1. Introduction

Scattering is a fundamental physical process that is important in a wide range of applications. For example, most experimental work in particle physics involves scattering, and a large part of what is known about the properties of particles, both elementary and composite, has been obtained through scattering experiments. For another example, scattering of nuclear species in a hot plasma is important in determining thermonuclear reaction rates in stars or in the early universe. For yet another, one of the current experimental techniques for investigating carbon nanotubes is the scattering of photons. A long list of examples could be accumulated.

We have previously considered some scattering processes from the standpoint of time-dependent perturbation theory, in Notes 33 and 34. There the general idea was to take a simple initial condition describing the incident particle (for example, a plane wave), and to solve the time-dependent Schrödinger equation to find transitions to final states in which there is a scattered particle. In these notes we begin a more systematic study of scattering theory, taking a mostly time-independent approach. That is, we will solve the time-independent Schrödinger equation, looking for scattering solutions of a given energy. As we will see, there is an interplay in scattering and decay processes between the time-dependent and the time-independent approaches.

2. Classical and Quantum Potential Scattering

In this introduction we will concentrate mostly on potential scattering in three dimensions, that is, the scattering of particles from a localized potential $V = V(\mathbf{x})$. The potential should go to zero as $r = |\mathbf{x}| \to \infty$; this is normally understood in scattering theory. Initially we will take a somewhat intuitive approach to the theoretical development, but some of the mathematical arguments are simpler if we assume that the potential rigorously vanishes outside some cut-off radius $r = r_{co}$. If the potential is cut off in this way then the wave function $\psi(\mathbf{x})$ satisfies the free particle Schrödinger equation for $r > r_{co}$.

We will draw certain conclusions about the asymptotic form of the wave function when the potential rigorously vanishes for $r > r_{co}$, but then the question arises as to whether these conclusions

† Links to the other sets of notes can be found at:
still hold for realistic potentials that only go to zero gradually as \( r \to \infty \). We will address this question in Sec. 8, where we will find that the main conclusions still hold as long as the potential goes to zero faster than \( 1/r \) as \( r \to \infty \). Of course, the potential that goes to zero precisely as \( 1/r \) is the Coulomb potential, which is important in applications. Its treatment, however, requires special techniques which (some day) will appear in a separate set of notes. In the meantime, a discussion of Coulomb scattering may be found in Schiff's or Sakurai's book on quantum mechanics.

We will speak of the scattering of a particle by a potential \( V(x) \), as if it were a fixed potential in space, but in reality the beam particle interacts with a target, which often is another particle. Then a proper treatment requires us to take into account the dynamics of both particles. The changes necessary to do this were discussed in some detail in Notes 33. For now we simply note that if the target is very massive, then it can be thought of as producing a potential for the beam particle that is fixed in space (that is, in an inertial frame), as we shall assume in these notes.

For simplicity, we will assume that there are no spin-dependent forces, so that the Hamiltonian for the scattering problem has the kinetic-plus-potential form.

![Fig. 1. Classical scattering. A beam of particles, all with the same momentum \( p \), is directed against a target.](image)

To gain insight into scattering in quantum mechanics, we first consider classical scattering, which is illustrated in Fig. 1. A beam of particles, all of the same momentum \( p \), is directed against a target. When the beam is first turned on, it takes some time for the beam to reach the target, after which particles are scattered in various directions. Potential scattering is elastic, that is, when particles gain kinetic energy by falling into a potential well, they lose the same amount when climbing back out again, so the kinetic energy of the scattered particles at a large distance from the scatterer is the same as the kinetic energy in the incident beam. Only the direction of motion has changed. If we sit at an observation point some distance from the scatterer, it takes some time for the first scattered particles to reach us, after which the flux of particles coming from the scatterer reaches a steady state.

Let us now consider how this picture changes in quantum scattering. In quantum mechanics a state of a definite momentum \( p \) is a plane wave \( Ce^{ik \cdot x} \), where \( C \) is a constant and \( p = \hbar k \), so it is natural to associate the incident beam in a scattering experiment with a plane wave. This involves
some idealization, since a real plane wave fills up all of space and, in particular, it extends to infinity in the transverse direction, while real beams are always of finite extent in the transverse direction.

As in our picture of classical scattering, let us imagine that the beam is turned on at some time, that is, the plane wave is cut off in the longitudinal direction, with a front that advances from the source (at a large distance from the scatterer) toward the scatterer. When the wave reaches the scatterer it interacts with it, producing a scattered wave which radiates out in all directions, as illustrated in Fig. 2. If we sit at an observation point at some distance from the scatterer, then, as in the case of classical scattering, after a while a steady state is reached, in which there is a definite flux of scattered particles at our observation point. Observers further out will have to wait longer for the steady state to be reached, but after sufficient time a steady state of scattered particles is reached at any fixed observation point. Meanwhile parts of the incident wave that have not interacted with the scatterer (speaking somewhat loosely) continue forward, progressively filling space in the longitudinal direction with the incident wave. Speaking a little more precisely, since we are imagining that the incident wave fills all of space in the transverse direction, we can imagine that as it passes around the scatterer, the scatterer effectively punches a hole in the incident beam, that is, it creates a shadow, into which the incident beam will gradually diffract as it proceeds downstream. The diffracted waves have their own flux which is not exactly in the same direction as the incident wave, and so must be regarded as representing scattered particles. In any case, the fact remains that at any given distance from the scatterer, including in the forward direction, there is some time after which a steady state is reached.

![Fig. 2. Quantum scattering by a potential $V(x)$. Incident and scattered waves are shown.](image)

In quantum mechanics an energy eigenstate, a solution of the time-independent Schrödinger equation of definite energy $E$, is sometimes called a “stationary state,” because the probability density $\rho = |\psi|^2$ and the probability current $J$ (see Secs. 5.14 and 5.15) are independent of time. In the picture of scattering described above, the initial state, a truncated plane wave approaching the scatterer from some distance, is not a stationary state, because it has a nontrivial time evolution. Nevertheless, the intuitive picture suggests that if we sit at some observation point $x$ and wait long enough, then the wave function $\Psi(x,t)$ will approach an energy eigenfunction, that is, it will take
on the form $\psi_E(x)e^{-iEt/\hbar}$ in the neighborhood of our observation point, where $\psi_E(x)$ is a solution of the time-independent Schrödinger equation of energy $E$.

Recall that in the analysis of scattering in Notes 33 we took an initial state (a plane wave filling all of space) that was not an energy eigenstate of the total Hamiltonian $H_0 + H_1 = p^2/2m + V(x)$, only an eigenstate of the unperturbed Hamiltonian $H_0 = p^2/2m$. Then we studied the time evolution of this initial state under the full Hamiltonian, and derived from it the scattering rate and from that the cross section. Although the initial state considered in Notes 33 is not the same as the truncated plane wave we are considering here, nevertheless in both cases the same idea applies, that an energy eigenstate can be extracted from the long time evolution of the initial state.

3. The Time-Independent Approach

A more direct approach, however, which we shall pursue in the rest of these notes, is simply to look for an energy eigenstate, that is, a solution of the time-independent Schrödinger equation,

$$ -\frac{\hbar^2}{2m} \nabla^2 \psi(x) + V(x)\psi(x) = E\psi(x). \quad (1) $$

The solution should have the right boundary conditions at large distances from the scatterer to represent both the incident plane wave and the scattered wave. At distances outside the cut-off of the potential, that is, when $r > r_{co}$, the potential vanishes (as we are assuming) and the wave function $\psi(x)$ must satisfy the free particle Schrödinger equation with energy $E$. In particular, this must apply to both the incident wave and the scattered wave. Since the incident wave is a plane wave, which is already a solution of the free particle Schrödinger equation, we must have $E = \hbar^2 k^2/2m$, that is, the energy eigenvalue in the Schrödinger equation (1) is the same as the kinetic energy of the incident beam. Since the experimenter is free to give the incident particles any positive kinetic energy, we see that $E$ is not quantized, that is, the scattering solutions that we shall find belong to the continuous spectrum with $E > 0$. Note, however, that the energy $E$ that appears in (1) applies at all points of space, even where the potential is nonzero. Wave functions of the continuous spectrum are not normalizable, which is reasonable in the present case because the incident plane wave is not normalizable.

The intuitive picture we have developed suggests that there is a unique solution of the Schrödinger equation (1) of energy $E > 0$, given the momentum of the incident plane wave $p$. This must be the energy eigenfunction that is obtained in the long time limit from the time-dependent solution when a truncated plane wave is directed at the target, as discussed above. This intuitive idea can be translated into a theorem, that there is a unique solution of the time-independent Schrödinger equation (1) of energy $E > 0$, given that the boundary conditions at $r \to \infty$ include the incident plane wave of given momentum $p$ and outgoing scattered waves. We will see more rigorously how this unique solution is obtained in the case of central force potentials in this set of notes, and in the case of arbitrary potentials (and other generalizations) in subsequent notes.
However, the solution so obtained is degenerate, that is, for the given $E$ there is more than one linearly independent solution of the Schrödinger equation (1). This follows simply from the fact that we can change the direction of $p$ (the direction of the incident beam) without changing $E$, thereby generating a class of linearly independent solutions of the same energy. In three dimensions, these solutions are parameterized by the direction of the incident momentum, so there is a continuous infinity of them. Note that in one dimension, there are only two linearly independent solutions, corresponding to an incident wave directed at the scatterer from the right or from the left.

4. Boundary Conditions

To be more precise about the incident and scattered waves, let $\psi(x)$ be an exact solution of the Schrödinger equation (1) of energy $E$, and define the incident wave by

$$\psi_{\text{inc}}(x) = e^{ikx}$$  \hspace{1cm} (2)

where the wave vector $k$ is related to the energy eigenvalue in the Schrödinger equation by the free particle relation,

$$E = \frac{\hbar^2 k^2}{2m}.$$  \hspace{1cm} (3)

The incident wave does not satisfy the Schrödinger equation (1) everywhere, only in the region $r > r_{co}$ where the potential vanishes. Then define the scattered wave by

$$\psi_{\text{scatt}}(x) = \psi(x) - \psi_{\text{inc}}(x),$$  \hspace{1cm} (4)

so that

$$\psi(x) = \psi_{\text{inc}}(x) + \psi_{\text{scatt}}(x),$$  \hspace{1cm} (5)

exactly. Notice that since $\psi$ satisfies the Schrödinger equation exactly, and since $\psi_{\text{inc}}$ does also in the region $r > r_{co}$ where $V = 0$, then so does $\psi_{\text{scatt}}$ in this region. But neither $\psi_{\text{inc}}$ nor $\psi_{\text{scatt}}$ satisfies the Schrödinger equation (1) in the scattering region, where $V \neq 0$.

We will be interested in the asymptotic form of the scattered wave, that is, when $r \to \infty$, because this is where the experimenter will locate the detection apparatus. In particular, $r \to \infty$ means $r \gg r_{co}$ (continuing with the simplification that $V = 0$ for $r > r_{co}$).

It is possible to guess the asymptotic form of the scattered wave. The intuitive picture we have developed suggests that in the asymptotic region the scattered wave will have the form of a spherical wave traveling outward from the scatterer. At distances $r \gg r_{co}$ the scatterer subtends only a small solid angle as seen from an observation point, and so it defines an almost unique direction in which the waves must be propagating (that is, away from the scatterer, in the radial direction). Since the probability density in quantum mechanics is $|\psi|^2$, we expect the scattered wave to fall off with distance $r$ from the scatterer as $1/r^2$, since as the scattered particles travel outward they are spread over a sphere of increasing radius $r$ and area proportional to $r^2$. This means that the scattered wave function $\psi_{\text{scatt}}$ should fall off as $1/r$. This is only an asymptotic form, that is, it is the leading
behavior of $\psi_{\text{scatt}}$ in an asymptotic expansion. In addition, we must allow $\psi_{\text{scatt}}$ to have an angular dependence to account for the different scattering rates in different directions. Finally, we require it to be proportional to $e^{ikr}$, since this (when multiplied by the time dependence $e^{-iE_t/\hbar}$) produces an outwardly propagating spherical wave. Overall, we guess that the asymptotic form of the scattered wave is

$$
\psi_{\text{scatt}}(x) \sim \frac{e^{ikr}}{r} f(\theta, \phi),
$$

where the function $f(\theta, \phi)$ accounts for the angular dependence.

We emphasize that this is only an asymptotic form, valid when $r$ is large. In these notes the symbol $\sim$, when used in an equation such as (6), will mean that the left hand side equals the right hand side, plus terms that go to zero faster than the right hand side as $r \to \infty$. In other words, the right hand side is the leading term of an asymptotic expansion of the left hand side. Notice that the $k$ parameter in the asymptotic form of the scattered wave is the same as $|k|$, where $k$ is the wave number appearing in the incident wave (2). This corresponds to the fact that the scattering is elastic, that is, the classical fact that in the asymptotic region the scattered particles have the same kinetic energy as the incident particles.

We should check that our guess (6) for the asymptotic form of the scattered wave satisfies the Schrödinger equation at large $r$, at least to leading order in powers of $1/r$. Since the potential is negligible at large $r$ we are talking about the free-particle Schrödinger equation. We see that it does if we compute the Laplacian of (6),

$$
\nabla^2 \left[ \frac{e^{ikr}}{r} f(\theta, \phi) \right] = -k^2 \left[ \frac{e^{ikr}}{r} f(\theta, \phi) \right] + O\left(\frac{1}{r^3}\right),
$$

where the dominant term comes from the radial term of the Laplacian in spherical coordinates (see Eq. (D.23)). Thus the kinetic energy term in the Schrödinger equation balances the total energy term $E\psi$, to leading order in $1/r$.

5. The Scattering Amplitude and Cross Section

The function $f(\theta, \phi)$ is called the scattering amplitude. It is in general a complex function of the angles. A good deal of scattering theory is devoted to determining the scattering amplitude, since it bears a simple relation to the differential cross section.

Cross sections and differential cross sections were defined in Notes 33, where the relation between cross sections and transition rates was discussed. In the present case let us imagine an experimental situation such as illustrated in Fig. 3. A detector, located at some distance from the scatterer, intercepts all scattered particles coming out in a small cone of solid angle $\Delta \Omega$, centered on some direction $\hat{n} = (\theta, \phi)$. The counting rate is the scattered current $J_{\text{scatt}}$, integrated across the aperture to the detector.

The probability density $\rho = |\psi|^2$ and probability current $J$ were discussed in Secs. 5.14 and 5.15. Note that the expression for $J$ depends on the form of the Hamiltonian. In the present context,
we are interested in Hamiltonians of the kinetic-plus-potential type, for which the current can be written
\[ J = \frac{\hbar}{m} \text{Im}(\psi^* \nabla \psi), \tag{8} \]
which is a version of Eqs. (5.56) and (5.57).

In Notes 5, we were thinking of normalized wave functions, for which \( \rho \) and \( J \) are interpreted as the probability density and current. In the present context, however, the wave functions are scattering solutions that are not normalizable. It is best in this context to think of \( \rho \) and \( J \) as a particle density and current (with dimensions of particles/volume and particles/area-time, respectively).

The particle density in the incident beam is \( |\psi_{\text{inc}}|^2 \), or,
\[ n_{\text{inc}} = 1. \tag{9} \]
There is one particle per unit volume in the incident beam. Similarly, the incident current is easy to compute. It is
\[ J_{\text{inc}} = \frac{\hbar k}{m} = v, \tag{10} \]
where \( v \) is the velocity of the incident beam. In magnitude, \( J_{\text{inc}} = v \).

We will also need the scattered current to get the counting rate. We first compute the gradient of the scattered wave (6) in spherical coordinates (see Eq. (D.20)),
\[ \nabla \psi_{\text{scatt}}(x) = \mathbf{\hat{r}} \left[ \frac{ik e^{ikr}}{r} f(\theta, \phi) \right] + O\left( \frac{1}{r^2} \right), \tag{11} \]
where we only carry the result to leading order in \( 1/r \). Substituting this into (8), we find
\[ J_{\text{scatt}} \sim \frac{\hbar k}{m} \frac{|f(\theta, \phi)|^2}{r^2} \mathbf{\hat{r}}. \tag{12} \]
To leading order, the asymptotic form of the scattered current is purely in the outward radial direction, as we expect. Terms in \( J_{\text{scatt}} \) that go to zero faster than \( 1/r^2 \) as \( r \to \infty \) will not contribute to the counting rate, since the area of the aperture to the detector, for fixed \( \Delta \Omega \), is proportional to \( r^2 \).
Now we integrate the scattered current over the aperture to the detector, which we assume is at large distance $r$ from the scatterer, and which has area $r^2 \Delta \Omega$. Then the counting rate is

$$\frac{dw}{d\Omega} \Delta \Omega = \int_{\text{aperture}} J_{\text{scatt}} \cdot da = v|f(\theta, \phi)|^2 \Delta \Omega,$$

(13)

where $da$ is the area element of the aperture and where we have used $v = \hbar k/m$. Now dividing this by $J_{\text{inc}} = v$, we obtain

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

(14)

a simple result. This equation explains the interest in finding $f(\theta, \phi)$, since it leads immediately to the differential cross section, which is measurable. Notice that the counting rate, which is physically observable in a scattering experiment, depends only on the leading asymptotic form of the scattered wave function. One does not need to know the exact form of the scattered wave (at smaller values of $r$ where correction terms to the asymptotic expansion of the scattered wave are important, or in the scattering region where the potential is nonzero).

Now for some comments about this calculation. Notice that we computed the flux of the scattered particles intercepted by the detector, but we ignored the incident particles. In realistic scattering experiments the detector is usually located outside the beam, so incident particles do not enter it. Our incident wave (2) fills all of space, but that is an artifact of our simplified model. In reality the beam will be cut off at some finite transverse size, and if the scattering angle is not too small, the detector can be located outside the beam.

If the scattering angle is very small, however, then the detector will have to be inside the beam and it will detect incident particles as well as scattered ones. The counting rate is still the particle flux intercepted by the aperture of the detector, but the flux is neither the incident flux nor the scattered flux nor the sum of the two, but rather the flux computed from the total wave function $\psi = \psi_{\text{inc}} + \psi_{\text{scatt}}$. Since the current is quadratic in the wave function, there are cross terms or interference terms between the incident wave and the scattered wave. Taking all these effects into account leads to the optical theorem, which we take up in Sec. 14.

6. Central Force Scattering

We now specialize to the important case of a central force potential, $V = V(r)$. The main simplification in this case is that the Schrödinger equation (1) is separable in spherical coordinates (see Notes 16), so the solutions can be written in the form

$$\psi_{k\ell m}(x) = \psi_{k\ell m}(r, \theta, \phi) = R_{k\ell}(r)Y_{\ell m}(\theta, \phi),$$

(15)

where $R_{k\ell}(r)$ is a solution of version one of the radial Schrödinger equation, Eq. (16.7). The radial eigenfunction $R_{k\ell}(r)$ is parameterized by $\ell$ because the radial Schrödinger equation contains $\ell$ in the centrifugal potential. It is also parameterized by the energy $E$, which we will normally indicate by an equivalent wave number $k$, given by $E = \hbar^2 k^2/2m$. The three-dimensional solution $\psi$ depends on $k,$
\( \ell \) and \( m \), as indicated in Eq. (15). The radial eigenfunction \( R_{k\ell}(r) \) is related to an alternative version of the radial eigenfunction \( u_{k\ell}(r) = rR_{k\ell}(r) \), which satisfies version two of the radial Schrödinger equation, Eq. (16.11). (Function \( u \) was called \( f \) in Notes 16.)

For our present purposes we rearrange these two versions of the radial Schrödinger equation as

\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR_{k\ell}}{dr} \right) + k^2 R_{k\ell}(r) = W(r)R_{k\ell}(r) \tag{16}
\]

and

\[
u''_{k\ell}(r) + k^2 u_{k\ell}(r) = W(r)u_{k\ell}(r), \tag{17}
\]

where

\[ W(r) = \frac{\ell(\ell + 1)}{r^2} + \frac{2m}{\hbar^2} V(r). \tag{18}\]

The solution \( \psi_{k\ell m} \) of the Schrödinger equation is a simultaneous eigenfunction of \( (H, L^2, L_z) \), with quantum numbers \( (k\ell m) \), of which \( k > 0 \) is continuous and \( \ell \) and \( m \) are discrete. This solution does not satisfy the boundary conditions we require for a scattering problem. Such solutions do, however, form a complete set, so any solution of a given energy \( E \) can be expressed as a linear combinations of solutions of the form (15) of the same value of \( E \). That is, the most general solution of the Schrödinger equation of a given \( E = \hbar^2 k^2 / 2m > 0 \) is given by

\[
\psi(x) = \sum_{\ell m} C_{\ell m} R_{k\ell}(r) Y_{\ell m}(\theta, \phi), \tag{19}
\]

where \( C_{\ell m} \) are the expansion coefficients. The freedom in the choice of the coefficients \( C_{\ell m} \) indicates that there is a large degeneracy in the solutions of the Schrödinger equation of a given energy \( E > 0 \), a fact that we have already noted. In moment we will find the expansion coefficients for our desired scattering solution, in terms of some simple parameters that characterize the potential (the parameters turn out to be the phase shifts \( \delta_\ell \)).

7. Free Particle Solutions

In the special case of the free particle, \( V(r) = 0 \), the radial wave function \( R_{k\ell}(r) \) is a linear combination of the two types of spherical Bessel functions, \( j_\ell(kr) \) and \( y_\ell(kr) \), as discussed in Secs. 16.6–16.8. You may wish to review the contents of those sections of Notes 16. Here we just note a slightly modified version of Eqs. (16.29) and (16.30),

\[
j_\ell(\rho) \approx \frac{1}{\rho} \sin \left( \rho - \ell \frac{\pi}{2} \right), \tag{20}
\]

\[
y_\ell(\rho) \approx -\frac{1}{\rho} \cos \left( \rho - \ell \frac{\pi}{2} \right), \tag{21}
\]

valid when \( \rho \gg \ell \).

Sometimes we are interested in solutions for a particle that is free everywhere, that is, where the potential \( V(r) = 0 \) for all \( r \), all the way down to \( r = 0 \). In that case the \( y \)-type Bessel functions
are not allowed, and \( R_{k\ell}(r) = j_\ell(kr) \). Then the most general free particle solution of energy \( E \) is a sum of the form (19), that is,

\[
\psi_{\text{free}}(x) = \sum_{\ell m} C_{\ell m} j_\ell(kr) Y_{\ell m}(\theta, \phi),
\]

for some expansion coefficients \( C_{\ell m} \).

In particular, it must be possible to express the incident wave \( e^{i\mathbf{k} \cdot \mathbf{x}} \) in this form. The problem of determining the expansion coefficients \( C_{\ell m} \) in this case is discussed in Sakurai’s book, and will not be repeated here. The derivation involves some use of recursion relations satisfied by the spherical Bessel functions and the Legendre polynomials, and is straightforward but not particularly illuminating. (A more illuminating derivation uses group theory, which, however, is outside the scope of this course.) The result, however, is very useful. It is

\[
e^{i\mathbf{k} \cdot \mathbf{x}} = 4\pi \sum_{\ell m} i^\ell j_\ell(kr) Y_{\ell m}^*(\hat{k}) Y_{\ell m}(\hat{r}),
\]

where \( \hat{r} \) and \( \hat{k} \) refer to the directions of the vectors \( \mathbf{x} \) and \( \mathbf{k} \) on the left hand side, and where \( Y_{\ell m}(\hat{r}) \) means the same as \( Y_{\ell m}(\theta, \phi) \). This expansion can be rewritten with the use of the addition theorem for spherical harmonics, Eq. (15.71), which for present purposes we write in the form

\[
P_\ell(\hat{r} \cdot \hat{k}) = P_\ell(\cos \gamma) = \frac{4\pi}{2\ell + 1} \sum_m Y_{\ell m}^*(\hat{k}) Y_{\ell m}(\hat{r}),
\]

where \( \gamma \) is the angle between \( \mathbf{x} \) and \( \mathbf{k} \). Then the expansion (23) becomes

\[
e^{i\mathbf{k} \cdot \mathbf{x}} = \sum_{\ell} i^\ell (2\ell + 1) j_\ell(kr) P_\ell(\cos \gamma).
\]

Notice that if we take \( \mathbf{k} \) to lie in the \( z \)-direction, \( \mathbf{k} = k\hat{z} \), then \( \gamma \) is the same as \( \theta \), the usual spherical coordinate. In that case, the incident plane wave becomes

\[
e^{i\mathbf{k} \cdot \mathbf{x}} = e^{ikr \cos \theta},
\]

that is, it is independent of the azimuthal angle \( \phi \), and the sum (25) is the expansion of the plane wave in Legendre polynomials of \( \cos \theta \).

8. Asymptotic Form of the Radial Wave Functions

If the potential \( V(r) \) is nonzero but vanishes outside a cut-off radius \( r = r_{\text{co}} \), then the radial eigenfunctions \( R_{k\ell}(r) \) in the region \( r > r_{\text{co}} \) are linear combinations of both \( j_\ell(kr) \) and \( y_\ell(kr) \). The \( y_\ell \)-type solutions are allowed because there is no attempt to extend them down to \( r = 0 \). Then, in view of Eqs. (18) and (19), we can write the leading asymptotic form of \( R_{k\ell}(r) \) as a linear combination of two functions,

\[
R_{k\ell}(r) \sim \frac{\sin(kr - \ell\pi/2)}{kr}, \quad \frac{\cos(kr - \ell\pi/2)}{kr}.
\]
Equivalently, the leading asymptotic form of $u_{k\ell}(r)$ is a linear combination of two simple exponentials,

$$u_{k\ell}(r) \sim e^{\pm ikr}. \quad (28)$$

What about when the potential does not cut off at a finite radius, but goes to zero gradually? One might guess that if it goes to zero fast enough, then when $r \to \infty$ the potential would not matter, and the leading asymptotic forms (27) and (28) would still be valid. Let us examine the asymptotic form of the radial wave functions more carefully to see if this is true.

We now allow $V(r)$ to go to zero gradually as $r \to \infty$, with no rigorous cut-off. We cannot find an explicit form of the radial eigenfunctions $R_{k\ell}(r)$ or $u_{k\ell}(r)$ without knowing the potential and solving the radial Schrödinger equation, but determining just the asymptotic form does not require this. It is easier to work with the $u$-form of the radial Schrödinger equation (17) for this analysis.

Since both the true potential and the centrifugal potential go to zero as $r \to \infty$, the function $W(r)$, defined by Eq. (18), also goes to zero as $r \to \infty$. So as a first stab at analyzing the asymptotic form of $u_{k\ell}(r)$, let us neglect $W(r)$ altogether on the right hand side of the radial Schrödinger equation (17). Then the solution for $u_{k\ell}(r)$ is simply a linear combination of the exponentials (28).

To take into account the effects of $W(r)$, let us write the solution of Eq. (17) as

$$u_{k\ell}(r) = e^{g(r) \pm ikr}, \quad (29)$$

where $g(r)$ is a correction that will account for the effects of the function $W(r)$. If we can show that $g(r) \to 0$ as $r \to \infty$, then the correct asymptotic forms of $u_{k\ell}(r)$ will be a linear combination of the solutions (28). That is, the function $W(r)$ on the right hand side will make no difference in the asymptotic form of the solution. Substituting Eq. (29) into the radial Schrödinger equation (17), we obtain an equation for $g$,

$$g'' + g'^2 + 2ikg' = W(r). \quad (30)$$

This is rigorously equivalent to Eq. (17).

Now we consider the behavior of $W(r)$ as $r \to \infty$. If the true potential $V(r)$ goes to zero faster than $1/r^2$, then $W(r)$ is dominated by the centrifugal potential and also goes to zero as $1/r^2$. We assume $\ell \neq 0$, so the centrifugal potential does not vanish. If the true potential goes to zero more slowly than $1/r^2$, let us assume that it does so as a power law, $1/r^p$, where $1 < p \leq 2$. This excludes the case of the Coulomb potential, for which $p = 1$, but it approaches the Coulomb potential as $p \to 1$. Then $W(r)$ has the asymptotic form,

$$W(r) \sim \frac{a}{r^p}, \quad (31)$$

where $1 < p \leq 2$ and $a$ is a constant. The case $\ell = 0$ can be handled as a special case, but it does not change any of the conclusions that we shall draw.

We are interested in solving Eq. (30) in the asymptotic region when $W$ has the asymptotic behavior (31). Let us assume that $g$ is asymptotically given by a power law,

$$g(r) \sim \frac{b}{r^s}, \quad (32)$$
where \( b \) is another constant and \( s > 0 \). Then the three terms on the left hand side of Eq. (30) go as \( 1/r^{s+2}, 1/r^{2s+2} \) and \( 1/r^{s+1} \), in that order. The third term dominates, so to leading order we have \( s = p - 1 \), so that \( 0 < s \leq 1 \), and the power law ansatz for \( g \) has a solution. That is, \( g(r) \sim b/r^{p-1} \), \( g(r) \) goes to zero as \( r \to \infty \), and thus the asymptotic form of \( u_{k\ell}(r) \) is a linear combination of \( e^{\pm ikr} \).

But in the case of the Coulomb potential, \( W(r) \sim a/r \), that is, with \( p = 1 \). Then taking the dominant term in Eq. (30), we have

\[
\pm 2ikg'(r) = \frac{a}{r},
\]

or,

\[
g(r) = \mp \frac{ia}{2k} \ln(kr).
\]

The logarithm does not go to zero as \( r \to \infty \), in fact, it increases without bound (although very slowly). Thus, in the case of the Coulomb potential, the asymptotic form of the radial wave function is

\[
u_{k\ell}(r) \sim \exp\left\{ \pm i\left[ kr - \frac{a}{2k} \ln(kr) \right] \right\}.
\]

The Coulomb potential gives rise to long range, logarithmic phase shifts that do not approach the free particle phases as \( r \to \infty \).

In summary, if the potential \( V(r) \) goes to zero faster than \( 1/r \), then the asymptotic form of the radial wave function is given by the linear combinations shown in Eq. (27) (for \( R_{k\ell} \)) or in Eq. (28) (for \( u_{k\ell} \)). For the rest of these notes we will assume that \( V(r) \) does satisfy this condition, thereby excluding the Coulomb potential.

9. Partial Waves

With this assumption about \( V(r) \), we can write the asymptotic form of \( R_{k\ell}(r) \) as a linear combination of the functions (27), that is,

\[
R_{k\ell}(r) \sim \frac{A\sin(kr - \ell\pi/2) + B\cos(kr - \ell\pi/2)}{kr},
\]

where \( A \) and \( B \) are constants. Since the radial Schrödinger equation (16) is a real equation, we can choose the functions \( R_{k\ell}(r) \) to be real, and thus the coefficients \( A \) and \( B \) are real. We have not specified the normalization we will use for the radial wave function, but if we change the normalization it amounts to multiplying \( A \) and \( B \) by a common constant. The ratio \( A/B \) or \( B/A \), however, can only be determined by solving the radial Schrödinger equation.

We multiply Eq. (36) by a constant to make the new values of \( A \) and \( B \) satisfy \((A^2 + B^2)^{1/2} = 1\). Then by using trigonometric identities Eq. (36) can be written

\[
R_{k\ell}(r) \sim \frac{\sin(kr - \ell\pi/2 + \delta_\ell)}{kr},
\]

where \( \cos\delta_\ell = A, \sin\delta_\ell = B \). The phase \( \delta_\ell \) depends on both \( \ell \) and \( k \), but we suppress the \( k- \) (or energy-) dependence in the notation.
The resulting asymptotic form has a single parameter, the phase shift $\delta_\ell$. Knowledge of $\delta_\ell$ is equivalent to knowledge of the ratio $A/B$ or $B/A$. We should compare the asymptotic form (37), which applies in the case of a potential $V(r)$, to the asymptotic form for the free particle, for which $R_{k\ell}(r) = j_\ell(kr)$. Using Eq. (20), we can write the latter as

$$R_{k\ell}(r) \sim \frac{\sin(kr - \ell\pi/2) - j_\ell(kr)}{kr} \quad \text{(free particle)}.$$  

(38)

Thus the phase shift $\delta_\ell$ in Eq. (37) is measured relative to the free particle phase.

The phases that occur in the asymptotic forms of the radial wave function in the case of any $V(r)$, Eq. (37), and in the case of the free particle, Eq. (38), can be visualized as follows. The solutions in both cases apply in the asymptotic region (large $r$), and both solutions are linear combinations of the spherical waves $e^{\pm ikr}/r$, of which $e^{-ikr}/r$ is inward traveling, and $e^{ikr}/r$ is outward traveling. We can imagine sending in an inward traveling spherical wave from a large distance, which collapses toward $r = 0$, then bounces back out as an outward going spherical wave. We can then measure the phase difference between the inward and outward going waves. We get a certain phase difference in the case of a free particle, and a different one in the case of the potential. The effect of the potential is to introduce a phase shift in the reflected wave, which is measured by $\delta_\ell$.

Now let us return to Eq. (19), the expansion of a general solution of the Schrödinger equation of energy $E$ as a linear combination of eigenfunctions of $H$, $L^2$ and $L_z$, and let us split a factor of $4\pi i^\ell$ from the coefficients $C_{\ell m}$ in order to make the sum look more like the plane wave expansion, Eq. (23). That is, let us write the general solution as

$$\psi(x) = 4\pi \sum_{\ell m} i^\ell C_{\ell m} R_{k\ell}(r) Y_{\ell m}(\hat{r}).$$  

(39)

We wish to determine the coefficients $C_{\ell m}$ such that the solution (39) will incorporate the incident plane wave and outgoing scattered wave of the desired scattering solution.

Interpreting (39) as the desired scattering solution of the Schrödinger equation (1), we subtract Eq. (23) from this and use Eq. (4), obtaining an expansion of the scattered wave,

$$\psi_{\text{scatt}}(x) = \psi(x) - e^{ikr} = 4\pi \sum_{\ell m} i^\ell \left[ C_{\ell m} R_{k\ell}(r) - j_\ell(kr) Y_{\ell m}(\hat{k}) \right] Y_{\ell m}(\hat{r}).$$  

(40)

At large distances, the scattered wave must consist of purely outgoing spherical waves. Taking the large $r$ limit and using Eqs. (37) and (38), the quantity in the square brackets in Eq. (40) becomes

$$[\ldots] = \frac{1}{kr} \left[ C_{\ell m} \sin(kr - \ell\pi/2 + \delta_\ell) - Y_{\ell m}^*(\hat{k}) \sin(kr - \ell\pi/2) \right].$$  

(41)

This is a linear combination of incoming and outgoing waves that are proportional to $e^{-ikr}/r$ and $e^{+ikr}/r$, respectively. The incoming part is

$$-\frac{1}{kr} \frac{1}{2i} \left[ C_{\ell m} e^{-i(kr - \ell\pi/2 + \delta_\ell)} - Y_{\ell m}^*(\hat{k}) e^{-i(kr - \ell\pi/2)} \right].$$  

(42)
But the scattered wave must be purely outgoing, so this must vanish. This implies
\[ C_{\ell m} = e^{i\delta_\ell} Y_{\ell m}(\mathbf{k}). \]  

(43)

We see that the exact expansion coefficients of the scattering solution (39) can be determined in terms of the asymptotic phase shifts of the radial eigenfunctions. Now substituting this back into the outgoing part of Eq. (41), we find, for the quantity in the square brackets in Eq. (40),
\[ \ldots = \frac{1}{kr} Y_{\ell m}^*(\mathbf{k}) e^{i(kr-\ell \pi/2)} \left( \frac{e^{2i\delta_\ell} - 1}{2i} \right). \]

(44)

Then the asymptotic form of the scattered wave (40) becomes
\[ \psi_{\text{scatt}}(x) \sim 4\pi e^{ikr} kr \sum_{\ell m} e^{i\delta_\ell} \sin \delta_\ell Y_{\ell m}^*(\mathbf{k}) Y_{\ell m}(\mathbf{r}), \]

(45)

where we have used \( i^{\ell} e^{-i\ell \pi/2} = 1. \) Using the addition theorem for spherical harmonics (24), this can also be written,
\[ \psi_{\text{scatt}}(x) \sim \frac{e^{ikr}}{kr} \sum_{\ell} (2\ell + 1) e^{i\delta_\ell} \sin \delta_\ell P_\ell(\cos \theta), \]

(46)

where we have assumed that \( k = k\hat{z} \) so that the angle between \( \mathbf{k} \) and \( \mathbf{r} \) is the usual spherical angle \( \theta. \) Since \( \mathbf{k} \) is the direction of the incident beam, and since \( \mathbf{r} \) is the direction to some distant observation point, \( \theta \) can be interpreted as the scattering angle.

Equation (46) is called the partial wave expansion of the scattered wave, that is, its angular dependence is expanded in spherical harmonics or Legendre polynomials with coefficients given in terms of the asymptotic phase shifts of the radial eigenfunctions. Comparing this with Eq. (6) we obtain the partial wave expansion of the scattering amplitude,
\[ f(\theta, \phi) = \frac{4\pi}{k} \sum_{\ell m} e^{i\delta_\ell} \sin \delta_\ell Y_{\ell m}^*(\mathbf{k}) Y_{\ell m}(\theta, \phi), \]

(47)

or, setting \( k = k\hat{z} \) and using the addition theorem for spherical harmonics,
\[ f(\theta) = \frac{1}{k} \sum_{\ell} (2\ell + 1) e^{i\delta_\ell} \sin \delta_\ell P_\ell(\cos \theta). \]

(48)

In the latter case it is obvious from symmetry that the scattered wave and hence the scattering amplitude are independent of the azimuthal angle \( \phi, \) as indicated by the expansion (48). This is a consequence of the rotational invariance of the potential \( V(r). \)

Squaring the scattering amplitude we obtain the differential cross section,
\[ \frac{d\sigma}{d\Omega}(\theta, \phi) = \left( \frac{4\pi}{k} \right)^2 \sum_{\ell m \ell' m'} e^{i(\delta_\ell - \delta_{\ell'})} \sin \delta_\ell \sin \delta_{\ell'} Y_{\ell m}^*(\mathbf{k}) Y_{\ell' m'}(\mathbf{k}) Y_{\ell m}(\mathbf{r}) Y_{\ell' m'}(\mathbf{r}), \]

(49)

or, with \( k = k\hat{z}, \)
\[ \frac{d\sigma}{d\Omega}(\theta) = \frac{1}{k^2} \sum_{\ell \ell'} (2\ell + 1)(2\ell' + 1) e^{i(\delta_\ell - \delta_{\ell'})} \sin \delta_\ell \sin \delta_{\ell'} P_\ell(\cos \theta) P_{\ell'}(\cos \theta). \]

(50)
These expressions have cross terms that do not simplify, but which show up experimentally as oscillations in the angular dependence of the differential cross section.

On the other hand, when we integrate over all angles to obtain the total cross section, the cross terms integrate to zero. This is easiest to see in the form (49), due to the orthonormality of the $Y_{\ell m}$’s. The result is

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = \left(\frac{4\pi}{k}\right)^2 \sum_{\ell m} \sin^2 \delta_{\ell} Y_{\ell m}^*(\hat{k}) Y_{\ell m}(\hat{k}),$$

or, with another application of the addition theorem (and noting that $\hat{k} \cdot \hat{k} = 1$ and $P_\ell(1) = 1$),

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell} (2\ell + 1) \sin^2 \delta_{\ell}.$$  

This is the partial wave expansion of the total cross section.

10. Hard Sphere Scattering

As an example of the partial wave expansion, let us consider scattering from a hard sphere. The potential is

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

where $a$ is the radius of the sphere. In the region $r > a$ the solution is a linear combination of the $j$- and $y$-type spherical Bessel functions, which we write as

$$R_{k\ell}(r) = A j_{\ell}(kr) - B y_{\ell}(kr),$$

for some constants $A$ and $B$. The radial wave function $R_{k\ell}$ is labeled by both the angular momentum $\ell$ and effective wave number $k$, where $E = \hbar^2 k^2 / 2m$. The wave function must vanish at $r = a$, so we have

$$0 = A j_{\ell}(ka) - B y_{\ell}(ka),$$

which determines the ratio of $B$ and $A$,

$$\frac{B}{A} = \frac{j_{\ell}(ka)}{y_{\ell}(ka)}.$$  

To obtain the actual values of $A$ and $B$ we must specify a normalization convention for $R_{k\ell}(r)$. We will choose a normalization so that

$$A^2 + B^2 = 1,$$

which specifies $A$ and $B$ to within a sign. We fix the sign by setting

$$A = -\frac{y_{\ell}(ka)}{D} = \cos \delta_{\ell},$$

$$B = -\frac{j_{\ell}(ka)}{D} = \sin \delta_{\ell},$$

where $D = \sqrt{\cos^2 \delta_{\ell} + \sin^2 \delta_{\ell}}$. The result is

$$\sigma = \frac{4\pi}{k^2} \sum_{\ell} (2\ell + 1) \sin^2 \delta_{\ell}.$$  

This is the partial wave expansion of the total cross section.
where the denominator $D$ is given by

$$D = \sqrt{j_\ell(ka)^2 + y_\ell(ka)^2}.$$  

Equation (58) also defines the angle $\delta_\ell$ modulo $2\pi$, which will turn out to be the phase shift. With these definitions, the solution in the region $r > a$ is

$$R_{k\ell}(r) = \frac{1}{D} \det \begin{bmatrix} j_\ell(ka) & y_\ell(ka) \\ j_\ell(kr) & y_\ell(kr) \end{bmatrix} = \cos\delta_\ell j_\ell(kr) - \sin\delta_\ell y_\ell(kr).$$  

Now taking the asymptotic forms (16.29) and (16.30), valid when $kr \gg \ell$, we find

$$R_{k\ell}(r) \sim \frac{1}{kr} \sin\left(kr - \frac{\ell\pi}{2} + \delta_\ell\right),$$  

confirming that $\delta_\ell$ is the phase shift.

Knowledge of the $\delta_\ell$ implies knowledge of the scattering amplitude and differential cross section. We will consider two limiting cases, in which the limiting forms of the spherical Bessel functions $j_\ell$ and $y_\ell$ can be used.

11. The limit $ka \ll 1$

In the first case we assume $ka \ll 1$. This is equivalent to $\lambda \gg a$, where $\lambda = 2\pi/k$ is the wavelength of the incident waves, that is, the scatterer is much smaller than a wavelength. The small argument forms of $j_\ell$ and $y_\ell$, Eqs. (16.27) and (16.28), show that in this case $y_\ell(ka)$ is large and negative and $j_\ell(ka)$ is small and positive. Then Eq. (58) shows that $\cos\delta_\ell$ is near 1 and $\sin\delta_\ell$ is small and negative for all values of $\ell$. Thus, to a good approximation,

$$\sin\delta_\ell \approx \delta_\ell \approx -\frac{(ka)^{2\ell+1}}{(2\ell - 1)!!(2\ell + 1)!!}.$$  

This shows that not only is the lowest phase shift $\delta_0$ small, the higher phase shifts $\delta_\ell$ for $\ell \geq 1$ are even smaller. In this limit

$$\delta_0 = -ka,$$  

and the series (48) for the scattering amplitude is dominated by the single term $\ell = 0$. Thus we have

$$f(\theta) = \frac{1}{k}(-ka) = -a, \quad ka \ll 1,$$  

since $e^{i\delta_0} \approx 1$ and $P_0(\cos\theta) = 1$. We see that the differential cross section is independent of angle,

$$\frac{d\sigma}{d\Omega} = a^2,$$  

and the total cross section is

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega} = 4\pi a^2.$$  

The total cross section is four times as large as the geometrical cross-sectional area of the small sphere. The classical cross section is just this cross-sectional area, $\pi a^2$, but the regime $\lambda \gg a$ is the one in which we expect classical mechanics to be a poor approximation to quantum mechanics, so we should not be surprised by the difference.
12. \( s \)-wave Scattering

When the partial wave \( \ell = 0 \) dominates the expansion of the scattering amplitude, we speak of \( s \)-wave scattering. The scattered wave is isotropic and has an equal intensity in all directions, including the forward direction. Since \( a \ll \lambda \) the sphere is too small to create a shadow; instead, the incident wave effectively wraps all the way around the scatterer. As we will see later, \( s \)-wave scattering applies to any localized potential whose characteristic size \( a \) satisfies \( a \ll \lambda \), that is, \( ka \gg 1 \) (not just hard spheres). The fundamental reason is that the radial wave functions must tunnel through the centrifugal potential to reach the scatterer, and the tunneling is deeper the higher the \( \ell \) value. Thus, the effect of the scatterer, as measured by the phase shift, is an exponentially decreasing function of \( \ell \). Recall that the phase shift \( \delta_\ell \) is a measure of the deviation from the behavior of a free particle in the \( \ell \)-th partial wave.

There are many physical examples in which \( s \)-wave scattering is important. For example, a Bose-Einstein condensate is a dilute gas of atoms at a temperature at which the de Broglie wavelength \( \lambda \) of the atoms due to their thermal motion is larger than the interparticle separation. Since the gas is dilute, the interparticle separation in turn is much larger than the atomic size, call it \( a \), so we have \( \lambda \gg a \), or \( ka \ll 1 \). Thus the interactions of the atoms with one another is described by \( s \)-wave scattering, and scattering of atoms by atoms, in all its complexity, is described by a single parameter, which is the phase shift \( \delta_0 \).

In \( s \)-wave scattering any two potentials that give the same phase shift \( \delta_0 \) will have the same effect. Therefore in theoretical models the exact potential can be replaced by a simpler one, as long as the phase shift is the same. Delta function potentials are popular for this purpose, which explains their appearance in the models of Bose-Einstein condensates such as the Gross-Pitaevski equation.

When light scatters from particles that are much smaller than the wavelength, for example, when optical radiation is scattered by atoms in a gas, is this \( s \)-wave scattering, and is the scattered wave isotropic? (This is a tricky question.) The answer is no, because electromagnetic waves are vector waves, not scalar waves as we have been discussing in these notes. In the case of electromagnetic waves, the scattering when \( ka \ll 1 \) is dominated by dipole radiation, which has a nontrivial angular dependence. Electromagnetic waves have no monopole radiation (that is, \( s \)-wave radiation), and the next higher term in the multipole series is the first one to appear. It is the one that dominates at small \( ka \).

13. The Limit \( ka \gg 1 \)

The second case we consider is the opposite extreme, \( ka \gg 1 \), that is, \( \lambda \ll a \). In this case the sphere is much larger than a wavelength. Now there are many \( \ell \) values that contribute to the partial wave sum. For small \( \ell \), for which \( \ell \ll ka \), we can use the asymptotic forms for \( j_\ell(ka) \) and \( y_\ell(ka) \), Eqs. (16.29) and (16.30). Substituting these into Eqs. (58) and (59) we find \( D = 1/ka \) and

\[
\delta_\ell = -ka + \frac{\ell\pi}{2}.
\]
This says that $\delta_\ell$ advances by $\pi/2$ when $\ell$ increases by 1, but this is an approximation that is only valid when $\ell \ll ka$. As $\ell$ increases toward $ka$, the increment in $\delta_\ell$ gradually gets smaller. When $\ell$ reaches and exceeds $ka$, the phase shifts $\delta_\ell$ rapidly approach zero, and the partial wave expansion (48) effectively cuts off. The same is true for the expansion (52) of the total cross section.

An intuitive explanation for the cutoff at $\ell \approx ka$ is illustrated in Fig. 4. We imagine particles of fixed energy $E = \hbar^2 k^2 / 2m$ emitted in various directions from a point on the surface of a sphere of radius $a$. These represent the waves scattered by the sphere. The angular momentum of the particles depends on the direction of emission; its minimum value is $L = 0$ when the particles are launched in the radial direction, and its maximum value $L = pa = \hbar ka$ is when the particles are launched tangentially to the sphere. The maximum value of $L$ corresponds to a maximum angular momentum quantum number, $\ell = L/\hbar = ka$. The same reasoning works for any short-range potential with an effective range of $a$; the partial wave expansion cuts off near $\ell \approx ka$.

The phase shift $\delta_\ell$ is determined by Eqs. (58) to within a multiple of $2\pi$. Thus each $\delta_\ell$ corresponds to a point on a circle with coordinates $x = \cos \delta_\ell$, $y = \sin \delta_\ell$. As $\ell$ increases away from $\ell = 0$, this point advances by a phase angle around the circle, where for $\ell \ll ka$ the increment is $\pi/2$, as indicated by Eq. (67). As mentioned, this increment decreases as $\ell$ increases toward $ka$. Finally, when $\ell \approx ka$, the phase shifts approach zero. This behavior is illustrated in Figs. 5 and 6.

While the points representing the $\delta_\ell$ are orbiting their circle as in Figs. 5 and 6, the average value of $\sin^2 \delta_\ell$ is $1/2$. Since the series cuts off near $\ell \approx ka$, the total cross section (52) can be estimated by

$$\sigma \approx \frac{4\pi}{k^2} \sum_{\ell=0}^{ka} (2\ell + 1) \frac{1}{2}. \quad (68)$$

Using the sum

$$\sum_{\ell=0}^{L} (2\ell + 1) = (L + 1)^2, \quad (69)$$
we obtain the estimate

$$\sigma \approx \frac{4\pi (ka)^2}{k^2} = 2\pi a^2,$$

(70)

where we ignore the difference between $ka$ and $ka + 1$. We see that the cross section is twice the classical value in the case $ka \gg 1$.

These conclusions are confirmed by detailed calculations, which show that $\sigma \to 4\pi a^2$ as $ka \to 0$ and $\sigma \to 2\pi a^2$ as $ka \to \infty$. See Fig. 7.

If we think of the classical limit as one in which the de Broglie wavelength $\lambda$ is much smaller than the scale of the potential, then it is surprising that the limit $\sigma \to 2\pi a^2$ as $ka \to \infty$ since this is twice the classical cross section, $\pi a^2$. To see how this “extra” cross-section is distributed in angle we refer to Fig. 8, a plot of the differential cross section for various values of $ka$.

Figure 8 shows that for small values of $ka$, the differential cross section is nearly independent of angle, confirming that we have $s$-wave scattering. The cross section $d\sigma/d\Omega$ is nearly $a^2$ in this range, confirming Eq. (65). As $ka$ increases, $d\sigma/d\Omega$ decreases at large angles toward the classical value, but at small angles a forward peak rises up, growing narrower and higher. At the edge of forward peak there also arise oscillations. Figure 9 is a similar plot except that $d\sigma/d\Omega$ has been multiplied by $\sin \theta$, which makes the integrated cross section proportional to area under the curve. This makes it easier to see that the total cross section in the forward peak is about the same as the classical cross section. In fact, detailed calculations (see Prob. 1) show that both the forward peak and the classical cross section contribute $\pi a^2$ to the total. The “extra” cross section comes entirely from the forward peak.

This peak is due to diffraction. As the waves pass by the edge of the sphere they are bent
Fig. 7. Total cross section $\sigma$ as a multiple of $\pi a^2$ for hard sphere scattering as a function of $ka$. The total cross section has the limits $\sigma \to 4\pi a^2$ as $ka \to 0$ and $\sigma \to 2\pi a^2$ as $ka \to \infty$.

in an inward direction, that is, the direction necessary to close in the shadow behind the sphere. Diffraction theory shows that if we move far enough downstream, the shadow is completely filled by diffracted waves. Of course the differential cross section is defined in the limit $r \to \infty$, so there is

Fig. 8. Differential cross section in hard sphere scattering, as a multiple of $a^2$. Curves are labeled by the value of $ka$, which increases from 0.1 to 8. Scattering angle $\theta$ is measured in degrees.

Fig. 9. Same as Fig. 8 except multiplied by $\sin \theta$. Area under curves in a given angle range is proportional to the total cross section in that range.
no shadow in the differential cross section. Diffraction causes the direction of the waves to change from the incident direction, and so must be counted as part of the scattering.

14. The Optical Theorem

The optical theorem is an exact relationship between the total cross section $\sigma$ and the scattering amplitude $f$. In the context of potential scattering that we have considered in these notes, the optical theorem is

$$\sigma = \frac{4\pi}{k} \text{Im} f(0), \quad (71)$$

where $f(0)$ refers to the scattering amplitude in the forward direction.

The optical theorem is trivial to prove in the case of scattering by central force potentials. We place the $z$-axis along the direction of the beam so that the usual polar angle $\theta$ is the scattering angle. Then Eq. (48) implies

$$\frac{4\pi}{k} \text{Im} f(0) = \frac{4\pi}{k^2} \text{Im} \sum_{\ell=0}^{\infty} (2\ell + 1) e^{i\delta_{\ell}} \sin \delta_{\ell} P_{\ell}(1) = \frac{4\pi}{k^2} \sum_{\ell=0}^{\infty} (2\ell + 1) \sin^2 \delta_{\ell} = \sigma, \quad (72)$$

where we have used Eqs. (52) and (15.75). This proof is straightforward but it gives no insight into what the theorem means.

The theorem (71) actually applies to scattering by any potential $V(x)$ that dies off faster than $1/r$ as $r \to \infty$, so that the asymptotic wave function is

$$\psi(x) \sim e^{ik\cdot x} + \frac{e^{ikr}}{r} f(\theta, \phi), \quad (73)$$
as indicated by Eqs. (5) and (6). That is, we need not assume that the potential is rotationally invariant. The two terms in Eq. (73) are the incident and scattered waves, respectively.

Since the wave function $\psi(x)$ is a solution of the time-independent Schrödinger equation, the current

$$J = \text{Re} \psi^*(x) \left( -\frac{i\hbar \nabla}{m} \right) \psi(x) \quad (74)$$

satisfies $\nabla \cdot J = 0$, so by Stokes’ theorem the integral of $J$ over any closed surface vanishes. See Eqs. (5.55)–(5.57). We will integrate $J$ over a large sphere of radius $r$ centered at the origin of the coordinates, which we assume is inside the region occupied by the potential as in Fig. 2. We will take the limit $r \to \infty$, so that the asymptotic form (73) of the wave function can be used.

Thus the asymptotic form of the current is

$$J \sim \text{Re} \left[ e^{-ikx} + \frac{e^{-ikr}}{r} f^*(\theta, \phi) \right] \left( -\frac{i\hbar \nabla}{m} \right) \left[ e^{ikx} + \frac{e^{ikr}}{r} f(\theta, \phi) \right]$$

$$= v \text{Re} \left[ e^{-ikr \cos \theta} + \frac{e^{-ikr}}{r} f^*(\theta, \phi) \right] \left[ \hat{z} \ e^{ikr \cos \theta} + \hat{r} \ e^{ikr} f(\theta, \phi) \right], \quad (75)$$

where we have set $\mathbf{k} = kg \hat{z}$ and $v = \hbar k/m$ and retained only the leading term in the gradient of the scattered wave, as in Eq. (11). The neglected terms will not contribute to the integral over the sphere when we take the limit $r \to \infty$. 
The current is quadratic in the wave function $\psi(x)$, so in addition to the incident current and scattered current there is a contribution coming from the cross terms, which represent the interference between the incident wave and the scattered wave. We write

$$J = J_{\text{inc}} + J_{\text{scatt}} + J_x,$$  \hspace{1cm} (76)

where $J_x$ is the interference current. By Stokes’ theorem we have

$$\int_{\text{sphere}} J \cdot d\mathbf{a} = 0,$$  \hspace{1cm} (77)

where $d\mathbf{a} = r^2 \hat{r} d\Omega$ is the area element of the sphere.

The incident current is

$$J_{\text{inc}} = v \Re \left( e^{-ikr \cos \theta} \hat{z} e^{ikr \cos \theta} \right) = v \hat{z},$$  \hspace{1cm} (78)

It is a constant vector whose integral over sphere vanishes,

$$\int_{\text{sphere}} J_{\text{inc}} \cdot d\mathbf{a} = 0,$$  \hspace{1cm} (79)

as is obvious from Fig. 10.

The scattered current was already computed in Sec. 5. It is

$$J_{\text{scatt}} = v \Re \left( \frac{e^{-ikr}}{r} f^*(\theta, \phi) \hat{r} \frac{e^{ikr}}{r} f(\theta, \phi) \right) = v \hat{r} \frac{r}{r^2} |f(\theta, \phi)|^2,$$  \hspace{1cm} (80)

whose integral over the sphere is

$$\int_{\text{sphere}} J \cdot d\mathbf{a} = v \int_{\text{sphere}} |f(\theta, \phi)|^2 d\Omega = \sigma v,$$  \hspace{1cm} (81)
where \(\sigma\) is the total cross section and where we have used Eq. (14). The scattered wave gives a net outgoing flux, proportional to the cross section, which is no surprise. See Fig. 11.

Therefore the interference current must provide a net inward flux that cancels the scattered flux. From Eq. (75) we have

\[
\mathbf{J}_x = \frac{v}{r} \Re \left[ \mathbf{\hat{z}} e^{-ikr(1-\cos \theta)} f^* (\theta, \phi) + \mathbf{\hat{r}} e^{ikr(1-\cos \theta)} f (\theta, \phi) \right].
\]

But the real part of a complex number is the same as the real part of its complex conjugate, so we can replace the first term in Eq. (82) by its complex conjugate to obtain

\[
\mathbf{J}_x = \frac{v}{r} \Re \left[ (\mathbf{\hat{z}} + \mathbf{\hat{r}}) e^{ikr(1-\cos \theta)} f (\theta, \phi) \right].
\]

Now the interference flux is

\[
\int_{\text{sphere}} \mathbf{J}_x \cdot d\mathbf{a} = \frac{vr}{k} \Re \int_0^{2\pi} d\phi \int_0^\pi \sin \theta \, d\theta \, (1 + \cos \theta) \, e^{ikr(1-\cos \theta)} f (\theta, \phi).
\]

We wish to evaluate this integral in the limit \(r \to \infty\), which is slightly delicate. The prefactor of \(r\) would tend to make the integral diverge, but the factor \(e^{ikr(1-\cos \theta)}\) in the integrand oscillates ever more rapidly in \(\theta\) as \(r\) gets larger, thereby chopping up the integrand and tending to make the integral vanish. To clarify the competition between these tendencies, we integrate by parts in \(\theta\), obtaining

\[
\int_{\text{sphere}} \mathbf{J}_x \cdot d\mathbf{a} = \frac{vr}{k} \Re \int_0^{2\pi} d\phi \int_0^\pi \sin \theta \, d\theta \, (1 + \cos \theta) \, e^{ikr(1-\cos \theta)} f (\theta, \phi)
\]

\[
= \frac{v}{k} \Re \int_0^{2\pi} d\phi \left\{ -ie^{ikr(1-\cos \theta)} (1 + \cos \theta) f (\theta, \phi) \bigg|_{\theta=0}^{\theta=\pi} + i \int_0^\pi d\theta \, e^{ikr(1-\cos \theta)} \frac{d}{d\theta} [(1 + \cos \theta) f (\theta, \phi)] \right\}.
\]

The integration by parts has eliminated the prefactor of \(r\), so now the final integral oscillates itself to death as \(r \to \infty\) and can be dropped. Evaluating the remaining term under the \(\phi\)-integral at the limits \(\theta = 0, \pi\), we see that it vanishes at \(\theta = \pi\) and that at \(\theta = 0\) it is proportional to \(f(0, \phi)\) which is what we are writing simply as \(f(0)\) and which is independent of \(\phi\). Thus we find

\[
\int_{\text{sphere}} \mathbf{J}_x \cdot d\mathbf{a} = \frac{v}{k} \Re \int_0^{2\pi} d\phi \, 2i f(0) = -\frac{4\pi v}{k} \Im f(0).
\]

The sum of this plus the scattered flux \(\sigma v\) vanishes, which produces the optical theorem (71).

We see that the interference flux comes in from the forward direction, where it partially cancels the incident flux going in the other direction.

The optical theorem has many generalizations. One version of it applies for the scattering of classical electromagnetic waves (vector waves, in contrast to the scalar waves considered here). Another applies to inelastic scattering in quantum mechanics, in which \(\sigma\) is the total cross section,
including both elastic and inelastic scattering, while \( f(0) \) refers only to the forward amplitude for elastic scattering. This is because only the wave for elastic scattering can interfere with the incident wave. There are many other applications in fields ranging from quantum mechanics to black hole physics.

**Problems**

1. The strange thing about scattering from a hard sphere in the limit \( ka \gg 1 \) is that the total cross section is \( 2\pi r^2 \), not \( \pi r^2 \), the geometrical cross section. When the wavelength is short, we expect quantum mechanics to agree with classical mechanics, but it does not in this case.

   (a) Work out the classical differential cross section \( d\sigma/d\Omega \) for a hard sphere of radius \( a \), and integrate it to get the total cross section \( \sigma \).

   (b) In problem 9.1, you worked out the far field wave function \( \psi(x, y, z) \), for \( z \gg ka^2 \), when a plane wave \( e^{ikz} \) traveling in the positive \( z \)-direction strikes a screen in the \( x-y \) plane with a circular hole of radius \( a \) cut out. In that problem the hole was centered on the origin. The solution was worked out for \( \theta = \rho/z \ll 1 \) (the paraxial approximation), where \( \rho = \sqrt{x^2 + y^2} \).

   By subtracting this solution from the incident wave \( e^{ikz} \), you get the far field wave function when a plane wave \( e^{ikz} \) strikes the complementary screen, that is, just a disk of radius \( a \) at the origin.

   It turns out this wave field is the same as the wave field in hard sphere (of radius \( a \)) scattering in the limit \( ka \gg 1 \), if measured in the forward direction. That is because for forward scattering from a hard scatterer, the physics is dominated by diffraction, so it is only the projection of the scatterer onto the \( x-y \) plane that matters.

   Write the scattered wave as \( (e^{ikr}/r)f(\theta) \), express \( r \) as a function of \( z \) and \( \theta \) for small \( \theta \), expand out to lowest order in \( \theta \), and compare to the asymptotic wave field to get an expression for the scattering amplitude for small angles \( \theta \). According to the optical theorem, the total cross section is given in terms of the imaginary part of the forward scattering amplitude by

   \[
   \sigma = \frac{4\pi}{k} \text{Im} f(0). \quad (87)
   \]

   Use this formula to compute \( \sigma \).

   (c) Show that \( d\sigma/d\Omega \) in the forward direction has a narrow peak of width \( \Delta\theta \sim 1/ka \ll 1 \). Write down an integral giving the contribution of this forward peak to the total cross section in terms of the first root \( b \) of the Bessel function \( J_1 \). You can approximate \( \sin \theta = \theta \) in this integral, since \( \theta \) is small. It turns out that the value of this integral does not change much if the upper limit is extended to infinity. Use the integral

   \[
   \int_0^\infty \frac{dx}{x} J_1(x)^2 = \frac{1}{2}, \quad (88)
   \]
to find the contribution of the forward peak to the total cross section. (See Gradshteyn and Ryzhik, integral number 6.538.2.)

2. This problem is borrowed from Sakurai. Consider a potential

\[ V(r) = \begin{cases} V_0 = \text{const}, & r < a, \\ 0, & r > a, \end{cases} \]  

(89)

where \( V_0 \) may be positive or negative. Using the method of partial waves, show that for \( |V_0| \ll E = \hbar^2 k^2 / 2m \) and \( ka \ll 1 \) the differential cross section is isotropic and that the total cross section is given by

\[ \sigma_{\text{tot}} = \frac{16 \pi m^2 V_0^2 a^6}{9 \hbar^4}. \]  

(90)

Suppose the energy is raised slightly. Show that the angular distribution can then be written as

\[ \frac{d\sigma}{d\Omega} = A + B \cos \theta. \]  

(91)

Obtain an approximate expression for \( B/A \).

3. This problem is best done after some experience with scattering of particles with spin, such as Problem 33.2.

Consider the scattering of a polarized, spin \( \frac{1}{2} \) particle by a target, such as a neutron by the nucleus of an atom (we may assume that the nucleus is polarized, too). There is some amplitude for scattering that does not flip the spin, and some for scattering that does.

Suppose the incident particle is polarized spin up, so that the incident wave function can be taken to be

\[ \psi_{\text{inc}} = e^{i k r} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \]  

(92)

The asymptotic form for the scattered wave is

\[ \psi_{\text{scatt}} \sim \frac{e^{i k r}}{r} \begin{pmatrix} f_+(\theta, \phi) \\ f_-(\theta, \phi) \end{pmatrix}, \]  

(93)

where \( f_\pm \) are the scattering amplitudes with and without spin flip.

Find a generalization of the optical theorem in this case. Recall Eq. (18.30) for the probability current for particles with spin. Is it possible that some target could cause the spin to flip with 100% probability? How do your answers change if a magnetization term such as seen in (18.33) is included in the probability current?