Answer on Question #44189, Physics, Quantum Mechanics

Question:

a) Calculate the components of energy along x, y and z axes and the total energy for an electron in a cubical box of length 10^-9 m, if nx = 3, ny =nz =1. State the values of nx, ny and nz for two other energy states which are degenerate with this level.

Hint: Use the principle of calculation of energy of a particle in the three dimensional box. (5)

Answer:

The time-independent Schrodinger equation:

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

Since we are dealing with a 3-dimensional figure, we need to add the 3 different axes into the Schrodinger equation:

$$-\frac{\hbar^2}{2m}\left(\frac{d^2\psi(r)}{dx^2} + \frac{d^2\psi(r)}{dy^2} + \frac{d^2\psi(r)}{dz^2}\right) = E\psi(r)$$

The easiest way in solving this partial differential equation is by having the wave function equal to each individual function for its individual variable:

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

Now each function has its own variable:

Now substitute $\Psi(x, y, z)$into Schrodinger equation and divide it by the product, $X(x)Y(y)Z(z)$:

$$-\frac{\hbar^2}{2m}\left(\frac{1}{X(x)}\frac{d^2\psi(r)}{dx^2} + \frac{1}{Y(y)}\frac{d^2\psi(r)}{dy^2} + \frac{1}{Z(z)}\frac{d^2\psi(r)}{dz^2}\right) = E$$

Now separate each term in last equation to equal zero:

$$\frac{d^2X}{dx^2} + \frac{2m}{\hbar^2}E_x X = 0$$

$$\frac{d^2Y}{dx^2} + \frac{2m}{\hbar^2}E_y X = 0$$

$$\frac{d^2Z}{dx^2} + \frac{2m}{\hbar^2} E_z X = 0$$

Solution for this equation is (the same for variables y and z):

$$E_x = \frac{n_x^2 h^2}{8ma^2}$$

Now we can add all the energies together to get the total energy:

$$E = E_x + E_y + E_z = \frac{h^2}{8ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

The component of energy along x axis:

$$E_x = \frac{n_x^2 h^2}{8ma^2} \cong 3.39\ eV$$

The components of energy along y and z axes:

$$E_y = E_z = \frac{n_x^2 h^2}{8ma^2} = \frac{h^2}{8ma^2} \cong 0.38\ eV$$

Total energy equals:

$$E = E_x + E_y + E_z \cong 4.15\ eV$$

Other 2 states with the same energy are:

$$n_x^2 + n_y^2 + n_z^2 = 3^2 + 1 + 1 = 11$$

$$n_x = 1, n_y = 1, n_z = 3$$

$$n_x = 1, n_y = 3, n_z = 1$$