)[l(l+1)/r^2]$ versus r . For $l \neq 0$ the barrier can be due to $(\hbar^2/2m)[l(l+1)/r^2]$; for $l = 0$ barrier must be due to V itself.

In the more realistic case of a finite barrier, the particle can be trapped inside, but it cannot be trapped forever. Such a trapped state has a finite lifetime due to quantum-mechanical tunneling. In other words, a particle leaks through the barrier to the outside region. Let us call such a state **quasi-bound state** because it would be an honest bound state if the barrier were infinitely high.

The corresponding scattering phase shift δ_l rises through the value $\pi/2$ as the incident energy rises through that of the quasi-bound state, and at the same time the corresponding partial-wave cross section passes through its maximum possible value $4\pi(2l + 1)/k^2$. [Editor's Note: Such a sharp rise in the phase shift is, in the time-dependent Schrödinger equation, associated with a delay of the emergence of the trapped particles, rather than an unphysical advance, as would be the case for a sharp decrease through $\pi/2$.]

It is instructive to verify this point with explicit calculations for some known potential. The result of a numerical calculation shows that a resonance behavior is in fact possible for $l \neq 0$ with a spherical-well potential.

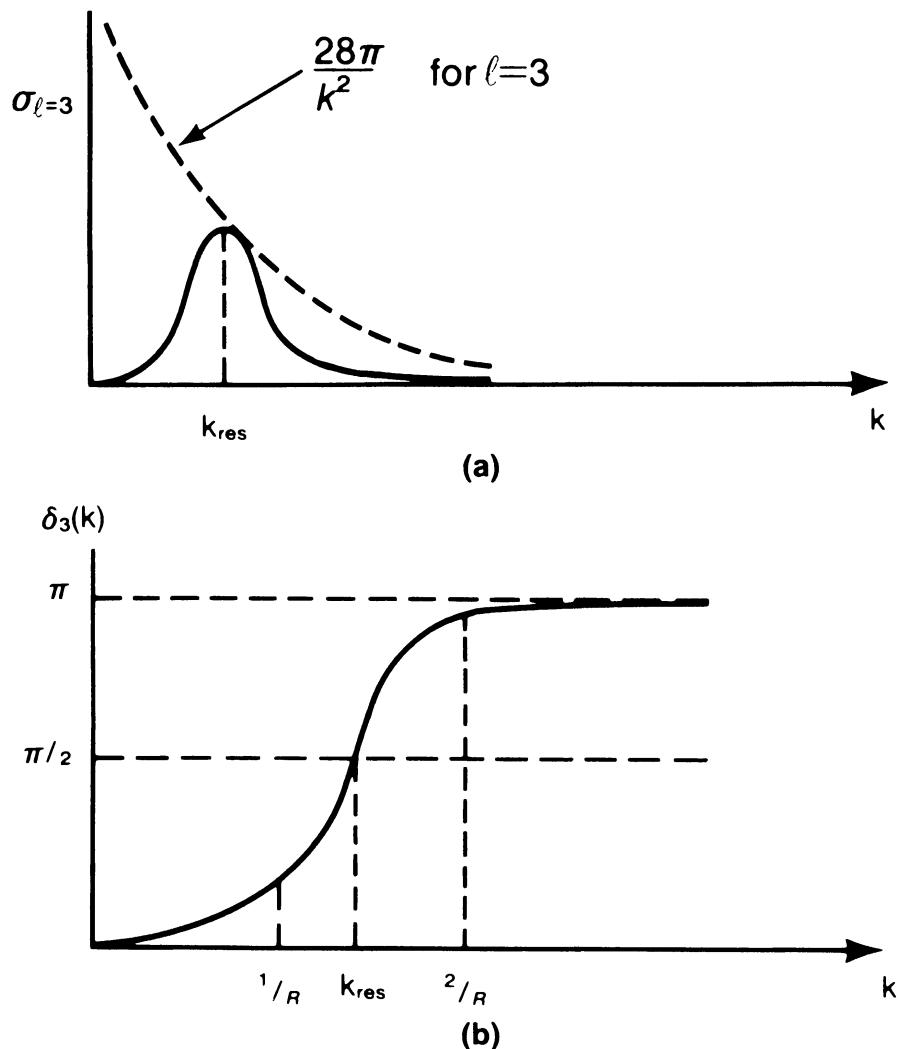


FIGURE 7.12. Plots of (a) $\sigma_{l=3}$ versus k , where at resonance $\delta_3(k_{\text{res}}) = \pi/2$ and $\sigma_{l=3} = (4\pi/k_{\text{res}}^2) \times 7 = 28\pi/k_{\text{res}}^2$ and (b) $\delta_3(k)$ versus k . The curves are for a spherical well with $2mV_0R^2/\hbar^2 = 5.5$.

To be specific we show the results for a spherical well with $2mV_0R^2/\hbar^2 = 5.5$ and $l = 3$ in Figure 7.12. The phase shift (Figure 7.12b), which is small at extremely low energies, starts increasing rapidly past $k = 1/R$, and goes through $\pi/2$ around $k = 1.3/R$.

Another very instructive example is provided by a repulsive δ -shell potential that is exactly soluble (see Problem 9 in this chapter):

$$\frac{2m}{\hbar^2} V(r) = \gamma \delta(r - R). \quad (7.8.1)$$

Here resonances are possible for $l = 0$ because the δ -shell potential itself can trap the particle in the region $0 < r < R$. For the case $\gamma = \infty$, we expect a series of bound states in the region $r < R$ with

$$kR = \pi, 2\pi, \dots; \quad (7.8.2)$$

this is because the radial wave function for $l = 0$ must vanish not only at $r = 0$ but also at $r = R$ – in this case. For the region $r > R$, we simply have hard-sphere scattering with the S -wave phase shift, given by

$$\delta_0 = -kR. \quad (7.8.3)$$

With $\gamma = \infty$, there is no connection between the two problems because the wall at $r = R$ cannot be penetrated.

The situation is more interesting with a finite barrier, as we can show explicitly. The scattering phase shift exhibits a resonance behavior whenever

$$E_{\text{incident}} \approx E_{\text{quasi-bound state}}. \quad (7.8.4)$$

Moreover, the larger the γ , the sharper the resonance peak. However, away from the resonance δ_0 looks very much like the hard-sphere phase shift. Thus we have a situation in which a resonance behavior is superimposed on a smoothly behaving background scattering. This serves as a model for neutron-nucleus scattering, where a series of sharp resonance peaks are observed on top of a smoothly varying cross section.

Coming back to our general discussion of resonance scattering, we ask how the scattering amplitudes vary in the vicinity of the resonance energy. If we are to have any connection between σ_l being large and the quasi-bound states, δ_l must go through $\pi/2$ (or $3\pi/2, \dots$) from below, as discussed above. In other words $\cot \delta_l$ must go through zero from above. Assuming that $\cot \delta_l$ is smoothly varying near the vicinity of resonance, that is,

$$E \approx E_r, \quad (7.8.5)$$

we may attempt to expand $\cot \delta_l$ as follows:

$$\cot \delta_l = \underbrace{\cot \delta_l|_{E=E_r}}_0 - c(E - E_r) + 0[(E - E_r)^2]. \quad (7.8.6)$$

This leads to

$$\begin{aligned} f_l(k) &= \frac{1}{k \cot \delta_l - ik} = \frac{1}{k} \frac{1}{[-c(E - E_r) - i]} \\ &= -\frac{\Gamma/2}{k \left[(E - E_r) + \frac{i\Gamma}{2} \right]}, \end{aligned} \quad (7.8.7)$$

where we have defined the *width* Γ by

$$\frac{d(\cot \delta_l)}{dE} \Big|_{E=E_r} = -c \equiv -\frac{2}{\Gamma} \quad (7.8.8)$$

Notice that Γ is very small if $\cot \delta_l$ varies rapidly. If a simple resonance dominates the l th partial-wave cross section, we obtain a one-level resonance formula (the Breit-Wigner formula):

$$\sigma_l = \frac{4\pi}{k^2} \frac{(2l+1)(\Gamma/2)^2}{(E - E_r)^2 + \Gamma^2/4}. \quad (7.8.9)$$

So it is legitimate to regard Γ as the full width at half-maximum, provided the resonance is reasonably narrow so that variation in $1/k^2$ can be ignored.

7.9. IDENTICAL PARTICLES AND SCATTERING

As an example to illustrate the phase of the scattering amplitude, let us consider the scattering of two identical spinless charged particles via the Coulomb potential (which we discuss further in Section 7.13). The space-wave function must now be symmetric, so the asymptotic wave function must look like

$$e^{i\mathbf{k} \cdot \mathbf{x}} + e^{-i\mathbf{k} \cdot \mathbf{x}} + [f(\theta) + f(\pi - \theta)] \frac{e^{ikr}}{r}, \quad (7.9.1)$$

where $\mathbf{x} = \mathbf{x}_1 - \mathbf{x}_2$ is the relative position vector between the two particles 1 and 2. This results in a differential cross section,

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= |f(\theta) + f(\pi - \theta)|^2 \\ &= |f(\theta)|^2 + |f(\pi - \theta)|^2 + 2 \operatorname{Re}[f(\theta)f^*(\pi - \theta)]. \end{aligned} \quad (7.9.2)$$

The cross section is enhanced through constructive interference at $\theta \approx \pi/2$.

In contrast, for spin $\frac{1}{2}$ – spin $\frac{1}{2}$ scattering with unpolarized beam and V independent of spin, we have the spin-singlet scattering going with space-symmetrical function and the spin triplet going with space-antisymmetrical wave function (see Section 6.3). If the initial beam is unpolarized,

we have the statistical contribution $\frac{1}{4}$ for spin singlet and $\frac{3}{4}$ for spin triplet; hence

$$\begin{aligned}\frac{d\sigma}{d\Omega} &= \frac{1}{4}|f(\theta) + f(\pi - \theta)|^2 + \frac{3}{4}|f(\theta) - f(\pi - \theta)|^2 \\ &= |f(\theta)|^2 + |f(\pi - \theta)|^2 - \text{Re}[f(\theta)f^*(\pi - \theta)].\end{aligned}\quad (7.9.3)$$

In other words, we expect destructive interference at $\theta \approx \pi/2$. This has, in fact, been observed.

7.10. SYMMETRY CONSIDERATIONS IN SCATTERING

Suppose V and H_0 are both invariant under some symmetry operation. We may ask what this implies for the matrix element of T or for the scattering amplitude $f(\mathbf{k}', \mathbf{k})$.

If the symmetry operator is unitary (for example, rotation and parity), everything is quite straightforward. Using the explicit form of T as given by (7.2.20), we see that

$$UH_0U^\dagger = H_0, \quad UVU^\dagger = V \quad (7.10.1)$$

implies that T is also invariant under U —that is,

$$UTU^\dagger = T. \quad (7.10.2)$$

We define

$$|\tilde{\mathbf{k}}\rangle \equiv U|\mathbf{k}\rangle, \quad |\tilde{\mathbf{k}}'\rangle \equiv U|\mathbf{k}'\rangle. \quad (7.10.3)$$

Then

$$\begin{aligned}\langle \tilde{\mathbf{k}}' | T | \tilde{\mathbf{k}} \rangle &= \langle \mathbf{k}' | U^\dagger U T U U^\dagger U | \mathbf{k} \rangle \\ &= \langle \mathbf{k}' | T | \mathbf{k} \rangle.\end{aligned}\quad (7.10.4)$$

As an example, we consider the specific case where U stands for the parity operator

$$\pi|\mathbf{k}\rangle = |-\mathbf{k}\rangle, \quad \pi|-\mathbf{k}\rangle = |\mathbf{k}\rangle. \quad (7.10.5)$$

Thus invariance of H_0 and V under parity would mean

$$\langle -\mathbf{k}' | T | -\mathbf{k} \rangle = \langle \mathbf{k}' | T | \mathbf{k} \rangle. \quad (7.10.6)$$

Pictorially, we have the situation illustrated in Figure 7.13a.

We exploited the consequence of angular-momentum conservation when we developed the method of partial waves. The fact that T is diagonal in the $|Elm\rangle$ representation is a direct consequence of T being invariant under rotation. Notice also that $\langle \mathbf{k}' | T | \mathbf{k} \rangle$ depends only on the relative orientation of \mathbf{k} and \mathbf{k}' , as depicted in Figure 7.13b.

When the symmetry operation is antiunitary (as in time reversal), we must be more careful. First, we note that the requirement that V as well as

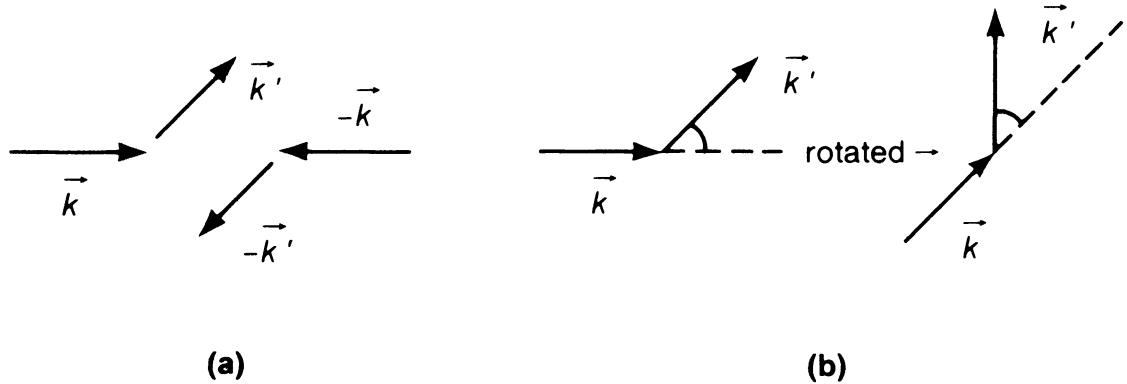


FIGURE 7.13. (a) Equality of T matrix elements between $\mathbf{k} \rightarrow \mathbf{k}'$ and $-\mathbf{k} \rightarrow -\mathbf{k}'$. (b) Equality of T matrix elements under rotation.

H_0 be invariant under time reversal invariance requires that

$$\Theta T \Theta^{-1} = T^\dagger. \quad (7.10.7)$$

This is because the antiunitary operator changes

$$\frac{1}{E - H_0 + i\epsilon} \text{ into } \frac{1}{E - H_0 - i\epsilon} \quad (7.10.8)$$

in (7.2.20). We also recall that for an antiunitary operator [see (4.4.11)],

$$\langle \beta | \alpha \rangle = \langle \tilde{\alpha} | \tilde{\beta} \rangle, \quad (7.10.9)$$

where

$$|\tilde{\alpha}\rangle \equiv \Theta |\alpha\rangle \quad \text{and} \quad |\tilde{\beta}\rangle \equiv \Theta |\beta\rangle. \quad (7.10.10)$$

Let us consider

$$|\alpha\rangle = T|\mathbf{k}\rangle, \quad \langle \beta| = \langle \mathbf{k}'|; \quad (7.10.11)$$

then

$$\begin{aligned} |\tilde{\alpha}\rangle &= \Theta T |\mathbf{k}\rangle = \Theta T \Theta^{-1} \Theta |\mathbf{k}\rangle = T^\dagger |-\mathbf{k}\rangle \\ |\tilde{\beta}\rangle &= \Theta |\mathbf{k}'\rangle = |-\mathbf{k}'\rangle. \end{aligned} \quad (7.10.12)$$

As a result (7.10.9) becomes

$$\langle \mathbf{k}' | T | \mathbf{k} \rangle = \langle -\mathbf{k} | T | -\mathbf{k}' \rangle. \quad (7.10.13)$$

Notice that the initial and final momenta are interchanged, in addition to the fact that the directions of the momenta have been reversed.

It is also interesting to combine the requirements of time reversal [(7.10.13)] and parity [(7.10.6)]:

$$\langle \mathbf{k}' | T | \mathbf{k} \rangle \stackrel{\text{under } \Theta}{=} \langle -\mathbf{k} | T | -\mathbf{k}' \rangle \stackrel{\text{under } \pi}{=} \langle \mathbf{k} | T | \mathbf{k}' \rangle; \quad (7.10.14)$$

that is, from (7.2.19) and (7.2.22) we have

$$f(\mathbf{k}, \mathbf{k}') = f(\mathbf{k}', \mathbf{k}), \quad (7.10.15)$$

which results in

$$\frac{d\sigma}{d\Omega}(\mathbf{k} \rightarrow \mathbf{k}') = \frac{d\sigma}{d\Omega}(\mathbf{k}' \rightarrow \mathbf{k}). \quad (7.10.16)$$

Equation (7.10.16) is known as **detailed balance**.

It is more interesting to look at the analogue of (7.10.14) when we have spin. Here we may characterize the initial free-particle ket by $|\mathbf{k}, m_s\rangle$, and we exploit (4.4.79) for the time-reversal portion:

$$\begin{aligned} \langle \mathbf{k}', m'_s | T | \mathbf{k}, m_s \rangle &= i^{-2m_s + 2m'_{s'}} \langle -\mathbf{k}, -m_s | T | -\mathbf{k}', -m'_{s'} \rangle \\ &= i^{-2m_s + 2m'_{s'}} \langle \mathbf{k}, -m_s | T | \mathbf{k}', -m'_{s'} \rangle. \end{aligned} \quad (7.10.17)$$

For unpolarized initial states, we sum over the initial spin states and divide by $(2s+1)$; if the final polarization is not observed, we must sum over final states. We then obtain detailed balance in the form

$$\overline{\frac{d\sigma}{d\Omega}}(\mathbf{k} \rightarrow \mathbf{k}') = \overline{\frac{d\sigma}{d\Omega}}(\mathbf{k}' \rightarrow \mathbf{k}), \quad (7.10.18)$$

where we understand the bar on the top of $d\sigma/d\Omega$ in (7.10.18) to mean that we average over the initial spin states and sum over the final spin states.

7.11. TIME-DEPENDENT FORMULATION OF SCATTERING

Our discussion of scattering so far has been based on the time-independent formulation. It is also possible to develop a formalism of scattering based on the time-dependent Schrödinger equation. We show that this formalism leads to the same Lippmann-Schwinger equation, (7.1.6).

In the time-dependent formulation we conceive of a scattering process as a change in the state ket from a free-particle ket to a state ket influenced by the presence of the potential V . The basic equation of motion is

$$\left(i\hbar \frac{\partial}{\partial t} - H_0 \right) |\psi; t\rangle = V |\psi; t\rangle, \quad (7.11.1)$$

where $|\psi; t\rangle$ is the time-dependent Schrödinger ket in the presence of V . The boundary condition appropriate for the scattering problem is that in the remote past ($t \rightarrow -\infty$), the particle was free. This requirement is automatically accomplished if we turn on the potential adiabatically—that is, very slowly—as in Section 5.8:

$$V \rightarrow \lim_{\eta \rightarrow 0} V e^{\eta t}. \quad (7.11.2)$$

Just as the partial differential equation with an inhomogeneous term is solved by introducing a Green's function [see (7.1.18)], the operator

Schrödinger equation (7.11.1) is solved by introducing the Green's operator $G_+(t, t')$ satisfying

$$\left(i\hbar \frac{\partial}{\partial t} - H_0 \right) G_+(t, t') = \delta(t - t'). \quad (7.11.3)$$

The *causality* requirement we impose on G_+ is that the interaction of a particle at t' has an effect only for $t > t'$. We therefore impose the *retarded* boundary condition

$$G_+(t, t') = 0 \quad \text{for } t < t'. \quad (7.11.4)$$

We claim that the solution to (7.11.3) and (7.11.4) is

$$G_+(t, t') = -\frac{i}{\hbar} \theta(t - t') e^{-iH_0(t-t')/\hbar}. \quad (7.11.5)$$

For $t > t'$, a constant times $e^{-iH_0(t-t')/\hbar}$ clearly satisfies the differential equation (7.11.3) because the δ -function on the right-hand side is inoperative. For $t < t'$, we obviously have the desired condition (7.11.4) because $G_+(t, t')$ here is identically zero. At $t = t'$, we note that there is an extra contribution due to the discontinuity of the θ -function that just balances the right-hand side of (7.11.3):

$$i\hbar \frac{\partial}{\partial t} \left[-\frac{i}{\hbar} \theta(t - t') \right] = \delta(t - t'). \quad (7.11.6)$$

The solution to the full problem can now be written as follows:

$$|\psi^{(+)}; t\rangle = |\phi; t\rangle + \int_{-\infty}^{+\infty} G_+(t, t') V |\psi^{(+)}; t'\rangle dt', \quad (7.11.7)$$

where

$$\left(i\hbar \frac{\partial}{\partial t} - H_0 \right) |\phi; t\rangle = 0 \quad (7.11.8)$$

and the upper limit of the integration in (7.11.7) may as well be t because G_+ vanishes for $t' > t$. As $t \rightarrow -\infty$, $|\psi^{(+)}; t\rangle$ coincides with $|\phi; t\rangle$ just as required; this is because $G_+(t, t')$ vanishes as $t \rightarrow -\infty$ for any finite value of t' . To see that (7.11.7) satisfies the t -dependent Schrödinger equation (7.11.1), we merely apply the operator $[i\hbar(\partial/\partial t) - H_0]$ to $|\psi^{(+)}; t\rangle$. The $|\phi; t\rangle$ ket makes no contribution; as for its effect on the second term, $[i\hbar(\partial/\partial t) - H_0]$ acting on G_+ just gives $\delta(t - t')$, by means of which the integration is immediately evaluated to be $V|\psi^{(+)}; t\rangle$.

So far we have not even required $|\psi^{(+)}; t\rangle$ to be an energy eigenket. If it is, we can separate the time dependence as usual:

$$\begin{aligned} |\phi; t\rangle &= |\phi\rangle e^{-iEt/\hbar} \\ |\psi; t\rangle &= |\psi\rangle e^{-iEt/\hbar}. \end{aligned} \quad (7.11.9)$$

Here there is the implicit assumption that E does not change if V is

switched on adiabatically according to (7.11.2). Equations (7.11.5) and (7.11.7), evaluated at $t = 0$, now yield

$$|\psi^{(+)}\rangle = |\phi\rangle - \frac{i}{\hbar} \int_{-\infty}^0 dt' e^{iH_0 t'/\hbar} e^{-iEt'/\hbar} V |\psi^{(+)}\rangle. \quad (7.11.10)$$

The integral may appear to oscillate indefinitely. However, we recall that V is really to be understood as $Ve^{\eta t}$. As a result, the time integration is straightforward:

$$\begin{aligned} |\psi^{(+)}\rangle &= |\phi\rangle - \frac{i}{\hbar} \lim_{t'' \rightarrow -\infty} \int_{t''}^0 dt' e^{i(H_0 - E - i\eta\hbar)t'/\hbar} V |\psi^{(+)}\rangle \\ &= |\phi\rangle - \frac{1}{H_0 - E - i\eta\hbar} \left[1 - \lim_{t'' \rightarrow -\infty} e^{[i(H_0 - E)/\hbar + \eta]t''} \right] V |\psi^{(+)}\rangle. \end{aligned} \quad (7.11.11)$$

But as $t'' \rightarrow -\infty$, this is just the Lippmann-Schwinger equation (7.1.6).

The reader should note carefully how the $i\varepsilon$ prescription appears in the two formalisms. Earlier, using the time-independent formalism we saw that the choice of positive sign of the $i\varepsilon$ -term (see Section 7.1) corresponds to the statement that the scatterer affects only outgoing spherical waves. In the t -dependent formulation presented here, the presence of $i\varepsilon$ ($\varepsilon = \eta\hbar$) in (7.11.11) arises from the requirement that the particle was free in the remote past.

One may argue that the slow switch-on of the potential (7.11.2) on which we have relied is somewhat artificial. But let us suppose that we are using a wave-packet formalism to describe scattering. When the wave packet is well outside the range of the potential, it does not matter whether the potential is zero or finite. In particular, V may be zero in the remote past, which then leads to no difficulty.

Connection With Time-Dependent Perturbation Theory

Inasmuch as scattering can be discussed using the time-dependent formulation, which is based on the time-dependent Schrödinger equation (7.11.1), we should be able to apply an approximation scheme based on (7.11.1). In particular we should be able to deploy the methods of time-dependent perturbation theory developed earlier in Section 5.6 to the scattering problem—provided, of course, the potential can be regarded as weak in some sense.

First we will show how the golden rule can be applied to compute $d\sigma/d\Omega$, leading to the results of the Born approximation of Section 7.2.

We assume in the remote past that the state ket is represented by a momentum eigenket $|\mathbf{k}\rangle$. When the interaction is slowly switched on, as in (7.11.2), momentum eigenkets other than $|\mathbf{k}\rangle$ —for example, $|\mathbf{k}'\rangle$ —are

populated. As we have seen (see Section 5.6), the transition probability is (to first order) evaluated in the following manner. First we write

$$\langle \mathbf{k}' | U_I^{(1)}(t, -\infty) | \mathbf{k} \rangle = -\frac{i}{\hbar} \int_{-\infty}^t \langle \mathbf{k}' | V_I(t') | \mathbf{k} \rangle dt', \quad (7.11.12)$$

where $V_I(t') = e^{iH_0 t' / \hbar} V e^{-iH_0 t' / \hbar} e^{\eta t'}$ and $E_{\mathbf{k}} = \hbar^2 k^2 / 2m$. The transition probability of finding $|\mathbf{k}'\rangle$ at time t is then

$$|\langle \mathbf{k}' | U_I^{(1)}(t, -\infty) | \mathbf{k} \rangle|^2 = \frac{|\langle \mathbf{k}' | V | \mathbf{k} \rangle|^2}{\hbar^2} \frac{e^{2\eta t}}{\left[(E_{\mathbf{k}} - E_{\mathbf{k}'})^2 / \hbar^2 + \eta^2 \right]}. \quad (7.11.13)$$

As $\eta \rightarrow 0$ (t finite), the transition rate is just what we expect from the golden rule:

$$\frac{d}{dt} |\langle \mathbf{k}' | U_I^{(1)}(t, -\infty) | \mathbf{k} \rangle|^2 = \frac{2\pi}{\hbar} |\langle \mathbf{k}' | V | \mathbf{k} \rangle|^2 \delta(E_k - E_{k'}), \quad (7.11.14)$$

where we have used (5.8.5). Note that the right-hand side of (7.11.14) is independent of t .

It is important here to review the normalization conventions used for plane-wave states. In Section 1.7 we used the δ -function normalization

$$\langle \mathbf{k}' | \mathbf{k} \rangle = \delta^{(3)}(\mathbf{k} - \mathbf{k}'). \quad (7.11.15)$$

The completeness relation is then written as

$$1 = \int d^3k | \mathbf{k} \rangle \langle \mathbf{k} |. \quad (7.11.16)$$

In applying t -dependent perturbation theory to scattering processes, it is more helpful to use box normalization,

$$\langle \mathbf{k}' | \mathbf{k} \rangle = \delta_{\mathbf{k}', \mathbf{k}}, \quad (7.11.17)$$

where the allowed values for \mathbf{k} are given by

$$k_{x, y, z} = \frac{2\pi n_{x, y, z}}{L}. \quad (7.11.18)$$

The wave function is given by

$$\langle \mathbf{x} | \mathbf{k} \rangle = \frac{1}{L^{3/2}} e^{i\mathbf{k} \cdot \mathbf{x}} \quad (7.11.19)$$

instead of $[1/(2\pi)^{3/2}] e^{i\mathbf{k} \cdot \mathbf{x}}$. The completeness relation is

$$1 = \sum_{\mathbf{k}} | \mathbf{k} \rangle \langle \mathbf{k} |, \quad (7.11.20)$$

but for a very large box we might as well treat the variables $k_{x, y, z}$ as

continuous, so

$$1 = \left(\frac{L}{2\pi} \right)^3 \int d^3k |\mathbf{k}\rangle \langle \mathbf{k}|. \quad (7.11.21)$$

This looks like (7.11.16) except for the presence of $(L/2\pi)^3$. A very useful relation that enables us to go from the δ -function normalization convention to that of box normalization is

$$(2\pi)^3 \langle \mathbf{k}' | V | \mathbf{k} \rangle_{\substack{\delta-fn \\ \text{normalization}}} = L^3 \langle \mathbf{k}' | V | \mathbf{k} \rangle_{\substack{\text{box} \\ \text{normalization}}} \quad (7.11.22)$$

as the reader may easily verify by inserting a complete set of states in the position representation.

The box normalization is very convenient for evaluating the density of states. For this reason it is used more often in a treatment of scattering based on time-dependent perturbation theory. Thus if we are interested in scattering into the solid angle $d\Omega$, the relevant formula is

$$n^2 dn d\Omega = \left(\frac{L}{2\pi} \right)^3 \frac{km}{\hbar^2} dE d\Omega \quad (7.11.23)$$

[see (5.7.31)].

Coming back to scattering, which we view as a transition rate w from $|\mathbf{k}\rangle$ into a group of states $|\mathbf{k}'\rangle$ subtending the solid-angle element $d\Omega$, we have w given by (for elastic scattering $k' = k$)

$$w = \frac{2\pi}{\hbar} |\langle \mathbf{k}' | V | \mathbf{k} \rangle|^2 \left(\frac{L}{2\pi} \right)^3 \frac{km}{\hbar^2} d\Omega \quad (7.11.24)$$

from the golden rule (5.6.34) and (7.11.14). This must be equated to

$$(\text{Incident flux}) \times \frac{d\sigma}{d\Omega} d\Omega. \quad (7.11.25)$$

As for the incident flux, we obtain [from $\mathbf{j} = (\hbar/m)\text{Im}(\psi^* \nabla \psi)$]

$$|\mathbf{j}| = \frac{\hbar}{m} \left| \text{Im} \left(\frac{e^{-i\mathbf{k} \cdot \mathbf{x}}}{L^{3/2}} \nabla \frac{e^{i\mathbf{k} \cdot \mathbf{x}}}{L^{3/2}} \right) \right| = \frac{\hbar k}{m L^3}. \quad (7.11.26)$$

Alternatively, incident flux = velocity/volume = $\hbar k / mL^3$. Putting everything together

$$\begin{aligned} \frac{d\sigma}{d\Omega} &= \left(\frac{mL^3}{\hbar k} \right) \left(\frac{2\pi}{\hbar} \right) \left(\frac{L}{2\pi} \right)^3 \left(\frac{km}{\hbar^2} \right) \left| \frac{1}{L^3} \int d^3x V(\mathbf{x}) e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{x}} \right|^2 \\ &= \left| \frac{1}{4\pi} \frac{2m}{\hbar^2} \int d^3x V(\mathbf{x}) e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{x}} \right|^2. \end{aligned} \quad (7.11.27)$$

But this is precisely the result of the first-order Born approximation [(7.2.22)]. Higher-order Born terms can be obtained in a similar manner.

To sum up, the time-dependent formulation based on the time-dependent Schrödinger equation [(7.11.1)] enables us to derive easily the results we obtained earlier using the time-independent formalism—the Lippmann-Schwinger equation, the Born approximation, and so on. Furthermore, it turns out that the time-dependent formalism is more suitable for discussing more-general reaction processes other than elastic scattering. As a concrete example to illustrate this point, we now turn to a discussion of the inelastic scattering of electrons by atoms.

7.12. INELASTIC ELECTRON-ATOM SCATTERING

Let us consider the interactions of electron beams with atoms assumed to be in their ground states. The incident electron may get scattered elastically with final atoms unexcited:

$$e^- + \text{atom (ground state)} \rightarrow e^- + \text{atom (ground state)}. \quad (7.12.1)$$

This is an example of *elastic scattering*. To the extent that the atom can be regarded as infinitely heavy, the kinetic energy of the electron does not change. It is also possible for the target atom to get excited:

$$e^- + \text{atom (ground state)} \rightarrow e^- + \text{atom (excited state)}. \quad (7.12.2)$$

In this case we talk about **inelastic scattering** because the kinetic energy of the final outgoing electron is now less than that of the initial incoming electron, the difference being used to excite the target atom.

The initial ket of the electron plus the atomic system is written as

$$|\mathbf{k}, 0\rangle \quad (7.12.3)$$

where \mathbf{k} refers to the wave vector of the incident electron and 0 stands for the atomic ground state. Strictly speaking (7.12.3) should be understood as the direct product of the incident electron ket $|\mathbf{k}\rangle$ and the ground-state atomic ket $|0\rangle$. The corresponding wave function is

$$\frac{1}{L^{3/2}} e^{i\mathbf{k} \cdot \mathbf{x}} \psi_0(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_z) \quad (7.12.4)$$

where we use the box normalization for the plane wave.

We may be interested in a final-state electron with a definite wave vector \mathbf{k}' . The final-state ket and the corresponding wave function are

$$|\mathbf{k}', n\rangle \quad \text{and} \quad \frac{1}{L^{3/2}} e^{i\mathbf{k}' \cdot \mathbf{x}} \psi_n(\mathbf{x}_1, \dots, \mathbf{x}_z), \quad (7.12.5)$$

where $n = 0$ for elastic scattering and $n \neq 0$ for inelastic scattering.

Assuming that time-dependent perturbation theory is applicable, we can immediately write the differential cross section, as in the previous