**Particle in a Box (1 Dimension)**

The time independent Schrödinger equation for a particle equation moving in one dimension:

Where:

|  |  |
| --- | --- |
|  |  (reduced Plank’s constant) |
|  | Plank’s constant (describes size of quanta in quantum mechanics) |
|  | mass of particle |
|  | wave function (replaces the concept of trajectory in classical mechanics) |
|  | potential energy of particle |
|  | total energy of particle |



For a particle in a one-dimensional box of length ,the potential energy function is

.

This implies that the particle can only exist inside the box where .

Therefore:

.

Let:

We have now reduced that equation to a homogeneous second order differential equation with constant coefficients. We have shown earlier that the general solution to this equation is:

The infinite potential outside of the box implies the following boundary conditions:

Furthermore, we can consider that for any point outside the box. Applying the first boundary condition:

Applying the second boundary condition:

where n is an integer. Therefore:

Note that the subscript on indicates that there are different solutions for different values of n. We now need to determine . Recall that:

Since represents the probability distribution function and we know that the particle will be somewhere in the box, we know that =1 for , i.e. there is a 100% probability that the particle is somewhere inside the box. Therefore:

We can show that:

This is the solution as it appears on the TI Voyage 200, but since n is an integer,. Hence:

and:

thus:

This is the solution to the wave equation for the particle in a one dimensional box.

We now turn our attention to the total energy. Recall:

Since:

 and

We get:

Thus the energy is quantized (since n=1,2,3, … and all other terms are constant). The wave functions and probability functions are plotted below for a box with length for corresponding energy levels. Note that the plots have been shifted up by for display purposes.



With regards to the wave functions, we define a node as a location other that the endpoint where . Note that there are nodes that correspond to each energy level. Consider , there is one node. If we consider the probability distribution function for , we see that it equals 0 at . If this is the case, how can a particle get from the left-half to the right-half of the box? You will discuss a phenomenon called “tunneling” in subsequent chemistry classes to explain this behavior.

Example:

What is the probability that a particle in the ground state will be found between L/2 and 2L/3? (note: ground state means

**Homework**

1. For the potential well describes in these notes, what is the probability that a particle in the 2nd energy level will be found between *L/2* and *2L/3*.
2. Assume that for the particle-in-box described in these notes that the potential energy inside the box V(x)=1. Assume that the box goes from x=0 to x=2L. Find . Find an expression for E in terms of *n, h, m*, and *L*.
3. In problem 2, what is the probability that a particle in the 3rd energy level will be found between *L/2* and *2L/3*.