Gasiorowicz 3rd edition April 22, 2008

P8-1.

Consider a special case of eq. (8-5) in which each of the potentials V_1, V_2 and V_3 are identical, in each case of the form

$$V(x) = 0 \qquad 0 \le x \le a$$
$$V(x) = \infty \qquad x > a$$
$$V(x) = \infty \qquad x < 0$$

and similarly for y and z. Use what you learned about the one-dimensional potential in Chapter 3 to find the eigenvalues and eigenfunctions for a particle in such a box.

[Eq. (8-5):

$$V(x,y,z)= V_1(x)+ V_2(y) + V_3(z) \qquad]$$

Solution:

Schrödinger equation :

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

Let $\psi = X(z)Y(y)Z(z)$

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right]X(z)Y(y)Z(z) = EX(z)Y(y)Z(z)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\left[YZ\frac{\partial^2 X}{\partial x^2}+XZ\frac{\partial^2 Y}{\partial y^2}+XY\frac{\partial^2 Z}{\partial z^2}\right] = EXYZ$$

$$\Rightarrow \left[\frac{1}{X}\frac{\partial^2 X}{\partial x^2}+\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}+\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}\right] = -\frac{2mE}{\hbar^2}$$

$$\Rightarrow \frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -\frac{2mE}{\hbar^2}-\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}-\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}$$

Since left hand side depends on x and right hand side depends on y and z. The only possibility is both sides equal to a constant, say, $-\frac{2mE_x}{\hbar^2}$

$$\therefore \frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -\frac{2mE_x}{\hbar^2} \qquad ----(1)$$

$$-\frac{2mE}{\hbar^2}-\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}-\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}=-\frac{2mE_x}{\hbar^2}$$

$$\Rightarrow \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}=\frac{2mE_x}{\hbar^2}-\frac{2mE}{\hbar^2}-\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}$$

Since left hand side depends on y and right hand side depends on z. The only possibility is both sides equal to a constant, say, $-\frac{2mE_y}{\hbar^2}$

$$\therefore \frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}=-\frac{2mE_y}{\hbar^2} \qquad ----(2)$$

$$\frac{2mE_x}{\hbar^2}-\frac{2mE}{\hbar^2}-\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}=-\frac{2mE_y}{\hbar^2}$$

$$\Rightarrow \frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}=\frac{2mE_x}{\hbar^2}+\frac{2mE_y}{\hbar^2}-\frac{2mE}{\hbar^2}$$

Let $\frac{2mE_x}{\hbar^2}+\frac{2mE_y}{\hbar^2}-\frac{2mE}{\hbar^2}=-\frac{2mE_z}{\hbar^2} \Rightarrow \frac{2mE}{\hbar^2}=\frac{2mE_x}{\hbar^2}+\frac{2mE_y}{\hbar^2}+\frac{2mE_z}{\hbar^2}$

$$\Rightarrow E=E_x+E_y+E_z \qquad ----(*)$$

Then we have

$$\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}=-\frac{2mE_z}{\hbar^2} \qquad ----(3)$$

Solving for (1):

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2}=-\frac{2mE_x}{\hbar^2} \quad \Rightarrow \frac{1}{X}\frac{\partial^2 X}{\partial x^2}=-k_x^{\ 2} \quad \text{where } k_x=\sqrt{\frac{2mE_x}{\hbar^2}}$$

$$\Rightarrow X=A\sin k_x x+B\cos k_x x$$

$X(0)=0 \Rightarrow B=0$

$X=A\sin k_x x$

$X(a)=0 \Rightarrow k_x a=n_x\pi \qquad n_x=1,2,3,.......$

$$\Rightarrow k_x=\frac{n_x\pi}{a}$$

$$\therefore X(x)= \quad A\sin\frac{n_x\pi}{a}x \qquad \text{and } E_x=\frac{\hbar^2 k_x^{\ 2}}{2m}=\frac{\hbar^2}{2m}\left(\frac{n_x\pi}{a}\right)^2 \qquad ----(4)$$

Solving (2) and (3) in a similar way, we have

$$Y(y)= \quad B\sin\frac{n_y\pi}{a}y \qquad \text{and } E_y=\frac{\hbar^2 k_y^{\ 2}}{2m}=\frac{\hbar^2}{2m}\left(\frac{n_y\pi}{a}\right)^2 \qquad ----(5)$$

$$Z(z)= \quad A\sin\frac{n_z\pi}{a}z \qquad \text{and } E_z=\frac{\hbar^2 k_z^{\ 2}}{2m}=\frac{\hbar^2}{2m}\left(\frac{n_z\pi}{a}\right)^2 \qquad ----(6)$$

$$(*) \;\Rightarrow\; E = E_x + E_y + E_z = \frac{\hbar^2}{2m}\left[\left(\frac{n_x\pi}{a}\right)^2 + \left(\frac{n_y\pi}{a}\right)^2 + \left(\frac{n_z\pi}{a}\right)^2\right]$$

$$\Psi(x,y,z) = X(x)Y(y)Z(z)$$

$$= ACE\sin\frac{n_x\pi}{a}x\sin\frac{n_y\pi}{a}y\sin\frac{n_z\pi}{a}z$$

$$= K\sin\frac{n_x\pi}{a}x\sin\frac{n_y\pi}{a}y\sin\frac{n_z\pi}{a}z \qquad (K = ACE)$$

K is determined by normalization condition :

$$K^2\int_0^a \sin^2\frac{n_x\pi}{a}x\,dx\int_0^a \sin^2\frac{n_y\pi}{a}y\,dy\int_0^a \sin^2\frac{n_z\pi}{a}z\,dz = 1$$

$$\Rightarrow\; K^2\int_0^a\left(\frac{1-\cos\frac{2n_x\pi}{a}}{2}\right)dx\int_0^a\left(\frac{1-\cos\frac{2n_y\pi}{a}}{2}\right)dy\int_0^a\left(\frac{1-\cos\frac{2n_z\pi}{a}}{2}\right)dz = 1$$

$$\Rightarrow\; K^2\,\frac{a}{2}\cdot\frac{a}{2}\cdot\frac{a}{2} = 1$$

$$\Rightarrow\; K = \left(\frac{2}{a}\right)^{\frac{3}{2}}$$

$$\therefore\; \Psi(x,y,z) = \left(\frac{2}{a}\right)^{\frac{3}{2}}\sin\frac{n_x\pi}{a}x\,\sin\frac{n_y\pi}{a}y\,\sin\frac{n_z\pi}{a}z \qquad n_x, n_y, n_z = 1, 2, 3, 4, \ldots\ldots$$

$$E_{n_x,n_y,n_z} = \frac{\hbar^2}{2m}\left[\left(\frac{n_x\pi}{a}\right)^2 + \left(\frac{n_y\pi}{a}\right)^2 + \left(\frac{n_z\pi}{a}\right)^2\right]$$