Potential Wells and Barriers

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Abstract

In this write-up, we'll consider and analyse different situations of potential wells and barrier. The analysis aims to apply Schrodinger's wave equation in various situations and analyse the resultant equations with justified boundary conditions. We would be taking up three introductory, yet non-trivial situations for the analysis in this write-up. These should demonstrate the application of Schrodinger's wave equation in analysing potential wells and barriers.

1 Introduction

Before we begin our analysis, it's important to lay down what are we trying to analyse and why is it relevant. Firstly, the definition of the most relevant terms that we shall use are as follows:

Definition 1.1. *A potential well is a region surrounding a local minimum of potential energy.*

Definition 1.2. *A potential barrier is a region surrounding a local maximum of potential energy.*

Furthermore, note that we shall investigate the variation of potential energy in one-dimension throughout this write-up. Now consider the stated problem classically. The total energy associated with a particle is the sum of its kinetic energy and potential energy. If the total energy E of a particle is smaller than the potential at some point x

$$\mathrm{E} = \mathrm{KE} + \mathrm{PE} < \mathrm{V}(x)$$

then according to classical mechanics, the particle can never reach point x. However, due to the probabilistic characteristic of quantum mechanics, a quantum particle might be able to reach point x without gaining extra energy.

Without the loss of generality, we shall assume our well or barrier to be located in the region

$$0 \leq x \leq \mathrm{L}$$

to simplify our calculations. Any other situation maybe derived by performing the linear transformation $x \mapsto x - \alpha$ where the well or barrier is assumed to be located in

$$\alpha \leq x \leq \mathrm{L} + \alpha$$

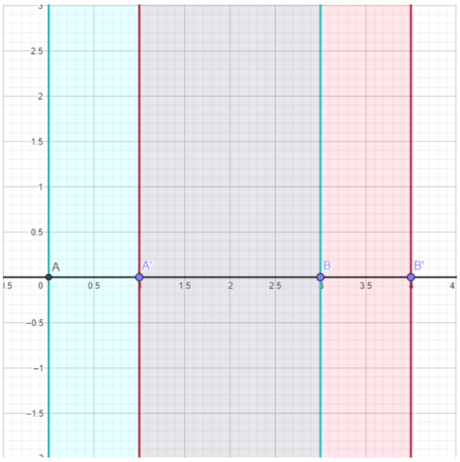

Figure 1: A linear transformation from $x = 0$ to $x = 1$

We shall also recall the characteristics of the wave function

- ⋆ $\Psi\left(x, t\right)$ is a finite, differentiable, continuous and a single valued function.
- ⋆ $\Psi\left(x, t\right)$ must satisfy the Schrodinger wave equation.

and we shall make use of them while posing the boundary conditions

2 Infinite Potential Well

In this section, we'll consider the infinite potential well. Explicitly, the variation of the potential with position is given by

$$\mathrm{V}(x) = \begin{cases} \infty & \text{if } x < 0 \\ 0 & \text{if } 0 \leq x \leq \mathrm{L} \\ \infty & \text{if } x > \mathrm{L} \end{cases}$$

Assuming time-independence, the Schrodinger's wave equation reduces to

$$-\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial x^2} + \mathrm{V}(x)\psi\left(x\right) = \mathrm{E}\psi\left(x\right) \tag{1}$$

Since, V is infinite the region outside the well $\implies$ $\psi(x) = 0$ for $x < 0$ and $x >$ L. For the region inside the well, $\mathrm{V} = 0$, thus the wave equation reduces further to

$$-\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial x^2} = E\psi \implies \frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi \tag{2}$$

Since the term $\frac{2mE}{\hbar^2}$ is positive, hence the wave equation has a trigonometric solution of the form

$$\psi\left(x\right) = \mathrm{A}\sin\left(kx\right) + \mathrm{B}\cos\left(kx\right) \tag{3}$$

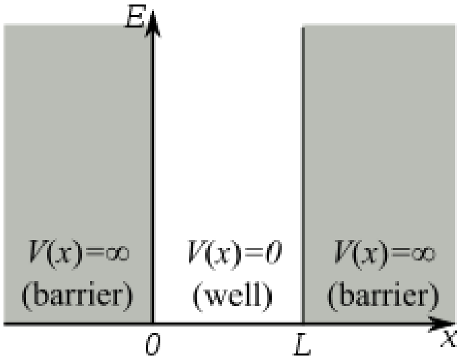

Figure 2: Potential V as a function of x

where $k = \sqrt{\frac{2mE}{\hbar^2}}$. Now let us try imposing the boundary conditions. Since ψ must be continuous all over the region

$$\psi\left(x = 0^-\right) = \psi\left(x = 0^+\right) \implies B = 0 \tag{4}$$

Thus our wave function takes the form

$$\boxed{\psi\left(x\right) = A\sin\left(\sqrt{\frac{2mE}{\hbar^2}}\right)} \tag{5}$$

We may determine the coefficient A using the normalisation condition

$$1 = \int\limits_{x=-\infty}^{x=+\infty} \psi\psi^* \,\mathrm{dx} = \int\limits_{x=0}^{x=\mathrm{L}} \mathrm{A}^2\sin^2 kx \,\mathrm{dx} = \mathrm{A}^2 \int\limits_{0}^{\mathrm{L}} \sin^2 kx \,\mathrm{dx} \tag{6}$$

which upon simplification yields $A = \sqrt{\frac{2}{\mathrm{L}}}$. Applying the boundary condition on the other side of the boundary $x = \mathrm{L}$ gives us

$$\psi\left(x = \mathrm{L}^-\right) = \psi\left(x = \mathrm{L}^+\right) \implies \sqrt{\frac{2mE}{\hbar^2}}\mathrm{L} = n\pi \tag{7}$$

from here we can obtain the wave function of the particle

$$\psi(x) = \begin{cases} 0 & \text{if } x < 0 \\ \sqrt{\frac{2}{\mathrm{L}}}\sin\left(\frac{n\pi x}{\mathrm{L}}\right) & \text{if } 0 \leq x \leq \mathrm{L} \\ 0 & \text{if } x > \mathrm{L} \end{cases}$$

We can also compute the energies of the particle in the nth states using

$$\sqrt{\frac{2mE}{\hbar^2}}\mathrm{L} = n\pi \implies \boxed{\mathrm{E}_n = \frac{n^2\pi^2\hbar^2}{2m\mathrm{L}^2}} \tag{8}$$

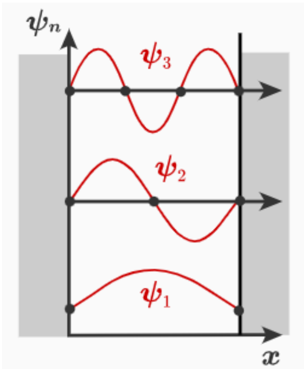

Figure 3: Wavefunction for different states

3 Finite Potential Well

In the previous section, we analysed the infinite potential situation. In this section, we would investigate what changes are brought when the potential well is finite. Suppose E is the total energy of the particle and let V_0 be the height of the potential well (where V_0 is a finite value). Classically, if $V_0 < E$, then the particle can definitely cross the well and in the other case it cannot cross the well. However, if we consider a quantum particle the probability of the particle being found anywhere in the region is not strictly zero. Let us begin by stating the time-independent Schrodinger's wave equation again.

$$-\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial x^2} + \mathrm{V}(x)\psi(x) = \mathrm{E}\psi(x)$$

which could be re-written as

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{2m}{\hbar^2}\left(\mathrm{V}(x) - \mathrm{E}\right)\psi(x) \tag{9}$$

Again, let us divide the line into three regions and state the potential function explicitly

$$\mathrm{V}(x) = \begin{cases} \mathrm{V}_0 & \text{if } x < 0 \\ 0 & \text{if } 0 \leq x \leq \mathrm{L} \\ \mathrm{V}_0 & \text{if } x > \mathrm{L} \end{cases}$$

In the first and the third region, the wave equation can be written as

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{2m}{\hbar^2}\left(\mathrm{V}_0 - \mathrm{E}\right)\psi(x) \tag{10}$$

For the purpose of non-trivial analysis, we shall assume that $E < V_0$. Thus, the solution to the wave equation is exponential. Explicitly stated as

$$\psi_{\mathrm{I}} = \mathrm{A}_1 e^{-k_1 x} + \mathrm{B}_1 e^{k_1 x} \tag{11}$$

$$\psi_{\mathrm{III}} = \mathrm{A}_3 e^{-k_1 x} + \mathrm{B}_3 e^{k_1 x} \tag{12}$$

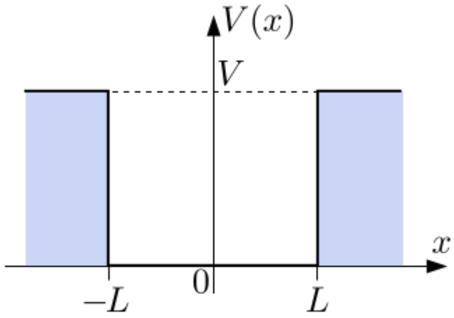

Figure 4: Finite Potential Well (transformed to $x = -\mathrm{L}$)

where $k_1 = \sqrt{\frac{2m}{\hbar^2}\left(\mathrm{V}_0 - E\right)}$. Moreover, we can observe that taking limits

$$x \longmapsto +\infty \text{ and } x \longmapsto -\infty$$

respectively reduce B_3 and A_1 to zero. Thus,

$$\boxed{\psi_{\mathrm{I}} = \mathrm{B}_1 e^{k_1 x} \text{ and } \psi_{\mathrm{III}} = \mathrm{A}_3 e^{-k_1 x}} \tag{13}$$

In the second region, the Schrodinger's wave equation reduces to (and thus implies):

$$-\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial x^2} = \mathrm{E}\psi\left(x\right) \implies \boxed{\psi_{\mathrm{II}} = \mathrm{A}_2 \sin\left(k_2 x\right) + \mathrm{B}_2 \cos\left(k_2 x\right)} \tag{14}$$

where $k_2 = \sqrt{\frac{2m\mathrm{E}}{\hbar^2}}$. Now, let's try to apply the boundary conditions. Since ψ must be continuous, at $x = 0$ we have

$$\psi\left(x = 0^-\right) = \psi\left(x = 0^+\right) \implies \mathrm{B}_1 = \mathrm{B}_2 \tag{15}$$

which reduces the number of unknown coefficients to three. Similarly, at $x = \mathrm{L}$ we have

$$\psi\left(x = \mathrm{L}^-\right) = \psi\left(x = \mathrm{L}^+\right) \implies \mathrm{A}_2 \sin\left(k_2 \mathrm{L}\right) + \mathrm{B}_2 \cos\left(k_2 \mathrm{L}\right) = \mathrm{A}_3 e^{-k_1 \mathrm{L}} \tag{16}$$

Since the wave function must be differentiable at $x = 0$, we get

$$\psi^{'}\left(x = 0^-\right) = \psi^{'}\left(x = 0^+\right) \implies \mathrm{B}_1 k_1 = \mathrm{A}_2 k_2 \tag{17}$$

which eliminates another variable $\mathrm{B}_1 = \mathrm{A}_2 \frac{k_2}{k_1}$. Similarly, we can do the same at $x = \mathrm{L}$

$$\psi^{'}\left(x = \mathrm{L}^-\right) = \psi^{'}\left(x = \mathrm{L}^+\right)$$

$$\mathrm{A}_2 k_2 \cos\left(k_2 \mathrm{L}\right) - \mathrm{B}_2 k_2 \sin\left(k_2 \mathrm{L}\right) = -\mathrm{A}_3 k_1 e^{-k_1 \mathrm{L}} \tag{18}$$

We can now carefully exploit equation (16) and (18) by first substituting values from equation (15) and (17) and dividing the equation

$$\left(k_2^2 - k_1^2\right) \tan\left(k_2 \mathrm{L}\right) = 2k_1 k_2 \tag{19}$$

From here, we can solve for E using numerical methods (since, it's a transcendental equation and cannot be solved using the high school algebra) and that would eventually replace k_1 and k_2 in the wave function terms. All the coefficients of the terms in the wave function can be expressed in the form of a single variable. To determine the exact value of this variable, we need to normalise our wave function. This can be achieved by solving the following equation

$$\int_{x=-\infty}^{x=+\infty} \psi\psi^* \,\mathrm{dx} = \int_{-\infty}^{0} \psi_{\mathrm{I}}\psi_{\mathrm{I}}^* \,\mathrm{dx} + \int_{0}^{\mathrm{L}} \psi_{\mathrm{II}}\psi_{\mathrm{II}}^* \,\mathrm{dx} + \int_{\mathrm{L}}^{\infty} \psi_{\mathrm{III}}\psi_{\mathrm{III}}^* \,\mathrm{dx} = 1$$

4 Finite Potential Barrier

In this final section we shall analyse the finite potential barrier problem. We omit the infinite potential barrier section, as the treatment is trivial and similar to the infinite treatment of the potential well problem. Moreover, we could set the limit of V in this situation to obtain the results for the infinite potential barrier problem. Let us now consider that the total energy of our particle is E and the barrier potential is V_0. If $\mathrm{V}_0 \leq \mathrm{E}$, then the particle can cross the barrier (even classically). However, if $\mathrm{E} < \mathrm{V}_0$ even though classically our particle cannot cross this potential barrier, quantum mechanics predicts that there is a non-zero probability that a quantum particle crosses the potential barrier even when $\mathrm{V}_0 > \mathrm{E}$. We shall omit the trivial cases $\mathrm{E} \geq \mathrm{V}_0$ and assume $\mathrm{E} < \mathrm{V}_0$ further onwards.

Again we start out by writing the time-independent form of Schrodinger's wave equation

$$-\frac{\hbar^2}{2m} \cdot \frac{\partial^2 \psi}{\partial x^2} + \mathrm{V}(x)\psi\left(x\right) = \mathrm{E}\psi\left(x\right)$$

and the potential function can be explicitly stated as

$$\mathrm{V}(x) = \begin{cases} 0 & \text{if } x < 0 \\ \mathrm{V}_0 & \text{if } 0 \leq x \leq \mathrm{L} \\ 0 & \text{if } x > \mathrm{L} \end{cases}$$

In the first and the third region, the Schrodinger's equation reduces to

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi$$

without loss of generality, we may assume that the particle moves from left to right across the region and thus the solutions to the above differential equation are

$$\psi_{\mathrm{I}} = \mathrm{A}_1 e^{ik_1 x} + \mathrm{B}_1 e^{-ik_1 x} \text{ and } \psi_{\mathrm{III}} = \mathrm{A}_3 e^{ik_1 x} \tag{20}$$

where $k_1 = \sqrt{\frac{2m\mathrm{E}}{\hbar^2}}$. In the second region, we would similarly have

$$\psi_{\mathrm{II}} = \mathrm{A}_2 e^{k_2 x} + \mathrm{B}_2 e^{-k_2 x} \tag{21}$$

where $k_2 = \sqrt{\frac{2m}{\hbar^2}\left(\mathrm{V}_0 - \mathrm{E}\right)}$. We could use the boundary conditions to obtain

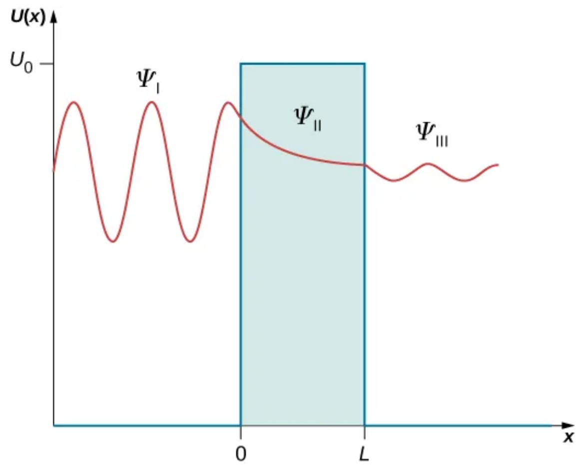

Figure 5: Finite Potential Barrier

the following four equations

$$\begin{aligned}
\psi\left(x = 0^-\right) = \psi\left(0^+\right) &\implies \mathrm{A}_1 + \mathrm{B}_1 = \mathrm{A}_2 + \mathrm{B}_2 && (22)\\
\psi\left(x = \mathrm{L}^-\right) = \psi\left(\mathrm{L}^+\right) &\implies ik_1\mathrm{A}_1 - ik_1\mathrm{B}_1 = -k_2\mathrm{A}_2 + k_2\mathrm{B}_2 && (23)\\
\psi^{'}\left(x = 0^-\right) = \psi^{'}\left(0^+\right) &\implies \mathrm{A}_2 e^{k_2\mathrm{L}} + \mathrm{B}_2 e^{k_2\mathrm{L}} = \mathrm{A}_3 e^{ik_1\mathrm{L}} && (24)\\
\psi^{'}\left(x = \mathrm{L}^-\right) = \psi^{'}\left(\mathrm{L}^+\right) &\implies k_2\mathrm{A}_2 e^{k_2\mathrm{L}} - \mathrm{B}_2 k_2 e^{-k_2\mathrm{L}} = ik_1\mathrm{A}_3 e^{ik_1\mathrm{L}} && (25)
\end{aligned}$$

We can eliminate three out of these five variables using the above four equations and doing some algebra. Combining these with the normalization conditions and then solving the equations entirely is again not possible using the high school algebra tools, as the simplified equations are transcendental equations (numerical approximation methods would be required to further obtain a solution). However, there's something interesting that we could still do.

Definition 4.1. *The transmission probability is the ratio of the transmitted intensity through a surface to the incident intensity onto the surface.*

From the equations, (22), (23), (24) and (25) we can obtain

$$\frac{\mathrm{A}_1}{\mathrm{A}_3} = \left(\frac{1}{2} + \frac{i}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)\right) e^{(ik_1+k_2)\mathrm{L}} + \left(\frac{1}{2} - \frac{i}{4}\left(\frac{k_2}{k_1} - \frac{k_1}{k_2}\right)\right) e^{(ik_1-k_2)\mathrm{L}} \tag{26}$$

If we assume the length of the barrier potential to be significant then

$$k_2\mathrm{L} >> 1 \implies e^{k_2\mathrm{L}} >> e^{-k_2\mathrm{L}} \tag{27}$$

and if we assume that the barrier potential $V_0 >> E$ then

$$\frac{k_2}{k_1} - \frac{k_1}{k_2} \approx \frac{k_2}{k_1} \tag{28}$$

Using the approximations (27) and (28) in equation (26)

$$\frac{A_1}{A_3} = \left(\frac{1}{2} + \frac{i}{4} \cdot \frac{k_2}{k_1}\right) e^{(ik_1 + k_2)L} \tag{29}$$

taking the conjugate of the above equation

$$\left(\frac{A_1}{A_3}\right)^* = \left(\frac{1}{2} - \frac{i}{4} \cdot \frac{k_2}{k_1}\right) e^{(-ik_1 + k_2)L} \tag{30}$$

We can multiply equation (29) and (30) to obtain

$$\frac{A_1 A_1^*}{A_3 A_3^*} = \left(\frac{1}{4} + \frac{k_2^2}{16k_1^2}\right) e^{2k_2 L} \tag{31}$$

If we carefully observe, we have obtained the inverse of the transmission probability. Since the transmission probability is the ratio of the transmitted intensity (which is $A_3 A_3^*$) to the incident intensity (which is $A_1 A_1^*$), therefore

$$T = \left(\frac{A_1 A_1^*}{A_3 A_3^*}\right)^{-1} = \boxed{\left(\frac{16}{4 + (k_2/k_1)^2}\right) e^{-2k_2 L}} \tag{32}$$

All of this discussion is incorporated in the topic Quantum Tunnelling. Note that if we hadn't used the approximations (27) and (28) then we could have obtained

$$T = \frac{\exp\left(-2\int_0^L dx \sqrt{\frac{2m}{\hbar^2}(V(x) - E)}\right)}{\left(1 + \frac{1}{4}\exp\left(-2\int_0^L dx \sqrt{\frac{2m}{\hbar^2}(V(x) - E)}\right)\right)^2},$$

but that's a story for some another day :)

5 References

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