Quantum Mechanics

Square well potential

Problem 1.- The functions $\psi_n(x)$ are eigen functions of the problem of a particle of mass "m" in a square well potential of length "a". You are given the solution at time t=0:

$$\psi(\mathrm{x},0) = \frac{1}{\sqrt{2}}[\psi_1(x) + \psi_2(x)]$$

Find the solution for time "t".

Solution: Following the prescription to get wave functions as a function of time, if at t=0

$$\psi(\mathrm{x},0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

You multiply each eigen function by a phase factor:

$$\psi(\mathrm{x},\mathrm{t}) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-i\frac{E_n t}{\hbar}}$$

In the present case, the summation is only over two elements, so we only need to multiply each of those two by their phase factors:

$$\psi(\mathrm{x},0) = \frac{1}{\sqrt{2}}(\psi_1(x) + \psi_2(x)) \rightarrow \psi(\mathrm{x},\mathrm{t}) = \frac{1}{\sqrt{2}}\left(\psi_1(x) e^{-i\frac{E_1 t}{\hbar}} + \psi_2(x) e^{-i\frac{E_2 t}{\hbar}}\right)$$

The eigen energies for a square well potential are well known. So, explicitly:

$$\psi(\mathrm{x},\mathrm{t}) = \frac{1}{\sqrt{2}}\left(\psi_1(x) e^{-i\frac{\hbar\pi^2 t}{2ma^2}} + \psi_2(x) e^{-i\frac{2\hbar\pi^2 t}{ma^2}}\right)$$

Problem 1a.- $\psi_n(x)$ are the eigen functions of a particle of mass "m" in a square well potential of length "a". You are given the solution at time t=0:

$$\psi(\mathrm{x},0) = A[\psi_1(x) - \psi_2(x) + \psi_3(x)]$$

Normalize the wave function and find the solution for time "t".

Problem 2.- Calculate the minimum kinetic energy of an electron (mass = 9.1×10^{-31}kg) confined in an infinite square well potential of 65nm length.

Solution: The minimum energy of a particle in a square potential well (the ground state) is:

$$E_1 = \frac{\hbar^2\pi^2}{2ma^2} = \frac{(1.05\times10^{-34}\,Js)^2(3.1416)^2}{2(9.1\times10^{-31}\,kg)(65\times10^{-9}\,m)^2} = \mathbf{1.42\times10^{-23}J}$$

Problem 2a.- Calculate the minimum kinetic energy of a proton (mass = 1.67×10^{-27} kg) confined in an infinite square well potential of 193nm length.

Problem 3.- A particle is confined in a one-dimensional box 0 < x < a with an initial (t=0) wave function given by

$$A\sin^3\left(\frac{\pi x}{a}\right)$$

a) Find the value of A that normalizes the wavefunction.
b) Find the expectation value of x as a function of time.
c) Find the expectation value of the energy.

Solution

a) To find the normalization constant we need to make sure that: $\int_{-\infty}^{\infty}\psi^*\psi dx = 1$, so:

$$\int_0^a\left[A\sin^3(\pi x/a)\right]^2 dx = \int_0^a A^2\sin^6(\pi x/a)dx = 1$$

Recall the Euler equation $e^{ix} = \cos x + i\sin x$, so:

$$\sin x = \frac{e^{ix}-e^{-ix}}{2i} \rightarrow \sin^6 x = \left[\frac{e^{ix}-e^{-ix}}{2i}\right]^6 = \frac{e^{6ix}-6e^{4ix}+15e^{2ix}-20+15e^{-2ix}-6e^{-4ix}+e^{-6ix}}{-64} =$$

$$\frac{\left[e^{6ix}+e^{-6ix}\right]-\left[6e^{4ix}+6e^{-4ix}\right]+\left[15e^{2ix}+15e^{-2ix}\right]-20}{-64} = \frac{-2\cos6x+12\cos4x-30\cos2x+20}{64} =$$

$$= \frac{-\cos6x+6\cos4x-15\cos2x+10}{32}$$

Plugging this result in the integral:

$$\int_{-\infty}^{\infty}\psi^*\psi dx = \int_0^a A^2\left[\frac{-\cos6(\pi x/a)+6\cos4(\pi x/a)-15\cos2(\pi x/a)+10}{32}\right]dx = \frac{5aA^2}{16} = 1$$

Then $A = \frac{4\sqrt{5a}}{5a}$

To find $\psi(x,t)$ we should write the wave function as a linear combination of eigen functions as follows:

$$\psi(x,0) = A\sin^3(\pi x/a) = A\left[\frac{3\sin(\pi x/a) - \sin(3\pi x/a)}{4}\right] = \frac{3\sqrt{5a}}{5a}\sin(\pi x/a) - \frac{\sqrt{5a}}{5a}\sin(3\pi x/a)$$

Which can also be written as:

$$\psi(x,0) = \frac{3}{\sqrt{10}}\psi_1(x,0) + \frac{1}{\sqrt{10}}\psi_3(x,0)$$

To get the general solution we need the eigen energies, which are given by:

$$E_1 = \frac{\pi^2\hbar^2}{2ma^2} \quad \text{and} \quad E_3 = \frac{9\pi^2\hbar^2}{2ma^2},$$

so $\quad \psi(x,t) = \frac{3\sqrt{5a}}{5a}e^{-i\frac{\pi^2\hbar t}{2ma^2}}\sin(\pi x/a) - \frac{\sqrt{5a}}{5a}e^{-i\frac{9\pi^2\hbar t}{2ma^2}}\sin(3\pi x/a)$

b) To find the expectation value of x we need to integrate: $\langle x\rangle = \int_{-\infty}^{\infty}\psi^* x\psi dx =$

$$\int_0^a\left(\frac{3\sqrt{5a}}{5a}e^{-i\frac{\pi^2\hbar t}{2ma^2}}\sin\left(\frac{\pi x}{a}\right) - \frac{\sqrt{5a}}{5a}e^{-i\frac{9\pi^2\hbar t}{2ma^2}}\sin n\left(\frac{3\pi x}{a}\right)\right)^* x\left(\frac{3\sqrt{5a}}{5a}e^{-i\frac{\pi^2\hbar t}{2ma^2}}\sin\left(\frac{\pi x}{a}\right) - \frac{\sqrt{5a}}{5a}e^{-i\frac{9\pi^2\hbar t}{2ma^2}}\sin\left(\frac{3\pi x}{a}\right)\right)dx$$

$$= \int_0^a\left(\frac{3\sqrt{5a}}{5a}e^{i\frac{\pi^2\hbar t}{2ma^2}}\sin\left(\frac{\pi x}{a}\right) - \frac{\sqrt{5a}}{5a}e^{i\frac{9\pi^2\hbar t}{2ma^2}}\sin\left(\frac{3\pi x}{a}\right)\right)x\left(\frac{3\sqrt{5a}}{5a}e^{-i\frac{\pi^2\hbar t}{2ma^2}}\sin\left(\frac{\pi x}{a}\right) - \frac{\sqrt{5a}}{5a}e^{-i\frac{9\pi^2\hbar t}{2ma^2}}\sin\left(\frac{3\pi x}{a}\right)\right)dx$$

$$= \int_0^a\left(\frac{9}{5a}\sin^2\left(\frac{\pi x}{a}\right) + \frac{1}{5a}\sin^2\left(\frac{3\pi x}{a}\right) - \frac{3}{5a}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{3\pi x}{a}\right)\left\{e^{i\frac{8\pi^2\hbar t}{2ma^2}} + e^{-i\frac{8\pi^2\hbar t}{2ma^2}}\right\}\right)xdx$$

$$= \int_0^a\left(\frac{9}{5a}\sin^2\left(\frac{\pi x}{a}\right) + \frac{1}{5a}\sin^2\left(\frac{3\pi x}{a}\right) - \frac{3}{5a}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{3\pi x}{a}\right)\left\{2\cos\left(\frac{8\pi^2\hbar t}{2ma^2}\right)\right\}\right)xdx$$

$$= \frac{9}{5a}\int_0^a x\sin^2\left(\frac{\pi x}{a}\right)dx + \frac{1}{5a}\int_0^a x\sin^2\left(\frac{3\pi x}{a}\right)dx - \frac{6\cos\left(\frac{8\pi^2\hbar t}{2ma^2}\right)}{5a}\int_0^a x\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{3\pi x}{a}\right)dx$$

$$= \frac{9}{5a}\frac{a^2}{4} + \frac{1}{5a}\frac{a^2}{4} - \frac{6\cos\left(\frac{8\pi^2\hbar t}{2ma^2}\right)}{5a}[0] = \frac{a}{2}$$

c) To get the expectation value of the energy, we use the equation:

$$\langle E\rangle = \int_{-\infty}^{\infty}\psi^* H\psi dx = \int_{-\infty}^{\infty}\left(\frac{3}{\sqrt{10}}\psi_1^* + \frac{1}{\sqrt{10}}\psi_3^*\right)H\left(\frac{3}{\sqrt{10}}\psi_1 + \frac{1}{\sqrt{10}}\psi_3\right)dx =$$

$$\int_{-\infty}^{\infty}\left(\frac{3}{\sqrt{10}}\psi_1^* + \frac{1}{\sqrt{10}}\psi_3^*\right)\left(\frac{3E_1}{\sqrt{10}}\psi_1 + \frac{E_3}{\sqrt{10}}\psi_3\right)dx = \frac{9E_1 + E_3}{10}$$

$$\langle E\rangle = \frac{9\pi^2\hbar^2}{10ma^2}$$

Problem 4.- A particle is confined in the one-dimensional box 0<x<a in the ground state. But suddenly the potential well gets expanded to 0<x<2a.

a) If an experiment is done to measure the energy, find the most probable value and its probability.
b) Find the next likely energy and its probability.
c) Find the expectation value of the energy

Solution: When the particle is in the ground state of the infinite well with length "a" the wave function is

$$\psi = \sqrt{\frac{2}{a}}\sin(\pi x/a) \quad \text{for } 0<x<a \text{ and zero elsewhere.}$$

After the expansion this wave function is no longer an eigen function of the new potential well, but it can be written as a linear combination of the new eigen functions:

$$\psi = \sum_{n=1}^{\infty} c_n\psi_n = \sum_{n=1}^{\infty} c_n\sqrt{\frac{1}{a}}\sin(n\pi x/2a)$$

To find the coefficients we can use Fourier series:

$$\psi\sqrt{\frac{1}{a}}\sin(m\pi x/2a) = \sum_{n=1}^{\infty} c_n\frac{1}{a}\sin(m\pi x/2a)\sin(n\pi x/2a)$$

$$\int_0^{2a}\psi\sqrt{\frac{1}{a}}\sin(m\pi x/2a)dx = \sum_{n=1}^{\infty}\int_0^{2a} c_n\frac{1}{a}\sin(m\pi x/2a)\sin(n\pi x/2a)dx = c_m$$

$$c_m = \int_0^{a}\psi\sqrt{\frac{1}{a}}\sin(m\pi x/2a)dx = \int_0^{a}\frac{\sqrt{2}}{a}\sin(\pi x/a)\sin(m\pi x/2a)dx =$$

$$= \int_0^{a}\frac{\sqrt{2}}{2a}\left(\cos((m-2)\pi x/2a) - \cos((m+2)\pi x/2a)\right)dx = \sqrt{2}\left[\frac{\sin((m-2)\pi/2)}{(m-2)\pi} - \frac{\sin((m+2)\pi/2)}{(m+2)\pi}\right]$$

This last result is only valid if m≠2. In the especial case where m=2, we get:

$c_2 = \int_0^a \frac{\sqrt{2}}{a}\sin^2(\pi x/a)dx = \frac{\sqrt{2}}{2}$, which is certainly the largest coefficient.

The most probable result corresponds to the energy of ψ_2 of the new potential well, which is:

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

This is the same energy that it had initially, so it is not surprising.
The probability of getting this result is $c_2{}^2 = 1/2$

To find the next probable energy, let us find the other coefficients:

For m even $c_m = \frac{\sqrt{2}}{\pi}\left[\frac{\sin((m-2)\pi/2)}{(m-2)} - \frac{\sin((m+2)\pi/2)}{(m+2)}\right] = 0$

For m odd, we can distinguish two possibilities:
Case 1: m= 4k+1:

$$c_m = \frac{\sqrt{2}}{\pi}\left[\frac{\sin((4k-1)\pi/2)}{4k-1} - \frac{\sin((4k+3)\pi/2)}{4k+3}\right] = \frac{\sqrt{2}}{\pi}\left[\frac{-1}{4k-1} + \frac{1}{4k+3}\right] = -\frac{4\sqrt{2}}{\pi}\frac{1}{(4k-1)(4k+3)}$$

Case 2: m= 4k+3:

$$c_m = \frac{\sqrt{2}}{\pi}\left[\frac{\sin((4k+1)\pi/2)}{4k+1} - \frac{\sin((4k+5)\pi/2)}{4k+5}\right] = \frac{\sqrt{2}}{\pi}\left[\frac{1}{4k+1} - \frac{1}{4k+5}\right] = \frac{4\sqrt{2}}{\pi}\frac{1}{(4k+1)(4k+5)}$$

Given these equations we get:

$$c_1 = \frac{4\sqrt{2}}{3\pi},\ c_3 = \frac{4\sqrt{2}}{5\pi}, c_5 = -\frac{4\sqrt{2}}{21\pi}, c_7 = \frac{4\sqrt{2}}{45\pi}$$

The largest coefficient corresponds to the ground state of the new potential well, whose energy is $E_1 = \frac{\pi^2\hbar^2}{2m(2a)^2} = \frac{\pi^2\hbar^2}{8ma^2}$ and with a probability equal to $c_1{}^2 = \frac{32}{9\pi^2} \approx 0.36$

To get the expectation value of the energy:

$\langle E\rangle = \int_{-\infty}^{\infty}\psi * H\psi dx$, but notice that the Hamiltonian and the wave function remain the same at t=0,

so the expectation value should be the same as before: $\langle E\rangle = \dfrac{\pi^2\hbar^2}{2ma^2}$

Problem 5.- Find the expectation value of position, momentum and momentum squared of the particle in a box 0<x<a with the wave function:

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

Additionally find the uncertainties σ_x, σ_p and $\sigma_x\sigma_p$

Solution:

$$\langle x\rangle = \int_0^a \psi^* x\psi dx = \int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)x\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)dx = \int_0^a x\frac{2}{a}\sin^2\left(\frac{n\pi x}{a}\right)dx =$$

$$\frac{a}{n^2\pi^2}\int_0^a n\pi x\frac{2}{a}\sin^2\left(\frac{n\pi x}{a}\right)dx\frac{n\pi}{a} = \frac{2a}{n^2\pi^2}\int_0^{n\pi} y\sin^2(y)dy = \frac{a}{n^2\pi^2}\int_0^{n\pi} y[1-\cos(2y)]dy = \frac{a}{n^2\pi^2}\int_0^{n\pi} y - y\cos(2y)dy =$$

$$\frac{a}{n^2\pi^2}\int_0^{n\pi} y - y\cos(2y)dy = \frac{a}{n^2\pi^2}\left[\frac{y^2}{2} - \frac{y\sin(2y)}{2}\bigg|_0^{n\pi} + \frac{1}{2}\int_0^{n\pi}\sin 2y dy\right] = \frac{a}{n^2\pi^2}\frac{n^2\pi^2}{2} = \frac{a}{2}$$

$$\langle x^2\rangle = \int_0^a \psi^* x^2\psi dx = \int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)x^2\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)dx = \int_0^a x^2\frac{2}{a}\sin^2\left(\frac{n\pi x}{a}\right)dx =$$

$$\frac{a^2}{n^3\pi^3}\int_0^a n^2\pi^2 x^2\frac{2}{a^2}\sin^2\left(\frac{n\pi x}{a}\right)dx\frac{n\pi}{a} = \frac{2a^2}{n^3\pi^3}\int_0^{n\pi} y^2\sin^2(y)dy =$$

$$\frac{a^2}{n^3\pi^3}\int_0^{n\pi} y^2\left[1-\cos(2y)\right]dy = \frac{a}{n^2\pi^2}\int_0^{n\pi} y^2 - y^2\cos(2y)dy =$$

$$\frac{a^2}{n^3\pi^3}\int_0^{n\pi} y^2 - y^2\cos(2y)dy = \frac{a^2}{n^3\pi^3}\left[\frac{y^3}{3} - \frac{y^2\sin(2y)}{2}\bigg|_0^{n\pi} + \frac{1}{2}\int_0^{n\pi}\sin 2y dy^2\right] = \frac{a^2n^3\pi^3}{3n^3\pi^3} = \frac{a^2}{3}$$

$$\langle p\rangle = \int_0^a \psi^* p\psi dx = \int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\left(-\frac{i\hbar\partial}{\partial x}\right)\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)dx = -\frac{2i\hbar n\pi}{a^2}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{n\pi x}{a}\right)dx =$$

$$= -\frac{i\hbar n\pi}{a^2}\int_0^a \sin\left(\frac{2n\pi x}{a}\right)dx = 0$$

$$\langle p^2\rangle = \int_0^a \psi^* p\psi dx = \int_0^a \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)\left(-\frac{\hbar^2\partial}{\partial x^2}\right)\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)dx = \frac{2\hbar^2n^2\pi^2}{a^3}\int_0^a \sin^2\left(\frac{n\pi x}{a}\right)dx =$$

$$= \frac{\hbar^2 n^2 \pi^2}{a^3} \int_0^a 1 - \cos\left(\frac{2n\pi x}{a}\right) dx = \frac{\hbar^2 n^2 \pi^2}{a^2}$$

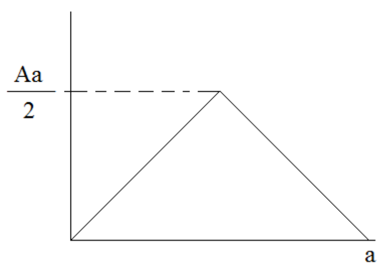
Uncertainties:

$$\sigma_x{}^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{a^2}{3} - \frac{a^2}{4} = \frac{a^2}{12} \rightarrow \sigma_x = \frac{\sqrt{3}a}{6}$$

$$\sigma_p{}^2 = \langle p^2 \rangle - \langle p \rangle^2 = \frac{n^2\pi^2\hbar^2}{a^2} \rightarrow \sigma_p = \frac{n\pi\hbar}{a}$$

$$\sigma_p \sigma_x = \frac{n\pi\hbar}{a} \frac{\sqrt{3}a}{6} = \frac{\sqrt{3}n\pi\hbar}{6} \geq \frac{\hbar}{2}$$

Problem 6.- A particle confined in a box defined as 0<x<a has an initial wave function:



Find A to normalize the wave function.

Express the wave function as a superposition of eigen states of the potential and find the probability of finding the particle in the ground state.

Find the expectation value of the energy.

Solution: To normalize: $\frac{A^2 a^3}{12} = 1 \rightarrow A = \sqrt{\frac{12}{a^3}}$

$$C_n = \frac{4A}{a} \int_0^{a/2} x \sin\left(\frac{n\pi x}{a}\right) dx$$

$$C_n = -\frac{4A}{n\pi} \int_0^{a/2} x d \cos\left(\frac{n\pi x}{a}\right) = -\frac{4A}{n\pi}\left[x\cos\left(\frac{n\pi x}{a}\right)\Bigg|_0^{a/2} - \int_0^{a/2} \cos\left(\frac{n\pi x}{a}\right) dx \right]$$

$$C_n = \frac{4A}{n\pi} \int_0^{a/2} \cos\left(\frac{n\pi x}{a}\right) dx = \pm \frac{4Aa}{n^2\pi^2}$$

$\psi(x,t) = \frac{4Aa}{\pi^2} \sum_{\substack{n=1 \\ odd}}^{\infty} \pm \frac{1}{n^2} \sin\left(\frac{n\pi x}{a}\right) \exp\left[-i\frac{n^2\pi^2\hbar}{2ma^2}t\right]$… sign alternates starting positive.

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

$$\psi(x) = \frac{4Aa}{\pi^2}\left\{\sin\left(\frac{n\pi x}{a}\right) + \sum_{\substack{n=3 \\ odd}}^{\infty} \pm \frac{1}{n^2}\sin\left(\frac{n\pi x}{a}\right)\right\} = \frac{4Aa}{\pi^2}\sqrt{\frac{a}{2}}\psi_1 + \frac{4Aa}{\pi^2}\left\{\sum_{\substack{n=3 \\ odd}}^{\infty} \pm \frac{1}{n^2}\sin\left(\frac{n\pi x}{a}\right)\right\}$$

$$P_1 = \left[\frac{4Aa}{\pi^2}\sqrt{\frac{a}{2}}\right]^2 = \frac{8A^2a^3}{\pi^4} = \frac{8\times 12}{\pi^4} = \frac{96}{\pi^4} = 98.55\%$$

$$\langle e\rangle = \frac{96}{\pi^4}\frac{\hbar^2\pi^2}{2ma^2} + \frac{96}{\pi^4 3^4}\frac{\hbar^2\pi^2 3^2}{2ma^2} + \frac{96}{\pi^4 3^4}\frac{\hbar^2\pi^2 3^2}{2ma^2} + \ldots$$

$$\langle e\rangle = \frac{96\hbar^2}{\pi^2 2ma^2}\left(1 + \frac{1}{3^2} + \frac{1}{5^2} + \ldots\right) = \frac{96\hbar^2}{\pi^2 2ma^2}\left(\frac{\pi^2}{8}\right) = \frac{6\hbar^2}{ma^2}$$