22.101 Applied Nuclear Physics (Fall 2006)
Lecture 7 (10/2/06)

Overview of Cross Section Calculation

References –

P. Roman, *Advanced Quantum Theory* (Addison-Wesley, Reading, 1965), Chap 3.

A. Foderaro, *The Elements of Neutron Interaction Theory* (MIT Press, 1971), Chap 4.

The interaction of radiation with matter is a cornerstone topic in 22.101. Since all radiation interactions can be described in terms of cross sections, clearly the concept of a cross section and how one can go about calculating such a quantity are important considerations in our studies. To keep the details, which are necessary for a deeper understanding, from getting in the way of an overall picture of cross section calculations, we attach two appendices at the end of this Lecture Note, *Appendix A Concepts of Cross Section* and *Appendix B, Cross Section Calculation: Method of Phase Shifts*. The students regard the discussions there as part of the lecture material.

We begin by referring to the definition of the cross section σ for a general interaction as discussed in Appendix A. One sees that σ appears as the proportionality constant between the probability for the reaction and the number of target nuclei exposed per unit area, (which is why σ has the dimension of an area). We expect that σ is a dynamical quantity which depends on the nature of the interaction forces between the radiation (which can be a particle) and the target nucleus. Since these forces can be very complicated, it may then appear that any calculation of σ will be quite complicated as well. It is therefore fortunate that methods for calculating σ have been developed which are within the grasp of students who have had a few lectures on quantum mechanics as is the case of students in 22.101.

The method of phase shifts, which is the subject of Appendix B, is a well-known elementary method worthy of our attention.. Here we will discuss the key steps in this method, going from the introduction of the scattering amplitude $f(\theta)$ to the expression for the angular differential cross section $\sigma(\theta)$.

Expressing $\sigma(\theta)$ in terms of the Scattering Amplitude $f(\theta)$

We consider a scattering scenario sketched in Fig.7.1.

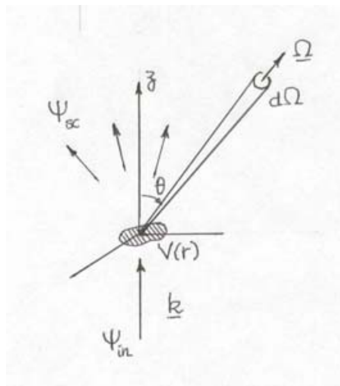

Fig.7.1. Scattering of an incoming plane wave by a potential field V(r), resulting in spherical outgoing wave. The scattered current crossing an element of surface area $d\Omega$ about the direction $\underline{\Omega}$ is used to define the angular differential cross section $d\sigma / d\Omega \equiv \sigma(\theta)$, where the scattering angle θ is the angle between the direction of incidence and direction of scattering.

We write the incident plane wave as

$$\Psi_{in} = be^{i(\underline{k}\cdot\underline{r}-\omega t)} \tag{7.1}$$

where the wavenumber k is set by the energy of the incoming effective particle E, and the scattered spherical outgoing wave as

$$\Psi_{sc} = f(\theta)b\frac{e^{i(kr-\omega t)}}{r} \tag{7.2}$$

where $f(\theta)$ is the scattering amplitude. The angular differential cross section for scattering through $d\Omega$ about $\underline{\Omega}$ is

$$\sigma(\theta) = \frac{\underline{J}_{sc} \cdot \underline{\Omega}}{J_{in}} = \left| f(\theta) \right|^2 \tag{7.3}$$

where we have used the expression (see (2.24)),

$$\underline{J} = \frac{\hbar}{2\mu i}\left[\Psi^*(\underline{\nabla}\Psi) - \Psi(\underline{\nabla}\Psi^*) \right] \tag{7.4}$$

Calculating $f(\theta)$ from the *Schrödinger* wave equation

The *Schrödinger* equation to be solved is of the form

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(r) \right)\psi(\underline{r}) = E\psi(\underline{r}) \tag{7.5}$$

where $\mu = m_1 m_2/(m_1 + m_2)$ is the reduced mass, and $E = \mu v^2/2$, with v being the relative speed, is positive. To obtain a solution to our particular scattering set-up, we impose the boundary condition

$$\psi_k(\underline{r}) \to_{r >> r_o} e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \tag{7.6}$$

where r_o is the range of force, V(r) = 0 for r > r_o. In the region beyond the force range the wave equation describes a free particle. This free-particle solution to is what we want to match up with the RHS of (7.6). The most convenient form of the free-particle wave function is an expansion in terms of partial waves,

$$\psi(r,\theta) = \sum_{\ell=0}^{\infty} R_\ell(r) P_\ell(\cos\theta) \tag{7.7}$$

where $P_\ell(\cos\theta)$ is the Legendre polynomial of order ℓ. Inserting (7.7) into (7.5), and setting $u_\ell(r) = rR_\ell(r)$, we obtain

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{2\mu}{\hbar^2}V(r) - \frac{\ell(\ell+1)}{r^2}\right)u_\ell(r) = 0\,, \tag{7.8}$$

Eq.(7.8) describes the wave function everywhere. Its solution clearly depends on the form of V(r). Outside of the interaction region, $r > r_o$, Eq.(7.8) reduces to the radial wave equation for a free particle,

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right)u_\ell(r) = 0 \tag{7.9}$$

with general solution

$$u_\ell(r) = B_\ell r j_\ell(kr) + C_\ell r n_\ell(kr) \tag{7.10}$$

where B_ℓ and C_ℓ are integration constants, and j_ℓ and n_ℓ are spherical Bessel and Neumann functions respectively (see Appendix B for their properties).

Introduction of the Phase Shift δ_ℓ

We rewrite the general solution (7.10) as

$$u_\ell(r) \rightarrow_{kr>>1} (B_\ell / k)\sin(kr - \ell\pi/2) - (C_\ell / k)\cos(kr - \ell\pi/2)$$

$$= (a_\ell / k)\sin[kr - (\ell\pi/2) + \delta_\ell] \tag{7.11}$$

where we have replaced B and C by two other constants, a and δ, the latter is seen to be a *phase shift*. Combining (7.11) with (7.7) the partial-wave expansion of the free-particle wave function in the asymptotic region becomes

$$\psi(r,\theta) \to_{kr>>1} \sum_{\ell} a_{\ell} \frac{\sin[kr-(\ell\pi/2)+\delta_{\ell}]}{kr} P_{\ell}(\cos\theta) \qquad (7.12)$$

This is the LHS of (7.6). Now we prepare the RHS of (7.6) to have the same form of partial wave expansion by writing

$$f(\theta) = \sum_{\ell} f_{\ell} P_{\ell}(\cos\theta) \qquad (7.13)$$

and

$$e^{ikr\cos\theta} = \sum_{\ell} i^{\ell}(2\ell+1) j_{\ell}(kr) P_{\ell}(\cos\theta)$$

$$\to_{kr>>1} \sum_{\ell} i^{\ell}(2\ell+1) \frac{\sin(kr-\ell\pi/2)}{kr} P_{\ell}(\cos\theta) \qquad (7.14)$$

Inserting both (7.13) and (7.14) into the RHS of (7.6), we match the coefficients of exp(ikr) and exp(-ikr) to obtain

$$f_{\ell} = \frac{1}{2ik}(-i)^{\ell}[a_{\ell}e^{i\delta_{\ell}} - i^{\ell}(2\ell+1)] \qquad (7.15)$$

$$a_{\ell} = i^{\ell}(2\ell+1)e^{i\delta_{\ell}} \qquad (7.16)$$

Combing (7.15) and (B.13) we obtain

$$f(\theta) = (1/k)\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_{\ell}} \sin\delta_{\ell} P_{\ell}(\cos\theta) \qquad (7.17)$$

Final Expressions for $\sigma(\theta)$ and σ

In view of (7.17), the angular differential cross section (7.3) becomes

$$\sigma(\theta) = \lambda\!\!\!^{-2} \left| \sum_{\ell=0}^{\infty} (2\ell+1) e^{i\delta_\ell} \sin\delta_\ell P_\ell(\cos\theta) \right|^2 \tag{7.18}$$

where $\lambda\!\!\!^{-} = 1/k$ is the reduced wavelength. Correspondingly, the total cross section is

$$\sigma = \int d\Omega \sigma(\theta) = 4\pi \lambda\!\!\!^{-2} \sum_{\ell=0}^{\infty} (2\ell+1) \sin^2 \delta_\ell \tag{7.19}$$

S-wave scattering

We have seen that if kr_o is appreciably less than unity, then only the ℓ = 0 term contributes in (7.18) and (7.19). The differential and total cross sections for s-wave scattering are therefore

$$\sigma(\theta) = \lambda\!\!\!^{-2} \sin^2 \delta_o(k) \tag{7.20}$$

$$\sigma = 4\pi \lambda\!\!\!^{-2} \sin^2 \delta_o(k) \tag{7.21}$$

Notice that s-wave scattering is spherically symmetric, or $\sigma(\theta)$ is independent of the scattering angle. This is true in CMCS, but not in LCS. From (7.15) we see $f_o = (e^{i\delta_o} \sin\delta_o)/k$. Since the cross section must be finite at low energies, as k $\rightarrow 0$ f_o has to remain finite, or $\delta_o(k) \rightarrow 0$. We can set

$$\lim_{k\rightarrow 0} [e^{i\delta_o(k)} \sin\delta_o(k)] = \delta_o(k) = -ak \tag{7.22}$$

where the constant *a* is called the *scattering length*. Thus for low-energy scattering, the differential and total cross sections depend only on knowing the scattering length of the target nucleus,

$$\sigma(\theta) = a^2 \tag{7.23}$$

$$\sigma = 4\pi a^2 \tag{7.24}$$

Physical significance of the sign of the scattering length

Fig. 7.2 shows two sine waves, one is the reference wave $\sin kr$ which has not had

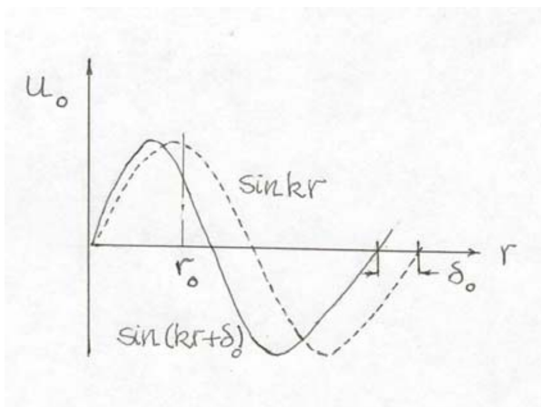

Fig. 7.2. Comparison of unscattered and scattered waves showing a phase shift δ_o in the asymptotic region as a result of the scattering.

any interaction (unscattered) and the other one is the wave $\sin(kr + \delta_o)$ which has suffered a phase shift by virtue of the scattering. The entire effect of the scattering is seen to be represented by the phase shift δ_o, or equivalently the scattering length through (7.22).

In the vicinity of the potential, we take kr_o to be small (this is again the condition of low-energy scattering), so that $u_o \sim k(r-a)$, in which case *a becomes the distance at which the wave function extrapolates to zero* from its value and slope at $r = r_o$. There are two ways in which this extrapolation can take place, depending on the value of kr_o. As shown in Fig. 7.3, when $kr_o > \pi/2$, the wave function has reached more than a quarter of its wavelength at $r = r_o$. So its slope is downward and the extrapolation gives a distance a which is positive. If on the other hand, $kr_o < \pi/2$, then the extrapolation gives a distance a which is negative. The significance is that a > 0 means the potential is such that it can have a bound state, whereas a < 0 means that the potential can only give rise to a virtual state.

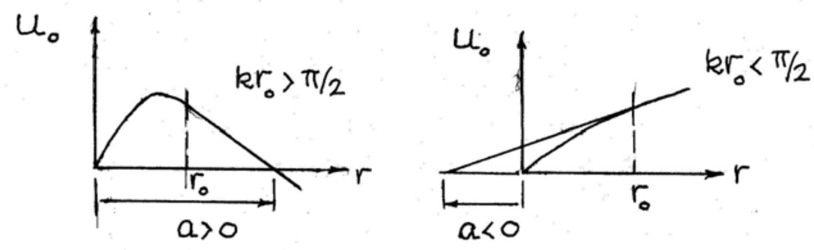

Fig. 7.3. Geometric interpretation of positive and negative scattering lengths as the distance of extrapolation of the wave function at the interface between interior and exterior solutions, for potentials which can have a bound state and which can only virtual state respectively.

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Appendix A: Concepts of Cross Sections

It is instructive to review the physical meaning of a cross section σ, which is a measure of the probability of a reaction. Imagine a beam of neutrons incident on a thin sample of thickness Δx covering an area A on the sample. See Fig. A.1. The intensity of the beam hitting the area A is I neutrons per second. The incident flux is therefore I/A.

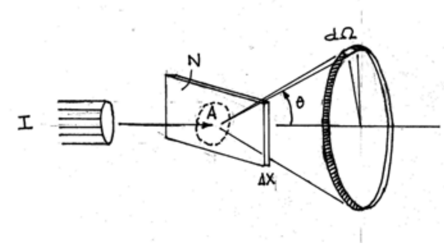

Fig. A.1. Schematic of an incident beam striking a thin target with a particle emitted into a cone subtending an angle θ relative to the direction of incidence, the 'scattering' angle. The element of solid angle $d\Omega$ is a small piece of the cone (see also Fig. A.2).

If the nuclear density of the sample is N nuclei/cm^3, then the no. nuclei exposed is NA Δx (assuming no effects of shadowing, i.e., the nuclei do not cover each other with respect to the incoming neutrons). We now write down the probability for a collision-induced reaction as

$$\{\text{reaction probability}\} = \Theta / I = \left(\frac{NA\Delta x}{A}\right) \bullet \sigma \qquad \text{(A.1)}$$

where Θ is the no. reactions occurring per sec. Notice that σ simply appears in the definition of reaction probability as *a proportionality constant*, with no further justification. Sometimes this simple fact is overlooked by the students. There are other ways to introduce or motivate the meaning of the cross section; they are essentially all equivalent when you think about the physical situation of a beam of particles colliding with a target of atoms. Rewriting (A.1) we get

$$\sigma = \{\text{reaction probability}\} / \{\text{no. exposed per unit area}\}$$

$$= \frac{\Theta}{IN\Delta x} = \frac{1}{I}\left[\frac{\Theta}{N\Delta x}\right]_{\Delta x \to 0} \qquad \text{(A.2)}$$

Moreover, we define $\Sigma = N\sigma$, which is called the *macroscopic cross section*. Then (A.2) becomes

$$\Sigma \Delta x = \frac{\Theta}{I}, \qquad \text{(A.3)}$$

or $\quad \Sigma \equiv \{\text{probability per unit path for small path that a reaction will occur}\} \qquad \text{(A.4)}$

Both the *microscopic cross section* σ , which has the dimension of an area (unit of σ is the **barn** which is 10^{-24} cm^2 as already noted above) , and its counterpart, the macroscopic cross section Σ , which has the dimension of reciprocal length, are fundamental to our study of radiation interactions. Notice that this discussion can be applied to any radiation or particle, there is nothing that is specific to neutrons.

We can readily extend the present discussion to an **angular differential** cross section $d\sigma / d\Omega$. Now we imagine counting the reactions per second in an angular cone subtended at angle θ with respect to the direction of incidence (incoming particles), as shown in Fig. A.1. Let $d\Omega$ be the element of solid angle, which is the small area through which the unit vector $\underline{\Omega}$ passes through (see Fig. A.2). Thus, $d\Omega = \sin\theta d\theta d\varphi$.

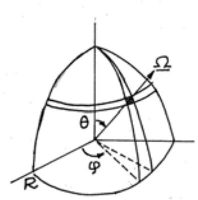

Fig. A.2. The unit vector $\underline{\Omega}$ in spherical coordinates, with θ and φ being the polar and azimuthal angles respectively (R would be unity if the vector ends on the sphere).

We can write

$$\frac{1}{I}\left(\frac{d\Theta}{d\Omega}\right) = N\Delta x\left(\frac{d\sigma}{d\Omega}\right) \tag{A.5}$$

Notice that again $d\sigma / d\Omega$ appears as a proportionality constant between the reaction rate per unit solid angle and a product of two simple factors specifying the interacting system - the incient flux and the number of nuclei exposed (or the number of nuclei available for reaction). The normalization condition of the angular differential cross section is $\int d\Omega (d\sigma/d\Omega) = \sigma$, which makes it clear why $d\sigma / d\Omega$ is called the *angular differential cross section*.

There is another differential cross section which we can introduce. Suppose we consider the incoming particles to have energy E and the particles after reaction to have energy in dE' about E'. One can define in a similar way as above an *energy differential cross section*, $d\sigma / dE'$, which is a measure of the probability of an incoming particle with energy E will have as a result of the reaction outgoing energy E'. Both $d\sigma / d\Omega$ and $d\sigma / dE'$ are *distribution functions*, the former is a distribution in the variable $\underline{\Omega}$, the solid angle, whereas the latter is a distribution in E', the energy after scattering. Their dimensions are barns per steradian and barns per unit energy, respectively.

Combining the two extensions above from cross section to differential cross sections, we can further extend to a *double differential cross section* $d^2\sigma / d\Omega dE'$, which is a quantity that has been studied extensively in thermal neutron scattering. This cross section contains the most fundamental information about the structure and dynamics of the scattering sample. While $d^2\sigma / d\Omega dE'$ is a distribution in two variables, the solid angle and the energy after scattering, it is not a distribution in E, the energy before scattering.

In 22.106 we will be concerned with all three types of cross sections, σ , the two differential cross sections., and the double differential cross section for neutrons, whereas the double differential cross section is beyond the scope of 22.101.

There are many important applications which are based on neutron interactions with nuclei in various media. We are interested in both the cross sections and the use of these cross sections in various ways. In diffraction and spectroscopy we use neutrons to probe the structure and dynamics of the samples being measured. In cancer therapy we use neutrons to preferentially kill the cancerous cells. Both involve a *single collision* event between the neutron and a nucleus, for which a knowledge of the cross section is all that required so long as the neutron is concerned. In contrast, for reactor and other nuclear applications one is interested in the effects of *a sequence of collisions or multiple collisions*, in which case knowing only the cross section is not sufficient. One needs to follow the neutrons as they undergo many collisions in the media of interest. This then requires the study of **neutron transport** - *the distribution of neutrons in configuration space, direction of travel, and energy*. In 22.106 we will treat transport in two ways, theoretical discussion and direct simulation using the Monte Carlo method, and the general purpose code MCNP (Monte Carlo Neutron and Photon).

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Appendix B: Cross Section Calculation: Method of Phase Shifts

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References --

P. Roman, *Advanced Quantum Theory* (Addison-Wesley, Reading, 1965), Chap 3.

A. Foderaro, *The Elements of Neutron Interaction Theory* (MIT Press, 1971), Chap 4.

We will study a method of analyzing potential scattering; it is called the method of partial waves or the method of phase shifts. This is the quantum mechanical description of the two-body collision process. In the center-of-mass coordinate system the problem is to describe the motion of an effective particle with mass μ, the reduced mass, moving in a central potential V(r), where r is the separation distance between the two colliding particles. We will solve the *Schrödinger* wave equation for the spatial distribution of this effective particle, and extract from this solution the information needed to determine the angular differential cross section $\sigma(\theta)$. For a discussion of the concepts of cross sections, see Appendix A.

The Scattering Amplitude $f(\theta)$

In treating the potential scattering problem quantum mechanically the standard approach is to do it in two steps, first to define the cross section $\sigma(\theta)$ in terms of the scattering amplitude $f(\theta)$, and then to calculate $f(\theta)$ by solving the *Schrödinger* equation. For the first step we visualize the scattering process as an incoming beam impinging on a potential field V(r) centered at the origin (CMCS), as shown in Fig. B.1. The incident beam is represented by a traveling plane wave,

$$\Psi_{in} = be^{i(\underline{k}\cdot\underline{r}-\omega t)} \tag{B.1}$$

where b is a coefficient determined by the normalization condition, and the wave vector $\underline{k} = k\hat{\underline{z}}$ is directed along the z-axis (direction of incidence). The magnitude of k is set by

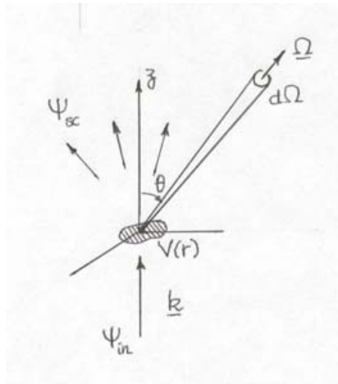

Fig.B.1. Scattering of an incoming plane wave by a potential field V(r), resulting in spherical outgoing wave. The scattered current crossing an element of surface area $d\Omega$ about the direction $\underline{\Omega}$ is used to define the angular differential cross section $d\sigma / d\Omega \equiv \sigma(\theta)$, where the scattering angle θ is the angle between the direction of incidence and direction of scattering.

the energy of the effective particle $E = \hbar^2 k^2 / 2\mu = \hbar\omega$ (the relative energy of the colliding particles). For the scattered wave which results from the interaction in the region of the potential V(r), we will write it in the form of an outgoing spherical wave,

$$\Psi_{sc} = f(\theta) b \frac{e^{i(kr - \omega t)}}{r} \tag{B.2}$$

where $f(\theta)$, which has the dimension of length, denotes the amplitude of scattering in a direction indicated by the polar angle θ relative to the direction of incidence (see Fig. B.1). It is clear that by representing the scattered wave in the form of (B.2) our intention is to work in spherical coordinates.

Once we have expressions for the incident and scattered waves, the corresponding current (or flux) can be obtained from the relation (see (2.24))

$$\underline{J} = \frac{\hbar}{2\mu i}\left[\Psi^* (\underline{\nabla}\Psi) - \Psi(\underline{\nabla}\Psi^*) \right] \tag{B.3}$$

The incident current is $J_{in} = v|b|^2$, where $v = \hbar k / \mu$ is the speed of the effective particle.

For the number of particles per sec scattered through an element of surface area $d\Omega$ about the direction $\underline{\Omega}$ on a unit sphere, we have

$$\underline{J} \cdot \underline{\Omega} d\Omega = v \left| f(\theta) \right|^2 d\Omega \qquad \text{(B.4)}$$

The angular differential cross section for scattering through $d\Omega$ about $\underline{\Omega}$ is therefore (see Appendix A),

$$\sigma(\theta) = \frac{\underline{J} \cdot \underline{\Omega}}{J_{in}} = \left| f(\theta) \right|^2 \qquad \text{(B.5)}$$

This is the fundamental expression relating the scattering amplitude to the cross section; it has an analogue in the analysis of potential scattering in classical mechanics.

Method of Partial Waves

To calculate $f(\theta)$ from the *Schrödinger* wave equation we note that since this is not a time-dependent problem, we can look for a separable solution in space and time, $\Psi(\underline{r},t) = \psi(\underline{r})\tau(t)$, with $\tau(t) = \exp(-itE/\hbar)$. The *Schrödinger* equation to be solved then is of the form

$$\left(-\frac{\hbar^2}{2\mu} \nabla^2 + V(r) \right) \psi(\underline{r}) = E \psi(\underline{r}) \qquad \text{(B.6)}$$

For two-body scattering through a central potential, this is the wave equation for an effective particle with mass equal to the reduced mass, $\mu = m_1 m_2 / (m_1 + m_2)$, and energy E equal to the sum of the kinetic energies of the two particles in CMCS, or equivalently

$E = \mu v^2/2$, with v being the relative speed. The reduction of the two-body problem to the effective one-body problem (B.6) is a useful exercise, which is quite standard. For those in need of a review, a discussion of the reduction in classical as well as quantum mechanics is given at the end of this Appendix.

As is well known, there are two kinds of solutions to (B.6), bound-state solutions for E < 0 and scattering solutions for E > 0. We are concerned with the latter situation. In view of (B.2) and Fig. B.1, it is conventional to look for a particular solution to (B.6), subject to the boundary condition

$$\psi_k(\underline{r}) \to_{r>>r_o} e^{ikz} + f(\theta)\frac{e^{ikr}}{r} \tag{B.7}$$

where r_o is the range of force, V(r) = 0 for r > r_o. The subscript k is a reminder that the entire analysis is carried out at constant k, or at fixed incoming energy $E = \hbar^2 k^2/2\mu$. It also means that $f(\theta)$ depends on E, although this is commonly not indicated explicitly. For simplicity of notation, we will suppress this subscript henceforth.

According to (B.7) at distances far away from the region of the scattering potential, the wave function is a superposition of an incident plane wave and a *spherical outgoing* scattered wave. In the far-away region, the wave equation is therefore that of a free particle since V(r) = 0. This free-particle solution is what we want to match up with (B.7). The form of the solution that is most convenient for this purpose is the expansion of $\psi(\underline{r})$ into a set of partial waves. Since we are considering central potentials, interactions which are spherically symmetric, or V depends only on the separation distance (magnitude of $\underline{r}$) of the two colliding particles, the natural coordinate system in which to find the solution is spherical coordinates, $\underline{r} \to (r,\theta,\varphi)$. The azimuthal angle φ is an ignorable coordinate in this case, as the wave function depends only on r and θ. The partial wave expansion is

$$\psi(r,\theta) = \sum_{\ell=0}^{\infty} R_\ell(r) P_\ell(\cos\theta) \tag{B.8}$$

where $P_\ell(\cos\theta)$ is the Legendre polynomial of order ℓ. Each term in the sum is a partial wave of a definite orbital angular momentum, with ℓ being the quantum number. The set of functions $\{P_\ell(x)\}$ is known to be orthogonal and complete on the interval (-1, 1). Some of the properties of $P_\ell(x)$ are:

$$\int_{-1}^{1} dx P_\ell(x) P_{\ell'}(x) = \frac{2}{2\ell+1}\delta_{\ell\ell'}$$

$$P_\ell(1) = 1,\ P_\ell(-1) = (-1)^\ell \tag{B.9}$$

$$P_0(x) = 1\,,\ P_1(x) = x\ \ P_2(x) = (3x^2 - 1)/2\ \ P_3(x) = (5x^3 - 3x)/2$$

Inserting (B.8) into (B.6), and making a change of the dependent variable (to put the 3D problem into 1D form), $u_\ell(r) = rR_\ell(r)$, we obtain

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{2\mu}{\hbar^2}V(r) - \frac{\ell(\ell+1)}{r^2}\right)u_\ell(r) = 0\,, \quad r < r_o \tag{B.10}$$

This result is called the radial wave equation for rather obvious reasons; it is a one-dimensional equation whose solution determines the scattering process in three dimensions, made possible by the properties of the central potential V(r). Unless V(r) has a special form that admits analytic solutions, it is often more effective to integrate (B.10) numerically. However, we will not be concerned with such calculations since our interest is not to solve the most general scattering problem.

Eq.(B.10) describes the wave function in the interaction region, $r < r_o$, where V(r) = 0, $r > r_o$. The solution to this equation clearly depends on the form of V(r). On the other hand, outside of the interaction region, $r > r_o$, Eq.(B.10) reduces to the radial wave equation for a free particle. Since this equation is universal in that it applies to all scattering problems where the interaction potential has a finite range r_o, it is worthwhile to discuss a particular form of its solution. Writing Eq.(B.10) for the exterior region this time, we have

$$\left(\frac{d^2}{dr^2} + k^2 - \frac{\ell(\ell+1)}{r^2}\right)u_\ell(r) = 0 \tag{B.11}$$

which is in the standard form of a second-order differential equation whose general solutions are spherical Bessel functions. Thus,

$$u_\ell(r) = B_\ell r j_\ell(kr) + C_\ell r n_\ell(kr) \tag{B.12}$$

where B_ℓ and C_ℓ are integration constants, to be determined by boundary conditions, and j_ℓ and n_ℓ are spherical Bessel and Neumann functions respectively. The latter are tabulated functions; for our purposes it is sufficient to note the following properties.

$$j_o(x) = \sin x / x\,, \qquad n_o(x) = -\cos x / x$$

$$j_1(x) = \frac{\sin x}{x} - \frac{\cos x}{x}\,, \qquad n_1(x) = -\frac{\cos x}{x^2} - \frac{\sin x}{x}$$

$$j_\ell(x) \to_{x\to 0} \frac{x^\ell}{1\cdot 3\cdot 5 ... (2\ell+1)} \qquad n_\ell(x) \to_{x\to 0} \frac{1\cdot 3\cdot 5 ... (2\ell-1)}{x^{\ell+1}} \tag{B.13}$$

$$j_\ell(x) \to_{x>>1} \frac{1}{x}\sin(x - \ell\pi/2) \qquad n_\ell(x) \to_{x>>1} -\frac{1}{x}\cos(x - \ell\pi/2)$$

The Phase Shift δ

Using the asymptotic expressions for j_ℓ and n_ℓ we rewrite the general solution (B.12) as

$$u_\ell(r) \rightarrow_{kr>>1} (B_\ell / k)\sin(kr - \ell\pi/2) - (C_\ell / k)\cos(kr - \ell\pi/2)$$

$$= (a_\ell / k)\sin[kr - (\ell\pi/2) + \delta_\ell] \qquad \text{(B.14)}$$

The second step in (B.14) deserves special attention. Notice that we have replaced the two integration constant B and C by two other constants, a and δ, the latter being introduced as a *phase shift*. The significance of the phase shift will be apparent as we proceed further in discussing how one can calculate the angular differential cross section through (B.5). In Fig. B.2 below we give a simple physical explanation of how the sign of the phase shift depends on whether the interaction is attractive (positive phase shift) or repulsive (negative phase shift).

Combining (B.14) with (B.8) we have the partial-wave expansion of the wave function in the asymptotic region,

$$\psi(r,\theta) \rightarrow_{kr>>1} \sum_\ell a_\ell \frac{\sin[kr - (\ell\pi/2) + \delta_\ell]}{kr} P_\ell(\cos\theta) \qquad \text{(B.15)}$$

This is the left-hand side of (B.7). Our intent is to match this description of the wave function with the right-hand side of (B.7), also expanded in partial waves, thus relating the scattering amplitude to the phase shift. Both terms on the right-hand side of (B.7) are seen to depend on the scattering angle θ. Even though the scattering amplitude is still unknown, we nevertheless can go ahead and expand it in terms of partial waves,

$$f(\theta) = \sum_\ell f_\ell P_\ell(\cos\theta) \qquad \text{(B.16)}$$

where the coefficients f_ℓ are the quantities to be determined in the present calculation. The other term in (B.7) is the incident plane wave. It can be written as

$$e^{ikr\cos\theta} = \sum_{\ell} i^{\ell}(2\ell+1)\, j_{\ell}(kr) P_{\ell}(\cos\theta)$$

$$\to_{kr>>1} \sum_{\ell} i^{\ell}(2\ell+1)\frac{\sin(kr-\ell\pi/2)}{kr} P_{\ell}(\cos\theta) \qquad \text{(B.17)}$$

Inserting both (B.16) and (B.17) into the right-hand side of (B.7), we see that terms on both sides are proportional to either exp(ikr) or exp(-ikr). If (B.7) is to hold in general, the coefficients of each exponential have to be equal. This gives

$$f_{\ell} = \frac{1}{2ik}(-i)^{\ell}[a_{\ell}e^{i\delta_{\ell}} - i^{\ell}(2\ell+1)] \qquad \text{(B.18)}$$

$$a_{\ell} = i^{\ell}(2\ell+1)e^{i\delta_{\ell}} \qquad \text{(B.19)}$$

Eq.(B.18) is the desired relation between the ℓ-th component of the scattering amplitude and the ℓ-th order phase shift. Combining it with (B.16), we have the scattering amplitude expressed as a sum of partial-wave components

$$f(\theta) = (1/k)\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_{\ell}}\sin\delta_{\ell} P_{\ell}(\cos\theta) \qquad \text{(B.20)}$$

This expression, more than any other, shows why the present method of calculating the cross section is called the method of partial waves. Now the angular differential cross section, (B.5), becomes

$$\sigma(\theta) = \lambda\!\!\!^{-2}\left|\sum_{\ell=0}^{\infty}(2\ell+1)e^{i\delta_{\ell}}\sin\delta_{\ell} P_{\ell}(\cos\theta)\right|^2 \qquad \text{(B.21)}$$

where $\lambda\!\!\!^{-} = 1/k$ is the reduced wavelength. Correspondingly, the total cross section is

$$\sigma = \int d\Omega \sigma(\theta) = 4\pi ƛ^2 \sum_{\ell=0}^{\infty} (2\ell + 1)\sin^2 \delta_\ell \qquad \text{(B.22)}$$

Eqs.(B.21) and (B.22) are very well known results in the quantum theory of potential scattering. They are quite general in that there are no restrictions on the incident energy. Since we are mostly interested in calculating neutron cross sections in the low-energy regime ($kr_o << 1$), it is only necessary to take the leading term in the partial-wave sum.

The $\ell = 0$ term in the partial-wave expansion is called the s-wave. One can make a simple semiclassical argument to show that at a given incident energy $E = \hbar^2 k^2 / 2\mu$, only those partial waves with $\ell < kr_o$ make significant contributions to the scattering. If it happens that furthermore $kr_o << 1$, then only the $\ell = 0$ term matters. In this argument one considers an incoming particle incident on a potential at an impact parameter b. The angular momentum in this interaction is $\hbar\ell$ = pb, where $p = \hbar k$ is the linear momentum of the particle. Now one argues that there is appreciable interaction only when b < r_o, the range of interaction; in other words, only the ℓ values satisfying b = ℓ/k < r_o will have significant contriubution to the scattering. The condition for a partial wave to contribute is therefore $\ell < kr_o$

S-wave scattering

We have seen that if kr_o is appreciably less than unity, then only the $\ell = 0$ term contributes in (B.21) and (B.22). What does this mean for neutron scattering at energies around $k_BT \sim 0.025$ eV? Suppose we take a typical value for r_o at ~ 2 x 10 $^{-12}$ cm, then we find that for thermal neutrons $kr_o \sim 10^{-5}$. So one is safely under the condition of low-energy scattering, $kr_o << 1$, in which case only the s-wave contribution to the cross section needs to be considered. The differential and total scattering cross sections become

$$\sigma(\theta) = ƛ^2 \sin^2 \delta_o(k) \qquad \text{(B.23)}$$

$$\sigma = 4\pi \lambda\!\!\!^{-2} \sin^2 \delta_o(k) \tag{B.24}$$

It is important to notice that s-wave scattering is spherically symmetric in that $\sigma(\theta)$ is manifestly independent of the scattering angle (this comes from the property $P_o(x) = 1$). One should also keep in mind that while this is so in CMCS, it is not true in LCS. In both (B.23) and (B.24) we have indicated that s-wave phase shift δ_o depends on the incoming energy E. From (B.18) we see that $f_o = (e^{i\delta_o} \sin \delta_o)/k$. Since the cross section must be finite at low energies, as k $\rightarrow 0$ f_o has to remain finite, or $\delta_o(k) \rightarrow 0$. Thus we can set

$$\lim_{k\rightarrow 0}[e^{i\delta_o(k)} \sin \delta_o(k)] = \delta_o(k) = -ak \tag{B.25}$$

where the constant a is called the *scattering length*. Thus for low-energy scattering, the differential and total cross sections depend only on knowing the scattering length of the target nucleus,

$$\sigma(\theta) = a^2 \tag{B.26}$$

$$\sigma = 4\pi a^2 \tag{B.27}$$

We will see in the next lecture on neutron-proton scattering that the large scattering cross section of hydrogen arises because the scattering length depends on the relative orientation of the neturon and proton spins.

Reduction of two-body collision to an effective one-body problem

We conclude this Appendix with a supplemental discussion on how the problem of two-body collision through a central force is reduced, in both classical and quantum mechanics, to the problem of scattering of an effective one particle by a potential field V(r) [Meyerhof, pp. 21]. By central force we mean the interaction potential is only a function of the separation distance between the colliding particles. We will first go through the argument in classical mechanics. The equation describing the motion of particle 1 moving under the influence of particle 2 is the Newton's equation of motion,

$$m_1 \ddot{\underline{r}}_1 = \underline{F}_{12} \tag{B.28}$$

where $\underline{r}_1$ is the position of particle 1 and $\underline{F}_{12}$ is the force on particle 1 exerted by particle 2. Similarly, the motion of motion for particle 2 is

$$m_2 \ddot{\underline{r}}_2 = \underline{F}_{21} = -\underline{F}_{12} \tag{B.29}$$

where we have noted that the force exerted on particle 2 by particle 1 is exactly the opposite of $\underline{F}_{12}$. Now we transform from laboratory coordinate system to the center-of-mass coordinate system by defining the center-of-mass and relative positions,

$$\underline{r}_c = \frac{m_1 \underline{r}_1 + m_2 \underline{r}_2}{m_1 + m_2}, \qquad \underline{r} = \underline{r}_1 - \underline{r}_2 \tag{B.30}$$

Solving for $\underline{r}_1$ and $\underline{r}_2$ we have

$$\underline{r}_1 = \underline{r}_c + \frac{m_2}{m_1 + m_2} \underline{r}, \qquad \underline{r}_2 = \underline{r}_c - \frac{m_1}{m_1 + m_2} \underline{r} \tag{B.31}$$

We can add and subtract (B.28) and (B.29) to obtain equations of motion for $\underline{r}_c$ and $\underline{r}$. One finds

$$(m_1 + m_2) \ddot{\underline{r}}_c = 0 \tag{B.32}$$

$$\mu \ddot{\underline{r}} = \underline{F}_{12} = -dV(r) / d\underline{r} \tag{B.33}$$

with $\mu = m_1 m_2 / (m_1 + m_2)$ being the reduced mass. Thus the center-of-mass moves in a straight-line trajectory like a free particle, while the relative position satisfies the equation of an effective particle with mass μ moving under the force generated by the potential V(r). Eq.(B.33) is the desired result of our reduction. It is manifestly the one-body problem of an effective particle scattered by a potential field. Far from the interaction field the particle has the kinetic energy $E = \mu(\dot{\underline{r}})^2 / 2$

The quantum mechanical analogue of this reduction proceeds from the *Schrödinger* equation for the system of two particles,

$$\left(-\frac{\hbar^2}{2m_1}\nabla_1^2 - \frac{\hbar^2}{2m_2}\nabla_2^2 + V(|\underline{r}_1 - \underline{r}_2|)\right)\Psi(\underline{r}_1, \underline{r}_2) = (E_1 + E_2)\Psi(\underline{r}_1, \underline{r}_2) \qquad \text{(B.34)}$$

Transforming the Laplacian operator ∇^2 from operating on ($\underline{r}_1$, $\underline{r}_2$) to operating on $(\underline{r}_c, \underline{r})$, we find

$$\left(-\frac{\hbar^2}{2(m_1 + m_2}\nabla_c^2 - \frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right)\Psi(\underline{r}_c, \underline{r}) = (E_c + E)\Psi(\underline{r}_c, \underline{r}) \qquad \text{(B.35)}$$

Since the Hamiltonian is now a sum of two parts, each involving either the center-of-mass position or the relative position, the problem is separable. Anticipating this, we have also divided the total energy, previously the sum of the kinetic energies of the two particles, into a sum of center-of-mass and relative energies. Therefore we can write the wave function as a product, $\Psi(\underline{r}_c, \underline{r}) = \psi_c(\underline{r}_c)\psi(\underline{r})$ so that (B.35) reduces to two separate problems,

$$-\frac{\hbar^2}{2(m_1 + m_2)}\nabla_c^2\psi_c(\underline{r}_c) = E_c\psi_c(\underline{r}_c) \qquad \text{(B.36)}$$

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2 + V(r)\right)\psi(\underline{r}) = E\psi(\underline{r}) \qquad \text{(B.37)}$$

It is clear that (B.36) and (B.37) are the quantum mechanical analogues of (B.32) and (B.33). The problem of interest is to solve either (B.33) or (B.37). As we have been discussing in this Appendix we are concerned with the solution of (B.37).