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 32 and 33. 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 $V = V(x)$. The potential should go to zero as $r = |x| \to \infty$; 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 $\psi(x)$ 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 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
Notes 34: Introduction to Scattering Theory

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 are discussed in Sakurai’s book, and which (some day) will appear in a separate set of notes.

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 32. 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, for example, 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.

\[
p = \hbar k
\]

Fig. 2. Quantum scattering by a potential \( V(x) \). Incident and scattered waves are shown.

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. 5.12 and 5.13) 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 32 we took an initial state (a plane wave filling
Notes 34: Introduction to Scattering Theory

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 32 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,

\[
-\frac{\hbar^2}{2m} \nabla^2 \psi(x) + V(x)\psi(x) = E\psi(x).
\]

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
solution 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 scatter 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

$$\psi_{\text{inc}}(x) = e^{ikx},$$

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

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

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

$$\psi_{\text{scatt}}(x) = \psi(x) - \psi_{\text{inc}}(x),$$

so that

$$\psi(x) = \psi_{\text{inc}}(x) + \psi_{\text{scatt}}(x),$$

exactly. Notice that since $\psi$ satisfies the Schrödinger equation exactly, and since $\psi_{\text{inc}}$ does also in the region $r > r_{\text{co}}$ 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 $r \gg r_{\text{co}}$ (continuing with the simplification that $V = 0$ for $r > r_{\text{co}}$).

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 $r \gg r_{\text{co}}$ 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 $e^{-iEt/\hbar}$) produces an
outwardly propagating spherical wave. Overall, we guess that the asymptotic form of the scattered wave is

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

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),

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

(7)

where the dominant term comes from the radial term of the Laplacian in spherical coordinates (see Eq. (D.21)). 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.

![Diagram](image_url)

Fig. 3. A particle detector intercepts a small solid angle \( \Delta\Omega \) which defines a cone as seen from the scatterer. Particles scattered into this cone will enter the detector.
Cross sections and differential cross sections were defined in Notes 32, 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 flux $J_{\text{scatt}}$, integrated across the aperture to the detector.

The probability density $\rho = |\psi|^2$ and probability flux $J$ were discussed in Secs. 5.12 and 5.13. 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 flux can be written

$$J = \hbar m \Im(\psi^* \nabla \psi),$$

which is a version of Eqs. (5.50) and (5.51).

In Notes 5, we were thinking of normalized wave functions, for which $\rho$ and $J$ are interpreted as the probability density and flux. 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 flux (with dimensions of particles/volume and particles/area-time, respectively).

The particle density in the incident beam is $|\psi_{\text{inc}}|^2$, or,

$$n_{\text{inc}} = 1.$$ (9)

There is one particle per unit volume in the incident beam. Similarly, the incident flux is easy to compute. It is

$$J_{\text{inc}} = \hbar k m = v,$$ (10)

where $v$ is the velocity of the incident beam. In magnitude, $J_{\text{inc}} = v$.

We will also need the scattered flux to get the counting rate. We first compute the gradient of the scattered wave (6) in spherical coordinates (see Eq. (D.18)),

$$\nabla \psi_{\text{scatt}}(x) = \hat{r} \left[ \frac{ik e^{ikr}}{r} f(\theta, \phi) \right] + O\left( \frac{1}{r^2} \right),$$ (11)

where we only carry the result to leading order in $1/r$. Substituting this into (8), we find

$$J_{\text{scatt}} \sim \frac{\hbar k}{m} \frac{|f(\theta, \phi)|^2}{r^2} \hat{r}. $$ (12)

To leading order, the asymptotic form of the scattered flux 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 flux 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

$$\frac{dv}{d\Omega} \Delta \Omega = \int_{\text{aperture}} J_{\text{scatt}} \cdot da = v|f(\theta, \phi)|^2 \Delta \Omega, $$ (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 integrated over 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 flux 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 will consider later.

### 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 \( E = \hbar^2k^2/2m \). 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

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

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 \( E \) is given by

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

where \( A_{\ell m} \) are the expansion coefficients. The freedom in the choice of the coefficients \( A_{\ell m} \) 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,

\[
\psi_{\text{free}}(x) = \sum_{\ell m} A_{\ell m} j_\ell(kr) Y_{\ell m}(\theta, \phi), \tag{22}
\]
for some expansion coefficients $A_{\ell m}$.

In particular, it must be possible to express the incident wave $e^{ik \cdot x}$ in this form. The problem of determining the expansion coefficients $A_{\ell m}$ 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

$$e^{ik \cdot x} = 4\pi \sum_{\ell m} i^\ell j^\ell(kr) Y^*_{\ell m}(\hat{k}) Y_{\ell m}(\hat{r}),$$

where $\hat{r}$ and $\hat{k}$ refer to the directions of the vectors $x$ and $k$ 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. (15.69), 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 $x$ and $k$. Then the expansion (23) becomes

$$e^{ik \cdot x} = \sum_{\ell} i^\ell (2\ell + 1) j^\ell(kr) P_\ell(\cos \gamma).$$

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

$$e^{ik \cdot x} = e^{ikr \cos \theta},$$

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 $r = r_{co}$, then the radial eigenfunctions $R_{k\ell}(r)$ in the region $r > r_{co}$ 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,

$$R_{k\ell}(r) \sim \frac{\sin(kr - \ell\pi/2)}{r}, \quad \frac{\cos(kr - \ell\pi/2)}{r}.$$

Equivalently, the leading asymptotic form of $u_{k\ell}(r)$ is a linear combination of two simple exponentials,

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

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

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

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 $g$,

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

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,

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

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,

$$g(r) \sim \frac{b}{r^s},$$

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, $g(r) \sim b/r^{p-1}$,
$g(r)$ does go 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

$$2ikg'(r) = \frac{a}{r},$$

or,

$$g(r) = \pm \frac{ia}{2k} \ln(kr).$$

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

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

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

$$R_{k\ell}(r) \sim \frac{\sin(kr - \ell\pi/2)}{kr} \quad \text{(free particle)}. \quad (38)$$

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 $A_{\ell m}$ in order to make the sum look more like the plane wave expansion, Eq. (23). That is, let us write the general solution as

$$\psi(x) = 4\pi \sum_{\ell m} i^\ell A_{\ell m} R_{k\ell}(r) Y_{\ell m}(\hat{r}). \quad (39)$$

We wish to determine the coefficients $A_{\ell m}$ 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,

$$\psi_{\text{scatt}}(x) = \psi(x) - e^{ikr} = 4\pi \sum_{\ell m} i^\ell [A_{\ell m} R_{k\ell}(r) - j\ell(kr)Y_{\ell m}^*(\hat{k})] Y_{\ell m}(\hat{r}). \quad (40)$$

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

$$[\ldots] = \frac{1}{kr} \left[ A_{\ell m} \sin(kr - \ell\pi/2 + \delta_\ell) - Y_{\ell m}^*(\hat{k}) \sin(kr - \ell\pi/2) \right]. \quad (41)$$

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

$$-\frac{1}{kr} \frac{1}{2i} \left[ A_{\ell m} e^{-i(kr-\ell\pi/2+\delta_\ell)} - Y_{\ell m}^*(\hat{k}) e^{-i(kr-\ell\pi/2)} \right]. \quad (42)$$

But the scattered wave must be purely outgoing, so this must vanish. This implies

$$A_{\ell m} = e^{i\delta_\ell} Y_{\ell m}^*(\hat{k}). \quad (43)$$
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),

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

(44)

Then the asymptotic form of the scattered wave (40) becomes

\[ \psi_{\text{scatt}}(x) \sim 4\pi e^{ikr} \sum_{\ell m} e^{i\delta_{\ell}} \sin \delta_{\ell} Y_{\ell m}^*(\hat{k}) Y_{\ell m}(\hat{r}), \]  

(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 \( \hat{k} \) and \( \hat{r} \) is the usual spherical angle \( \theta \). Since \( \hat{k} \) is the direction of the incident beam, and since \( \hat{r} \) 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,

\[ f(\theta, \phi) = \frac{4\pi}{k} \sum_{\ell m} e^{i\delta_{\ell}} \sin \delta_{\ell} Y_{\ell m}^*(\hat{k}) Y_{\ell m}(\theta, \phi), \]  

(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,

\[ \frac{d\sigma}{d\Omega}(\theta, \phi) = \left( \frac{4\pi}{k} \right)^2 \sum_{\ell m \ell' m'} e^{i(\delta_{\ell} - \delta_{\ell'})} \sin \delta_{\ell} \sin \delta_{\ell'} Y_{\ell m}^*(\hat{k}) Y_{\ell' m'}(\hat{k}) Y_{\ell m}(\hat{r}) Y_{\ell' m'}^*(\hat{r}), \]  

(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

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

(51)

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

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

(52)

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

**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 wave length 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 differential cross section by

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

(53)

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
\[ \int_0^\infty \frac{dx}{x} J_1(x)^2 = \frac{1}{2}, \]
(54)
to find the contribution of the forward peak to the total cross section. (See Gradshteyn and Ryzhik, integral number 6.538.2.)