Modern Homework 4
'11

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1. a) $E = \frac{1}{2m}\left(|P_x|^2 + |P_y|^2 + |P_z|^2\right)$

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$$= \frac{1}{2m}\left(\left(\hbar\frac{n_1\pi}{L_1}\right)^2 + \left(\hbar\frac{n_2\pi}{L_2}\right)^2 + \left(\hbar\frac{n_3\pi}{L_3}\right)^2\right)$$

$$= \frac{\hbar^2\pi^2}{2mL^2}\left(n_1^2 + \frac{n_2}{4} + \frac{n_3}{9}\right)$$

using excel to plug in n_1, n_2, n_3 and sort by the sum in the parentheses:

	n_1	n_2	n_3	$E\left(\frac{\hbar^2\pi^2}{2mL^2}\right)$
1	1	1	1	1.361
2	1	1	2	1.472
3	1	1	3	1.583
4	1	2	1	1.611
5	1	1	4	1.694
6	1	2	2	1.722
7	~~1~~	~~1~~	~~5~~	~~1.806~~
8	1	2	3	1.833
9	1	3 1, 3, 2	1	1.861
10	~~1~~	~~1~~	~~6~~	~~1.917~~
11	1	2	4	1.944

where n_1 is the x-dir
n_2 y-dir
n_3 z-dir

there are no repeats (in the first 11), so there are no degenerate energy levels.

We cannot use $n^2 = n_1^2 + n_2^2 + n_3^2$ because it assumes a cube, we're use a rectangular prism with non-identical edges, so we have to make it fit the new boundary conditions.

b) Now for some derivations of a new equation.

$$\psi(x,y,z) = \begin{cases} A\sin(k_1 x)\sin(k_2 y)\sin(k_3 z) & \text{in box} \\ 0 & \text{out box} \end{cases}$$

$$= \begin{cases} A\sin\left(\frac{n_1\pi}{L}x\right)\sin\left(\frac{n_2\pi}{2L}y\right)\sin\left(\frac{n_3\pi}{3L}z\right) \\ 0 \end{cases}$$

$$1 = \int|\psi|^2 dV = \int |A|^2 \sin^2\left(\frac{n_1\pi}{L}x\right)\sin^2\left(\frac{n_2\pi}{2L}y\right)\sin^3\left(\frac{n_3\pi}{3L}z\right)dV$$

Quick math detour:

$$\int \sin^2\theta \, d\theta = \int \underbrace{\tfrac{1}{2} - \tfrac{1}{2}\cos 2\theta}\, d\theta$$

Since we constructed boundary conditions to be zero at sin, for all integers this will be 0-0

$$\int \sin^2\theta \, d\theta = \tfrac{1}{2}\theta \Big|_0^L$$

So, for this setup the bounds are 0 to $\frac{L}{2}n$

$$\int_0^{L/2\, n} \sin^2\theta \, d\theta = \tfrac{1}{2}\left(n\tfrac{L}{2}\right)$$

$$1 = \int |\psi|^2 dv = \int |A|^2 \sin^2\left(\tfrac{n_1\pi}{L}x\right)\sin^2\left(\tfrac{n_2\pi}{2L}y\right)\sin^2\left(\tfrac{n_3\pi}{3L}y\right) dv$$

$$= |A|^2\left(\tfrac{1}{2}n_1\tfrac{L}{2}\right)\left(\tfrac{1}{2}n_2\tfrac{2L}{2}\right)\left(\tfrac{1}{2}n_3\left(\tfrac{3L}{2}\right)\right)$$

$$= |A|^2\left(\tfrac{3}{32}L^3\right)(n_1 n_2 n_3)$$

$$A = \cancel{\sqrt{\frac{32}{3L^3 n_1 n_2 n_3}}} \quad 4/3L^3$$

I will call it satisfactory to say

$$\psi(x,y,z) = \begin{cases} \sqrt{\frac{32}{3L^3 n_1 n_2 n_3}}\, \sin\left(\frac{n_1\pi}{L}x\right)\sin\left(\frac{n_2\pi}{2L}y\right)\sin\left(\frac{n_3\pi}{3L}z\right) & \text{in box} \\ 0 & \text{out of box.} \end{cases}$$

For the first five energy levels uses

	n_1	n_2	n_3
1.	1	1	1
2.	1	1	2
3.	1	1	3
4.	1	2	1
5.	1	1	4

We assumed a separable equation, so

$\Psi(\vec{r},t) = \psi(r)e^{-i\omega t}$ What is ω?

this will require a complex plot to graph, but $|\Psi|^2$ looks just like $|\psi|^2$, just constant in time.

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$$-\frac{\hbar^2}{2m}\nabla^2\psi + u\psi = E\psi$$

$$\frac{\nabla^2\psi}{A} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\psi\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\psi\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\left(\frac{1}{a}e^{-r/2a} - \frac{1}{2a^2}e^{-r/2a}\right)\right)\cos\theta + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta(-\sin\theta)\frac{r}{a}e^{-r/2a}$$

$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(\frac{r^2}{a}e^{-r/2a} - \frac{r^3}{2a^2}e^{-r/2a}\right)\cos\theta + \frac{1}{r^2\sin\theta}(-2\sin\theta\cos\theta)\frac{r}{a}e^{-r/2a}$$

$$= \frac{1}{r^2}\left(\frac{2r}{a}e^{-r/2a} - \frac{r^2}{2a^2}e^{-r/2a} - \frac{3r^2}{2a^2}e^{-r/2a} + \frac{r^3}{4a^3}e^{-r/2a}\right)\cos\theta - \frac{2}{r}\cos\theta\frac{1}{a}e^{-r/2a}$$

$$= \left[\frac{2}{ar} - \frac{1}{2a^2} - \frac{3}{2a^2} + \frac{r}{4a^3}\right]e^{-r/2a}\cos\theta - \frac{2}{ra}\cos\theta e^{-r/2a}$$

$$= \left[-\frac{1}{2a^2} - \frac{3}{2a^2} + \frac{r}{4a^3}\right]e^{-r/2a}\cos\theta$$

$$= \left[\frac{r}{4a^3} - \frac{2}{a^2}\right]e^{-r/2a}\cos\theta = \left[\frac{1}{4a^2} - \frac{2}{ar}\right]\frac{r}{a}e^{-r/2a}\cos\theta = \left[\frac{1}{4a^2} - \frac{2}{ar}\right]\psi/A$$

we left out the A since it is a constant

$$-\frac{\hbar^2}{2m}\nabla^2\psi + u\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\left[\frac{1}{4a^2} - \frac{2}{ar}\right]\psi + u\psi = E\psi$$

it will be helpful to remember

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$$

$$k = \frac{1}{4\pi\varepsilon_0}$$

$$-\frac{\hbar^2}{2m}\left[\frac{1}{4a^2} - \frac{2}{ar}\right] - \frac{ke^2}{r} = E$$

$$-\frac{\hbar^2}{2m}\left[\frac{1}{4a^2} - \frac{2}{\left(\frac{4\pi\varepsilon_0\hbar^2}{me^2}\right)r}\right] - \frac{e^2}{4\pi\varepsilon_0 r} = E$$

$$-\frac{\hbar^2}{2m}\frac{1}{4a^2} + \frac{2\hbar^2 me^2}{(2m)(4\pi\varepsilon_0\hbar^2)r} - \frac{e^2}{4\pi\varepsilon_0 r} = E$$

$$-\frac{\hbar^2}{2m}\frac{1}{4a^2} + \frac{e^2}{4\pi\varepsilon_0 r} - \frac{e^2}{4\pi\varepsilon_0 r} = E \quad (A)$$

$$\boxed{-\frac{\hbar}{2m}\frac{1}{4a^2} = E}$$

We also see that the final E is not reliant on any variables, as it should be (as it / it shouldn't have variables, and it doesn't)

Grabbing the derived point (A) above, the explicit solution looks like

$$\left[\frac{-\hbar^2}{8ma^2} + \frac{e^2}{4\pi\varepsilon_0 r}\right]\psi = (E-U)\psi$$

$$\left[\frac{-\hbar^2}{8ma^2} + \cancel{\frac{e^2}{4\pi\varepsilon_0 r}}\right]\psi = \left(E + \cancel{\frac{e^2}{4\pi\varepsilon_0 r}}\right)\psi$$

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b) Now for this bugger... Hey, it's good for you.

$$1 = \int |\psi|^2 dv = \int |A|^2 \left(\frac{r}{a}\right)^2 e^{-r/a}\cos^2\theta\, dv = \int |A|^2\left(\frac{r^2}{a^2}\right)e^{-r/a}\cos^2\theta\, r^2\sin\theta\, dr\, d\theta\, d\phi$$

$$= |A|^2 \int_0^\infty \frac{r^4}{a^2}e^{-r/a}dr \int_0^{\pi} \cos^2\theta\sin\theta\, d\theta \int_0^{2\pi} d\phi$$

$$= |A|^2 \int_0^\infty \frac{r^4}{a^2}e^{-r/a}dr \left(-\frac{1}{3}\cos^3\theta\Big|_0^\pi\right)(2\pi)$$

$$= |A|^2 \left(\frac{2}{3}\right)(2\pi)\int_0^\infty \frac{r^4}{a^2}e^{-r/a}dr$$

$$\int_0^\infty \frac{r^4}{a^2}e^{-r/a}dr = -\frac{r^4}{a}e^{-r/a} + \int \frac{4r^3}{a}e^{-r/a}dr$$

$$= -\frac{r^4}{a}e^{-r/a} - 4r^3e^{-r/a} + \int 12r^2e^{-r/a}dr$$

$$= -\frac{r^4}{a}e^{-r/a} - 4r^3e^{-r/a} - 12r^2ae^{-r/a} + \int 24rae^{-r/a}dr$$

$$= -\frac{r^4}{a}e^{-r/a} - 4r^3e^{-r/a} - 12r^2ae^{-r/a} - 24ra^3 + \int 24a^2e^{-r/a}dr$$

$$= -\frac{r^4}{a}e^{-r/a} - 4r^3e^{-r/a} - 12r^2ae^{-r/a} - 24ra^3 - 24a^3e^{-r/a}$$

$$1 = |A|^2\left(\frac{2}{3}\right)(2\pi)\left[\left(-\frac{r^4}{a} - 4r^3 - 12r^2a - 24ra^2 - 24a^3\right)e^{-r/a}\right]\Big|_0^\infty$$

Using L'hopitals to figure out limit at ∞

$$\lim_{r\to\infty}\left(-\frac{r^4}{a} - 4r^3 - 12r^2a - 24ra^2 - 24a^3\right)e^{-r/a}$$

$$= \lim_{r\to\infty}\frac{\frac{1}{a}e^{r/a}}{\frac{-4r^3}{a} - 12r^2 - 24ra - 24} = \lim_{r\to\infty}\frac{\frac{-12r^2}{a} - 24r - 24a}{\frac{1}{a^2}e^{+r/a}}$$

$$= \lim_{r\to\infty}\frac{\frac{1}{a^3}e^{r/a}}{\frac{-24r}{a} - 24} = \lim_{r\to\infty}\frac{\frac{-24}{a}}{\frac{1}{a^4}e^{r/a}} = \lim_{r\to\infty} 24a^3e^{-r/a} \to 0$$

$$1 = |A|^2 \left(\frac{2}{3}\right)(2\pi)(0 + 24a^3)$$

$$1 = |A|^2 (32\pi a^3)$$

$$\boxed{A = \sqrt{\frac{1}{32\pi a^3}}}$$

Units $\frac{1}{\sqrt{V}}$