Solutions - HW7

Problem 4.2 (15pts)

6pts (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: $\psi(x,y,z) = X(x)Y(y)Z(z)$. Put this in, and divide by XYZ:

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

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

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

Solution:

$$X(x) = A_x\sin k_xx + B_x\cos k_xx; \quad Y(y) = A_y\sin k_yy + B_y\cos k_yy; \quad Z(z) = A_z\sin k_zz + B_z\cos k_zz.$$

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

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

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

$$\boxed{\psi(x,y,z) = \left(\frac{2}{a}\right)^{3/2}\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{a}y\right)\sin\left(\frac{n_z\pi}{a}z\right); \quad E = \frac{\pi^2\hbar^2}{2ma^2}(n_x^2+n_y^2+n_z^2); \quad n_x,n_y,n_z = 1,2,3,\ldots}$$

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

3pts **(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 (6pts)

$$\text{Eq. 4.32} \Rightarrow Y_0^0 = \frac{1}{\sqrt{4\pi}}P_0^0(\cos\theta);\ \text{Eq. 4.27} \Rightarrow P_0^0(x) = P_0(x);\ \text{Eq. 4.28} \Rightarrow P_0(x) = 1.\quad \boxed{Y_0^0 = \frac{1}{\sqrt{4\pi}}.}$$

$$Y_2^1 = -\sqrt{\frac{5}{4\pi}\frac{1}{3\cdot 2}}\,e^{i\phi}P_2^1(\cos\theta);\quad P_2^1(x) = \sqrt{1-x^2}\frac{d}{dx}P_2(x);$$

$$P_2(x) = \frac{1}{4\cdot 2}\left(\frac{d}{dx}\right)^2\left(x^2-1\right)^2 = \frac{1}{8}\frac{d}{dx}\left[2(x^2-1)2x\right] = \frac{1}{2}\left[x^2-1+x(2x)\right] = \frac{1}{2}\left(3x^2-1\right);$$

$$P_2^1(x) = \sqrt{1-x^2}\frac{d}{dx}\left[\frac{3}{2}x^2 - \frac{1}{2}\right] = \sqrt{1-x^2}\,3x;\ P_2^1(\cos\theta) = 3\cos\theta\sin\theta.\ \boxed{Y_2^1 = -\sqrt{\frac{15}{8\pi}}\,e^{i\phi}\sin\theta\cos\theta.}$$

Normalization: $\iint |Y_0^0|^2 \sin\theta \, d\theta \, d\phi = \frac{1}{4\pi}\left[\int_0^{\pi} \sin\theta \, d\theta\right]\left[\int_0^{2\pi} d\phi\right] = \frac{1}{4\pi}(2)(2\pi) = 1.$ ✓

$$\iint |Y_2^1|^2 \sin\theta \, d\theta \, d\phi = \frac{15}{8\pi}\int_0^{\pi} \sin^2\theta \cos^2\theta \sin\theta \, d\theta \int_0^{2\pi} d\phi = \frac{15}{4}\int_0^{\pi} \cos^2\theta(1-\cos^2\theta)\sin\theta \, d\theta$$

$$= \frac{15}{4}\left[-\frac{\cos^3\theta}{3} + \frac{\cos^5\theta}{5}\right]\Bigg|_0^{\pi} = \frac{15}{4}\left[\frac{2}{3} - \frac{2}{5}\right] = \frac{5}{2} - \frac{3}{2} = 1 \checkmark$$

Orthogonality: $\iint Y_0^{0*} Y_2^1 \sin\theta \, d\theta \, d\phi = -\frac{1}{\sqrt{4\pi}}\sqrt{\frac{15}{8\pi}}\underbrace{\left[\int_0^{\pi} \sin\theta\cos\theta\sin\theta \, d\theta\right]}_{(\sin^3\theta)/3|_0^{\pi}=0}\underbrace{\left[\int_0^{2\pi} e^{i\phi} d\phi\right]}_{(e^{i\phi})/i|_0^{2\pi}=0} = 0.$ ✓

Problem 4.16 (3pts)

$$\psi = \frac{1}{\sqrt{\pi a^3}} e^{-r/a}; \quad P = |\psi|^2 4\pi r^2\, dr = \frac{4}{a^3} e^{-2r/a} r^2\, dr = p(r)\, dr; \quad p(r) = \frac{4}{a^3} r^2 e^{-2r/a}.$$

$$\frac{dp}{dr} = \frac{4}{a^3}\left[2re^{-2r/a} + r^2\left(-\frac{2}{a}e^{-2r/a}\right)\right] = \frac{8r}{a^3}e^{-2r/a}\left(1 - \frac{r}{a}\right) = 0 \Rightarrow \boxed{r = a.}$$

SP7 (8 pts)

a) The eigenstates are the same as the eigenstates of $\hat{L}^2$, which are the spherical harmonics. The eigenvalues are the eigenvalues of $\hat{L}^2$ divided by $4Ma^2$, so

$$\frac{\hbar^2 l(l+1)}{4Ma^2}$$

with l an integer.

b) The first excited state corresponds to $l = 1$. Plugging in numbers, we find

$$\frac{\hbar^2 1(1+1)}{4Ma^2} = \frac{\hbar^2}{2Ma^2}$$

= 6.7e-22 J = 0.004 eV