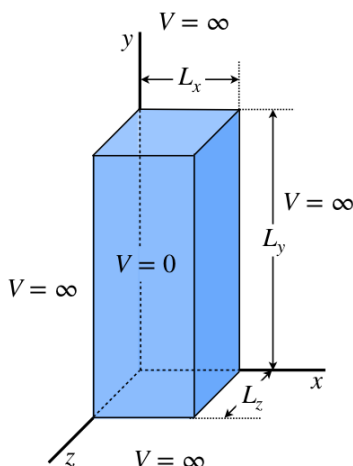


7.2: 3-Dimensional Models

Particle in a 3D Infinite Square Well

The infinite square well in three dimensions has the same property as the one-dimensional box – the potential is zero everywhere inside, and instantly becomes infinity at the boundaries. The one-dimensional case had a specified length, but we will not saddle this infinite well with the same width in all three directions, meaning we will confine the particle to a rectangular prism, not a cube. We will define our coordinate system so that the walls are parallel to the three planes, and we will place the origin at one of the box corners. The lengths of the walls along the x , y , and z axes we will call L_x , L_y , L_z , respectively.

Figure 7.2.1 Three-Dimensional Infinite Square Well



Mathematically, the potential is written:

$$V(x, y, z) = \begin{cases} 0 & 0 < x < L_x \text{ and } 0 < y < L_y \text{ and } 0 < z < L_z \\ \infty & \text{elsewhere} \end{cases} \quad (7.2.1)$$

As we saw for the one-dimensional box, we can use a combination of two oppositely-moving plane waves (for each of the three axes) to construct a wave function of definite energy that vanishes at the walls (i.e. sinusoidal functions). The individual solutions to the differential equations in x , y , and z are the same as before, with two exceptions: Each dimension involves a separate harmonic number n , so like the 1-dimensional well, all the wave functions are sines:

$$X(x) = A_x \sin \frac{n_x \pi x}{L_x} \quad Y(y) = A_y \sin \frac{n_y \pi y}{L_y} \quad Z(z) = A_z \sin \frac{n_z \pi z}{L_z}, \quad n_x, n_y, n_z = 1, 2, \dots \quad (7.2.2)$$

Before we move on to the energy spectrum, let's construct the spatial full wave function by multiplying the partial wave functions. We also have to deal with normalizing the full wave function. Normalization does not tell us anything about the values of A_x , A_y , and A_z , but their product must equal the normalization constant for the full wave function. The normalization integral is over all three dimensions and integrals over x will only affect $X(x)$, and similarly for y and z , so the normalization constant for the full wave function turns out to be the same as the product of the normalization constants for the three separate one-dimensional wave functions.

$$\psi_{n_x n_y n_z}(x, y, z) = \sqrt{\frac{8}{L_x L_y L_z}} \sin \frac{n_x \pi x}{L_x} \sin \frac{n_y \pi y}{L_y} \sin \frac{n_z \pi z}{L_z}, \quad n_x, n_y, n_z = 1, 2, \dots \quad (7.2.3)$$

In keeping with our notation of labeling the wave function with the quantum numbers, we have labeled the energy eigenstate wave function accordingly.

Plugging the wave function back into the stationary-state Schrödinger equation, we get the following energy spectrum:

$$E_{n_x n_y n_z} = \left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right) \frac{h^2}{8m}, \quad n_x, n_y, n_z = 1, 2, \dots \quad (7.2.4)$$

Alert

One might be tempted to think that the ground state energy of this particle occurs when the n along the longest dimension is 1, while the others are zero, but It should be emphasized that the minimum value of all three n values is 1. None of the three modes can provide a zero contribution to the energy.

Another way that the three-dimensional case differs from the one-dimensional case is apparent if we consider the hierarchy of the energy spectrum. Suppose for example, we wanted to draw an energy-level diagram for this spectrum. We know that ψ_{111} is the ground state, but which quantum state would be the first excited state? The answer depends upon the dimensions of the well. If the L_x is greater than the other two box dimensions, then the smallest increase in the total energy will come from incrementing n_x from 1 to 2, and the first excited state would be ψ_{211} . What about the second excited state? Well, now we need even more information. If L_x is only slightly greater than L_y dimension (and both are longer than L_z), then the second excited state would be ψ_{221} . But if L_x is significantly longer than the other dimensions, then the second excited state would be ψ_{311} . In other words, with three quantum numbers, we have lost the ability (at least for this case) to express the energy levels with a single integer.

The 3D Harmonic Oscillator

As our final example of a potential that allows for separation of variables in Cartesian coordinates, we consider the three dimensional harmonic oscillator, which has a potential that is a sum of functions purely of x , y , and z . In general, the spring constants are different for each direction, so:

$$V(x, y, z) = \frac{1}{2}\kappa_x x^2 + \frac{1}{2}\kappa_y y^2 + \frac{1}{2}\kappa_z z^2 \quad (7.2.5)$$

This sort of model might be useful for crystal lattices where the bonds differ along the different dimensions. Plugging this into [Equation 7.1.10](#) results in an equation with three separated functions again:

$$\left[\frac{1}{X} \frac{\partial^2 X}{\partial x^2} + \frac{\kappa_x m}{\hbar^2} x^2 \right] + \left[\frac{1}{Y} \frac{\partial^2 Y}{\partial y^2} + \frac{\kappa_y m}{\hbar^2} y^2 \right] + \left[\frac{1}{Z} \frac{\partial^2 Z}{\partial z^2} + \frac{\kappa_z m}{\hbar^2} z^2 \right] = -\frac{2mE}{\hbar^2} \quad (7.2.6)$$

Following the same procedure as before gives us three separate differential equations. This decoupling maneuver once again leaves us with three wave function pieces, which are multiplied together to get the full wave function. As with the case of the square well, the energy contributions of the partial wave functions are added together to give the total energy of the state:

$$E_{n_x n_y n_z} = \left(n_x + \frac{1}{2} \right) \hbar \sqrt{\frac{\kappa_x}{m}} + \left(n_y + \frac{1}{2} \right) \hbar \sqrt{\frac{\kappa_y}{m}} + \left(n_z + \frac{1}{2} \right) \hbar \sqrt{\frac{\kappa_z}{m}} \quad (7.2.7)$$

This gives us a nice way to describe bonds along different axes in general, but of particular interest is the *isotropic harmonic oscillator*, which involves equal spring constants (κ) in all three directions. In this case, the energy spectrum reduces to:

$$E_{n_x n_y n_z} = \left(n_x + n_y + n_z + \frac{3}{2} \right) \hbar \omega_c, \quad \omega_c = \sqrt{\frac{\kappa}{m}} \quad (7.2.8)$$

Notice that even with the simplification of isotropy, three quantum numbers are required to define the state.

Degeneracy

Notice that unlike one-dimensional potentials, in these cases a single quantum number does not define the energy. But there is even more to it than that. Looking at the case of the three-dimensional box again, suppose it has three equal sides: $L_x = L_y = L_z = L$. In this case, there exist three distinct quantum states that possess the same total energy, namely ψ_{211} , ψ_{121} , and ψ_{112} . These states clearly possess equal energies, and yet they are distinct because, for example, the states ψ_{211} and ψ_{121} yield different uncertainties in the x -component of the particle's position (ψ_{211} has two antinodes along the x axis, while ψ_{121} has only one). A similar thing occurs (only more dramatically) for the isotropic harmonic oscillator, as any combination of n_x , n_y , and n_z that gives the same sum will result in the same energy.

When multiple quantum states yield the same energy, they are said to be *degenerate*, and if there are a total of j distinct states for the same energy, that energy level is said to be *j-fold degenerate*. Typically degeneracy comes about due to obvious symmetries, such as in the cases mentioned above. All we need to do is rename our axes, and the states morph into each other, so naturally the energies are the same. But occasionally degeneracies arise unexpectedly, through what can only really be described as a coincidence. These are called *accidental degeneracies*. An example of one of these for the three-dimensional square well with all

three sides of equal length arises for the states ψ_{511} , ψ_{151} , ψ_{115} , and ψ_{333} – this energy level is 4-fold degenerate, rather than the "expected" 3-fold degeneracy. Naturally the first three states are not unexpectedly degenerate, but the fourth seems to come from out of nowhere.

Symmetric quantum systems are common in physics, and degeneracy follows them everywhere. This can cause difficulty in developing theory, as some internal structure can be obscured when different configurations result in the same energy spectrum. The trick then is to introduce an external perturbation that breaks the symmetry, thereby separating otherwise degenerate states. The analogous case for the cubical box would be squeezing or stretching one of the dimensions slightly. This also can work in the other direction – we might see unexpected additional spectral lines that indicate that there is additional structure present that breaks the symmetry we thought existed. So the analogous case for this is an infinite well that we think should be cubical, but provides a spectrum with energy levels landing between those that we compute.

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