PHAS2441 FINAL ASSIGNMENT 2017

The infinite "unsquare" potential

Last revision February 6, 2017
louise.dash@ucl.ac.uk

Contents

Introduction

In the course so far we've used a wide variety of techniques to give you a flavour of the sort of problems that can be tackled using computational approaches.

In session 10, we're going to look at one more new aspect of this, including boundary values in the solving of differential equations. You

will then apply this to the problem for the PHAS2441 final assignment: solving the quantum-mechanical problem of a particle in an infinite potential well. You will first solve for an infinite square potential well, and use the known solutions for this system to check that your results are correct. You will then be able to extend this to calculate for systems where there is no simple analytical solution.

Before commencing any of the tasks below, make sure you have gone through and understood the contents of the Jupyter Notebook script for session 10, which will guide you through the process of finding roots of a function using the secant method, and hence solving differential equations with boundary value conditions, both of which you will need to solve this problem.

Boundary value problems: eigenvalue solutions

In this task we are going to be applying our new knowledge of boundary value problems to the one-dimensional time-independent Schrödinger equation,

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

Initially, we're going to consider one of the most well-known solutions of this—for a particle in a square potential well of width $2a$ with infinitely high walls. This is shown in Fig. 1, and the potential $V(x)$ takes the form

$$V_x = \begin{cases} 0 & \text{if } -a < x < +a, \\ \infty & \text{if } |x| > a. \end{cases} \tag{2}$$

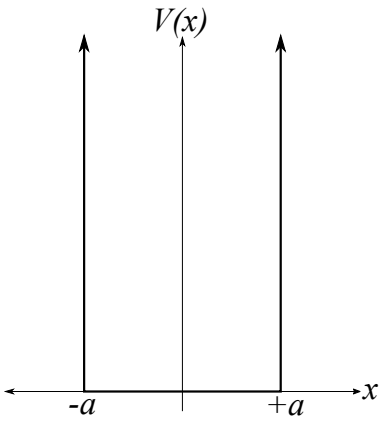

Figure 1: The infinite square well potential. Within the well, the potential is zero, everywhere else the potential is infinite.

You have all studied this in PHAS2222 (or an equivalent course) and should be familiar with the solutions. These solutions show that the probability of finding the particle in the region where $V(x) = \infty$ is zero, and thus the wavefunction must be subject to the boundary conditions of $\psi = 0$ at $x = -a$ and $x = +a$.

Therefore this would seem to be an ideal system to solve using the same approach as we used to calculate the trajectory of a thrown ball in the Jupyter Notebook for Session 10—we could transform Eq. (1) into two first-order equations, guess some initial values, and iterate until we find a solution that fulfils the boundary condition at $x = +a$.

Separating out the Schrödinger equation into two first-order equa-

tions yields

$$\frac{d\psi}{dx} = \phi, \tag{3}$$

$$\frac{d\phi}{dx} = \frac{2m}{\hbar^2}\left[V(x) - E\right]\psi(x). \tag{4}$$

We know one initial boundary condition, that $\psi = 0$ at $x = -a$. We would therefore need to guess an initial condition for ϕ, and then vary this with the secant method (or another root-finding method) until we find a solution where $\psi(x = +a) = 0$.

Unfortunately, this approach won't work. The Schrödinger equation is a linear equation, so if we have a solution ψ, any multiple of ψ will also be a solution. Conversely, a multiple of any candidate wavefunction ψ that *doesn't* fulfil the boundary condition of $\psi(x = +a) = 0$ will also not fulfil the condition.

This is because the Schrödinger equation is an *eigenvalue* equation—it only has solutions at particular values of the energy E. For other values, there are no solutions that fulfil the boundary conditions.

The approach we will adopt, therefore, is not to search for an initial condition on ϕ that will give us the required solution, but instead to search on values of E. As the only effect of ϕ's initial condition is to multiply the wavefunction by a constant, we can choose any starting value. We can then normalize the wavefunction once we have found a solution if needed.

Infinite square well

You now have all the information you need to start on the task. The first part of the task is to calculate the energy of the ground state. You should be able to do this by the end of Session 10, and you can get help from the demonstrators for this part of the task during the session.

Start by creating a new notebook from scratch. You will need to define the following physical constants.

- electron mass $m = 9.1094 \times 10^{-31}$ kg
- $\hbar = 1.0546 \times 10^{-34}$ J.s
- electron charge $e = 1.6022 \times 10^{-19}$ C

You can include more digits of precision than this if you wish, but please work in SI units. When quoting energies however, you will find

it more convenient to convert to electronvolts (eV) by dividing the value in Joules (J) by e.

Set the half-width of the potential well a, to be 5×10^{-11} m, so that the well will be $2a = 10^{-10}$ m wide. Use $N = 1000$ for the number of Runge-Kutta calculation points.

For an infinite square well, we know that the particle will never be outside the well, where $V(x) = \infty$, and as $V(x) = 0$ inside the well, we could just ignore this in the calculations. However, later in the task you will calculate for other forms of $V(x)$, so write a suitably-named and documented function that will, for the moment, return a value of $V(x) = 0$ for all values of x, the function input[1].

We've already split the Schrödinger equation into two first order equations, Eqs. (3) and (4). You will need to write another function, just like the ones you used in Sessions 7 and 8, to calculate the right-hand side of these equations[2].

Now you need a Runge Kutta function. Use the fourth-order function you already have, but you will probably want to make some changes. In particular, you can put the initial conditions within the function. You can use any initial condition you choose for ϕ, but `phi = 1.0` is probably a good choice. Instead of running over an array of time-points, the loop will now run over an array of N x-points starting at $x = -a$ and finishing at $x = +a$, with step size $h = 2a/N$. The Runge Kutta function will need to return an array of the wavefunction values representing $\psi(x)$, although note that we *don't* actually need to return an array to represent $\phi(x) = d\psi/dx$.

[1] Hint: you just need one line in the function at the moment: `return 0.0`. Make sure you remember the docstring as well though.

[2] Hint: Unlike the previous functions, this one will need three arguments as inputs: a vector `r` of ψ and ϕ, a value of `x`, and a value for the energy `E`, which appears in the RHS of equation (4).

Finding the ground state energy

As in the script for Session 10, you will need to set up a code cell to iterate using the secant method until you find a value of E that gives the required $\psi(x) = 0$ at $x = a$. To do this, you'll need two initial guesses for the energy (I'd suggest using variable names `E1` and `E2`)[3], then calculate corresponding wavefunction arrays using the Runge Kutta function. Check the *final* element of these wavefunction arrays—are they equal to zero? If not, update the guesses `E1` and `E2` using the secant method until you find an energy that does fulfil the boundary conditions[4].

If all has gone well, your code will converge on the ground state reasonably quickly. To check your result, compare it with the known ground state energy, by recalling that the eigenvalues of this system

[3] Hint: choose initial guesses that are close to the initial ground state energy, otherwise you may find the eigenvalue of one of the excited states instead!

[4] Hint: You will need to set an appropriate value for the tolerance, $e/1000$ is probably a good choice.

are given by:

$$E_n = \frac{\pi^2 \hbar^2 n^2}{2m(2a)^2}. \tag{5}$$

***This is the point that we anticipate most of you will be able to reach by the end of Session 10. From this point onwards, you have to complete the task entirely on your own, with no help from demonstrators* or from your peers.**

Finding the ground state wavefunction

Now calculate and plot, on an appropriately labelled plot, the ground state wavefunction. You may wish to represent the walls of the infinite square well potential on the plot as well[5].

[5] Hint: `plt.axvline(x=-a, c='k',ls='-',lw=2)` will plot a thick black vertical line at $x = -a$. Adapt this as required.

As we noted earlier when discussing the arbitrary choice of initial condition for ϕ, our wavefunction as calculated is not normalised. It would be useful to write a function that will normalize the wavefunction, so that

$$\int |\psi(x)|^2 \mathrm{d}x = 1. \tag{6}$$

You can achieve this by calculating the value of the integral on the left-hand side of Eq. (6), and then dividing the wavefunction through by the square root of this value. The easiest way of calculating the integral is to use the trapezoidal rule[6] , where an integral with limits a and b can be evaluated as

[6] Note that our wavefunction is already in a convenient form to do this, as it is a numpy array

$$I(a,b) = h\left[\frac{1}{2}f(a) + \frac{1}{2}f(b) + \sum_{k=1}^{n-1} f(x+kh)\right]. \tag{7}$$

Having done this, compare your calculated wavefunction with the known ground state wavefunction, remembering that the normalized wavefunctions of the system are given by

$$\psi_n(x) = \frac{1}{\sqrt{a}} \cos\left(\frac{n\pi x}{2a}\right) \qquad n \text{ odd}, \tag{8a}$$

$$\psi_n(x) = \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi x}{2a}\right) \qquad n \text{ even}. \tag{8b}$$

If all has gone well, you should find a perfect match between your numerical results and the analytical solutions we already knew.

Finding the higher energy states

Once you are satisfied that your ground state solutions are correct, try finding the first few excited states ($n = 2, 3, 4$, as a minimum), and verify that these are also correct. Comment on how you chose the initial guesses for the energies for these states. Once more, plot these solutions and compare with the known solutions.

Does your method also work to find eigenstates for large n (for example, $n \sim 20$?

The infinite "unsquare" well

Hopefully now you have code that works well to solve for the eigenstates of the infinite square well. However, you probably found it a fair amount of work to calculate answers that we already knew from a relatively simple analytical solution. In fact, the main point of doing this was to confirm that your numerical version does indeed work as expected, before going on to calculate for systems that aren't easily solvable analytically. This is what you will do now, and then compare your results to the systems you have already met.

We are going to keep the infinite square walls of the potential well, which guarantee that the particle cannot be found in the $V(x) = \infty$ region. This means we can keep the boundary conditions of the original problem.

However, we are going to change the *base* of the potential well so that it is no longer square—in effect we are going to embed another potential within the square well. An example of this is shown in Fig. 2.

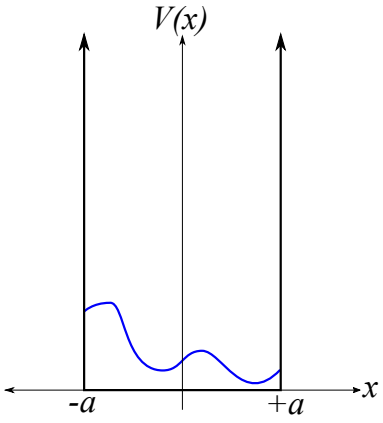

Figure 2: Potentials can be embedded within our infinite square well, as shown by the blue line. We can calculate for any arbitrary potential defined within the surrounding infinite square well.

This opens up the possibility of solving for a wide range of systems for which there is no simple analytical solution. By starting with embedded potentials with familiar forms, you will be able to explore the similarities and differences from the analytical solutions and get a feel for the physics of the new, embedded system. You will then be able to extend this to any (arbitrary) embedded potential.

You can implement this simply by changing the form of the potential defined in the Python function earlier. Start with the suggestions here, but if you want, try some other potentials as well. Give reasons for your choice, and describe the physics of what you observe.

In each case, try to calculate the lowest three or so eigenstates, and plot the wavefunctions. It's also useful to plot the potential itself, with

the energy eigenvalues as horizontal lines.

Compare these results qualitatively to the form of the wavefunctions you'd expect for the standard form of these potentials—explain the similarities and differences in your text cell commentary. You may also want to attempt a quantitative comparison using the known eigenvalues and wavefunctions

I. Harmonic potential: Set the potential to have the form

$$V(x) = V_0 \frac{x^2}{a^2}. \tag{9}$$

This will give you a harmonic potential embedded within the infinite square well, as shown in Fig. 3. You'll need to pick an appropriate value for V_0. $800e$ is a good starting point, as it gives a fairly deep harmonic potential, but experiment to find a value you think is most suitable. In what way do your results differ from the known results for a simple harmonic oscillator potential? Why?

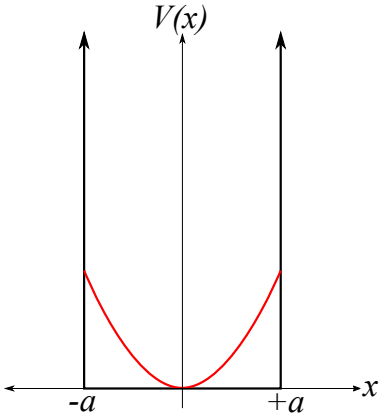

Figure 3: A harmonic potential embedded in the infinite well. Note that the particle is still constrained within the infinite walls indicated by the black lines.

II: Finite square well: Set the potential to have the form

$$V_x = \begin{cases} 0 & \text{if } -a/2 < x < +a/2, \\ V_0 & \text{if } |x| > a/2, \end{cases} \tag{10}$$

Again, you'll need to adjust V_0, and you may also want to experiment with the width of the finite square well. How do your results differ from the known results for a normal finite square well, and why?

III. Other potentials: Now try this for your own choice(s) of potential. There's no need to choose one for which the analytical results of the non-embedded potential are known—in fact it would be more interesting to choose one which is *not* solvable analytically. Make sure you include an interpretation of the physics of your results in your notebook.

General assignment advice

Submit your work as a fully self-contained Jupyter Notebook. Your notebook should have a similar writing style to a formal report, and should not include any interactive code requiring user input. Pay particular attention to your text cell commentary. Because this task is fairly open-ended, we'll only be able to tell what you've done, and

why you've chosen to do it in that way, if you use the text cells to tell us. Likewise, make sure your code is fully commented, as you may not get full credit if we can't figure out what it does.

Assessment

In this assignment, most of the available marks (65%) are for successfully calculating the eigenvalues and eigenfunctions, and analysing and discussing these results in the text commentary.

The remaining marks will be allocated for the overall quality of your plots (10%), the overall quality of your coding style and code comments (10%), and the overall quality of your discussion in the text cells (including grammar and spelling) (15%).

As a guide: if you have *successfully* completed only the first part of the task (i.e. calculation of the ground state energy), including a reasonable text cell commentary etc., you would receive a maximum grade of around 45%. A complete, fully correct solution of the low-lying eigenstates of the infinite square well would expect to receive a grade of no more than 60%. Higher grades than this will only be achieved if you have extended your code for other potentials, and given a sensible description of the physics.

It's better to do the early parts of the task well, but not get as far as the later parts, than it is to attempt all of the task but not do any of it well.

Submission

This is an individual assignment. You must work on this on your own, with no help or input from staff or other students. Everything in your submission must be either completely your own work, or have the source explicitly acknowledged and suitably referenced. We will be using several methods to check for any plagiarised or copied assignments, including but not limited to the Turnitin similarity score.

This assignment will be graded anonymously. Please make sure that:

- your name does not appear anywhere in your submission;
- your submission title starts with your student number; and
- you include your student number at the start of your submitted Jupyter Notebook.

If you have an e-sticker from Student Disability Services please copy and paste the wording (but not your name!) into a clearly labelled text cell at the top of your Jupyter Notebook.

You can only submit one file to Turnitin, so it will not be possible to upload additional figure files. You may include images as linked URLs (as, for example, in the script for session 10), and make sure that the original source of the image is made clear. If you want to include figures you have created yourself, you will need to upload these to an external hosting service (e.g. Imgur, Flickr, etc) and ensure that the images are public. In this case please make it clear in the accompanying text that you have created this image yourself.

You are advised to include a suitably-formatted bibliography or reference section if you refer to any textbooks, lecture notes (eg PHAS2222) or other sources of information.

Page limit

This year we have introduced a page limit of the equivalent of ***60 sides of A4 paper*** for the final assignment.

You can find out how to determine the page count for your completed notebook by following the procedure laid out at the bottom of the Moodle page for Session 10.