

13.7: Particle in a 2-dimensional box

We learned from solving Schrödinger's equation for a particle in a *one*-dimensional box that there is a set of solutions, the stationary states, for which the time dependence is just an overall rotating phase factor, and these solutions correspond to definite values of the energy. An alternative way of finding that set of solutions is *separation of variables*. The basic strategy is to assume that the solution to the wave equation can be factored into a product of two functions, one depending only on time, the other on the spatial variable,

$$\Psi(x, t) = \psi(x)\varphi(t) \quad (13.7.1)$$

If this solution is substituted in the Schrödinger equation, and the result divided by $\Psi(x, t)$, we find

$$i\hbar \frac{\frac{\partial \phi(t)}{\partial t}}{\phi(t)} = \frac{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x)}{\psi(x)} \quad (13.7.2)$$

On writing the equation in this form, it is clear that the left hand side is only a function of t , not of x , and the right hand side is only a function of x ! This can only make sense if in fact both sides are the same constant. If we denote this constant by E , we can write two equations:

$$i\hbar \frac{\partial \phi(t)}{\partial t} = E\phi(t) \quad (13.7.3)$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x) \quad (13.7.4)$$

The solution to the first equation just gives the phase time dependence,

$$\varphi(t) = Ae^{-iEt/\hbar} \quad (13.7.5)$$

and the second is the time independent Schrödinger equation as before. The solutions to this equation are determined by the boundary conditions on ψ , in general there is a sequence of such eigenstates labeled by a quantum number $n = 0, 1, 2, 3, \dots$, with corresponding values E_0, E_1, \dots , which are put in the corresponding $\varphi(t)$.

A Two Dimensional Box

Let us now consider the Schrödinger equation for an electron confined to a two dimensional box, $0 < x < a$ and $0 < y < b$. That is to say, within this rectangle the electron wavefunction behaves as a free particle ($V(x, y) = 0$), but the walls are impenetrable so the wavefunction $\Psi(x, y, t) = 0$ at the walls. What do we expect the wavefunction to look like?

First notice that the separation of variables trick given above for one dimension works equally well here, writing

$$\Psi(x, y, t) = \psi(x, y)\varphi(t) \quad (13.7.6)$$

gives

$$i\hbar \frac{\partial \phi(t)}{\partial t} = E\phi(t) \quad (13.7.7)$$

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{\partial^2 \psi(y)}{\partial y^2} \right) = E\psi(x) \quad (13.7.8)$$

The surprising thing at this point is that we can do the separation of variables trick *again*—we can write

$$\psi(x, y) = f(x)g(y) \quad (13.7.9)$$

and substitute in the above equation to find

$$-\frac{\hbar^2}{2m} \left(\frac{\frac{\partial^2 f(x)}{\partial x^2}}{f(x)} + \frac{\frac{\partial^2 g(y)}{\partial y^2}}{g(y)} \right) = E \quad (13.7.10)$$

Again, we have an equation in which only one term is x -dependent, so it must be a constant (which we take to be negative for future convenience),

$$\frac{\frac{\partial^2 f(x)}{\partial x^2}}{f(x)} = -C \quad (13.7.11)$$

so

$$\frac{\partial^2 f(x)}{\partial x^2} = -Cf(x) \quad (13.7.12)$$

This is exactly the same equation we dealt with in the one dimensional case, so we know

$$f(x) = A \sin \frac{n\pi x}{a} \quad (13.7.13)$$

with n an integer, and the constant C is equal to $n^2\pi^2/a^2$. Hence the energy levels in this rectangular well are given by

$$E_n = \frac{\hbar^2}{2m} \left(\frac{n_x^2\pi^2}{a^2} + \frac{n_y^2\pi^2}{b^2} \right) \quad (13.7.14)$$

with n_x and n_y are the two quantum numbers needed to label each state.

The first nice probability distributions for a particle in a 2D box are viewable below.

`wiki.page("Visualizations_and_Simulations/CalcPlot3D/Probability_Wave_Function")`

Figure 13.7.1: Visualization of the probability for a particle in a 2D box. The quantum numbers (n_x and n_y) can be varied in the upper left.

Degeneracy

Two distinct wavefunctions are said to be *degenerate* if they correspond to the same energy. If the sides a , b of the rectangle are such that a/b is irrational (the general case), there will be no degeneracies. The *most* degenerate case is the square, $a = b$, for which clearly $E_{m,n} = E_{n,m}$. Degeneracies in quantum physics are most often associated with symmetries in this way.

Figure 13.7.2: Contours of the $n_x = 2$ and $n_y = 3$ wavefunction (left) and $n_x = 3$ and $n_y = 2$ wavefunction (right).

We give here examples of wavefunctions (3,2) and (2,3) for a rectangle. These are contour maps for the time-independent solution, with white being the highest point. These two wavefunctions do not correspond to the same energy, although they would, of course, for a square.

Contributors and Attributions

- Michael Fowler (Beams Professor, [Department of Physics, University of Virginia](#))

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