Group Problems #31 - Solutions

<p style="text-align:center">Monday, November 14</p>

Problem 1 *3D Infinite Square Well*

A particle is confined to a 3D box with sides of length $L_x = L$, $L_y = 2L$, and $L_z = 4L$.

(a) Give the sets of quantum numbers, n_x, n_y, and n_z that correspond to the lowest 10 energy levels of this box.

The energy eigenvalues for the 3D infinite well are given by:

$$E_{n_x,n_y,n_z} = \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)\frac{\pi^2\hbar^2}{2m}. \tag{1}$$

Substituting $L_x = L$, $L_y = 2L$, and $L_z = 4L$, yields:

$$E_{n_x,n_y,n_z} = \left(\frac{n_x^2}{L^2} + \frac{n_y^2}{4L^2} + \frac{n_z^2}{16L^2}\right)\frac{\pi^2\hbar^2}{2m} \tag{2}$$

$$\tag{3}$$

$$= \left(16n_x^2 + 4n_y^2 + n_z^2\right)\frac{\pi^2\hbar^2}{32mL^2} = \left(16n_x^2 + 4n_y^2 + n_z^2\right)E_0. \tag{4}$$

Let's make a table of the 10 lowest energy levels and their degeneracy:

(n_x, n_y, n_z)	E/E_0	Degeneracy
(1,1,1)	21	1
(1,1,2)	24	1
(1,1,3)	29	1
(1,2,1)	33	1
(1,2,2) (1,1,4)	36	2
(1,2,3)	41	1
(1,1,5)	45	1
(1,2,4)	48	1
(1,3,1)	53	1
(1,3,2) (1,1,6)	56	2

<p style="text-align:center">1</p>

(b) What sets of quantum numbers correspond to degenerate energy levels?

As the table shows, the two states $(n_x, n_y, n_z) = (1, 2, 2)$ and $(1, 1, 4)$ both have the same energy $E = 36E_0$ and thus this level has a degeneracy of 2. Similarly, $(n_x, n_y, n_z) = (1, 3, 2)$ and $(1, 1, 6)$ both have energy $E = 56E_0$, with a degeneracy of 2.

(c) For the state, $n_x = 1$, $n_y = 1$, and $n_z = 4$, where is the probability of finding the particle the largest?

The wavefunctions for the 3D infinite well are given by:

$$\psi_{n_x, n_y, n_z}(x, y, z) \quad = \quad A \sin \frac{n_x \pi x}{L_x} \sin \frac{n_y \pi y}{L_y} \sin \frac{n_z \pi z}{L_z} \tag{5}$$

$$\tag{6}$$

$$= \quad A \sin \frac{n_x \pi x}{L} \sin \frac{n_y \pi y}{2L} \sin \frac{n_z \pi z}{4L}. \tag{7}$$

For the state $(n_x, n_y, n_z) = (1, 1, 4)$, the wave function becomes:

$$\psi_{1,1,4}(x, y, z) = A \sin \frac{\pi x}{L} \sin \frac{\pi y}{2L} \sin \frac{\pi z}{L}, \tag{8}$$

and the probability density is thus given by:

$$\frac{dp}{dV} = |\psi_{1,1,4}(x, y, z)|^2 = A^2 \sin^2 \frac{\pi x}{L} \sin^2 \frac{\pi y}{2L} \sin^2 \frac{\pi z}{L}. \tag{9}$$

The maximum values of $\sin^2$ occur at odd-integer multiples of $\pi/2$: $\pi/2$, $3\pi/2$, etc. So ψ^2 is maximum at $x = L/2$, $y = L$, and $z = L/2$, $3L/2$, $5L/2$, $7L/2$. The particle is most likely to be found at these locations.

(d) Repeat part (c) for any state with the same energy as in part (c).

The table above shows that the state $(n_x, n_y, n_z) = (1, 2, 2)$ has the same energy as $(1, 1, 4)$. For the state $(1, 2, 2)$, the probability density is:

$$\frac{dp}{dV} = |\psi_{1,2,2}(x, y, z)|^2 = A^2 \sin^2 \frac{\pi x}{L} \sin^2 \frac{\pi y}{L} \sin^2 \frac{\pi z}{2L}. \tag{10}$$

For this state, the maximum values of ψ^2 occur at $x = L/2$, $y = L/2$, $3L/2$, and $z = L$, $3L$.