1 Scattering in 3D - Exact Solution

We consider elastic scattering of an incoming particle in the presence of a potential $V(\vec{r})$ that is constrained to a finite volume centered on the origin: $V(\vec{r}) = 0$ for $|\vec{r}| > a$. (We ignore for now inelastic scattering and particle production; however, the results we will obtain can be easily applied to elastic scattering of one particle off another by transforming the problem into center-of-mass and relative coordinates; $V(\vec{r})$ then becomes the interaction potential between the two particles depending on their relative coordinate while the center of mass motion is trivial). To solve the scattering problem in 3D, we are looking for solutions of the Schrödinger equation that asymptotically approach free eigenfunctions of H_0 at large distance r from the origin (where the potential is zero).

The incoming particle is once again described by a Gaussian wave packet, this time in three dimension - let's assume it travels along the z-axis. Following the same procedure as for 1D scattering, we can take the asymptotic limit where this becomes a plane wave with momentum $\hbar k$ along the z-axis: $\psi_{in}(\vec{r}) = \exp(i\vec{p}\cdot\vec{r}/\hbar) = \exp(ikz)$ (the normalization is arbitrarily chosen to make the wave function as simple as possible, but it will cancel in the end).

In the "frequentist interpretation" of quantum mechanics, where the wave function describes a large number of identical particles, the cross section can be expressed as the ratio between the rate of events dN/dt in a detector of area A at distance R from the origin, spanning a solid angle $\Delta\Omega = A/R^2$, divided by the probability current density j_z of the incoming particles. Note: $dN/dt = Aj_r = \Delta\Omega R^2 j_r$ where j_r is the radial current density, and $j_z = \hbar k/m$. Since we expect the cross section to depend only on the energy E of the incoming particle and the direction of the detector (θ, ϕ), it is best to use spherical coordinates to describe the outgoing (scattered) asymptotic wave function.

We have seen the previous semester that for a free Hamiltonian $H_0 = \frac{\vec{p}^2}{2m} = \frac{-\hbar^2}{2m}\nabla^2$, expressing ∇^2 in polar coordinates we obtain the following eigenfuctions:

$$\psi_{Elm} = R_{E,l}(r)Y_l^m(\theta,\phi) = \frac{u_{E,l}(r)}{r}Y_l^m(\theta,\phi) \quad E = \frac{\hbar^2 k^2}{2m}, \tag{1}$$

where $R_{E,l}(r)$ can be a Neumann function $\eta_l(kr)$ (singular at $r = 0$) or a Bessel function $j_l(kr)$ (regular at $r = 0$).. (We cannot discard the Neumann functions since the free Hamiltonian is only applicable for $r > a$ where they behave perfectly fine.)

The general solution for the Schrödinger Equation with eigenvalue (energy) E anywhere outside of the sphere of radius a around the origin will be a superposition of the eigenfunctions of H_0 with the same energy E:

$$\psi_E(r,\theta,\phi) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l}[A_{lm}j_l(kr) + B_{lm}\eta_l(kr)]Y_l^m(\theta,\phi)]. \tag{2}$$

We remember that asymptotically for $r \to \infty$ we have:

$$\begin{cases} j_l(kr) \to \frac{1}{kr}\sin(kr - l\pi/2) = \frac{1}{2ikr}(e^{i(kr-l\pi/2)} - e^{-i(kr-l\pi/2)}) \\ \eta_l(kr) \to -\frac{1}{kr}\cos(kr - l\pi/2) = -\frac{1}{2kr}(e^{i(kr-l\pi/2)} + e^{-i(kr-l\pi/2)}) \end{cases}$$

Inserting these expressions in ψ_E we obtain:

$$\psi_E(r \to \infty, \theta, \phi) = \qquad (3)$$
$$\frac{1}{2kr} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \quad [(-iA_{lm} - B_{lm}) e^{i(kr - l\pi/2)} + (iA_{lm} - B_{lm}) e^{-i(kr-l\pi/2)}] Y_l^m(\theta, \phi)] \quad .$$

For the scattered wave function, we are looking for solutions that represent an outgoing wave (meaning that j_r is positive). Therefore, the second coefficient must be zero, meaning $A_{lm}/B_{lm} = -i$, so we arrive at the following expression for the asymptotic outgoing wave function:

$$\psi_E(r, \theta, \phi) = \frac{1}{kr} e^{ikr} \sum_{l,m} (-i)^l (-B_{lm}) Y_l^m(\theta, \phi) = \frac{1}{r} e^{ikr} f(\theta, \phi). \qquad (4)$$

The last equality defines the *scattering amplitude* $f(\theta, \phi)$.

We combine this with the incoming plane wave. So asymptotically the wave function for the $3D$ scattering problem is:

$$\psi(r \to \infty) = e^{ikz} + \frac{e^{ikr}}{r} f(\theta, \phi). \qquad (5)$$

We can now calculate the outgoing probability current density:

$$j_r = \frac{\hbar k}{m} \frac{1}{r^2} |f(\theta, \phi)|^2. \qquad (6)$$

This follows from the gradient in spherical coordinates; it is

$$\hat{r} \frac{\partial}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial}{\partial \theta} + \hat{\phi} \frac{1}{r \sin\theta} \frac{\partial}{\partial \phi} \qquad (7)$$

but we discard all terms that fall off faster than $1/r^2$ and are therefore suppressed at the large distance R of the detector.

We therefore get for the rate into the detector

$$dN/dt = \Delta\Omega R^2 j_r(R) = \Delta\Omega R^2 \frac{\hbar k}{m} \frac{1}{R^2} |f(\theta, \phi)|^2 = \Delta\Omega \frac{\hbar k}{m} |f(\theta, \phi)|^2 \qquad (8)$$

which is indeed independent of R as expected. Dividing by j_z, we obtain the following expression for the elastic differential cross section:

$$\frac{\Delta\sigma}{\Delta\Omega} \to \frac{d\sigma}{d\Omega} = \frac{1}{j_z} \frac{\hbar k}{m} |f(\theta, \phi)|^2 = |f(\theta, \phi)|^2. \qquad (9)$$

Therefore, our task is to find a solution of the Schrödinger Equation with the asymptotic form Eqs. 4-5 for $r > a$ and then we can calculated the cross section from $f(\theta, \phi)$.

For this purpose, it is convenient to solve the Schrödinger equation in spherical coordinates. Therefore, we have to write the incoming plane wave in spherical coordinates also:

$$e^{ikz} = e^{ikr\cos\theta} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos\theta). \qquad (10)$$

(This is at least plausible given that a plane wave along the z-axis must be spherically symmetric - so only the Y_l^m with $m = 0$ contribute, which are proportional to the Legendre polynomials $P_l(\cos\theta)$. Furthermore, only the Bessel functions can be present since a plane wave must be regular at the origin. The exact magnitude of each coefficient can be obtained using various properties of the Legendre polynomials, including the fact that they form an orthonormal basis).

At very large $r \to \infty$ this becomes (using again the asymptotic form of j_l:

$$e^{ikz} \to \frac{1}{2ikr} \sum_{l=0}^{\infty} (2l+1)(e^{ikr} - i^{2l} e^{ikr}) P_l(\cos\theta). \tag{11}$$

If the potential is invariant under rotations along the z axis, $\frac{\partial V}{\partial \phi} = 0$, the outgoing wave should be symmetric as well (independent of ϕ) and takes the form:

$$\frac{1}{kr} e^{ikr} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} (-i)^l (-B_{lm}) Y_l^m = \frac{e^{ikr}}{r} \sum_{l=0}^{\infty} (2l+1) a_l(k) P_l(\cos\theta) = f(\theta) \frac{e^{ikr}}{r}\ , \tag{12}$$

where we define a_l appropriately to get this convenient form (again, $Y_l^0 \sim P_l(\cos\theta)$ and $P_l(1) = 1$.)

So the total wave function at large r can be rewritten in this way:

$$\psi_E(r \to \infty, \theta, \phi) = e^{ikz} + \frac{e^{ikr}}{r} f(\theta, \phi) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1) \left((1 + 2ika_l) \frac{e^{ikr}}{r} - i^{2l} \frac{e^{-ikr}}{r} \right) P_l(\cos\theta). \tag{13}$$

Now all we need to do is find a solution of the full Schrödinger equation for all r with the same eigenvalue E. We can do this in 2 parts: Outside of $r = a$, we know that the solution will be simply the free one, of the same form as Eq. 2. Inside ($r < a$), we need to come up with the correct solution $R_{E,l}(r)$ for the given potential, for each value of l. The two solutions must be matched (in value and in their first derivatives) at $r = a$. We can make use of the fact that any such solution can be written as a purely real function of r. Therefore, we can replace the sum of j_l and η_l for each l in Eq. 2 by a Bessel function only, but shifted by a certain amount (called “phase shift”):

$$\psi_E(r > a, \theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} [C_{lm} j_l(kr + \delta_l) Y_l^m(\theta, \phi)], \tag{14}$$

just like $A\cos\theta + B\sin\theta$ can always be replaced with $C\sin(\theta + \delta)$.

Asymptotically for $r \to \infty$, once again we have:

$$j_l(kr + \delta_l) \to \frac{1}{kr} \sin(kr - l\pi/2 + \delta_l) = \frac{1}{2ikr} (e^{i(kr - l\pi/2 + \delta_l)} - e^{-i(kr - l\pi/2 + \delta_l)}) \tag{15}$$

Inserting this expressions in ψ_E we obtain:

$$\psi_E(r \to \infty, \theta, \phi) = \frac{1}{2ikr} \sum_{l=0}^{\infty} D_l [(-i)^l e^{i\delta_l} e^{ikr} - (i)^l e^{-i\delta_l} e^{-ikr}] P_l(\cos\theta) \quad . \tag{16}$$

where we once again made use of the cylindrical symmetry.

Comparing with Eq. 13, we can read off from the terms proportional to $\exp(-ikr)$ that

$$-(2l+1)i^{2l} = -D_l i^l e^{-i\delta_l} \Rightarrow D_l = (2l+1)i^l e^{i\delta_l} \tag{17}$$

Plugging this in and comparing the terms proportional to $\exp(ikr)$ in both equations, we see that

$$(2l+1)(1+2ika_l) = D_l(-i)^l e^{i\delta_l} = (2l+1)e^{2i\delta_l}. \tag{18}$$

We see that, as a consequence of the solution being real, the factor in front of the "outgoing wave" in Eq. 13 is has the same magnitude and only differs in phase from the factor in front of the "incoming spherical wave". This can also be understood from the point of view of probability conservation: If the factors had different magnitude, we would have a "net flow of probability" inwards or outwards for specific angular momenta, which is inconsistent with a stationary solution (and angular momentum conservation).

Solving for the constants a_l we obtain:

$$a_l = \frac{e^{2i\delta_l}-1}{2ik} = \frac{\sin\delta_l}{k}e^{i\delta_l} \Rightarrow f(\theta) = \frac{1}{k}\sum_{l=0}^{\infty}(2l+1)\sin\delta_l e^{i\delta_l} P_l(\cos\theta). \tag{19}$$

This form is in particular useful if only a few angular momenta l contribute; in general, only angular momenta up to $l \approx ka$ need to be considered, since the "centrifugal barrier" suppresses higher orbital angular momenta.

Note, in summary, that once we have determined the phase shifts $\delta_l(k)$ from solving and matching the Schrödinger equation at $r = a$ for all values of k, we have a complete description of the elastic cross section at all energies and in all directions.