

Lecture 5

Potentials

5.1 Potentials

In this lecture we will solve Schrödinger's equation for some simple one-dimensional potentials, and discuss the physical interpretation of the results.

The Schrödinger equation for these problems is:

$$i\hbar \frac{\partial}{\partial t} \Psi(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi(x, t) + V(x) \Psi(x, t). \quad (5.1)$$

Thus the time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi(x) + V(x) \psi(x) = E \psi(x). \quad (5.2)$$

This is a second order differential equation for the function ψ , which has two linearly independent solutions. Remember that ψ must be single-valued and continuous, and its first derivative with respect to x must also be continuous if the potential is not singular - see Sect. 3.2.3.

5.1.1 Potential step

The simplest case we can think of is a *potential step*:

$$V(x) = \begin{cases} 0, & \text{for } x < 0, \\ V > 0, & \text{for } x > 0, \end{cases} \quad (5.3)$$

as shown in Fig. 5.1.

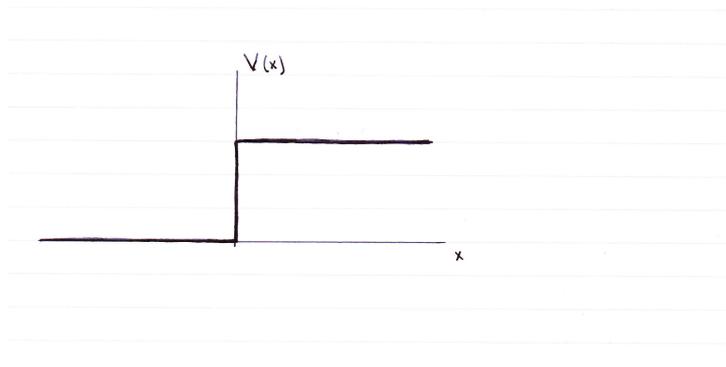


Figure 5.1: Potential step.

Note that the energy eigenvalues are always larger than the minimum of the potential, and hence in this case $E > 0$. There are two distinct cases that need to be analyzed.

Case 1. We shall start from the case where the total energy E is greater than V . We can then rewrite Eq. (5.2) as:

$$\begin{cases} \psi'' = -(p/\hbar)^2\psi(x), & \text{for } x < 0, \\ \psi'' = -(\bar{p}/\hbar)^2\psi(x), & \text{for } x > 0, \end{cases} \quad (5.4)$$

where we have introduced the real numbers:

$$p = \sqrt{2mE}, \quad \bar{p} = \sqrt{2m(E - V)}, \quad (5.5)$$

and the double prime symbol denotes two derivatives with respect to the position x .

In classical mechanics when a particle moving from left to right arrives at $x = 0$ potential energy increases. In order for energy to be conserved, the kinetic energy of the particle has to decrease, i.e. the particle continues to move to the right, at a smaller velocity. The classical momenta of the particle to the left and to the right of the well are given respectively by p and \bar{p} . There is clearly no reflection when $E > V$ in classical mechanics.

The solutions of the eigenvalue equation for the energy in the quantum system are :

$$\psi(x) = \begin{cases} Ae^{ipx/\hbar} + Be^{-ipx/\hbar}, & \text{for } x < 0, \\ Ce^{i\bar{p}x/\hbar} + De^{-i\bar{p}x/\hbar}, & \text{for } x > 0. \end{cases} \quad (5.6)$$

They represent a superposition of plane waves travelling to the right and to the left.

We want to consider the case of an incident particle from the left that hits the barrier. Hence for $x > 0$ we do not expect to have a wave travelling to the left, and we can set $D = 0$.

We are now left with three unknown coefficients in Eq. (5.6), namely A, B , and C . One of them determines the overall normalization of the wave function, while the other two can be determined imposing the continuity of the wave function and its derivative at the origin:

$$\lim_{x \rightarrow 0^-} \psi(x) = \lim_{x \rightarrow 0^+} \psi(x), \quad (5.7)$$

$$\lim_{x \rightarrow 0^-} \psi'(x) = \lim_{x \rightarrow 0^+} \psi'(x). \quad (5.8)$$

You can readily check that:

$$\text{Eq. (5.7)} \Rightarrow A + B = C \quad (5.9)$$

$$\text{Eq. (5.8)} \Rightarrow p(A - B) = \bar{p}C. \quad (5.10)$$

The system can be easily solved:

$$B = \frac{p - \bar{p}}{p + \bar{p}}A, \quad (5.11)$$

$$C = \frac{2p}{p + \bar{p}}A. \quad (5.12)$$

Let us now discuss the physical content of this solution. To the right of the step, $x > 0$, we have a wave propagating to the right. C is the relative amplitude for the particle to be in the transmitted wave. To the left of the step, $x < 0$, we find a superposition of the incident wave and a *reflected* wave. The relative amplitudes for the particle to be in each of these states are respectively A and B . We have found a phenomenon that has no classical analogue: there is a possibility for the particle to be reflected by the potential step even if its energy is greater than the height of the barrier!!

Case 2. Let us now discuss the case where $E < V$. In classical mechanics this situation corresponds to an incident particle that does not have enough kinetic energy to get past the potential barrier, and therefore is reflected at $x = 0$. Formally the eigenvalue equations are the same as Eq. (5.4), but now \bar{p} is a purely imaginary number. In order to have a probability density that is bounded for $x > 0$, we need to choose the solution that yields a decreasing exponential:

$$\bar{p} = i\sqrt{2m(V - E)} \equiv i\tilde{p}, \quad (5.13)$$

$$\psi(x) = Ce^{-\tilde{p}x/\hbar}. \quad (5.14)$$

Note that in this case:

$$B = \frac{p - i\tilde{p}}{p + i\tilde{p}}A, \quad (5.15)$$

and therefore $|A|^2 = |B|^2$. The magnitudes of the incident and the reflected waves are the same. The two amplitudes are related by a simple phase shift:

$$\frac{p - i\tilde{p}}{p + i\tilde{p}} = -e^{2i\delta(E)}. \quad (5.16)$$

The phase shift can be expressed as a function of p and \tilde{p} :

$$\tilde{p} = p \cot \delta, \quad (5.17)$$

which shows that $\delta \rightarrow 0$ as $E \rightarrow 0$.

It is crucial to remark here that there is a non-vanishing probability to find the particle in the classically forbidden region $x > 0$. However this probability decays exponentially as x is increased. The typical range in which we can expect to find the particle is of the order of \hbar/p .

In the region where $E > V(x)$, the wave function has an oscillatory behaviour. On the other hand, in the classically forbidden region the amplitude of the wave function falls off exponentially.

5.1.2 Tunneling

We have seen in the previous Section that a quantum particle can access regions that are classically forbidden. This fact leads to a very important phenomenon called *tunneling*, which is characteristic of quantum mechanics.

A step potential of height V and size a as shown in Fig. 5.2 yields a simple example of tunneling that we can solve analytically.

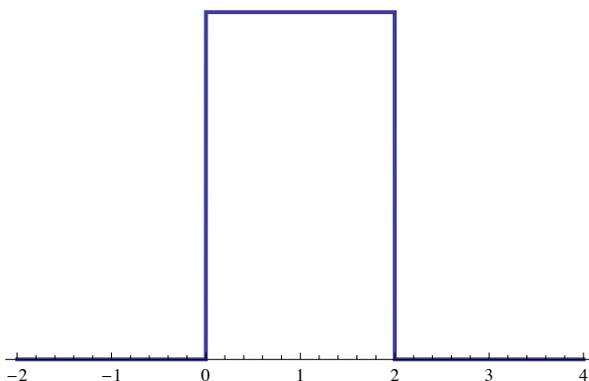


Figure 5.2: Potential step of height V and size a ($a = 2$ in this example) that allows the system to tunnel from one side to the other.

We are looking for solutions that would not penetrate the barrier classically, hence $0 < E < V$. In this case, following the method used in the previous Section, we can write the most general function for the wave function representing a wave incident from the left:

$$\psi(x) = \begin{cases} Ae^{ipx/\hbar} + Be^{-ipx/\hbar}, & \text{for } x < 0, \\ Ce^{-\tilde{p}x/\hbar} + De^{\tilde{p}x/\hbar}, & \text{for } 0 < x < a, \\ AS(E)e^{ip(x-a)/\hbar}, & \text{for } x > a. \end{cases} \quad (5.18)$$

Note that in this case we can keep the exponentially growing solution in the interval $0 < x < a$. Since this interval is finite, the wave function remains bounded. The fact that we have an incident wave from the left is encoded in the fact that there is no left-propagating wave for $x > a$, i.e. no term of the form $e^{-ipx/\hbar}$.

In this case we have a system with 5 unknown variables A , B , C , D , and $S(E)$. We have to impose the continuity equations at $x = 0$, and $x = a$. The latter are four equations, which enable us to determine the unknown coefficients up to an overall normalization. In particular here we are interested in computing the transition amplitude $S(E)$, i.e. the ratio of the probability amplitude for the outgoing wave at $x > a$ to the probability amplitude for

the incoming wave at $x < 0$. The computation is not difficult, but rather lengthy, and will be discussed in problem sheet 3.

The solution for the transmission amplitude is:

$$S(E) = \frac{2ip\tilde{p}}{(p^2 - \tilde{p}^2) \sinh(\frac{\tilde{p}a}{\hbar}) + 2ip\tilde{p} \cosh(\frac{\tilde{p}a}{\hbar})}. \quad (5.19)$$

The transmissivity T is defined as the probability for the particle to tunnel through the barrier:

$$T = |S(E)|^2 = \left[1 + \frac{\sinh^2(\tilde{p}a/\hbar)}{4(E/V)(1 - E/V)} \right]^{-1}. \quad (5.20)$$

This is a monotonically increasing function of E , as long as $E < V$. On the other hand, if the energy of the state is fixed, we see from Eq. (5.20) that T decreases exponentially with the size of the barrier a :

$$T \propto \exp \left[-2\sqrt{2m(V - E)}a/\hbar \right]. \quad (5.21)$$

Tunneling is a phenomenon that has no classical analogue. Its experimental observation is one of the many strong confirmations that the quantum-mechanical framework yields correct predictions. Tunneling has numerous applications in physics at the atomic and subatomic scale.

1. The α decay of nuclei can be modeled as a tunneling process. The α particle inside the nucleus can be described as quantum mechanical system with the potential depicted in Fig. 5.3. A particle with energy E would be confined inside the nucleus - i.e. inside the dip in the potential - according to classical mechanics. However, in quantum mechanics, the particle has a finite probability of tunneling to the right.

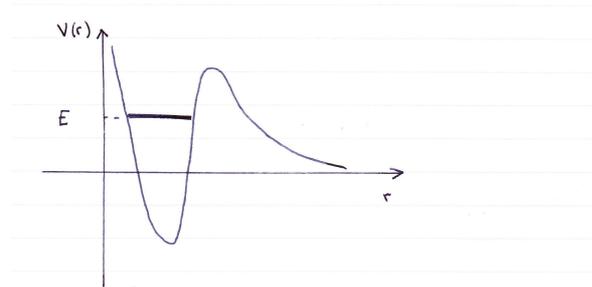


Figure 5.3: Potential felt by an α particle in the nucleus.

2. In solid state physics, if we separate two metals with a thin insulator layer, and apply a voltage across the metals, then the insulator will act as a potential barrier. Any

current observed in such an experiment is due to the tunneling of the electrons across the potential barrier.

3. The scanning tunneling microscope (STM) allows individual atoms at the surface of a metal to be imaged. The layer of air between the surface of the metal and the STM's needle can be seen as a potential barrier that the electrons need to tunnel through. Since the tunneling probability depends exponentially on the distance between the STM's needle and the surface, one can determine such distance very precisely by measuring the current of electrons that are actually tunneling.

5.2 Summary

As usual, we summarize the main concepts introduced in this lecture.

- Solution of the Schrödinger equation for simple potentials.
- Potential step and continuity equations.
- Reflected and transmitted waves.
- Tunneling.
- Experimental observation of tunneling phenomena.

