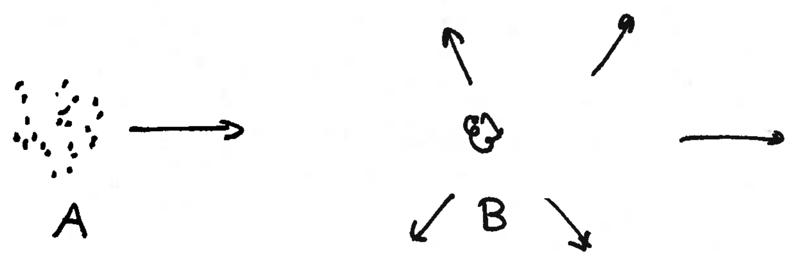
April 2

Basic Notions of Scattering Theory

To begin our discussion of scattering theory, we must first ask, what is it that we measure in a scattering experiment. Roughly, we set up a scattering experiment by considering a collection of some particles B as target, taking a handful of particles A, and throwing them at the target. We then measure the energies and momenta of any particles that result from the interaction.



It would be good to make this description more systematic, so that we can quote properties of the interaction between A and B that are independent of the details of how we set up the experiment.

First, I will almost always assume in this course that the target particles B can be treated independently of one another. If B is an atom in a block of solid, we typically have to correct the results of the scattering experiment for the energy lost by particles as they move through to solid block toward and then away from B. In some circumstances, waves or quantum mechanical particles scatter from many atoms in the solid coherently. The canonical example of this is X-ray diffraction. In this course, I will typically ignore these effects and treat the scattering target as an isolated atom or other particle.

Second, instead of thinking of the projectiles A as a cloud of particles, I will think of them as a uniform beam of particles moving in the $\hat{z}$ direction. Remember that our target atoms are very small. Then, whatever the shape of the cloud of A particles, it is well approximated by a uniform density of particles raining on the target.

With these idealizations, we can define an observable of AB scattering that do not depend on the details of the experiment. This quantity is called the *cross section.* We measure the rate for some outcome, in events/sec. The outcome in question might be that anything happens, or that an A particle scatters elastically, or that A scatters elastically in a given direction. In any case, the rate of the outcome is proportional to the number of A particles that hit the target. This in turn is proportional to the *flux* of A particles

$$\Phi = \#\text{ of particle}/\text{cm}^2\text{sec} = \underset{\text{density}\cdot}{\rho}\ \underset{\text{velocity}}{v}$$

Then we can define the cross section σ by

$$\sigma = \frac{\#\text{ of scattering events/sec}}{\Phi}$$

The cross section has units of area, cm^2. It is the effective area that the target presents to the incoming flux of A particles to produce the given outcome.

If what we measure is the total rate for any scattering event, the result is the *total cross section*, σ_{tot}. Alternatively, we might measure the counting rate for an A atom to scatter into a given instrumented area of solid angle $\Delta\Omega$.

The can express this counting rate as an integral over the solid angle

$$\frac{\text{events/sec into }\Delta\Omega}{\text{flux}} = \int_{\Delta\Omega} d^2\Omega \ \frac{d\sigma}{d^2\Omega}$$

The *integrand* of this expression is called the *differential cross section.* If the scattering can be inelastic, we might want to measure both the angle and the energy of the final-state A particle. Then we can measure a triply-differential quantity

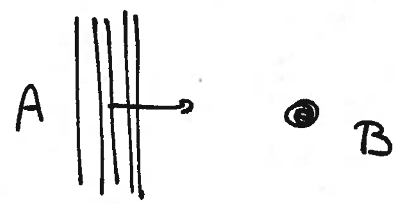
$$\frac{\text{events/sec into }\Delta\Omega,\ \Delta E'}{\text{flux}} = \int d^2\Omega \int dE' \ \frac{d\sigma}{d^2\Omega\, dE'}$$

The integration over all variables should give back the total cross section σ_{tot}.

Note that the total cross section includes only events in which something actually happens. Since the target B is very small, most particles A in the beam miss the target. These should not be counted in the cross section.

In classical mechanics, we are used to analyzing dynamics by following the individual trajectories of particles. However, we can discuss the cross section for scattering of classical particles. We compute the scattering angle or final state for each particular incoming trajectory and then *average* over a class of trajectories that characterize, statistically, the incoming beam. The description in terms of the cross section is not necessary, but it is convenient in many circumstances.

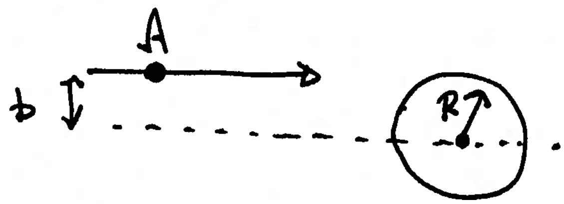
In quantum mechanics, the setup of a scattering experiment and the measurement of a cross section must be considered more carefully. To get the most information from a scattering experiment, we want to define the beam in momentum and measure the momenta and energies of scattered particles as precisely as possible. That means that the initial wavefunctions of the beam particles should be highly localized in momentum. But then, by the Heisenberg uncertainty principle, the initial particles should occupy wavefunctions that are extremely extended in space. In particular, the initial wavefunctions will extend transversely over distances much larger than the size of the target atom B.



The question of whether any given A particle will interact with B is then a matter of probability. We are thus forced to use an observable that averages over many scattering events. The cross section fills this necessary place in the formalism.

To get a feeling for the cross section, I will compute it classically for a simple example. Let B be a hard sphere of radius R, and let A be a very small particle that can scatter elastically from the sphere. I will follow the route appropriate for classical mechanics, first following a given trajectory into and out of the scattering process, and then averaging over the results on different trajectories.

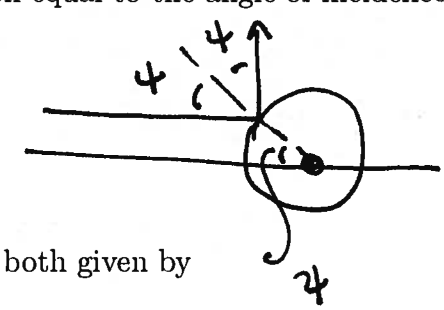
The particles of the initial beam come in along the $\hat{z}$ axis at some displacement from the line through the center of the sphere. The perpendicular distance from the initial trajectory to the center of the sphere is called the *impact parameter*, denoted b.



Particles with $b > R$ miss hitting the sphere and are not counted in the cross section. If $b < R$, the particle is scattered. So the total cross section is

$$\sigma = \int_{b<R} d^2b = \pi R^2$$

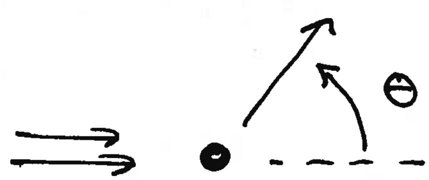
Now we look more differentially. A particle that hits the sphere will rebound with an angle of reflection equal to the angle of incidence.



These angles ψ are both given by

$$\sin\psi = \frac{b}{R}$$

The scattering angle θ is defined as the angle of deflection of a particle from the beam.



Comparing the pictures, we see that θ is related to ψ by

$$\theta = \pi - 2\psi$$

Then

$$b = R \sin \psi = R \sin \left(\frac{\pi}{2} - \frac{\theta}{2} \right)$$

$$b = R \cos \frac{\theta}{2}$$

Assuming a uniform flux $\Phi = \rho v$, the number of particles arriving at the sphere per second is

$$\rho v \int_{b<R} db \, 2\pi b$$

The cross section is given by dividing this by the flux. Thus,

$$\sigma = \int 2\pi \, b(\theta) \, db$$

This can be written

$$\sigma = \int_{b=0}^{b=R} 2\pi \, b(\theta) \, \frac{db}{d\theta} \, d\theta$$

and now the integrand gives the cross section differential in θ. Since

$$\frac{db}{d\theta} = -\frac{R}{2} \sin \frac{\theta}{2}$$

we find

$$\sigma = \int_0^\pi 2\pi \, R\cos\frac{\theta}{2} \; \frac{R}{2}\sin\frac{\theta}{2} \, d\theta = \int_0^\pi \frac{\pi}{2} R^2 \sin\theta \, d\theta$$

$$= \int \frac{\pi}{2} R^2 \, d\cos\theta$$

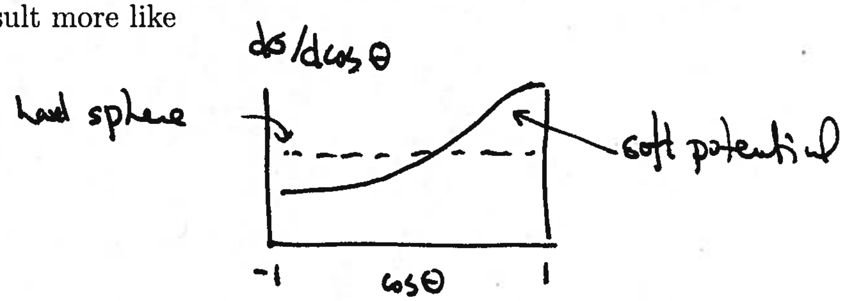
or

$$\frac{d\sigma}{d\cos\theta} = \frac{1}{2}\pi R^2$$

Since $d^2\Omega = d\phi d\cos\theta$, the quantity $d\sigma/d\cos\theta$ is proportional to the scattering rate per unit of solid angle and so provides a very useful way to present the dependence of the cross section on scattering angle. The integral of this quantity over $\cos\theta$ should give the total cross section, and, indeed,

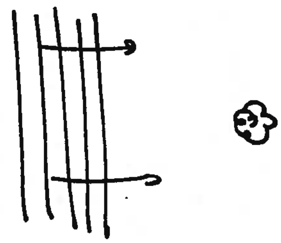
$$\sigma = \int_{-1}^{1} d\cos\theta \; \frac{1}{2}\pi R^2 = \pi R^2$$

In the case of classical scattering from a hard sphere, the differential cross section $d\sigma/d\cos\theta$ is a constant. A potential well that deflects particles less strongly might give a result more like

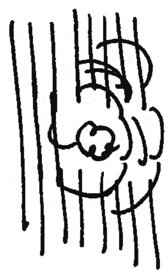


If we could understand precisely how the form of the potential leads to a definite form for the differential cross section, we could work backwards to infer the potential from the scattering data. This is what we will have to do to understand the microscopic forces that act between quantum particles.

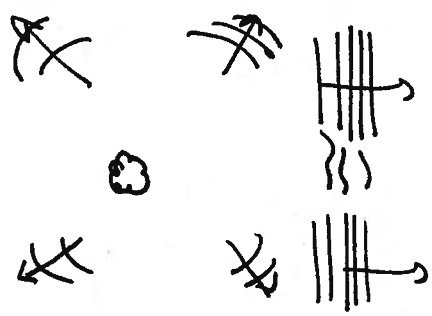
The generalization of this calculation to quantum mechanics is not so simple. In fact, at first sight, it is extremely complex. Even if the target B is described by a static potential, the beam particle A must be described by a Schrödinger wavefunction that is much larger than the scattering center.



The wave will interact with the scattering center



and different pieces of the wave will go in different directions



Most of the wave will go forward and should be ignored. The small pieces that are reflected into new directions, when squared, give the differential scattering cross section. It would seem that, to analyze this process, we need to directly integrate the Schrödinger equation, as a partial differential equation, through this complicated process.

There must be an easier way, and, indeed, there is. In the next few lectures, I will present some more tractable strategies to compute the scattering cross section. What we would like to do is to analyze the scattering process using methods similar to those we used to find bound states, splitting the Schrödinger wavefunction to into states of definite angular momentum, and then solving an ordinary differential equation for each angular momentum state. What is not clear about this is how to join these solutions onto the large initial and final wavefunctions set up at distances very far from the scattering center.

I would now like to address that question. It is simplest to carry out the analysis first for scattering problems in 1 space dimension. For both the 1- and 3-dimensional cases, I will need a basic mathematical tool, the description of a large but ultimately localized wavefunction. We can build such a wavefunction as a superposition of free particle states, called a *wavepacket*. In the remainder of this lecture, I will work out the basic formulae for wavepackets in 1 dimension.

We are dealing with free particles, so the Hamiltonian is

$$\underset{\sim}{H} = \frac{\underset{\sim}{P}^2}{2m}$$

The eigenstates of H are uniform exponentials

$$\psi(x) = e^{ikx}$$

with

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

(This is the last time you will see $\hbar$ in a formula that will not be evaluated numerically.)

To construct a localized state, we superpose states with different values of k. I will try to maintain a small spread in k. Thus, write

$$\psi(x) = \int \frac{dk}{2\pi}\, e^{ikx} \cdot e^{-ikx_0} (4\pi\Delta)^{1/4}\, e^{-\frac{\Delta}{2}(k-k_0)^2}$$

with $\Delta \gg k_0^2$. The integral here is a simple Gaussian, so we can evaluate it explicitly to see what this function looks like in x space. Let

$$\bar{k} = k - k_0$$

Then

$$\psi(x) = \int \frac{d\bar{k}}{2\pi}\, e^{ik_0(x-x_0)} (4\pi\Delta)^{1/4}\, e^{i\bar{k}(x-x_0)}\, e^{-\frac{\Delta}{2}\bar{k}^2}$$

$$= \int \frac{d\bar{k}}{2\pi}\, e^{ik_0(x-x_0)} (4\pi\Delta)^{1/4}\, e^{-\frac{\Delta}{2}\left(\bar{k} - i\frac{x-x_0}{\Delta}\right)^2}\, e^{-\frac{1}{2\Delta}(x-x_0)^2}$$

The final result is

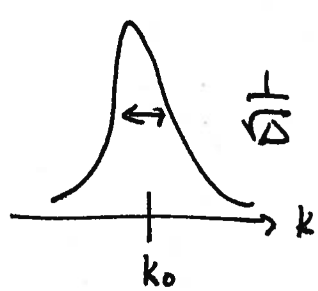
$$= \frac{1}{2\pi} (4\pi\Delta)^{1/4} \left(\frac{2\pi}{\Delta}\right)^{1/2} e^{ik_0(x-x_0)}\, e^{-\frac{1}{2\Delta}(x-x_0)^2}$$

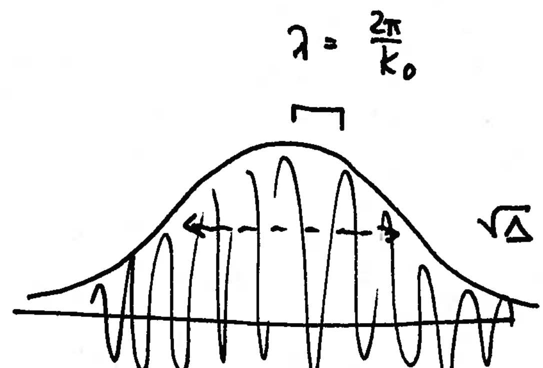
$$\psi(x) = \frac{1}{(\pi\Delta)^{1/4}}\, e^{-\frac{1}{2\Delta}(x-x_0)^2}\, e^{ik_0(x-x_0)}$$

This wavefunction is localized near x_0, but not too near if Δ is large. The wavefunction is properly normalized to

$$\int dx\, |\psi(x)|^2 = 1$$

In k space and in x space, it has the form





The reciprocal relation of the sizes of the wavefunctions reflects the Heisenberg uncertainty principle.

The function $\psi(x)$ is a static wavepacket, but we can easily compute its time dependence. The pure exponentials extend to time-dependent wavefunctions

$$e^{ikx}\, e^{-i\frac{k^2}{2m}t}$$

that are solutions of the time-dependent Schrödinger equation. Any superposition of these will also be a solution of the time-dependent Schrödinger equation. Thus,

$$\begin{aligned}
\psi(x,t) &= \int \frac{dk}{2\pi}\, e^{ik(x-x_0)} (4\pi\Delta)^{1/4}\, e^{-\frac{\Delta}{2}(k-k_0)^2} \cdot e^{-i\frac{k^2}{2m}t} \\
&= \int \frac{d\bar{k}}{2\pi}\, (4\pi\Delta)^{1/4} e^{ik_0(x-x_0)}\, e^{-i\frac{k_0^2}{2m}t}\, e^{-\frac{\Delta}{2}\bar{k}^2}\, e^{-i\frac{t}{2m}(\bar{k}^2+2\bar{k}k_0)}\, e^{i\bar{k}(x-x_0)} \\
&= \int \frac{d\bar{k}}{2\pi}\, (4\pi\Delta)^{1/4} e^{ik_0(x-x_0)}\, e^{-i\frac{k_0^2}{2m}t} \exp\left[-\frac{1}{2}\left(\Delta+i\frac{t}{m}\right)\left(\bar{k}-i\,\frac{x-x_0-\frac{k_0t}{m}}{\Delta+it/m}\right)^2\right] \\
&\qquad \cdot \exp\left[-\frac{1}{2(\Delta+it/m)}\left(x-x_0-\frac{k_0t}{m}\right)^2\right]
\end{aligned}$$

or, finally,

$$\psi(x,t) = \left(\frac{\Delta}{\pi}\right)^{1/4} \frac{1}{\boldsymbol{\Delta}^{1/2}}\, e^{ik_0(x-x_0)}\, e^{-i\frac{k_0^2t}{2m}}\, e^{-\frac{1}{2\boldsymbol{\Delta}}\left(x-x_0-\frac{k_0t}{m}\right)^2}$$

The time evolution of the wavepacket shows two effects. First, the wavepacket spreads with time according to

$$|\boldsymbol{\Delta}| = \left|\Delta + i\frac{t}{m}\right| = \left(\Delta^2 + t^2/m^2\right)^{1/2}$$

If the initial value of Δ is very large, this is not a qualitatively important effect. The spreading is, in any case, only at second order in t. In the use I make of wavepackets, there will be no mistake if we ignore this effect.

The more important effect is that the wavepacket moves with t. The center of the packet evolves according to

$$x = x_0 + \frac{k_0}{m} t$$

This will allow us to set up a wavepacket at a position x_0 very far from the scattering center, with $|x_0| > \Delta^{1/2}$, and let the packet naturally evolve into interaction with the scattering potential. If we then follow the evolution of the wavepacket through a time

$$2 \frac{|x_0|}{(k_0/m)}$$

we can watch the packet come out of the interaction and interpret the result in terms of the scattering cross section. I will set up an analysis of this type in the next lecture.