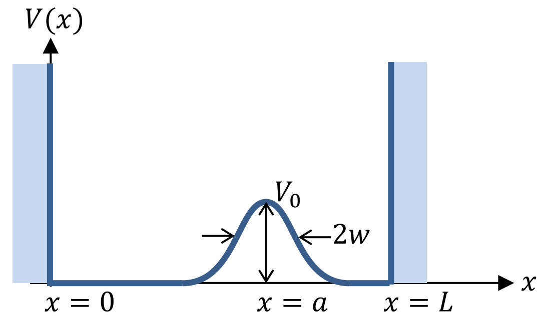
PHYS 260 – Programming Assignment 9

1. Modified Infinite Square Well and Quantum Tunneling



In this problem you will modify the program for the infinite square well and investigate the phenomenon known as tunneling, where a quantum particle can occupy a region of space that is forbidden by classical physics, and tunnel through an energy barrier. Tunneling has important applications in electronics and microscopy. Consider an infinite square well of width L with a Gaussian-shaped "bump" of width $2w$ and height V_0 centered at $x = a$. The potential of this modified infinite square well is

$$V(x) = \begin{cases} V_0 e^{-(x-a)^2/(2w^2)} & 0 \le x \le L \\ \infty & \text{otherwise} \end{cases}$$

The goal of this problem is to solve Schrödinger's Equation for this potential to determine the allowed energy levels and normalized wave functions. No exact solutions can be obtained analytically (although there are analytical methods for obtaining approximate solutions), so this is a good application of numerical methods. Start with the program we wrote for the infinite square well.

(a) Modify the function `V(x)` to include the potential of the bump. Use $a = \frac{2}{3}L$, $w = \frac{L}{10}$, and $V_0 = 1.0 \times 10^{-17}$ J. Move `V(x)` so that it is outside the `solvepsi(E)` function so that you can easily access `V(x)` from your main code. Make a plot of $V(x)$ for $0 \le x \le L$. Try adjusting V_0, a and w to observe what effect those parameters have. Imagine that you have a classical particle and place it to the left of the bump and give it kinetic energy $E < V_0$. How would the classical particle move as it encounters the bump? Keep this in mind as you solve this problem for a quantum particle.

(b) Now, you will determine the allowed energies for an electron placed in this potential. Recall that the `solvepsi(E)` function solves the Schrödinger Equation for an energy guess `E` and returns the wave function $\psi(x)$ evaluated at each value in the array `xvalues`. Allowed energies are those that yield a wave function that matches the boundary conditions: $\psi(0) = \psi(L) = 0$. Since our solution starts at $x = 0$, we have already enforced $\psi(0) = 0$, and our solution is guaranteed to obey the left boundary condition. The goal here is to determine the approximate values of the energy levels by graphing. Make an array of energy values for $0 \le E \le 1000$ eV where 1 eV $= 1.6022 \times 10^{-19}$ J. Recall that 1 eV is the amount of energy an electron obtains when accelerated through a potential difference of 1 V. Now make a plot of ψ_L vs. E where ψ_L is the value of ψ at $x = L$ for energy guess E. Recall that ψ_L is simply the last element of the `psiList` array that is returned by the `solvepsi(E)` function. From your graph, what are approximate values of the first three energy levels?

(c) Here you will determine accurate values for the energy levels using the secant method within `solve(E)`. Use the approximate values obtained from (b) as guesses and pass them to `solve(E)` to obtain values of the first three energy levels that are accurate to 10^{-3} eV.

(d) Use the energies from (c) to obtain normalized wave functions for the first three energy levels. Plot ψ vs. x for the first three wave functions on the same graph. On a separate graph, plot ψ^2 vs. x, also for the first three wave functions. Recall that $\psi^2 dx$ is the probability of finding the electron in between x and $x + dx$. How are the wave functions and probabilities different than those for the original infinite square well? Pay special attention to ψ_1, the wave function for the ground state (lowest) energy. What does its shape tell you about the probability of finding the electron at various places relative to the bump? How does this match your intuition?

(e) Now let's focus attention on the ground state energy E_1 and wave function ψ_1. What is the ground state energy and how does it compare to V_0, the height of the bump? You should have found that E_1 is smaller than V_0. Now imagine that the electron behaved classically and that it is initially close to $x = 0$. You give it a push to the right so that it has kinetic energy given by E_1. Since $E_1 < V_0$, it will not be able to surmount the bump. However, it will still move up the bump, converting its kinetic energy into potential energy, and come to a brief rest when $E_1 = V(x_{\text{turn}})$. Here, x_{turn} is the classical turning point. It is the location on the x-axis where a classical particle would turn around (i.e. come to rest) when encountering a potential barrier. Solve $E_1 = V(x_{\text{turn}})$ for x_{turn} to show that it is given by

$$x_{\text{turn}} = a \pm \sqrt{2w^2 \ln\left(\frac{V_0}{E_1}\right)}$$

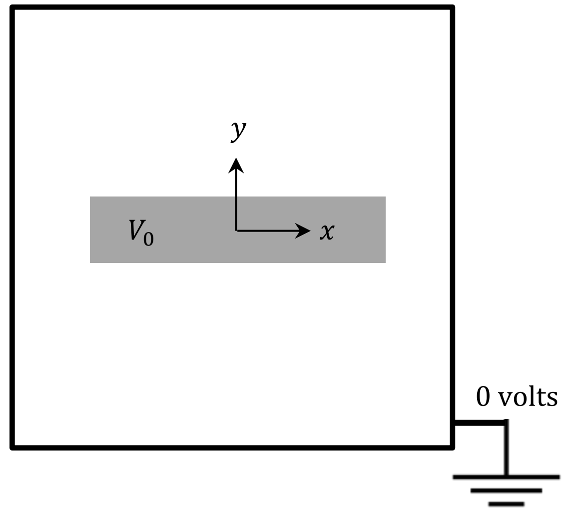
There are two solutions because there are two sides of the bump (i.e. a particle that starts off close to $x = L$ will travel up the right side of the bump and turn around at $a + \sqrt{2w^2 \ln\left(\frac{V_0}{E_1}\right)}$). Plug in the values of a, w, V_0 and E_1 to obtain numerical values for x_{turn}. If the electron was a classical particle, the probability P of finding it in the region between the turning points would be zero. This region is called a "classically forbidden region". Notice from your graph that ψ_1 is NOT zero in this region. Therefore, a quantum particle could occupy a region of space that is forbidden by classical physics. And because of this phenomenon, a quantum particle initially on the left side of the square well can pass through, or "tunnel" through the energy barrier to arrive on the right side. Let's calculate the probability of finding the electron in the classically forbidden region. Create a function `probability(x1, x2, psi)` that calculates and returns the value of the integral

$$P = \int_{x_1}^{x_2} |\psi(x)|^2 dx$$

using the trapezoid rule. Use the left and right turning points for x_1 and x_2 to calculate the probability of finding the electron in the classically forbidden region for ψ_1. The fact that this probability is nonzero is quite interesting because it cannot be explained with classical physics. This gives rise to the phenomenon known as tunneling where a particle of energy E can pass through an energy barrier of height $V_0 > E$. Note tunneling only occurs for E_1 in this case. The electron can also be found in between these turning points for ψ_2 and ψ_3. However, those aren't quite as interesting because E_2 and E_3 are both greater than V_0. Thus, it is not surprising that the particle can pass over the bump in excited energy states.

2. Rectangular Conductor

This problem illustrates why electrostatic fields outside a conductor concentrate at a sharp point – the principle of the lightning rod. It is also relevant to apertureless nearfield scanning optical microscopy.



Consider a conducting beam centered at $(x, y) = (0,0)$ with a rectangular cross-section. The length of the beam along the x and y axes is L_x and L_y, respectively. Consider the following cases:

1) $L_x = L_y = 50$
2) $L_x = 50, L_y = 10$
3) $L_x = 50, L_y = 2$

The conductor is held at a constant electrostatic potential $V_0 = 1\ \text{V}$. It sits in the center of a 101×101 square conducting box held at 0 V.

(a) Write a program to find the potential in the space between the conductor and the walls of the box by the relaxation method until the calculation converges to within 1×10^{-6}. Consider each of the three conductor shapes described above. For each make a contour plot showing the potential in the xy plane.

(b) Calculate the electric field using forward and backward differences along the edges and using central differences for points on the interior. Plot the electric field on the same plot as the potential. For each shape, where is the electric field the largest? Calculate the ratio between the maximum and minimum electric field just outside the conductor. For what shape is the ratio the largest?

3. Waves on a String

A string of length $L = 1.00$ m is fixed at both ends. The string has linear mass density $\mu = 1.00 \times 10^{-2}$ kg/m and is under tension $T = 100$ N, so that the wave speed is $v = \sqrt{T/\mu} = 100$ m/s. At $t = 0$ the string has a profile given by $\psi(x, 0)$. It is released from rest at $t = 0$ so $\partial\psi(x, 0)/\partial t = 0$. Therefore, the general solution to the wave equation can by written as

$$\psi(x,t) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{n\pi v t}{L}\right)$$

In practice, we can't take the sum all the way to ∞, but can instead take a large number N of terms. Using a discrete Fourier sine series, solve for the Fourier coefficients b_n using $N = 500$ for the following initial wave functions

1) $\psi_1(x, 0) = \sin\left(\frac{\pi x}{L}\right)$

2) $\psi_2(x, 0) = \frac{1}{2}\sin\left(\frac{\pi x}{L}\right) + \frac{1}{2}\sin\left(\frac{3\pi x}{L}\right)$

3) $\psi_3(x, 0) = \begin{cases} e^{-\left(x-\frac{L}{2}\right)^2/2\sigma^2}, & \text{if } \left|x - \frac{L}{2}\right| \le 4\sigma, \text{ where } \sigma = L/10 \\ 0, & \text{otherwise} \end{cases}$

4) $\psi_4(x, 0) = \begin{cases} \frac{3}{L}x, & \text{if } x \le \frac{L}{3} \\ -\frac{3}{2L}(x - L), & \text{if } \frac{L}{3} \le x \le L \end{cases}$

(a) For each initial wave function, make a plot of $|b_n|$ vs. n. You may find it useful to make the plot as a bar graph using the `gvbar` function from `vpython`. Based on the graphs for ψ_1 and ψ_2 above, what is the physical meaning of the Fourier coefficients b_n?

(b) Make an animation in VPython of $\psi(x, t)$.

(c) You should observe ψ_3 clearly separate into two smaller Gaussian profiles that move in opposite directions. Why does this happen? Can you observe a similar phenomenon happening in the other wave functions?

(d) ψ_4 is similar to the initial shape of a plucked guitar string. You have probably seen an audio waveform from a musical instrument at some point. Based on your analysis, why do such waveforms never appear to be perfectly sinusoidal?

4. Quantum Harmonic Oscillator (optional)

Consider the one-dimensional, time independent Schrödinger equation in a harmonic (i.e. quadratic) potential $V(x) = \frac{1}{2}kx^2$, where k is a constant..

(a) Write down the Schrödinger equation for this problem and convert it from a second-order equation to two first-order ones as in Infinite Square Well in-class exercise. Write a program to find the energies of the ground state ($n = 0$) and the first two excited states ($n = 1,2$) for these equations when m is the electron mass, $k = m\omega^2$ is the force constant and $\omega = 4.20 \times 10^{17}$ Hz is the natural frequency of oscillation. Find the energies to an accuracy of 10^{-8} eV ($1 \text{ eV} = 1.60 \times 10^{-19}$ J). Note that in theory the wavefunction goes all the way out to $x = \pm\infty$, but you can get good answers by using a large but finite interval. Use $x = -10a$ to $+10a$, with $a = 10^{-11}$ m with the wavefunction $\psi = 0$ at both boundaries. (In effect, you are putting the harmonic oscillator in a box with impenetrable walls.) The wavefunction is real everywhere, so you don't need to use complex variables, and you can use evenly spaced points for the solution – there is no need to use an adaptive method for this problem.

The quantum harmonic oscillator is known to have energy states that are given by

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0,1,2,\ldots$$

Check that your calculated energies obey this formula, to the precision of your calculation.

(b) Now modify your program to calculate the properly normalized wavefunctions for the three states and make a plot of them, all on the same graph, as a function of x over $x = -10a$ to $x = 10a$ using $N = 1000$ data points. Plot the data points using dots.

To normalize the wavefunctions you will have to calculate the value of the integral $\int_{-\infty}^{\infty}|\psi(x)|^2 dx$ and then rescale ψ appropriately to ensure that the area under the square of each of the wavefunctions is 1. Either the trapezoidal rule or Simpson's rule will give you a reasonable value for the integral.

(c) The wavefunctions can be written analytically as

$$\psi_n(x) = \frac{(-1)^n}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right), \quad n = 0,1,2,\ldots$$

where $H_n(z)$ are Hermite polynomials, which can be determined by the recursion relation

$$H_n(z) = 2zH_{n-1}(z) - 2(n-1)H_{n-2}(z)$$

with $H_0(z) = 1$ and $H_1(z) = 2z$. Add plots for the first three wavefunctions given by the equation above to your graph using the line representation. You should obtain pretty good agreement between the analytic functions and the numeric ones. In order to distinguish the two functions, you can use the plot option `markevery=10` for your numerical functions so that it only displays every 10th data point.

(d) The maximum displacement from equilibrium for a classical particle occurs when all of its kinetic energy is converted into potential energy. That is when

$$E = \frac{1}{2}kx_{\max}^2$$

where E is the total energy of the particle, k is the force constant and $x_{\max}$ is the maximum displacement of the particle. Therefore, we can write

$$x_{\max} = \sqrt{\frac{2E}{k}}$$

Classically, the particle can never obtain a displacement larger than $x_{\max}$ (i.e. the probability of finding the particle with displacements larger than this is zero). The probability $P(x_1, x_2)$ of finding a quantum particle in between x_1 and x_2 is given by

$$P(x_1, x_2) = \int_{x_1}^{x_2} |\psi(x)|^2 dx$$

Calculate the probability of the quantum particle being found inside a region that is forbidden by classical physics. That is, calculate the probability of finding the particle in the regions $[-10a, -x_{\max}]$ and $[+x_{\max}, +10a]$. Note that, since $|\psi(x)|^2$ is symmetric about $x = 0$, you only have to calculate one integral and multiply it by two to calculate the total probability. For the ground state, the probability should be around 15%. What happens to the probability when E increases?