1. A particle is in the ground state of an infinite square well potential given by

$$V(x) = \begin{cases} 0 & \text{for } -a \le x \le a \\ \infty & \text{otherwise} \end{cases}$$

What is the probability to find the particle in the interval between –a/2 and a/2?

Ans.

The 1D Schrödinger equation is:

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2} E\psi(x) = 0 \qquad \text{for} \qquad -a < x < a$$

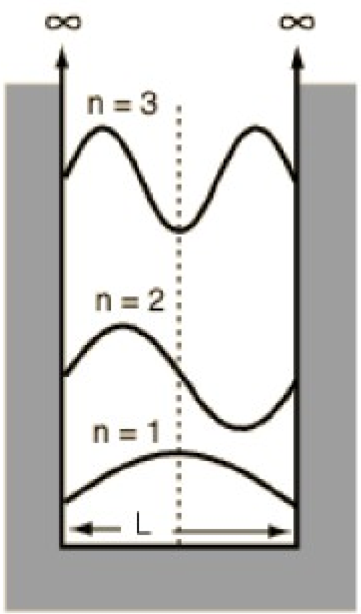
$$= A\cos kx + B\sin kx \qquad\qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

The wave function must be zero at both walls of well:

$$A\cos(ka)+B\sin(ka)=0$$

$$A\cos(-ka)+B\sin(-ka)=0 \quad \Rightarrow \quad A\cos(ka)-B\sin(ka)=0$$

$$\Rightarrow \quad A\cos(ka)=0 \quad \text{and} \quad B\sin(ka)=0$$




$$\psi_n(x)=\frac{1}{\sqrt{a}}\cos\left(\frac{n\pi}{2a}x\right), \quad n=1,3,5,\ldots$$

$$\psi_n(x)=\frac{1}{\sqrt{a}}\sin\left(\frac{n\pi}{2a}x\right), \quad n=2,4,6,\ldots$$

$$P=\int_{-a/2}^{a/2}\sqrt{\frac{2}{2a}}\cdot\sqrt{\frac{2}{2a}}\cos\frac{\pi x}{2a}\cdot\cos\frac{\pi x}{2a}\,dx=\int_{-a/2}^{a/2}\frac{1}{a}\cos^2\frac{\pi x}{2a}\,dx=\frac{1}{a}\times\frac{1}{2}\left[\int_{-a/2}^{a/2}\left(1+\cos\frac{2\pi x}{2a}\right)dx\right]$$

$$=\frac{1}{2a}\left[x+\frac{a}{\pi}\sin\frac{\pi x}{a}\right]_{-a/2}^{a/2}=\frac{1}{2a}\left[\frac{a}{2}+\frac{a}{2}+\frac{a}{\pi}(1+1)\right]=\frac{1}{2a}\left[a+\frac{2a}{\pi}\right]=\left(\frac{1}{2}+\frac{1}{\pi}\right)$$

2.

Consider the box potential

$$V(x) = \begin{cases} 0, & 0 < x < a, \\ \infty, & \text{elsewhere.} \end{cases} \quad .$$

(a) Estimate the energies of the ground state as well as those of the first and the second excited states for (i) an electron enclosed in a box of size $a = 10^{-10}$ m (express your answer in electron volts; you may use these values: $\hbar c = 200\,\text{MeV fm}$, $m_e c^2 = 0.5\,\text{MeV}$); (ii) a 1 g metallic sphere which is moving in a box of size $a = 10$ cm (express your answer in joules).

(b) Discuss the importance of the quantum effects for both of these two systems.

(c) Use the uncertainty principle to estimate the velocities of the electron and the metallic sphere.

Ans.

The energy of a particle of mass $m$ in a box having perfectly rigid walls is given by

$$E_n = \frac{n^2 h^2}{8ma^2}, \qquad n = 1, 2, 3, \ldots,$$

where $a$ is the size of the box.

(a) (i) For the electron in the box of size $10^{-10}$ m, we have

$$\begin{aligned} E_n &= \frac{\hbar^2 c^2}{m_e c^2 a^2} \frac{4\pi^2 n^2}{8} \equiv \frac{4 \times 10^4 \,(\text{MeV fm})^2}{0.5\,\text{MeV} \times 10^{10}\,\text{fm}^2} \frac{\pi^2}{2} n^2 \\ &= 4\pi^2 n^2\,\text{eV} \simeq 39 n^2\,\text{eV}. \end{aligned}$$

Hence $E_1 = 39\,\text{eV}$, $E_2 = 156\,\text{eV}$, and $E_3 = 351\,\text{eV}$.

(ii) For the sphere in the box of side 10 cm we have

$$E_n = \frac{(6.6 \times 10^{-34}\,\text{J s})^2}{10^{-3}\,\text{kg} \times 10^{-2}\,\text{m}^2} n^2 = 43.6 \times 10^{-63} n^2\,\text{J}$$

Hence $E_1 = 43.6 \times 10^{-63}$ J, $E_2 = 174.4 \times 10^{-63}$ J, and $E_3 = 392.4 \times 10^{-63}$ J.

(b) The differences between the energy levels are

$$(E_2 - E_1)_{electron} = 117\,\text{eV}, \qquad (E_3 - E_2)_{electron} = 195\,\text{eV},$$

$$(E_2 - E_1)_{sphere} = 130.8 \times 10^{-63}\,\text{J}, \qquad (E_3 - E_2)_{sphere} = 218 \times 10^{-63}\,\text{J}.$$

- The spacing between the energy levels of the electron are quite large; the levels are far apart from each other. Thus, the quantum effects are important.

- The energy levels of the sphere are practically indistinguishable; the spacing between the levels are negligible. The energy spectrum therefore forms a continuum; hence the quantum effects are not noticeable for the sphere.

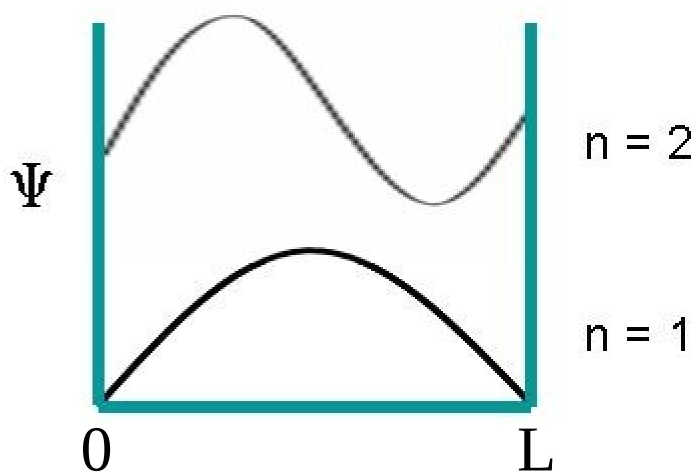
(c)

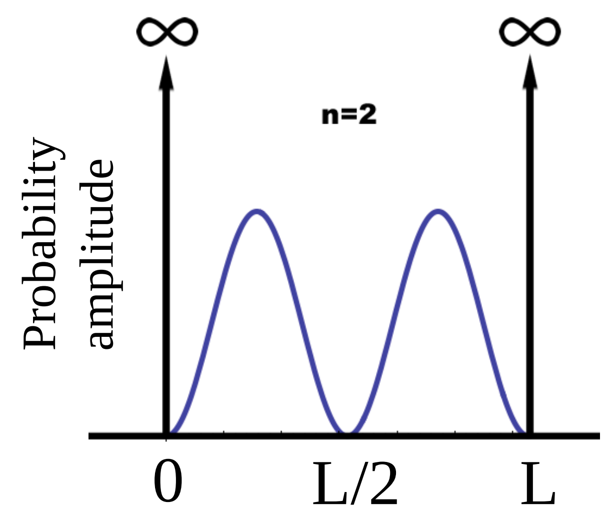
$$\Delta x \, \Delta p \geq \frac{\hbar}{2}$$

The electron moves quite fast and the sphere is practically at rest.

3. If the wave function of a particle trapped in space between x = 0 and x = L is given by , where A is a constant, for which value(s) of x will the probability of finding the particle be the maximum?

Ans.




The probability will be maximum at L/4 and 3L/4.

You can also find it out by taking first derivative of probability density and put that equal to zero.

4.

A particle of mass $m$ is in the state

Where $A$ and $a$ are positive real constants.

(a) Find $A$.

(b) For what potential energy function $V(x)$ does $\Psi$ satisfy the Schrödinger equation?

(c) Calculate the expectation values of $x$, $x^2$, $p$, and $p^2$.

Ans. (a) Normalization condition:

;

If  is normalized at t = 0, it stays normalized for all future time.

$$\boxed{\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x,t)|^2\,dx = 0}$$

Proof:

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x,t)|^2\,dx = \int_{-\infty}^{+\infty}\frac{\partial}{\partial t}|\Psi(x,t)|^2\,dx$$

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{\partial}{\partial t}(\Psi^*\Psi) = \Psi^*\frac{\partial\Psi}{\partial t} + \frac{\partial\Psi^*}{\partial t}\Psi$$

Using Schrödinger Equation

$$\frac{\partial\Psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}V\Psi$$

Taking Complex conjugate

$$\frac{\partial\Psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2} + \frac{i}{\hbar}V\Psi^*$$

On substituting

$$\frac{\partial}{\partial t}|\Psi|^2 = \frac{i\hbar}{2m}\left(\Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial^2 \Psi^*}{\partial x^2}\Psi\right) = \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\right]$$

$$\frac{d}{dt}\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\, dx = \frac{i\hbar}{2m}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)\Bigg|_{-\infty}^{+\infty}$$

$$\boxed{\frac{d}{dt}\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\, dx = 0} \qquad \text{(Proved)}$$

Putting t = 0 and using the normalization condition

$$1 = 2|A|^2 \int_0^\infty e^{-2amx^2/\hbar} dx = 2|A|^2 \frac{1}{2}\sqrt{\frac{\pi}{(2am/\hbar)}} = |A|^2 \sqrt{\frac{\pi\hbar}{2am}}; \quad \boxed{A = \left(\frac{2am}{\pi\hbar}\right)^{1/4}.}$$

(b) Schrödinger Equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi$$

$$\frac{\partial\Psi}{\partial t} = -ia\Psi; \quad \frac{\partial\Psi}{\partial x} = -\frac{2amx}{\hbar}\Psi$$

$$\frac{\partial^2\Psi}{\partial x^2} = -\frac{2am}{\hbar}\left(\Psi + x\frac{\partial\Psi}{\partial x}\right) = -\frac{2am}{\hbar}\left(1 - \frac{2amx^2}{\hbar}\right)\Psi$$

$$V\Psi = i\hbar(-ia)\Psi + \frac{\hbar^2}{2m}\left(-\frac{2am}{\hbar}\right)\left(1 - \frac{2amx^2}{\hbar}\right)\Psi$$

$$= \left[\hbar a - \hbar a\left(1 - \frac{2amx^2}{\hbar}\right)\right]\Psi = 2a^2mx^2\Psi$$

$$\boxed{V(x) = 2ma^2x^2.}$$

(c) Expectation Value:

$$\langle x \rangle = \int \Psi^*(x)\Psi \, dx,$$

$$\langle p \rangle = \int \Psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi \, dx \; ; \; \langle p \rangle = m\frac{d\langle x \rangle}{dt} = -i\hbar \int \left(\Psi^* \frac{\partial \Psi}{\partial x}\right) dx$$

$$\langle x \rangle = \int_{-\infty}^{\infty} x|\Psi|^2 dx = \boxed{0.} \qquad \text{[Odd integrand.]}$$

$$\langle x^2 \rangle = 2|A|^2 \int_0^{\infty} x^2 e^{-2amx^2/\hbar} dx = 2|A|^2 \frac{1}{2^2(2am/\hbar)}\sqrt{\frac{\pi\hbar}{2am}} = \boxed{\frac{\hbar}{4am}.}$$

$$\langle p \rangle = m\frac{d\langle x \rangle}{dt} = \boxed{0.}$$

$$\langle p^2\rangle = \int \Psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \Psi dx = -\hbar^2 \int \Psi^* \frac{\partial^2 \Psi}{\partial x^2} dx$$

$$= -\hbar^2 \int \Psi^* \left[-\frac{2am}{\hbar}\left(1 - \frac{2amx^2}{\hbar}\right)\Psi\right] dx = 2am\hbar \left\{\int |\Psi|^2 dx - \frac{2am}{\hbar}\int x^2 |\Psi|^2 dx\right\}$$

$$= 2am\hbar \left(1 - \frac{2am}{\hbar}\langle x^2\rangle\right) = 2am\hbar \left(1 - \frac{2am}{\hbar}\frac{\hbar}{4am}\right) = 2am\hbar\left(\frac{1}{2}\right) = \boxed{am\hbar.}$$

5. At $t = 0$ a particle is represented by the wave function

$$\Psi(x,0) = \begin{cases} Ax/a, & \text{if } 0 \le x \le a \\ A(b-x)/(b-a), & \text{if } a \le x \le b \\ 0, & \text{otherwise} \end{cases}$$

where $a$ and $b$ are constants, and $A$ is a normalization constant.

(a) Normalize $\Psi(x,0)$.

(b) Sketch $\Psi(x,0)$ as a function of $x$.

(c) Where is the particle most likely to be found at $t = 0$?

(d) What is the probability of finding the particle to the left of the point $a$?

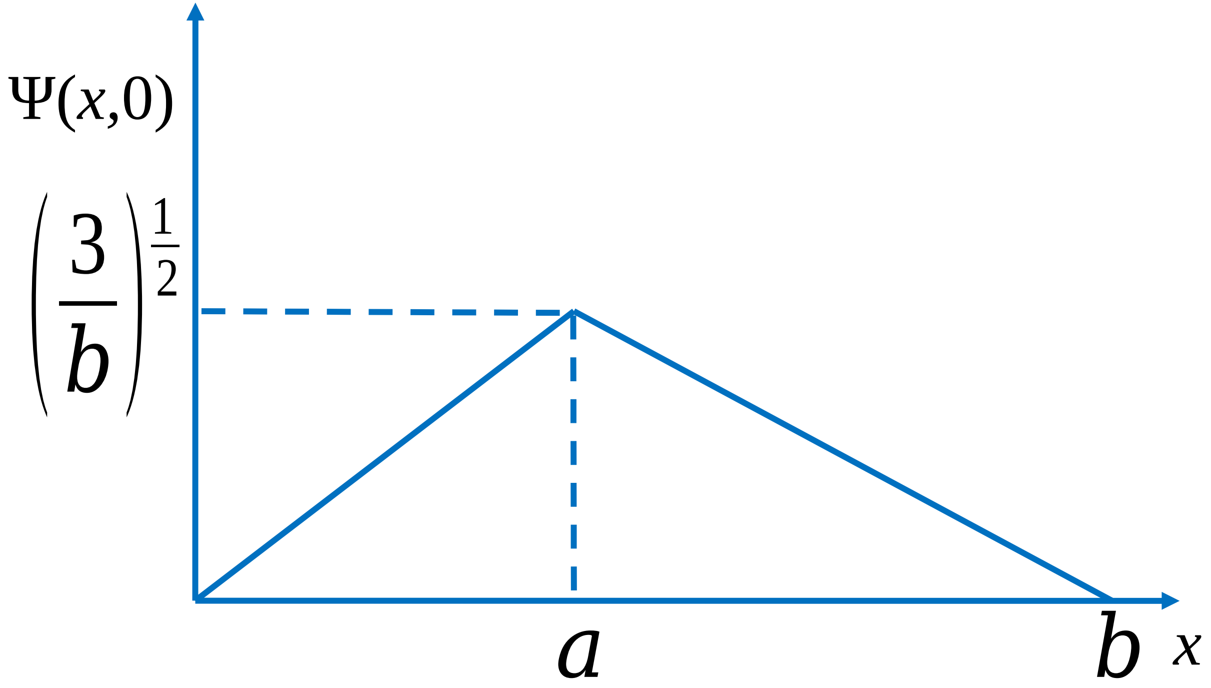
Ans.

(a) Using normalization condition: ;

$|A|^2$

$$A=\left(\frac{3}{b}\right)^{\frac{1}{2}}$$

(b)



(c) The particle is most likely to be found at  since amplitude of wave function is maximum there and hence, the probability of finding the particle is maximum there.

(d) Probability, :

$$\boxed{P = \frac{a}{b}}$$

6. A proton is confined in an infinite square well of width 10 fm. (The nuclear potential that binds protons and neutrons in the nucleus of an atom is often approximated by an infinite square well potential.)

- Calculate the energy and wavelength of the photon emitted when the proton undergoes a transition from the first excited state ($n = 2$) to the ground state ($n = 1$).
- In what region of the electromagnetic spectrum does this wavelength belong?

Ans. The energy $E_n$ of a particle of mass m in the nth energy state of an infinite square well potential with width L:

$$E = n^2h^2/8mL^2$$

The energy $E$ and wavelength λ of a photon emitted as the particle makes a transition from the $n = 2$ state to the $n = 1$ state are

$E = E_2 - E_1 = E = 3h^2/8mL^2$

$= hc/E$

For a proton ($m = 938\ \mathrm{MeV}/c^2$), $E = 6 \triangleright 15\mathrm{MeV}$ and $\lambda = 202\mathrm{fm}$. The wavelength is in the gamma ray region of the spectrum.

7. A particle with mass m is in an infinite square well potential with walls at $x = -L/2$ and $x = L/2$.
Write the wave functions for the states $n = 1$, $n = 2$ and $n = 3$

Ans. To obtain the wavefunctions $\psi_n(x)$ for a particle in an infinite square potential with walls at $x = -L/2$ and $x = L/2$

$$\psi_n(x) = \sin\left(\frac{n\pi\left(x+\frac{L}{2}\right)}{L}\right)$$

which satisfies $\psi_n(-L/2) = \psi_n(L/2) = 0$ as required. Thus,

$$\psi_1(x) = \cos\left(\frac{\pi x}{L}\right)$$

$$\psi_2(x) = \sin\left(\frac{2\pi x}{L}\right)$$

$$\psi_3(x) = \cos\left(\frac{3\pi x}{L}\right)$$

8. An electron is confined to a 1 micron thin layer of silicon. Assuming that the semiconductor can be adequately described by a one-dimensional quantum well with infinite walls, calculate the lowest possible energy within the material in units of electron volt. If the energy is interpreted as the kinetic energy of the electron, what is the corresponding electron velocity? (The effective mass of electrons in silicon is $m^* = 0.26\ m_0$, where $m_0 = 9.11 \times 10^{-31}$ kg is the free electron rest mass).

Ans.

The lowest energy in a quantum well is

$$E_1 = \frac{h^2}{2m^*}\left(\frac{1}{2L}\right)^2 = \frac{(6.626\times10^{-34})^2}{2\times0.26\times9.11\times10^{-31}}\left(\frac{1}{2\times10^{-6}}\right)^2$$

$= 2.32 \times 10^{-25}$ Joules $= 1.45$ meV.

The velocity of an electron with this energy equals:

$$v = \sqrt{\frac{2E_1}{m^*}} = \sqrt{\frac{2\times2.32\times10^{-25}}{0.26\times9.11\times10^{-31}}} = 1.399 \text{ km/s.}$$

9. A particle in a 1-D box has a minimum allowed energy of 2.5 eV.
(a) What is the next higher energy it can have? And the next higher after that? Does it have a maximum allowed energy?
(b) If the particle is an electron, how wide is the box?
(c) The fact that particles in a 1-D box have a minimum energy is not completely unrelated to the uncertainty principle. Find the minimum momentum of a particle, with mass m, trapped in a 1-D box of size L. How does this compare with the momentum uncertainty required by the uncertainty principle, if we assume $\Delta x = L$ ?

## Ans.

(a) $E_n = n^2\pi^2\hbar^2/(2mL^2)$
$E_1 = 2.5$ eV, $E_2 = 4*2.5$ eV $= 10$ eV, $E_3 = 9*2.5$ eV $= 22.5$ eV. There is no upper limit

(b) $2.5 \text{ eV}*1.6*10^{-19} \text{ J/eV} = \pi^2(1.05*10^{-34} \text{ Js})^2/(2*9.109*10^{-31} \text{ kg}*L^2)$
$L = 3.86*10^{-10}$ m.
The box has a width that is comparable to the typical size of an atom.

(c) $E_1 = p_{min}^2/(2m)$, $p_{min}^2 = (2*9.109*10^{-31} \text{ kg}*2.5 \text{ eV}*1.6*10^{-19} \text{ J/eV})$, $p_{min} = 8.5*10^{-25}$ kg m/s.
$\Delta p = \hbar/\Delta x = (1.05*10^{-34} \text{ Js})/(3.86*10^{-10} \text{ m}) = 2.7*10^{-25}$ kg m/s. The minimum momentum required by the uncertainty principle is approximately equal to $\Delta p$.
$\Delta p$ and $p_{min}$ have the same order of magnitude.

10.

An electron is traded in a one-dimensional potential well of length  m. Find the longest wavelength photons emitted by the electron as it changes energy levels in the well.

Ans. The allowed energy states of a particle of mass m trapped in an infinite potential well of length L are

$$E = n^2 \frac{(hc)^2}{8mc^2 L^2}$$

Therefore, the electron has allowed energy levels given by

$$\begin{aligned} E &= n^2 \frac{(hc)^2}{8mc^2 L^2} \\ E &= n^2 \frac{(1240)^2}{8(511000\text{eV})(0.4\text{nm})^2} \\ E &= n^2(2.35\text{eV}) \end{aligned}$$

As the electron changes energy levels, the energy released by the electron is in the form of a photon.

$$E_{photon} = E_{initial\ electron} - E_{final\ electron}$$
$$E_{photon} = (n_i^2 - n_f^2)2.35\text{eV}$$

Thus, the emitted wavelengths are

$$\lambda = \frac{hc}{E_{photon}}$$
$$\lambda = \frac{1240\text{eV nm}}{(n_i^2 - n_f^2)2.35\text{eV nm}}$$
$$\lambda = \frac{528\text{ nm}}{(n_i^2 - n_f^2)}$$

The longest wavelength photons involve the smallest value of $n_i^2 - n_f^2$. These are:

| $n_i$ | $n_f$ | $\lambda$ |
|---|---|---|
| 2 | 1 | 176nm |
| 3 | 2 | 106 nm |
| 4 | 3 | 75.6 nm |