Lecture 8:
Solved problems on the Schrödinger equation

Case 1: Potential barrier of infinite height:

Let us consider a particle of mass m in the one-dimensional potential:

$$\begin{cases} V(x) = 0 \quad 0 < x < a \ II \\ V(x) = \infty \quad x \le 0 \ \ \text{I}, \ x \ge a \ III, \end{cases} \tag{1}$$

The solution in regions I and III is trivially: $\psi = 0$.

In region II, we need to solve the Schrödinger equation for a free particle:

$$\frac{p^2}{2m}\psi_{II} = E\psi_{II} \quad \text{with} \quad p = -i\hbar\frac{\partial}{\partial \text{x}} \tag{2}$$

It is easy to see that the solution of this equation is:

$$\psi_{II} = A\sin(kx+\delta) \qquad , \quad k = \frac{\sqrt{2mE}}{\hbar} \tag{3}$$

where A and δ are complex constants to be defined using the boundary conditions. In order to determine A and δ, we need to make sure that the overall wave function and its first derivative are continuous in the whole region of space. In particular, we need to satisfy the boundary conditions: $\psi_{\text{I}}(0) = \psi_{\text{II}}(0)$, $\psi'_{\text{I}}(0) = \psi'_{\text{II}}(0)$ for the boundary I $\leftrightarrow$ II, and $\psi_{\text{II}}(a) = \psi_{\text{III}}(a)$, $\psi'_{\text{II}}(a) = \psi'_{\text{III}}(a)$ for the boundary II $\leftrightarrow$ III.

At $x = 0$, we obtain:

$$A\sin\delta = 0 \quad \rightarrow \quad \sin\delta = 0 \quad \rightarrow \quad \delta = 0 \tag{4}$$

At $x = a$ we obtain the condition of quantisation:

$$\sin(ka+\delta) = 0 \quad \rightarrow \quad k_n a = n\pi \quad \text{with} \quad n = 0, 1, 2, 3.... \tag{5}$$

This condition implies that the energy levels E_n are:

$$E_n = \frac{k_n^2\hbar^2}{2m} = \frac{\pi^2\hbar^2}{2ma^2}n^2, \tag{6}$$

and the wavefunction is:

$$\psi_n(x) = C\sin\left(\frac{\pi n}{a}x\right), \tag{7}$$

with C being a complex constant (remember that two wavefunctions which differ only by a multiplying constant are physically equivalent). If we want to find the normalised wavefunction, we have to include the condition that the integral of the square of the wavefunction over space must be one. This is physically equivalent to the trivial condition that the particle must be located somewhere in space:

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 \,\mathrm{d}\,x = 1, \tag{8}$$

however $\psi(x) = 0$ for $x < 0$ or $x > a$. The integral is then equivalent to:

$$\int_0^a |\psi(x)|^2 \,\mathrm{d}\,x = 1, \quad \rightarrow \quad C = \sqrt{\frac{2}{a}} \quad \rightarrow \quad \psi(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi n}{a} x\right) \tag{9}$$

Case 2: Tunnel effect through a potential barrier of finite height:

Let us assume a potential well of the form:

$$\begin{cases} V(x) = V_0 & 0 < x < a \ \mathrm{II} \\ V(x) = 0 & x \leq 0 \ \ \mathrm{I},\ x \geq a \ \mathrm{III}, \end{cases} \tag{10}$$

and a particle incident from $x = -\infty$. We would like to calculate the probability of transmission/reflection as a function of E (initial energy of the the particle) and V_0. We will start by considering $E > V_0$. Being the particle initially free, it will arrive as a plane wave ($\psi = e^{ikx}$). Classically, the probability of reflection is zero, being the particle more energetic than the potential barrier. However, the situation is significantly different in Quantum Mechanics. The wavefunctions in the three different regions of space (I, II, and III) will assume the form:

$$\begin{cases} \psi_{\mathrm{I}} = e^{ikx} + Ae^{-ikx} & k = \frac{\sqrt{2mE}}{\hbar} \\ \psi_{\mathrm{II}} = Be^{ik'x} + B'e^{-ik'x} & k' = \frac{\sqrt{2m(E-V_0)}}{\hbar} \\ \psi_{\mathrm{III}} = Ce^{ikx} \end{cases} \tag{11}$$

Again, the wavefunction and its first derivative must be continuous over the entire space and, in particular, across $x = 0$ and $x = a$:

$$\begin{cases} 1 + A = B + B' \\ ik(1 - A) = ik'(B - B') & I \leftrightarrow II \\ Be^{ik'a} + B'e^{-ik'a} = Ce^{ika} \\ ik'(Be^{ik'a} - B'e^{-ik'a}) = ikCe^{ika} & II \leftrightarrow III \end{cases} \tag{12}$$

The probability of transmission T is equal to the square of the ratio between the coefficient for the transmitted wave C and that of the arriving wave (1), whereas the probability of reflection R is equal to the square of the ratio between the coefficient for the reflected wave

A and that of the arriving wave (1):

$$\begin{cases} D = |C|^2 \\ R = |A|^2 \end{cases} \tag{13}$$

By using the boundary conditions, and applying a bit of tedious algebra:

$$\begin{cases} D = \frac{4k^2k'^2}{4k^2k'^2+(k^2-k'^2)^2\sin^2(k'a)} \\ R = \frac{(k^2-k'^2)^2\sin^2(k'a)}{4k^2k'^2+(k^2-k'^2)^2\sin^2(k'a)} \end{cases} \tag{14}$$

Regardless of the particular expression of D and R, it is important to note the following properties:

1 $D + R = 1$, i.e. it is certain that the particle is either transmitted or reflected.

2 $R \neq 0$. Despite the particle's energy be greater than the potential, there is still a non-negligible probability that the particle be reflected, in clear contrast to what predicted by Classical Dynamics.

3 Only for certain values: $\sqrt{2m(E - V_0)}a/\hbar = n\pi$, the probability of transmission is exactly equal to 1.

For the case where the particle's energy is lower than the potential height, we can find the probability of transmission and reflection simply noting that the equations are identical if we perform the transformation: $k' \to i\kappa$, being $\kappa = \frac{\sqrt{2m(V_0-E)}}{\hbar}$.

$$\begin{cases} D = \frac{4k^2\kappa^2}{4k^2\kappa^2+(k^2+\kappa^2)^2\sinh^2(\kappa a)} \\ R = \frac{(k^2+\kappa^2)^2\sinh^2(\kappa a)}{4k^2\kappa^2+(k^2+\kappa^2)^2\sinh^2(\kappa a)} \end{cases} \tag{15}$$

In this case, we note that:

1 again $D + R = 1$, i.e. it is certain that the particle is either transmitted or reflected.

2 $D \neq 0$. Despite the particle's energy be smaller than the potential, there is still a non-negligible probability that the particle be transmitted, in clear contrast to what predicted by Classical Dynamics.

3 Even in the case of an arbitrarily large potential barrier ($V_0 \to \infty$ and $a \to \infty$), the probability of transmission is not zero, even though exponentially small:

$$D \simeq e^{-2\sqrt{2m(V_0-E)}a/\hbar} \tag{16}$$