It is in fact the $1/r$ behavior of the outgoing spherical wave term that ensures that the flux in a solid angle $\Delta\Omega$ is independent of r. The definition (12.1) of the differential cross section permits the following identification for $n_t = 1$:

$$\boxed{\frac{d\sigma}{d\Omega} = |f(\Omega)|^2}. \tag{12.12}$$

12.2 Partial waves and phase shifts

12.2.1 The partial-wave expansion

In Section 10.4.1 we presented a method for solving the Schrödinger equation when the potential $V(r)$ is spherically symmetric. The method consists of expanding the wave function in spherical harmonics as in (10.77):

$$\psi(r, \theta, \phi) = \sum_{l,m_l} \frac{u_l(r)}{r} Y_l^{m_l}(\theta, \phi).$$

The cylindrical symmetry about Oz in the present problem allows us to limit ourselves to terms independent of ϕ, $m_l = 0$, and take into account the proportionality (10.62) of the spherical harmonics with $m_l = 0$ to the Legendre polynomials. We can then write[4]

$$\psi(r, \theta) = \sum_{l=0}^{\infty} \frac{u_l(r)}{r} P_l(\cos\theta), \tag{12.13}$$

where $u_l(r)$ is the solution of the radial equation (10.78):

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2} + V(r)\right] u_l(r) = E_l u_l(r), \tag{12.14}$$

with the boundary condition $u_l(0) = 0$, or, more precisely using (10.82),

$$r \to 0 : u_l(r) \propto r^{l+1}. \tag{12.15}$$

Since the Legendre polynomials form a basis for functions defined on the interval $[-1, +1]$, we can write the following series expansion for $f(\theta)$:

$$f(\theta) = \sum_{l=0}^{\infty} f_l P_l(\cos\theta), \quad f_l = \frac{2l+1}{2} \int_{-1}^{+1} f(\theta) P_l(\cos\theta)\, d\cos\theta. \tag{12.16}$$

The series (12.16) is called *the partial-wave expansion of the scattering amplitude*.

[4] We have modified the normalization of $u_l(r)$ by the unimportant factor $\sqrt{4\pi/(2l+1)}$ in going from one equation to the other.

If $V(r)$ tends to zero sufficiently rapidly for $r \to \infty$,[5] we can neglect $V(r)$ and the centrifugal barrier term in (12.14). The asymptotic behavior of $u_l(r)$ will then be

$$r \to \infty : u_l(r) \propto \sin(kr + \hat{\delta}_l).$$

Let us compare this behavior to that of a plane wave. A plane wave $\exp(ikz) = \exp(ikr\cos\theta)$ is a cylindrically symmetric solution of the Schrödinger equation when $V(r) = 0$. We can then expand $\exp(ikz)$ in a series of Legendre polynomials of the type (12.13). The coefficients of this series are calculated using (12.16) and are called the *spherical Bessel functions* $j_l(kr)$:

$$e^{ikz} = \sum_{l=0}^{\infty}(2l+1)i^l j_l(kr)P_l(\cos\theta). \tag{12.17}$$

The spherical Bessel functions can be expressed in terms of sines and cosines and are given by the recursion relation

$$j_l(x) = (-1)^l x^l \left(\frac{1}{x}\frac{d}{dx}\right)^l \frac{\sin x}{x} = (-1)^l x^l \left(\frac{1}{x}\frac{d}{dx}\right)^l j_0(x). \tag{12.18}$$

When $r \to 0$ we have $krj_l(kr) \propto (kr)^{l+1}$, which is a special case of the behavior (12.15) since $rj_l(kr)$ is a solution of the radial Schrödinger equation with $V(r) = 0$. When $r \to \infty$ it can be shown that[6]

$$r \to \infty : j_l(kr) \simeq \frac{1}{kr}\sin\left(kr - \frac{1}{2}l\pi\right). \tag{12.19}$$

Comparison with the behavior of $u_l(r)$ leads to the definition

$$\delta_l = \hat{\delta}_l - \frac{1}{2}l\pi,$$

which allows us to write down the asymptotic behavior of $u_l(r)$:

$$r \to \infty : u_l(r) \simeq a_l \sin\left(kr - \frac{1}{2}l\pi + \delta_l\right). \tag{12.20}$$

The number δ_l is the *phase shift* in the lth partial wave, and is a function of k: $\delta_l(k)$. To express $f(\theta)$ as a function of the phase shifts, it is sufficient to compare the asymptotic expansions of (12.9) and (12.13) at $r \to \infty$, choosing $A = 1$. Taking into account (12.17), the series (12.9) can be written as

$$e^{ikz} + f(\theta)\frac{e^{ikr}}{r} = \sum_{l=0}^{\infty} X_l(r)\,P_l(\cos\theta),$$

$$X_l(r) = (2l+1)i^l j_l(kr) + f_l\frac{e^{ikr}}{r}.$$

[5] This restriction on the potential should be made more precise. All the results of the present chapter are valid if $V(r)$ has finite range $[V(r) = 0$ if $r > R]$ or decreases at infinity faster than any power. If $V(r)$ falls off at infinity as $r^{-\alpha}$, certain results will be valid only if $\alpha \geq \alpha_0$. The discussion of this problem is rather technical, and we refer the reader to the references cited in Further Reading.

[6] See, for example, Cohen-Tannoudji *et al.* [1977], Complement A_{VIII}.

The asymptotic form (12.19) of the j_l gives

$$\mathrm{i}^l j_l(kr) \simeq \frac{1}{2\mathrm{i}kr}\left[(-1)^{l+1}\mathrm{e}^{-\mathrm{i}kr} + \mathrm{e}^{\mathrm{i}kr}\right],$$

and we obtain

$$X_l = \frac{2l+1}{2\mathrm{i}kr}\left[(-1)^{l+1}\mathrm{e}^{-\mathrm{i}kr} + \left(1 + \frac{2\mathrm{i}k}{2l+1} f_l\right)\mathrm{e}^{\mathrm{i}kr}\right]. \tag{12.21}$$

The function $X_l(r)$ must asymptotically be equal to $u_l(r)/r$, and so according to (12.20)

$$\frac{u_l(r)}{r} \simeq \frac{a_l}{2\mathrm{i}r}\left[(-1)^{l+1}\mathrm{e}^{-\mathrm{i}kr} + \mathrm{e}^{2\mathrm{i}\delta_l}\mathrm{e}^{\mathrm{i}kr}\right]. \tag{12.22}$$

The expressions (12.21) and (12.22) can be equal only if

$$\mathrm{e}^{2\mathrm{i}\delta_l} = 1 + \frac{2\mathrm{i}k}{2l+1} f_l$$

or

$$f_l = \frac{2l+1}{2\mathrm{i}k}\left(\mathrm{e}^{2\mathrm{i}\delta_l} - 1\right) = \frac{2l+1}{k}\,\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l. \tag{12.23}$$

This equation gives the *partial wave expansion* for $f(\theta)$) as a function of the phase shifts:

$$\boxed{f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\mathrm{e}^{\mathrm{i}\delta_l}\sin\delta_l P_l(\cos\theta)}\,. \tag{12.24}$$

We can obtain the differential cross section from (12.12) and then the total cross section by integrating over angles using the orthogonality relation of the Legendre polynomials derived from (10.62) and the orthogonality (10.55) of the spherical harmonics:

$$\int \mathrm{d}\Omega\, P_l(\cos\theta)\, P_{l'}(\cos\theta) = \frac{4\pi}{2l+1}\,\delta_{ll'}.$$

The result for σ_{tot} can be written as

$$\boxed{\sigma_{\text{tot}} = \frac{4\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)\sin^2\delta_l}\,. \tag{12.25}$$

The function

$$\boxed{S_l(k) = \mathrm{e}^{2\mathrm{i}\delta_l(k)}}\,, \tag{12.26}$$

where we have noted explicitly the dependence on k, is called the *S-matrix element in the lth partial wave*. It plays an important role in scattering, which can be understood by comparing the behavior (12.21) of a free spherical wave $j_l(kr)$ with that of the wave function in the presence of a potential (12.22):

$$j_l(kr) \;\propto\; \left[(-1)^{l+1}\mathrm{e}^{-\mathrm{i}kr}+\mathrm{e}^{\mathrm{i}kr}\right],$$
$$u_l(r) \;\propto\; \left[(-1)^{l+1}\mathrm{e}^{-\mathrm{i}kr}+\mathrm{e}^{2\mathrm{i}\delta_l}\mathrm{e}^{\mathrm{i}kr}\right].$$

The effect of the potential is to multiply the outgoing spherical wave by the phase factor $S_l=\exp(2\mathrm{i}\delta_l)$ while not affecting the incoming wave. This is a result of the boundary conditions that have been imposed, since the incident plane wave is composed of an incoming spherical wave and an outgoing spherical wave. The outgoing part is modified by the scattering, because the particles are scattered by the target and diverge from it. However, the incoming wave is not modified by the interaction with the target. In Section 12.3.1 we shall show that the condition $|S_l|=1$ takes into account the fact that the number of particles entering a sphere of large radius drawn about the target is equal to the number of particles leaving the sphere when the scattering is elastic.

Each term of (12.25) corresponds to the scattering cross section in the lth partial wave. It is obviously impossible to identify the contribution of each partial wave except in the total cross section, because the various partial waves interfere in the differential cross section. We note that the contribution to the total cross section from each partial wave is bounded:

$$\sigma_l=\frac{4\pi}{k^2}\,(2l+1)\sin^2\delta_l\le\sigma_l^{\max}=\frac{4\pi}{k^2}\,(2l+1). \tag{12.27}$$

Let us give a semi-classical interpretation of this result. Classically, the angular momentum $\hbar l$ and the impact parameter are related as $l=kb$, and so

$$\frac{l}{k}\le b\le\frac{l+1}{k}.$$

The maximum classical cross section is the area between the circles of radii l and $l+1$:

$$\sigma_l\le\frac{\pi}{k^2}\left[(l+1)^2-l^2\right]=\frac{\pi}{k^2}\,(2l+1)=\frac{1}{4}\,\sigma_l^{\max}.$$

The *classical* cross section is at most a quarter of the maximum quantum cross section. If the potential has finite range, $V(r)=0$ for $r>R$, then, from the classical point of view, an incident particle can interact only if its impact parameter is less than R, $b<R$, and only partial waves with $l\lesssim kR$ will contribute. We see that the phase-shift method will work well if the energy is low, because in this case only a limited number of partial waves will contribute. In particular, only the s-wave ($l=0$) will contribute appreciably when $k\to 0$. In quantum mechanical terms, the probability density $\propto r^2 j_l^2(kr)$ of a free spherical wave is negligible for $kr\lesssim[l(l+1)]^{1/2}$, and this wave does not penetrate into regions where the potential is important for small k unless $l=0$, when $r^2 j_0^2(kr)\propto\mathrm{const}$

omit r^2

if $r \to 0$. It can be rigorously shown[7] that for a potential of finite range the phase shift δ_l behaves as

$$\delta_l(k) \propto (kR)^{2l+1} \tag{12.28}$$

when $k \to 0$ or $l \to \infty$.

12.2.2 Low-energy scattering

When the potential has finite range, the s-wave will be the only one to contribute significantly to the low-energy cross section, and so the latter will be isotropic. In the rest of this section we shall take into account only the $l=0$ wave and use the notation $\delta_{l=0}(k)=\delta(k)$, $S_{l=0}(k)=S(k)$, $f_{l=0}(k)=f(k)$, $u_{l=0}(r)=u(r)$. Using the behavior (12.28) for $l=0$, $\delta(k) \propto k$, we can define the *scattering length* a as

$$\boxed{a = -\lim_{k\to 0} \frac{\delta(k)}{k}}\ . \tag{12.29}$$

The minus sign is chosen by convention and will be justified below.

As an example of a calculation of the phase shift and scattering length, let us consider the spherical well (Fig. 12.4):

$$V(r) = -V_0, \quad 0 \le r \le R,$$
$$V(r) = 0, \qquad r > R.$$

Such a spherical well gives an approximate description of neutron–proton scattering with the following parameters (Exercises 10.7.8 and 12.5.3):

$$R \simeq 2 \text{ fm}, \quad V_0 \simeq 26 \text{ MeV}.$$

The radial Schrödinger equation is written as

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{2m}{\hbar^2}V(r)\right)u(r) = \frac{2m}{\hbar^2}Eu(r), \tag{12.30}$$

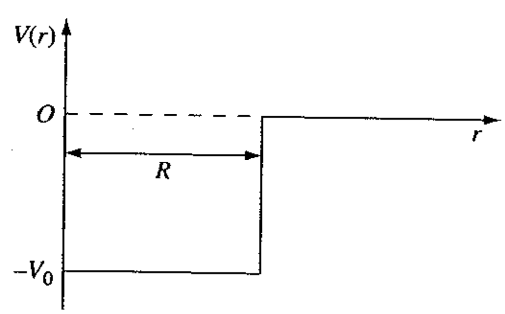

Fig. 12.4. The spherical well.

[7] See, for example, Messiah [1999], Chapter X.

which gives

$$r > R : \left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k^2\right) u(r) = 0,$$

$$r < R : \left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} + k'^2\right) u(r) = 0,$$

with $k^2 = 2mE/\hbar^2$ and $k'^2 = 2m(E + V_0)/\hbar^2$, from which, taking into account the condition $u(r = 0) = 0$, we find

$$r > R : u(r) = C \sin(kr + \delta),$$

$$r < R : u(r) = D \sin k'r.$$

The continuity of the logarithmic derivative of $u(r)$ at $r = R$ imposes the condition

$$k' \cot k'R = k \cot(kR + \delta). \tag{12.31}$$

The equation

$$\cot x = \mathrm{i}\,\frac{\mathrm{e}^{2\mathrm{i}x} + 1}{\mathrm{e}^{2\mathrm{i}x} - 1}$$

can be used to determine the S-matrix element $S(k)$. An easy calculation gives

$$S(k) = \mathrm{e}^{2\mathrm{i}\delta(k)} = \mathrm{e}^{-2\mathrm{i}kR}\,\frac{\cos k'R + \mathrm{i}\dfrac{k}{k'}\sin k'R}{\cos k'R - \mathrm{i}\dfrac{k}{k'}\sin k'R}. \tag{12.32}$$

As expected, the expression for $S(k)$ has unit modulus. The phase shift is determined only up to a factor of π, and to learn the "true" value of the phase shift it is necessary to allow the potential to increase from 0 to V_0 while following the evolution of δ between zero and its final value.

As in the one-dimensional case (cf. Section 9.4.3), there exists a remarkable relation between the S-matrix and bound states. Let us set $k = \mathrm{i}\kappa$ (in an instant we shall see that we must choose $k = \mathrm{i}\kappa$, $\kappa > 0$ and not $k = -\mathrm{i}\kappa$). The function $S(k)$ has poles for

$$\cos k'R + \frac{\kappa}{k'}\sin k'R = 0, \tag{12.33}$$

but this is also just the equation that determines the bound states. The wave function of a bound state of energy $E = -B < 0$ is given by

$$r > R : u(r) = C\mathrm{e}^{-\kappa r},$$

$$r < R : u(r) = D \sin k'r,$$

with $\kappa = (2mB/\hbar^2)^{1/2}$ and $k' = [2m(V_0 - B)]^{1/2}/\hbar$, and the continuity of the logarithmic derivative at $r = R$ is written as

$$-\kappa = k' \cot k'R, \tag{12.34}$$

which is exactly the equation for the poles of $S(k)$. The result is general for potentials that fall off sufficiently rapidly at infinity and is valid for any partial wave: the poles of $S_l(k)$ for $k = \mathrm{i}\kappa$ give the position of the bound states in the lth partial wave.

It is easy to derive the scattering length from (12.31). This equation can also be written as

$$\tan(kR + \delta) = \frac{k}{k'} \tan k'R.$$

In the limit $k \to 0$ and $kR \to 0$, $\delta \to 0$ and $k' \to k_0 = (2mV_0/\hbar^2)^{1/2}$, from which we have

$$kR + \delta(k) \simeq \frac{k}{k_0} \tan k_0 R,$$

or

$$\delta(k) \simeq -k\left(R - \frac{\tan k_0 R}{k_0}\right),$$

which according to the definition (12.29) gives

$$a = R\left(1 - \frac{\tan k_0 R}{k_0 R}\right). \tag{12.35}$$

Another case of particular interest is that of hard-sphere scattering: $V(r) = 0$ if $r > R$ and $V(r) = +\infty$ if $r < R$. The radial wave function $u(r)$ must vanish at $r = R$:

$$r > R : u(r) = C \sin(kR + \delta),$$ should be r

$$r < R : u(r) = 0,$$

so that $kR + \delta = n\pi$ and for k sufficiently small,

$$\delta = -kR, \quad a = R. \tag{12.36}$$

The minus sign in the definition (12.29) has been chosen such that the scattering length of a hard sphere is $+R$ rather than $-R$. From the qualitative behavior of $u(r)$ in Fig. 12.5 we see that $a > 0$ for any repulsive potential. The situation is more complicated for an attractive potential. When there is no bound state an attractive potential gives a negative scattering length. The appearance of a bound state changes the sign of a, which becomes positive. The sign changes again with the appearance of a second bound state, and so on. This is confirmed by (12.35): the condition for the appearance of a first bound state is $k_0 R = \pi/2$ and the scattering length is negative for $k_0 R < \pi/2$. It becomes infinite when $k_0 R = \pi/2$, positive when $k_0 R > \pi/2$, and remains positive for $\pi/2 < k_0 R < 3\pi/2$. The appearance of a second bound state corresponds to $k_0 R = 3\pi/2$, and the scattering length is negative beyond this value after having again become infinite. A large positive scattering length indicates the presence of a low-energy bound state, and a scattering length that is large and negative indicates that a bound state is about to appear. It is sometimes said that there is an antibound or virtual state.

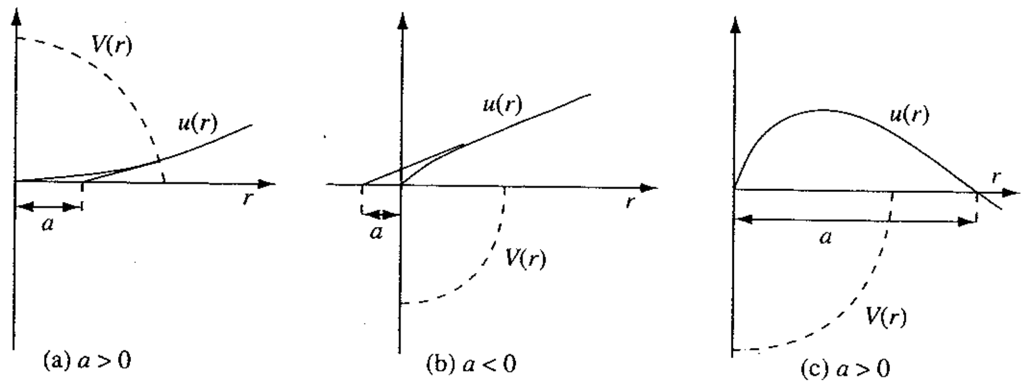

Fig. 12.5. Behavior of the wave function and the scattering length for various potentials: (a) a repulsive potential; (b) an attractive potential without a bound state; (c) an attractive potential with a single bound state.

According to (12.12) the low-energy cross section is isotropic, and the total cross section is

$$\sigma_{\text{tot}} = 4\pi a^2. \tag{12.37}$$

It is interesting to note that the quantum cross section of a hard sphere ($a = R$) is four times the classical cross section πR^2, in agreement with the inequality mentioned previously. Measurement of the total cross section gives only the absolute value of a. However, the sign of the scattering length is an important quantity. For example, the effective potential which we shall define in the following paragraph is attractive for $a < 0$ and repulsive for $a > 0$, which has direct consequences, for example, for the possibility of forming Bose–Einstein condensates of atomic gases. Another important case is neutron–proton scattering (Section 12.2.4).

The low-energy form $\delta(k) \simeq -ka$ is actually the first term of an expansion of the phase shift in powers of k^2. Exercise 12.5.3 shows that the function $k\cot\delta(k)$ is an analytic function[8] of k^2 for which we can write down a Taylor series for $k^2 \to 0$:

$$k\cot\delta(k) = -\frac{1}{a} + \frac{1}{2}\, r_0 k^2 + O(k^4). \tag{12.38}$$

The distance r_0 is called the *effective range*. We often use the low-energy form of the scattering amplitude:

$$f(k) = \frac{\mathrm{e}^{2\mathrm{i}\delta(k)} - 1}{2\mathrm{i}k} = \frac{1}{k[\cot\delta(k) - \mathrm{i}]},$$

or, expressing $\cot\delta(k)$ as a function of a if $r_0 k \ll 1$,

$$\boxed{f(k) = \frac{-a}{1 + \mathrm{i}ka}}\,. \tag{12.39}$$

[8] If $V(r)$ falls off at least as fast as $\exp(-\mu r)$. Equation (12.38) is valid provided that $V(r)$ falls off at least as r^{-5}.

This form can be made more precise by using the effective-range approximation (12.38):

$$f(k) = \frac{-a}{1 + ika - \frac{1}{2}\, r_0 a k^2}. \tag{12.40}$$

12.2.3 The effective potential

The scattering length makes it possible to introduce the very useful concept of effective potential, not to be confused with the effective potential $V_l(r)$ of (10.79). When studying a system of low-energy particles, it is convenient to be able to replace the actual potential $V(r)$ by a simpler potential $V_{\text{eff}}(r)$, called the *effective potential*, which gives the same results for low-energy scattering. An effective potential is used, for example, for the theoretical study of low-energy neutron scattering or Bose–Einstein condensates of atomic gases. We shall show that low-energy scattering is described by choosing an effective potential proportional to a δ function:

$$V_{\text{eff}}(r)\psi(r) = g\delta(\vec{r})\, \frac{\mathrm{d}}{\mathrm{d}r}\,[r\psi(r)], \tag{12.41}$$

where g is a constant to be determined. To justify this potential and find g, let us examine the Schrödinger equation for a wave function $\psi(r) = u(r)/r$. The expression for the Laplacian applied to a function of r

$$\nabla^2 f(r) = \frac{1}{r}\,\frac{\mathrm{d}^2}{\mathrm{d}r^2}\,[rf(r)] \tag{12.42}$$

is valid only for a function $f(r)$ that is regular at $r = 0$, and for $f(r) \propto 1/r$ the familiar equation from electrostatics is used:

$$\nabla^2 \frac{1}{r} = -4\pi\delta(\vec{r}). \tag{12.43}$$

Let us study the Schrödinger equation taking (12.41) as the potential:

$$-\frac{\hbar^2}{2m}\,\nabla^2 \frac{u(r)}{r} + V_{\text{eff}}(r)\,\frac{u(r)}{r} = \frac{\hbar^2 k^2}{2m}\,\frac{u(r)}{r},$$

and write down the kinetic energy term

$$\begin{aligned}\nabla^2 \frac{u(r)}{r} &= \nabla^2 \left[\frac{u(r) - u(0)}{r}\right] + u(0)\nabla^2 \frac{1}{r} \\ &= \frac{1}{r}\,\frac{\mathrm{d}^2}{\mathrm{d}r^2}\, r \left[\frac{u(r) - u(0)}{r}\right] - 4\pi u(0)\delta(\vec{r}) = \frac{1}{r}\,\frac{\mathrm{d}^2 u(r)}{\mathrm{d}r^2} - 4\pi u(0)\delta(\vec{r}),\end{aligned}$$

where we have noted that $[u(r) - u(0)]/r$ is a regular function at $r = 0$. Moreover, if we write

$$u(r) = a + br + cr^2 + \cdots,$$

then

$$\frac{1}{r}\,\frac{\mathrm{d}^2 u}{\mathrm{d}r^2} = \frac{2c}{r} + \cdots$$

and the integral of this term in a sphere of radius R about the origin tends to zero with R. We then have

$$-\frac{\hbar^2}{2mr}\frac{\mathrm{d}^2u(r)}{\mathrm{d}r^2}-\frac{\hbar^2k^2}{2m}\frac{u(r)}{r}=\left[-\frac{4\pi\hbar^2}{2m}u(0)-gu'(0)\right]\delta(\vec{r}).$$

The two sides of this equation must vanish separately, which for the left-hand side implies

$$u(r)=C\sin(kr+\delta(k)),\qquad r>0,$$

and so $u'(0)/u(0)=k\cot\delta(k)$. The vanishing of the coefficient of $\delta(\vec{r})$ imposes the condition

$$-\frac{2\pi\hbar^2}{m}=gk\cot\delta(k),$$

and the $k\to 0$ limit of this equation makes it possible to relate g and a:[9]

$$\boxed{g=\frac{2\pi\hbar^2}{m}a,\qquad V_{\text{eff}}(\vec{r})=\frac{2\pi\hbar^2a}{m}\delta(\vec{r})\frac{\mathrm{d}}{\mathrm{d}r}r}\,. \tag{12.44}$$

The effective potential depends on a single parameter, the scattering length a; we take it to be that of a more realistic potential or simply use the experimental value. Let us also study the bound states of the effective potential. The radial wave function of a bound state must have the form

$$u(r)=C\mathrm{e}^{-\kappa r},$$

and so $u'(0)/u(0)=-\kappa$. We can derive a relation between the binding energy B and the scattering length:

$$\kappa=\sqrt{\frac{2mB}{\hbar^2}}=\frac{2\pi\hbar^2g}{m}=\frac{1}{a}. \tag{12.45}$$

The bound state of the effective potential is unique, and we again find that $a>0$ for a single bound state. In summary, an effective potential for which $a>0$ may correspond either to a hard sphere or to an attractive potential with a single bound state. These two potentials lead to the same behavior for an ensemble of low-energy particles, but the behavior will be different if $a<0$: it is the sign of the scattering length that is crucial. The function $k\cot\delta(k)$ is a constant:

$$k\cot\delta(k)=-\frac{2\pi\hbar^2}{mg}=-\frac{1}{a},$$

and the scattering amplitude of the effective potential is given *exactly* by (12.39):

$$f_{\text{eff}}(k)=\frac{-a}{1+ika}.$$

9 It should be born in mind that if we consider the scattering of identical particles of mass M, the reduced mass is $m=M/2$ and $g=(4\pi\hbar^2/M)\,a$.

12.2.4 Low-energy neutron–proton scattering

Low-energy neutron–proton scattering provides a very important practical example of the formalism we have just developed. The proton and the neutron are spin-1/2 particles and the scattering is spin-dependent, and so we shall generalize the above results to take this into account. In low-energy scattering the total spin $\vec{S}_{tot}$ is conserved. The orbital angular momentum is zero, because the scattering occurs in the s-wave, and the conservation of total angular momentum is equivalent to the conservation of total spin. The scattering amplitude can be written as an operator $\hat{f}$ acting in the four-dimensional space $\mathcal{H}$, the tensor product of the two spaces of spin-1/2 states, as a function of the projectors $\mathcal{P}_s = \mathcal{P}_0$ and $\mathcal{P}_t = \mathcal{P}_1$ on the singlet (total spin zero) and triplet (total spin one) states given in (10.128):

$$\hat{f}(k) = f_s(k)\mathcal{P}_s + f_t(k)\mathcal{P}_t.$$

This form of $\hat{f}$ ensures that the total spin remains unchanged in the scattering: a singlet state remains a singlet and a triplet state remains a triplet. We shall limit ourselves to the case $ka \ll 1$. According to (12.39),

$$f_s(k) = -a_s, \quad f_t(k) = -a_t,$$

where a_s and a_t are the scattering lengths in the singlet and triplet states. When the condition $ka \ll 1$ is not satisfied, it is possible to use expressions analogous to (12.39), or even (12.40), for $f_s(k)$ and $f_t(k)$, thus introducing the effective ranges r_{0s} and r_{0t}. In summary, in the approximation where $ka \ll 1$

$$\hat{f} = -a_s\mathcal{P}_s - a_t\mathcal{P}_t, \tag{12.46}$$

or, introducing the Pauli matrices $\vec{\sigma}_p$ and $\vec{\sigma}_n$ acting in the space of the proton and neutron spin states,

$$-\hat{f} = \hat{a} = \frac{1}{4}(a_s + 3a_t)I + \frac{1}{4}(a_t - a_s)\vec{\sigma}_p \cdot \vec{\sigma}_n. \tag{12.47}$$

The differential cross section is isotropic and the total cross section for a state of initial spin $|i\rangle$ and final spin $|f\rangle$ is

$$\sigma_{fi} = 4\pi|\langle f|\hat{a}|i\rangle|^2. \tag{12.48}$$

If the final spins are not measured and the initial state is a mixture for which we know only the probability p_i of finding the initial spins in the state $|i\rangle$, it is necessary to sum over the states $|f\rangle$ and the probabilities p_i:

$$\sigma = 4\pi\sum_i \mathsf{p}_i \sum_f \langle i|\hat{a}|f\rangle\langle f|\hat{a}|i\rangle$$

$$= 4\pi\sum_i \mathsf{p}_i\langle i|\hat{a}^2|i\rangle = 4\pi\,\mathrm{Tr}\,(\rho_{init}\,\hat{a}^2),$$

where we have used the completeness relation in $\mathcal{H}$, $\sum_f |f\rangle\langle f| = I$, and the definition of the state operator of the initial state:

$$\rho_{\text{init}} = \sum_i \mathrm{p}_i |i\rangle\langle i|.$$

The most frequently encountered case is that of unpolarized initial state, so that the states $|++\rangle$, $|+-\rangle$, $|-+\rangle$, and $|--\rangle$ have the same probability. In this case $\rho_{\text{init}} = I/4$ and

$$\begin{aligned}\sigma_{\text{unpol}} &= \pi \operatorname{Tr} \hat{a}^2 = \pi \operatorname{Tr}\left(a_s^2 \mathcal{P}_s + a_t^2 \mathcal{P}_t\right) \\ &= 4\pi \left(\frac{1}{4} a_s^2 + \frac{3}{4} a_t^2\right) = \frac{1}{4}\sigma_s + \frac{3}{4}\sigma_t.\end{aligned} \tag{12.49}$$

The physical interpretation is straightforward: if the initial state is unpolarized, the probability of having a singlet state is 1/4 and that of having a triplet state is 3/4, which gives the weights 1/4 and 3/4 of the singlet and triplet cross sections in (12.49).

The unpolarized cross section gives only the combination $a_s^2 + 3a_t^2$ of the scattering lengths. Additional information can be obtained from the existence of a bound state in the triplet state, the deuteron, which allows the approximate determination of a_t. A precise relation between the deuteron parameters and the low-energy scattering parameters in the triplet state is obtained in Exercise 12.5.3 using the effective-range approximation. An approximate expression is obtained by noting that the deuteron wave function extends far beyond the range of the potential, $\kappa^{-1} \gg R$, which makes it possible to use the effective potential and the relation (12.45). Using the fact that $B \simeq 2.22\,\text{MeV}$, we obtain $\kappa^{-1} \simeq 4.2\,\text{fm}$, while the exact value of a_t is 5.4 fm. However, this argument is sufficient for determining the sign of a_t: $a_t > 0$.

Knowledge of a_t from the deuteron parameters and measurement of the unpolarized cross section make it possible to determine the modulus of the scattering length in the singlet state $|a_s|$, but not its sign. A possible method for finding the sign of a_s is to use neutron scattering on a hydrogen molecule; this is studied in Exercise 12.5.2. It is found that the scattering length a_s is negative, consistent with the fact that there is no singlet bound state. The experimental values of the scattering lengths and effective ranges are

$$a_t = 5.40\,\text{fm}, \quad r_{0t} = 1.73\,\text{fm}, \quad a_s = -23.7\,\text{fm}, \quad r_{0s} = 2.5\,\text{fm}.$$

It can be observed that a_s is large and negative, and that the neutron–proton system in the singlet state is very close to forming a bound state, showing the presence of a virtual state.

12.3 Inelastic scattering

12.3.1 The optical theorem

In general, in a collision particles can undergo not only elastic, but also inelastic scattering. For example, the scattering of a photon on an atom A in its ground state E_0 can leave the atom in an excited level A^* of energy E_1:

$$\gamma + A \to \gamma' + A^*,$$

the final photon having lost an energy $(E_1 - E_0)$ compared with the initial one (if the atomic recoil is neglected). It is also possible for the final particles to be different from the initial ones, as in

$$\pi^- + p \rightarrow K^0 + \Lambda$$

or

$$\pi^- + p \rightarrow \pi^- + \pi^+ + n.$$

We have seen that $|S_l(k)| = 1$ in the case of elastic scattering. We shall show that it is possible to generalize the expression for the scattering amplitude $f(\Omega)$ to the inelastic case if we allow $|S_l(k)| \leq 1$. This inequality follows from the condition that the modulus of the amplitude of the outgoing wave be smaller than that of the incoming wave, that is, the number of particles N_{out} leaving a large sphere of radius r enclosing the target must be smaller than the number N_{in} entering the sphere, because incident particles can only *disappear* in inelastic scattering. As we shall show below, this inequality holds for each partial wave, $N^l_{\text{out}} \leq N^l_{\text{in}}$, because the integration over the surface of the sphere eliminates interference between partial waves. If the scattering is purely elastic in the lth partial wave, $N^l_{\text{in}} = N^l_{\text{out}}$ and $|S_l(k)| = 1$. Let us evaluate N^l_{in} and N^l_{out} using the asymptotic form (12.22) of the wave function at $r \rightarrow \infty$. As in elastic scattering, only the outgoing wave term can be modified:

$$\frac{e^{ikr}}{r} \rightarrow S_l(k)\frac{e^{ikr}}{r},$$

from which we find the asymptotic behavior of $\psi(\vec{r})$:

$$\psi \simeq \frac{iA}{2kr}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)\left[(-1)^l e^{-ikr} - S_l e^{ikr}\right],$$

which gives for $f(\theta)$

$$f(\theta) = \frac{1}{2ik}\sum_{l=0}^{\infty}(2l+1)P_l(\cos\theta)(S_l - 1).$$

The total elastic cross section then is

$$\sigma_{\text{el}} = \int d\Omega |f(\theta)|^2$$

and the result of the integration over Ω generalizes (12.25):

$$\boxed{\sigma_{\text{el}} = \frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)|1 - S_l|^2}. \qquad (12.50)$$

Let us calculate the number of incoming particles in the lth partial wave, N^l_{in}, by integrating the current entering through the surface of a sphere of radius $r \rightarrow \infty$ about the target.

Since the Legendre polynomials are orthogonal, there are no interference terms between different partial waves. We find

$$N_{\rm in}^{l}=\left[\frac{(2l+1)^2|A|^2}{4k^2}\right]\left[\frac{2}{2l+1}\right]\left[\frac{\hbar k}{m}\right][2\pi]=\frac{\pi\hbar(2l+1)|A|^2}{mk}.$$

The first term comes from the normalization of $|\psi|^2$, the second from the orthogonality relation of the Legendre polynomials, the third from the expression for the current of the incoming wave, and the last from the integration over ϕ. A similar calculation gives $N_{\rm out}^{l}$:

$$N_{\rm out}^{l}=\frac{\pi\hbar(2l+1)|A|^2}{mk}\,|S_l|^2.$$

The condition $N_{\rm out}^{l}\le N_{\rm in}^{l}$ implies that $|S_l|\le 1$. The inelastic cross section in the lth partial wave is, up to the flux factor $\mathcal{F}=\hbar k|A|^2/m$, just the difference between the numbers of incoming and outgoing particles:

$$\sigma_{\rm inel}^{l}=\frac{1}{\mathcal{F}}\left(N_{\rm in}^{l}-N_{\rm out}^{l}\right)=\frac{\pi\hbar(2l+1)|A|^2}{k^2}(1-|S_l|^2),$$

and the total inelastic cross section becomes

$$\boxed{\sigma_{\rm inel}=\frac{\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(1-|S_l|^2)}\,. \tag{12.51}$$

If $N_{\rm in}^{l}=N_{\rm out}^{l}$, the number of outgoing particles is equal to the number of incoming ones, the scattering is elastic in the lth partial wave, and $|S_l(k)|=1$, $S_l(k)=\exp[2{\rm i}\delta_l(k)]$. The condition $|S_l|\le 1$ implies $\sigma_{\rm inel}^{l}\ge 0$, as it should. The sum of the elastic and inelastic cross sections is the total cross section:

$$\boxed{\sigma_{\rm tot}=\frac{2\pi}{k^2}\sum_{l=0}^{\infty}(2l+1)(1-{\rm Re}\,S_l)}\,. \tag{12.52}$$

The presence of inelastic channels implies that $(1-S_l)\ne 0$, and so in quantum physics it is not possible to have purely inelastic scattering, whereas in classical physics particles can be sent onto perfectly absorbing targets, without undergoing elastic scattering. If the absorption in the lth partial wave is total, which corresponds to $N_l^{\rm out}=0$ and therefore to $S_l=0$, then

$$\sigma_{\rm el}=\sigma_{\rm inel}^{l}=\frac{\pi}{k^2}(2l+1). \tag{12.53}$$

By comparison, the maximum elastic cross section is

$$\sigma_{\rm el,max}^{l}=\frac{4\pi}{k^2}(2l+1).$$

An important consequence of the intertwining of elastic and inelastic scattering is the optical theorem. Let us calculate the imaginary part of the forward scattering amplitude[10] Im $f(\theta=0)$ using $P_l(1)=1$:

$$\mathrm{Im}\, f(\theta=0)=\frac{1}{2k}\sum_{l=0}^{\infty}(2l+1)(1-\mathrm{Re}\, S_l).$$

Comparing this with (12.52) for σ_{tot}, we see that

$$\boxed{\sigma_{\mathrm{tot}}=\frac{4\pi}{k}\,\mathrm{Im} f(\theta=0)}\,. \tag{12.54}$$

This relation is the *optical theorem*, which relates the total cross section to the imaginary part of the forward scattering. The proof of the theorem shows that it follows from probability conservation.

12.3.2 The optical potential

Inelastic scattering can be taken into account by introducing a complex potential in the Schrödinger equation. Actually, if we repeat the proof in Section 9.2.2 of the continuity equation for the current $\vec{\nabla}\cdot\vec{j}=0$ in the case of a stationary wave $\psi_{\vec{k}}(\vec{r})$, we see that this equation is not satisfied if the potential is complex:

$$\vec{\nabla}\cdot\vec{j}=\frac{2}{\hbar}\,\mathrm{Im}\, V(\vec{r})|\psi_{\vec{k}}(\vec{r})|^2. \tag{12.55}$$

Of course, we recover the result $\vec{\nabla}\cdot\vec{j}=0$ in the case of the real potential used in Section 9.2.2. The number of particles absorbed per unit time is equal to the incident flux multiplied by the inelastic cross section. To calculate the number of absorbed particles, we imagine that the target is surrounded by a large sphere and calculate the flux of $\vec{j}$ through the surface $\mathcal{S}$ of the sphere:

$$-\int_{\mathcal{S}}\vec{j}\cdot\mathrm{d}\vec{\mathcal{S}}=-\int_{\mathcal{V}}\vec{\nabla}\cdot\vec{j}\,\mathrm{d}^3r=-\frac{2}{\hbar}\int_{\mathcal{V}}\mathrm{Im}\, V(\vec{r})|\psi_{\vec{k}}(\vec{r})|^2\,\mathrm{d}^3r,$$

where $\mathcal{V}$ is the volume of the sphere and the minus sign corresponds to the fact that $\mathrm{d}\vec{\mathcal{S}}$ points toward the outside. We then have

$$\sigma_{\mathrm{in}}=-\frac{2m}{\hbar^2k}\int \mathrm{Im}\, V(\vec{r})|\psi_{\vec{k}}(\vec{r})|^2\,\mathrm{d}^3r, \tag{12.56}$$

where we have integrated over all space because the potential is assumed to have finite range or to fall off sufficiently rapidly at infinity. From now on to the end of this chapter the potential $V(\vec{r})$ will be arbitrary, not necessarily invariant under rotation. Equation (12.56) implies that the imaginary part of $V(\vec{r})$ must be negative, Im $V(\vec{r})\le 0$.

[10] This quantity cannot be measured directly, because in the forward direction one finds mostly incident particles which have not undergone a collision. It is necessary to take the $\theta\to 0$ limit of $f(\theta)$. See also Footnote 3.

A complex potential with negative imaginary part $V(\vec{r})$ is called an *optical potential*. Such a potential is useful when we are interested not in the details of inelastic processes, but only in their effects on elastic processes. It is often used, in particular, in neutron–nucleus scattering. At low energies this complex potential can be represented as an effective potential of the type (12.41) with a complex scattering length $a = a_1 + \mathrm{i}a_2$, $a_2 < 0$. Under these conditions $\mathrm{Im}\, f = -a_2$ and the total cross section is very large compared with the elastic cross section:

$$\sigma_{\mathrm{tot}} \simeq \sigma_{\mathrm{in}} \simeq \frac{4\pi}{k}\,|a_2| \gg \sigma_{\mathrm{el}} = 4\pi a_1^2.$$

The proportionality of σ_{in} to $1/k$, or to $1/v$, where v is the speed of the incident neutrons, is an extremely important result: *the cross section for neutron absorption grows as* $1/v$ *when* $v \to 0$. This implies, for example, that neutrons must be slowed down in order to obtain sizable cross sections for uranium fission in a nuclear reactor. Another example is the use of cadmium to absorb neutrons: the scattering length is complex, with $a_1 = -3.8\,\mathrm{fm}$ and $a_2 = -1.2\,\mathrm{fm}$.

Let us rewrite the optical theorem using (12.56):

$$\mathrm{Im}\, f(\theta = 0) = \frac{k}{4\pi}\int |f(\Omega)|^2\,\mathrm{d}\Omega - \frac{m}{2\pi\hbar^2}\int \mathrm{Im}\, V(\vec{r})|\psi_{\vec{k}}(\vec{r})|^2\,\mathrm{d}^3 r. \qquad (12.57)$$

This equation can be generalized. We define the scattering amplitude $f(k\hat{r}, \vec{k})$ using the solution (12.9) of the Schrödinger equation:

$$\psi_{\vec{k}}^{(+)}(\vec{r}) = \mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}} + f(k\hat{r}, \vec{k})\frac{\mathrm{e}^{\mathrm{i}kr}}{r}.$$

Since the potential is not assumed to be invariant under rotation, the scattering amplitude depends on $\hat{r}$ and $\vec{k}$, and not only on k and the angle between $\hat{r}$ and $\hat{k}$. It is then possible to prove the *unitarity relation*:[11]

$$\frac{1}{2\mathrm{i}}\left[f(\vec{k}\,', \vec{k}) - f^*(\vec{k}, \vec{k}\,')\right] = \frac{k}{4\pi}\int f^*(k\hat{r}, \vec{k}\,')f(k\hat{r}, \vec{k})\,\mathrm{d}^2\hat{r}$$
$$-\frac{m}{2\pi\hbar^2}\int \mathrm{Im}\, V(\vec{r})\,[\psi_{\vec{k}'}^{(+)}(\vec{r})]^*\psi_{\vec{k}}^{(+)}(\vec{r})\mathrm{d}^3 r. \qquad (12.58)$$

Invariance under time reversal implies that $f(\vec{k}\,', \vec{k}) = f(-\vec{k}, -\vec{k}\,')$, and invariance under parity implies that $f(\vec{k}\,', \vec{k}) = f(-\vec{k}\,', -\vec{k})$. If these two invariances are valid, $f(\vec{k}\,', \vec{k}) = f(\vec{k}, \vec{k}\,')$ and

$$\frac{1}{2\mathrm{i}}\left[f(\vec{k}\,', \vec{k}) - f^*(\vec{k}, \vec{k}\,')\right] = \mathrm{Im}\, f(\vec{k}\,', \vec{k})$$

in (12.58). We then recover (12.57) by taking $\vec{k}\,' = \vec{k}$.

[11] See, for example, Landau and Lifschitz [1958], Section 124.