PHYSICS 115B HWK 1

1 Inside the box $-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi$

(a)
$$-\frac{\hbar}{2m}\left[\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+\frac{\partial^2\psi}{\partial z^2}\right] = E\psi \qquad (1)$$

Separation of variables $\psi(x,y,z) = X(x)Y(y)Z(z)$

Substituting into (1), dividing by ψ, multiplying by $-\frac{2m}{\hbar}$:

$$\underbrace{\frac{1}{X}\frac{d^2X}{dx^2}}_{\text{function of } x} + \underbrace{\frac{1}{Y}\frac{d^2Y}{dy^2}}_{\text{function of } y} + \underbrace{\frac{1}{Z}\frac{d^2Z}{dz^2}}_{\text{function of } z} = \underbrace{-\frac{2m}{\hbar}E}_{\text{just a number}}$$

In order for this equation to be satisfied for all (x,y,z) each individual term must be equal to a constant.

Let's write $\frac{1}{X}\frac{d^2X}{dx^2} = -k_x^2 \quad \frac{1}{Y}\frac{d^2Y}{dy^2} = -k_y^2 \quad \frac{1}{Z}\frac{d^2Z}{dz^2} = -k_z^2$

with $k_x^2+k_y^2+k_z^2 = \frac{2mE}{\hbar} \Rightarrow \boxed{E = \frac{\hbar^2}{2m}\left(k_x^2+k_y^2+k_z^2\right)}$

The solution of the X equation is

$X(x) = A_x \sin k_x x + B_x \cos k_x x$

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The boundary conditions are $X(0) = X(a) = 0$

This gives $B_x = 0$ and $k_x = \frac{n_x \pi}{a}$ n_x is integer

Similarly for the y and z equations.

Solution then is $\boxed{\psi(x,y,z) = C \sin \frac{n_x \pi}{a} \sin \frac{n_y \pi}{a} \sin \frac{n_z \pi}{a}}$

Normalization of the wavefunction $\int_0^a dx \int_0^a dy \int_0^a dz\, |\psi|^2 = 1$

gives $\boxed{C = \left(\frac{2}{a}\right)^{3/2}}$

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

(b) Lowest energy all n's = 1 $E_1 = \frac{3\hbar^2\pi^2}{2ma^2}$ only 1 combination

Next lowest $(n_x\, n_y\, n_z) = (2,1,1)$ and 3 permutations $E_2 = \frac{6\pi^2\hbar^2}{2ma^2}$ degeneracy = 3

3rd lowest $(n_x\, n_y\, n_z) = (2,2,1)$ and 3 permutations $E_3 = \frac{9\pi^2\hbar^2}{2ma^2}$ degeneracy = 3

4th lowest $(n_1 n_2 n_3) = (3,1,1)$ and 3 permutations $E_4 = \frac{11\pi^2\hbar^2}{2ma^2}$ degeneracy = 3

5th lowest $(n_1 n_2 n_3) = (2,2,2)$ $E_5 = \frac{12\pi^2\hbar^2}{2ma^2}$ degeneracy = 1

6th lowest $(n_1 n_2 n_3) = (1,2,3)$ 6 permutations $E_6 = \frac{14\pi^2\hbar^2}{2ma^2}$ degeneracy = 6

② $-\frac{\hbar^2}{2m}\nabla^2\psi + \frac{1}{2}m\omega^2(x^2+y^2+z^2)\psi = E\psi$

(a) Using the same method as in problem 1, we obtain 3 different equations that look exactly like 1D oscillators, eg

$$-\frac{\hbar^2}{2m}\frac{d^2X}{dx^2} + \frac{1}{2}m\omega^2x^2X(x) = E_x X(x)$$

This has solutions (from last quarter) $E_x = (n_x+\frac{1}{2})\hbar\omega$

Same for the y and z coordinates, and

$$E = E_x + E_y + E_z = (n_x+n_y+n_z+3/2)\hbar\omega = \boxed{(n+3/2)\hbar\omega}$$

Note: in this case the n_x, n_y, n_z can be $=0$

(b) The degeneracy of the state with eigenenergy $E_n = (n+3/2)\hbar\omega$ is equal to the number of ways that 3 integers can add up to n. For a given n_x, in order to have $n_x+n_y+n_z = n$, I can pick $n_y = 0, 1, \dots, n-n_x$. (Note, once n_x & n_y are fixed, so is $n_z = n-n_x-n_y$). So, at a given n_x there are $n-n_x+1$ choices of n_y. But, since n_x can be anything from 0 to n, the degeneracy $d(n)$ will be

$$d(n) = \sum_{n_x=0}^{n}(n-n_x+1) = (n+1)\sum_{n_x=0}^{n}1 - \sum_{n_x=0}^{n}n_x$$

$$d(n) = (n+1)^2 - \frac{1}{2}n(n+1) = \boxed{\frac{1}{2}(n+1)(n+2) = d(n)}$$

(c) Any linear combination of degenerate eigenstates is an eigenstate. So $\frac{1}{\sqrt{3}}\left[\psi_{100} + \psi_{010} + \psi_{001}\right]$ and $\frac{1}{\sqrt{2}}\left[\psi_{100} + i\psi_{001}\right]$ are eigenstates, whereas $\frac{1}{\sqrt{2}}\left[\psi_{000} + \psi_{010}\right]$ is not

3. Same as 2, except now

$$\boxed{E = \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y + \left(n_z + \frac{1}{2}\right)\hbar\omega_z}$$

There is no degeneracy except in special cases

4. For $l=0$, there is no angular dependence $Y_0^0(\theta,\phi) = \sqrt{\frac{1}{4\pi}}$

The radial equation becomes $\frac{d^2u}{dr^2} = -k^2 u$

with $u(r) = rR(r)$ and $k = \frac{\sqrt{2mE}}{\hbar}$ [see equations 4.41 and 4.42 in Griffiths]

The solution is $u(r) = Ae^{ikr} + Be^{-ikx}$

or equivalently $u(r) = C\sin kr + D\cos kr$

Let's take the exponential solution

$$R(r) = \frac{u(r)}{r} = A\frac{e^{ikr}}{r} + B\frac{e^{-ikr}}{r}$$

Note This is a free particle. There is no way to normalize it. You should have seen this last quarter. See Griffiths page 56. In analogy to the 1D case, the two solutions correspond to ingoing and outgoing waves (see Griffiths page 55)

(5) $P_\ell^m(z) = (1-z^2)^{m/2} F(z)$

$$\frac{dP_\ell^m}{dz} = -mz(1-z^2)^{\frac{m}{2}-1} F(z) + (1-z^2)^{m/2}\frac{dF(z)}{dz}$$

Then the associated Legendre equation in term of $F(z)$

$$\frac{d}{dz}\left[(1-z^2)\left[-mz(1-z^2)^{\frac{m}{2}-1}F(z) + (1-z^2)^{m/2}\frac{dF}{dz}\right]\right] +$$

$$+\left[\ell(\ell+1) - \frac{m^2}{1-z^2}\right](1-z^2)^{m/2} F(z) = 0$$

$$\frac{d}{dz}\left[-mz(1-z^2)^{m/2}F(z)+(1-z^2)^{m/2+1}\frac{dF}{dz}\right]+$$

$$+\ell(\ell+1)(1-z^2)^{m/2}F(z)-m^2(1-z^2)^{m/2-1}F(z)=0$$

$$-m(1-z^2)^{m/2}F(z)+m^2z^2(1-z^2)^{m/2-1}F(z)-mz(1-z^2)^{m/2}\frac{dF}{dz}+$$

$$-2z\left(\frac{m}{2}+1\right)(1-z^2)^{m/2}\frac{dF}{dz}+(1-z^2)^{m/2+1}\frac{d^2F}{dz^2}+$$

$$+\ell(\ell+1)(1-z^2)^{m/2}F(z)-m^2(1-z^2)^{m/2-1}F(z)=0$$

Cancel out a factor of $(1-z^2)^{m/2}$

$$-mF(z)+\frac{m^2z^2}{1-z^2}F(z)-mz\frac{dF}{dz}-mz\frac{dF}{dz}-2z\frac{dF}{dz}+(1-z^2)\frac{d^2F}{dz^2}+$$

$$+\ell(\ell+1)F(z)-\frac{m^2}{1-z^2}F(z)=0$$

$$\boxed{(1-z^2)\frac{d^2F}{dz^2}-2z(m+1)\frac{dF}{dz}+\left[\ell(\ell+1)-m(m+1)\right]F(z)=0} \quad 1$$

Now take Legendre equation

$$\frac{d}{dz}\left[(1-z^2)\frac{dP_\ell}{dz}\right]+\ell(\ell+1)P_\ell(z)=0$$

$$(1-z^2)\frac{d^2P_\ell}{dz^2}-2z\frac{dP_\ell}{dz}+\ell(\ell+1)P_\ell(z)=0$$

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Differentiate this equation m-times - Look at the 3 terms, one by one

First term: $(1-z^2)\frac{d^{2+m}P_\ell}{dz^{2+m}} - 2mz\frac{d^{1+m}P_\ell}{dz^{1+m}} - 2\frac{m(m-1)}{2}\frac{d^mP_\ell}{dz^m}$

Second Term: $-2z\frac{d^{1+m}P_\ell}{dz^{1+m}} - 2m\frac{d^mP_\ell}{dz^m}$.

Third term: $\ell(\ell+1)\frac{d^mP_\ell}{dz^m}$

Putting it together

$$(1-z^2)\frac{d^{2+m}P_\ell}{dz^{2+m}} - 2(m+1)z\frac{d^{1+m}P_\ell}{dz^{1+m}} + \left[\ell(\ell+1) - m(m+1)\right]\frac{d^mP_\ell}{dz^m} = 0$$

But this is the same as equation (1) for $F(z)$

So $\frac{d^mP_\ell}{dz^m} = F_z = (1-z^2)^{-m/2} P_\ell^m(z)$.

And $\boxed{P_\ell^m(z) = (1-z^2)^{m/2}\frac{d^mP_\ell}{dz^m}}$ (The additional factor of $(-1)^m$ is conventional)

This was done for $m>0$. Because the associated Legendre equation depends on m^2 not m, this will also work for $m<0$ provided $m \to |m|$.