Scattering in Three Dimensions

Scattering experiments are an important source of information about quantum systems, ranging in energy from very low energy chemical reactions to the highest possible energies at the LHC. This set of notes gives a brief treatment of some of the main ideas of scattering of a single particle in three dimensions from a static potential.

Partial Wave Expansion A partial wave expansion is useful for scattering from a spherically symmetric potential at low energy. The basic move is to expand the wave function into states of definite orbital angular momentum. Experiments never input waves of definite angular momentum, rather the input is a beam of particles, along a certain direction, almost always taken to be the $z-$axis. Therefore, one of the first results needed is the expansion of a plane wave along the $z-$axis into partial waves. (The word "partial wave" is synonymous with a state of definite angular momentum.) Setting $z = r\cos\theta$, the expansion reads

$$e^{ikr\cos\theta} = \sum_l (i)^l j_l(kr)(2l+1)P_l(\cos\theta).$$

The $P_l(\cos\theta)$ are the Legendre polynomials. The $j_l(kr)$ are the so-called "spherical Bessel functions." They are actually simple functions, involving $\sin kr$ and $\cos kr$ and inverse powers of kr. The main properties of the j_l are the following:

$$j_l(kr) \to \frac{\sin(kr - \frac{l\pi}{2})}{kr} \text{ as } kr \to \infty,$$

and

$$j_l(kr) \to C_l(kr)^l \text{ as } r \to 0.$$

The factor i^l in the expansion is for convenience. With this factor pulled out, the j_l are real. The j_l satisfy the free radial Schrödinger equation,

$$\left(\frac{1}{r^2}\partial_r(r^2\partial_r) - \frac{l(l+1)}{r^2} + k^2\right) j_l(kr) = 0$$

Turning to the case when a potential is present, we can represent the full continuum wave function by the formula

$$\Psi_k(\vec{x}) = e^{ikr\cos\theta} + \Psi_{sc}(\vec{x}),$$

where Ψ_{sc} is the part of the wave function directly coming from the potential. It should be noted that for the notion of scattering to make sense, the potential must vanish sufficiently rapidly as $|\vec{x}| \to \infty$. We may expand the full wave function in partial waves in a similar manner to the expansion of a plane wave;

$$\Psi_k(\vec{x}) = \sum_l (i)^l R_l(r)(2l+1)P_l(\cos\theta),$$

where $R_l(r)$ is the radial wave function and satisfies the following radial Schrödinger equation,

$$\left(\frac{1}{r^2}\partial_r(r^2\partial_r) - \frac{l(l+1)}{r^2} - U(r) + k^2\right) R_l = 0,$$

where $U(r) = 2mV(r)/\hbar^2$. As will be seen below, the radial wave function R_l is not real in general. However, it is useful in dealing the the radial wave function to solve it using a real function, $\tilde{R}_l$. The function $\tilde{R}_l$ satisfies the same equation as R_l,

$$\left(\frac{1}{r^2}\partial_r(r^2\partial_r) - \frac{l(l+1)}{r^2} - U(r) + k^2\right) \tilde{R}_l = 0.$$

As $r \to \infty$, $\tilde{R}_l$ approaches a real solution of the free Schrödinger equation. This is written as follows,

$$\tilde{R}_l(r) \to \frac{\sin(kr - \frac{l\pi}{2} + \delta_l)}{kr} \quad \text{as } r \to \infty,$$

where δ_l is an angle called the **phase shift**. In a low energy experiment, usually only a few partial waves are needed, and the goal of the experiment will be to determine the phase shifts.

Now since R_l and $\tilde{R}_l$ satisfy the same Schrödinger equation, they must be related by a constant factor. This factor can be determined by comparing the ingoing waves of each function. (An ingoing wave has radial dependence $\exp(-ikr)$, while an outgoing wave has radial dependence $\exp(ikr)$.)

Using the formula for $\sin kr$ in terms of exponentials, we have for the ingoing wave of $\tilde{R}_l$,

$$\tilde{R}_l \to \frac{1}{2ikr}\exp(-i(kr - \frac{l\pi}{2} + \delta_l)) \text{ as } r \to \infty.$$

Meanwhile for R_l the ingoing wave must be exactly the ingoing wave of the plane wave, since the scattering process only produces outgoing waves. We have for the ingoing wave of R_l :

$$R_l \to \frac{1}{2ikr}\exp(-i(kr - \frac{l\pi}{2}))$$

From this we see that the two functions are related by a factor involving the phase shift,

$$R_l = e^{i\delta_l}\tilde{R}_l$$

To summarize, using the information that the functions must be related by a constant since they both satisfy the same differential equation, we have gone to a region where both functions take a simple form (large r) and found the factor by comparing the ingoing wave in each function.

Having found the needed factor, it will be useful in what follows to note that the *outgoing* wave of R_l is for large r given by:

Outgoing wave of $i^l R_l$:

$$i^l R_l \to \frac{1}{2ikr}\exp(i(kr + 2\delta_l))$$

Example for $l = 0$ An example where many details can be worked out is the δ shell potential, discussed in much more detail in the earlier edition of Gottfried's book. We have

$$U(r) = \lambda\delta(r - r_0)$$

Here we will work out the problem for $l = 0$ only. The radial Schrödinger equation becomes simpler if we define a modified radial wave function,

$$\tilde{R}_0 = \frac{u_0}{r}$$

The function u_0 satisfies

$$(\partial_r^2 - U(r) + k^2)u_0(r) = 0.$$

To keep $\tilde{R}_0$ finite at $r = 0$, u_0 must vanish at $r = 0$. Now the potential is only active at $r = r_0$, so u_0 satisfies the free Schrödinger equation for $r < a$ and $r > a$. We have

$$\begin{array}{rcll} u_0(r) & = & A\sin(kr) & r < r_0 \\ u_0(r) & = & B\sin(kr + \delta_0) & r > r_0 \end{array}$$

Demanding that u_0 be continuous and its derivative have the jump required by a δ function potential gives

$$A\sin(kr_0) = B\sin(kr_0 + \delta_0),$$

and

$$kB\cos(kr_0 + \delta_0) - kA\cos(kr_0) = \lambda A\sin(kr_0)$$

Taking the ratio of these two equations gives

$$\tan(kr_0 + \delta_0) = \frac{\tan(kr_0)}{1 + \frac{\lambda}{k}\tan(kr_0)}.$$

Using standard trigonometric identities, we have

$$\frac{\tan(\delta_0)}{k} = \frac{-\frac{\lambda}{k^2}\sin^2(kr_0)}{1 + \frac{\lambda}{k}\sin(kr_0)\cos(kr_0)}. \tag{1}$$

We note that $\tan\delta_0 \to k$ as $k \to 0$. This behavior generalizes to higher values of l as follows:

$$\tan\delta_l \to k^{2l+1} \text{ as } k \to 0$$

The origin of this small k behavior is that for a fixed l as $k \to 0$, to keep the angular momentum fixed, the region where the wave function is appreciable must move to larger and larger r. This can be easily seen by making the classical estimate $\hbar l \sim \hbar k r_m$, where r_m is the position of the wave function maximum. Clearly as $k \to 0$, r_m must get larger and larger.

Scattering Length For $l = 0$ scattering at very low energy, the scattering is dominated by a quantity called the *scattering length*. The scattering length a (or sometimes a_s) is defined by

$$\lim_{k\to 0} \frac{\tan\delta_0}{k} = -a.$$

(An equivalent formula for $1/a$ is often written using the $\cot\delta_0$ instead of $\tan\delta_0$.) In the example of the delta shell potential, we have from Eq.(1)

$$a = \frac{\lambda r_0}{1+\lambda r_0} r_0 \tag{2}$$

From this formula, we have

$$\begin{array}{lll} a>0 & \lambda>0 & \\ a<0 & \lambda<0, & 1+\lambda r_0>0 \\ a>0 & \lambda<0, & 1+\lambda r_0<0 \end{array}$$

We see that if the delta shell potential is repulsive ($\lambda > 0$), then $a > 0$. However, if the delta shell potential is attractive, a can have either sign. Roughly speaking, *weak attraction* leads to $a < 0$, and *strong attraction* leads to $a > 0$. It is possible to gain insight into these results by considering the equation for $u_0(r)$ for $k^2 = 0$. This is

$$\partial_r^2 u_0(r) = U(r) u_0(r)$$

For the delta shell potential we can solve this equation very easily. We have

$$\begin{array}{rcll} u_0(r) & = & Ar, & r<r_0 \\ u_0(r) & = & B(r-a), & r>r_0 \end{array} \tag{3}$$

It is not obvious at this point that the parameter a in Eq.(3) is the scattering length as given in Eq.(2). This will be justified shortly. Demanding continuity and the correct delta function jump condition at $r = r_0$ gives

$$\begin{array}{rcl} Ar_0 & = & B(r_0-a) \\ A(1+\lambda r_0) & = & B. \end{array}$$

Taking the ratio of these equations leads to Eq.(2) for a, which establishes that the a in Eq.(3) is indeed the scattering length.

Now consider a generic short range potential, which is either zero or vanishes very rapidly for $r \geq r_0$, where r_0 is a parameter characterizing the range of the potential. (The delta shell is certainly an example, but now we want to discuss an arbitrary short range potential.) For $r > r_0$, the $k = 0$ wave function $u_0(r)$ will certainly approach a straight line of the form $B(r - a)$, and it can be established that this a is indeed the scattering length. At this point, we see that the scattering length is defined by taking the large r form of the $k = 0$ wave function $u_0(r)$, and asking where does this form reach 0? The value of this intercept is the scattering length.

Finally, we can understand the sign of a, by looking at the $k = 0$ equation for $r < r_0$,

$$\partial_r^2 u_0(r) = U(r) u_0(r).$$

We must have $u_0(0) = 0$, and we can certainly start off from $r = 0$ with $u_0(r) > 0$. Then for an attractive ($U(r) < 0$), we have $\partial_r^2 u_0(r) < 0$, i.e. the potential is trying to curve $u_0(r)$ toward the $u_0 = 0$ axis. For a strongly attractive potential, by the time $r > r_0$, $u_0(r)$ will have developed a negative slope and the straight line it matches onto must cross the axis at $r > 0$. For a weakly attractive potential, the slope of $u_0(r)$ will still be positive at $r = r_0$, and the scattering length will be negative. The boundary between weak and strong attraction comes when the potential becomes strong enough to have a bound state. A striking example of this is in the scattering of a neutron and a proton. The scattering length is large by nuclear standards, $a \sim +5.2fm$, and there is a bound state in the system, the deuteron.

It is easy to show using formulas from the next section that at very low values of k, the total crossection is given in terms of the scattering length by

$$\sigma_{tot} = 4\pi a^2.$$

Resonant Scattering Resonant scattering is an important phenomenon in low energy scattering. It occurs when the system in question has an "almost bound" state. The system has an attractive potential, and may have bound states, but a resonance occurs in the actual scattering region. A true resonance corresponds to a particle with a finite lifetime. Resonances abound in particle physics, nuclear physics, and atomic physics. They are hard to model with simple potentials, so only a basic description is given here. A typical example is a resonance in an $l = 1$ partial wave. If the scattering energy is E, the resonance energy is E_r and the so-called width of the resonance is $\Gamma/2$. then the formula for $\exp(2i\delta_1)$ would be

$$e^{2i\delta_1} = \frac{E - E_r - i\frac{\Gamma}{2}}{E - E_r + i\frac{\Gamma}{2}}$$

or equivalently,

$$e^{i\delta_1} \sin\delta_1 = -\frac{\frac{\Gamma}{2}}{E - E_r + i\frac{\Gamma}{2}}$$

From these two formulas, it is easy to see that a resonance corresponds to a phase shift that is positive for $E < E_R$, rises rapidly and reaches $\pi/2$ at the resonance, and then continues on. A sharp resonance corresponds to a a relatively small value of Γ. In many cases, even though several partial waves may be active, a resonance in one of them can lead to a sharp peak in the total crossection. This is the way many resonances were discovered. Another hallmark of a resonance is the location of the pole in the complex energy plane. We see that this occurs at $E = E_r - i\Gamma/2$. Considerations of causality require that the pole occur in the *lower half* of the complex energy plane.

Partial waves and the full scattering amplitude As $r \to \infty$, the scattering part of the wave function becomes proportional to the *scattering amplitude*,

$$\Psi_{sc} \to \frac{f(\theta,\phi)}{r} e^{ikr} \text{ as } r \to \infty$$

From our formula for the partial wave expansion of the full scattering wave function along with the outgoing wave term in R_l, we have for the outgoing wave of the full scattering wave function,

$$\Psi_k^{out} \to \frac{1}{2ikr} e^{ikr} \sum_l e^{2i\delta_l}(2l+1)P_l(\cos\theta) \text{ as } r \to \infty.$$

Similarly, the outgoing wave part of the plane wave is, from our previous formulas,

$$(e^{ikz})^{out} \to \frac{1}{2ikr} e^{ikr} \sum_l (2l+1)P_l(\cos\theta) \text{ as } r \to \infty.$$

Now the scattering outgoing wave comes from the *difference* between the outgoing wave of the full wave function and the plane wave,

$$\frac{f(\theta,\phi)}{r} e^{ikr} = \Psi_k^{out} - (e^{ikz})^{out}$$

Using the two formulas above, we have

$$\frac{f(\theta,\phi)}{r} e^{ikr} = \frac{1}{r} e^{ikr} \sum_l \frac{1}{2ik}(e^{2i\delta_l} - 1)(2l+1)P_l(\cos\theta),$$

which finally gives for the scattering amplitude,

$$f(\theta,\phi) = \sum_l e^{i\delta_l} \frac{\sin\delta_l}{k}(2l+1)P_l(\cos\theta).$$

(For a spherically symmetric potential, the scattering amplitude depends only on the polar angle θ.)

It is of interest to see how the optical theorem is satisfied by the partial wave expansion. The optical theorem is

$$\frac{4\pi}{k} Im(f(\theta=0)) = \sigma_T = \int |f(\theta,\phi)|^2 d\Omega$$

From our formula for the partial wave expansion of f, and $P_l(\cos\theta = 1) = 1$, we have for the left hand side of the optical theorem,

$$\frac{4\pi}{k} Im(f(\theta=0) = \frac{4\pi}{k} \sum_l \frac{\sin^2\delta_l}{k}(2l+1).$$

For the integral on the right hand side, we have

$$\int |f(\theta,\phi)|^2 d\Omega = \int d\Omega \frac{1}{k^2} \left(\sum_{l,l'} (e^{i\delta}\sin\delta)_l (e^{i\delta}\sin\delta)_{l'} \ (2l+1)(2l'+1) P_l(\cos\theta) P_{l'}(\cos\theta) \right)$$

Using the orthogonality properties of the Legendre polynomials, we have

$$\int d\Omega P_l(\cos\theta) P_{l'}(\cos\theta) = \frac{4\pi}{2l+1}.$$

This reduces the double sum on l, l' to a single sum and we have

$$\sigma_T = \frac{4\pi}{k^2} \sum_l \sin^2\delta_l (2l+1),$$

which is the same as the left hand side we calculated above. It is important to note that the optical theorem is satisfied *partial wave by partial wave.* This makes sense, since the optical theorem is ultimately a statement of probability conservation, and says that for a given partial wave, the outgoing wave must have the same strength as the incoming wave, and therefore can only differ by a phase factor, which in terms of δ_l is $\exp(2i\delta_l)$.

The full scattering amplitude **NOTE** In the equations of this section x and x' are three dimensional vectors.

The Schrödinger equation for the full scattering wave function is

$$(\nabla^2 + k^2)\Psi_k(x) = U(x)\Psi_k(x).$$

In scattering theory, it is useful to turn this into an integral equation,

$$\Psi_k(x) = \Psi_k^0(x) + \int G_k(x-x') U(x') \Psi_k(x') d^3x'$$

The function Ψ_k^0 is the free plane wave input, and satisfies

$$(\nabla^2 + k^2)\Psi_k^0(x) = 0.$$

The function $G_k(x-x')$ is the scattering Green function, and must satisfy

$$(\nabla^2 + k^2) G_k(x-x') = \delta^3(x-x').$$

This is necessary so that Ψ_k satisfies the full Schrödinger equation.

The scattering Green function can be found by Fourier transform,

$$G_k(x-x') = \int e^{k'\cdot(x-x')} \tilde{G}_k(k') \frac{d^3k'}{(2\pi)^3}.$$

Applying $(\nabla^2 + k^2)$ to $G_k(x-x')$ gives

$$(k^2 - (k')^2)\tilde{G}_k(k') = 1$$

The correct form of $G_k(x-x')$ is obtained from the Fourier transform by adding $i\epsilon$ to k^2 in the denominator of the integral. (This insures that $G_k(x-x')$ involves only outgoing waves.) We have

$$G_k(x-x') = \int e^{k'\cdot(x-x')} \frac{1}{k^2 + i\epsilon - (k')^2} \frac{d^3k'}{(2\pi)^2}.$$

The result of computing the Fourier transform can be obtained by contour integration and is

$$G_k(x-x') = \frac{-1}{4\pi|x-x'|} e^{ik|x-x'|}$$

The scattering integral equation now takes the form,

$$\Psi_k(x) = \Psi_k^0(x) - \frac{1}{4\pi} \int \frac{e^{ik|x-x'|}}{|x-x'|} U(x')\Psi_k(x') d^3x'.$$

For reading off the scattering amplitude, we want to take the coordinates very large compared to the range of $U(r)$. We have

$$\frac{1}{|x-x'|} \to \frac{1}{r} \text{ as } r \to \infty \text{ where } r = |x|,$$

and

$$|x-x'| = \sqrt{x^2 - 2x\cdot x' + (x')^2} \to r - \hat{r}\cdot x' \text{ as } r \to \infty.$$

Using these formulas to get the large distance form of Ψ_{sc}, we have

$$\Psi_k(x) \to e^{ikz} - \frac{e^{ikr}}{4\pi r} \int e^{-ik\hat{r}\cdot x'} U(x')\Psi_k(x')$$

By definition, the scattering amplitude is the coefficient of $\exp(ikr)/r$, so the scattering amplitude is then

$$f(\theta,\phi) = -\frac{1}{4\pi} \int e^{-ik\hat{r}\cdot x} U(x)\Psi_k(x)$$

This is an exact formula, and requires the knowledge of the exact scattering wave function. It is a useful formula nevertheless, since it only requires that the exact wave function be known inside the range of $U(r)$. It is also useful for formulating approximations to $f(\theta,\phi)$.

Born approximation The Born approximation is extremely useful for scattering at high energy, in particular for $U(r) << k^2$. In using the Born approximation, it is convenient to think of the scattering as going from an initial wave vector to a final wave vector, where these are defined by

$$k_f = k\hat{r}, \quad k_i = k\hat{z}.$$

The Born approximation involves replacing the exact wave function in the integral for the scatting amplitude by the plane wave, so we have

$$f_B(k_f, k_i) = -\frac{1}{4\pi} \int e^{-ik\hat{r}\cdot x} U(x) e^{ikz} d^3x$$

To see how a calculation of f_B goes, take the potential

$$U(r) = \gamma \frac{e^{-\beta r}}{r}.$$

This so-called Yukawa potential can also be used to model a Coulomb potential for β very small. The Born approximation is

$$f_B(k_f, k_i) = -\frac{1}{4\pi} \int e^{i(k_i - k_f)\cdot x} \, \gamma \frac{e^{-\beta r}}{r} d^3x$$

It is seen that the Born approximation only depends on the difference of initial and final wave vectors. Setting

$$q = k_i - k_f,$$

and doing the elementary solid angle integral, we have

$$f_B = -\gamma \int \frac{\sin qr}{qr} \frac{e^{-\beta r}}{r} r^2 dr.$$

This radial integral is also elementary and we obtain

$$f_B(k_f, k_i) = -\frac{\gamma}{\beta^2 + q^2}$$

Note that if we take an attractive potential, $\gamma < 0$, the Born amplitude is positive.

The differential cross section in Born approximation is given by

$$\frac{d\sigma_B}{d\Omega} = |f_B|^2 = \frac{\gamma^2}{|\beta^2 + q^2|^2}$$

Writing out q^2 in terms of the scattering angle, we have

$$q^2 = k_f^2 - 2k_f \cdot k_i + k_i^2 = 2k^2(1 - \cos\theta) = 4k^2 \sin^2 \frac{\theta}{2},$$

so the differential cross section in Born approximation is given by

$$\frac{d\sigma_B}{d\Omega} = |f_B|^2 = \frac{\gamma^2}{|\beta^2 + 4k^2 \sin^2 \frac{\theta}{2}|^2}$$

For large k^2, this formula shows a sharp peak as $\theta \to 0$. The scattering at large angles is dominated by the $4k^2 \sin^2 \frac{\theta}{2}$ factor in the denominator, and is the way Rutherford demonstrated that the nucleus of an atom looks like a point charge to α particle scattering at the energy he was using.