Fri: Read 7.3

Next HW Tues

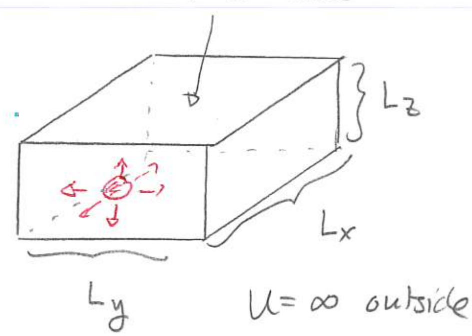
Particle in a three dimensional infinite well

Consider a particle restricted to a rectangular region inside of which it is free. The region is bounded by

$0 \le x \le L_x$

$0 \le y \le L_y$

$0 \le z \le L_z$



Then the wavefunction satisfies:

outside: $\psi(x,y,z) = 0$

inside: $$-\frac{\hbar^2}{2M}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) = E\,\psi(x,y,z)$$

boundary: $\psi = 0$

The strategy for solving the TISE is to assume that

$$\psi(x,y,z) = F(x)\,G(y)\,H(z)$$

where F, G, H are unknown single variable functions. This is called the separation of variables and general schemes, as illustrated in the text, eventually result in specific expressions for the unknown functions.

1 Three-dimensional infinite well

A particle is in a three-dimensional infinite well for which

$$0 \leqslant x \leqslant L_x$$
$$0 \leqslant y \leqslant L_y$$
$$0 \leqslant z \leqslant L_z$$

Consider the following candidate as a solution to the time-independent SChrödinger equation:

$$\psi(x, y, z) = A \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

where k_x, k_y, k_z and A are constants.

a) Verify that this is a solution and find an expression for the energy.

b) Use the boundary conditions to find permissible values for k_x, k_y and k_z. Determine the possible energies.

Suppose that $L_x = L_y = L_z = L$

c) List the seven states with lowest energies.

Answer a) $\frac{\partial \psi}{\partial x} = A \frac{\partial}{\partial x} \sin(k_x x) \sin(k_y y) \sin(k_z z)$

$= + k_x A \cos(k_x x) \sin(k_y y) \sin(k_z z)$

$\frac{\partial^2 \psi}{\partial x^2} = + k_x A (-k_x) \sin(k_x x) \sin(k_y y) \sin(k_z z)$

$= -k_x^2 \psi$

Similarly

$\frac{\partial^2 \psi}{\partial y^2} = -k_y^2 \psi$

$\frac{\partial^2 \psi}{\partial z^2} = -k_z^2 \psi$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right) = -\frac{\hbar^2}{2m}\left(-k_x^2-k_y^2-k_z^2\right)\psi$$

$$= \underbrace{\frac{\hbar^2}{2m}\left(k_x^2+k_y^2+k_z^2\right)}_{E}\psi$$

It is a solution and

$$E = \frac{\hbar^2}{2m}\left(k_x^2+k_y^2+k_z^2\right)$$

b) $\psi(0,y,z) = 0 \Rightarrow A\,\cancel{\sin(k_x 0)}^{\,0}\sin(k_y y)\sin(k_z z) = 0$ true

$\psi(L_x,y,z) = 0 \Rightarrow A\sin(k_x L_x)\sin(k_y y)\sin(k_z z) = 0$

$$\Rightarrow \sin(k_x L_x) = 0 \quad \Rightarrow \quad k_x L_x = n_x\pi$$

$$\Rightarrow \quad k_x = \frac{n_x\pi}{L_x}$$

$\hookrightarrow n_x = 1,2,3$

Similarly $k_y = \dfrac{n_y\pi}{L_y}$

$k_z = \dfrac{n_z\pi}{L_z}$

$$\Rightarrow \quad E = \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{L_x^2}+\frac{n_y^2}{L_y^2}+\frac{n_z^2}{L_z^2}\right)$$

$n_x = 1,2,3,\ldots$

$n_y = 1,2,3,\ldots$

$n_z = 1,2,3,\ldots$

c) Here

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

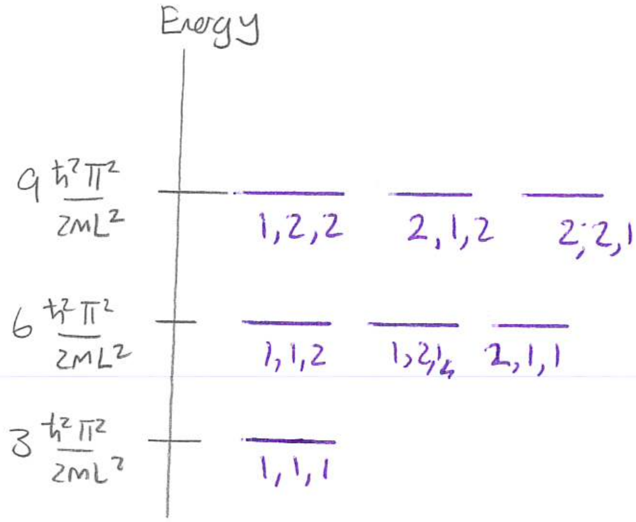
The possibilities are:

n_x	n_y	n_z	E
1	1	1	$3 \frac{\hbar^2 \pi^2}{2mL^2}$
1	1	2	
1	2	1	$6 \frac{\hbar^2 \pi^2}{2mL^2}$
2	1	1	
1	2	2	
2	1	2	$9 \frac{\hbar^2 \pi^2}{2mL^2}$
2	2	1	

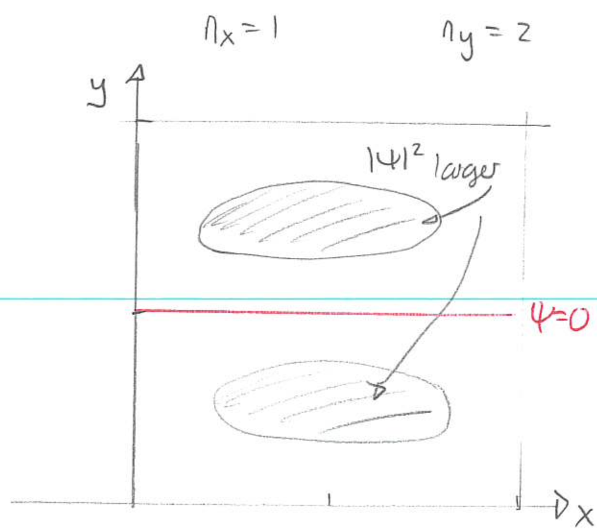
Degeneracy

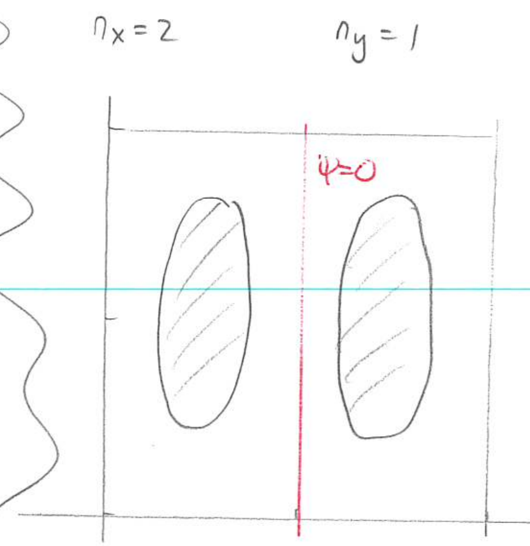
The example illustrates the fact that there are distinct states which have the same energy. A system that has this property is called degenerate and any energy level with more than one state is called degenerate.

Although multiple states can provide the same energy, their spatial wavefunctions reveal that they are distinct



Consider a two dimensional version.





$$\psi = A \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{2\pi y}{L}\right)$$

$$P = |\psi|^2 = A^2 \sin^2\left(\frac{\pi x}{L}\right) \sin^2\left(\frac{2\pi x}{L}\right)$$

$$\psi = A \sin\left(\frac{2\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right)$$

$$P = |\psi|^2 = A^2 \sin^2\left(\frac{2\pi x}{L}\right) \sin^2\left(\frac{\pi y}{L}\right)$$

Quiz 1