

HARMONIC OSCILLATOR IN 3-D - RECTANGULAR COORDINATES

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.38.

The 3-d harmonic oscillator can be solved in rectangular coordinates by separation of variables. The Schrödinger equation to be solved for the 3-d harmonic oscillator is

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

To use separation of variables we define

$$\psi(x, y, z) = \xi(x)\eta(y)\zeta(z) \quad (2)$$

Dividing 1 through by this product we get

$$-\frac{\hbar^2}{2m}\frac{\xi''}{\xi} + \frac{1}{2}m\omega^2x^2 - \frac{\hbar^2}{2m}\frac{\eta''}{\eta} + \frac{1}{2}m\omega^2y^2 - \frac{\hbar^2}{2m}\frac{\zeta''}{\zeta} + \frac{1}{2}m\omega^2z^2 = E \quad (3)$$

where the double prime notation indicates the second derivative of a function with respect to its independent variable, so $\xi'' = d^2\xi/dx^2$, etc.

We now have three groups of two terms each of which depends on only one of the variables x , y and z , and the sum of all these terms is the constant E . We can therefore use the usual argument that each group of two terms must be a constant on its own, so the 3-d equation reduces to the sum of three 1-d harmonic oscillators. From the analysis of the 1-d harmonic oscillator, we know that each of these will contribute $(n + 1/2)\hbar\omega$ to the total energy, with the ground state at $n = 0$. Thus the ground state for the 3-d oscillator will have energy $3\hbar\omega/2$, and the general energy level will increase in steps of $\hbar\omega$ so the energy levels are given by

$$E_n = \left(n + \frac{3}{2}\right)\hbar\omega \quad (4)$$

Unlike the 1-d case, the energies of the 3-d oscillator are degenerate. A given value of n is composed of the sum of 3 quantum numbers: $n = n_x + n_y + n_z$ where all numbers are non-negative integers. Suppose we choose a value for n_x so that $n_y + n_z = n - n_x$. The number of pairs of integers that

can be used for $n_y + n_z$ is $n - n_x + 1$ (since n_y can be anything between 0 and $n - n_x$). Since n_x itself can range between 0 and n , the total number of combinations of quantum states that can make up state n is

$$d(n) = \sum_{n_x=0}^n (n - n_x + 1) \quad (5)$$

$$= (n+1) \sum_{n_x=0}^n 1 - \sum_{n_x=0}^n n_x \quad (6)$$

$$= (n+1)^2 - \frac{1}{2}n(n+1) \quad (7)$$

$$= \frac{1}{2}(n+1)(n+2) \quad (8)$$

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