Harmonic Oscillator

$$\frac{d^2\phi(x)}{dx^2}+\frac{2m}{\hbar^2}\left[E-\frac{1}{2}kx^2\right]\phi(x)=0$$

The ground state Eigen function is of the following form.

$$\phi(x)=Ae^{-\alpha x^2}$$

Derivatives

$$\phi(x)=Ae^{-\alpha x^2}$$

$$\frac{d\phi}{dx}=Ae^{-\alpha x^2}\times(-2\alpha x)$$

$$\frac{d^2\phi}{dx^2}=Ae^{-\alpha x^2}\times(-2\alpha x)^2+Ae^{-\alpha x^2}\times(-2\alpha)$$

Substitution

$$Ae^{-\alpha x^2}\times(-2\alpha x)^2+Ae^{-\alpha x^2}\times(-2\alpha)$$
$$+\frac{2m}{\hbar^2}\left(E-\frac{1}{2}kx^2\right)\times Ae^{-\alpha x^2}=0$$

$$(-2\alpha x)^2+(-2\alpha)+\frac{2m}{\hbar^2}\left(E-\frac{1}{2}kx^2\right)=0$$

Reorganizing Terms

$$(-2\alpha x)^2+(-2\alpha)+\frac{2m}{\hbar^2}\left(E-\frac{1}{2}kx^2\right)=0$$

$$\left(4\alpha^2-\frac{mk}{\hbar^2}\right)x^2+\left(\frac{2mE}{\hbar^2}-2\alpha\right)=0$$

Equating Coefficients to Zero

$$\left(4\alpha^2-\frac{mk}{\hbar^2}\right)x^2+\left(\frac{2mE}{\hbar^2}-2\alpha\right)=0$$

$$4\alpha^2-\frac{mk}{\hbar^2}=0\Rightarrow\alpha=\frac{\sqrt{mk}}{2\hbar}$$

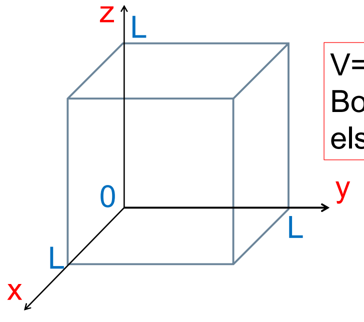
$$\frac{2mE}{\hbar^2}-2\alpha=0\Rightarrow E=\frac{\alpha\hbar^2}{m}$$

Energy Eigen Value

$$\alpha=\frac{\sqrt{mk}}{2\hbar}$$

$$E=\frac{\alpha\hbar^2}{m}=\frac{\sqrt{mk}}{2\hbar}\times\frac{\hbar^2}{m}=\frac{1}{2}\hbar\sqrt{\frac{k}{m}}=\frac{1}{2}\hbar\omega$$

A particle in a 3-d Cubical Box



V=0 within Box, V=∞, elsewhere.

$$\nabla^2\phi+\frac{2m}{\hbar^2}(E-V)\phi=0$$

$$\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}+\frac{\partial^2\phi}{\partial z^2}+\frac{2m}{\hbar^2}E\phi=0$$

We solve by using method of separation of variables. Let us try the following.

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

Substituting in the Schrödinger Equation we get

$$YZ\frac{d^2X}{dx^2} + XZ\frac{d^2Y}{dy^2} + XY\frac{d^2Z}{dz^2}$$
$$+\frac{2mE}{\hbar^2}XYZ = 0$$

$$YZ\frac{d^2X}{dx^2} + XZ\frac{d^2Y}{dy^2} + XY\frac{d^2Z}{dz^2}$$
$$+\frac{2mE}{\hbar^2}XYZ = 0$$
$$\frac{1}{X}\frac{d^2X}{dx^2} + \frac{1}{Y}\frac{d^2Y}{dy^2} + \frac{1}{Z}\frac{d^2Z}{dz^2} = -\frac{2mE}{\hbar^2}$$

Could separate all the three variables in one shot.

This gives

$$\frac{1}{X}\frac{d^2X}{dx^2} = -k_x^{\ 2}$$
$$\frac{1}{Y}\frac{d^2Y}{dy^2} = -k_y^{\ 2}$$
$$\frac{1}{Z}\frac{d^2Z}{dz^2} = -k_z^{\ 2}$$

$$\boxed{k_x^{\ 2} + k_y^{\ 2} + k_z^{\ 2} = \frac{2mE}{\hbar^2}}$$

Solution for X

The general solution

$$X = A_x \sin(k_x x) + B_x \cos(k_x x)$$

Boundary Conditions

$$\phi(0,y,z) = 0; \quad \phi(L,y,z) = 0$$

irrespective of the values of y and z. This implies

$$X(0)=0; \quad X(L)=0$$

Like before this gives

$$B_x=0$$
$$k_xL=n_x\pi$$
$$X=A_x\sin(k_xx)$$

In a similar way, we shall find out

$$k_yL=n_y\pi$$
$$Y=A_y\sin(k_yy)$$
$$k_zL=n_z\pi$$
$$Z=A_z\sin(k_zz)$$

$$\boxed{k_x{}^2+k_y{}^2+k_z{}^2=\frac{2mE}{\hbar^2}}$$

$$E=\frac{\hbar^2}{2m}\left(k_x{}^2+k_y{}^2+k_z{}^2\right)$$
$$=\frac{\pi^2\hbar^2}{2mL^2}\left(n_x{}^2+n_y{}^2+n_z{}^2\right)$$

The wave function is

$$\phi(x,y,z)=A\sin\left(\frac{n_x\pi x}{L}\right)\sin\left(\frac{n_y\pi y}{L}\right)\sin\left(\frac{n_z\pi z}{L}\right)$$

The constant A has to be found from normalization.

Comments

- There are three independent quantum numbers which determine energy.
- The quantum numbers n_x=1, n_y=1, n_z=1gives the ground state energy.

- There are different set of quantum numbers which give the same energy, even though different wave functions.
- The first excited state is triply degenerate (2,1,1), (1,2,1), (1,1,2).

Can k_x be imaginary?

Is there a possibility that one of the k_i^2 is negative and others are positive, such that sum is positive?

$$X = A_x e^{\alpha x} + B_x e^{-\alpha x}; \alpha = \sqrt{-k_x^{\ 2}}$$

The boundary conditions yield the following.

$$A_x + B_x = 0$$

$$A_x e^{\alpha L} + B_x e^{-\alpha L} = 0$$

$$A_x e^{\alpha L} = A_x e^{-\alpha L}$$

A_x=0 or $\alpha L = 0$

If $\alpha = 0$

$X = A_x + B_x = 0$