

Problem 4.46

Consider the **three-dimensional harmonic oscillator**, for which the potential is

$$V(r) = \frac{1}{2}m\omega^2 r^2. \quad (4.215)$$

- (a) Show that separation of variables in cartesian coordinates turns this into three one-dimensional oscillators, and exploit your knowledge of the latter to determine the allowed energies. *Answer:*

$$E_n = \left(n + \frac{3}{2}\right) \hbar\omega. \quad (4.216)$$

- (b) Determine the degeneracy $d(n)$ of E_n .

Solution

Schrödinger's equation governs the time evolution of a wave function.

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi$$

Here the aim is to solve it in all of space with the potential energy function,

$$V(x, y, z) = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2).$$

Since $V = V(x, y, z)$, expand the Laplacian operator in Cartesian coordinates.

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} + \frac{\partial^2 \Psi}{\partial z^2} \right) + V(x, y, z)\Psi(x, y, z, t), \quad -\infty < x, y, z < \infty, \quad t > 0$$

Because Schrödinger's equation and its associated boundary conditions ($\Psi \rightarrow 0$ as $|\mathbf{x}| \rightarrow \infty$) are linear and homogeneous, the method of separation of variables can be applied: Assume a product solution of the form $\Psi(x, y, z, t) = X(x)Y(y)Z(z)T(t)$ and plug it into the PDE.

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} [X(x)Y(y)Z(z)T(t)] &= -\frac{\hbar^2}{2m} \left\{ \frac{\partial^2}{\partial x^2} [X(x)Y(y)Z(z)T(t)] \right. \\ &\quad + \frac{\partial^2}{\partial y^2} [X(x)Y(y)Z(z)T(t)] \\ &\quad \left. + \frac{\partial^2}{\partial z^2} [X(x)Y(y)Z(z)T(t)] \right\} \\ &\quad + \frac{1}{2}m\omega^2(x^2 + y^2 + z^2)[X(x)Y(y)Z(z)T(t)] \\ i\hbar X(x)Y(y)Z(z)T'(t) &= -\frac{\hbar^2}{2m} [X''(x)Y(y)Z(z)T(t) + X(x)Y''(y)Z(z)T(t) + X(x)Y(y)Z''(z)T(t)] \\ &\quad + \frac{1}{2}m\omega^2(x^2 + y^2 + z^2)[X(x)Y(y)Z(z)T(t)] \end{aligned}$$

Divide both sides by $X(x)Y(y)Z(z)T(t)$ in order to separate variables.

$$i\hbar \frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2m} \left[\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} \right] + \frac{1}{2}m\omega^2(x^2 + y^2 + z^2)$$

The only way a function of t can be equal to a function of x , y , and z is if both are equal to a constant.

$$i\hbar \frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2m} \left[\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} \right] + \frac{1}{2}m\omega^2(x^2 + y^2 + z^2) = E$$

Bring the terms with y and z to the right side.

$$-\frac{\hbar^2}{2m} \frac{X''(x)}{X(x)} + \frac{1}{2}m\omega^2 x^2 = E + \frac{\hbar^2}{2m} \left[\frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} \right] - \frac{1}{2}m\omega^2(y^2 + z^2)$$

The only way a function of x can be equal to a function of y and z is if both are equal to another constant.

$$-\frac{\hbar^2}{2m} \frac{X''(x)}{X(x)} + \frac{1}{2}m\omega^2 x^2 = E + \frac{\hbar^2}{2m} \left[\frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} \right] - \frac{1}{2}m\omega^2(y^2 + z^2) = F$$

Bring the terms with y to one side.

$$-\frac{\hbar^2}{2m} \frac{Y''(y)}{Y(y)} + \frac{1}{2}m\omega^2 y^2 = E - F + \frac{\hbar^2}{2m} \frac{Z''(z)}{Z(z)} - \frac{1}{2}m\omega^2 z^2$$

The only way a function of y can be equal to a function of z is if both are equal to another constant.

$$-\frac{\hbar^2}{2m} \frac{Y''(y)}{Y(y)} + \frac{1}{2}m\omega^2 y^2 = E - F + \frac{\hbar^2}{2m} \frac{Z''(z)}{Z(z)} - \frac{1}{2}m\omega^2 z^2 = G$$

As a result of using the method of separation of variables, Schrödinger's equation has reduced to four ODEs—one in x , one in y , one in z , and one in t .

$$\left. \begin{aligned} i\hbar \frac{T'(t)}{T(t)} &= E \\ -\frac{\hbar^2}{2m} \frac{X''(x)}{X(x)} + \frac{1}{2}m\omega^2 x^2 &= F \\ -\frac{\hbar^2}{2m} \frac{Y''(y)}{Y(y)} + \frac{1}{2}m\omega^2 y^2 &= G \\ E - F + \frac{\hbar^2}{2m} \frac{Z''(z)}{Z(z)} - \frac{1}{2}m\omega^2 z^2 &= G \end{aligned} \right\}$$

The strategy is to solve the second and third eigenvalue problems for F and G , then to solve the fourth eigenvalue problem for E , and then finally to solve the first eigenvalue problem for $T(t)$.

Since $-\infty < x, y, z < \infty$, the method of operator factorization can be used to solve the latter three (as was done in Problem 2.10).

$$F = \left(j + \frac{1}{2}\right) \hbar\omega, \quad j = 0, 1, 2, \dots$$

$$G = \left(k + \frac{1}{2}\right) \hbar\omega, \quad k = 0, 1, 2, \dots$$

$$E - F - G = \left(l + \frac{1}{2}\right) \hbar\omega, \quad l = 0, 1, 2, \dots$$

Substitute the formulas for F and G into the third equation.

$$E - \left(j + \frac{1}{2}\right) \hbar\omega - \left(k + \frac{1}{2}\right) \hbar\omega = \left(l + \frac{1}{2}\right) \hbar\omega$$

Solve for E .

$$E_{jkl} = \left(j + k + l + \frac{3}{2}\right) \hbar\omega, \quad \begin{cases} j = 0, 1, 2, \dots \\ k = 0, 1, 2, \dots \\ l = 0, 1, 2, \dots \end{cases}$$

Evaluate the energy for many values of j , k , and l .

$$E_{000} = \left(0 + 0 + 0 + \frac{3}{2}\right) \hbar\omega = \left(\frac{3}{2}\right) \hbar\omega = E_0$$

$$E_{100} = \left(1 + 0 + 0 + \frac{3}{2}\right) \hbar\omega = \left(\frac{5}{2}\right) \hbar\omega = E_1$$

$$E_{010} = \left(0 + 1 + 0 + \frac{3}{2}\right) \hbar\omega = \left(\frac{5}{2}\right) \hbar\omega$$

$$E_{001} = \left(0 + 0 + 1 + \frac{3}{2}\right) \hbar\omega = \left(\frac{5}{2}\right) \hbar\omega$$

$$E_{110} = \left(1 + 1 + 0 + \frac{3}{2}\right) \hbar\omega = \left(\frac{7}{2}\right) \hbar\omega = E_2$$

$$E_{101} = \left(1 + 0 + 1 + \frac{3}{2}\right) \hbar\omega = \left(\frac{7}{2}\right) \hbar\omega$$

$$E_{011} = \left(0 + 1 + 1 + \frac{3}{2}\right) \hbar\omega = \left(\frac{7}{2}\right) \hbar\omega$$

$$E_{200} = \left(2 + 0 + 0 + \frac{3}{2}\right) \hbar\omega = \left(\frac{7}{2}\right) \hbar\omega$$

$$E_{020} = \left(0 + 2 + 0 + \frac{3}{2}\right) \hbar\omega = \left(\frac{7}{2}\right) \hbar\omega$$

$$E_{002} = \left(0 + 0 + 2 + \frac{3}{2}\right) \hbar\omega = \left(\frac{7}{2}\right) \hbar\omega$$

Evaluate the energy for more values of j , k , and l .

$$E_{111} = \left(1 + 1 + 1 + \frac{3}{2}\right) \hbar\omega = \left(\frac{9}{2}\right) \hbar\omega = E_3$$

$$E_{210} = \left(2 + 1 + 0 + \frac{3}{2}\right) \hbar\omega = \left(\frac{9}{2}\right) \hbar\omega$$

$$E_{201} = \left(2 + 0 + 1 + \frac{3}{2}\right) \hbar\omega = \left(\frac{9}{2}\right) \hbar\omega$$

$$E_{120} = \left(1 + 2 + 0 + \frac{3}{2}\right) \hbar\omega = \left(\frac{9}{2}\right) \hbar\omega$$

$$E_{021} = \left(0 + 2 + 1 + \frac{3}{2}\right) \hbar\omega = \left(\frac{9}{2}\right) \hbar\omega$$

$$E_{012} = \left(0 + 1 + 2 + \frac{3}{2}\right) \hbar\omega = \left(\frac{9}{2}\right) \hbar\omega$$

$$E_{102} = \left(1 + 0 + 2 + \frac{3}{2}\right) \hbar\omega = \left(\frac{9}{2}\right) \hbar\omega$$

$$E_{300} = \left(3 + 0 + 0 + \frac{3}{2}\right) \hbar\omega = \left(\frac{9}{2}\right) \hbar\omega$$

$$E_{030} = \left(0 + 3 + 0 + \frac{3}{2}\right) \hbar\omega = \left(\frac{9}{2}\right) \hbar\omega$$

$$E_{003} = \left(0 + 0 + 3 + \frac{3}{2}\right) \hbar\omega = \left(\frac{9}{2}\right) \hbar\omega$$

Therefore, following the pattern,

$$E_n = \left(n + \frac{3}{2}\right) \hbar\omega, \quad n = 0, 1, 2, \dots$$

The degeneracy is the number of states that have the same energy. As a result, $d_0 = 1$, $d_1 = 3$, $d_2 = 6$, and $d_3 = 10$. Notice that to get d_1 , 2 needs to be added to d_0 ; to get d_2 , 3 needs to be added to d_1 ; and to get d_3 , 4 needs to be added to d_2 . The pattern is apparent for d_{n+1} .

$$d_{n+1} = (n + 2) + d_n, \quad d_0 = 1$$

This is a recurrence relation, more specifically an inhomogeneous first-order linear difference equation with constant coefficients. Bring d_n to the left side.

$$d_{n+1} - d_n = n + 2$$

The left side is how the discrete derivative of a function d_n of the integers is defined.

$$Dd_n = n + 2$$

Take the discrete antiderivative of both sides by summing from 0 to $n - 1$.

$$\sum_{q=0}^{n-1} Dd_q = \sum_{q=0}^{n-1} (q + 2)$$

$$Dd_0 + Dd_1 + Dd_2 + \cdots + Dd_{n-2} + Dd_{n-1} = \sum_{q=0}^{n-1} q + \sum_{q=0}^{n-1} 2$$

$$(d_1 - d_0) + (d_2 - d_1) + \cdots + (d_{n-1} - d_{n-2}) + (d_n - d_{n-1}) = 0 + \sum_{q=1}^{n-1} q + 2 \sum_{q=0}^{n-1} 1$$

$$d_n - d_0 = \frac{(n-1)[(n-1)+1]}{2} + 2[(n-1)+1]$$

$$d_n - 1 = \frac{(n-1)n}{2} + 2n$$

$$d_n - 1 = \frac{n^2 + 3n}{2}$$

$$d_n = \frac{n^2 + 3n + 2}{2}$$

Therefore, the degeneracy of energy E_n is

$$d_n = \frac{(n+2)(n+1)}{2}.$$