Lecture 21 Highlights Phys 402

Scattering experiments are one of the most important ways to gain an understanding of the microscopic world that is described by quantum mechanics. The idea is to take a known entity (for example an electron), give it a known energy and initial momentum (magnitude and direction), and send it on a "collision course" with an object whose structure and properties are not fully known. The known entity will interact with the particles making up the unknown substance through a (hopefully simple) interaction force. In the simplest experiments one then measures the energy and momentum of the known entity as it exits from the interaction region. It is assumed that the interactions take place only in a limited region around the target particles. This experiment is repeated many times for a given initial energy and momentum, and statistics of exiting energy and momentum are compiled. This exercise is repeated for other values of initial energy and momentum, resulting in a "big data" set. No wonder that the World Wide Web was invented by physicists trying to share this data with all of their colleagues around the world.

We began by reviewing scattering in <u>one dimension</u>, where the particle has the choice of either being reflected or transmitted. The results can be summarized nicely using the Scattering matrix *S*. In three dimensions, the scattered particles can go off in any direction, so it is useful to put the scattering center at the origin and use spherical coordinates to describe the scattered particle direction. Note that in all cases we are now considering only scattering states (as opposed to bound states), and these have energy E > 0.

Examples of scattering experiments include <u>Rutherford scattering</u> and angleresolved photoemission spectroscopy (ARPES), which is basically the photoelectric effect on steroids. The language of quantum scattering theory is used throughout physics, including high energy physics, nuclear physics, quantum optics, condensed matter physics, etc. Although it is rather technical, it is worth learning this theory...



Classical Scattering Theory

In classical mechanics it is appropriate to consider point particles that follow welldefined trajectories. The starting point for thinking about scattering is having a light particle incident from infinity on a heavy stationary target particle. Classically, the incident particle is travelling in a straight line as it approaches the potential created by the target particle. If it feels no interaction force, then it will travel by in an un-deviated straight line trajectory. The distance between its incident direction and the trajectory that sends it into a "head-on" collision with the target particle is called the "impact parameter" and often denoted with the symbol b. The extension of the "head-on" direction to infinity is defined as the z-axis. As the incident particle approaches the target it experiences a force that causes it to deviate away from its initial trajectory. After this interaction the light particle will be free once again of the target potential and move off in a straight line trajectory. We define this outgoing trajectory direction using spherical angular coordinates (θ, φ) from the above-defined z-axis. To describe the results of many such experiments with different impact parameters and outgoing directions, we establish a differential relationship between a finite-size incident beam area and an outgoing beam of particles into a differential solid angle $d\Omega$.

The only quantity not controlled in a typical scattering experiment is the impact parameter b of the projectile with respect to the target particle. The impact parameter is the distance of closest approach to the target particle, assuming no forces of interaction cause the projectile to change from its initial direction. Because we cannot control the impact parameter, we have to perform many experiments in which all possible values of b are employed for the incident beam of projectiles. We then give a (classical) statistical description of the resulting scattering. With such a description, we can write the number of particles scattered N_{scatt} in terms of the number of particles incident N_{inc} as $N_{scatt} =$ $N_{inc}n_{target}\sigma$, where n_{target} is the density of target particles projected into the twodimensional plane ($n_{target} \sim 1/m^2$) and σ is defined as the scattering cross section of each particle. σ is often measured in units of 'barns', which is $10^{-28}m^2$. We can generalize the concept of cross section to any process, including capture ($\sigma_{capture}$), ionization ($\sigma_{ionization}$), fission ($\sigma_{fission}$), etc. This is done by using the definition $N_{scatt,x} =$ $N_{inc}n_{target}\sigma_x$ for process "x". Here we will consider only *elastic* (energy conserving) scattering.

Experiments start with a beam of projectile particles of identical structure and equal initial momenta and energy. The projectiles enter the target with all possible values of impact parameter. One then measures how many particles come out with angle of exit θ, φ and also the energy and momentum of the exiting particle. Our job is to identify the force of interaction between the projectile and target particles from the number of particles scattered through angle θ, φ , for all possible angles. We write the 'angle-resolved' scattering cross section as $N_{scatt}(into d\Omega \ around \theta, \varphi) = N_{inc}n_{target}\frac{d\sigma}{d\Omega}(\theta,\varphi)d\Omega$, where $\frac{d\sigma}{d\Omega}(\theta,\varphi)$ is called the **differential scattering cross section (DSCS)**. Note that the element of differential solid angle is $d\Omega = \sin \theta \ d\theta d\varphi$. We expect that if this quantity is integrated over all possible exiting angles, we should recover the total scattering cross section for this process: $\sigma = \iint \frac{d\sigma}{d\Omega}(\theta,\varphi) \ d\Omega$. We shall assume that all scattering potentials are spherically symmetric, hence there will be no dependence on the φ coordinate.

To find $\frac{d\sigma}{d\Omega}(\theta, \varphi)$ we compare the area covered by the incident particles at impact parameters between *b* and *b* + *db* in an angle $d\phi$ (i.e. $d\sigma = b \, db \, d\phi$) to the solid angle subtended by the exiting beam of particles (i.e. $d\Omega = \sin \theta \, d\theta \, d\phi$) to arrive at $\frac{d\sigma}{d\Omega} = \frac{b}{\sin \theta} \left| \frac{db}{d\theta} \right|$. To find the DSCS, we need to calculate the trajectory of a projectile particle for every possible impact parameter. We then did the example of a point particle elastically scattering from a fixed hard sphere of radius *R* and found that $b = R \cos\left(\frac{\theta}{2}\right)$, $\frac{d\sigma}{d\Omega} = \frac{R^2}{4}$, which is independent of angle! The total scattering cross section is just $\sigma = \pi R^2$, which is the cross-sectional area presented by the sphere.

Another famous case of classical scattering theory is Rutherford scattering associated with a Coulomb interaction. This type of scattering experiment was used to deduce that most of the mass of the atom was concentrated in a small volume known as the nucleus. The DSCS was deduced to be : $D(\theta) = \frac{d\sigma}{d\Omega} = \left(\frac{qQ/4\pi\varepsilon_0}{4E\sin^2(\theta/2)}\right)^2$, where *E* is the energy of the incident particle of charge *q* approaching a target of charge *Q* and scattering through angle θ . The DSCS has a distinctive $\frac{1}{\sin^4(\theta/2)}$ angular dependence, which was clearly observed by Geiger and Marsden using α -particles scattering from thin Au foils. They also showed that the scattering rate scaled with n_{target} (by varying the thickness of the foil), scaled as $1/E^2$ (by varying the energy of the incident alpha particles), scaled as $\frac{1}{\sin^4(\theta/2)}$ (by measuring the number of particles scattered vs. outgoing angle), and scaled as Z^2 , where Q = +Ze is the nuclear charge.

Note that because $\frac{d\sigma}{d\Omega} \sim q^2 Q^2$, the scattered particle distribution is insensitive to whether the Coulomb interaction is attractive or repulsive. Also, the agreement for the angular dependence of $\frac{d\sigma}{d\Omega}$ with data suggests that the Coulomb force has the simple 1/r² dependence even down to nuclear length scales. Finally, the total scattering cross section calculated from this $\frac{d\sigma}{d\Omega}$ diverges. This is because the bare Coulomb force is infinitely long ranged. In reality, the Coulomb force of the nucleus is screened out by the electron cloud of the atom, on the length scale of one nm, or less. When this screening is taken into account the total scattering cross section becomes finite, as observed.

These calculations assume that the alpha particle only undergoes one scattering event in the material (the Born scattering approximation). In addition, because of the electron screening, when an alpha particle is near one nucleus, it is insensitive to all the other nuclei because they are 'cloaked' by their neutralizing electron clouds.

Quantum Scattering Theory

In **quantum mechanics** one does not describe the particles in terms of trajectories, but as waves. We replace the incident particle trajectory with a plane wave moving in the z-direction $\psi_{incident} = A e^{ikz}$, where the energy of the particle is $E = \hbar^2 k^2 / (2m)$.



As implied by this picture, a plane wave essentially sends 'particles' of every possible impact parameter at the target at once!

This wave interacts with the scattering center and sends out a collection of <u>outgoing</u> <u>spherical waves</u> centered on the scatterer, as shown in the picture above. We expect solutions at large distances from the scattering center of the form,

$$\psi(r,\theta) = A\left\{e^{ikz} + f(\theta)\frac{e^{ikr}}{r}\right\},\tag{1}$$

where the first term in the bracket is the incoming plane wave and the second term is an outgoing spherical wave with a direction-dependent coefficient $f(\theta)$. Since the scattering potential is assumed to be spherically symmetric we expect no dependence on the azimuthal spherical coordinate, ϕ .

Instead of calculating a trajectory and an impact parameter for this wave (which makes no sense) we instead deal with probability flow through the scattering region. Equating the probability of the incident particle being in a differential volume of size $d\sigma v dt$ (where v is the speed) to the outgoing scattered wave being in a differential volume $r^2 d\Omega v dt$ described by the wavefunction above, yields the DSCS $D(\theta) = \frac{d\sigma}{d\Omega} = |f(\theta)|^2$.

One can proceed using **Partial Wave Analysis**. This process decomposes the scattering by breaking it into a series of scattering events of progressively higher angular momentum scattering states. This is essentially analogous to considering classical particles with larger and larger values of the impact parameter.

We wish to solve the full Schrodinger equation for a spherically symmetric potential V(r). From previous studies of the 3D Schrodinger equation in chapter 4 we know the successful ansatz for this case is $\psi(r, \theta, \phi) = R(r) Y_{\ell,m}(\theta, \phi)$, where $Y_{\ell,m}(\theta, \phi)$ are the spherical harmonics. This separates the problem into angular equations (already solved by the spherical harmonics) and a radial equation. Defining $u(r) \equiv rR(r)$, we find that the radial equation reduces to

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[V(r) + \frac{\ell(\ell+1)\hbar^2}{2mr^2}\right]u = Eu$$
(2)

We divide the problem into 3 regions. First is the asymptotic region where both $V(r) \rightarrow 0$ and the centrifugal term $\frac{\ell(\ell+1)\hbar^2}{2mr^2}$ can be ignored. In this **Radiation zone** one has $kr \gg 1$. The radial Schrödinger equation becomes quite simple:

 $-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} = Eu, \text{ or } \frac{d^2u}{dr^2} = -k^2u, \text{ with solutions } u(r) \sim e^{\pm ikr}. \text{ This gives an outgoing wave}$ of the form $R(r) = \frac{u}{r} = A\frac{e^{ikr}}{r}$, which was the form posited above in Eq. (1).

The next domain is the **Intermediate region** where we can assume that $V(r) \rightarrow 0$ but the centrifugal term cannot be neglected. This assumes that the scattering potential is localized, which means effectively that it falls off faster than $\frac{1}{r^2}$. In this region the radial Schrodinger equation becomes $-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[\frac{\ell(\ell+1)\hbar^2}{2mr^2}\right]u = Eu$, or $\frac{d^2u}{dr^2} - \left[\frac{\ell(\ell+1)}{r^2}\right]u = -k^2u$. The solutions are of the form of spherical Bessel functions: $u(r) = A r j_\ell(kr) + B r n_\ell(kr)$, where the $j_\ell(x)$ remain finite as $x \rightarrow 0$, while the $n_\ell(x)$ do not. Roughly speaking $j_\ell(kr)$ is analogous to sin x, while $n_\ell(kr)$ is analogous to cos x. As with trigonometric functions, it is sometimes useful to consider their complex sum, which are called the spherical Hankel functions of the first and second kind, defined as $h_\ell^{(1)}(kr) = j_\ell(kr) + in_\ell(kr)$ and $h_\ell^{(2)}(kr) = j_\ell(kr) - in_\ell(kr)$. The spherical Hankel function of the first kind has the useful property that it turns into an outgoing spherical wave for large argument: $h_\ell^{(1)}(kr) \approx 1$) $\rightarrow \frac{e^{ikr}}{r}$. The solution for the radial wavefunction now becomes $R(r) = h_\ell^{(1)}(kr)$.