Problem 4.2 Griffith's Q.M.

Use separation of variables in Cartesian coordinates to solve the infinite cubical well.

$$V(x,y,z) = \begin{cases} 0, & \text{if } x,y,z \text{ are all between } 0 \text{ and } a \\ \infty, & \text{otherwise} \end{cases}$$

Questions: 1. Find the stationary states, and the corresponding energies.

2. Call the distinct energies $E_1, E_2, \ldots$ in order of increasing energy.

Find E_1 and E_2 and their degeneracies.

Solutions: 1. As always, we are solving the time-independent Schrödinger equation.

Inside of the box, $V(x,y,z) = 0$.

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\nabla^2 \Psi(x,y,z) = E\Psi(x,y,z) \qquad \text{where } \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\left[\frac{\partial^2\Psi}{\partial x^2} + \frac{\partial^2\Psi}{\partial y^2} + \frac{\partial^2\Psi}{\partial z^2}\right] = E\Psi$$

Perfect case for separation of variables!

Assume solution of the form: $\Psi(x,y,z) = A(x)B(y)C(z)$

Try out the solution.

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\left[\frac{\partial^2 A}{\partial x^2}BC + A\frac{\partial^2 B}{\partial y^2}C + AB\frac{\partial^2 C}{\partial z^2}\right] = EABC \qquad \text{Divide by } ABC.$$

$$\frac{1}{A}\frac{\partial^2 A}{\partial x^2} + \frac{1}{B}\frac{\partial^2 B}{\partial y^2} + \frac{1}{C}\frac{\partial^2 C}{\partial z^2} = -\frac{2mE}{\hbar^2}$$

$$\Rightarrow \quad f(x) + g(y) + h(z) = \#$$

$$f(x) \equiv \frac{1}{A}\frac{\partial^2 A}{\partial x^2} \qquad g(y) \equiv \frac{1}{B}\frac{\partial^2 B}{\partial y^2} \qquad h(z) \equiv \frac{1}{C}\frac{\partial^2 C}{\partial z^2}$$

Each function $f(x)$, $g(y)$, and $h(z)$ must be equal to a constant. If they weren't equal to constants, they would depend on the other spatial variables.

Let $f(x) = -K_x^2$, $g(y) = -K_y^2$, $h(z) = -K_z^2$

$$\Rightarrow \quad K_x^2 + K_y^2 + K_z^2 = \frac{2mE}{\hbar^2}$$

also: $\frac{1}{A}\frac{d^2A}{dx^2} = -K_x^2 \qquad \frac{1}{B}\frac{d^2B}{dy^2} = -K_y^2 \qquad \frac{1}{C}\frac{d^2C}{dz^2} = -K_z^2$

We know the solutions to these from the one-dimensional case.

$$A(x) = \sqrt{\tfrac{2}{a}}\sin(K_x x) \quad B(y) = \sqrt{\tfrac{2}{a}}\sin(K_y y) \quad C(z) = \sqrt{\tfrac{2}{a}}\sin(K_z z)$$

Where $K_x = \frac{n_x \pi}{a}$, $K_y = \frac{n_y \pi}{a}$, $K_z = \frac{n_z \pi}{a}$

$$\therefore \quad A(x) = \sqrt{\tfrac{2}{a}}\sin\left(\frac{n_x \pi x}{a}\right) \quad , \text{ etc.}$$

Full solution is: $\psi(x,y,z) = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{n_x \pi x}{a}\right)\sin\left(\frac{n_y \pi y}{a}\right)\sin\left(\frac{n_z \pi z}{a}\right)$

What about the energies? $K_x^2 + K_y^2 + K_z^2 = \frac{2mE}{\hbar^2}$

$$\Rightarrow \left(\frac{n_x \pi}{a}\right)^2 + \left(\frac{n_y \pi}{a}\right)^2 + \left(\frac{n_z \pi}{a}\right)^2 = \frac{2mE}{\hbar^2}$$

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

Now have 3 quantum numbers labelling each energy.

2. E_1 comes from $n_x = n_y = n_z = 1$ and is non-degenerate.

E_2 comes from some combination of 2, 1, 1.

	n_x	n_y	n_z
#1	2	1	1
#2	1	2	1
#3	1	1	2

} 3 times degeneracy.

$\Rightarrow$ 3 combinations give the same energy