Infinite potential well

Let's say that a particle is in a potential defined by following:

$$V(x) = 0 \ \text{ for } 0 < x < L, \qquad V(x) = \infty \ \text{ otherwise} \tag{1}$$

This potential is called infinite potential. To understand the dynamics of this particle, let's solve Schrödinger equation. For $0 < x < L$, we have:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + 0 \cdot \psi(x) = E\psi(x) \tag{2}$$

whose solution is given by:

$$\psi(x) = A\sin(k_x x) + B\cos(k_x x), \quad \text{for } x < 0 \tag{3}$$

where $E = \hbar^2 k_x^2/(2m)$.

On the other hand, for $x < 0$, or $x > L$, the potential is infinity, so the particle cannot enter this region. This statement is true not only in the classical case but also in the quantum case. There is no way to satisfy the following equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + \infty \cdot \psi(x) = E\psi(x) \tag{4}$$

without $\psi(x)$ being zero. Therefore, we have:

$$\psi(x) = 0 \text{ for } x < 0 \text{ or } x > L \tag{5}$$

which implies:

$$\psi(x = 0) = \psi(x = L) = 0 \tag{6}$$

since $\psi(x)$ is a continuous function. Notice that this is the same condition as the oscillating string stretched between two clamps considered in our earlier article "standing wave." There, the end-points were fixed. Anyhow, we can impose these conditions to (3). Then, we have:

$$B = 0, \qquad k_x L = n_x \pi \tag{7}$$

for some positive integer n_x. In other words, this is the same condition as $\lambda_x = 2L/n$ as in the earlier article, since $\lambda = 2\pi/k_x$. In any case, the momentum of the particle is given by:

$$p_x = h/\lambda_x = \hbar k_x = \frac{n\pi}{L} \tag{8}$$

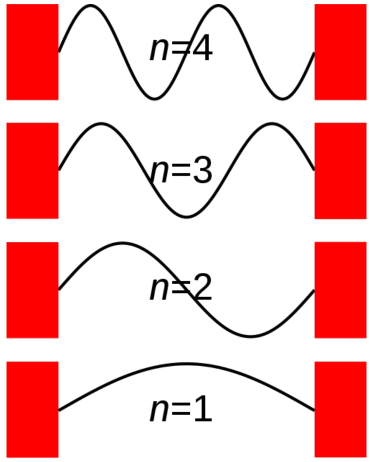

Figure 1: Standing waves in infinite potential well

and $E = p_x^2/2m$ implies

$$E = \frac{\hbar^2 k^2}{2m} = \frac{n_x^2 \pi^2}{2mL^2} \tag{9}$$

Therefore, we see that the possible energy in infinite potential well admits only discrete values labeled by positive integer n_x. This was a problem in 1 dimension. What would be the 3d-analog of this problem?

The potential for the 3d-infinite potential well is given as follows:

$$V(x,y,z) = 0 \text{ for } 0 < x < L,\ 0 < y < L, 0 < z < L, \qquad V(x) = \infty \text{ otherwise} \tag{10}$$

You see that the potential is zero, inside the cube, and infinity outside the cube. As before, $\psi(x,y,z)$ is zero, when the particle is outside the cube, and inside the cube, the Schrödinger equation is given by:

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right)\psi = E\psi \tag{11}$$

If we use the separation of variables method, the solution is given by:

$$\psi = (A_1\sin(k_x x) + B_1\cos(k_x x))(A_2\sin(k_x x) + B_2\cos(k_x x))(A_3\sin(k_x x) + B_3\cos(k_x x)) \tag{12}$$

where $E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$. As before, the boundary conditions imply:

$$B_1 = B_2 = B_3 = 0, \qquad k_x L = n_x\pi, \quad k_y L = n_y\pi, \quad k_z L = n_z\pi \tag{13}$$

for some positive ns. This condition implies:

$$E = \frac{\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) \tag{14}$$

We see that the energy in 3d-potential well admits only discrete values as in 1-d case.

Problem 1. Consider (10). Let's say that a particle is initially in a state ($n_x = 1, n_y = 2, n_z = 0$), and by emitting a photon finds itself in a state ($n_x = 0, n_y = 1, n_z = 0$). What is the wavelength of the emitted photon? (Hint[1])

Problem 2. Consider (1). Let's say that a particle is in the lowest possible energy state (also called "ground state") of such an infinite potential well. What is the probability that it will be found in the region $0 < x < L/3$? (Hint[2])

Summary

- In an infinite potential well, the wave function must satisfy the boundary condition that it vanishes at the wall.
- This condition implies that the standing waves allowed in the well has the wavelength $2L/n$ where L is the width of well, and n an integer.

(The figure is from `http://en.wikipedia.org/wiki/File:Particle_in_a_box_wavefunctions_2.svg`)

[1] Use (14) and Planck's relation. To find the relation between the frequency and the wavelength consult our earlier article "Travelling wave."

[2] Lowest possible energy state implies $n_x = 1$. Then, we can obtain the corresponding k_x. Also, while B is zero, A in (3) can be obtained by normalizing the wave function. To calculate the probability, you also need $\sin^2\theta = (1 - \cos 2\theta)/2$, since you will need to integrate a square of a sine function.