Scattering Problems in One Dimension

S Uma Sankar

Department of Physics
Indian Institute of Technology Bombay
Mumbai, India

Scattering in Quantum Mechanics

Ref: Chapter-7 of Serway

- 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 as it is pushed by 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

- 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.
- We consider the simplest potential in one dimension,

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

- 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 $\exp(ikx)$.
- 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 is time independent. 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.
- For $x \leq 0$ (on the left side of the barrier) 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 represents the incident wave and the second term represents the reflected wave.

Scattering in One dimension

- For $x > 0$ (on the right side of the barrier) the time independent Schroedinger's equation is

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

  $(E - V_0) < 0$ 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 can solve these two equations obtain the two ratios
$$\begin{aligned} \frac{B}{A} &= \frac{k - i\kappa}{k + i\kappa} \\ \frac{D}{A} &= \frac{2k}{1 + i\kappa} \end{aligned}$$

- The reflection coefficient $R = |B/A|^2 = 1$, meaning that the probability for reflection is 100%. However $D \neq 0$, which means that the particle actually penetrates the potential barrier upto a depth of about $1/\kappa = \hbar/\sqrt{2m(V_0 - E)}$.
- How can the particel both penetrate the barrier and also get reflected from it?
- We have to take the point of view that the particle is getting reflected, partly from the edge of the barrier and also partly from inside the barrier.
- Can we detect the particle inside the barrier? It is possible. But to detect it, we have to localize it to the size a of the experimental probe. Which would lead to imparting a momentum $\hbar/a$ to the particle. This will lead to an increase in kinetic energy $\hbar^2/2ma^2$. The particle is detectable only if this increase makes the net kinetic energy positive.

Scattering in One dimension

- Let us now consider another scattering problem with the same potential. But now we take a projectile with a large 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

$$\begin{aligned} \psi_L(x) &= Ae^{ik_1 x} + Be^{-ik_1 x} \\ \psi_R(x) &= De^{-ik_2 x}, \end{aligned}$$

where $k_2^2 = 2m(E - V_0)/\hbar^2$.

- There is no $e^{ik_2 x}$ 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.
- My initial condition is that I have a source at $x \to -\infty$ which is shooting a constant stream of particles at the barrier. Hence I must have $\exp(ik_1 x)$ in ψ_L.
- When these particles hit the barrier, they are either reflected back or transmitted. So the barrier acts as a source for $\exp(-ik_1 x)$ in ψ_L and for $\exp(ik_2 x)$ for ψ_R.
- But there is no possible source for $\exp(-ik_2 x)$ for ψ_R.
- We impose the conditions that the wave function and its first derivative should be continuous at $x = 0$ and we get the conditions

$$\begin{aligned} A + B &= D \\ ik_1(A - B) &= ik_2 D. \end{aligned}$$

- We solve these equations to obtain the ratios

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}$$
$$\frac{D}{A} = \frac{2k_1}{k_1 + k_2}$$

- Note that B and the reflection coefficient $R = |B/A|^2 \neq 0$.
- The transmission coefficient T is defined as $(k_2/k_1)|D/A|^2$.
- The additional (k_2/k_1) factor in T arises due to the following reason.
- We assumed that the scattering process is time independent. Which means that the following equation must hold:
- The rate at which incident particles approach the barrier = the rate at which particles are reflected + the rate at which they are transmitted.

Scattering in One dimension

- The rate of approach is the probability of the left moving wave multiplied by its speed $= (\hbar k_1/m)|A|^2$. Similarly, the rate at which they are reflected $= (\hbar k_1/m)|B|^2$ and the rate at which they are transmitted $= (\hbar k_2/m)|D|^2$.
- Conservation of particles equation becomes

$$\frac{\hbar k_1}{m}\left(|A|^2 - |B|^2\right) = \frac{\hbar k_2}{m}|D|^2.$$

Rewriting this equation in terms of the reflection and transmission coefficients, we get

$$R + T = 1.$$