INFINITE SQUARE WELL IN THREE DIMENSIONS

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References: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.2.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Chapter 10, Exercise 10.2.1.

The three-dimensional particle in a box problem is a fairly straightforward extension of the one dimensional case. The 3-d time-independent Schrödinger equation in rectangular coordinates is

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

Using separation of variables, we can assume that the spatial wave function is the product of three individual functions, each dependent on only one spatial coordinate:

$$\psi(\mathbf{r}) = \xi(x)\eta(y)\zeta(z) \tag{2}$$

Plugging this into the 3-d Schrödinger equation and dividing through by $\xi(x)\eta(y)\zeta(z)$ gives

$$-\frac{\hbar^2}{2m}\left(\frac{\xi_{xx}}{\xi}+\frac{\eta_{yy}}{\eta}+\frac{\zeta_{zz}}{\zeta}\right) = E \tag{3}$$

where a subscript indicates a derivative with respect to that variable, so $\xi_{xx} = d^2\xi/dx^2$ etc.

Since E is a constant (independent of position), and each term in the sum depends on a different independent variable, each term in the sum must itself be a constant. In order to be able to use the analysis from the one-dimensional case, we therefore introduce three constants k_x, k_y and k_z so that

$$\xi_{xx} = -k_x^2\xi \tag{4}$$

$$\eta_{yy} = -k_y^2\eta \tag{5}$$

$$\zeta_{zz} = -k_z^2\zeta \tag{6}$$

From 3 the constants satisify the condition:

$$k_x^2 + k_y^2 + k_z^2 = \frac{2mE}{\hbar^2} \tag{7}$$

From here, we can use the analysis of the infinite square well in one dimension, to get:

$$\begin{aligned}
\xi(x) &= \sqrt{\frac{2}{a}} \sin \frac{n_x \pi}{a} x & (8)\\
\eta(y) &= \sqrt{\frac{2}{a}} \sin \frac{n_y \pi}{a} y & (9)\\
\zeta(z) &= \sqrt{\frac{2}{a}} \sin \frac{n_z \pi}{a} z & (10)
\end{aligned}$$

where each of n_x, n_y and n_z can take any positive integer value. From 7, the energies are given by

$$E_i = \frac{\pi^2 \hbar^2}{2ma^2} \left(n_x^2 + n_y^2 + n_z^2\right) \tag{11}$$

The various energies can be found by listing the values of n_x, n_y and n_z such that the sums $n_x^2 + n_y^2 + n_z^2$ are listed in ascending order. The degeneracy of each combination of ns can be found by noting that if all three ns are the same, the degeneracy is 1, if two are the same, the degeneracy is 3, and if all three are different, the degeneracy is 6. Thus in the following table, we list only one combination of ns for each degenerate set. The energies are given in units of $\frac{\pi^2 \hbar^2}{2ma^2}$

n_x	n_y	n_z	Energy	Degeneracy
1	1	1	$E_1 = 3$	1
2	1	1	$E_2 = 6$	3
2	2	1	$E_3 = 9$	3
3	1	1	$E_4 = 11$	3
2	2	2	$E_5 = 12$	1
3	2	1	$E_6 = 14$	6
3	2	2	$E_7 = 17$	3
4	1	1	$E_8 = 18$	3
3	3	1	$E_9 = 19$	3
4	2	1	$E_{10} = 21$	6
3	3	2	$E_{11} = 22$	3
4	2	2	$E_{12} = 24$	3
4	3	1	$E_{13} = 26$	6
3	3	3	$E_{14} = 27$	4
5	1	1	“	“

The case of E_{14} has a degeneracy of 4, since it can arise from two distinct combinations of ns, as shown. It's an interesting question as to whether this case is unique. Not obvious from a superficial analysis how this could be proved one way or the other.

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