14 Step potential and quantum tunneling

"Scientific knowledge is a body of statements of varying degrees of certainty – some most unsure, some nearly sure, none absolutely certain." $\sim$ *Richard Feynman*

14.1 Step potential

The next system that we discuss quantum mechanically is the step potential, that is the potential energy of a particle is constant but at some point abruptly changes to another value. Our final goal will be to calculate with what probability the particle will be reflected by that step and with what probability it will pass. The step potential is an idealization, in reality the potential energy always changes smoothly, but we discuss the simplified version in order to be able to find a solution.

The potential energy of the particle is given by

$$U(x) = \begin{cases} 0, & \text{if } x < 0 \\ U_0, & \text{if } x \geq 0 \end{cases} \tag{14.1}$$

and is depicted in fig. 13.

A particle is coming from the left and encounters the step. We will assume that the particle has energy $E > U_0$, and that the energy is exact, i.e. the particle is in an eigenstate of the energy operator. This means that the wavefunction describing the particle has to satisfy the time-independent Schrödinger equation. We will solve the equation in the two regions (left of the step, right of the step) separately, then will combine the solutions. Let us first discuss the case $x < 0$. The Schrödinger equation takes the form

$$-\frac{\hbar^2}{2m}\psi''(x) = E\psi(x)$$
$$\psi''(x) + k_1^2\psi(x) = 0$$

where

$$k_1 = \frac{\sqrt{2mE}}{\hbar} \tag{14.2}$$

The general solution of this equation is

$$\psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \tag{14.3}$$

where A and B are constants.

Since we are interested in the motion of particle, let us look at the full time-dependent wavefunction. As we saw in the previous lecture, if we have an energy eigenstate, to get the full time-dependent solution we just need to multiply it by $e^{-\frac{iEt}{\hbar}}$, see equation (12.14). Denoting

$$\omega_1 = \frac{E}{\hbar}$$

in agreement with de Broglie frequency, we get

$$\Psi_1(x,t) = Ae^{ik_1x - i\omega_1 t} + Be^{-ik_1x - i\omega_1 t}$$

This is simply a sum of two waves, the first one moving to the right, the second one moving to the left[23]. Since we have a particle coming in from the left, the first term represents the incoming wave, the second term - the reflected wave.

[23] Remember that $e^{i\alpha} = \cos\alpha + i\sin\alpha$, so each of the exponents is nothing but a sine wave.

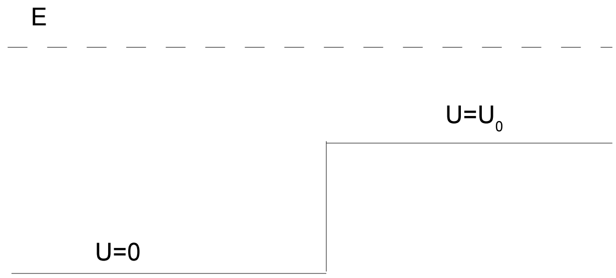

Figure 13: The step potential.

Let us now solve the Schrödinger equation to the right of the wall. It takes the form

$$-\frac{\hbar^2}{2m}\psi''(x) + U_0\psi(x) = E\psi(x)$$
$$\psi''(x) + k_2^2\psi(x) = 0$$

where

$$k_2 = \frac{\sqrt{2m(E-U_0)}}{\hbar}$$

The solution is

$$\psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \tag{14.4}$$

If we again consider time-dependence, we can see that the first term in (14.4) is a wave moving to the right, while the second term is a wave moving to the left. The first term has to represent the transmitted wave, and the second term has to be 0 since there is no particle coming towards the step from the right. Next, we need to make sure that the wavefunction is continuous, and so is its derivative (the potential energy is not infinite anywhere, so the derivative of the wavefunction has to be continuous as well). Since we get two different solutions on two sides of point 0, which are both continuous by themselves, all we need to worry about is the continuity at point 0. The continuity of wavefunction gives

$$\psi_1(0) = \psi_2(0)$$
$$A + B = C \tag{14.5}$$

The continuity of the derivative of the wavefunction gives

$$\psi_1'(0) = \psi_2'(0)$$
$$ik_1A - ik_1B = ik_2C \tag{14.6}$$

Equations (14.5) and (14.6) can be used to express B and C in terms of A. Plugging (14.5) in (14.6) we get

$$k_1A - k_1B = k_2(A+B)$$
$$B = \frac{k_1-k_2}{k_1+k_2}A \tag{14.7}$$

From (14.5)

$$C = \frac{2k_2}{k_1 + k_2} A \tag{14.8}$$

We can now find the probability R of the particle being reflected back, and the probability T of the particle being transmitted. R is just the ratio of the probability of getting the reflected wave (second term in (14.3)) to the probability of the incoming wave (first term in (14.3)). To get the probabilities we need to take the absolute value of the wavefunction squared, then integrate. The absolute value of the reflected wave squared gives $|B|^2$, while for the incoming wave we have $|A|^2$, so we do not really need to worry about integrating (see below about some problems with the integrals), we can just divide these numbers

$$R = \frac{|B|^2}{|A|^2}$$

Using (14.7) we get

$$R = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2} \tag{14.9}$$

To find the transmission coefficient directly is slightly more tricky since the transmitted wave and reflected wave have different wavelengths[24], but we know that the particle is either reflected or transmitted with total probability 1, so the transmission and reflection probabilities should add to 1

$$T + R = 1 \tag{14.10}$$

$$T = 1 - R \tag{14.11}$$

R and T are also called the *reflection coefficient* and the *transmission coefficient* respectively.

Problem 48 1000 *electrons* ($m_e = 0.511 MeV/c^2$) *with energy* $10eV$ *are incident on a step potential of height* $7eV$. *How many electrons are transmitted and how many are reflected back?*

The wavefunction in the whole space can be written as

$$\psi(x) = \begin{cases} Ae^{ik_1x} + Be^{-ik_1x}, & \text{if } x < 0 \\ Ce^{ik_2x}, & \text{if } x \geq 0 \end{cases} \tag{14.12}$$

Although we expressed B and C in terms of A, we did not find A (we did not really need that to calculate the reflection and transmission coefficients). A should be found from the normalization condition, however the wavefunction (14.12) cannot be normalized, the integral is infinite. The reason why this happens is because in an infinite space the particle cannot have exact energy, since that implies exact momentum, which means that the uncertainty in position is infinite! So we cheated a little bit by considering an idealization. The proper way to solve this problem would be to consider an incoming wave packet of finite spatial extent and solve the full time-dependent Schrödinger equation for it. However, our idealization does give the transmission and reflection coefficients correctly, so we are fine as long as we do not worry about overall normalization.

[24] That means that we cannot divide the constants in front of the wavefunctions directly, they will get modified when integrated.

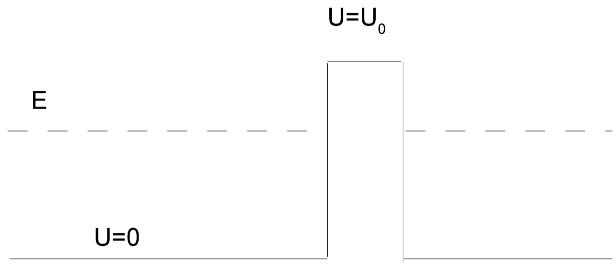

Figure 14: Potential barrier.

14.2 Quantum tunneling

Let us now assume that $E < U_0$, i.e. the energy of the particle is not enough to pass to the right of the step. The Schrödinger equation to the right of the step now takes the form

$$-\frac{\hbar^2}{2m}\psi''(x) + U_0\psi(x) = E\psi(x)$$
$$\psi''(x) - \alpha_2^2\psi(x) = 0$$

where

$$\alpha = \frac{\sqrt{2m(U_0 - E)}}{\hbar} \tag{14.13}$$

The solution is

$$\psi(x) = Ae^{-\alpha x} + Be^{\alpha x} \tag{14.14}$$

The second term increases to infinity as $x \to \infty$, but we know that the wavefunction has to decrease to 0. This means that B has to be set to 0. Then the wavefuncion becomes

$$\psi(x) \propto e^{-\alpha x} \tag{14.15}$$

which exponentially decreases to 0. So if we go far enough right of the step the probability of finding the particle there becomes essentially 0, the particle has to be reflected back with probability 1. But what if we have a potential barrier instead of a step? A barrier means some finite region where the potential energy is bigger than the total energy of the particle, as depicted in fig. 14. Let us assume a particle is coming from the left. As soon as it hits the barrier the wavefunction will start decreasing exponentially as given by (14.15), but it will not decrease completely to 0 since the barrier has finite length. Assuming the length of the barrier is l, on the other side of the barrier the wavefunction will have decreased by about $e^{-\alpha l}$. The probability of finding the particle on the other side of the barrier will have decreased by

$$T \sim e^{-2\alpha l} \tag{14.16}$$

since the probability distribution is the square of the absolute value of the wavefunction. We can see that the particle can be found on the other side of the barrier with finite probability! This phenomenon is called *tunneling* and is only possible in quantum mechanics. Classically, the particle can never go to regions where its total energy is less than the potential energy, so the particle can never climb up the barrier, therefore it can never go to the other side. Tunneling is made possible

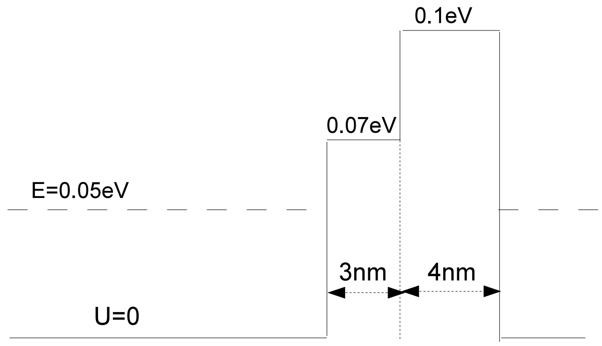

Figure 15: Problem 49.

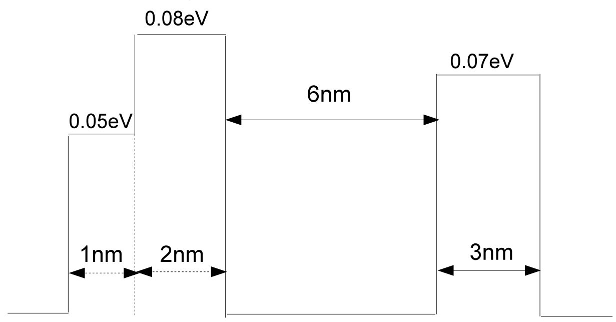

Figure 16: Problem 50.

in quantum mechanics because of the fact that the position of the particle is not precise, it can be at different places at the same time with different probabilities!

T in (14.16) is called the *transmission coefficient* or the *tunneling coefficient*. Note that (14.16) is only an estimate because we did not worry about the constants in front of the exponents. It is still a good estimate because the exponential decay is the most important part in that coefficient. To find the transmission coefficient exactly we would need to solve the Schrödinger equation in all three regions (left side of the barrier, the barrier, right side of the barrier), impose the continuity conditions on the wavefunction and relate the constants in front of the exponents to each other, just like we did for the step potential. However, the algebra becomes tedious without telling much new about the physics, so we will restrict ourselves to the estimate (14.16).

We found the transmission coefficient in the simplest case of a rectangular barrier. If the barrier has a more complex shape, we can always divide it into a bunch of small barriers, find the transmission coefficient through each one of the barriers, then multiply them together (the probability of passing through multiple barriers is equal to the product of probabilities of passing through each barrier)

$$T = T_1 \cdot T_2 \cdot T_3 \cdot ... \cdot T_n \tag{14.17}$$

Problem 49 *An electron ($m_e = 0.511MeV/c^2$) with energy $0.05eV$ is incident on a barrier which consists of two rectangular portions. The first portion has height $0.07eV$ and length $3nm$, the second portion has height $0.1eV$ and length $4nm$, see fig. 15. Estimate the transmission coefficient.*

Problem 50 *An electron ($m_e = 0.511MeV/c^2$) is stuck between two barriers, as depicted in fig. 16. The first barrier consists of two rectangular portions - $0.05eV$ by $1nm$ and $0.08eV$ by $2nm$. The second barrier is rectangular, $0.07eV$ by $3nm$. The distance between the barriers is $6nm$. We*

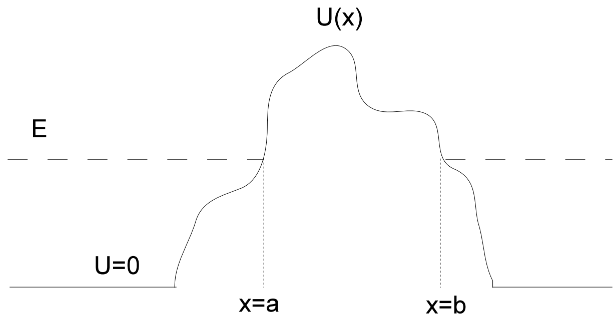

Figure 17: Potential barrier of arbitrary shape $U(x)$.

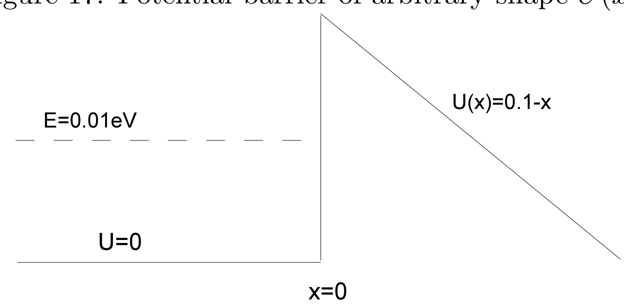

Figure 18: Problem 51. $U(x)$ is in eV, x is in nm.

will treat that region as an infinite square well and assume that the electron is in the ground state. Find the energy of the electron. Estimate the tunneling coefficients through both barriers. Is it more probable that the electron will tunnel to the left or to the right?

If the barrier has some arbitrary shape $U(x)$, the transmission coefficient takes the form

$$T \sim e^{-\frac{2\sqrt{2m}}{\hbar}\int_a^b \sqrt{U(x)-E}dx} \tag{14.18}$$

where a indicates the beginning of the barrier, b is the end of the barrier, see fig. 17. These points are determined by the condition

$$U(a) = U(b) = E \tag{14.19}$$

Problem 51 100 *electrons* ($m_e = 0.511MeV/c^2$) *with energy* $0.01eV$ *are incident on a potential barrier that has the shape depicted in fig. 18. The potential energy is given by*

$$U(x) = \begin{cases} 0, & \textit{if } x < 0 \\ 0.1 - x, & \textit{if } x \geq 0 \end{cases}$$

where $U(x)$ *is measured in* eV, x *is measured in* nm. *Estimate the number of transmitted electrons.*

Lots of physical phenomena (one example is radioactive decay) involve quantum tunneling. The nuclear reactions that are responsible for the radiation of the sun happen thanks to tunneling!