Zero of energy is arbitrary

The normal definition of a potential energy is somewhat arbitrary. Consider where a potential comes from: It appears when the total energy (potential plus kinetic) is constant. But if something is constant, we can add a number to it, and it is still constant! Thus whether we define the gravitational potential at the surface of the earth to be 0 or 100 J does not matter.

Only differences in potential energies play a rôle. It is customary to define the potential ``far away", as $|x| \to \infty$ to be zero. That is a very workable definition, except in one case: if we take a square well and make it deeper and deeper, the energy of the lowest state decreases with the bottom of the well. As the well depth goes to infinity, the energy of the lowest bound state reaches $-\infty$, and so does the second, third etc. state. It makes much more physical sense to define the bottom of the well to have zero energy, and the potential outside to have value V_0, which goes to infinity.

Solution

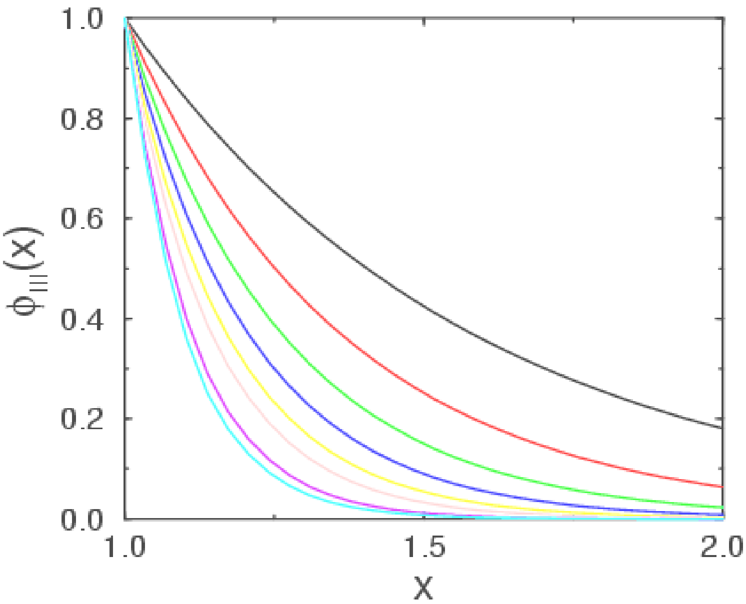

Figure 3.1: The change in the wave function in region III, for the lowest state, as we increase the depth of the potential well. We have used $a = 10^{-10} m$, and $k_0 a = 2,3,4,5,6,7,8,9$ and 10.

As stated before the continuity arguments for the derivative of the wave function do not apply for an infinite jump in the potential energy. This is easy to understand as we look at the behaviour of a low energy solution in one of the two outside regions (I or III). In this case the wave function can be approximated as

$$e^{\pm kr}, \quad k = \sqrt{\frac{2m}{\hbar^2} V_0}, \tag{3.1}$$

which decreases to zero faster and faster as V_0 becomes larger and larger. In the end the wave function can no longer penetrate the region of infinite potential energy. Continuity of the wave function now implies that $\varphi(a)=\varphi(-a)=0$. Defining

$$\kappa = sqrt \frac{2m}{\hbar^2} E, \tag{3.2}$$

we find that there are two types of solutions that satisfy the boundary condition:

$$\phi_{2n+1}(x) = \cos(\kappa_{2n+1} x), \phi_{2n}(x) = \sin(\kappa_{2n} x). \tag{3.3}$$

Here

$$\kappa_l = \frac{\pi l}{2a}. \tag{3.4}$$

We thus have a series of eigen states $\phi_l(x), \quad l = 0,1,2,\ldots$. The energies are

$$E_l = \frac{\hbar^2 \pi^2 l^2}{8a^2}. \tag{3.5}$$

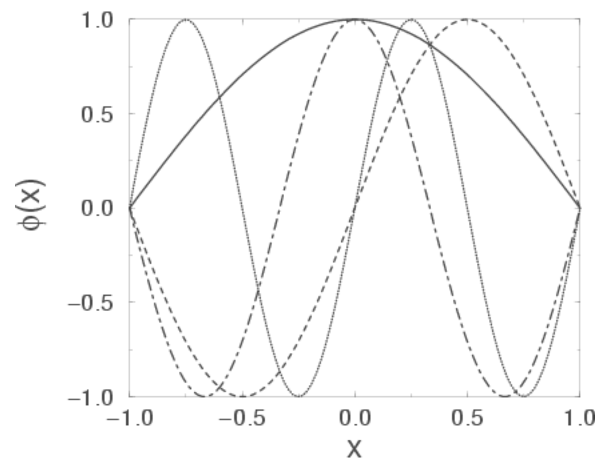

Figure 3.2: A few wave functions of the infinite square well.

These wave functions are very good to illustrate the idea of normalization. Let me look at the normalization of the ground state (the lowest state), which is

$$\phi_0(x) = A_1 \cos\left(\frac{\pi x}{2a}\right) \tag{3.6}$$

For $-a < x < a$, and 0 elsewhere.

We need to require

$$\int_{-\infty}^{\infty} |\phi_0(x)|^2 dx = 1, \tag{3.7}$$

where we need to consider the absolute value since $\phi(x)$ can be complex. We only have to integrate from $-a$ to a, since the rest of the integral is zero, and we have

$$\begin{aligned}
\int_{-\infty}^{\infty} |\phi_0(x)|^2 dx &= |A|^2 \int_{-a}^{a} \cos^2\left(\frac{\pi x}{2a}\right) dx = \\
= \quad |A|^2 \frac{2a}{\pi} \int_{-\pi/2}^{\pi/2} \cos^2(y)\, dy \quad &= \quad |A|^2 \frac{2a}{\pi} \int_{-\pi/2}^{\pi/2} \tfrac{1}{2}(1+\cos(2y))dy \quad = \\
= \quad |A|^2 \frac{2a}{\pi} \pi.
\end{aligned} \tag{3.8}$$

Here we have changed variables from x to $y = \pi x / 2a$. We thus conclude that the choice

$$A = \sqrt{\frac{1}{2a}} \tag{3.9}$$

leads to a normalized wave function.

Non-normalisable wave functions

I have argued that solutions to the time-independent Schrödinger equation must be normalised, in order to have a the total probability for finding a particle of one. This makes sense if we think about describing a single Hydrogen atom, where only a single electron can be found. But if we use an accelerator to send a beam of electrons at a metal surface, this is no longer a requirement: What we wish to describe is the flux of electrons, the number of electrons coming through a given volume element in a given time.

Let me first consider solutions to the ``free'' Schrödinger equation, i.e., without potential, as discussed before. They take the form

$$\phi(x) = Ae^{ikx} + Be^{-ikx}. \tag{3.10}$$

Let us investigate the two functions. Remembering that $p = \frac{\hbar}{i}\frac{\partial}{\partial x}$ we find that this represents the sum of two states, one with momentum $\hbar k$, and the other with momentum $-\hbar k$. The first one describes a beam of particles going to the right, and the other term a beam of particles traveling to the left.

Let me concentrate on the first term, that describes a beam of particles going to the right. We need to define a probability current density. Since current is the number of particles times their velocity, a sensible definition is the probability density times the velocity,

$$|\phi(x)|^2 \frac{\hbar k}{m} = |A|^2 \frac{\hbar k}{m}. \tag{3.11}$$

This concept only makes sense for states that are not bound, and thus behave totally different from those we discussed previously.

Potential step

Consider a potential step $$V(x) = \begin{cases} V_0 & x < 0 \\ V_1 & x > 0 \end{cases} \tag{3.12}$$

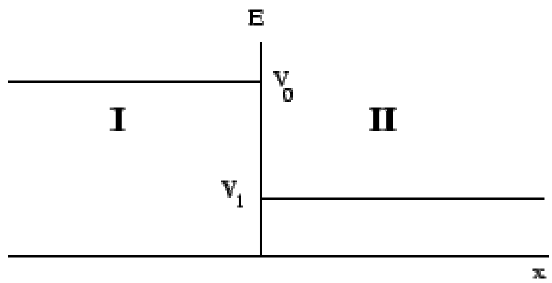

Figure 3.3 : The step potential

Let me define

$$k_0 = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} \qquad \text{and} \qquad k_1 = \sqrt{\frac{2m}{\hbar^2}(E - V_1)}$$

We assume a beam of particles comes in from the left,

$$\phi(x) = A_0 e^{ik_0 x}, \quad x < 0. \tag{3.13}$$

At the potential step the particles either get reflected back to region I, or are transmitted to region II. There can thus only be a wave moving to the right in region II, but in region I we have both the incoming and a reflected wave,

$$\phi_I(x) = A_0 e^{ik_0 x} + B_0 e^{-ik_0 x}, \tag{3.14}$$

$$\phi_{II}(x) = A_1 e^{ik_1 x}. \tag{3.15}$$

We define a transmission and reflection coefficient as the ratio of currents between reflected or transmitted wave and the incoming wave, where we have canceled a common factor

$$R = \frac{|B_0|^2}{|A_0|^2} \quad T = \frac{k_1 |A_1|^2}{k_0 |A_0|^2}. \tag{3.16}$$

Even though we have given up normalisability, we still have the two continuity conditions. At $x = 0$ these imply, using continuity of $\phi(x)$ and $\frac{d\phi(x)}{dx}$,

$$A_0 + B_0 = A_1 \ , \quad \text{and} \quad ik_0(A_0 - B_0) = ik_1 A_1 \tag{3.17}$$

We thus find

$$A_1 = \frac{2k_0}{k_0 + k_1} A_0 \tag{3.18}$$

$$B_0 = \frac{k_0 - k_1}{k_0 + k_1} A_0 \tag{3.19}$$

and the reflection and transmission coefficients can thus be expressed as

$$R = \left(\frac{k_0 - k_1}{k_0 + k_1} \right)^2 \tag{3.20}$$

$$T = \frac{4 k_0 k_1}{(k_0 + k_1)^2} \tag{3.21}$$

Notice that $R + T = 1$!

In Fig. 3.3 we have plotted the behaviour of the transmission and reflection of a beam of Hydrogen atoms impinging on a barrier of height 2 meV.

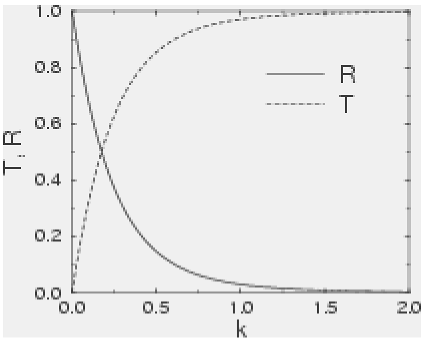

Figure 3.4: The transmission and reflection coefficients for a square barrier.

Square barrier

A slightly more involved example is the square potential barrier, an inverted square well, see Fig. 3.4

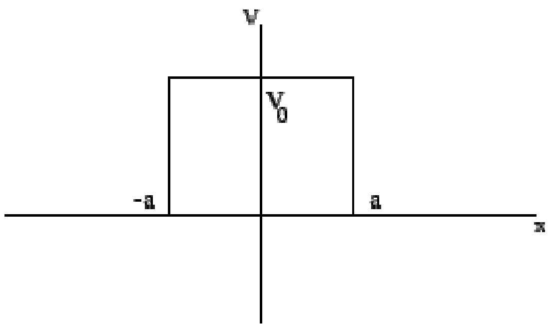

Figure 3.5: The square barrier.

We are interested in the case that the energy is below the barrier height, $0 < E < V_0$. If we once again assume an incoming beam of particles from the right, it is clear that the solutions in the three regions are

$$\phi_I(x) = A_1 e^{ikx} + B_1 e^{-ikx}, \tag{3.22}$$

$$\phi_{II}(x) = A_2 \cosh(\kappa x) + B_2 \sinh(\kappa x), \tag{3.23}$$

$$\phi_{III}(x) = A_3 e^{ikx}. \tag{3.24}$$

Here

$$k = \sqrt{\frac{2m}{\hbar^2} E}, \quad \kappa = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)}. \tag{3.25}$$

Matching at $x = -a$ and $x = a$ gives (use $\sinh(-x) = -\sinh(x)$ and $\cosh(-x) = \cosh(x)$)

$$A_1 e^{-ika} + B_1 e^{ika} = A_2 \cosh(\kappa a) - B_2 \sinh(\kappa a) \tag{3.26}$$

$$ik(A_1 e^{-ika} - B_1 e^{ika}) = \kappa(-A_2 \sinh(\kappa a) + B_2 \cosh(\kappa a)) \tag{3.27}$$

$$A_3 e^{ika} = A_2 \cosh(\kappa a) + B_2 \sinh(\kappa a) \tag{3.28}$$

$$ikA_3 e^{ika} = \kappa(A_2 \sinh(\kappa a) + B_2 \cosh(\kappa a)) \tag{3.29}$$

These are four equations with five unknowns. We can thus express for of the unknown quantities in one other. Let us choose that one to be A_1, since that describes the intensity of the incoming beam.

We are not interested in A_2 and B_2, which describe the wave function in the middle. We can combine the equation above so that they either have A_2 or B_2 on the right hand side, which allows us to eliminate these two variables, leading to two equations with the three interesting unknowns A_3, B_1 and A_1. These can then be solved for A_3 and B_1 in terms of A_1:

The way we proceed is to add eqs. (3.26) and (3.28), subtract eqs. (3.27) from (3.29), subtract (3.28) from (3.26), and add (3.27) and (3.29).

We find

$$A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika} = 2A_2 \cosh(\kappa a) \tag{3.30}$$

$$ik(-A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika}) = 2\kappa\, A_2 \sinh(\kappa a) \tag{3.31}$$

$$A_1 e^{-ika} + B_1 e^{ika} - A_3 e^{ika} = -2B_2 \sinh(\kappa a) \tag{3.32}$$

$$ik(A_1 e^{-ika} - B_1 e^{ika} + A_3 e^{ika}) = 2\kappa\, B_2 \cosh(\kappa a) \tag{3.33}$$

We now take the ratio of equations (3.30) and (3.31) and of (3.32) and (3.33), and find (i.e., we take ratios of left- and right hand sides, and equate those)

$$\frac{A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika}}{ik(-A_1 e^{-ika} + B_1 e^{ika} + A_3 e^{ika})} = \frac{1}{\kappa \tanh(\kappa a)} \tag{3.34}$$

$$\frac{A_1 e^{-ika} + B_1 e^{ika} - A_3 e^{ika}}{ik(A_1 e^{-ika} - B_1 e^{ika} + A_3 e^{ika})} = -\frac{\tanh(\kappa a)}{\kappa} \tag{3.35}$$

These equations can be rewritten as (multiplying out the denominators, and collecting terms with A_1, B_1 and A_3),

$$A_1\left(1+\frac{ik}{\kappa \tanh(\kappa a)}\right)e^{-2ika} + B_1\left(1-\frac{ik}{\kappa \tanh(\kappa a)}\right) + A_3\left(1-\frac{ik}{\kappa \tanh(\kappa a)}\right) = 0 \tag{3.36}$$

$$A_1\left(1-\frac{ik \tanh(\kappa a)}{\kappa}\right)e^{-2ika} + B_1\left(1+\frac{ik \tanh(\kappa a)}{\kappa}\right) + A_3\left(-1+\frac{ik \tanh(\kappa a)}{\kappa}\right) = 0 \tag{3.37}$$

Now eliminate A_3 and find

$$\begin{aligned} &A_1 e^{-ika}[(\kappa - ik\tanh\kappa a)(\kappa\tanh\kappa a + ik) + (\kappa\tanh\kappa a - ik)(\kappa - ik\tanh\kappa a)] + \\ &+ B_1 e^{ika}[(\kappa - ik\tanh\kappa a)(\kappa\tanh\kappa a - ik) + (\kappa\tanh\kappa a - ik)(\kappa + ik\tanh\kappa a)] = 0 \end{aligned} \tag{3.38}$$

Thus we find

$$B_1 = -A_1 e^{-2ika} \frac{(\kappa^2 + k^2)^* \tanh \kappa a}{(\kappa \tanh \kappa a - ik)(\kappa - ik \tanh \kappa a)} \tag{3.39}$$

and we find, after using some of the angle-doubling formulas for hyperbolic functions, that the absolute value squared, i.e., the reflection coefficient, is

$$R = \frac{(\kappa^2 + k^2)^2 \sinh^2 2\kappa a}{4\kappa^2 k^2 + (\kappa^2 - k^2)^2 \sinh^2 2\kappa a} \quad ((3.40)$$

In a similar way we can express A_3 in terms of A_1, or use $T = 1 - R$!

Alternative approach. The equation can be given in matrix form !

Can you invert the right matrices and find the same answer?

We now consider a particle of the mass of a hydrogen atom, m=1.67*$10^{-27} kg$, and use a barrier of height $4meV$ and of width 10^{-10} m. The picture for reflection and transmission coefficients can seen in Fig. 6.4a. We have also evaluated R and T for energies larger than the height of the barrier (the evaluation is straightforward).

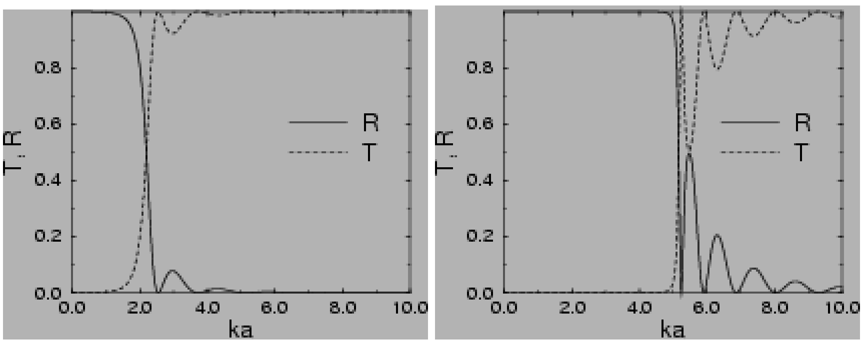

Figure 3.6: The reflection and transmission coefficients for a square barrier of height 4 meV (left) amd 50 meV (right) and width 10^{-10} m.

If we heighten the barrier to 50 meV, we find a slightly different picture, see Fig. 3.6 b.

Notice the oscillations (resonances) in the reflection. These are related to an integer number of oscillations fitting exactly in the width of the barrier, $\sin 2\kappa a = 0$.