of matter that every matter is associated with de-Broglie wave $\lambda=\frac{h}{mv}$. According to Heisenberg Uncertainty Principle, it is impossible to determine both the momentum and position of a particle simultaneously. Position and Momentum are complimentary variables and we cannot measure complementary variables of matter at same time to certainty.

Erwin Schrödinger thought that the quantum mechanical description of a particle can be done if we set up an equation involving the wave function as a function of *'r'* and *'t'*. It's a complex quantity whose representation in x-direction can be given as $\Psi = Ae^{\frac{-i}{\hbar(Et-Px)}}$. Being a complex quantity, it doesn't have a physical significance of its own but when it is multiplied with its complex conjugate, it gives us the probability amplitude $|\Psi(\vec{r},t)|^2$, the probability of finding the particle at that time and position (*Aharonov et al.* 1993).The wave function at a particular time contains all the information about the particle at any point '$\vec{r}$' at an instant of time 't'. Wavefunction ψ can have many possible solutions but only those solutions are acceptable in which $\psi(x)$ and $d\psi/dx$ are finite, single – valued, continuous and square integrable. Equations governing this wavefunction is called Schrödinger equation (*Verma, 2009*). The two types of Schrödinger equation are time independent and time dependent Schrödinger equation. Time dependent equation explains the behavior of the wave function with time and time independent describes the allowed energy state of the particle or probability of transition. However, these two are not different form, rather the time independent Schrödinger equation can be derived from time dependent Schrödinger equation(*Verma, 2009*).

For solving the problem of particle in a 3-D box, time independent Schrödinger equation is used. This research is a review of previous research work. We have calculated the energy of the particle inside the box for different quantum values of ***'n'***. Then the probability from ground state, up-to second excitation state and expectation value at different varied length for each mentioned state.

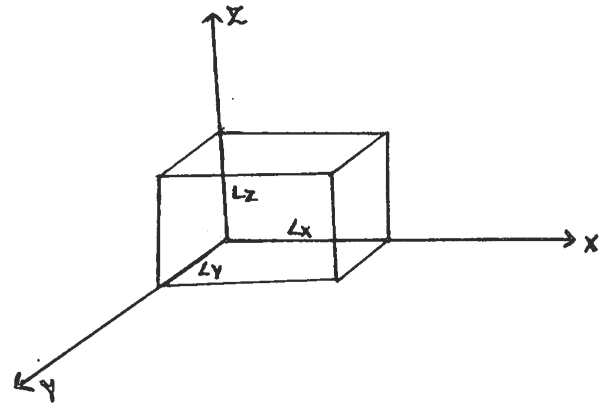

Fig. 1. Three - dimensional box

Materials and Methods :

We considered a 3-dimensionalboxhaving dimension L_x, L_y, L_z in x,y,z directions respectively (*Prakash, 2007*).

The potential energy V is zero inside the box and is infinity inside the box. Particle can be anywhere inside this box and the probability of finding the particle outside this box is zero.

The total energy E of the particle can be written assum of its kinetic energy and potential energy

$$E = K + V \qquad ...(1)$$

$$K = \frac{P^2}{2m}$$

For particle in 3-D box, kinetic energy

$$K = \left(\frac{P_x^2 + P_y^2 + P_z^2}{2m}\right)$$

The momentum operator P can be written as

$$P = -i\hbar\nabla$$

So,

$$p_x^2 + p_y^2 + p_z^2 = (-i\hbar\nabla)^2$$

$$K = \frac{(-i\hbar\nabla)^2}{2m}$$

So,

$$E = \left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) + \mathrm{V(x,y,z)}\right]$$

$$E\Psi(x,y,z) = \left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\right.\right.$$
$$\mathrm{V(x,y,z)}\,\Psi(x,y,z)\ldots\ (2)$$

From the independent Schrodinger's equation in 3-dimensions, we have

$$\left(\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}+\frac{\partial^2\Psi}{\partial z^2}\right)+\frac{2m}{\hbar^2}(E-V)\Psi(x,y,z) = 0 \qquad \ldots(3)$$

$$V(x,y,z) = V_x(x)+V_y(y)+V_z(z)$$

$$V_x(x) = 0 \ \ if\ 0<x<L_x, \text{else infinity;}$$

$$V_y(y) = 0 \ \ if\ 0<y<L_y, \text{else infinity;}$$

$$V_z(z) = 0 \ \ if\ 0<z<L_z, \text{else infinity;}$$

Using variables separation method ***Ψ****(x,y,z)* can be written as

$$\Psi(x,y,z) = X(x)Y(y)Z(z)$$

Hence, equation (3) becomes

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right) + \mathrm{V_x(x)} + \mathrm{V_y(y)} + \mathrm{V_z(z)}\right] X(x)Y(y)Z(z) = E\,X(x)Y(y)Z(z)$$

$$-\frac{\hbar^2}{2m}\mathrm{Y(y)Z(z)}\frac{\partial^2X(x)}{\partial x^2}+Y(y)Z(z)V_x(x)X(x) -\frac{\hbar^2}{2m}X(x)Z(z)\frac{\partial^2Y(y)}{\partial y^2} + X(x)Z(z)V_y(y)Y(y) -\frac{\hbar^2}{2m}X(x)Y(y)\frac{\partial^2Z(z)}{\partial z^2} + Y(y)X(x)\,V_z(z)Z(z)] = EX(x)Y(y)Z(z)$$

Dividing throughout by *X(x)Y(y)Z(z)*

$$-\frac{\hbar^2}{2m}\frac{1}{X(x)}\left(\frac{\partial^2X(x)}{\partial x^2}\right)+V_x(x) -\frac{\hbar^2}{2m}\frac{1}{Y(y)}\left(\frac{\partial^2Y(y)}{\partial x^2}\right)+V_y(y) -\frac{\hbar^2}{2m}\frac{1}{Z(z)}\left(\frac{\partial^2Z(z)}{\partial x^2}\right)+V_z(z) = E$$

$$E = E_x+E_y+E_z$$

Let,

$$-\frac{\hbar^2}{2m}\frac{1}{X(x)}\left(\frac{\partial^2X(x)}{\partial x^2}\right)+V_x(x) = E_x$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2X(x)}{\partial x^2}\right)+V_x(x)X(x) = E_xX(x)$$

Since $V_x(x) = 0$ if $0<x<L_x$, else infinity;

$$\text{So,}\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}\right)+\mathrm{V_x(x)}\right]X(x) = E_xX(x) \quad \ldots(4)$$

Equation (4) represents particle in 1-dimension,

For $V_x(x)=0$, equation (4) becomes

$$\left(\frac{\partial^2X(x)}{\partial x^2}\right)+\frac{2m}{\hbar^2}ExX(x) = 0 \qquad \ldots(5)$$

In order to solve equation (5),we put

$$\frac{2m}{\hbar^2}E = K^2$$

$$K = \frac{\sqrt{2mE}}{\hbar^2} \qquad \ldots(6)$$

$$\left(\frac{\partial^2X(x)}{\partial x^2}\right)+K^2X(x) = 0$$

The general solution of this second order differential equation is

$$X(x) = A\sin k_xx + B\cos k_xx$$

where,*A* and B are arbitrary constants.

Applying boundary conditions : $x=0$

$$X(x) = 0$$

$$Asin0 + Bcos0 = 0 + B$$

Therefore $B = 0$

Hence, $X(x) = A\sin k_x x$

At $x = L_x, X(x) = 0$

$$AsinK_xL_x = 0 \; as \; A \neq 0$$

$$\text{So,} \quad sinK_xL_x = 0$$

$$K_xL_x = 0, \pm x, \pm 2x, \pm 3x \dots$$

Since $K \neq 0$ and $L_x \neq 0$ and also will not be equal to any negative value so, in general

$$K_xL_x = n_x\pi$$

$$K_x = \frac{n_x\pi}{L_x} \qquad \dots (7)$$

Similarly,

$$\frac{\partial^2 Y(y)}{\partial y^2} + \frac{2m}{\hbar^2}E_yY(y) = 0$$

And the solution,

$$Y(y) = CsinK_yY + DcosK_yY$$

$$K_y = \frac{n_y\pi}{L_y} \qquad \dots (8)$$

Again

$$\frac{\partial^2 Z(z)}{\partial z^2} + \frac{2m}{\hbar^2}E_zZ(z) = 0$$

with solution,

$$Z(z) = EsinK_zZ + FcosK_zZ$$

$$K_z = \frac{n_z\pi}{L_z} \qquad \dots (9)$$

$$K_x = \frac{n_x\pi}{L_x} = \frac{\sqrt{2mE_x}}{\hbar^2}$$

from equations(6)and(7).

$$E_x = \frac{n_x^2\pi^2\hbar^2}{2mL_x^2} \qquad \dots (10a)$$

Similarly,

$$E_y = \frac{n_y^2\pi^2\hbar^2}{2mL_y^2} \qquad \dots (10b)$$

$$Ez = \frac{n_z^2\pi^2\hbar^2}{2mL_z^2} \qquad \dots (10c)$$

So total energy

$$E = E_x + E_y + E_z$$

$$E = \frac{\pi^2\hbar^2}{2m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right) \qquad \dots (11)$$

Also,

$$X(x) = AsinK_xX = Asin\left(\frac{n_x\pi}{L_x}\right)X$$

$$Y(y) = CsinK_yY = Csin\left(\frac{n_y\pi}{L_y}\right)Y$$

$$Z(z) = EsinK_zZ = Esin\left(\frac{n_z\pi}{L_z}\right)Z$$

So,

$$\Psi(x,y,z) = ACE\, sin\left(\frac{n_x\pi}{L_x}\right)X\, sin\left(\frac{n_y\pi}{L_y}\right)Y\, sin\left(\frac{n_z\pi}{L_z}\right)Z \qquad \dots (12)$$

According to normalization condition,

$$\int \Psi^*(x)\Psi(x)dx = 1$$

For

$$X(x) = A\, sinK_xX$$

$$\int_0^{L_x}(A\, sinK_xX \cdot A\, sinK_xX)\, dx = 1$$

$$A^2 \int_0^{Lx} sin^2 K_x X = 1$$

$$A^2 \left|\frac{K_x}{2}\right|_0^{L_x} = 1$$

$$A = \sqrt{\frac{2}{L_x}}$$

So,

$$X(x) = \sqrt{\frac{2}{L_x}}\, sin\left(\frac{n_x \pi}{L_x}\right) X$$

Similarly,

$$Y(y) = \sqrt{\frac{2}{L_y}}\, sin\left(\frac{n_y \pi}{L_y}\right) Y$$

$$Z(z) = \sqrt{\frac{2}{L_z}}\, sin\left(\frac{n_z \pi}{L_z}\right) Z$$

So, equation (12) becomes,

$$\Psi(x, y, z) = \sqrt{\frac{8}{L_x L_y L_z}}\, sin\left(\frac{n_x \pi}{L_x}\right) X\, sin\left(\frac{n_y \pi}{L_y}\right) Y\, sin\left(\frac{n_z \pi}{L_z}\right) Z \quad ...(13)$$

After obtaining the wave function ψ *(x,y,z)*, theprobability of finding the particle in the box can be calculated. Since the particle is surely presentanywhere inside the box and probability of finding it outside the box is zero so it can be calculated by the formula(Arvind et al., 2018)

$$P = \int\int\int [\Psi(x, y, z)]^2 d\tau$$

where $d\tau = dxdydz$

$$P = \int\int\int \left[\sqrt{\frac{8}{L_x L_y L_z}}\, \sin\left(\frac{n_x \pi}{L_x}\right) X \sin\left(\frac{n_y \pi}{L_y}\right) Y \sin\left(\frac{n_z \pi}{L_z}\right) Z\right]^2 dxdydz \quad ...(14)$$

$$P = \int\int\int \left[\sqrt{\frac{8}{V}}\, \sin\left(\frac{n_x \pi}{L_x}\right) X \sin\left(\frac{n_y \pi}{L_y}\right) Y \sin\left(\frac{n_z \pi}{L_z}\right) Z\right]^2 dxdydz \quad ...(15)$$

where V = volume of the box = $L_x L_y L_z$

The Expectation value of the particle can be calculated by

$$\langle V\rangle = \sqrt{\frac{8}{V}} \iiint \left[\sin\left(\frac{n_x \pi}{L_x}\right) X \sin\left(\frac{n_y \pi}{L_y}\right) Y \sin\left(\frac{n_z \pi}{L_z}\right) Z\right]^2 xyz\, dxdydz$$

where $V = L^3$ = volume of the box.

Results and Discussion :

As we saw earlier, to find the value of energy levels of particle in 1-dimensional box, we have the following relation (*Polkinghorne,* 2002)

$$E = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

Substituting $\hbar = h/2\pi$ wehavethefollowing relation:

$$E = \frac{h^2}{8mL^2} n^2 \qquad (\because a = L)$$

Further generalization of this equation gives us theresult as:

$$E = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$$

Now we are considering a cube, therefore

$$L_x = L_y = L_z = L$$

The values ofvarious energy levels were calculated

as

$$E_{n_x, n_y, n_z} = \frac{h^2}{8mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

For ground zero state we have$n_x = n_y = n_z = 1$

$$E_{1,1,1} = \frac{3h^2}{8mL^2}$$

where $\frac{h^2}{8mL^2}$ being a constant, because h- Planck's constant whose value is 6.626 × 10^{-34} m^2 -kg/sec

$$h^2 = 43.90 \times 10^{-68} m^2 - kg/sec$$

$$m = 9.11 \times 10^{-31}\, kg$$

$$L = 0.5\ \text{Å}$$

Therefore,

$$\frac{h^2}{8mL^2} = \frac{43.90 \times 10^{-68}}{8 \times 9.11 \times 10^{-31} \times 0.5 \times 0.5 \times 10^{-20}}$$

$$= 2.409 \times 10^{17}$$

$$E_{1,1,1} = \frac{3h^2}{8mL^2} = 3 \times 2.409 \times 10^{17}$$

$$E_{1,1,1} = 7.228 \times 10^{-17}\, J$$

Degeneracy

The energy of a state dependson the sum of square of quantum numbers. If the particles arehaving different wavefunctions(can be stationary) at a particular value of energy, then these states are said to be degenerate.

For example, for the first excited state there are three sets of quantum numbers possible. They are – (1,1,2), (1,2,1), (2,1,1). The sum of squares of these sets of quantum numbers is 6. Each wavefunction has same energy *i.e.*

$$E\,(1,1,2) = E(1,2,1) = E(2,1,1) = \frac{6h^2}{8mL^2}\, J$$

Hence the number of independent wavefunction for an energy level is called degree of degeneracy of the energy level (Supriadi et al.2019).

Table 1. The result of particle energy levels in three-dimensional boxes

$n_x^2 + n_y^2 + n_z^2$	Possible Combinat-ions	Energy	Energy Value (in×10^{-17} J)	Degree of degeneracy
3	(1,1,1)	$\frac{3h^2}{8mL^2}$	7.228	1
6	(1,1,2) (1,2,1) (2,1,1)	$\frac{6h^2}{8mL^2}$	14.454	3
9	(2,2,1) (2,1,2) (1,2,2)	$\frac{9h^2}{8mL^2}$	21.681	3
11	(3,1,1) (1,3,1) (1,1,3)	$\frac{11h^2}{8mL^2}$	26.499	3
12	(2,2,2)	$\frac{12h^2}{8mL^2}$	28.908	1

Therefore, we saw that energy level of a particle depends on the value of n^2 *i.e.* square of quantum number (*Lal et al. 2008*).

Calculation of probability

We calculated the probability of a particle in a 3-dimensional box using the following equation-

$$P = \iiint \left[\sqrt{\frac{8}{V}} \sin\left(\frac{n_x\pi}{L_x}\right) X \sin\left(\frac{n_y\pi}{L_y}\right) Y \sin\left(\frac{n_z\pi}{L_z}\right) Z \right]^2 dxdydz$$

We have: $V = Lx\,Ly\,Lz$

$Lx = Ly = Lz = L$ (sides of a cube)

we have used variation in the width of cube which are, $\frac{L}{4}, \frac{L}{2}, \frac{3L}{4}, L.$ We kept the quantum number same which is $n_x = n_y = n_z$.

We obtained the following table based on our calculation.

Table 2. The result of mathematical data on particle probability values in a three-dimensional box

State	Box Width	Probability
(1,1,1)	$\frac{L}{4}$	0.00075
	$\frac{L}{2}$	0.125
	$\frac{3L}{4}$	0.206
	L	1
(2,2,2)	$\frac{L}{4}$	0.016
	$\frac{L}{2}$	0.125
	$\frac{3L}{4}$	0.421
	L	1
(3,3,3)	$\frac{L}{4}$	0.028
	$\frac{L}{2}$	0.125
	$\frac{3L}{4}$	0.339
	L	1

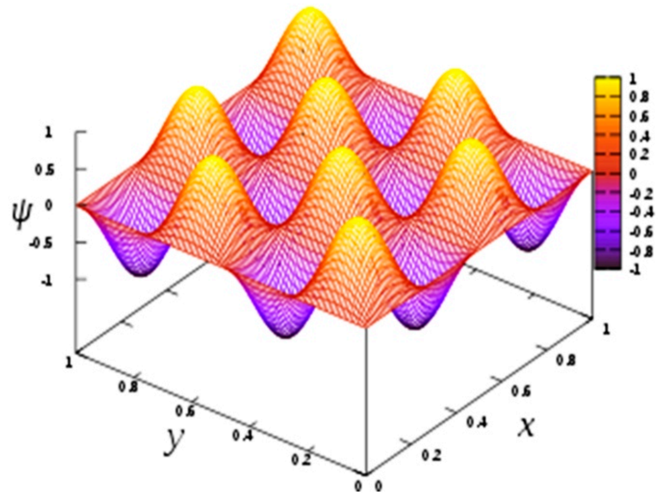

Fig. 2. Wavefunction representing probability of a particle in a 3D box

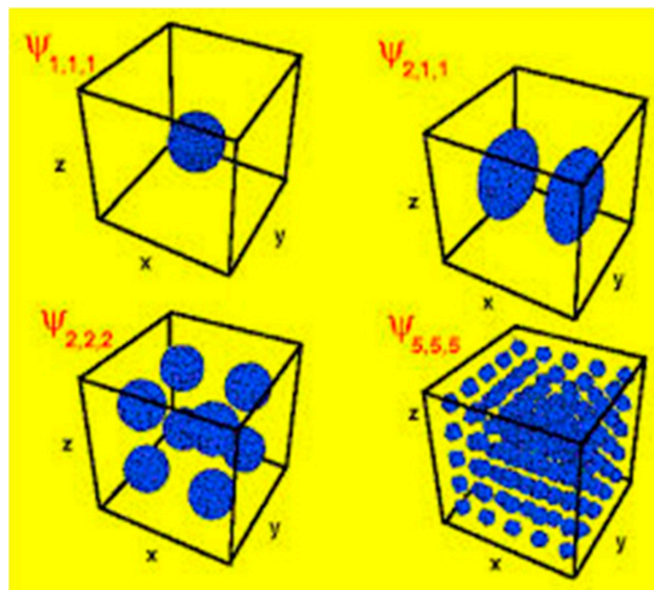

Fig. 3. Visualizing the probability of a particle in a 3D box

Calculation of expectation value

For the calculation of expectation values of a particle in 3-dimensional box we have used the formula(Supriadi et al.2019):

$$\langle V \rangle =$$

$$= \sqrt{\frac{8}{V}} \iiint \left[\sin\left(\frac{n_x\pi}{L_x}\right) X \sin\left(\frac{n_y\pi}{L_y}\right) Y \sin\left(\frac{n_z\pi}{L_z}\right) Z \right]^2 xyzdxdydz$$

where $V = L_x L_y L_z = L_3 =$ volume of the box.

Based on our calculation we have the following table:

Table 3. The result of mathematical data on particle expectation values in a three-dimensional box

State	Box Width	Expectation Values
(1,1,1)	$\frac{L}{4}$	0.0000047
	$\frac{L}{2}$	0.0054
	$\frac{3L}{4}$	0.077
	L	0.125
(2,2,2)	$\frac{L}{4}$	0.000084
	$\frac{L}{2}$	0.0019
	$\frac{3L}{4}$	0.025
	L	0.125
(3,3,3)	$\frac{L}{4}$	0.00012
	$\frac{L}{2}$	0.022
	$\frac{3L}{4}$	0.014
	L	0.125

Conclusions :

The probability value of particles depends on square of quantum number and the variation in width of the box. The probability of finding particles at the width of L/2 and L remains same for all the states. In addition to probability the report also tells us about the energy possessed by the particle. The analysis tells us about the variation of energy level with changing box width and quantum number. The expectation value of particles with box width L is same for all the values of quantum numbers.

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