INFINITE SQUARE WELL - CHANGE IN WELL SIZE

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Suppose a particle is in the ground state in an infinite square well in the interval $x \in [0, a]$. If the right wall suddenly moves to $x = 2a$, what effect does this have on the allowable energies?

The ground state for an infinite square well of width a is

$$\psi_1 = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \tag{1}$$

The stationary states for a well of width $2a$ are

$$\psi_n = \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi x}{2a}\right) \tag{2}$$

The initial wave function can be expanded as a series using the new states:

$$\psi_1 = \sum_{n=1}^{\infty} c_n \psi_n \tag{3}$$

where the c_n are found using the orthogonal property of the stationary states:

$$c_n = \frac{1}{\sqrt{a}} \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{n\pi x}{2a}\right) dx \tag{4}$$

For $n \neq 2$, this integral evaluates to (using Maple):

$$c_n = \frac{4\sqrt{2}}{\pi\left(4-n^2\right)} \sin\left(\frac{n\pi}{2}\right) \tag{5}$$

For $n = 2$, we have

$$c_2 = \frac{1}{\sqrt{a}} \sqrt{\frac{2}{a}} \int_0^a \sin^2\left(\frac{\pi x}{a}\right) dx \tag{6}$$

$$= \frac{1}{\sqrt{2}} \tag{7}$$

The first few probabilities for stationary states are then

$$|c_1|^2 = \frac{32}{9\pi^2} \tag{8}$$
$$= 0.36 \tag{9}$$
$$|c_2|^2 = 0.5 \tag{10}$$
$$|c_3|^2 = \frac{32}{25\pi^2} \tag{11}$$
$$= 0.13 \tag{12}$$

All higher coefficients are smaller, with all even coefficients from $n = 4$ upwards being zero.

The most probable energy is therefore

$$E_2 = \frac{2^2\pi^2\hbar^2}{2m(2a)^2} \tag{13}$$
$$= \frac{\pi^2\hbar^2}{2ma^2} \tag{14}$$

This happens to be the ground state of the original well, so, unsurprisingly, the most probable energy for the particle is the one it starts with.

The next most probable energy is

$$E_1 = \frac{\pi^2\hbar^2}{8ma^2} \tag{15}$$

The average energy *could* be found if we could sum the infinite series

$$\langle E\rangle = \frac{1}{2}E_2 + \sum_{\text{odd } n} \frac{32}{\pi^2(4-n^2)^2}E_n \tag{16}$$
$$= \frac{\pi^2\hbar^2}{8ma^2}\left[2 + \sum_{\text{odd } n} \frac{32n^2}{\pi^2(4-n^2)^2}\right] \tag{17}$$

Clearly this isn't an easy sum, but we can calculate the expectation value of the Hamiltonian directly as an integral to get the result

$$\langle E\rangle = \int_0^a \psi_1(x)\left(-\frac{\hbar^2}{2m}\right)\frac{d^2}{dx^2}\psi_1(x)dx \tag{18}$$

$$= -\frac{\hbar^2}{ma}\int_0^a \sin\left(\frac{\pi x}{a}\right)\frac{d^2}{dx^2}\sin\left(\frac{\pi x}{a}\right)dx \tag{19}$$

$$= \frac{\hbar^2\pi^2}{ma^3}\int_0^a \sin^2\left(\frac{\pi x}{a}\right)dx \tag{20}$$

$$= \frac{\hbar^2\pi^2}{2ma^2} \tag{21}$$

$$= E_2 \tag{22}$$

If you're interested, a side effect of this result is that we can evaluate the sum above:

$$\sum_{\text{odd } n}\frac{32n^2}{\pi^2\left(4-n^2\right)^2} = 2 \tag{23}$$

This series doesn't converge all that quickly (it goes as $1/n^2$). The sum of the first 100 terms gives 1.991893832.

A slight rearrangement gives yet another way of calculating π:

$$\sum_{\text{odd } n}\frac{16n^2}{\left(4-n^2\right)^2} = \pi^2 \tag{24}$$