4.3 Infinite Potential Well in Three Dimensions

Suppose region of three dimensions a, b, and c, the potential inside this region equals to zero, and the potential outside equals =∞.

$v = o \quad when$	$0 < x < a$ $o < y < b$ $o < z < c$	$v = \infty \quad when$	$o \geq x \geq a$ $o \geq y \geq b$ $o \geq z \geq c$

- Schrodinger equation of three dimensions
- $-\frac{\hbar^2}{2m}\ \nabla^2\psi\ (x,y,z) = \mathrm{E}\ \psi(x,y,z)$
- $-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\ \psi = \mathrm{E}\ \psi\ (x,y,z)$ …….(4.9)

The wave function of potential in3D potential box

- $\psi\ (n_x, n_y, n_z) = \sqrt{\frac{8}{abc}}\sin\frac{n_x\pi x}{a}\sin\frac{n_y\pi y}{b}\sin\frac{n_z\pi z}{c}.$
- $\psi_{nx,ny,nz}(x,y,z) = \sqrt{\frac{8}{a^3}}\sin\frac{n_x\pi x}{a}\sin\frac{n_{y\pi y}}{a}\sin\frac{n_z\pi z}{a}$

- The energies of particles in3D potential box
- $\mathrm{E} = \mathrm{T} + \mathrm{V} = \mathrm{T} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$
- $\mathrm{E} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 k_x^2 + \hbar^2 k_y^2 + \hbar^2 k_z^2}{2m} = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$
- $k_x = \frac{n_x \pi}{a}, k_y = \frac{n_y \pi}{b}, k_z = \frac{n_z \pi}{c}$
- $\therefore E = \frac{\hbar^2 \pi^2}{2m}\left[\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right]$
- If the potential box is cubic, then a= b= c
- $\therefore E = \frac{\hbar^2 \pi^2}{2ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$ ....(4.10)

- The energy of particle in 3D P.B. is quantized
- $\frac{3\pi^2\hbar^2}{2ma^2}, \frac{6\pi^2\hbar^2}{2ma^2}, \dots\dots\dots$
- The ground state ψ_{111}
- The first excited state is: $\psi_{211}, \psi_{221}, \psi_{112}$
- The second excited state is : $\psi_{221}, \psi_{212}, \psi_{122}$

ground stat	$\psi_{111} = \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{\pi z}{a}$
1st excited state	$\psi_{211} = \sqrt{\frac{8}{a^3}} \sin\frac{2\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{\pi z}{a}$ $\psi_{121} = \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{2\pi y}{a} \sin\frac{\pi z}{a}$ $\psi_{112} = \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{2\pi z}{a}$

The phenomena of number of different state having the same energy is called degeneracy or degeneracy state and the number of wave function called order of degeneracy.

Solved Example: What the energy of particle in potential box of three dimensions at second excited state? write the degeneracy state, and the order of degeneracy?

- **Solution:**
- $E_{ny,ny,nx} = \frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$
- $E_{ny,ny,nx} = E_{221} = E_{212} = E_{122} = \frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$
- $= \frac{\pi^2\hbar^2}{2ma^2}[(2)^2 + (2)^2 + (1)^2]$
- $= \frac{q\pi^2\hbar^2}{2ma^2}$

$\psi_{221} = \sqrt{\frac{8}{a^3}} \sin\frac{2\pi x}{a} \sin\frac{2\pi y}{a} \sin\frac{\pi z}{a}$ $\psi_{212} = \sqrt{\frac{8}{a^3}} \sin\frac{2\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{2\pi z}{a}$ $\psi_{122} = \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{2\pi y}{a} \sin\frac{2\pi z}{a}$	**Three wave function return to the same energy** $\mathrm{E} = \frac{9\pi^2\hbar^2}{2ma^2}$

The order of degenerate = 3

Solved Example: find the wave function, the energy, and the order of degenerate of a particle in P.B of 3D in the third excited state?

- **Solution:**
- $\psi_{nx,ny,nz}(x,y,z) = \sqrt{\frac{8}{a^3}} \sin\frac{n_x \pi x}{a} \sin\frac{n_y \pi y}{a} \sin\frac{n_z \pi z}{a}$
- $\psi_{113} = \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{3\pi z}{a}$
- $\psi_{131} = \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{3\pi y}{a} \sin\frac{\pi z}{a}$
- $\psi_{122} = \sqrt{\frac{8}{a^3}} \sin\frac{3\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{\pi z}{a}$
- **The energy**
- $\mathrm{E_{nx,ny,nz}} = \frac{\pi^2 \hbar^2}{2ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$
- $\mathrm{E_{113}} = \frac{\pi^2 \hbar^2}{2ma^2}(1^2 + 1^2 + 3^2)$
- $= \frac{11\pi^2 \hbar^2}{2ma^2}$
- The order of degenerate = 3
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The wave function of fifth excited state:

$$\psi_{123} = \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{2\pi y}{a} \sin\frac{3\pi z}{a}$$

$$\psi_{132} = \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{3\pi y}{a} \sin\frac{2\pi z}{a}$$

$$\psi_{213} = \sqrt{\frac{8}{a^3}} \sin\frac{2\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{3\pi z}{a}$$

$$\psi_{231} = \sqrt{\frac{8}{a^3}} \sin\frac{2\pi x}{a} \sin\frac{3\pi y}{a} \sin\frac{\pi z}{a}$$

$$\psi_{312} = \sqrt{\frac{8}{a^3}} \sin\frac{3\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{2\pi z}{a}$$

$$\psi_{321} = \sqrt{\frac{8}{a^3}} \sin\frac{3\pi x}{a} \sin\frac{2\pi y}{a} \sin\frac{\pi z}{a}$$

same energy

$$E = \frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

$$= \frac{14\pi^2\hbar^2}{2ma^2}$$

The order of degenerate = 6

The normalized condition $\int_{all\ space} \psi^* \, \psi \, dv = 1$

Solved Example: prove the wave function of a particle in P.B of 3D at ground state is normalized

- $\psi_{111} = \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{\pi z}{a}$
- $\int_{all\ space} \psi \, \psi \, dv = 1$ $\qquad dv = \ d_x \, d_y \, d_z$

- $= \int_o^a \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{\pi z}{a} \,.\, \sqrt{\frac{8}{a^3}} \sin\frac{\pi x}{a} \sin\frac{\pi y}{a} \sin\frac{\pi z}{a}\ d_x\, d_y\, d_z$
- $\frac{8}{a^3} \int_o^a sin^2 \frac{\pi x}{a}\ dx \int_o^a sin^2 \frac{\pi y}{a} dy\ \int_o^a sin^2 \frac{\pi z}{a}\ dz$
- $\frac{8}{a^3}\ \int_0^a \frac{1}{2}\left(1 - \cos\frac{2\pi x}{a}\right) d_x\ \int_0^a \frac{1}{2}\left(1 - \cos\frac{2\pi y}{a}\right) d_y\ \int_0^a \frac{1}{2}\left(1 - \cos\frac{2\pi z}{a}\right) d_z$
- $\frac{1}{a^3}\ \left[x - \frac{a}{2\pi}\sin\frac{2\pi x}{a}\right]_o^a \left[y - \frac{a}{2\pi}\sin\frac{2\pi y}{a}\right]_o^a \left[z - \frac{a}{2\pi}\sin\frac{2\pi z}{a}\right]_o^a$
- $\frac{1}{a^3}[a]\ [a]\ [a] = 1$
- $\therefore \psi_{111} = 1$ Normalized
- **Problem:** write the wave function of a particle in P.B of 3D at first excited state and prove it is normalized and orthogonal with the other functions.

- Thank You