Scattering and Resonances

Most of our knowledge of nuclei and of "elementary" particles and of the forces acting at the nuclear and subnuclear level comes from scattering experiments. In these experiments, a beam of particles is used to bombard a target, and the deflections of the incident particles upon collisions with the target particles are measured. If the energy of the incident particles is sufficiently large, the scattering process can become very complicated, with the creation of new particles in violent reactions.

In this chapter, we will discuss only the simple case of elastic scattering of a particle by a potential. This potential may be thought of as the potential exerted by the target particle on the incident particle; the coordinate x or r that we will use for the incident particle should therefore be thought of as a relative coordinate giving the distance between the particles. The recoil motion of the target particle can be taken into account by introducing the coordinates of the center of mass, as in Section 8.2; but we will not deal with this detail here.

We will first discuss scattering in one dimension. This frees us from the complications imposed by angular momentum, and permits us to bring many of the fundamental concepts into sharper focus.

Throughout this chapter, we will adopt the position representation, since this is the most convenient for scattering problems with potentials defined as functions of position.

11.1 Elastic Scattering in One Dimension

Consider a particle moving in one dimension in a potential that is different from zero only in some finite range. The particle is incident from a large distance, interacts with the potential, and then

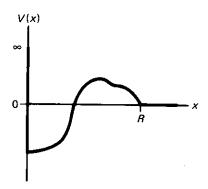


Fig. 11.1 A typical potential in one dimension. The range R of the potential is finite.

again moves out to a large distance. A typical potential is the following (see Fig. 11.1):

$$V = \begin{cases} V(x) & \text{for } 0 < x < R \\ 0 & \text{for } x < R \\ \infty & \text{for } x < 0 \end{cases}$$
 (1)

The quantity R is called the *range* of the potential.¹

It might seem strange to use a potential that restricts the motion of the particle to positive values of x. But this case of exceptional importance, because the effective potential for the radial motion of a particle moving in three dimensions often has the form given by Eq. (1). If the potential in three dimensions is a function of r only (a central potential), then we can separate the radial motion from the angular motion by assuming that the incident particle is in an eigenstate of angular momentum. The Schrödinger equation for three dimensions then reduces to a Schrödinger equation for one dimension, with r as the one-dimensional coordinate [we saw examples of this reduction of the Schrödinger equation in Eqs. (8.6) and (8.37)]. The radial motion of the particle then reduces to one-dimensional motion with a potential which may be taken as infinite at r = 0. Note that although the case of the Coulomb potential fits the pattern given in Eq. (1), the range of

 $^{^1}$ For potentials that tend to zero sufficiently quickly as r increases—such as potentials proportional to an exponentially decreasing function—the definition of the range can be relaxed somewhat. But in this section we will concentrate on piecewise constant potentials, for which the range is determined by the point at which the potential disappears.

this potential is infinite, and this introduces some exceptional complications in the scattering problem; we will not deal with the Coulomb potential or other potentials of infinite range.

First we will solve the scattering problem for the trivial case V(x) = 0. This means that we are dealing with a free particle which is reflected by the infinitely high barrier at x = 0. Suppose that the particle has energy E; then the magnitude of its momentum is $p = \sqrt{2mE}$ and the wave vector is $k = p/\hbar$. The wavefunction that represents the stationary state of positive energy E must have an *incoming* part e^{-ikx} and an *outgoing* part e^{ikx} . These parts describe, respectively, waves traveling to the left and to the right. In the total wavefunction $\phi(x)$, the incoming and outgoing waves must be superposed in such a way that the boundary condition $\phi(0) = 0$ is satisfied. This implies that the only viable superposition is

$$\phi(x) \propto e^{ikx} - e^{-ikx} \tag{2}$$

In writing this wavefunction, we have omitted the time dependence; it is given by the usual factor $e^{-iEt/\hbar}$.

The wavefunction (2) is not normalizable, but we find it convenient to insert an extra factor 1/2i, so

$$\phi(x) = \frac{1}{2i} (e^{ikx} - e^{-ikx}) = \sin kx$$
 (3)

Next, we must examine the scattering problem with a nonzero potential. We assume that the potential has a finite range R, as in Eq. (1). In the region x > R, the wavefunction will again have an incoming and an outgoing part, as in the case of zero potential. For the incoming part, we take $-(1/2i)e^{-ikx}$, exactly the same as in Eq. (3); this will make it easy to see what the effects of the potential are. The outgoing part must be e^{ikx} multiplied by some coefficient. We will use the notation $(1/2i)e^{2i\delta}$ for this coefficient. The wavefunction is then

$$\psi(x) = \frac{1}{2i} \left(e^{ikx + 2i\delta} - e^{-ikx} \right) \quad \text{for } x > R$$
 (4)

The quantity δ is real. Thus, $e^{2i\delta}$ is simply a phase factor, and the intensities of the incoming and outgoing waves are equal. This equality of incoming and outgoing intensities is required by the conservation of probability. The potential cannot destroy or create probability—it cannot destroy or create particles.

The value of δ depends on the potential V(x) and on the en-

ergy E; it can be calculated by solving the Schrödinger equation in the interior region, x < R. Before we proceed with such a calculation, we briefly consider some general properties of the quantity δ . This quantity is called the *phase shift* for the following reason: Suppose that we compare the probability densities given by Eq. (3) [corresponding to V(x) = 0] and by Eq. (4) [corresponding to $V(x) \neq 0$]. These probability densities are

$$|\phi(x)|^2 = \sin^2 kx \tag{5}$$

and

$$|\psi(x)|^2 = \sin^2(kx + \delta) \tag{6}$$

The comparison of these functions shows that, in the presence of the potential, the maxima and minima of the probability distribution are shifted toward the origin by a distance δ/k relative to their location in the absence² of the potential (see Fig. 11.2). As we will see, the value of δ is positive for an attractive potential; the maxima and minima are then shifted toward the origin. The value of δ is negative for a repulsive potential; the maxima are then shifted away from the origin.

We can define a scattered wave $\psi_S(x)$ as the difference between $\psi(x)$ and $\phi(x)$:

$$\psi_S(x) = \psi(x) - \phi(x) \qquad \text{for } x > R \tag{7}$$

The scattered wave tells us how much the potential changes the wave from what it is in the absence of the potential. The scattered wave is zero if the potential is absent, which means that there is no scattering.

We can also write $\psi_S(x)$ as follows:

$$\psi_{S}(x) = \frac{1}{2i} \left(e^{ikx + 2i\delta} - e^{-ikx} \right) - \frac{1}{2i} \left(e^{ikx} - e^{-ikx} \right)$$

$$= \frac{e^{ikx}}{2i} \left(e^{2i\delta} - 1 \right)$$
(8)

From this we see that the scattered wave is a purely outgoing wave. The amplitude of this outgoing wave is called the scatter-

² Absence of potential means that the function V(x) in Eq. (1) is zero; but the potential for x < 0 remains infinite.

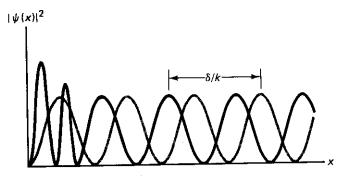


Fig. 11.2 Shift the maxima and minima of the probability distribution. The black curve is $|\psi(x)|^2$; the gray curve is $|\phi(x)|^2$.

ing amplitude:

[scattering amplitude] =
$$\frac{\psi_S}{e^{ikx}} = \frac{1}{2i} (e^{2i\delta} - 1)$$
 (9)

The modulus squared of the scattering amplitude is a measure of the probability of scattering, or the strength of scattering:

$$\begin{bmatrix} \text{probability} \\ \text{of scattering} \end{bmatrix} \propto \left| \begin{bmatrix} \text{scattering} \\ \text{amplitude} \end{bmatrix} \right|^2 = |\psi_S|^2 = \left| \frac{e^{2i\delta} - 1}{2i} \right|^2 = \sin^2 \delta \qquad (10)$$

As we will see in Section 11.4, in three dimensions the cross section is proportional to the square of scattering amplitude. This means that δ or, more precisely, $\sin^2 \delta$ is what we can measure by experiment. From the measured value of δ as a function of energy, we can then try to extract information about the interaction responsible for the scattering.

Another interesting property of δ is the following: $2\hbar d\delta/dE$ gives the time delay that the incident particle suffers by having to pass through the potential. To understand this, suppose that we send a wave packet toward the origin from some large distance. The packet then returns to us after a certain time, having passed through the potential and having been reflected at the origin. The time delay is defined as the difference between the times taken when there is a potential and when there is no potential. This time "delay" can be either positive or negative. A negative "delay" means that the particle spends less time in the region of the potential than a free particle. This can happen if the potential is attractive, and therefore increases the speed of the particle. But it can also happen for a repulsive potential, since then the particle's

path length can be shortened if it is reflected before it reaches the origin.

For the calculation of the time delay, we suppose that our wave packet has an average energy E_0 . The incoming wave packet is then

$$\psi_{\rm in}(x, t) = \int f(E) e^{-i\sqrt{2mE}x/\hbar} e^{-iEt/\hbar} dE$$
 (11)

where f(E) is some function peaked around $E=E_0$. Here we have written the wave packet as an integral over energies rather than an integral over momenta (as we did in Chapter 2), because it better suits our present purposes; of course, it is easy to change the variable of integration from p to E, or vice versa. According to Eq. (4), corresponding to an incoming wave $e^{-i\sqrt{2mE}\,x/\hbar}$, there is an outgoing wave $-e^{i\sqrt{2mE}\,x/\hbar+2i\delta(E)}$. In the latter wave, we have indicated the energy dependence of δ explicitly. Hence

$$\psi_{\text{out}}(x, t) = -\int f(E) e^{i\sqrt{2mE}x/\hbar + 2i\delta(E)} e^{-iEt/\hbar} dE$$
 (12)

Provided that the peak of f(E) at $E = E_0$ is sufficiently narrow, we can approximate $\delta(E) \simeq \delta(E_0) + \delta'(E_0)(E - E_0)$ and therefore

$$\psi_{\text{out}}(x, t) = -e^{2i\delta(E_0) - iE_0t/\hbar} \int f(E) e^{i\sqrt{2mE} x/\hbar} e^{-i(E - E_0)[t - 2\hbar\delta'(E_0)]/\hbar} dE \qquad (13)$$

Let us compare this with the corresponding wave packet in the absence of the potential. The latter is

$$\psi_{in}(x, t) = -e^{-iE_0t/\hbar} \int f(E) e^{i\sqrt{2mE}x/\hbar} e^{-i(E_0 - E)t/\hbar} dE \qquad (14)$$

Ignoring the overall phase factors that stand in front of these integrals, which have no effect on the motion of the envelope of the packets, we see that $t - 2\hbar\delta'(E_0)$ appears in Eq. (13), where t appears in Eq. (14). Hence the former packet is behind the latter by $2\hbar\delta'(E_0)$, that is,

[time delay] =
$$2\hbar \frac{d\delta}{dE}$$

Furthermore, according to Eqs. (13) and (14), this time delay is the only effect the potential has on the outgoing packet. Of course, this depends on the approximation that the packets have a very narrow energy distribution. In general, the packet will suffer both a time delay and a distortion of its shape as it passes through the potential.

11.2 Scattering by a Square Well

For a simple example of scattering in one dimension, we take the piecewise constant potential shown in Fig. 11.3:

$$V(x) = \begin{cases} \infty & \text{for } x < 0 \\ -V_0 & \text{for } 0 < x < a \\ 0 & \text{for } x > a \end{cases}$$
 (15)

The wavefunction in the exterior region, x > a, must have the form given in Eq. (4):

$$\psi(x) = e^{i\delta} \sin(kx + \delta)$$
 for $x > a$ (16)

with $k = \sqrt{2mE}/\hbar$. The wavefunction in the interior region, x < a, must be such as to vanish at x = 0:

$$\psi(x) = A \sin k' x \qquad \text{for } x < a \tag{17}$$

with $k' = \sqrt{2m(E + V_0)}/\hbar$.

The boundary conditions to be imposed at x = a are that the wavefunction and the derivative of the wavefunction are continuous (see Section 3.1). Thus,

$$A \sin k' a = e^{i\delta} \sin(ka + \delta) \tag{18}$$

$$k'A \cos k'a = ke^{i\delta} \cos(ka + \delta)$$
 (19)

These boundary conditions determine the wave amplitude A and the phase shift δ . The equation for the phase shift is

$$\cot \delta = \frac{\tan ka + \frac{k'}{k} \cot k'a}{1 - \frac{k'}{k} \cot k'a \tan ka}$$
 (20)

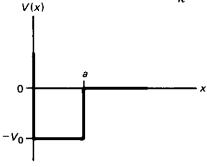


Fig. 11.3 A square potential well.

Exercise 1. Obtain this expression from Eqs. (18) and (19).

From cot δ we can readily evaluate factor $e^{2i\delta}$ that appears in the scattered wave [see Eq. (8)]:

$$e^{2i\delta} = \frac{\cot \delta + i}{\cot \delta - i}$$

$$= \frac{\tan ka + \frac{k'}{k} \cot k'a + i \left(1 - \frac{k'}{k} \cot k'a \tan ka\right)}{\tan ka + \frac{k'}{k} \cot k'a - i \left(1 - \frac{k'}{k} \cot k'a \tan ka\right)}$$
(21)

Figure 11.4a is a plot of δ as a function of ka for the case $V_0 = 3.4\hbar^2/(2ma^2)$. This particular value of V_0 is interesting because the nuclear force between a neutron and a proton with parallel spins (triplet state) can be approximately described by such a potential.³ Figures 11.4b, c, and d are plots of the square of the scattering amplitude, the wave amplitude |A| in the interior region, and $(1/a)d\delta/dk$. The time delay is related to $d\delta/dk$:

[time delay] =
$$2\hbar \frac{d\delta}{dE} = \frac{2m}{\hbar k} \frac{d\delta}{dk}$$
 (22)

which can also be written as

$$\frac{1}{a}\frac{d\delta}{dk} = \frac{\hbar k}{2am} \times [\text{time delay}]$$
 (23)

Since $\hbar k/m$ is the speed of the particle in the absence of the potential, Eq. (23) indicates that the quantity $(1/a)d\delta/dk$ plotted in Fig. 11.4d is the time delay expressed in units of the "free transit time" $2a/(\hbar k/m)$ that the free particle takes to cover the distance 2a. Note that for $k \to 0$, the time delay in our example tends to infinity; however, the ratio of the time delay to the free transit time remains finite.

 $^{^3}$ The values of V_0 and of a for the neutron-proton interaction in the triplet state are $38.5~{\rm MeV}$ and $1.93\times 10^{-15}~{\rm m}$, respectively. However, the interaction can be described by such a potential only at low energies ($E_{\rm cm}\ll 200~{\rm MeV}$). At higher energies, the hard repulsive core of the nuclear interaction as well as inelastic processes become important. Note that m is the reduced mass of the neutron-proton system.

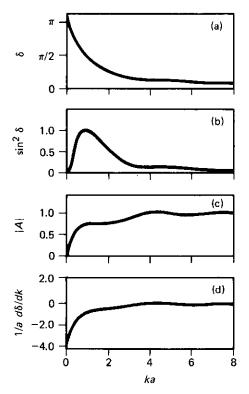


Fig. 11.4 Plots of (a) the phase shift, (b) the square of the scattering amplitude, (c) the wave amplitude |A| in the interior region, and (d) the derivative $(1/a)d\delta/dk$ of the phase shift versus k for $V_0 = 3.4\hbar^2/(2ma^2)$.

In the limit of large energy, Fig. 11.4 suggests that

$$\delta \to 0$$
 (24)

$$\sin^2 \delta \to 0 \tag{25}$$

$$A \to 1$$
 (26)

[time delay]
$$\rightarrow 0$$
 (27)

It is easy to understand how these limits arise. If the particle has a very large energy $(E \gg V_0)$, then it hardly notices the potential, and it behaves pretty much as a free particle, so the scattering tends to zero. In arriving at Eq. (24), we have made use of a convention for the phase shift. Obviously, Eq. (20) determines δ only modulo π , and we can say only that $\delta \to n\pi$ as $E \to \infty$. We adopt the convention that n is to be taken as zero.

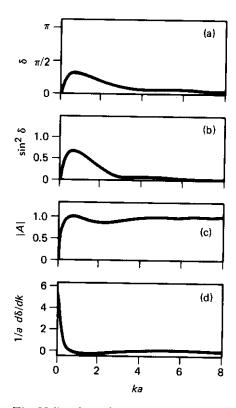


Fig. 11.5 Plots of (a) the phase shift, (b) the square of the scattering amplitude, (c) the wave amplitude |A| in the interior region, and (d) the derivative $(1/a)d\delta/dk$ of the phase shift versus k for $V_0 = 2.1\hbar^2/(2ma^2)$.

As a second example, Fig. 11.5 plots the results of a similar calculation for a somewhat weaker potential, with $V_0 = 2.1\hbar^2/(2ma^2)$. This happens to be the potential that describes the interaction between a neutron and a proton with antiparallel spins (singlet state).⁴ Comparing Figs. 11.4a and 11.5a, we see that the behavior of the phase shift at low energy is quite different. For the stronger potential, $\delta(0) = \pi$ and for the weaker potential $\delta(0) = 0$.

This difference between our two examples is a consequence of an interesting theorem that relates the net change of the phase shift between E = 0 and $E = \infty$ to the number of bound states in the

⁴ For the neutron-proton interaction in the singlet state, $V_0 = 14.3$ MeV and $a = 2.50 \times 10^{-15}$ m.

potential. This theorem, known as Levinson's theorem, asserts that the phase shift at zero energy is

$$\delta(0) = N\pi \tag{28}$$

where N is the number of possible bound states in the potential. According to the results of Section 3.4 [see Eq. (3.94)], the square well with $V_0 = 3.4\hbar^2/(2ma^2)$ has exactly one bound state; hence N = 1 and $\delta(0) = \pi$. The square well with $V_0 = 2.1\hbar^2/(2ma^2)$ is too shallow to have any bound states; hence N = 0 and $\delta(0) = 0$.

The proof of the theorem is very simple. Consider a particle moving in some potential, constrained to the region x > 0. Pretend that the particle is also constrained so x < L, where L is large (ultimately, the limit $L \to \infty$ will be taken). This means the particle is confined in an infinite potential well of width L; all the eigenstates are discrete, which makes it easy to count them. If the potential in the region 0 < x < L is zero, then the positive-energy eigenfunctions are $\phi \propto \sin kx$, and since they must vanish at x = L,

$$kL = n\pi \tag{29}$$

Hence the number of states in a small momentum interval Δk is

$$\Delta n = \frac{L}{\pi} \Delta k \tag{30}$$

If the potential is not zero, then the positive-energy eigenfunctions outside the range of the potential are $\psi \propto e^{i\delta} \sin(kx + \delta)$ [see Eq. (4)], and the condition that they vanish at x = L is

$$kL + \delta = n\pi \tag{31}$$

The number of states in a small momentum interval Δk is therefore

$$\Delta n = \frac{L}{\pi} \Delta k + \frac{1}{\pi} \delta'(k) \Delta k \tag{32}$$

where $\delta'(k) = d\delta/dk$. The change, caused by the potential, in the number of positive-energy eigenstates in the interval Δk is then $(1/\pi) \delta'(k) \Delta k$. The total change in the number of positive-energy states is

$$\Delta N = \frac{1}{\pi} \int_0^\infty \delta'(k) \ dk = \frac{1}{\pi} \left[\delta(\infty) - \delta(0) \right] \tag{33}$$

This equation for the change in the number of states is independent of L, and hence is also valid in the limit $L \rightarrow \infty$. The change in

the number of positive-energy states implies an opposite change in the number of negative-energy states, since states cannot appear or disappear as the strength of the potential is varied. When the potential is zero, there is a certain number of states; turning on the potential cannot change the *number* of states, only their energies (it can be shown quite generally that the energy of a state depends continuously on the strength of the potential). Some of the positive-energy states become negative-energy states (bound states), others are shifted to some different positive energy (see Fig. 11.6). The decrease in the number of positive-energy states must therefore be compensated by an increase in the number of bound states:

$$N = -\Delta N = \frac{1}{\pi} \left[\delta(0) - \delta(\infty) \right] \tag{34}$$

With the convention $\delta(\infty) = 0$, this completes the proof of Eq. (28).

As a corollary of this theorem we obtain another interpretation of the quantity $\delta'(k)$. According to Eq. (33), $(1/\pi)d\delta/dk$ is the change in the density of states caused by the potential. For example, Fig. 11.5d can be interpreted as a plot of the change in the density of states and shows that, near zero energy, the continuum states in the presence of the potential are much more densely packed than in the absence of potential.

Before we proceed with our discussion of scattering, let us look at the bound states of the potential given in Eq. (15). There is, of course, a well-known and straightforward procedure for solving the Schrödinger equation for this case (see Section 3.4). But here we will deal with a clever alternative method that makes use of the positive-energy solution we examined above.

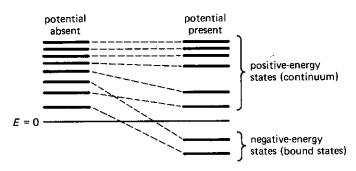


Fig. 11.6 Shifts in the energies of some states produced by the presence of the potential.

If E < 0, then

$$k' = \frac{\sqrt{2m(E + V_0)}}{\hbar} = \frac{\sqrt{2m(V_0 - |E|)}}{\hbar}$$
 (35)

and

$$k = \frac{\sqrt{2mE}}{\hbar} = i \frac{\sqrt{2m|E|}}{\hbar} \tag{36}$$

We will use the notation $\kappa = \sqrt{2m|E|}/\hbar$, so

$$k = i\kappa \tag{37}$$

Now, Eqs. (16) and (17), with δ and A determined by Eqs. (18) and (19), give a solution of the Schrödinger equation with the correct boundary conditions, irrespective of the sign of E. However, if E < 0, it is convenient to express this solution in terms of the real variable κ . Equation (16) then becomes

$$\psi(x) \frac{1}{2i} \left(e^{2i\delta} e^{-\kappa x} - e^{\kappa x} \right) \tag{38}$$

where, by Eq. (20),

$$\cot \delta = \frac{\tan i\kappa a + \frac{k'}{i\kappa} \cot k'a}{1 - \frac{k'}{i\kappa} \cot k'a \tan i\kappa a}$$
(39)

Although Eq. (38) is a solution of the Schrödinger equation, it is not an acceptable solution; it has the wrong behavior at infinity, with $\psi(x) \to \infty$ as $x \to \infty$. We must somehow get rid of the increasing exponential $e^{\kappa x}$. Since the normalization of the bound-state wavefunction must in any case be carried out after we have found an acceptable solution, we may as well ignore an overall factor of proportionality, and replace Eq. (38) by

$$\psi(x) \propto e^{-\kappa x} - e^{-2i\delta} e^{\kappa x} \tag{40}$$

From this, it is obvious that in order to get rid of the increasing exponential, we need only demand that

$$e^{-2i\delta} = 0 (41)$$

Since δ as given by Eq. (39) is complex,⁵ this equation has solutions. The equation can also be rewritten as a condition on cot δ :

⁵ Our previous argument requiring δ to be real applies only when E > 0.

$$\cot \delta = i \frac{e^{i\delta} + e^{-i\delta}}{e^{i\delta} - e^{-i\delta}} = i \frac{1 + e^{-2i\delta}}{1 - e^{-2i\delta}} = i$$
 (42)

Substituting this into Eq. (39), we obtain

$$\cot k'a = -\frac{\kappa}{k'} \tag{43}$$

or

$$\cot \frac{\sqrt{2m(V_0 - |E|)} \ a}{\hbar} = -\sqrt{\frac{|E|}{V_0 - |E|}} \tag{44}$$

This equation for the energy eigenvalues coincides with Eq. (3.89), obtained by other means.

Exercise 2. Derive Eq. (44) from Eq. (39).

As already mentioned above, the square well with $V_0 = 3.4\hbar^2/(2ma^2)$ has exactly one bound state. In the case of the triplet neutron-proton interaction, this bound state corresponds to the deuteron, with a binding energy |E| = 2.22 MeV.

The square well with $V_0 = 2.1\hbar^2/(2ma^2)$ has no bound state. However, it is customary to say that there is a virtual state, or an antibound state, in singlet neutron-proton scattering. By this is meant the following: We have seen that a bound state is obtained by eliminating the increasing exponential from Eq. (38). A virtual, antibound "state" is obtained by eliminating the decreasing exponential, so the wavefunction becomes a purely increasing exponential.⁶ This requires

$$e^{2i\delta} = 0 (45)$$

which implies that

$$\cot \frac{\sqrt{2m(V_0 - |E|)} \ a}{\hbar} = + \sqrt{\frac{|E|}{V_0 - |E|}} \tag{46}$$

Exercise 3. Derive Eq. (46).

⁶ There exists several other, slight different definitions of *virtual state*. The definition given here is the most straightforward. Note that the use of the word *virtual* in relativistic perturbation theory (Feynman diagrams) is unrelated to our use here.

The preceding equation yields a binding energy |E| = 170 keV for the virtual singlet state of the deuteron.

It must be emphasized that the presence of a virtual "state" means nothing but that Eq. (45) is satisfied. The virtual "state" is no more than a root of $e^{2i\delta}$; it is not a physical state (hence the name). The wavefunction increases exponentially at large distances and is therefore not acceptable; the system can never be put into this "state." Nevertheless, the presence of the virtual "state" makes itself felt by its influence on the scattering at small (positive) energies. Thus, the behavior of $\sin^2\delta$ near zero energy (see Fig. 11.5b) can be explained in terms of the presence of the nearby virtual "state" at small negative energy.

The quantity $e^{2i\delta}$ by which the outgoing wave is multiplied is usually called the *S-matrix*, or more precisely, an *S*-matrix element (*S* stands for scattering). In general, each scattering reaction $|\alpha\rangle \rightarrow |\beta\rangle$, where $|\alpha\rangle$ represents some initial state and $|\beta\rangle$ some final state, possibly with a different final set of particles, is assigned an *S*-matrix element $S_{\alpha\beta}$ which is related to the probability amplitude for the occurrence of the reaction. The *S*-matrix is the totality of all such elements.

We have seen that $e^{2i\delta} = \infty$ at a bound state. This means that the S-matrix has a pole (singularity) at the bound-state energy:

bound state
$$\Rightarrow$$
 pole in S-matrix (47)

This rule holds in general and is very important in attempts at constructing the S-matrix ("S-matrix theory"). The program of S-matrix theory is this: Since we often do not know the forces that act between particles, we cannot solve the Schrödinger equation or the relativistic version of this equation. But we can nevertheless find the S-matrix, which contains all the information about scattering, by somehow discovering all the singularities. This would determine the S-matrix completely, because if all the singularities of a function are known, at both real and complex values of its argument, then the function is determined. Since the singularities at both real and complex (unphysical) values of the energy must be discovered, the program of S-matrix theory is ambitious and difficult.

11.3 Resonances

A particle incident on the square well of Eq. (15) never suffers any large time delay. Neither does the wave amplitude |A| in the interior region ever become large. We will now examine the case of a

more complicated potential, consisting of a square well and a barrier:

$$V(x) = \begin{cases} -V_0 & \text{for } 0 < x < a \\ V_1 & \text{for } a < x < 2a \\ 0 & \text{for } x > a \\ \infty & \text{for } x < 0 \end{cases}$$

$$(48)$$

This potential is plotted in Fig. 11.7. The barrier in this potential can prevent the escape of a particle from the interior region for a fairly long time, provided the energy is just right, and this leads to the accumulation of a large wave amplitude in the interior region.

The solution of the Schrödinger equation for the potential (48) is of the form

$$\psi(x) = \begin{cases} A \sin k'x & \text{for } 0 < x < a \\ B \sin k''x + C \cos k''x & \text{for } a < x < 2a \\ e^{i\delta} \sin(kx + \delta) & \text{for } x > 2a \end{cases}$$
(49)

where $k' = \sqrt{2m(E+V_0)}/\hbar$ and $k'' = \sqrt{2m(E-V_1)}/\hbar$. Note that if $E < V_1$, then k'' will be imaginary, but it is not necessary to treat this case separately.

The usual boundary conditions at x = a and at x = 2a provide four equations that determine the four unknowns A, B, C, and δ . Of these unknowns, A and δ are the most interesting. The formulas for them are rather messy, and it is more instructive to examine plots of these quantities. Figure 11.8 shows plots of δ as a function of ka, and plots of the square of the scattering amplitude, the wave amplitude |A| in the interior region, and $(1/a) d\delta/dk$. These plots

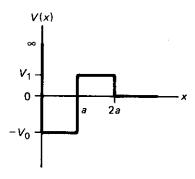


Fig. 11.7 A square well with a barrier.

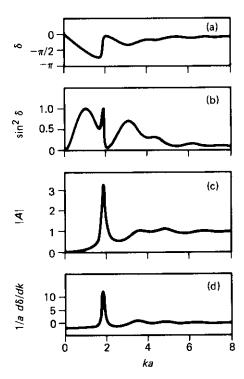


Fig. 11.8 Plots of (a) the phase shift, (b) the square of the scattering amplitude, (c) the wave amplitude |A| in the interior region, and (d) the derivative $(1/a) \ d\delta/dk$ of the phase shift vs. k for the square well with a barrier.

were prepared for $V_0 = 1.0\hbar^2/2ma^2$ and $V_1 = 5.0\hbar^2/2ma^2$. A striking feature of Fig. 11.8 is the resonance or quasi-stationary state that appears at ka = 1.8. At this energy

- i. the phase shift suddenly increases by (nearly) π and passes through $\pi/2$.
- ii. the square of the scattering amplitude has a sharp maximum and reaches $\sin^2\!\delta = 1$
- iii. the wave amplitude in the interior region has a sharp maximum
- iv. the derivative $d\delta/dk$ has a sharp maximum.

The quantity $d\delta/dk$ is related to the time delay by Eq. (23), which we can write as

$$\frac{d\delta}{dk} = R \times \frac{\text{[time delay]}}{\text{[free transit time]}}$$
 (50)

where R is the range of the potential, and the free transit time is $2R/(\hbar k/m)$. The time delay may be regarded as the lifetime of the resonant state. If this lifetime is very large, the resonance will resemble a stationary state (for the latter the lifetime is infinite). We can also express this in another way: the maximum in $d\delta/dk$ at the resonant energy means that the density of states is at a maximum. If this maximum is very large and very narrow, the density of states resembles that of a stationary state (for the latter, the density of states is infinite at the stationary state and zero elsewhere, that is, it is a delta function).

From our knowledge of classical oscillating systems, we expect that at the resonant energy, the amplitude of oscillation of the system should build up to a very large value. In the present case, the quantity |A| may be regarded as the amplitude of oscillation of the system, and it indeed has the expected behavior. Figure 11.9 is a plot of the absolute value squared of the wavefunction near resonance. Clearly, the amplitude of oscillation is large inside the potential well.

Unfortunately, in scattering experiments, measurements are performed on the incident particle only when it is far away from the scattering region; that is, the incident particle is observed only before and after the collision with the target particle. Hence the quantity |A| is not directly accessible in these experiments. What can be measured directly is the scattering probability $\sin^2\delta$. The measurement of $\sin^2\delta$ as a function of energy determines δ and $d\delta/dE$ as a function of energy, except perhaps for an ambiguity in sign.

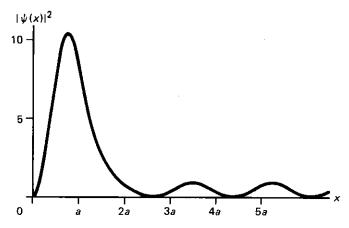


Fig. 11.9 Plot of $|\psi(x)|^2$ vs. x when the energy is near resonance.

The time delay $2\hbar d\delta/dE$ at resonance can be obtained directly by measurement of the time that a particle takes to move though the potential. The wave packet used for such a measurement must have a width Δk that is small compared with the width of the resonance. Since the latter width is approximately $\pi(d\delta/dk)^{-1}$, we need

$$\Delta k \ll \pi \left(\frac{d\delta}{dk}\right)^{-1} \tag{51}$$

and the packet must have a length

$$\Delta x \ge \frac{1}{2 \Delta k} \gg \frac{d\delta}{dk} \tag{52}$$

This means that the time of departure and of arrival of the particle is uncertain by

$$\Delta t = \frac{\Delta x}{v} \gg \frac{d\delta}{dk} \frac{m}{\hbar k} \tag{53}$$

or

$$\Delta t \gg \hbar \, \frac{d\delta}{dE} \tag{54}$$

Hence, Δt is much larger than the time delay that we seek to measure. This means that it will be impossible to perform the measurement by observation of a single particle. However, repeated measurements on identically prepared systems will give an average time delay which is not affected by the large uncertainties of the individual measurements. The time delay has, therefore, only a statistical significance.

We saw that in the case of the potential given by Eq. (48), the conditions (i)-(iv) all hold at resonance. We will now proceed in general, without any special assumption about the shape of the potential, and examine what relationships we can establish between the conditions (i)-(iv).

First, we show that condition (i) implies all the others. If δ increases sharply by about π in the vicinity of $k=\alpha$, passing through $\delta=\pi/2$ at $k=\alpha$, then we can approximate δ in this vicinity by

$$\delta \simeq \tan^{-1} \frac{\beta}{\alpha - k} \tag{55}$$

where β is a positive constant such that

$$\frac{1}{\beta} = \frac{d\delta}{dk} \bigg|_{k=\alpha} \tag{56}$$

The function (55) has the correct value of δ and the correct value of the derivative $d\delta/dk$ at $k = \alpha$; it is therefore effectively equivalent to a two-term Taylor-series expansion. According to Eq. (55),

$$e^{2i\delta} = \frac{1 + i \tan \delta}{1 - i \tan \delta} \simeq \frac{k - \alpha - i\beta}{k - \alpha + i\beta}$$
 (57)

and hence the square of the scattering amplitude is

$$|\psi_{\rm S}|^2 = \sin^2 \delta = \frac{1}{4} |{\rm e}^{2i\delta} - 1|^2 \simeq \frac{\beta^2}{(k - \alpha)^2 + \beta^2}$$
 (58)

This has a maximum at $k = \alpha$, as required by condition (ii).

If we write Eq. (58) as a function of the energy, with $E_{\alpha} = \alpha^2 \hbar^2 / 2m$ and with the approximation $(E - E_{\alpha}) \simeq (k - \alpha) \alpha \hbar^2 / m$, then the square of the scattering amplitude becomes

$$|\psi_S|^2 = \sin^2 \delta \simeq \frac{\frac{1}{4}\Gamma^2}{(E - E_\alpha)^2 + \frac{1}{4}\Gamma^2}$$
 (59)

where

$$\Gamma = \frac{2\alpha\beta\hbar^2}{m} \tag{60}$$

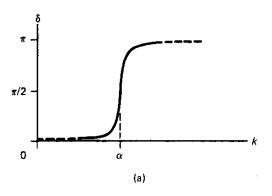
and the approximation has been made. Equation (59) is known as the *Breit–Wigner resonance formula*. It gives the behavior of the square of the scattering amplitude near resonance under the assumption that the nonresonant scattering can be neglected. Figure 11.10 shows plots of δ and of $\sin^2\delta$ near resonance, according to the Breit–Wigner formula; note that the shape of these plots is in agreement with Fig. 11.8.

It is obvious that condition (iv) is also satisfied since, with the approximation (55),

$$\frac{d\delta}{dk} = \frac{d}{dk} \tan^{-1} \frac{\beta}{\alpha - k} = \frac{\beta}{(k - \alpha)^2 + \beta^2}$$
 (61)

which, indeed, has a maximum at $k = \alpha$.

We will now give a simple, but not rigorous, argument that a maximum in $d\delta/dk$ is usually associated with a maximum in the wave amplitude in the interior region. If there is a time delay



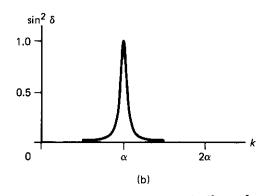


Fig. 11.10 Phase shift δ and square of the scattering amplitude $|\psi_S|^2 = \sin^2\!\delta$ near resonance.

 $2\hbar d\delta/dE$, the emergence of a wave train that enters the potential is delayed, and for a time $2\hbar d\delta/dE$ probability is flowing into the region of the potential, but there is no corresponding flow out of the region of the potential; thus, probability accumulates in this region. The incoming wave has a probability density $|e^{-ikx}/2i|^2 = 1/4$; its probability current is the product of this probability density and the speed $\hbar k/m$:

[probability current] =
$$\frac{1}{4} \frac{\hbar k}{m}$$

The accumulated probability is then

[probability current] × [time delay]
$$\simeq \frac{1}{4} \frac{\hbar k}{m} \times 2\hbar \frac{d\delta}{dE}$$
 (62)

However, we can also express the change of probability that the potential produces in the interior region as

$$\int_{0}^{R} (|\psi|^{2} - |\phi|^{2}) dx$$

where $\phi = \sin kx$ [see Eq. (3)] and ψ is the solution of the Schrödinger equation for the given potential. Hence⁸

⁷ The wavefunction is not normalizable, and hence this probability and all the probabilities in the following equations are relative, not absolute.

⁸ Equation (63) is not exact since, strictly, the time delay can be defined only for wave packets, and not for the harmonic waves used in the above argument. The exact equation has an extra term $[\sin 2kx - \sin 2(kx + \delta)]/2k$ added to the right side.

$$\frac{1}{2} \frac{\hbar^2 k}{m} \frac{d\delta}{dE} \simeq \int_0^R (|\psi|^2 - |\phi|^2) \ dx \tag{63}$$

that is,

$$\frac{d\delta}{dk} \simeq 2 \int_0^R (|\psi|^2 - |\phi|^2) dx \tag{64}$$

Since

$$\int_0^R |\phi|^2 dx = \int_0^R \sin^2 kx \, dx < R \tag{65}$$

we see that a large maximum in $d\delta/dk$ must correspond to a large maximum in $\int |\psi|^2 dx$, and conversely. This implies that the average wave amplitude in the interior is at maximum, in agreement with condition (iii).

Next we consider the implications of condition (ii). If the square of the scattering amplitude goes through its maximum value ($\sin^2\delta=1$), then δ must pass through $\pi/2$. However, such a maximum is not a resonance unless δ is increasing with energy. For example, the peak at ka=1.0 in Fig. 11.8b does not correspond to a resonance; the time delay is negative at this energy, and there is no quasi-stationary state. Maxima with negative time delays are not rare. In fact, the number of such maxima is never less than the number of resonances. Levinson's theorem tells us that, on the average, δ does not increase with energy $[\delta(0)-\delta(\infty)\geq 0]$; since at each resonance, δ increases through $\pi/2$, it must again decrease through $\pi/2$, and therefore give a nonresonant maximum in the square of the scattering amplitude.

Although in general the existence of a maximum in $\sin^2\delta$ is not a sufficient condition for the existence of a resonance, the existence of a narrow maximum is a sufficient condition. This is so because a narrow maximum implies that δ is passing through $\pi/2$ very quickly, that is, $|d\delta/dk|$ is large, and this is possible only if $d\delta/dk$ is positive. The reason for a positive value of $d\delta/dk$ is causality. If $d\delta/dk$ were negative, we would have a time advance. But, by causality, the largest possible time advance is 2R/v, which occurs if the incident particle is reflected at the outer edge of the potential (or, equivalently, transverses the potential with very large speed). Therefore, the time delay necessarily satisfies the condition

$$2\hbar \, \frac{d\delta}{dE} \ge - \, \frac{2R}{v}$$

$$\frac{d\delta}{dk} \ge -R \tag{66}$$

This is known as the Wigner condition.9

The Wigner condition tells us that if the peak of $\sin^2 \delta$ is so narrow that $|d\delta/dk|$ is larger than the range of the potential, then this peak will indeed correspond to a resonance; a peak that is not so narrow may or may not correspond to a resonance. This provides some justification for experimental physicists who, upon observing very narrow peaks in nuclear cross sections, immediately claim that they have found a resonance.

As a next step of our investigation of the relationships among the conditions (i)-(iv), we will show that a sufficiently sharp peak in the quantity $d\delta/dk$ —which is proportional to the time delay expressed in units of the free transit time [see Eq. (50)]—implies the existence of a resonance. If $d\delta/dk$ has a maximum at $k = \alpha$, we can approximate this function in the vicinity by

$$\frac{d\delta}{dk} \simeq \frac{\xi \beta}{(k-\alpha)^2 + \beta^2} \tag{67}$$

where ξ and β are positive constants. Equation (67) amounts to no more than the assumption that $(d\delta/dk)^{-1}$ can be expanded in a Taylor series about the point $k = \alpha$: 10

$$\left(\frac{d\delta}{dk}\right)^{-1} = \frac{\beta}{\xi} + \frac{1}{\beta\xi} (k - \alpha)^2 \tag{68}$$

We assume that the higher-order terms in this expansion can be neglected as long as $|k - \alpha| \le \beta$. Note that Eq. (61) is a special case of Eq. (67) with $\xi = 1$; it will be interesting to see how this special case arises.

The differential equation (67) can be integrated to give δ as a function of k:

$$\delta(k) = \int_{\alpha}^{k} \frac{\xi \beta}{(k - \alpha)^{2} + \beta^{2}} dk + \delta(\alpha)$$

$$\simeq \xi \tan^{-1} \frac{\beta}{\alpha - k} - \frac{\xi \pi}{2} + \delta(\alpha)$$
(69)

⁹ Our argument is not rigorous, and neither is the result (66). The exact Wigner condition is $d\delta/dk \ge -(R+1/k)$.

¹⁰ The Taylor series for $(d\delta/dk)^{-1}$ is more convenient than that for $d\delta/dk$, because $(d\delta/dk)^{-1}$ is small near resonance.

We must now take into account an important restriction on the possible values of ξ . It is obvious from Eq. (4) that δ is defined only modulo π , since an increase of δ by $n\pi$ leaves this equation unchanged. On the other hand, $\xi \tan^{-1} \beta/(\alpha - k)$ is defined modulo $\xi\pi$. For the sake of consistency of these two equations, we must therefore require that ξ is an integer:

$$\xi = 0, 1, 2, 3, \dots$$
 (70)

The case $\xi = 0$ is of no interest. The cases $\xi = 1, 2, 3, \ldots$ correspond to resonances of different types. We will for now assume that $\xi = 1$, because this type of resonance seems to be the one that usually occurs in nature. In this special case

$$\delta(k) \simeq \tan^{-1} \frac{\beta}{\alpha - k} - \frac{\pi}{2} + \delta(\alpha)$$
 (71)

which shows that δ increases by about π in the vicinity of $k = \alpha$. Hence δ must necessarily pass through $\pi/2$ (modulo π) in this vicinity, and we see that all the conditions (i)–(iv) are satisfied.

To simplify matters further, let us assume that the scattering off resonance is small, so the resonant peak in the scattering is well isolated from the nonresonant background. In terms of Eq. (71), this means that the constant term $-\pi/2 + \delta(\alpha)$ is small and that

$$\delta(k) \simeq \tan^{-1} \frac{\beta}{\alpha - k} \tag{72}$$

We conclude that under these circumstances δ passes through $\pi/2$ (modulo π) at $k \simeq \alpha$, so the maxima in $d\delta/dk$ and in $\sin^2\delta$ occur at nearly the same energy. The expression (72) is identical to (55) and leads to the familiar Breit–Wigner formula (59).

11.4 Elastic Scattering in Three Dimensions

Many of the concepts we introduced to describe the scattering in one dimension also apply to three dimension. Consider a particle incident on some three-dimensional region in which the potential $V(\mathbf{r})$ is different from zero. We will call this region the interaction region (see Fig. 11.11). The incident particle is represented by a plane wave, and this wave is scattered by the interaction with the potential, that is, the some portion of the wave is spread out over all angles.

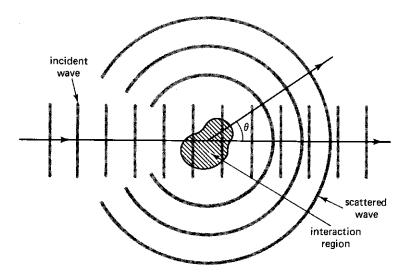


Fig. 11.11 Scattering of an incident plane wave by interaction with a potential. The scattering angle is measured relative to the incident direction.

For convenience, we assume that the incident wave approaches the interaction region from the negative z direction. Thus, the incident wave is

$$\phi(\mathbf{r}) = e^{ikz} \tag{73}$$

As in Section 11.1, we have omitted the time dependence of this wave; it is given by the usual factor $e^{-iEt/\hbar}$ for all our waves.

At large distances from the interaction region, the scattered wave consists of an outgoing spherical wave with a radial dependence of the form e^{ikr}/r . Here, we have included a factor of 1/r in this wavefunction because, when the wave travels outward, it spreads over an increasing area, and the probability density in the wave must decrease as $1/r^2$ (this decrease of the intensity of the spherical quantum-mechanical wave is entirely analogous to the decrease of the intensity of a spherical sound wave spreading out from a small source). Since the wave need not have the same intensity in all directions, we also want to include an angular dependence in the scattered wave. We describe this angular dependence by a function $f(\theta)$, where θ is the scattering angle, or the deflection angle, relative to the incident direction (see Fig. 11.11). The scattered wave then takes the form

$$\psi_S(\mathbf{r}) = f(\theta) \frac{e^{ikr}}{r} \tag{74}$$

The net wave is the sum of the incident wave and the scattered wave,

$$\psi(\mathbf{r}) = \phi(\mathbf{r}) + \psi_S(\mathbf{r}) = e^{ikz} + f(\theta) \frac{e^{ikr}}{r}$$
 (75)

In one-dimensional scattering, we defined the scattering amplitude as the amplitude of the scattered wave [see Eq. (9)]. In three-dimensional scattering, the amplitude of the scattered wave is $f(\theta)/r$ [see Eq. (74)]; however, since the factor 1/r is always present in three-dimensional scattering and conveys no distinctive information about the scattering, we will omit it from the definition of the scattering amplitude:

[scattering amplitude] =
$$f(\theta)$$
 (76)

We will see that the scattering probability and the scattering cross section can be expressed directly in terms of this scattering amplitude $f(\theta)$.

As in Section 10.6, we define the differential cross section $d\sigma$ as the ratio of the number of particles scattered per unit time into a solid angle $d\Omega$ to the flux of incident particles:

$$d\sigma = \frac{\begin{bmatrix} \text{number of particles scattered per unit time} \\ \text{into solid angle } d\Omega \text{ at } \theta, \phi \end{bmatrix}}{[\text{flux of incident particles}]}$$
(77)

The flux of incident particles is the product of the probability density of the incident wave and the speed. Since the incident wave (73) has a probability density $|e^{ikz}|^2 = 1$ and the particles have a speed $\hbar k/m$,

[flux of incident particles] =
$$1 \times \frac{\hbar k}{m}$$
 (78)

The number of scattered particles in a small volume (see Fig. 11.12) between r and r + dr in the solid angle $d\Omega$ is

$$\left| f(\theta) \frac{e^{ikr}}{r} \right|^2 r^2 dr d\Omega = |f(\theta)|^2 dr d\Omega$$
 (79)

These particles take a time $dt = dr/(\hbar k/m)$ to leave this volume; hence the number emerging per unit time is

$$|f(\theta)|^2 \frac{\hbar k}{m} d\Omega \tag{80}$$

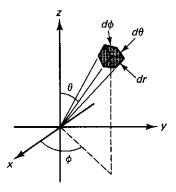


Fig. 11.12 A small volume between r and r + dr in the solid angle $d\Omega = \sin \theta \ d\theta \ d\phi$.

and the differential cross section (77) is

$$d\sigma = \frac{|f(\theta)|^2 \hbar k/m}{\hbar k/m} d\Omega \tag{81}$$

or

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 \tag{82}$$

The total cross section is obtained by integrating the differential cross section over all angles:

$$\sigma = \int d\sigma = \int \frac{d\sigma}{d\Omega} d\Omega = \int |f(\theta)|^2 d\Omega$$
 (83)

11.5 Partial Waves in a Central Potential; The Optical Theorem

For the calculation of the scattering amplitude $f(\theta)$ and the cross section, we need to specify the potential. Most of the potentials of interest in physics are central potentials, that is, potentials that depend only on the radial coordinate r. For such a central potential, the incident wave and the scattered wave can be expressed as superpositions of eigenfunctions of the orbital angular momentum, and each of these eigenfunctions is scattered independently of the other eigenfunctions. The angular-momentum eigenfunctions contained within the incident and the scattered wave are called

partial waves. Each partial wave is characterized by the value of its angular-momentum quantum number l. During the scattering each partial wave acquires a phase shift of its own, and these phase shifts determine the scattering amplitude and the cross section.

To construct the partial waves, we recall from Section 8.3 that the plane wave e^{ikz} can be written as a superposition of angular momentum eigenfunctions:

$$e^{ikz} = \sqrt{4\pi} \sum_{l=0}^{\infty} \sqrt{2l+1} \ i^l Y_l^{0}(\theta) j_l(kr)$$
 (84)

We want to examine the behavior of the wavefunctions at a large distance from the interaction region. Thus, we will assume that r is very large, and that the functions $j_l(kr)$ can be replaced by their asymptotic forms $(1/kr) \sin(kr - l\pi/2)$, according to Eq. (8.114). The plane wave e^{ikz} then becomes

$$e^{ikz} \simeq \sqrt{4\pi} \sum_{l=0}^{\infty} \sqrt{2l+1} i^l Y_l^0(\theta) \frac{1}{kr} \sin\left(kr - \frac{l\pi}{2}\right)$$
 (85)

or

$$e^{ikz} \simeq \frac{\sqrt{4\pi}}{k} \sum_{l=0}^{\infty} \sqrt{2l+1} i^{l} Y_{l}^{0}(\theta) \frac{1}{2i} \left(\frac{e^{i(kr-l\pi/2)}}{r} - \frac{e^{-i(kr-l\pi/2)}}{r} \right)$$
(86)

This shows that the lth partial wave consists of an incoming spherical wave

$$-\frac{\mathrm{e}^{-i(kr-l\pi/2)}}{r} \tag{87}$$

and an outgoing spherical wave

$$\frac{\mathrm{e}^{i(kr-l\pi/2)}}{r} \tag{88}$$

If the potential V(r) is zero, then the sum of these incoming and outgoing spherical waves [with the coefficients specified in Eq. (86)] provides us with the solution of the scattering problem.

If the potential is nonzero, then the solution of the scattering problem will still be a sum of incoming and outgoing spherical waves, but with somewhat different coefficients. From our discussion of scattering in one dimension, we know that the incoming wave is unchanged, but the outgoing wave acquires an extra phase factor $e^{2i\delta_i}$. Thus, the solution of the scattering problem is

$$\psi(\mathbf{r}) = \frac{\sqrt{4\pi}}{k} \sum_{l=0}^{\infty} \sqrt{2l+1} \ i^{l} Y_{l}^{0}(\theta) \frac{1}{2i} \left(\frac{e^{i(kr-l\pi/2+2\delta_{l})}}{r} - \frac{e^{-i(kr-l\pi/2)}}{r} \right)$$
(89)

According to Eq. (75), the scattered wave $f(\theta)e^{ikr}/r$ is the difference between the net wavefunction $\psi(\mathbf{r})$ and the incident wave e^{ikz} :

$$f(\theta) \frac{e^{ikr}}{r} = \psi(r) - e^{ikz}$$

$$= \frac{\sqrt{4\pi}}{k} \sum_{l=0}^{\infty} \sqrt{2l+1} i^{l} Y_{l}^{0}(\theta) \frac{1}{2i} \left(\frac{e^{(ikr-l\pi/2+2\delta_{l})}}{r} - \frac{e^{-i(kr-l\pi/2)}}{r} \right)$$

$$- \frac{\sqrt{4\pi}}{k} \sum_{l=0}^{\infty} \sqrt{2l+1} i^{l} Y_{l}^{0}(\theta) \frac{1}{2i} \left(\frac{e^{(ikr-l\pi/2)}}{r} - \frac{e^{-i(kr-l\pi/2)}}{r} \right)$$

$$= \frac{\sqrt{4\pi}}{k} \sum_{l=0}^{\infty} \sqrt{2l+1} i^{l} Y_{l}^{0}(\theta) \frac{1}{2i} (e^{2i\delta_{l}} - 1) \frac{e^{i(kr-l\pi/2)}}{r}$$
(90)

Hence,

$$f(\theta) = \frac{\sqrt{4\pi}}{k} \sum_{l=0}^{\infty} \sqrt{2l+1} Y_l^0(\theta) \frac{1}{2i} (e^{2i\delta_l} - 1)$$

$$= \frac{\sqrt{4\pi}}{k} \sum_{l=0}^{\infty} \sqrt{2l+1} Y_l^0(\theta) e^{i\delta_l} \sin \delta_l$$
 (91)

From this expression for $f(\theta)$, we can calculate the differential cross section [Eq. (82)] and the total cross section [Eq. (83)]. The latter takes an especially simple form, in consequence of the orthonormality relation for the spherical harmonics:

$$\sigma = \int |f\theta|^2 d\Omega = \frac{4\pi}{k^2} \sum_{l=0}^{\infty} (2l + 1) \sin^2 \delta_l$$
 (92)

Exercise 4. Derive this formula for the total cross section.

An interesting result emerges from Eq. (91) if we examine the imaginary part of the scattering amplitude at $\theta = 0$, called the forward scattering amplitude. With $Y_l^0(0) = \sqrt{(2l+1)/4\pi}$, we obtain

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$$\operatorname{Im}\left[f(0)\right] = \operatorname{Im}\left[\frac{\sqrt{4\pi}}{k} \sum_{l=0}^{\infty} \sqrt{2l+1} \sqrt{\frac{2l+1}{4\pi}} e^{i\delta_{l}} \sin \delta_{l}\right]$$
$$= \frac{1}{k} \sum_{l=0}^{\infty} (2l+1) \sin^{2} \delta_{l} \tag{93}$$

Comparison of this with Eq. (92) shows that

$$\sigma = \frac{4\pi}{k} \operatorname{Im} f(0) \tag{94}$$

This is called the *optical theorem*. (A similar theorem holds for light waves, and it was known long before its rediscovery in quantum mechanics.)

Finally, let us apply some of these results to a simple case of scattering by the potential of a hard elastic sphere of radius a. If the particles have low energy, the dominant contribution to the scattering comes from the partial wave l=0 (s wave scattering); this is so because if the particles have low energy, then they can attain a nonzero angular momentum only if they have a large impact parameter, and then they miss the sphere. Thus, for low-energy particles, the total cross section can be approximated by the first term in the sum (92):

$$\sigma \simeq \frac{4\pi}{k^2} \sin^2 \delta_0 \tag{95}$$

The phase shift δ_0 is easy to evaluate. In the presence of the hard-sphere potential, the wavefunction has a node at the surface of the sphere, that is, at r=a, whereas in the absence of the potential the wavefunction has a node at r=0. This means that the path of the wave coming in and then moving back out is shortened by 2a, and the phase of the outgoing wave is therefore shifted by 2ak relative to the outgoing wave in the absence of potential. Thus, $2\delta_0 = -2ak$, and Eq. (95) becomes

$$\sigma \simeq \frac{4\pi}{k^2} \sin^2{(-ak)}$$

or, since k is small,

¹¹ This simple method of calculating the phase shift for the hard sphere works for the l=0 partial wave only. The other partial waves experience an effective centrifugal potential, and their wavelengths are not constant and not equal to $2\pi/k$.

$$\sigma \simeq \frac{4\pi}{k^2} (ak)^2 = 4\pi a^2 \tag{96}$$

This quantum-mechanical scattering cross section is four times as large as the geometrical cross section of the hard sphere.

11.6 The Born Approximation; Rutherford Scattering

Equation (92) gives us the cross section if we know the phase shifts. However, the determination of the phase shifts requires the solution of the Schrödinger equation for each partial wave. As we saw in Section 11.1, such a determination of the phase shifts is quite tedious. Perturbation theory sometimes provides an alternative method for the calculation of the cross section. Here we will deal with a simple method of calculation based on Fermi's Golden Rule.

Suppose we regard the potential $V(\mathbf{r})$ that produces the scattering as a perturbation of the free-particle Hamiltonian. According to Fermi's Golden Rule, the rate of transitions from an initial momentum eigenstate $|\psi_{\mathbf{p}'}\rangle$ to a final momentum eigenstate $|\psi_{\mathbf{p}'}\rangle$ is then

$$W_{\mathbf{p} \to \mathbf{p}'} = \frac{2\pi}{\hbar} \langle \psi_{\mathbf{p}'} | V(\mathbf{r}) | \psi_{\mathbf{p}} \rangle \frac{dN(E)}{dE}$$
 (97)

With the box normalization for the wavefunctions and with the usual expression (10.79) for the number of states per unit energy interval, this transition rate becomes 12

$$W_{\mathbf{p}\to\mathbf{p}'} = \frac{2\pi}{\hbar} \left| \int \frac{e^{-i\mathbf{p}'\cdot\mathbf{r}/\hbar}}{\sqrt{V}} V(\mathbf{r}) \frac{e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}}{\sqrt{V}} d^3r \right|^2 \frac{V}{h^3} m\sqrt{2mE} d\Omega \qquad (98)$$

From this transition rate into the solid angle $d\Omega$, we immediately obtain the differential cross section by dividing by the incoming flux of particles [compare Eq. (10.101)]. Since the flux of particles associated with the incident wave is $(1/V)\sqrt{2E/m}$, the differential cross section is

$$d\sigma = \left(\frac{m}{2\pi\hbar^2}\right)^2 \left| \int V(\mathbf{r}) e^{i(\mathbf{p} - \mathbf{p}') \cdot \mathbf{r}/\hbar} d^3r \right|^2 d\Omega$$
 (99)

Accordingly, the scattering amplitude is

 $^{^{12}}$ Do not confuse the volume V with the potential V(r).

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \int V(\mathbf{r}) e^{i(\mathbf{p}-\mathbf{p}')\cdot\mathbf{r}/\hbar} d^3r$$
 (100)

Here, a minus sign has been inserted to bring Eq. (100) into conformity with the result obtained by an alternative calculation (via a Green's function) of the scattering amplitude. Equation (100) is called the *Born approximation* for the scattering amplitude.

If the potential is central, we can simplify the integral in Eq. (100) by introducing the vector

$$\mathbf{K} = \frac{\mathbf{p} - \mathbf{p}'}{\hbar} = \mathbf{k} - \mathbf{k}' \tag{101}$$

which is the difference between the wave vectors of the incident and the scattered particles. The magnitude of this vector is

$$K = |\mathbf{k} - \mathbf{k}'| = 2k \sin \frac{\theta}{2} \tag{102}$$

where θ is the scattering angle (see Fig. 11.13). The integration in Eq. (100) can then be performed by means of a change to spherical coordinates r, Θ , ϕ with a new z axis along the direction of K. This yields, with $\mu = \cos \Theta$,

$$f(\theta) = -\frac{m}{2\pi\hbar^2} \int_0^{2\pi} d\phi \int_0^{\infty} \int_0^{\pi} V(r) e^{iKr\cos\Theta} r^2 \sin\Theta d\Theta dr$$

$$= -\frac{m}{\hbar^2} \int_0^{\infty} r^2 V(r) \int_{-1}^1 e^{iKr\mu} d\mu dr$$

$$= -\frac{2m}{\hbar^2 K} \int_0^{\infty} rV(r) \sin Kr dr \qquad (103)$$

The Born approximation treats the potential as a perturbation of the free-particle Hamiltonian. Hence its validity is restricted to

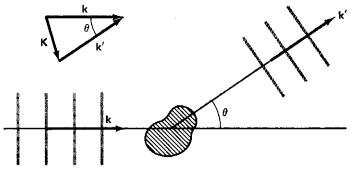


Fig. 11.13 Scattering of an incident plane wave by the interaction region.

kinetic energies that are large compared with the potential energy. This means that the Born approximation to some extent complements the method of partial waves. The Born approximation requires high energies, whereas the method of partial waves is best applied at low energies, where the angular momenta of the particles are small, and the first few terms in the infinite sum (92) suffice for an approximate evaluation of the cross section. Incidentally, the Born approximation fails to satisfy the optical theorem [according to Eq. (103), the scattering amplitude has no imaginary part]. This failure can be traced to the assumption of large kinetic energy and small potential energy implicit in this approximation.

Note that we cannot use the Born approximation for the Coulomb potential, since, with $V(r) \propto 1/r$, the integral (103) fails to converge. However, we can use it for the *screened Coulomb potential*, which has the form of the Coulomb potential with an extra exponential factor $e^{-r/b}$, where b is a positive constant:

$$V(r) = -\frac{Ze^2}{4\pi\varepsilon_0} \frac{e^{-r/b}}{r}$$
 (104)

This screened Coulomb potential approximately describes the potential experienced by an electron incident on an atom with many electrons, where the charge distribution of the electrons of the atom screens the nucleus from view. The appropriate value of the exponential decay length b for such an atom is approximately $4\pi\varepsilon_0\hbar^2/Z^{1/2}me^2$. A potential of the same mathematical form as (104)—but with a different value of b and a different overall constant of proportionality—also occurs in nuclear physics. This potential, called the Yukawa potential, describes the strong force acting between two nucleons.

For the screened Coulomb potential, the Born approximation gives us a scattering amplitude.

$$f(\theta) = \frac{2m}{\hbar^2 K} \frac{Ze^2}{4\pi\epsilon_0} \int_0^\infty e^{-r/b} \sin Kr \, dr$$
$$= \frac{2m}{\hbar^2} \frac{Ze^2}{4\pi\epsilon_0} \frac{1}{K^2 + 1/b^2}$$
(105)

¹³ This requirement can be relaxed if the potential is very shallow, roughly, if the potential is so shallow that it admits no bound state. For a simple discussion of the limitations of the Born approximation, see, for example, D. S. Saxon, *Elementary Quantum Mechanics*.

Hence the differential cross section is

$$\frac{d\sigma}{d\Omega} = |f(\theta)|^2 = \left(\frac{2m}{\hbar^2} \frac{Ze^2}{4\pi\epsilon_0}\right)^2 \frac{1}{(K^2 + 1/b^2)^2}$$
(106)

If we suppose that the incident electron has a high energy, so $K^2 \gg 1/b^2$, then we can neglect the term $1/b^2$ in the denominator of Eq. (106), and we obtain

$$\frac{d\sigma}{d\Omega} = \left(\frac{2m}{\hbar^2} \frac{Ze^2}{4\pi\epsilon_0}\right)^2 \frac{1}{K^4}$$

or, with $K = 2k \sin \frac{1}{2}\theta = 2(\sqrt{2mE}/\hbar) \sin \frac{1}{2}\theta$,

$$\frac{d\sigma}{d\Omega} = \left(\frac{Ze^2}{16\pi\varepsilon_0 E}\right)^2 \frac{1}{\sin^4 \frac{1}{2}\theta} \tag{107}$$

Here, the dependence on the exponential decay length has dropped out, because for a high-energy particle, most of the scattering occurs near the nucleus, where the potential is strongest and almost unscreened.

Equation (107) is the Rutherford cross section for the scattering of a particle of charge $\pm e$ by a nucleus of charge Ze. The cross section for the scattering of an alpha particle of charge 2e is four times as large as (107).

PROBLEMS

1. According to Eq. (3.48), the solutions of the time-dependent Schrödinger equation in one dimension satisfy the identity

$$\frac{\partial}{\partial t} \left(\psi^* \psi \right) = -\frac{\partial}{\partial x} \left[\frac{\hbar}{2im} \left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right) \right]$$

(a) Prove that if ψ is the wavefunction for a stationary state, then

$$\frac{\hbar}{2im}\left[\psi^*(x)\frac{\partial\psi(x)}{\partial x}-\psi(x)\frac{\partial\psi^*(x)}{\partial x}\right]=\text{constant}$$

- (b) Substitute the wavefunction (4) into this identity and thereby deduce that δ must be real.
- 2. (a) Prove that if ψ is a solution of the three-dimensional time-dependent Schrödinger equation, then

$$\frac{\partial}{\partial t} (\psi^* \psi) = -\nabla \cdot \left[\frac{\hbar}{2im} (\psi^* \nabla \psi - \psi \nabla \psi^*) \right]$$

(b) According to this equation, the quantity

$$\frac{\hbar}{2im} \left(\psi^* \; \nabla \psi - \psi \; \nabla \psi^* \right)$$

can be regarded as the probability current. Check that for a plane wave $\psi = e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}$, this probability current coincides with the product of probability density and velocity, that is, $\psi^*\psi \mathbf{p}/m$.

3. Figure 11.14 shows a potential barrier of height V_0 and width a placed adjacent to the origin. The potential is

$$V(x) = \begin{cases} \infty & \text{for } x < 0 \\ V_0 & \text{for } x < a \\ 0 & \text{for } x > a \end{cases}$$

Find the phase shift for this potential barrier, and plot as a function of the wave number k. Are there any resonances?

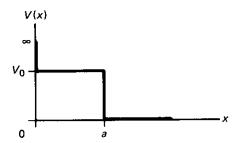


Fig. 11.14

- 4. Solve Eqs. (18) and (19) for the wave amplitude A in the interior of the square well.
- 5. Show that for scattering on a square well (see Fig. 11.3), the wave amplitude |A| can never exceed 1. Show that |A| equals 1 if $E = \hbar^2 \pi^2 (n + \frac{1}{2})^2 / 2ma^2 V_0$, and show that this condition corresponds to constructive interference of the de Broglie waves reflected back and forth across the well.
- 6. Show that the Wigner condition (66) implies that

$$\int_0^R |\psi|^2 dx \ge -\frac{1}{4k} \sin 2kR$$

7. Consider particles scattering on a hard sphere of radius a. If the particles have an energy $E = \hbar^2 k^2/2m$, roughly what impact parame-

ter is required to give angular momentum $l\hbar$? Roughly what range of values of l will contribute to the scattering on the hard sphere?

- 8. If the total cross section (92) is finite, show that δ_l must approach zero at least as fast as 1/l as $l \to \infty$.
- 9. In the scattering of particles of energy $E = \hbar^2 k/2m$ by a nucleus, an experimenter finds a differential cross section

$$\frac{d\sigma}{d\Omega} = \frac{1}{k^2} (0.86 + 3.07 \cos \theta + 2.77 \cos^2 \theta)$$

- (a) What partial waves are contributing to the scattering, and what are their phase shifts at the given energy?
- (b) What is the total cross section?
- 10. A free electron of momentum p initially directed along the positive z axis is perturbed by a potential

$$V(x, y, z) = \begin{cases} V_0 & \text{for } |x| < a, |y| < a, |z| < a \\ 0 & \text{for } |x| > a, |y| > a, |z| > a \end{cases}$$

where V_0 is a constant. Use Fermi's Golden Rule to find the scattering amplitude. Find the differential cross section $d\sigma$ (θ, ϕ) for transitions into a small solid angle $d\Omega$.

11. (a) In three dimensions, a particle is scattered elastically by a spherical potential well

$$V(r) = \begin{cases} -V_0 & \text{for } r < a \\ 0 & \text{for } r > a \end{cases}$$

where V_0 is positive. Use the one-dimensional results obtained in Section 11.2 to find the phase shift for the partial wave l = 0. If the energy of the particle is low, what is the differential cross section and what is the total cross section?

- (b) Footnote 3 gives the appropriate values of the parameters V_0 and a for the scattering of neutrons by protons in the triplet state. Evaluate the total cross section at an energy $E_{\rm cm} \ll 10$ MeV. (Note that the mass m in our equations must be interpreted as the reduced mass, $m \simeq \frac{1}{2}m_{\rm p}$.)
- (c) Footnote 4 gives the appropriate values of the parameters V_0 and a for the scattering of neutrons by protons in the singlet state. Evaluate the total cross section at an energy $E_{\rm cm} \ll 10$ MeV.
- 12. A particle is scattered elastically by a "soft sphere" with a repulsive spherical potential

$$V(r) = \begin{cases} V_0 & \text{for } r < a \\ 0 & \text{for } r > a \end{cases}$$

where V_0 is positive. Evaluate the phase shift for the partial wave l=0. If the energy of the particle is low, what is the differential cross section and what is the total cross section?

- 13. Integrate the differential cross section (106) over all angles and find the total cross section.
- 14. Consider the Gaussian potential

$$V(r) = V_0 \mathrm{e}^{-r^2/b^2}$$

Use the Born approximation to find the differential cross section and the total cross section.

15. The potential for a "soft sphere" is

$$V(r) = \begin{cases} V_0 & \text{for } r < a \\ 0 & \text{for } r > a \end{cases}$$

where V_0 is positive. Use the Born approximation to find the differential cross section and plot as a function of the scattering angle θ .