

Problem 4.2

(a) Equation 4.8 $\Rightarrow -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) = E\psi$ (inside the box). Separable solutions $X(x)Y(y)Z(z)$. Put this in, and divide by XYZ :

$$\frac{1}{X} \frac{d^2 X}{dx^2} + \frac{1}{Y} \frac{d^2 Y}{dy^2} + \frac{1}{Z} \frac{d^2 Z}{dz^2} = -\frac{2m}{\hbar^2} E.$$

The three terms on the left are functions of x , y , and z , respectively, so each must be a constant separation constants k_x^2 , k_y^2 , and k_z^2 (as we'll soon see, they must be positive). (c)

$$\frac{d^2 X}{dx^2} = -k_x^2 X; \quad \frac{d^2 Y}{dy^2} = -k_y^2 Y; \quad \frac{d^2 Z}{dz^2} = -k_z^2 Z, \quad \text{with} \quad E = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2).$$

Solution:

$$X(x) = A_x \sin k_x x + B_x \cos k_x x; \quad Y(y) = A_y \sin k_y y + B_y \cos k_y y; \quad Z(z) = A_z \sin k_z z + B_z \cos k_z z$$

But $X(0) = 0$, so $B_x = 0$; $Y(0) = 0$, so $B_y = 0$; $Z(0) = 0$, so $B_z = 0$. And $X(a) = 0 \Rightarrow \sin k_x a = 0 \Rightarrow k_x = n_x \pi/a$ ($n_x = 1, 2, 3, \dots$). [As before (page 31), $n_x \neq 0$, and negative values are redundant.] So $k_y = n_y \pi/a$ and $k_z = n_z \pi/a$. So

$$\psi(x, y, z) = A_x A_y A_z \sin \left(\frac{n_x \pi}{a} x \right) \sin \left(\frac{n_y \pi}{a} y \right) \sin \left(\frac{n_z \pi}{a} z \right), \quad E = \frac{\hbar^2}{2m} \frac{\pi^2}{a^2} (n_x^2 + n_y^2 + n_z^2)$$

We might as well normalize X , Y , and Z separately: $A_x = A_y = A_z = \sqrt{2/a}$. Conclusion:

$$\boxed{\psi(x, y, z) = \left(\frac{2}{a} \right)^{3/2} \sin \left(\frac{n_x \pi}{a} x \right) \sin \left(\frac{n_y \pi}{a} y \right) \sin \left(\frac{n_z \pi}{a} z \right); \quad E = \frac{\pi^2 \hbar^2}{2ma^2} (n_x^2 + n_y^2 + n_z^2)}$$

(b)

n_x	n_y	n_z	$(n_x^2 + n_y^2 + n_z^2)$
1	1	1	3
1	1	2	6
1	2	1	6
2	1	1	6
1	2	2	9
2	1	2	9
2	2	1	9
1	1	3	11
1	3	1	11
3	1	1	11
2	2	2	12
1	2	3	14
1	3	2	14
2	1	3	14
2	3	1	14
3	1	2	14
3	2	1	14

Energy	Degeneracy
$E_1 = 3 \frac{\pi^2 \hbar^2}{2ma^2}$	$d = 1$
$E_2 = 6 \frac{\pi^2 \hbar^2}{2ma^2}$	$d = 3.$
$E_3 = 9 \frac{\pi^2 \hbar^2}{2ma^2}$	$d = 3.$
$E_4 = 11 \frac{\pi^2 \hbar^2}{2ma^2}$	$d = 3.$
$E_5 = 12 \frac{\pi^2 \hbar^2}{2ma^2}$	$d = 1.$
$E_6 = 14 \frac{\pi^2 \hbar^2}{2ma^2}$	$d = 6.$

- (c) The next combinations are: $E_7(322)$, $E_8(411)$, $E_9(331)$, $E_{10}(421)$, $E_{11}(332)$, $E_{12}(422)$, $E_{13}(431)$, and $E_{14}(333 \text{ and } 511)$. The degeneracy of E_{14} is $\boxed{4}$. Simple combinatorics accounts for degeneracies of 1 ($n_x = n_y = n_z$), 3 (two the same, one different), or 6 (all three different). But in the case of E_{14} there is a numerical “accident”: $3^2 + 3^2 + 3^2 = 27$, but $5^2 + 1^2 + 1^2$ is also 27, so the degeneracy is greater than combinatorial reasoning alone would suggest.

Problem 4.4

$$\frac{d\Theta}{d\theta} = \frac{A}{\tan(\theta/2)} \frac{1}{2} \sec^2(\theta/2) = \frac{A}{2} \frac{1}{\sin(\theta/2) \cos(\theta/2)} = \frac{A}{\sin \theta}. \quad \text{Therefore } \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) = \frac{d}{d\theta} \left(\frac{A}{\sin \theta} \right).$$

With $l = m = 0$, Eq. 4.25 reads: $\frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) = 0$. So $A \ln[\tan(\theta/2)]$ does satisfy Eq. 4.25.

So $\Theta(0) = A \ln(0) = A(-\infty)$; $\Theta(\pi) = A \ln \left(\tan \frac{\pi}{2} \right) = A \ln(\infty) = A(\infty)$. Θ blows up at $\theta = 0$ and $\theta = \pi$.

Problem 4.5

$$Y_l^l = (-1)^l \sqrt{\frac{(2l+1)}{4\pi}} \frac{1}{(2l)!} e^{il\phi} P_l^l(\cos \theta). \quad P_l^l(x) = (1-x^2)^{l/2} \left(\frac{d}{dx} \right)^l P_l(x).$$

$$P_l(x) = \frac{1}{2^l l!} \left(\frac{d}{dx} \right)^l (x^2 - 1)^l, \quad \text{so } P_l^l(x) = \frac{1}{2^l l!} (1-x^2)^{l/2} \left(\frac{d}{dx} \right)^{2l} (x^2 - 1)^l.$$

Now $(x^2 - 1)^l = x^{2l} + \dots$, where all the other terms involve powers of x less than $2l$, and hence given when differentiated $2l$ times. So

$$P_l^l(x) = \frac{1}{2^l l!} (1-x^2)^{l/2} \left(\frac{d}{dx} \right)^{2l} x^{2l}. \quad \text{But } \left(\frac{d}{dx} \right)^n x^n = n!, \quad \text{so } P_l^l = \frac{(2l)!}{2^l l!} (1-x^2)^{l/2}.$$

$$\therefore Y_l^l = (-1)^l \sqrt{\frac{(2l+1)}{4\pi(2l)!}} e^{il\phi} \frac{(2l)!}{2^l l!} (\sin \theta)^l = \boxed{\frac{1}{l!} \sqrt{\frac{(2l+1)!}{4\pi}} \left(-\frac{1}{2} e^{i\phi} \sin \theta \right)^l}.$$