Scattering Problems in One Dimension

Scattering is a very important topic Quantum Mechanics because, in a number of cases, we study the properties of the interaction between two objects by means of **scattering**. We shoot projectiles (usually light objects) with a well defined momentum ($\vec{p}_{\rm in}$) at a target (usually a heavy object at rest). We observe how the projectiles are **scattered** by the target. That is we measure the momenum ($\vec{p}_{\rm fin}$) of each projectile after it interacts with the target. We parametrize the interaction between the projectile and the target in terms of a potential. By observing the pattern of the projectiles scattering off the target, we can figure out the potential. Some examples of scattering are

1. Rutherford Scattering: Shooting α particles off gold nuclei.
2. Compton Scattering: Shooting X-rays off electrons in metal.
3. Raman Scattering: Shooting light off electrons in molecules.

Raman Scattering is an important technique in finding energy levels in molecules.

Scattering in One dimension

Case A: $E < V_0$

Here we consider only the projectile. We will not worry about what the target is. We assume that the target gives rise to a potential $V(x)$ and the projectile is affected by this potential. First we consider the simplest potential in one dimension,

$$\begin{aligned} V(x) &= 0 \text{ for x} \leq 0 \\ &= V_0 \text{ for x} > 0, \text{ where } V_0 > 0. \end{aligned}$$

This is called *Step Potential*. As mentioned before, in scattering problems the projectile is assumed to have a well defined momentum and hence a well defined wave number k. Therefore we represent the projectile by a plane wave $\exp(ikx)$. That is the projectile has momentum in positve x direction. We also assume that a steady stream of projectiles come in and get scattered by the potential. The picture we have is of a steady flow. Even though things are moving, the problem we solve is time independent. Because we consider a situation where the flow does not change with time. So we do not explicitly consider the time dependence.

Let us assume that the wave number k of the projectile is small enough such that its energy $E = \hbar^2 k^2/2m < V_0$. In classical mechanics, such a particle is **always** reflected by the potential barrier at $x = 0$. Same thing happens in quantum mechanics too *but with a difference*. For $x \leq 0$ the time independent Schroedinger's equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_L(x)}{dx^2} = E\psi_L(x).$$

The most general solution is given by

$$\psi_L(x) = Ae^{ikx} + Be^{-ikx},$$

where $k^2 = 2mE/\hbar^2$. The first term is a wave with momentum in +ve x direction and it represents the **incident** wave. The second term is a wave with momentum in -ve x direction and it represents the **reflected** wave.

For $x > 0$ the time independent Schroedinger's equation is

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2\psi_R(x)}{dx^2} + V_0\psi_R(x) &= E\psi_R(x) \\ \frac{d^2\psi_R(x)}{dx^2} &= -\frac{2m(E - V_0)}{\hbar^S}\psi_R(x). \end{aligned}$$

$(E - V_0) < 0$ so the RHS is positive. For $x > 0$, the square of the wave number $k'^2 = 2m(E - V_0)/\hbar^2$, is negative, meaning k' is imaginary. We define $k' = i\kappa$. The most general wave function for $x > 0$ is

$$\psi_R(x) = Ce^{\kappa x} + De^{-\kappa x}.$$

Obviously $\kappa^2 = 2m(V_0 - E)/\hbar^2$ and κ is the positive square root. $e^{\kappa x}$ diverges as $x \to \infty$. It is not allowed. Hence $C = 0$.

The wave function should be continuous at $x = 0$. This gives us the condition

$$A + B = D.$$

The first derivative also should be continuous at $x = 0$. This gives us the condition

$$ik(A - B) = -\kappa D.$$

We have two equations and three unknowns. The normlisation condition,

$$\int_{-\infty}^{0} |\psi_L(x)|^2 dx + \int_{0}^{\infty} |\psi_R(x)|^2 dx = 1,$$

should provide us the third condition so that three constants A, B and D could be determined. But normalization of e^{ikx} is tricky! One simple way to handle this problem is the following: We consider the projectiles to come from $-L$ rather than $-\infty$. Similarly we expect the step potential V_0 to extend to $+L$ rather than $+\infty$. And we choose L such that it is much larger than $1/k$ so that the incident wave and the reflected wave look very similar to plane waves. For example, if $k = (cm)^{-1}$, we choose $L \geq 1\ m$. In this approximation, we get finite values for A, B and D. But we will see below that the physically relevant quantities are not A, B and D but the two ratios B/A and D/A. Hence the exact normalization of the wave function is needed in this problem.

We define the reflection coefficient R and transmission coefficient T based on the following point of view. We said in the beginning that we consider a steady state problem. That means that a particle incident on the potential should be either reflected or transmitted. Extending this argument we say that the rate at which the incident particles strike the barrier is equal to the rate at which they are reflected from the barrier plus the rate at which they are transimitted through the barrier to $+\infty$. The rate at which the incident particles approach the barrier is equal to $(\hbar k_1/m)|A|^2$ (that is, speed*probability of incident wave). The rate at which they are reflected from the barrier is $(\hbar k_1/m)|B|^2$ and the rate at which they are transmitted to $+\infty$ is zero because $\psi_R(x)$ approaches 0 as $x \to \infty$.

$$\begin{aligned} R &= \frac{\text{flux of particles with negative wave vector at x} \to -\infty}{\text{flux of particles with positive wave vector at x} \to -\infty} \\ T &= \frac{\text{flux of particles with positive wave vector at x} \to \infty}{\text{flux of particles with positive wave vector at x} \to -\infty} \end{aligned}$$

For the problem of step potential, we solve the two equations coming from the continuity of ψ and $d\psi/dx$. We obtain the two ratios

$$\begin{aligned} \frac{B}{A} &= \frac{k - i\kappa}{k + i\kappa} \\ \frac{D}{A} &= \frac{2k}{1 + i\kappa} \end{aligned}$$

From the definition of the reflection coefficient, we can work out $R = |B|^2/|A|^2$. From the above equation, we see that $R = 1$ meaning that the probability for reflection is 100%. That obviously means that the transmission coefficient is 0. This is true even if $D \neq 0$. The reason is that $\psi_R(x) \to 0$ as $x \to +\infty$ and the probability of finding the particle at $+\infty$ is 0. Since $D \neq 0$, it means that the particle actually **penetrates** the potential barrier upto a depth of about $1/\kappa = \hbar/\sqrt{2m(V_0 - E)}$. Because the exponential function falls very steeply for large x, we see that the probability of finding the particle at $x > 1/\kappa$ is quite small. In a steady state situation, any particle that does penetrate into the potential, will be reflected back from within the potential and will never reach $+\infty$.

Case B: $E > V_0$

Let us now consider another scattering problem with the same potential. But now we take a projectile with a larger wave number k_1 such that $E = \hbar^2 k_1^2/2m > V_0$. In classical mechanics such a particle always overcomes the potential barrier and goes off to $x \to \infty$. In quantum mechanics, the conditions of the continuity of the wave function and its derivative, lead to the conclusion that there is always a reflected wave. The allowed forms of the wave function are

$$\begin{aligned}\psi_L(x) &= Ae^{ik_1x} + Be^{-ik_1x} \\ \psi_R(x) &= Ce^{ik_2x},\end{aligned}$$

where $k_2^2 = 2m(E - V_0)/\hbar^2$. There is no e^{-ik_2x} term in $\psi_R(x)$ because the boundary conditions do not allow it. Another way of saying it is, there is no **source** for such a term. That is, we have a source at $-\infty$ which is shooting particles of wave vector $+k_1$. Such particles, when they interact with the potential at $x = 0$, will either be reflected back (wave vector $-k_1$) or be transmitted (wave vector $+k_2$). There is no possibility of of a wave with wave vector $-k_2$.

We impose the conditions that the wave function and its first derivative should be continuous at $x = 0$ and we get the conditions

$$\begin{aligned}A + B &= C \\ ik_1(A - B) &= ik_2C.\end{aligned}$$

We solve these equations to obtain the ratios

$$\begin{aligned}\frac{B}{A} &= \frac{k_1 - k_2}{k_1 + k_2} \\ \frac{C}{A} &= \frac{2k_1}{k_1 + k_2}\end{aligned}$$

Note that B and the reflection coefficient $R = |B/A|^2 \neq 0$. Using the definition of the transmission coefficient we find $T = (k_2/k_1)|D/A|^2$ leading to

$$\begin{aligned}R &= \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \\ T &= \frac{4k_1 k_2}{(k_1 + k_2)^2}.\end{aligned}$$

It is trivial to see that $R + T = 1$.