Eigenfunctions in Quantum Mechanics

We solve the stationary Schrödinger equation in one-space dimension

Objectives

To study slightly more complicated eigenfunction problems than the ones coming from solving the heat equation.

Introduction

The stationary Schrödinger equation in one space dimension is

$$-\frac{\hbar^2}{2m}\,\psi''(x) + V(x)\,\psi(x) = E\,\psi(x), \tag{1}$$

where $\psi(x)$ is the probability density of finding a particle at the position x, V is the potential function, $\hbar$ is the Planck constant divided by 2π, m is the particle mass, and E is the particle's energy.

The equation above is part of an eigenfunction problem, where $\hbar$, m and $V(x)$ are given, and one looks for the eigenfunctions ψ and the eigenvalues E. We said that the equation above is *part of* an eigenfunction problem, because to have an eigenfunction problem we still need to provide boundary conditions. These boundary conditions depend, among other things, on the particular type of the potential function V.

We start with the simplest case, a free particle a (one dimensional) infinite well. We then consider a more complicated situation, when one side of the well is half open.

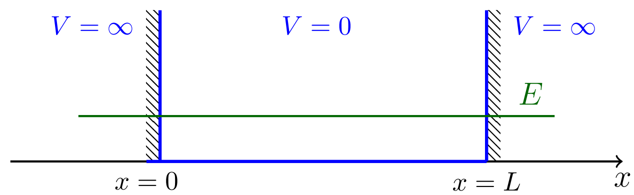
Particle in an Infinite Well

A one dimensional infinite square well is system where one quantum particle, for example an electron, can move freely inside a finite region, but it can never leave that region. Such a system is described by the eigenfunctions, ψ, and eigenvalues, E, of the Schrödinger equation (1). The potential vanishes inside the box, which means that the particle can move freely inside the box. The potential becomes infinite at the border of the box, which means that particle can never leave the box. This also means that the particle wave function must vanish at the border of the box.

We put all these conditions together into the following boundary value problem.

$$-\frac{\hbar^2}{2m}\,\psi''(x) = E\,\psi(x),$$

$$\psi(0) = 0, \qquad \psi(L) = 0.$$



Once you solve this problem you will find that the energy E of the quantum particle cannot be any real number. Instead, the energy must be one of the (discrete) allowed values. People say that the energy of the particle is quantized. A quantum particle cannot have an arbitrary velocity inside the box, instead it must have a velocity compatible with one of the allowed energies. This behavior of the quantum particle is in direct opposition with our intuition, which is based on the behavior of classical particles. A classical particle can move inside a box with any velocity, that is, it can have any energy. This is not the case for a quantum particle.

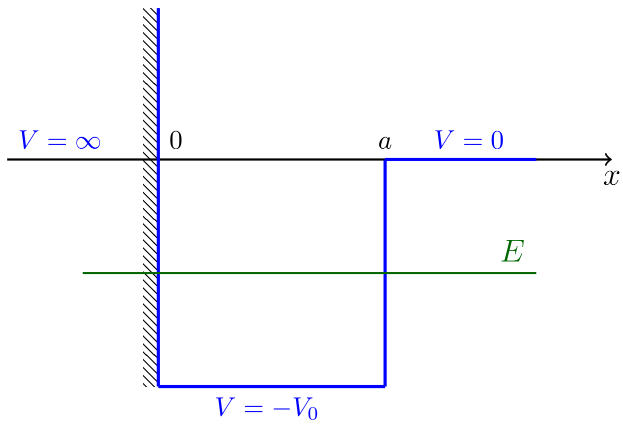
Question 1: *(2 points)* Find all the eigenvalues and eigenfunctions in the problem above.

Particle in a Semi-Infinite Well

We now describe the behavior of a quantum particle inside a box that has an infinite wall on one side but only a finite wall on the other. The quantum particle is again described by the eigenvalues and eigenfunctions of the Schrödinger equation (1).

In this case we choose the potential function $V(x)$ as follows

$$V(x) = \begin{cases} \infty & \text{for} \quad x \leqslant 0, \\ -V_0 & \text{for} \quad 0 < x < a, \\ 0 & \text{for} \quad x \geqslant a. \end{cases}$$



Potential functions $V(x)$ that differ by a constant describe the same physics. In this case we chose the potential so that inside the box it takes a negative value,$V(x) = -V_0$, for $0 < x < a$, instead of zero. The solution formulas for the eigenfunctions look a bit nicer with this choice of the additive constant in the potential function.

We want to study particles mostly confined inside this box $0 < x < a$. That's why we consider only the case where the particle energy is $E \leqslant 0$, equivalently $E = -|E|$. The boundary value problem satisfied by the quantum particle in this potential is

$$-\frac{\hbar^2}{2m}\,\psi''(x) + V(x)\,\psi(x) = E\,\psi(x), \quad E < 0,$$

$$\psi(0) = 0, \quad \lim_{x\to\infty} \psi(x) = 0.$$

The formula for the solution ψ in the region $0 < x < a$ is different form the formula in the region $x > a$. So it is convenient to split ψ and the whole problem into two regions, $0 < x < a$ and $x > a$. One finds the general solution ψ on each region and then imposes the boundary conditions on each region. The final step is to match the two solutions at $x = a$. The matching conditions are

$$\psi_{0<x<a}(a) = \psi_{x>0}(a), \qquad \psi'_{0<x<a}(a) = \psi'_{x>0}(a).$$

It is from these matching conditions that the energy of the quantum particle E gets quantized.

Once you answer Question 2 in the next pages, you should click on the **Interactive Graph**. In that graph we choose some arbitrary values for the potential $V_0 = 10$, the particle mass m, and the box size a, and we plot the function $\psi(x)$. We leave the energy $E \in [-10, 0]$ as a free parameter. The inside of the box is shaded in green, the outside in red. Since the energy E is a real number, the function displayed in the graph is not an eigenfunction of the Schrödinger equation above. This function becomes an eigenfunction for very specific values of the energy, which then become eigenvalues. Move the slider for the energy in the interactive graph, and see if you can find the energy values for which the function becomes and eigenfunction. How many eigenvalues E are in the range displayed in the interactive graph?

Question 2:

(2a) *(2 points)* Split the solution function ψ as follows,

$$\psi(x) = \begin{cases} \psi_1(x) & \text{for} \quad 0 \leqslant x \leqslant a, \\ \psi_2(x) & \text{for} \quad x \geqslant a, \end{cases}$$

Show that if you split the Schrödinger differential equation in the same way you can write it as

$$\psi_1'' = -k^2\,\psi_1, \qquad 0 \leqslant x \leqslant a,$$
$$\psi_2'' = \kappa^2\,\psi_2, \qquad x \geqslant a.$$

Find the formulas for $k > 0$ and $\kappa > 0$ in terms of the mass m, Planck constant $\hbar$, potential $V_0 > 0$, and energy $|E| > 0$. Also find one the boundary condition for ψ_1 and one boundary condition for ψ_2, obtained from the boundary conditions on ψ at $x = 0$ and at $x \to \infty$.

(2b) *(2 points)* The second part of the problem is to find all the solutions, ψ_1 and ψ_2, of their respective boundary value problems. Write these functions in terms of k and κ.

Note: So far there should be no condition on the values of the energy E.

(2c) *(2 points)* The third part of the problem is to match the functions ψ_1 and ψ_2 found in (2b) at $x = 0$. Impose the matching conditions

$$\psi_1(a) = \psi_2(a), \qquad \psi_1'(a) = \psi_2'(a),$$

and from these equations find a relation between k and κ and between c_1 and d_1 of the form

$$\frac{k}{\kappa} = -f(ka), \qquad d_1 = c_1\, g(k, \kappa, a).$$

Find the functions $f(ka)$ and $g(k, \kappa, a)$. These functions do not depend on c_1 or d_1.