Gasiorowicz 3rd edition April 25, 2008

P8-2.

What is the ground state energy for the potential in Problem 1? List the values of the lowest 10 energy levels and label them by their appropriate quantum numbers. What is the degeneracy pf the levels on your list?

[Problem 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):

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

]

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):

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

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

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

$X=A\sin k_x x$

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

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

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

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

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

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

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

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

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

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

K is determined by normalization condition :

$$K^2\int_0^a \sin^2\frac{n_x\pi}{a}xdx\int_0^a \sin^2\frac{n_y\pi}{a}ydy\int_0^a \sin^2\frac{n_z\pi}{a}zdz = 1$$

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

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

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

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

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

I use Excel to list out all possible combinations of n_x, n_y, and n_z, then calculate n_x^2+ n_y^2+n_z^2 in the fourth column. After this I sort the fourth column small smallest value to largest, and the first twelve energy levels are given as follow:

nx	ny	nz	nx^2+ny^2+nz^2	Energy level	Degeneracy
1	1	1	3	1st	1
2	1	1	6	2nd	3
1	2	1	6		
1	1	2	6		
2	2	1	9	3rd	3
2	1	2	9		
1	2	2	9		
3	1	1	11	4th	3
1	3	1	11		
1	1	3	11		
2	2	2	12	5th	1
3	2	1	14	6th	6
2	3	1	14		
3	1	2	14		
1	3	2	14		
2	1	3	14		
1	2	3	14		
3	2	2	17	7th	3
2	3	2	17		
2	2	3	17		
4	1	1	18	8th	3
1	4	1	18		
1	1	4	18		
3	3	1	19	9th	3
3	1	3	19		
1	3	3	19		
4	2	1	21	10th	6
2	4	1	21		
4	1	2	21		
1	4	2	21		
2	1	4	21		
1	2	4	21		
3	3	2	22	11th	3
3	2	3	22		
2	3	3	22		
4	2	2	24	12th	3
2	4	2	24		
2	2	4	24		

The energy of each level is given by

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