ENGINEERING PHYSICS

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Class #30

We have discussed the case of 1D infinite potential well (symmetrically located about the origin defined by $-\frac{a}{2} < x < \frac{a}{2}$) and what we get on Solving Schrodinger's equation are the

Eigen functions $\psi_n = \sqrt{\frac{2}{a}}\cos\left(\frac{n\pi}{a}x\right)$ *for n = 1,3,5,..*

$\psi_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$ *for n = 2,4,6,..* *and*

Eigen values $E_n = \frac{n^2h^2}{8ma^2}$

Infinite potential well (2D & 3D)

We have also discussed the case of 1D infinite potential well (located between $0 < x < a$) and what we get on Solving Schrodinger's equation are the

Eigen functions $\psi_n = \sqrt{\frac{2}{a}} sin\left(\frac{n\pi}{a}x\right)$ *for n = 1,2,3,4,5,.. and*

Eigen values $E_n = \frac{n^2h^2}{8ma^2}$

Now the natural question is how do we handle 2D and 3D infinite potential wells?

The starting point is to first define the wells

Infinite potential well (2D & 3D)

We will first handle the case of 3D well and then point to the changes that needs to be made for a 2D well

3D infinite potential well defined as follows (this well is cubical)

$$-\frac{a}{2} < x < \frac{a}{2}, \quad -\frac{a}{2} < y < \frac{a}{2}, \quad -\frac{a}{2} < z < \frac{a}{2}$$

Inside the well V = 0 and outside the well $V = \infty$

To obtain the eigen functions and eigen values we need to solve the Schrodinger's equation

Infinite potential well, 3D)

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Schrodinger's equation in 3D: $\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\psi = 0$

This can be written as $\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2} + \frac{2m}{\hbar^2}(E - V)\psi = 0$

This time we should be aware that ψ *is a function of x, y and z, i.e.* $\psi(x, y, z)$

This equation is a partial differential equation and can be solved by separation of variables as $\psi(x, y, z) = X(x)Y(y)Z(z)$

Infinite potential well, 3D

If we substitute $\psi(x,y,z) = X(x)Y(y)Z(z)$ in Schrodinger's equation, we get $\frac{\partial^2 XYZ}{\partial x^2} + \frac{\partial^2 XYZ}{\partial y^2} + \frac{\partial^2 XYZ}{\partial z^2} + \frac{2m}{\hbar^2}(E-V)XYZ = 0$

Remembering that V = 0 inside the well we have

$$\frac{\partial^2 XYZ}{\partial x^2} + \frac{\partial^2 XYZ}{\partial y^2} + \frac{\partial^2 XYZ}{\partial z^2} + \frac{2mE}{\hbar^2} XYZ = 0$$

The equation can be simplified as

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

Infinite potential well, 3D

Dividing throughout by XYZ we get

$$\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{1}{Z}\frac{d^2Z}{dz^2}+\frac{2mE}{\hbar^2}=0,\ \textit{Now}\ \frac{2mE}{\hbar^2}=k^2.$$

In 3D the propagation constant k is given by $k^2=k_x^2+k_y^2+k_z^2$

Thus $\frac{1}{X}\frac{d^2X}{dx^2}+\frac{1}{Y}\frac{d^2Y}{dy^2}+\frac{1}{Z}\frac{d^2Z}{dz^2}+k_x^2+k_y^2+k_z^2=0$ *or*

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

Infinite potential well, 3D

Comparing the LHS and RHS we have three 1D ordinary differential equations

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

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

The solutions to these are $X = A\cos(k_xx) + B\sin(k_xx)$

$Y = C\cos(k_yy) + D\sin(k_yy)$ *and* $Z = G\cos(k_zz) + H\sin(k_zz)$

Infinite potential well, 3D

Applying boundary conditions

$X = 0$ *at* $x = \pm\frac{a}{2}$, $Y = 0$ *at* $y = \pm\frac{a}{2}$ *and* $Z = 0$ *at* $z = \pm\frac{a}{2}$ *we get*

$k_x = \frac{n_x\pi}{a}$, $k_y = \frac{n_y\pi}{a}$ *and* $k_z = \frac{n_z\pi}{a}$

The eigen energies are then given by $E_{n_x n_y n_z} = \frac{(n_x^2+n_y^2+n_z^2)h^2}{8ma^2}$

The normalized eigen functions are given by

Infinite potential well, 3D

$X_n = \sqrt{\frac{2}{a}}\cos\left(\frac{n_x\pi}{a}x\right)$ for n_x = 1,3,5,.. **and** $X_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n_x\pi}{a}x\right)$ for n_x = 2,4,6,..

$Y_n = \sqrt{\frac{2}{a}}\cos\left(\frac{n_y\pi}{a}y\right)$ for n_y = 1,3,5,.. **and** $Y_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n_y\pi}{a}y\right)$ for n_y = 2,4,6,..

$Z_n = \sqrt{\frac{2}{a}}\cos\left(\frac{n_z\pi}{a}z\right)$ for n_z = 1,3,5,.. **and** $Z_n = \sqrt{\frac{2}{a}}\sin\left(\frac{n_z\pi}{a}z\right)$ for n_z = 2,4,6,..

Infinite potential well, 3D

If we define the well as $0 < x < a$, $0 < y < a$ and $0 < z < a$ and solve for the eigen functions then we get

$$X_n = \sqrt{\frac{2}{a}}\, sin\left(\frac{n_x\pi}{a}x\right),\ Y_n = \sqrt{\frac{2}{a}}\, sin\left(\frac{n_y\pi}{a}y\right) \text{ and } Z_n = \sqrt{\frac{2}{a}}\, sin\left(\frac{n_z\pi}{a}z\right),$$ *with*

n_x, n_y and n_z having values 1,2,3,4, …….

The eigen value expression remains the same.

Infinite potential well, 3D

Let us look at the eigen energies, $E_{n_x n_y n_z} = \frac{(n_x^2+n_y^2+n_z^2)h^2}{8ma^2}$

They are definitely quantized. Keep in mind that n_x, n_y, and n_z can take values 1,2,3,….

The lowest energy is given by $E_{111} = \frac{(3)h^2}{8ma^2}$. *The next energy is* $E_{211} = \frac{(6)h^2}{8ma^2}$. *We also have* $E_{121} = \frac{(6)h^2}{8ma^2}$ *and* $E_{112} = \frac{(6)h^2}{8ma^2}$. *The states corresponding to the energies can be written as* $\psi_{n_x n_y n_z}$. *For example* ψ_{211}, ψ_{121} *and* ψ_{112} *represent states corresponding to the energy* $\frac{(6)h^2}{8ma^2}$

Infinite potential well, 3D

- *Eigen functions represented for the states ψ_{211}, ψ_{121} and ψ_{112}*
- *For the well defined by $-\frac{a}{2} < x < \frac{a}{2}, -\frac{a}{2} < y < \frac{a}{2}$ and $-\frac{a}{2} < z < \frac{a}{2}$*
- $\psi_{211} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} \sin\left(\frac{2\pi}{a}x\right)\cos\left(\frac{\pi}{a}y\right)\cos\left(\frac{\pi}{a}z\right)$
- $\psi_{121} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} \cos\left(\frac{\pi}{a}x\right)\sin\left(\frac{2\pi}{a}y\right)\cos\left(\frac{\pi}{a}z\right)$
- $\psi_{112} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} \cos\left(\frac{\pi}{a}x\right)\cos\left(\frac{\pi}{a}y\right)\sin\left(\frac{2\pi}{a}z\right)$

Infinite potential well, 3D

- *For the well defined by* $0 < x < a, 0 < y <$*a and* $0 < z < 0$

- $\psi_{211} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} sin\left(\frac{2\pi}{a}x\right) sin\left(\frac{\pi}{a}y\right) sin\left(\frac{\pi}{a}z\right)$

- $\psi_{121} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} sin\left(\frac{\pi}{a}x\right) sin\left(\frac{2\pi}{a}y\right) sin\left(\frac{\pi}{a}z\right)$

- $\psi_{112} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} sin\left(\frac{\pi}{a}x\right) sin\left(\frac{\pi}{a}y\right) sin\left(\frac{2\pi}{a}z\right)$

Infinite potential well, 2D

Now let us go to the 2D infinite potential well and look at the eigen energies.

Starting from the 3D eigen energy expression, $E_{n_x n_y n_z} = \frac{(n_x^2+n_y^2+n_z^2)h^2}{8ma^2}$, *we now assume that there is no z variable. Thus, we have* $E_{n_x n_y} = \frac{(n_x^2+n_y^2)h^2}{8ma^2}$

As before the energy is quantized. The lowest energy is given by $E_{11} = \frac{(2)h^2}{8ma^2}$

The next energy is $E_{21} = \frac{(5)h^2}{8ma^2}$. *We also have* $E_{12} = \frac{(5)h^2}{8ma^2}$

Infinite potential well, 2D

Now what about the eigen functions? (for the well defined by $-\frac{a}{2} < x < \frac{a}{2}, and\ -\frac{a}{2} < y < \frac{a}{2}$*)*

Again, we start from the 3D case and this time eliminate the z variable to get

$X_n = \sqrt{\frac{2}{a}} cos\left(\frac{n_x \pi}{a} x\right)$ *for* n_x *= 1,3,5,.. and* $X_n = \sqrt{\frac{2}{a}} sin\left(\frac{n_x \pi}{a} x\right)$ *for* n_x *= 2,4,6,..*

$Y_n = \sqrt{\frac{2}{a}} cos\left(\frac{n_y \pi}{a} y\right)$ *for* n_y *= 1,3,5,.. and* $Y_n = \sqrt{\frac{2}{a}} sin\left(\frac{n_y \pi}{a} y\right)$ *for* n_y *= 2,4,6,..*

Infinite potential well, 2D

For the eigen functions for the well defined by $0 < x < a$, $and\ 0 < y < a$

Again, we start from the 3D case and this time eliminate the z variable to get

$$X_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n_x \pi}{a} x\right) \text{ for } n_x = 1,2,3,..$$

$$Y_n = \sqrt{\frac{2}{a}} \sin\left(\frac{n_y \pi}{a} y\right) \text{ for } n_y = 1,2,3,..$$

Infinite potential well, 2D

What then would the eigen function be for (1,2) and (2,1) states? To keep things simple, we will consider the well defined by $0 < x < a, and\ 0 < y < a$

The eigen functions are

$$\psi_{12} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} sin\left(\frac{\pi}{a}x\right) sin\left(\frac{2\pi}{a}y\right)$$ *Both states have energy given by* $E = \frac{(5)h^2}{8ma^2}$

$$\psi_{21} = \sqrt{\frac{2}{a}}\sqrt{\frac{2}{a}} sin\left(\frac{2\pi}{a}x\right) sin\left(\frac{\pi}{a}y\right)$$

Try to get the eigen functions for the well defined by $-\frac{a}{2} < x < \frac{a}{2}, and\ -\frac{a}{2} < y < \frac{a}{2}.$

Class #30 …….. Quiz….

If the dimensions of a 3D well were a_x, a_y and a_z, which of the following would be the correct expression for the energy?

- ❑ $E_{n_x n_y n_z} = \frac{(n_x^2+n_y^2+n_z^2)h^2}{8m(a_x^2+a_y^2+a_z^2)}$
- ❑ $E_{n_x n_y n_z} = \left(\frac{n_x^2}{a_x^2} + \frac{n_y^2}{a_y^2} + \frac{n_z^2}{a_z^2}\right)\frac{h^2}{8m}$
- ❑ $E_{n_x n_y n_z} = \left(n_x^2 a_x^2 + n_y^2 a_y^2 + n_z^2 a_z^2\right)\frac{h^2}{8ma^2}$
- ❑ $E_{n_x n_y n_z} = \left(\frac{n_x^2}{a_x} + \frac{n_y^2}{a_y} + \frac{n_z^2}{a_z}\right)\frac{h^2}{8m}$

THANK YOU

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