6.2: Particle in Box

Consider a particle of mass m trapped inside a cubic box of dimension a. (See Section [s5.2].) The particle's stationary wavefunction, $\psi(x,y,z)$, satisfies

$$\left(\frac{\partial^{\,2}}{\partial x^{\,2}}+\frac{\partial^{\,2}}{\partial y^{\,2}}+\frac{\partial^{\,2}}{\partial z^{\,2}}\right)\psi=-\frac{2\,m}{\hbar^{\,2}}\,E\,\psi, \tag{6.2.1}$$

where E is the particle energy. The wavefunction satisfies the boundary condition that it must be zero at the edges of the box.

Let us search for a separable solution to the previous equation of the form

$$\psi(x,y,z)=X(x)\,Y(y)\,Z(z). \tag{6.2.2}$$

The factors of the wavefunction satisfy the boundary conditions $X(0)=X(a)=0$, $Y(0)=Y(a)=0$, and $Z(0)=Z(a)=0$. Substituting Equation ([e6.22]) into Equation ([e6.21]), and rearranging, we obtain

$$\frac{X''}{X}+\frac{Y''}{Y}+\frac{Z''}{Z}=-\frac{2\,m}{\hbar^{\,2}}\,E, \tag{6.2.3}$$

where $'$ denotes a derivative with respect to argument. It is evident that the only way in which the previous equation can be satisfied at all points within the box is if

$$\frac{X''}{X}=-k_x^2,$$
$$\frac{Y''}{Y}=-k_y^2,$$
$$\frac{Z''}{Z}=-k_z^2,$$

where k_x^2, k_y^2, and k_z^2 are spatial constants. Note that the right-hand sides of the previous equations must contain negative, rather than positive, spatial constants, because it would not otherwise be possible to satisfy the boundary conditions. The solutions to the previous equations which are properly normalized, and satisfy the boundary conditions, are [see Equation ([e5.11])]

$$X(x)=\sqrt{\frac{2}{a}}\,\sin(k_x\,x),$$
$$Y(y)=\sqrt{\frac{2}{a}}\,\sin(k_y\,y),$$
$$Z(z)=\sqrt{\frac{2}{a}}\,\sin(k_z\,z),$$

where

$$k_x=\frac{l_x\,\pi}{a},$$
$$k_y=\frac{l_y\,\pi}{a},$$
$$k_z=\frac{l_z\,\pi}{a}.$$

Here, l_x, l_y, and l_z are positive integers. Thus, from Equations ([e7.28])–([e7.31]), the energy of the system is written [see Equation ([eenergy])]

$$E=\frac{l^{\,2}\,\pi^{\,2}\,\hbar^{\,2}}{2\,m\,a^{\,2}}. \tag{6.2.4}$$

where

$$l^{\,2}=l_x^2+l_y^2+l_z^2. \tag{6.2.5}$$

Contributors and Attributions

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