

PHAS0029 FINAL ASSIGNMENT 2021

The infinite “unsquare” potential

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Contents

<i>1</i>	<i>Introduction</i>	<i>2</i>
<i>2</i>	<i>Boundary value problems: eigenvalue solutions</i>	<i>2</i>
<i>3</i>	<i>Infinite square well</i>	<i>3</i>
<i>3.1</i>	<i>Task for session 8: Finding the ground state energy</i>	<i>3</i>
<i>3.2</i>	<i>Finding the ground state wavefunction</i>	<i>5</i>
<i>3.3</i>	<i>Finding the higher energy states</i>	<i>6</i>
<i>4</i>	<i>The infinite “unsquare” well</i>	<i>6</i>
<i>5</i>	<i>General assignment advice</i>	<i>8</i>
<i>5.1</i>	<i>Assessment</i>	<i>8</i>
<i>5.2</i>	<i>Referencing and bibliography</i>	<i>9</i>
<i>5.3</i>	<i>Submission</i>	<i>9</i>
<i>5.4</i>	<i>Page limit</i>	<i>10</i>

1 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 8, 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 PHAS0029 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 familiar analytical 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 8, 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. It is also recommended that you read this entire script through before commencing the Session 8 task outlined in section 3.1.

2 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,

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

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

$$V_x = \begin{cases} 0 & \text{if } -a \leq x \leq +a, \\ \infty & \text{if } |x| > a. \end{cases} \quad (2)$$

You have all studied this in PHAS0022 (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 $x = +a$.

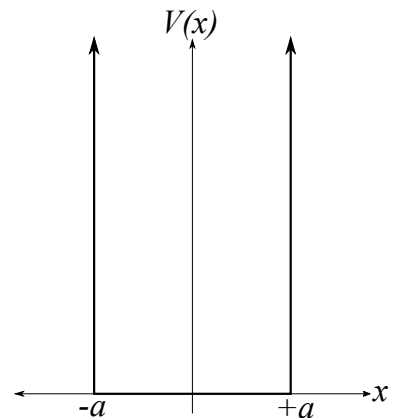


Figure 1: The infinite square well potential. Within the well, the potential is zero, everywhere else the potential is infinite.

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 8—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 equations yields

$$\frac{d\psi}{dx} = \phi, \quad (3)$$

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

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.

3 *Infinite square well*

3.1 *Task for session 8: Finding the ground state energy*

You now have all the information you need to start on the assignment. The first part of the assignment is to calculate the energy of the ground state, and this will form the task for Session 8. You can get help from the demonstrators for this part of the task during the Session 8 live session *only*. You must not share or discuss your work in any way with other students, and please make sure you are fully familiar with the [UCL guidance on academic integrity](#) before you start work.

You can find the rubric for the assessment for the session 8 task on the submission page on Moodle—for session 8 you will not be assessed on your text cells, but you will probably find it helpful to include at least some text so that both you and your marker can tell what you're doing. Your session 8 task will form the starting point of your final assignment, and you should implement the feedback from your session 8 task in your final version.

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

- electron mass $m = 9.109\,383\,702 \times 10^{-31}$ kg
- $\hbar = 1.054\,571\,817 \times 10^{-34}$ J.s
- electron charge $e = 1.602\,176\,634 \times 10^{-19}$ C

You can include more digits of precision than this if you wish, but please work in SI units. When quoting energies however, you should 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 return a value of $V(x) = 0$ for all values of x , the function input¹.

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 6 and 7, to calculate the right-hand side of these equations².

Now you need a Runge Kutta function. You can reuse the fourth-order function you already have (make sure this is clear in the comments), 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 —explain what effect this choice has in the text cell commentary. 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 $\phi(x) = d\psi/dx$.

As in the script for Session 8, you will need to write code to iterate using the secant method until you find a value of E that gives the required

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

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

$\psi(x) = 0$ 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 conditions⁴.

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

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

This is the point that we anticipate most of you will be able to reach by the end of Session 8, and this is what you should submit as your session 8 task. Make sure you read the submission instructions for the session 8 task on Moodle carefully.

From this point onwards, you have to complete the task entirely on your own, with no help from demonstrators, other students, or anyone else.

3.2 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 well⁵.

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

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 1. \quad (6)$$

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 rule⁶, where an integral with limits a and b can be evaluated as

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

³ Hint: choose initial guesses that are reasonably 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.

⁵ Hint: `plt.axvline(x=-a, c='#5f5f5f', ls='-', lw=2.5)` will plot a thick dark grey vertical line at $x = -a$. Adapt this as required.

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

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

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

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

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

3.3 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. Think about the best way to choose initial guesses for these states, bearing in mind that you want to come up with a general method that works for any potential, including ones where there is no analytical solution available for comparison. Comment on your chosen method for determining the initial guesses for the energies for these eigenstates. Once more, plot these solutions and compare with the analytical solutions.

Does your method also work to find eigenstates for large n ? Check this explicitly for at least two states in the range $18 \leq n \leq 28$.

4 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.

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 writing a new Python function for the form of the potential.

For each potential, calculate at least the lowest three eigenstates (include some of the higher eigenstates if you wish), and plot the wavefunctions. In a separate plot, plot the both the potential itself and the energy eigenvalues overlaid as horizontal lines.

Compare these results both qualitatively and quantitatively, where possible, to the form of the wavefunctions you'd expect for the standard form of these potentials. Make sure you fully analyse and explain the similarities and differences between the two forms in your text cell commentary.

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

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

This will give you a harmonic potential embedded within the infinite square well, as shown in Fig. 3. Again, you'll need to pick an appropriate value for V_0 . Around $700e$ is a good starting point for this, but experiment to find a value you think is most appropriate to demonstrate interesting physics. Compare your eigenvalue and wavefunction results explicitly with the analytical solutions for a pure harmonic potential. In what way do your results differ? Why? Fully discuss and interpret the similarities and differences in your text cells.

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

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

This will give you a finite square well embedded within the infinite square well. You'll need to pick an appropriate value for V_0 . Around

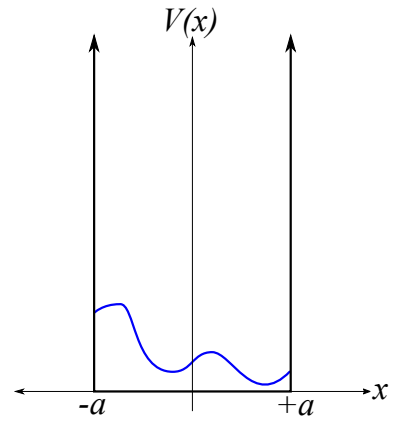


Figure 2: Potentials can be embedded within our infinite square well, as shown by the blue line. We can calculate for any arbitrary potential defined within the surrounding infinite square well.

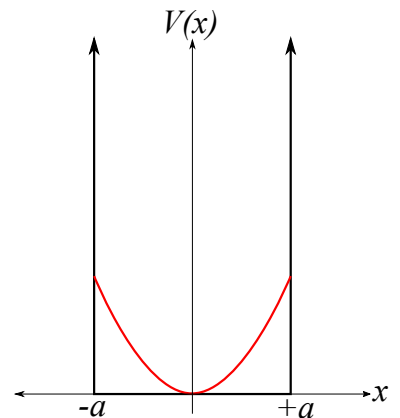


Figure 3: A harmonic potential embedded in the infinite well. Note that the particle is still constrained within the infinite walls indicated by the black lines.

$600e$ is a good starting point, but experiment to find a value you think gives the most interesting results. 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? Discuss and interpret the similarities and differences in your text cells.

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. Explain the reason for your choice in the text cells—what makes your chosen potential an interesting one to study? Make sure you include a full interpretation of the physics of your results in your notebook.

5 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—i.e. use complete and grammatically correct sentences, avoid bullet lists, and use formal scientific language.

Pay particular attention to your text cell commentary, which is highly weighted for assessment. Additionally, 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.

Your notebook should not include any interactive code requiring user input.

5.1 Assessment

You will find a preview of the marking rubric for the assignment on Moodle, where you can see the criteria that will be used to grade your work, their relative weightings, and most of the level descriptors for each criterion.

5.2 Referencing and bibliography

Everything in your submission must be either entirely your own original work, or have the source explicitly acknowledged and suitably referenced:

- If you re-use sections of code from the course scripts or your previous submissions, you *must* note this explicitly in the comments for that section of code. When referring to your own previous submissions, use your Student Number rather than your name, as this assignment is assessed anonymously.
- There is a separate notebook available on Moodle that contains the equations from this script typeset in \LaTeX form. You may copy and paste equations from this notebook, as long as they are referenced appropriately.
- **Use the Harvard bibliography style** to reference all external sources (for example textbooks, lecture notes, or websites) you refer to. An example of how to implement this in a Jupyter notebook is included in the notebook of equations. You should also refer to the “Harvard” section of the UCL referencing guide <http://www.ucl.ac.uk/library/docs/guides/references-plagiarism> for full examples of how to cite various different types of sources, or you may also find this [pdf reference guide](#) a useful, more concise, summary for how to cite various resources:.

5.3 Submission

This is an individual assignment.

- You must work on this on your own, with no help or input from staff, other students, or anyone else.
- You may not make any posts on social media or e-mail, consult in any way with any other person, or engage in any other form of academic misconduct.
- Everything in your submission must be *completely* your own work, or have the source explicitly acknowledged and suitably referenced as above

We will be using several methods to check for plagiarism, copying, and collusion.

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.

You can only submit one file on Moodle, 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 08), and make sure that the original source of the image is made very clear and included in your references. 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.

This is an individual assignment. You must work on this on your own, with no help from staff or other students.

5.4 *Page limit*

There is 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 08.