Homework #8

Problem 5 - 9.4.5:

We have to solve Schrödinger's equation for a particle in a box. The equations is:

$$-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi \tag{1}$$

with the boundary conditions: $\psi = 0$ for $x = 0$ and a, $y = 0$ and b, and $z = 0$ and c.

We will work in cartesian coordinates because the b.c.'s are given on planes and we propose:

$$\psi(x, y, z) = X(x)Y(y)Z(z). \tag{2}$$

This replacement was done in class (just replace k^2 by E in Helmholz equation). For X and Y we obtained the harmonic oscillator equation and, considering the boundary conditions for $x = y = 0$ we need to chose:

$$X(x) \propto sin(\alpha x), \tag{3}$$

and

$$Y(y) \propto sin(\beta y). \tag{4}$$

Since X has to vanish at a it means that

$$\alpha = \frac{\pi n_x x}{a}, \tag{5}$$

with $n_x = 1, 2, 3, ...$ and since $Y(b) = 0$ it means that

$$\beta = \frac{\pi n_y y}{b}, \tag{6}$$

with $n_y = 1, 2, 3, ...$ Finally for Z we were left with the equation:

$$\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = \alpha^2 + \beta^2 - \frac{2mE}{\hbar^2} = -\gamma^2. \tag{7}$$

Thus (7) is also the harmonic oscillator equation and from the b.c. for Z we find that

$$Z(z) \propto sin(\gamma z), \tag{8}$$

with

$$\gamma = \frac{\pi n_z z}{c}, \tag{9}$$

with $n_z = 1, 2, 3, ...$ Thus, collecting all the results, we obtain

$$\psi(x, y, z) = \sum_{n_x,n_y,n_x=1}^{\infty} A_{n_x,n_y,n_z} sin(\frac{\pi n_x x}{a}) sin(\frac{\pi n_y y}{b}) sin(\frac{\pi n_z z}{c}), \tag{10}$$

where A_{n_x,n_y,n_z} can be evaluated by requesting that ψ is normalized to 1. But the value of this constant is irrelevant for the question that we have to address. We need to find the lowest value of E. Replacing in (7) the values obtained for α, β and γ we find that

$$E = \frac{\hbar^2\pi^2}{2m}(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}). \tag{11}$$

Then the lowest value of E is obtained for $n_x = n_y = n_z = 1$ giving

$$E_{111} = \frac{\hbar^2\pi^2}{2m}(\frac{1}{a^2} + \frac{1}{b^2} + \frac{1}{c^2}). \tag{11}$$