LEARN: TUNNELLING - Advanced[1]

In the Discover description of quantum tunnelling we use as an analogy "a ball trying to roll over a hill". An example of a physical system displaying this behaviour is an electron that approaches another electron, fixed in some place, and encounters a potential barrier due to the mutual repulsive force exerted between the two. In the following, we will keep things as simple as possible, without worrying about how a potential barrier can be created. We will consider a one-dimensional problem, involving a particle moving in one dimension, say x, from left to right, and a square potential barrier $V(x)$, as represented in the picture below. In fact, despite being a particularly easy to solve case, this example illustrates the type of behaviour seen in more complex situations.

The energy eigenvalue equation for a particle with mass m moving in one dimension is

$$\hat{H}\,|\Psi\rangle = \left(\frac{1}{2m}\hat{P}^2 + V(\hat{X}\,)\right)|\Psi\rangle = E\,|\Psi\rangle,$$

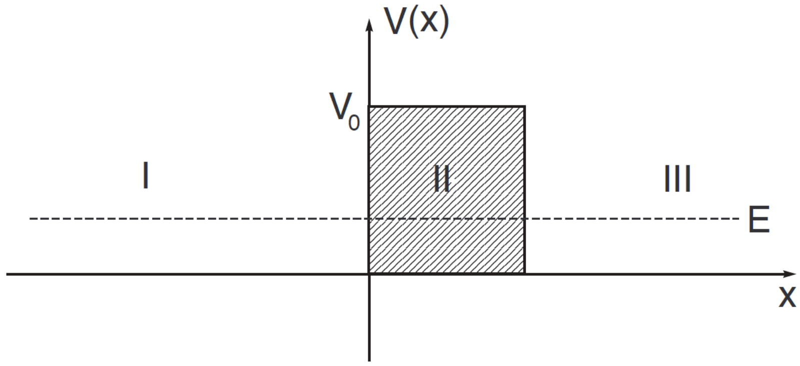
where $\hat{H}$ is the system Hamiltonian, $\hat{P}$ is the momentum operator, $V(\hat{X}\,)$ is the potential, depending on the position operator $\hat{X}$, and E is the energy of the system, i.e., the eigenvalue of the Hamiltonian. We can rewrite it in terms of the wave-function $\Psi(x)$ (see the Quest entry wave-like behaviour) as the time-independent Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx}\Psi(x) + V(x)\Psi(x) = E\,\Psi(x)$$

or

$$\Psi''(x) = -\frac{2m}{\hbar^2}\Big(E - V(x)\Big)\Psi(x). \tag{1}$$

This is an ordinary second-order differential equation, and if the potential $V(x)$ is everywhere continuous, then not only Ψ'', but also Ψ and Ψ', are continuous. Instead, if the potential is discontinuous, it may happen, in the worst case of an infinite discontinuity of $V(x)$, that the first derivative is discontinuous. However, Ψ will be continuous in any case, and therefore, we can always require continuity conditions for the wave-function $\Psi(x)$. This is actually what allows us to solve the Schrödinger equation, patching together the solutions in different potential regions. Moreover, it is easy to show (for instance considering a stationary state and then using $\{\,|p\rangle\}_{\mathscr{H}}$, the momentum states basis) that we can get meaningful solutions only when $E \geq 0$.



The propagation of a quantum particle on the other side of the barrier (region III) is known as tunnel effect or tunnelling.

The square potential barrier is a potential such that:

[1] There are many textbooks where you can find the calculations reported here. We refer to "Quantum processes systems, & information" B. Schumacher, M. D. Westmoreland, Cambridge University Press.

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \le x \le L \\ 0 & x > L \end{cases},$$

characterised by its "height" V_0 and its "width" L. We can therefore identify three different regions (*I*, *II* and *III*) with constant potential, for which we have to find the respective solutions of Eq. (1). A classical particle in region *I* with $E < V_0$ cannot access region *III*, since it is reflected by the barrier; if $E > V_0$ the particle can pass. But in Quantum Physics a particle with $E < V_0$ has a probability different from zero to be found in region *III*. Also, it can be found reflected in region *I* even if $E > V_0$. Notice that, since this a diffusion phenomenon, we should in principle solve a time-dependent problem; nonetheless by considering eigenstates of the energy, also known as *stationary states*, we can ignore the time-dependence, and therefore the problem is reduced to solving the one-dimensional time-independent Schrödinger equation reported above.

In any region where the potential is a constant, the mathematical solutions of Eq. (1) split into two groups:

- When $E < V_0$, the general solution is of the form

$$\Psi(x) = Ae^{bx} + Be^{-bx}, \quad \text{with} \quad b = \sqrt{\frac{2m}{\hbar^2}(V_0 - E)},$$

  that is, a superposition of increasing and decreasing exponential functions.

- When $E > V_0$, the general solution is of the form

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}, \quad \text{with} \quad k = \sqrt{\frac{2m}{\hbar^2}(E - V_0)},$$

  that is, a superposition of rightward and leftward moving plane waves.

Going back to our case, let us focus on a particle propagating from left to right with $E < V_0$: we want to determine whether the chance of finding the particle in region *III* is null. Choosing the coefficient $A = 1$ and requiring that, in the third region, only the rightward solution exists, the wave-function will be

$$\Psi(x) = \begin{cases} e^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{bx} + De^{-bx} & 0 \le x \le L \\ Fe^{ikx} & x > L \end{cases}.$$

For $x < 0$ the first part of the wave-function corresponds to the *incident wave* and the second one to the *reflected wave*, whereas for $x > L$ we have the part named *transmitted wave*. Via the continuity conditions of the wave-function $\Psi(x)$ and of its first derivative $\Psi'(x)$, we can determine the coefficients B, C, D, F. The continuity of the wave-function tells us that

$$\begin{aligned} \Psi_I(0) = \Psi_{II}(0) &\Rightarrow 1 + B = C + D \\ \Psi_{II}(L) = \Psi_{III}(L) &\Rightarrow Ce^{bL} + De^{-bL} = Fe^{ikL}, \end{aligned} \tag{2}$$

while the requirements on the first derivative lead to

$$\begin{aligned} \Psi_I'(0) = \Psi_{II}'(0) &\Rightarrow ik(1 - B) = b(C - D) \\ \Psi_{II}'(L) = \Psi_{III}'(L) &\Rightarrow b(Ce^{bL} - De^{-bL}) = ikFe^{ikL}. \end{aligned} \tag{3}$$

Such conditions provide us a system of four linear equations for the four unknown variables B, C, D, F; solving it, we can obtain the wave-function everywhere.

In particular, we want to verify if there is the chance of finding the particle in region *III;* in order to do so, we must introduce the *probability flux* j, defined as

$$j(x,t) = \frac{i\hbar}{2m}\left(\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right). \tag{4}$$

Exploiting this definition, we can then identify the reflection and transmission coefficient, R and T, via the ratios of the reflected flux to the incident flux and of the transmitted flux to the incident flux, respectively:

$$R = \frac{|j_{ref}|}{|j_{inc}|} \quad , \quad T = \frac{|j_{tran}|}{|j_{inc}|},$$

where j_{ref}, j_{inc} and j_{tran} are obtained via Eq. (4), considering the reflected, the incident and the transmitted waves. Since we chose $A = 1$, we get $R = |B|^2$ and $T = |F|^2$. Since we are interested in finding T, we have to determine F. Using equations (2) and (3), we can write C and D in terms of F:

$$C = \frac{1}{2} e^{-bL} \left(1 + \frac{ik}{b}\right) e^{ikL} F,$$

$$D = \frac{1}{2} e^{bL} \left(1 - \frac{ik}{b}\right) e^{ikL} F.$$

Substituting these in the first equations of relations (2) and (3) yields

$$F = \frac{4ikbe^{-ikL}}{(b+ik)^2 e^{-bL} - (b-ik)^2 e^{bL}} .$$

Now we can calculate T, and it is actually a bit easier to write down the inverse of the transmission coefficient:

$$\frac{1}{T} = 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 bL ,$$

where we have expressed b and k in terms of E and V_0. Even though $E < V_0$, being $T > 0$, the particle may "tunnel" through the barrier with some probability. Notice that if the barrier is very thin, so that $bL \ll 1$, then $T \simeq 1$ and the barrier is nearly "transparent." On the other hand, if the barrier is very wide, with $bL \gg 1$, the hyperbolic sine function can be approximated by $\sinh bL = \frac{1}{2} e^{bL} \gg 1$. In this case,

$$T \simeq \frac{4E(V_0 - E)}{V_0^2} \frac{4}{e^{2bL}} ,$$

that means, for wide barriers, the tunnelling probability decreases exponentially with L.