ENGINEERING PHYSICS

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Class #19

- **Eigen functions and eigen energy values in a 2D potential well**
- **Eigen functions and eigen energy values in a 3D potential well**

➢ *Suggested Reading*

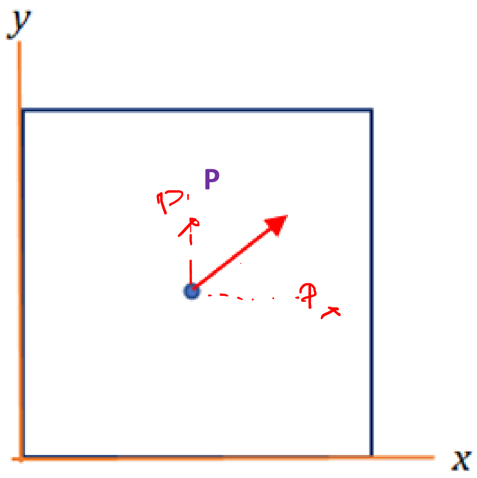
1. *Concepts of Modern Physics, Arthur Beiser, Chapter 5*
2. *Learning Material prepared by the Department of Physics*

➢ *Reference Videos*

1. *Video lectures : MIT 8.04 Quantum Physics I*
2. *Engineering Physics Class #17 & #18*

Particle bound in a 2D potential Box

- ***A particle in a 2D potential box has two degrees of freedom and bound by infinite potentials at the boundaries***



- ***The momentum P of a particle moving in the x y plane can be resolved into two independent momentum components P_x and P_y along the x and y directions.***

- ***Two independent problems for the x and y directions and the solutions would be similar to the one dimensional infinite potential well problem.***

Particle bound in a 2D potential Box

The Schrodinger's equation for motion in the x direction can be written as

$$\frac{\partial^2\psi}{\partial x^2} + \frac{2m}{\hbar^2}E\psi = 0 \quad or \quad \frac{\partial^2\psi}{\partial x^2} + {k_x}^2\psi = 0$$

where $k_x = \sqrt{\frac{2mE_x}{\hbar^2}}$ *and the solutions are*

$\psi_{n_x}(x) = \sqrt{\frac{2}{a}}\cos\left(\frac{n_x\pi}{a}x\right)$ $for\ n_x\ odd$ (even parity)

$\psi_{n_x}(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n_x\pi}{a}x\right)$ $for\ n_x\ even$ (odd parity)

with the eigen values for energy as $E_x = \frac{h^2{n_x}^2}{8ma^2}$

where n_x can take values 1,2,3,4,5

Particle bound in a 2D potential Box

The Schrodinger's equation for motion in the y direction can be written as

$$\frac{\partial^2\psi}{\partial y^2} + \frac{2m}{\hbar^2}E_y\psi = 0 \ or \ \frac{\partial^2\psi}{\partial y^2} + {k_y}^2\psi = 0$$

where $k_y = \sqrt{\frac{2mE_y}{\hbar^2}}$ *and the solutions are*

$$\psi_{n_y}(y) = \sqrt{\frac{2}{a}}cos\left(\frac{n_y\pi}{a}x\right) \quad for\ n_y\ odd \qquad \text{(even parity)}$$

$$\psi_{n_y}(y) = \sqrt{\frac{2}{a}}sin\left(\frac{n_y\pi}{a}x\right) \quad for\ n_y\ even \qquad \text{(odd parity)}$$

with the eigen values for energy as $E_y = \frac{h^2{n_y}^2}{8ma^2}$

where n_y can take values 1,2,3,4,5

Particle bound in a 2D potential Box

The eigen function of the system can be written as

$$\psi_{n_x n_y} = \psi_{n_x} \times \psi_{n_y}$$

The first allowed state with $n_x = n_y = 1$ *gives the wave function*

$$\psi_{11} = \frac{2}{a} cos\left(\frac{\pi}{a} x\right) \; cos\left(\frac{\pi}{a} y\right)$$

The next allowed state with $n_x = 2$ *and* $n_y = 1$ *gives the wave function*

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

The allowed state with $n_x = 1$ *and* $n_y = 2$ *gives the wave function*

$$\psi_{12} = \frac{2}{a} cos\left(\frac{\pi}{a} x\right) \; sin\left(\frac{2\pi}{a} y\right)$$

Particle bound in a 2D potential Box

The energy eigen values of the particle can be written as

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

where n_x *,* n_y *can take values* ***1,2,3,4,5***

The first allowed energy state of the system is

$E_{11} = 2\frac{h^2}{8ma^2} = 2E_o$ **where** $E_o = \frac{h^2}{8ma^2}$.

The next allowed energy state

$\mathrm{E}_{21} = 5\mathrm{E}_o$ *which is also the energy of the state* E_{12}

This energy state is degenerate !

Particle bound in a 2D potential Box

The states ψ_{21} *and* ψ_{12} *with energy* $5E_o$ *are degenerate states with a degeneracy factor of 2.*

In general, for a 2D system

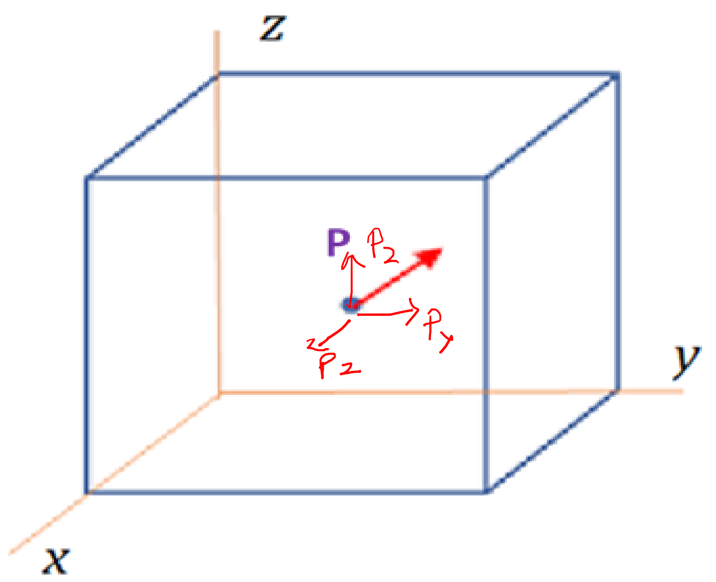
when $n_x = n_y$ *the energy state is a single state and*

when $n_x \neq n_y$ *the energy state has a degeneracy factor of 2*

Particle bound in a 3D potential Box

A particle bound by potentials at boundaries of a 3D box can be analyzed in a very similar manner

The particle has 3 degrees of freedom and the problem can be treated as three independent 1D problems



Particle bound in a 3D potential Box

The eigen functions for the x direction

$$\psi_{n_x}(x) = \sqrt{\frac{2}{a}} \cos\left(\frac{n_x \pi}{a} x\right) \quad for\ n_x\ odd$$

$$\psi_{n_x}(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_x \pi}{a} x\right) \quad for\ n_x\ even$$

The eigen functions for the y direction

$$\psi_{n_y}(y) = \sqrt{\frac{2}{a}} \cos\left(\frac{n_y \pi}{a} y\right) \quad for\ n_y\ odd$$

$$\psi_{n_y}(y) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_y \pi}{a} y\right) \quad for\ n_y\ even$$

The eigen functions for the z direction

$$\psi_{n_z}(z) = \sqrt{\frac{2}{a}} \cos\left(\frac{n_z \pi}{a} y\right) \quad for\ n_z\ odd$$

$$\psi_{n_z}(z) = \sqrt{\frac{2}{a}} \sin\left(\frac{n_z \pi}{a} y\right) \quad for\ n_z\ even$$

Particle bound in a 3D potential Box

The eigen function of the particle in the box

$$\psi_{n_x n_y n_z} = \psi_{n_x} \times \psi_{n_y} \times \psi_{n_z}$$

The wave functions of the first allowed state with $n_x = 1$, $n_y = 1$ *and* $n_z = 1$

$$\psi_{111} = \left(\frac{2}{a}\right)^{\frac{3}{2}} cos\left(\frac{\pi}{a}x\right)\ cos\left(\frac{\pi}{a}y\right)\ cos\left(\frac{\pi}{a}z\right)$$

which is a singleton state (no degeneracy)

Particle bound in a 3D potential Box

The wave function of the allowed state with $n_x = 2$, $n_y = 1$ and $n_z = 1$

$$\psi_{211} = \left(\frac{2}{a}\right)^{\frac{3}{2}} \sin\left(\frac{2\pi}{a}x\right) \cos\left(\frac{\pi}{a}y\right) \cos\left(\frac{\pi}{a}z\right)$$

The wave function of the allowed state with $n_x = 1$, $n_y = 2$ and $n_z = 1$

$$\psi_{121} = \left(\frac{2}{a}\right)^{\frac{3}{2}} \cos\left(\frac{\pi}{a}x\right) \sin\left(\frac{2\pi}{a}y\right) \cos\left(\frac{\pi}{a}z\right)$$

The wave function of the allowed state with $n_x = 1$, $n_y = 1$ and $n_z = 2$

$$\psi_{112} = \left(\frac{2}{a}\right)^{\frac{3}{2}} \cos\left(\frac{\pi}{a}x\right) \cos\left(\frac{\pi}{a}y\right) \sin\left(\frac{2\pi}{a}z\right)$$

Particle bound in a 3D potential Box

The energy of the particle in any state can be evaluated as

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

The first allowed state is the ground state of the system and has an energy

$$E_{111} = 3\frac{h^2}{8ma^2} = 3E_o \text{ where } E_o = \frac{h^2}{8ma^2}$$

The energy second allowed state of the system is given by

$$E_{211} = 6E_o$$

which is also the energy of the states $E_{121}\ and\ E_{112}$

There are three allowed states for the same energy value of $6E_o$. This state is then triply degenerate.

Particle bound in a 3D potential Box

The analysis of the first few states reveal that the states are non degenerate when $n_x = n_y = n_z$.

The states have a degeneracy factor of 3 whenever two of the numbers n_x, n_y *and* n_z are equal and not equal to the third.

When all the three numbers n_x, n_y *and* n_z are unequal then the energy state would have a degeneracy of 6.

The energy separation between the states is not an uniform or monotonic increase.

$\psi_{123}, \psi_{132}, \psi_{231}, \psi_{213}, \psi_{312}, \psi_{321}$

Class #19 …….. Quiz….

The concepts which are true of 2D and 3D quantum systems…

1. Many particles can be accommodated in a single energy state
2. The degeneracy of the states depend on the combination of n_x, n_y and n_z.
3. Particles with the same energy occupy degenerate states
4. The wave functions of the degenerate states are orthogonal
5. $n_x = n_y = n_z$ is a degenerate state
6. Wave functions of degenerate states are different for each of the states

THANK YOU

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