CHAPTER

14 Scattering in Three Dimensions

In this chapter an elementary description is offered of the quantum mechanical theory of scattering in three dimensions. Application of low-energy scattering is made to the Ramsauer effect, formerly encountered in Chapter 7, and scattering from a rigid sphere. The chapter continues with a discussion of the Born approximation. This important analysis permits certain scattering problems to be formulated in terms of harmonic perturbation theory developed previously in Chapter 13. The cross section of an atom interacting with a radiation field is obtained. For off-resonant incident phonons one encounters the line-shape factor. The chapter concludes with a description of the formal theory of scattering and derivation of the Lippmann–Schwinger equation in which the formalism of the interaction picture (Chapter 11) comes into play.

14.1 ■ PARTIAL WAVES

The Rutherford Atom

One of the most fundamental tools of physics used for probing atomic and subatomic domains involves scattering of known particles from a sample of the element in question. Thus, for example, the description of an atom as being comprised of a positively charged central core of radius $\simeq 10^{-13}$ cm, with external satellite electrons, is due to scattering experiments performed by E. Rutherford in 1911. In these experiments α particles in an incident beam were deflected in passing through a thin metal foil. The prevalent model for an atom at the time was J. J. Thomson's "plum pudding" model, in which negative electrons floated in a ball of positive charge. The relatively large angle suffered by a small fraction of the α

particles in the incident beam in Rutherford's experiments was found to be inconsistent with Thomson's model of the atom. For it is easily shown that α particles, after passing through hundreds of such spheres of distributed charge, are deflected at most only by a few degrees. On the other hand, the actual scattering data are consistent with an atomic model in which the positive charge is concentrated in a central core of small diameter. Large angle of scatter is then experienced by α particles which pass sufficiently close to the positive nucleus.

Scattering Cross Section

The typical configuration of a scattering experiment is shown in Fig. 14.1. A uniform monoenergetic beam of particles of known energy and current density $\mathbf{J}_{\text{inc}}$ (7.107) is incident on a target containing scattering centers. Such scattering centers might, for example, be the positive nuclei of atoms in a metal lattice. If the particles in the incident beam are, say, α particles, then when one such particle comes sufficiently close to one of the nuclei in the sample, it will be scattered. If the target sample is sufficiently thin, the probability of more than one such event for any particle in the incident beam is small and one may expect to obtain a valid description of the scattering data in terms of a single two-particle scattering event.

Let the scattered current density be $\mathbf{J}_{\text{sc}}$. Then the number of particles per unit time scattered through some surface element $d\mathbf{S}$ is $\mathbf{J}_{\text{sc}} \cdot d\mathbf{S}$. Let $d\mathbf{S}$ be at the radius $\mathbf{r}$ from the target. Then if $d\mathbf{\Omega}$ is the vector solid angle subtended by $d\mathbf{S}$ about the target origin, $d\mathbf{S} = r^2\, d\mathbf{\Omega}$ (see Figs. 9.9 and 14.1). The vector solid angle $d\mathbf{\Omega}$ is in the direction of $\mathbf{e}_r$; that is, $d\mathbf{\Omega} = \mathbf{e}_r\, d\Omega$. It follows that

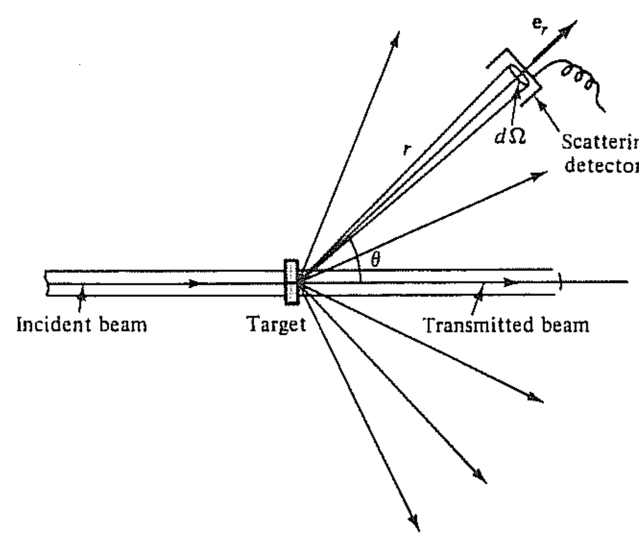


FIGURE 14.1 Scattering configuration.

$$\left.\begin{array}{l}\text{Number of particles}\\ \text{passing through } d\mathbf{S}\\ \text{per second}\end{array}\right\} = dN = \mathbf{J}_{sc} \cdot d\mathbf{S} = r^2 \mathbf{J}_{sc} \cdot d\mathbf{\Omega}$$

Since the number of such scattered particles will grow with the incident current $\mathbf{J}_{inc}$, one may assume this number to be proportional to $\mathbf{J}_{inc}$ and can equate

$$dN = r^2 \mathbf{J}_{sc} \cdot d\mathbf{\Omega} = \mathbf{J}_{inc}\, d\sigma \tag{14.1}$$

The proportionality factor $d\sigma$ is called the *differential scattering cross section* and has dimensions of cm^2. It may be interpreted as an obstructional area which the scatterer presents to the incident beam. Particles taken out of the incident beam by this obstructional area are scattered in $d\mathbf{\Omega}$. The *total scattering cross section* σ represents the obstructional area of scattering in all directions.

$$\sigma = \int d\sigma = \int_{4\pi} \left(\frac{d\sigma}{d\Omega}\right) d\Omega \tag{14.2}$$

Scattering cross section has a classical counterpart. Classically, the total cross section seen by a uniform beam of point particles incident on a fixed rigid sphere of radius a is $\sigma = \pi a^2$. If the incident beam has current $\mathbb{J}_{inc}$, the number per second scattered out of the beam in all directions is $\pi a^2 \mathbb{J}_{inc}$.

The Scattering Amplitude

Returning to quantum mechanics, let the particles in the incident beam be independent of each other so that prior to interaction with the target a particle in the incident beam may be considered a *free particle*. If the z axis is taken to coincide with the axis of incidence, then a particle in the incident beam with momentum $\hbar\mathbf{k}$ and energy $\hbar^2k^2/2m$ is in the plane-wave state,

$$\varphi_{inc} = e^{ikz} \tag{14.3}$$

When this wave interacts with a scattering center, an outgoing scattered wave φ_{sc} is initiated. If the scattering is *isotropic* so that scattering into all directions (all 4π steradians of solid angle) is equally probable, we can expect the scattered wave φ_{sc} to be a spherically symmetric outgoing wave. The specific form of an isotropic outgoing wave was described previously [(10.65) and Problem 10.6].

$$\varphi_{sc,\,iso} = \frac{e^{ikr}}{r}$$

More often, however, the scattered wave is anisotropic. Anisotropy of the scattering component wavefunction φ_{sc} may be described by a modulation factor $f(\theta)$, and in general we write

$$\varphi_{sc} = \frac{f(\theta)e^{ikr}}{r} \tag{14.4}$$

The modulation $f(\theta)$ is called the *scattering amplitude* and will be shown to determine the differential scattering cross section $d\sigma$.

The number of particles scattered into $d\mathbf{\Omega}$, which is in the direction of $\mathbf{e}_r$, is obtained from the radial component of $\mathbf{J}_{sc}$ [recall (7.107)]:

$$\begin{aligned}\mathbb{J}_{sc,\,r} &= \frac{\hbar}{2mi}\left(\varphi_{sc}{}^*\frac{\partial}{\partial r}\varphi_{sc} - \varphi_{sc}\frac{\partial}{\partial r}\varphi_{sc}{}^*\right) \\ &= \frac{\hbar k}{mr^2}|f(\theta)|^2\end{aligned} \tag{14.5}$$

Since the vector element of solid angle $d\mathbf{\Omega}$ is in direction $\mathbf{e}_r$, it follows that

$$r^2\mathbf{J}_{sc} \cdot d\mathbf{\Omega} = r^2\mathbb{J}_{sc,\,r}\, d\Omega = \mathbb{J}_{inc}\, d\sigma$$

In that the current vector of the incident beam only has a z component with magnitude $\hbar k/m$ [see Fig. 14.2], the preceding equation becomes

$$r^2\mathbb{J}_{sc,\,r}\, d\Omega = \frac{\hbar k}{m}\, d\sigma$$

Substituting (14.6) into this equation gives the desired relation,

$$\boxed{d\sigma = |f(\theta)|^2\, d\Omega} \tag{14.6}$$

Thus the problem of determining $d\sigma$ is equivalent to constructing the scattering amplitude $f(\theta)$.

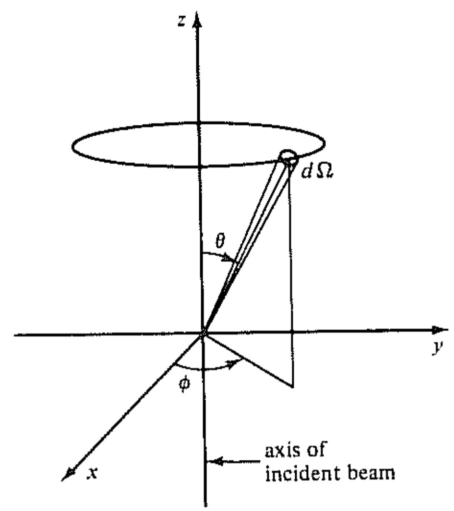


FIGURE 14.2 The scattering cross section is independent of the azimuthal angle ϕ for central potentials of interaction $V(r)$.

Owing to the rotational symmetry of the scattering configuration about the axis of the incident beam and the assumed radial quality of the interaction potential between incident particle and scatterer, the scattering cross section depends only on the scattering angle θ (and incident energy) and not on the azimuthal angle ϕ (see Fig. 14.2). It follows that, in integration (14.6) over all directions, the integration over $d\phi$ may be done separately to obtain 2π. There results

$$\sigma = \int d\sigma = 2\pi \int_0^{\pi} |f(\theta)|^2 \sin\theta \, d\theta \tag{14.7}$$

The total cross section is a simple integral over the square modulus of the scattering amplitude. Referring again to Fig. 14.2, we see that the same symmetry implies that $f(\theta)$ is an even function of θ or, equivalently, $f(\theta) = f(\cos\theta)$.

Partial-Wave Phase Shift

The form of the wavefunction for the steady-state scattering configuration described above, at positions far removed from the scattering target, will contain a plane-wave incident component and an "outgoing" scattered component:

$$\varphi(r, \theta) = e^{ikz} + \frac{f(\theta)e^{ikr}}{r} (r \to \infty) \tag{14.8}$$

(Fig. 14.3). The scattering amplitude is determined by matching (14.8) to the asymptotic form of the solution of the Schrödinger equation relevant to the configuration at hand. Such configuration includes a particle of mass m with known energy $\hbar^2k^2/2m$, interacting with a fixed scattering center through the central potential $V(r)$. The radial Schrödinger equation is given by (10.109).

$$\left[\frac{1}{r}\frac{d^2}{dr^2}r - \frac{l(l+1)}{r^2} + k^2 - \frac{2mV}{\hbar^2}\right] R_{kl}(r) = 0 \tag{14.9}$$

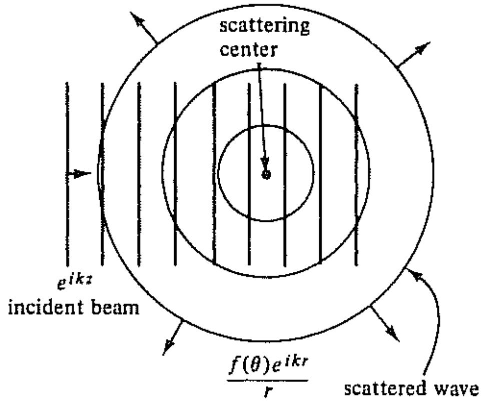


FIGURE 14.3 Incident plane wave and scattered outgoing spherical wave.

In the far field where $V(r)$ is rapidly approaching zero, one may expect the solution to this equation to be given approximately by the asymptotic form of the free-particle solution $j_l(kr)$ [see (10.55) and Table 10.1].

$$R_{kl} \sim \frac{1}{kr} \sin\left(kr - \frac{l\pi}{2}\right) \tag{14.10}$$

Provided that $V(r)$ decreases faster than r^{-1}, this free-particle asymptotic form remains intact[1] save for a change in argument through a phase shift δ_l.

$$R_{kl}{}^{\text{asm}} = \frac{1}{kr} \sin\left(kr - \frac{l\pi}{2} + \delta_l\right) \tag{14.11}$$

A superposition state comprised of these wavefunctions at fixed k has the form

$$\varphi_k(r, \theta) = \sum_{l=0}^{\infty} C_l R_{kl}{}^{\text{asm}} P_l(\cos\theta) \tag{14.12}$$

The lth term in the sum is called the lth *partial wave* and δ_l is the phase shift that the partial wave incurs in scattering.

We must now match the asymptotic form of the general solution (14.12) to the form (14.8). With the expansion of $\exp(ikz)$ given in Problem 10.12, we obtain the asymptotic expression

$$e^{ikz} \sim \sum_{l=0}^{\infty} (2l+1)i^l \frac{\sin(kr - l\pi/2)}{kr} P_l(\cos\theta)$$

The coefficients C_l and the scattering amplitude $f(\theta)$ are found from the matching equation

$$\sum_l C_l P_l(\cos\theta) \frac{\sin(kr - l\pi/2 + \delta_l)}{kr} = \sum_l (2l+1) i^l P_l(\cos\theta) \frac{\sin(kr - l\pi/2)}{kr} + \frac{f(\theta)e^{ikr}}{r}$$

Expanding $f(\theta)$ in a series of Legendre polynomials, one obtains, after some trigonometric gymnastics,

$$\begin{aligned} C_l &= i^l(2l+1)\exp(i\delta_l) \\ f(\theta) &= \frac{1}{k}\sum_{l=0}^{\infty} \frac{C_l}{i^l} \sin\delta_l P_l(\cos\theta) \end{aligned} \tag{14.13}$$

The problem of calculating $d\sigma$ or, equivalently, $f(\theta)$ is reduced to one of constructing the phase shifts of δ_l.

[1] For example, the analysis is not valid for the Coulomb potential $V(r) = r^{-1}$. Proof of the validity of the stated criterion may be found in L. Landau and E. Lifshitz, *Quantum Mechanics*, Addison-Wesley, Reading, Mass., 1958.

Two immediate results are evident: First, substituting the series (14.13) into (14.7) and taking advantage of the orthogonality of the $P_l(\cos\theta)$ polynomials, we obtain

$$\sigma = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l \tag{14.14}$$

The second result follows from setting $\theta = 0$ in (14.13), which yields

$$f(0) = \frac{1}{k}\sum_l (2l+1)\cos\delta_l \sin\delta_l + \frac{i}{k}\sum_l (2l+1)\sin^2\delta_l$$

Comparison with (14.14) reveals that

$$\sigma = \frac{4\pi}{k}\,\mathrm{Im}[f(0)] \tag{14.15}$$

This result is known as the *optical theorem*. It is a widely used relation connecting the forward scattering amplitude, $f(0)$, to the scattering in all directions, σ.[2]

Relative Magnitude of Phase Shifts

The problem of determining the partial wave phase shifts δ_l is often difficult. However, under certain conditions one may make simplifying assumptions which greatly facilitate calculation. In classical scattering one introduces the impact parameter. If L and p are the incident particle's angular momentum and linear momentum, respectively, then the impact parameter s is given by (see Fig. 14.4)

$$L = ps$$

Quite clearly, if the potential of interaction is appreciable only over the range r_0, then the interaction between incident particle and scatterer will be negligible for $s > r_0$. This criterion provides a useful rule of thumb applicable in quantum mechanics. With $L = \hbar\sqrt{l(l+1)} \simeq \hbar l$ and $p = \hbar k$, interaction will be negligible

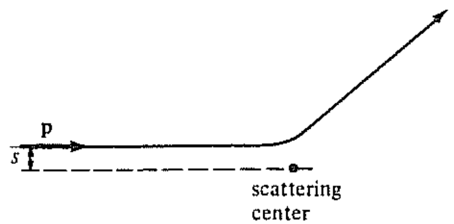


FIGURE 14.4 Classical trajectory and impact parameter s.

[2]For inelastic scattering, (14.15) is still valid with σ replaced by the total cross section, $\sigma_T = \sigma_S + \sigma_A$, where σ_S is the elastic cross section and σ_A is the absorption cross section.

if

$$l > r_0 k \tag{14.16}$$

The incident energy is $\hbar^2k^2/2m$.

Each partial wave in the superposition (14.12) represents a state of definite angular momentum. From (14.16) we can expect that partial waves with l values in excess of r_0k will suffer little or no shift in phase. In the corresponding expansion of the scattering amplitude $f(\theta)$ as given by (14.13) it follows that only those δ_l values will contribute for which $l < r_0k$. For low-energy scattering with $kr_0 \ll 1$, only the $l = 0$ phase shift will differ appreciably from zero. When such is the case (14.13) reduces to

$$f(\theta) = \frac{1}{k}e^{i\delta_0}\sin\delta_0 \tag{14.17}$$

which is independent of θ. The scattering is isotropic and is called S-wave scattering. Only the S partial wave ($l = 0$) contributes to the scattering. In the opposite extreme of large incident energies, $kr_0 \gg 1$, we can expect all partial waves to suffer phase shifts and the cross section to be anisotropic.

PROBLEMS

14.1 From (14.1) we find that the number of particles scattered into the solid angle $d\Omega$ per second is

$$dN = \mathbb{J}\,d\sigma$$

or, equivalently,

$$\frac{dN}{\mathbb{J}} = \left(\frac{d\sigma}{d\Omega}\right)d\Omega$$

The Coulomb cross section for the scattering of a charged particle of energy E and charge q from a fixed charge Q is

$$\frac{d\sigma}{d\Omega} = \left(\frac{qQ}{4E}\right)^2\frac{1}{\sin^4(\theta/2)}$$

(a) What is the expression for the fraction of particles scattered into the differential cone $(\theta, \theta + d\theta)$ from a target comprised of Λ scattering centers per unit area?

(b) Employ the expression you have obtained to find the fraction of α particles with incident energy 5 MeV which are scattered into a differential cone $(\theta, \theta + d\theta)$ at $\theta = \pi/2$, in passing through a gold sheet 1 μm thick.

Answers

(a) If we assume that each particle in the incident beam sees only one scatterer and that there is a scattering event for each scatterer, then

$$\delta N = \Lambda\left(\frac{d\sigma}{d\Omega}\right) d\Omega$$

e scattering into the cone $(\theta, \theta + d\theta)$

$$\delta N = \Lambda \int_0^{2\pi} d\phi \left(\frac{d\sigma}{d\Omega}\right) \sin\theta \, d\theta$$
$$= 2\pi\Lambda\left(\frac{d\sigma}{d\Omega}\right) \sin\theta \, d\theta$$

of mass density ρ, thickness l, comprised of atoms with atomic ass A,

$$\Lambda = \frac{\rho N_0 l}{A}$$

where N_0 is Avogadro's number (N_0 atoms have mass A grams). For a gold foil l cm thick with $\rho = 19.3\,\mathrm{g/cm^3}$ and $A = 197$, we obtain $\Lambda = 5.9 \times 10^{22}\, l$ atoms/cm^2. For α particles of energy 5 MeV scattered by the nuclei of gold atoms, $qQ/E = e^2 \cdot 2 \times 79/E = 4.6 \times 10^{-12}$ cm. Thus we obtain

$$\delta N(\pi/2) = \frac{\pi}{2}\left(\frac{qQ}{E}\right)^2 \frac{\rho N_0 l}{A}\, d\theta \simeq 2 \times 10^{-4}\, d\theta$$

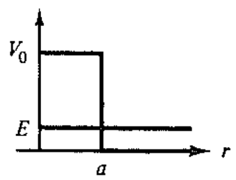
14.2 ■ S-WAVE SCATTERING

Let us consider the configuration of a low-energy beam of point particles of mass m scattering from a finite spherical attractive well of depth V_0 and radius a.

$$V(r) = \begin{cases} -V_0 & \text{for } r < a \\ 0 & \text{for } r > a \end{cases} \tag{14.18}$$

If we assume that energies are sufficiently small that $ka \ll 1$, we need only look at the S-wave scattering. The corresponding Schrödinger equation is obtained from (14.9). Setting $l = 0$ and $u \equiv rR$ there results, for $r < a$,

$$\frac{d^2u_1}{dr^2} + k_1 u_1 = 0$$
$$\frac{\hbar^2 k_1^2}{2m} = E + V_0$$



The solution to this equation which corresponds to $R(r)$ remaining finite at $r = 0$ is

$$u_1 = A \sin k_1 r \qquad (r < a)$$

For $r > a$, $V = 0$ and we obtain the general solution

$$u_2 = B \sin(kr + \delta_0) \qquad (r > a)$$
$$\frac{\hbar^2 k^2}{2m} = E$$

Boundary conditions require continuity of $d \ln u/dr$ at $r = a$, which gives

$$k_1 \cot k_1 a = k \cot(ka + \delta_0) \tag{14.19}$$

In that k_1 is finite, in the limit that k goes to zero,

$$\cot(ka + \delta_0) = \frac{k_1 \cot k_1 a}{k}$$

grows large so that $\sin(ka + \delta_0)$ grows small and we may set

$$\sin(ka + \delta_0) \simeq ka + \delta_0$$

Since $ka \ll 1$, this equation implies that $\delta_0 \ll 1$ as well. Under these conditions (14.19) reduces to

$$k_1 \cot k_1 a \simeq \frac{k}{ka + \delta_0}$$

or equivalently

$$\delta_0 = ka\left(\frac{\tan k_1 a}{k_1 a} - 1\right)$$

In that δ_0 is small, we may also set

$$\delta_0 \simeq \sin\,\delta_0 = ka\left(\frac{\tan k_1 a}{k_1 a} - 1\right)$$

We may now construct the scattering amplitude (14.17) and cross section (14.7).

$$\sigma = 4\pi a^2 \left(\frac{\tan k_1 a}{k_1 a} - 1\right)^2 \tag{14.20}$$

Two significant observations relevant to this study of attractive well scattering are discussed next.

S-Wave Resonances and Ramsauer Effect

First we note that when $k_1 a$ is an odd multiple of $(\pi/2)$, $\tan k_1 a$ is infinite and the cross section as given by (14.20) becomes singular. In that δ_0 is also infinite at these values of $k_1 a$, assumptions leading to (14.19) are violated and we must seek an alternative procedure to construct the cross section. Consider the relation (14.19), which assumes only that $ka \ll 1$. Let $k_1 a = n(\pi/2)$, where n is an odd number. At these values, (14.19) gives $\sin(\delta_0 + ka) = 1$, which with the condition $ka \ll 1$ yields $\sin \delta_0 \simeq 1$. Thus the maximum cross section at these *S-wave resonances* is

$$\sigma_{\max} = \frac{4\pi}{k^2}, \qquad k_1 a = n\left(\frac{\pi}{2}\right) \tag{14.21}$$

A more careful analysis pursued to higher angular momentum states, appropriate to larger incident energies, reveals corresponding resonances at $l = 1$, termed *P-wave resonances*, and so forth.

Whereas (14.20) suggests resonant scattering at odd multiples of $\pi/2$, it also indicates that the attractive scattering will become transparent to the incident beam at values of $k_1 a$ which satisfy the transcendental relation

$$\tan k_1 a = k_1 a$$

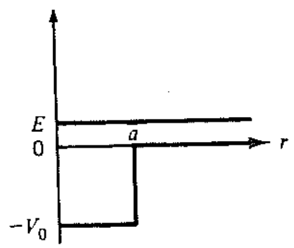
As noted in Section 7.8, such resonant transparency of an attractive well is experimentally corroborated in the scattering of low-energy electrons (~0.7 eV) by rare gas atoms and is termed the *Ramsauer effect*.

The Repulsive Sphere

The second observation related to our study of low-energy scattering by a scattering well is that merely changing the sign in the defining equations (14.18) produces the potential for a repulsive sphere of radius a. Solution for the corresponding scattering problem is effected by simply replacing k_1 by $i\kappa$, in the relations following (14.18). For the interior wavefunction we obtain

$$u_1 = A \sinh \kappa r \qquad (r < a)$$

$$\frac{\hbar^2 \kappa^2}{2m} = V_0 - E > 0$$



The exterior wavefunction u_2 maintains it sinusoidal dependence for $r > a$, as given in the equation preceding (14.19). Imposing boundary conditions at $r = a$ and, again assuming low-energy incident particles, we obtain the total scattering cross section,

$$\sigma = 4\pi a^2 \left(\frac{\tanh \kappa a}{\kappa a} - 1\right)^2 \tag{14.22}$$

In the limit that $V_0 \to \infty$, the sphere becomes impenetrable and the total cross section reduces to

$$\sigma = 4\pi a^2 \tag{14.23}$$

Since this formula does not contain $\hbar$, our suspicion is that it is also appropriate to the classical domain. However, the obstructional area imposed by a rigid sphere of radius a to an incident beam of classical particles has the value πa^2, so the quantum cross section is larger than the classical one by a factor of 4. Although the cross section (14.23) does not contain Planck's constant, nevertheless one might still object to considering it a classical result in that it is relevant to the strictly nonclassical domain of large de Broglie wavelength. If a classical result is to be obtained, it should emerge in the limit of large incident energy, $ka \gg 1$. Such analysis, which includes the phase shifts of all waves,[3] again yields a cross section independent of $\hbar$, namely

$$\sigma = 2\pi a^2, \qquad ka \gg 1$$

which is still larger than the classical result. Thus the classical cross section does not emerge in the limit of large incident energy. This discrepancy may be ascribed to the sharp edge of the spherical potential barrier for the configuration at hand. Across the sharp potential step, dV/dx is infinite and it is impossible for the classical criterion (7.166) to be satisfied.

PROBLEMS

14.2 The scattering amplitude for a certain interaction is given by

$$f(\theta) = \frac{1}{k}(e^{ika} \sin ka + 3ie^{i2ka} \cos \theta)$$

where a is a characteristic length of the interaction potential and k is the wavenumber of incident particles.

(a) What is the S-wave differential cross section for this interaction?

(b) Suppose that the above scattering amplitude is appropriate to neutrons incident on a species of nuclear target. Let a beam of 1.3-eV neutrons with current $10^{14}\ \mathrm{cm^{-2}\,s^{-1}}$ be incident on this target. What number of neutrons per second are scattered out of the beam into $4\pi \times 10^{-3}$ steradian about the forward direction?

14.3 Analysis of the scattering of particles of mass m and energy E from a fixed scattering center with characteristic length a finds the phase shifts

$$\delta_l = \sin^{-1}\left[\frac{(iak)^l}{\sqrt{(2l+1)l!}}\right]$$

[3]The calculation may be found in L. I. Schiff, *Quantum Mechanics*, 3d ed., McGraw-Hill, New York, 1968.

(a) Derive a closed expression for the total cross section as a function of incident energy E.

(b) At what values of E does S-wave scattering give a good estimate of σ?

Answer (partial)

(a)
$$\sigma = \frac{4\pi\hbar^2}{2mE}\exp\left(\frac{-2mEa^2}{\hbar^2}\right)$$

14.3 ■ CENTER-OF-MASS FRAME

In all of the preceding analysis, it has been assumed that the target particle remains fixed during the scattering process. This is the case if the mass of the target particle far exceeds that of the incident particle. More generally, however, the recoil motion of the target particle must be taken into account in any scattering analysis. Thus the general formulation of a scattering event involves two particles, of mass m_1 and m_2.

As described in Section 10.5, the motion of such two-particle systems may be described in terms of the motion of the center of mass and motion relative to the center of mass. The Hamiltonian of the relative motion (10.99) describes a single effective particle with reduced mass $\mu = m_1m_2/(m_1+m_2)$ at the radius $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$. This is the motion observed in a frame moving with the center of mass. So, in fact, in this center-of-mass frame, the scattering event may be described by a single particle of mass μ interacting with a potential $V(r)$ centered at a fixed origin. It follows that the preceding formulation of the cross section $\sigma(\theta)$ describing scattering from a fixed scattering center is appropriate to scattering in the center-of-mass frame. The only change is that the mass m of the incident particle is set equal to the reduced mass μ. In addition, we must note that the angle of deflection θ is measured in the center-of-mass frame. For example, in the expression (14.13) for the scattering amplitude, θ is the angle of scatter in the center-of-mass frame, which will henceforth be called θ_C. To obtain a relation between the scattering cross section $\sigma_L(\theta_L)$ in the frame of the experiment, or what is commonly called the *lab frame* and the cross section $\sigma_C(\theta_C)$ as measured in the center-of-mass frame, we note the following. The number of particles scattered into an element of solid angle in the lab frame $\mathbb{J}_{\text{inc}}(d\sigma_L/d\Omega_L)\,d\Omega_L$ is equal to the number scattered into the corresponding solid angle in the center-of-mass frame, $\mathbb{J}_{\text{inc}}(d\sigma_C/d\Omega_C)\,d\Omega_C$. This gives the equality

$$\frac{d\sigma_L}{d\cos\theta_L} = \frac{d\sigma_C}{d\cos\theta_C}\frac{d\cos\theta_C}{d\cos\theta_L} \tag{14.24}$$

The relation between $\cos\theta_C$ and $\cos\theta_L$ is obtained by examining the scattering in both frames. In transforming from one frame to the other, it is convenient to speak in terms of velocities. Such velocities are related to linear momentum through the prescription $\mathbf{v} = \hbar\mathbf{k}/m$. When one describes an "orbit" in this description, one has in mind a picture inferred by the direction of momentum $\mathbf{k}$ vectors. Thus,

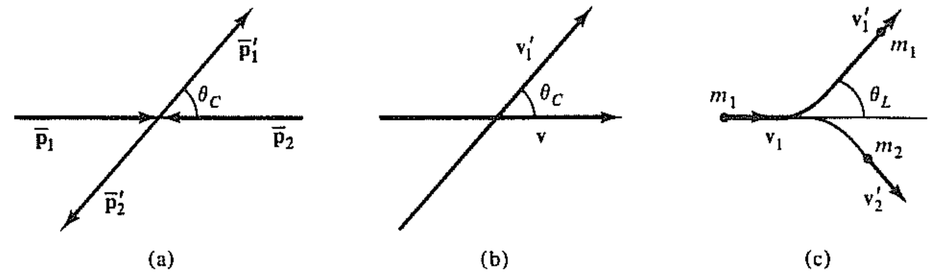


FIGURE 14.5 (a) In the center-of-mass frame, the total momentum is zero. (b) The relative velocity vector $\mathbf{v}$ rotates through the angle θ_C. (c) In the lab frame, m_2 is assumed to be at rest before collision.

before collision, m_2 is at rest and the incident particle has velocity $\mathbf{v}_1 = \hbar\mathbf{k}/m_1$. After collision, m_1 is scattered through the angle θ_L.

The center-of-mass frame is characterized by the property that *total momentum in that frame is zero before and after collision* (Fig. 14.5). Letting barred variables denote values in the center-of-mass frame, and $\mathbf{v}$ the *relative velocity*,

$$\mathbf{v} \equiv \mathbf{v}_1 - \mathbf{v}_2$$

one obtains, for before the collision

$$\bar{\mathbf{p}}_1 = m_1(\mathbf{v}_1 - \mathbf{v}_{\text{CM}}) = \mu\mathbf{v}$$

We may immediately conclude that

$$\bar{\mathbf{p}}_2 = -\mu\mathbf{v}$$

In a similar manner, after collision we write

$$\bar{\mathbf{p}}_1{}' = \mu\mathbf{v}'$$
$$\bar{\mathbf{p}}_2{}' = -\mu\mathbf{v}'$$

or, equivalently,

$$\bar{\mathbf{v}}_1{}' = \frac{\mu}{m_1}\mathbf{v}'$$
$$\bar{\mathbf{v}}_2{}' = -\frac{\mu}{m_2}\mathbf{v}'$$

The corresponding relations in the lab frame are obtained by adding $\mathbf{v}_{\text{CM}}$ to the right-hand sides of these equations. Multiplying the resulting equations by m_1 and m_2, respectively, gives

$$\mathbf{p}_1{}' = \mu\mathbf{v}' + \frac{\mu}{m_2}\mathcal{P}$$

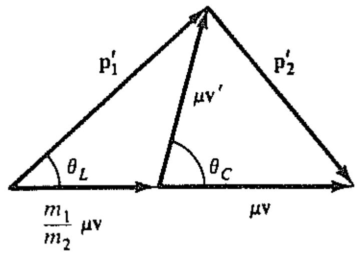


FIGURE 14.6 Orientation of momentum and relative velocity for $m_1/m_2 < 1$.

$$\mathbf{p}_2' = -\mu\mathbf{v}' + \frac{\mu}{m_1}\mathcal{P} \tag{14.25}$$

$$\mathcal{P} = \mathbf{p}_1 + \mathbf{p}_2$$

Since m_2 is at rest before scattering, $\mathbf{p}_1 = m_1\mathbf{v} = \mathcal{P}$. It follows that (14.25) may be rewritten

$$\begin{aligned} \mathbf{p}_1' &= \mu\mathbf{v}' + \frac{m_1}{m_2}\mu\mathbf{v} \\ \mathbf{p}_2' &= -\mu\mathbf{v}' + \mu\mathbf{v} \end{aligned} \tag{14.26}$$

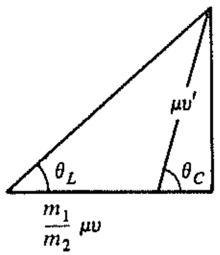


FIGURE 14.7 Triangle used to obtain relation between θ_L and θ_C.

These vector equations imply the vector diagrams shown in Fig. 14.6. The desired relation between θ_L and θ_C is obtained by constructing $\tan\theta_L$ from the partial diagram shown in Fig. 14.7:

$$\tan\theta_L = \frac{\mu v' \sin\theta_C}{(m_1/m_2)\mu v + \mu v' \cos\theta_C} \tag{14.27}$$

Now H_{rel} is a conserved quantity throughout the scattering. Prior to, and after collision, H_{rel} is purely kinetic and has the respective values $\mu v^2/2$, $\mu v'^2/2$. It follows that the magnitude of the relative velocity is maintained in scattering

$$v = v'$$

Substituting this equality into (14.27) gives the desired relation,

$$\tan\theta_L = \frac{\sin\theta_C}{\epsilon + \cos\theta_C} \qquad \left(\epsilon \equiv \frac{m_1}{m_2}\right) \tag{14.28}$$

This relation permits completion of (14.24):

$$\frac{d\sigma_L}{d\cos\theta_L} = \frac{d\sigma_C}{d\cos\theta_C}\frac{(1+\epsilon^2+2\epsilon\cos\theta_C)^{3/2}}{1+\epsilon\cos\theta_C} \tag{14.29}$$

If the mass of the scatterer is very much larger than that of the incident particle, we may set $\epsilon = 0$ and the cross sections in both frames are equal. From (14.28) in this same extreme we obtain $\theta_L = \theta_C$.

In general, as (14.29) implies, scattering that is isotropic in the center-of-mass frame is not isotropic in the lab frame. For example, the isotropic cross section obtained for S-wave scattering (14.17),

$$\left(\frac{d\sigma}{d\Omega}\right)_C = |f(\theta)|^2 = \frac{\sin^2\delta_0}{k^2}$$

when substituted in (14.29) yields [with (14.28)] an anisotropic cross section in the lab frame:

$$\left(\frac{d\sigma}{d\Omega}\right)_L = \frac{\sin^2\delta_0}{k^2}\frac{(1+\epsilon^2+2\epsilon\cos\theta_C)^{3/2}}{1+\epsilon\cos\theta_C} \tag{14.30}$$

Applications of results developed in this section appear in problems to follow. Whereas our primary example in the preceding analysis is relevant to low-energy scattering, where the potential of interaction plays a dominant role, the analysis to be developed in Section 14.4 addresses the case where the potential of interaction acts as a small perturbation on the incident plane-wave state. This analysis, known as the Born approximation, has many applications.

PROBLEMS

14.4 Assume that the differential cross section for a given interaction potential $d\sigma/d\Omega$ is isotropic in the center-of-mass frame. For mass ratio $\epsilon \ll 1$, what is the ratio of the differential cross section in the forward direction to that in the $\theta = \pi/2$ direction in the lab frame?

Answer

$$\frac{d\sigma(0)}{d\sigma(\pi/2)} = 1 + 2\epsilon$$

14.5 At what value of θ_C will the cross section vanish in the lab frame for S-wave scattering of two particles with mass ratio ϵ?

14.4 ■ THE BORN APPROXIMATION

Harmonic perturbation theory, developed in Chapter 13, includes as a special case the example of a constant potential that has been turned on for t seconds. The perturbation Hamiltonian[4] is then given by (13.53) with $\omega = 0$. As was shown in Section 13.6, the theory of harmonic perturbation leads naturally to Fermi's formula (13.64) for cases where final states comprise a continuum. Such, of course, is the situation for scattering problems.

[4] For the case $\omega = 0$, the factor 2 is deleted in (13.53).

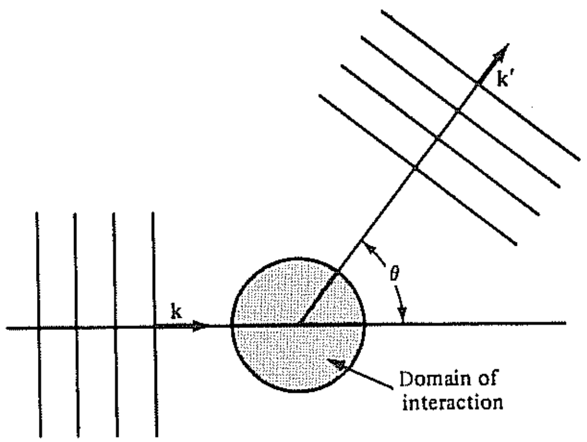


FIGURE 14.8 In the Born approximation, incident and scattered particles are in plane-wave states.

For these problems the perturbation Hamiltonian is the interaction potential, which is viewed as being "turned on" during the time that the incident particle is in the range of the potential. The incident particle enters the range of interaction with momentum $\hbar\mathbf{k}$ and leaves the range of interaction with momentum $\hbar\mathbf{k}'$. Such states of definite $\mathbf{k}$ before and after interaction correspond to plane-wave states (Fig. 14.8). Let us suppose that the scattering experiment is performed in a large cubical box of volume L^3. Normalized plane-wave states corresponding to $\mathbf{k}$ and $\mathbf{k}'$ are then given by

$$
\begin{aligned}
|\mathbf{k}\rangle &= \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{L^{3/2}} \\
|\mathbf{k}'\rangle &= \frac{e^{i\mathbf{k}'\cdot\mathbf{r}}}{L^{3/2}}
\end{aligned}
\tag{14.31}
$$

To apply Fermi's formula (13.64) for the rate of transition from the $\mathbf{k}$ to the $\mathbf{k}'$ state, caused by the perturbing potential $V(r)$,

$$\overline{w}_{\mathbf{k}\mathbf{k}'} = \frac{2\pi}{\hbar} g(E_{k'})|\langle\mathbf{k}'|V|\mathbf{k}\rangle|^2 \tag{14.32}$$

we must know the density of final states $g(E_{k'})$. Having prescribed that the scattering experiment is performed in a large box of volume L^3, we may employ the expression for $g(E)$ as given by (8.141). Written in terms of final momentum $\hbar k'$, this expression becomes for nonspinning particles[5]

$$g(E_{k'}) = \frac{mL^3k'}{2\pi^2\hbar^2} \tag{14.33}$$

[5]The g factor in Problem 2.42 represents density of states per unit volume.

Now we wish to use the rate formula (14.32) to obtain an expression for the differential scattering cross section $d\sigma$. This parameter was defined by (14.1) according to which the number of particles scattered into $d\boldsymbol{\Omega}$ per second is $\mathbb{J}_{\text{inc}}\, d\sigma$. To relate the transition rate $\overline{w}_{\mathbf{k}\mathbf{k}'}$ to $d\sigma$, we note that the incident plane wave $|\mathbf{k}\rangle$ given in (14.31) corresponds to an incident current

$$\mathbf{J}_{\text{inc}} = \frac{\hbar\mathbf{k}}{mL^3} \tag{14.34}$$

In that $g(E_k)$ as given by (14.33) is isotropic in $\mathbf{k}'$, it represents the density of final $\mathbf{k}'$ states in all 4π solid angle. To select those scattered states that lie in the direction $d\boldsymbol{\Omega}$ about $\mathbf{k}'$, we multiply g by the ratio $d\Omega/4\pi$. With $g(E_{k'})$ so augmented, $\overline{w}_{\mathbf{k}\mathbf{k}'}$ then represents the rate at which particles of the incident flux (14.34) are scattered into $d\boldsymbol{\Omega}$ in the direction of $\mathbf{k}'$. This rate is by definition the product $\mathbb{J}_{\text{inc}}\, d\sigma$. Thus we obtain the desired relation

$$\mathbb{J}_{\text{inc}}\, d\sigma = \frac{d\Omega}{4\pi}\overline{w}_{\mathbf{k}\mathbf{k}'}$$

Inserting previous expressions, we obtain

$$\frac{d\sigma}{d\Omega} = \left(\frac{mL^3}{2\pi\hbar^2}\right)^2 \frac{k'}{k}|\langle\mathbf{k}'|V|\mathbf{k}\rangle|^2 \tag{14.35}$$

Since particles suffer no loss in energy in the scattering process, we may equate

$$k = k'$$

The Scattering Amplitude

Recalling (14.6), which relates $d\sigma$ to the scattering amplitude $f(\theta)$, and inserting the explicit forms (14.31) for incident and scattered states into (14.35), allows the identification (with a conventional minus sign)

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\int V(r)e^{i\mathbf{r}\cdot(\mathbf{k}-\mathbf{k}')}\, d\mathbf{r} \tag{14.36}$$

This formula for the scattering amplitude may be further simplified through the substitution

$$\mathbf{K} = \mathbf{k} - \mathbf{k}'$$

As is evident in Fig. 14.9a, owing to the equal magnitudes of $\mathbf{k}$ and $\mathbf{k}'$, we may set

$$K = 2k\sin\left(\frac{\theta}{2}\right)$$

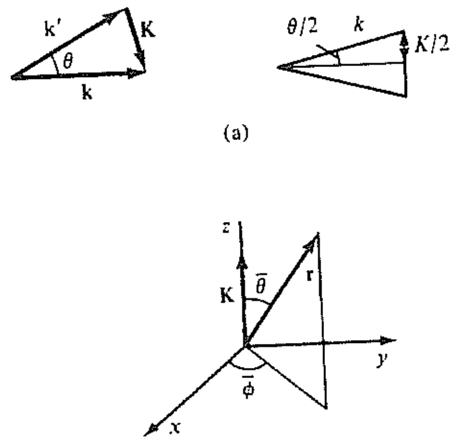


FIGURE 14.9 (a) Transformation $\mathbf{K} = \mathbf{k} - \mathbf{k}'$. (b) Spherical coordinate frame with $\mathbf{K}$ aligned with the polar axis.

where θ is the angle of scatter. With the differential volume of integration $d\mathbf{r}$ in (14.36) written in spherical coordinates and the polar axis taken to be coincident with $\mathbf{K}$ (Fig. 14.9b), we obtain

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

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

Integration over $\eta \equiv \cos\bar{\theta}$ gives

$$\boxed{f(\theta) = -\frac{2m}{\hbar^2 K}\int_0^{\infty} dr\, r V(r)\sin Kr} \qquad (14.37)$$

This expression for the scattering amplitude is called the *standard form of the Born approximation*.

In applying this formula for the scattering amplitude, one should keep in mind that it is derived on the basis of perturbation theory according to which the scattering potential should be small compared to the free-particle (unperturbed) Hamiltonian. This will be the case for sufficiently large incident energies or sufficiently weak strengths of potential.

The Shielded Coulomb Potential

Let us apply (14.37) to calculate the cross section for the shielded Coulomb potential,[6]

$$V(r) = -\frac{Ze^2\exp(-r/a)}{r}$$

The exponential factor for $r > a$ acts to shield the bar Coulomb potential Ze^2/r between two particles with respective charges Ze and e. Thus beyond the range a, the potential is exponentially small. Within the range, $r < a$, the potential is essentially Coulombic. Substituting the shielded Coulomb potential into (14.37) gives

$$f(\theta) = \frac{2mZe^2}{\hbar^2 K}\int_0^{\infty} e^{-r/a}\sin Kr\, dr$$

$$= \frac{2mZe^2}{\hbar^2}\frac{1}{K^2 + (1/a)^2}, \qquad K = 2k\sin\left(\frac{\theta}{2}\right)$$

The corresponding scattering cross section is obtained from (14.6).[7]

$$\frac{d\sigma}{d\Omega} = \frac{(2mZe^2/\hbar^2)^2}{[K^2 + (1/a)^2]^2} \qquad (14.38)$$

In the limit of large incident energies $K^2 \gg a^{-2}$, the predominant contribution to $d\sigma$ is due to the bare Coulomb potential. The resulting cross section, employed previously in Problem 14.1, appears as

$$\frac{d\sigma}{d\Omega} = \left[\frac{Ze^2}{4(\hbar^2 k^2/2m)\sin^2(\theta/2)}\right]^2 \qquad (14.39)$$

$$= \left(\frac{Ze^2}{4E}\right)^2\frac{1}{\sin^4(\theta/2)}, \qquad E = \frac{\hbar^2 k^2}{2m}$$

This is the precise expression for the Rutherford cross section for the scattering of a charged particle with charge e and mass m from a fixed charge Ze, which is seen to be dominated by forward scattering ($\theta \approx 0$). Furthermore, the classical evaluation of the Rutherford cross section also gives (14.40), with $E = p^2/2m$.

[6]This potential enters in three independent areas of physics, where it carries the following names: in plasma physics, the *Debye potential*; in high-energy physics, the *Yukawa potential*; in solid-state physics, the *Thomas–Fermi potential*.

[7]With m replaced by the reduced mass μ, (14.38) represents the cross section in the center-of-mass frame.

PROBLEMS

14.6 Using the Born approximation, evaluate the differential scattering cross section for scattering of particles of mass m and incident energy E by the repulsive spherical well with potential

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

Exhibit explicit E and θ dependence.

Answer

$$\frac{d\sigma}{d\Omega} = \left(\frac{2mV_0}{\hbar^2 K^3}\right)(\sin Ka - Ka\cos Ka)^2$$

$$\hbar K = 2\sqrt{2mE}\,\sin(\theta/2)$$

14.7 Using the Born approximation, obtain an integral expression for the total cross section for scattering of particles of mass m from the attractive Gaussian potential

$$V(r) = -V_0 \exp\left[-\left(\frac{r}{a}\right)^2\right]$$

14.8 An important parameter in scattering theory is the scattering length a. This length is defined as the negative of the limiting value of the scattering amplitude as the energy of the incident particle goes to zero.

$$a = -\lim_{k\to 0} f(\theta)$$

(a) For low-energy scattering and relatively small phase shift, show that

$$a = -\lim_{k\to 0}\frac{\delta_0}{k}$$

(b) For the same conditions as in part (a), show that

$$\sigma = 4\pi a^2$$

(c) What is the scattering length for point particles scattering from a rigid sphere of arbitrary radius $\bar{a}$?

14.5 ■ ATOMIC-RADIATIVE ABSORPTION CROSS SECTION

Returning to our analysis of Section 13.9, again we consider a flux of photons incident on an atom, carrying one photon per unit volume. Since the photon moves with speed c, this gives an incident photon current

$$J_{\text{inc}} = c \times \frac{1\text{ photon}}{\text{cm}^3} = c\left(\frac{\text{photons}}{\text{cm}^2\text{ s}}\right) \tag{14.40}$$

There is a probability rate for each photon in the incident current to be absorbed by the atom. The principle of microscopic reversibility allows us to equate this probability rate for absorption to the corresponding probability rate of atomic decay.

With Fermi's golden rule (13.64) we may then write the probability rate for atomic absorption as

$$w_{nn'} = \frac{2\pi}{\hbar}|\langle n', \mathbf{k}|\mathbb{H}_-|n\rangle|^2\frac{g(\omega)}{\hbar} \tag{14.41}$$

where we have made the replacement

$$g(E) = \frac{g(\omega)}{\hbar}$$

[See (13.111b) and recall that $g(E) = 8\pi\overline{g}(E)$ and that $V = 1$.] With (13.106), our preceding equation (14.41) becomes

$$w_{nn'} = \frac{2\pi}{\hbar}e^2(2\pi\hbar\omega)\frac{g(\omega)}{\hbar}|\langle n'|\mathbf{a}\cdot\mathbf{r}|n\rangle|^2 \tag{14.42}$$

If the polarization unit vector $\mathbf{a}$ of the incident field is randomly oriented, then as was previously demonstrated in our discussion of the Einstein B coefficient (Section 13.7), we may set

$$|\langle n'|\mathbf{a}\cdot\mathbf{r}|n\rangle|^2 = \frac{1}{3}r_{nn'}{}^2 = \frac{1}{3}\frac{d_{nn'}{}^2}{e^2} \tag{14.43}$$

Here we have reintroduced the dipole moment $\mathbf{d}$ (13.69).

With (14.43) placed into (14.42) we find

$$w_{nn'} = \frac{4}{3}\frac{\pi^2\omega\, d_{nn'}{}^2}{\hbar}g(\omega) \tag{14.44}$$

This is the probability rate for an atom to absorb a photon from an incident current carrying one photon per unit volume. Since the incident current in the present configuration is so normalized, $w_{nn'}$ represents the rate at which photons are absorbed by the atom from the incident beam. With our previous definition of cross section we may then write

$$J_{\text{inc}}\sigma_{nn'} = w_{nn'} \tag{14.45}$$

Note the dimensions:

$$J_{\text{inc}}\left(\frac{\text{photons}}{\text{cm}^2\text{ s}}\right) \times \sigma(\text{cm}^2) = W_{nn'}\left(\frac{1}{\text{s}}\right)$$

With (14.40) and (14.45) we obtain the total cross section,

$$\sigma_{nn'} = \frac{4}{3}\frac{\pi^2\omega\, d_{nn'}{}^2}{\hbar c}g(\omega) \tag{14.46}$$

bsorption at the incident frequency

$$\hbar\omega = E_n - E_{n'}$$

e description of this process includes the possibility of absorp-
tons which are off-resonance. For such cases, with $\varpi \equiv \omega_{nn'}$,
d to the form

$$\sigma(\varpi, \omega) = \frac{4}{3}\frac{\pi^2 d^2}{\hbar c}\varpi g(\varpi, \omega) \tag{14.47}$$

e we have set

$$g(\omega) \to g(\varpi, \omega)$$

The function $g(\varpi, \omega)$ is the so-called *line-shape factor*.

A realistic expression for $g(\varpi, \omega)$ which is appropriate to many line-broadening processes is the *Lorentzian line-shape factor*,

$$g_L(\varpi, \omega) = \frac{1}{\pi}\frac{\Delta\omega_L/2}{(\varpi - \omega)^2 + (\Delta\omega_L/2)^2} \tag{14.48}$$

See Fig. 14.10.

The spreading of an absorption line is attributed to relaxation processes—such as, for example, the relaxation of excited atomic states incurred in atomic collisions. If τ represents the decay time for such processes, then one sets

$$\frac{\Delta\omega_L}{2} = \frac{1}{\tau}$$

In the idealized limit that these states last indefinitely, $\Delta\omega_L \to 0$, and $g_L(\varpi, \omega)$ becomes sharply peaked about $\omega = \varpi$. In this limit (14.47) becomes

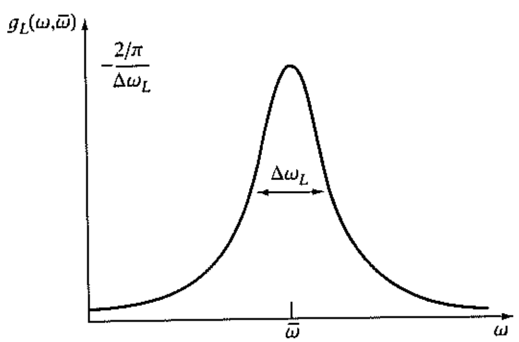


FIGURE 14.10 Lorentzian line shape.

$$\sigma(\varpi, \omega) = \frac{4}{3}\frac{\pi^2 d^2}{\hbar c}\varpi\,\delta(\omega - \varpi) \tag{14.49}$$

Here we have employed the delta-function representation (C.9).

14.6 ■ ELEMENTS OF FORMAL SCATTERING THEORY. THE LIPPMANN–SCHWINGER EQUATION

In this concluding section we present a brief introduction to the formal theory of scattering, central to which is the Lippmann–Schwinger equation.[8] An elementary derivation of this equation is presented based on the interaction picture described previously in Section 11.12. The Lippmann–Schwinger equation so derived appears in a form independent of representation. Writing this equation in coordinate representation is found to give an integral equation for scattered states, which in turn gives a general expression for the scattering amplitude. In the Born approximation this relation returns our previous expression for $f(\theta)$ given by (14.36).

We consider the Hamiltonian

$$\hat{H} = \hat{H}_0 + \hat{V}e^{-\varepsilon|t|/\hbar} \tag{14.50}$$

where $\hat{H}_0$ is the free-particle Hamiltonian and the infinitesimal parameter ε has dimensions of energy. The interaction $\hat{V}$ is assumed to be independent of time. For small ε the exponential factor has the effect of "turning on" the interaction $\hat{V}$ in the interval about $t = 0$. We will also find that the presence of this factor insures convergence of integration in the derivative to follow (in both limits $t \to \pm\infty$).

Recall that the Schrödinger equation in the interaction picture has the integral form (11.144),[9]

$$|\psi_I(t)\rangle = |\psi_I(t_0)\rangle + \frac{1}{i\hbar}\int_{t_0}^{t}\hat{V}_I(t')|\psi_I(t')\rangle\,dt' \tag{14.51}$$

where, we recall,

$$|\psi_I(t)\rangle = e^{it\hat{H}_0/\hbar}|\psi(t)\rangle \tag{14.52a}$$

$$\hat{V}_I(t) = e^{it\hat{H}_0/\hbar}\hat{V}e^{-itH_0/\hbar} \tag{14.52b}$$

As we wish to apply (14.51) to scattering theory, we stipulate that $\hat{V}_I(t) \to 0$ in the limits $t \to \pm\infty$. At these asymptotic values, with the interaction vanishingly small, $|\psi_I(t)\rangle$ loses its time dependence, and we define

[8]For further discussion, see E. Merzbacher, *Quantum Mechanics*, 2d ed., Wiley, New York, 1970, Chapter 19.

[9]Ket notation is employed to obtain a relation independent of representations.

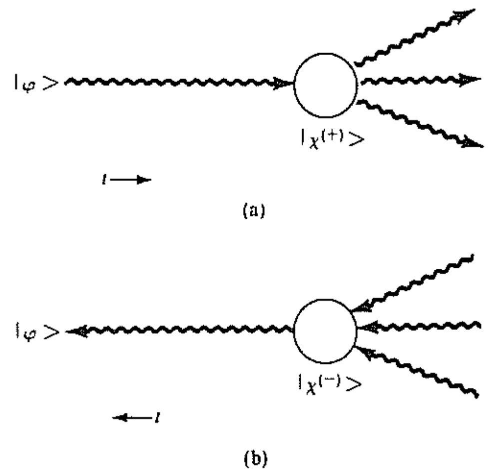


FIGURE 14.11 (a) "In" solution. (b) "Out" solution.

$$|\varphi\rangle \equiv |\psi_I(\pm\infty)\rangle \tag{14.53}$$

which may be identified as free-particle states.

Rewriting (14.51) over the interval $t_0 = \pm\infty$, $t = 0$, and identifying the scattering states

$$|\psi^{(\pm)}\rangle \equiv |\psi(0)\rangle \tag{14.54}$$

gives the equation

$$|\psi^{(\pm)}\rangle = |\varphi\rangle + \frac{1}{i\hbar}\int_{\mp\infty}^{0} \hat{V}_I(t)|\psi_I(t)\rangle\, dt \tag{14.55}$$

Note that with this choice of interval, $|\psi^{(\pm)}\rangle$, given by (14.54), represents scattered states in the domain of interaction. Furthermore, as $|\psi^{(+)}\rangle$ is relevant to the time interval $(-\infty \le t \le 0)$, we may identify it with incoming incident waves, commonly called the "in" solution. As $|\psi^{(-)}\rangle$ relates to the interval $(\infty, 0)$, it is the time-reversed state of $|\psi^{(+)}\rangle$ and is commonly called the "out" solution. See Fig. 14.11. In the limit $\varepsilon \to 0$ we take $|\psi^{(\pm)}\rangle$ to be an eigenstate of the total Hamiltonian and write

$$\hat{H}|\psi^{(\pm)}\rangle = E|\psi^{(\pm)}\rangle \tag{14.56}$$

Reduction of Interaction Integral

Consider the integrand in (14.55). With (14.52a,b) we write

$$\begin{aligned}\hat{V}_I(t)|\psi_I(t)\rangle &= e^{i\hat{H}_0 t/\hbar}\hat{V}e^{-\varepsilon|t|/\hbar}e^{-i\hat{H}_0 t/\hbar}e^{i\hat{H}_0 t/\hbar}|\psi(t)\rangle \\ &= e^{i\hat{H}_0 t/\hbar}\hat{V}e^{-\varepsilon|t|/\hbar}e^{-i\hat{H}t/\hbar}|\psi(0)\rangle\end{aligned} \tag{14.57}$$

and note

$$|\psi(0)\rangle = |\psi_I(0)\rangle = |\psi^{(\pm)}\rangle$$

Substituting this identification into (14.57) followed by replacement of (14.57) into (14.55) gives

$$|\psi^{(\pm)}\rangle = |\varphi\rangle + \frac{1}{i\hbar}\int_{\mp\infty}^{0} e^{i\hat{H}_0 t/\hbar}\hat{V}e^{-\varepsilon|t|/\hbar}e^{-i\hat{H}t/\hbar}|\psi^{(\pm)}\rangle\, dt \tag{14.58}$$

With (14.56) the preceding becomes

$$|\psi^{(\pm)}\rangle = |\varphi\rangle + \frac{1}{i\hbar}\int_{\mp\infty}^{0} e^{i\hat{H}_0 t/\hbar}\hat{V}e^{-\varepsilon|t|/\hbar}e^{-iEt/\hbar}|\psi^{(\pm)}\rangle\, dt \tag{14.59}$$

For "in" solutions we encounter the integral

$$\begin{aligned}\hat{G}^{(+)} &= \frac{1}{i\hbar}\int_{-\infty}^{0} dt \exp\left[\frac{-t(i\hat{H}_0 - iE + \varepsilon)}{\hbar}\right] \\ &= \frac{1}{E - \hat{H}_0 + i\varepsilon}\end{aligned}$$

Similarly,

$$\hat{G}^{(-)} = \frac{1}{E - \hat{H}_0 - i\varepsilon}$$

Note that without the presence of ε the integrals $\hat{G}^{(\pm)}$ do not converge. Substituting these expressions for $\hat{G}^{(\pm)}$ into (14.59) gives the *Lippmann–Schwinger equation*,

$$\boxed{|\psi^{(\pm)}\rangle = |\varphi\rangle + \frac{1}{E - \hat{H}_0 \pm i\varepsilon}|\psi^{(\pm)}\rangle} \tag{14.60}$$

which, as previously noted, is independent of specific representation.

Scattering Amplitude Revisited

In Problem 14.11 you are asked to show that the coordinate representation of the "in" solution to (14.60) assumes the form

$$\psi_{\mathbf{k}}^{(+)}(\mathbf{r}) = \varphi_{\mathbf{k}}(r) - \frac{m}{2\pi\hbar^2}\int \frac{\exp(ik|\mathbf{r} - \mathbf{r}'|)}{|\mathbf{r} - \mathbf{r}'|} V(\mathbf{r}')\psi_{\mathbf{k}}^{+}(\mathbf{r}')\, d\mathbf{r}' \tag{14.61}$$

Here we have made the identifications

$$\langle \mathbf{r}|\varphi\rangle = \varphi_{\mathbf{k}}(\mathbf{r}) \tag{14.62a}$$

$$\langle \mathbf{r}|\psi^{(+)}\rangle = \psi_{\mathbf{k}}{}^{(+)}(\mathbf{r}) \tag{14.62b}$$

$$\langle \mathbf{r}|\hat{V}\psi^{(+)}\rangle = V(\mathbf{r})\psi^{(+)}(\mathbf{r}) \tag{14.62c}$$

At large distances from the interaction domain we may write

$$\frac{1}{|\mathbf{r}-\mathbf{r}'|} \simeq \frac{1}{r} + \cdots$$

and

$$k|\mathbf{r}-\mathbf{r}'| = kr\left[1 + \left(\frac{r'}{r}\right)^2 - \frac{2\mathbf{r}\cdot\mathbf{r}'}{r^2}\right]^{1/2}$$

$$\simeq kr\left[1 - \frac{\mathbf{r}\cdot\mathbf{r}'}{r^2} + \cdots\right] = kr - \mathbf{k}'\cdot\mathbf{r}'$$

where we have set

$$\mathbf{k}' \equiv \frac{k\mathbf{r}}{r}$$

Substituting these expansions in (14.61) gives

$$\psi_{\mathbf{k}}{}^{(+)}(\mathbf{r}) = \varphi_{\mathbf{k}}(\mathbf{r}) - \frac{m}{2\pi\hbar^2}\frac{e^{ikr}}{r}\langle\varphi_{\mathbf{k}'}|V|\psi_{\mathbf{k}}^{(+)}\rangle \tag{14.63}$$

Comparison with (14.7) gives the following expression for the scattering amplitude:

$$f(\theta) = -\frac{m}{2\pi\hbar^2}\langle\varphi_{\mathbf{k}'}|V|\psi_{\mathbf{k}}{}^{(+)}\rangle \tag{14.64}$$

In the Born approximation

$$\psi_{\mathbf{k}}{}^{+} \rightarrow \varphi_{\mathbf{k}}$$

and (14.64) returns our previous finding (14.36). However, one should bear in mind that (14.63) is, more generally, an integral equation for $\psi_{\mathbf{k}}{}^{(+)}$, solution to which gives a more accurate expression for the scattering amplitude through (14.64).

PROBLEMS

14.9 A beam of photons at a given frequency propagates into a medium of atoms with density $n(\text{cm}^{-3})$. The cross section for absorption of photons at this frequency by

the atoms is σ. If J is incident photon flux, then argue that the decrease in J in the distance dx due to absorption is

$$dJ = -\kappa J\,dx$$

where

$$\kappa = n\sigma$$

14.10 A monochromatic beam of photons at frequency $\nu = 10^{14}$ Hz and intensity $1.4\,\text{keV/cm}^2$ s is incident on a gas of atoms of density $n = 10^{18}\,\text{cm}^{-3}$. At the given frequency the radiation is very near resonance of the atoms. The related transition dipole moment of atoms in the gas has magnitude $0.4a_0e$. At what distance (cm) into the gas will the intensity of the beam be e^{-1} times its starting value? (*Hint:* Use results of the preceding problem.)

14.11 Working in the coordinate representation, employ the Lippmann–Schwinger equation (14.60) to derive its coordinate representation (14.61).

Answer
Let us label

$$\hat{G}_{\pm} \equiv \lim_{\varepsilon\to 0} G^{(\pm)}$$

The Lippmann–Schwinger equation (14.60) may then be written

$$|\psi^{(\pm)}\rangle = |\varphi\rangle + \hat{G}_{\pm}\hat{V}|\psi^{(\pm)}\rangle$$

To obtain the coordinate representation of this equation, we operate on it from the left with $\langle\mathbf{r}|$ to obtain [see (14.62)]

$$\psi_{\mathbf{k}}{}^{(\pm)}(\mathbf{r}) = \varphi_{\mathbf{k}}(\mathbf{r}) + \langle\mathbf{r}|\hat{G}_{\pm}\hat{V}|\psi^{(\pm)}\rangle \equiv \varphi_{\mathbf{k}}(\mathbf{r}) + I_{\pm}$$

which serves to define the interaction term $I_{\pm}$. Developing this term, we obtain[10]

$$I_{\pm} = \int d\mathbf{r}' \int d\bar{\mathbf{k}}\langle\mathbf{r}|\bar{\mathbf{k}}\rangle\langle\bar{\mathbf{k}}|\hat{G}_{\pm}|\mathbf{r}'\rangle\langle\mathbf{r}'|\hat{V}|\psi^{(\pm)}\rangle$$

We recall[11]

$$\langle\mathbf{r}|\mathbf{k}\rangle = \frac{1}{(2\pi)^{3/4}}e^{i\mathbf{k}\cdot\mathbf{r}}$$

and

$$\hat{H}_0|\mathbf{k}\rangle = \frac{\hbar^2k^2}{2m}|k\rangle$$

[10]Here we employ the spectral resolution of unity (see Problem 11.1).
[11]Note that this form gives the proper normalization

$$\int d\mathbf{k}\langle\mathbf{r}|\mathbf{k}\rangle\langle\mathbf{k}|\mathbf{r}'\rangle = \delta(\mathbf{r}-\mathbf{r}')$$

See (C.11).

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whence

$$\langle \bar{\mathbf{k}}|\hat{G}_{\pm}|\mathbf{r}'\rangle = \lim \frac{1}{E - (\hbar^2\bar{k}^2/2m) \pm i\varepsilon}\langle \bar{\mathbf{k}}|\mathbf{r}'\rangle$$

Thus we obtain

$$I_{\pm} = \frac{1}{(2\pi)^3}\int d\mathbf{r}' \int d\bar{\mathbf{k}} \frac{e^{i\bar{\mathbf{k}}\cdot(\mathbf{r}-\mathbf{r}')}}{E - (\hbar^2\bar{k}^2/2m) \pm i\varepsilon}\langle \mathbf{r}'|\hat{V}|\psi^{(\pm)}\rangle$$

Consider the $\bar{\mathbf{k}}$ integration,

$$\Phi_{\pm} \equiv \int d\bar{\mathbf{k}} \frac{e^{i\bar{\mathbf{k}}\cdot\Delta\mathbf{r}}}{R_{\pm}}$$

where

$$\Delta\mathbf{r} \equiv \mathbf{r} - \mathbf{r}'$$

$$R_{\pm} = E - \frac{\hbar^2\bar{k}^2}{2m} \pm i\varepsilon$$

With

$$\int d\bar{\mathbf{k}} = 2\pi \int_0^{\infty} \bar{k}^2\, d\bar{k} \int_{-1}^{1} d\mu$$

$$\mu \equiv \cos\theta = \frac{\bar{\mathbf{k}}\cdot\Delta\mathbf{r}}{|\bar{\mathbf{k}}\cdot\Delta\mathbf{r}|}$$

integration over μ gives

$$\int_{-1}^{1} d\mu \exp(i\bar{k}\Delta r\mu) = \frac{1}{i\bar{k}\,\Delta r}[\exp(i\bar{k}\,\Delta r) - \exp(-i\bar{k}\,\Delta r)]$$

As $\bar{k}/R_{\pm}$ is an odd function of $\bar{k}$, we find

$$\begin{aligned}\Phi_{\pm} &= 2\pi \int_0^{\infty} d\bar{k}\,\bar{k}^2 \frac{1}{i\bar{k}\,\Delta r}\frac{[\exp(i\bar{k}\,\Delta r) - \exp(-i\bar{k}\,\Delta r)]}{R_{\pm}} \\ &= \frac{2\pi}{i\,\Delta r}\int_{-\infty}^{\infty} \frac{d\bar{k}\,\bar{k}e^{i\bar{k}\,\Delta r}}{R_{\pm}}\end{aligned}$$

Next we set

$$E = \frac{\hbar^2 k^2}{2m}$$

which, by conservation of energy, is the same as the free-particle energy of the incident wave, $\varphi_{\mathbf{k}}(\mathbf{r})$. We obtain

$$\begin{aligned}\frac{2m}{\hbar^2}R_{\pm} &= \left(k^2 - \bar{k}^2 \pm i\frac{2m\varepsilon}{\hbar^2}\right) \\ &= (k - \bar{k} \pm i\bar{\varepsilon})(k + \bar{k} \pm i\bar{\varepsilon})\end{aligned}$$

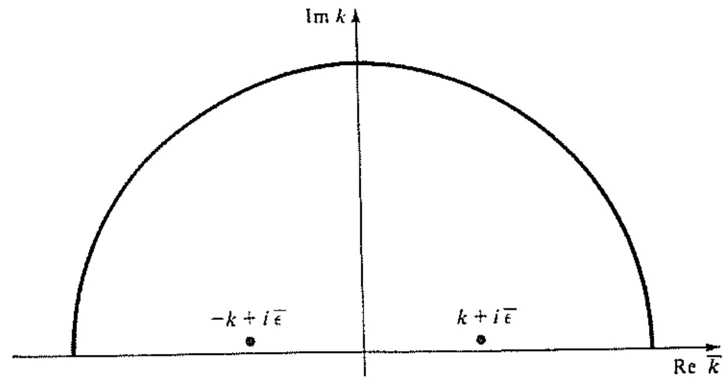

FIGURE 14.12 The contour for the integration in $\Phi_{\pm}$. The pole at $k + i\varepsilon'$ contributes to $\psi^{(+)}$ and the one at $-k + i\varepsilon'$ contributes to $\psi^{(-)}$.

where $\bar{\varepsilon} \equiv m\varepsilon/\hbar^2 k$. Thus

$$\frac{\bar{k}}{R_{\pm}} = -\frac{2m}{\hbar^2}\left(\frac{1/2}{\bar{k} - k \mp i\bar{\varepsilon}} + \frac{1/2}{\bar{k} + k \pm i\bar{\varepsilon}}\right)$$

We are now prepared to integrate over $\bar{k}$ by contour integration. As the integrand contains the factor $\exp i\bar{k}\,\Delta r$, it must be closed in the domain $\mathrm{Im}\,\bar{k} > 0$, that is, the upper half $\bar{k}$ plane. For Φ_+ there is a pole at

$$\bar{k} = k + i\bar{\varepsilon}$$

whereas for Φ_- there is a pole at

$$\bar{k} = -k + i\bar{\varepsilon}$$

See Fig. 14.12.

Passing to the limit $\bar{\varepsilon} \to 0$, we obtain

$$\begin{aligned}\Phi_{\pm} &= -\frac{2\pi}{i\,\Delta r}\frac{2m}{\hbar^2}2\pi i\left(\frac{1}{2}\right)e^{\pm ik\,\Delta r} \\ &= \frac{4\pi^2 m}{\hbar^2}\frac{e^{\pm ik\,\Delta r}}{\Delta r}\end{aligned}$$

whence

$$I_+ = -\frac{1}{(2\pi)^3}\frac{4\pi^2 m}{\hbar^2}\int d\mathbf{r}' \frac{e^{ik\,\Delta r}}{\Delta r}\langle \mathbf{r}'|\hat{V}|\psi^{(+)}\rangle$$

which when inserted in our starting relation

$$\psi_{\mathbf{k}}^{(+)} = \varphi_{\mathbf{k}}(r) + I_+$$

returns (14.61).

14.12 Is (14.61) a valid relation for inelastic collisions—for example, an ionizing collision in which an electron is emitted from an atom due to, say, electron scattering?

Answer
As the energy of the incident electron is not conserved (it loses energy in releasing the bound electron), one cannot equate energy of the scattered electron to its incident free-particle value, and the derivation in the preceding problem is invalid.

CHAPTER 15 Relativistic Quantum Mechanics

In this chapter we present a description of relativistic quantum mechanics. The chapter begins with a review of basic relativistic notions and continues with derivation of the Klein–Gordon equation relevant to relativistic bosons. Incorporating elements of this equation, the Dirac equation appropriate to fermions is obtained. Plane-wave solutions to this equation for a free particle are constructed, components of which are shown to correspond to "spin up" and "spin down" wavefunctions. The energy spectrum of these solutions is noted to have a forbidden gap and an infinite sea of negative values. These properties imply the existence of positrons. The Dirac equation is then shown to imply the correct magnetic dipole moment of the electron. The chapter continues with a derivation of the four-dimensional spin operator in the Dirac formalism and closes with a brief introduction to the covariant formulation of relativistic quantum mechanics.

15.1 PRELIMINARY REMARKS

Postulates, World Lines, and the Light Cone

The two postulates of special relativity are as follows:

1. The laws of physics are invariant under inertial transformations.
2. The speed of light is independent of the motion of the source.

The first postulate states that the result of an experiment in a given inertial frame of reference is independent of the constant translational motion of the system as a whole. An inertial frame is one in which a mass at rest experiences no force. Thus there is no absolute frame in the universe with respect to which motion