Square step potential

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1 Introduction

The inherent difference between quantum and classical mechanics is that energies have discrete values. This was determined through studying the infinite and finite square wells. The problem assessed in this write up addresses the question of a square step potential well of the form

$$U(x) = \begin{cases} -U_0 & -l < x < 0 \\ -U_0 + \epsilon_s & 0 < x < l \\ 0 & |x| > l \end{cases} \tag{1}$$

and the effect, should there be any, of ϵ_s on the wavefunction.

This problem was analysed numerically, using the method of finite differences and selecting specific values for the potential $-U_0$ and ϵ_s. The values of three different cases of ϵ_s are analysed, and the wavefunctions are computed. The values of ϵ_s were chosen so that in the first case, $\epsilon_s < 0$, in the second case, $0 > \epsilon_s > -U_0$ and the third case where $\epsilon_s > 0$.

2 The numerical method

The square step well of the potential given in equation 1 was solved numerically using the method of finite differences. Instead of analysing Schrödinger's equation for infinitesimal points, we choose a discretized number of points (i.e. x_n where n = 1, 2,...,N).

Schrödingers equation is given by

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + U(x)\psi(x) = E\psi(x) \tag{2}$$

In taking the derivatives, we approximate the values by assuming small but discrete values of x. Thus, using the standard definition of the derivatives, the first derivative gives

$$\frac{\partial\psi(x)}{\partial x} \approx \frac{\psi(x+\delta x) - \psi(x)}{\delta x}$$

And for the second derivative, we get

$$\frac{\partial^2 \psi(x)}{\partial x^2} \approx \frac{\psi(x+\delta x) - 2\psi(x) + \psi(x-\delta x)}{(\delta x)^2}$$

Thus, for the Schrodinger equation, we get

$$\frac{-\hbar}{2m}\frac{N^2}{L^2}\psi(x_{n+1}) + (-\frac{\hbar}{2m}\frac{N^2}{L^2} + U(x_n)) - \frac{\hbar}{2m}\frac{N^2}{L^2}\psi(x_{n-1}) = E\psi(x_n) \quad (3)$$

In the model being studied, three different cases will be analysed. As the potential changed by a factor of ϵ_s, we can study the cases for where $\epsilon_s < 0$, $0 > \epsilon_s > -U_0$ and $\epsilon_s > U_0$, in the following section.

3 Results and discussion

3.1 Case 1: $\epsilon_s < 0$

In the first case, a value of $\epsilon_s < 0$ is examined. That is, the value of ϵ gives a total potential less than U_0.

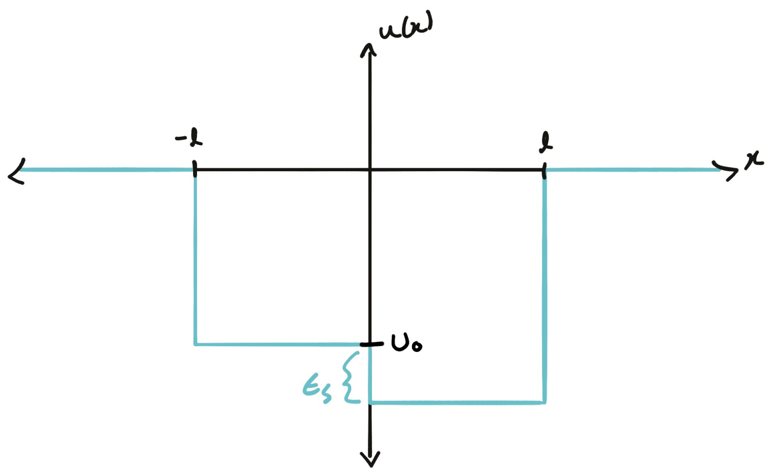


Figure 1: Potential well of square step function for $\epsilon_s < 0$

In examining the wavefunctions of this form, the probability of where the electron is found is dependant on the eigenenergies of the function as well as the chosen values of U_0 and ϵ_s. Initial values of $U_0 = 1$ and $\epsilon_s = -3$ were examined. Through studies of the finite and infinite potential wells, it is known that there cannot be energies less than the lowest potential energy. In this case, that is $-U_0 + \epsilon_s = -1 + -3 = -4$. So the lowest possible eigenenergy for these values is E = -4. Between $-U_0$ and $-U_0 + \epsilon_s$, the particle can only exist between 0 and l. This is seen in the graphs of figure 2 where for values between -4 and -1, the particle is most likely to be found between 0 and l. For energy eigenvalues greater than U_0, the particle is now more likely to be found on between $-l$ and 0, although the probability of finding the particle in the other half of the well is small, but not zero.

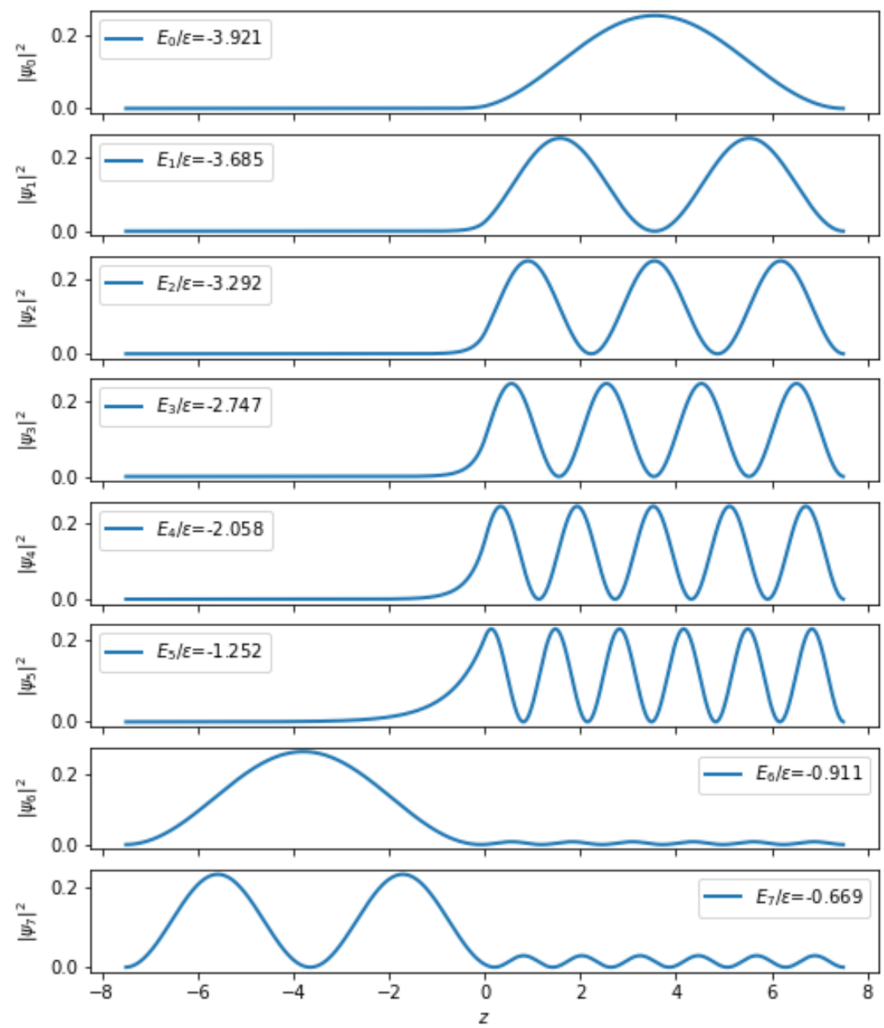


Figure 2: Wavefunctions of the potential square step for values $U_0 = 1$ and $\epsilon_s = -3$.

These results can stem from the fact that it requires less energy for the particle to be in the left side of the well as the energies cross U_0. Upon further analysis of different values of ϵ_s, a similar pattern follows.

3.2 Case 2: $0 > \epsilon_s > -U_0$

The second case examined is the case where $0 > \epsilon_s > -U_0$. The wavefunctions of this case will follow a similar pattern to that of the previous case.

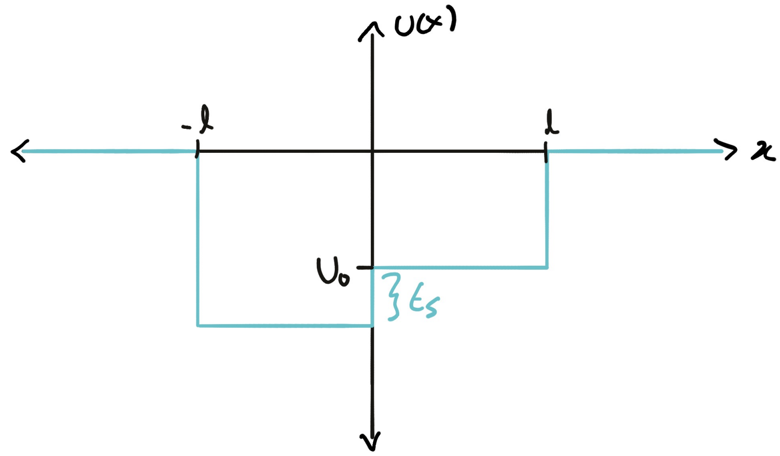


Figure 3: Potential well of square step function for $0 > \epsilon_s > -U_0$

The wavefunctions for this value of ϵ_s as shown in figure 4, depends on the eigenenergies of the function. In this case, the energy of $-U_0$ is less than the energy of ϵ_s and so for values between these two potentials, the particle can only be found between $-l$ and 0. The values this was tested at was $U_0 = 5$ and $\epsilon_s = 1$. The lowest possible energy eigenstate in this case is -5. So for energies between -5 and -4, the particle can only be found on the left side of the well. For values greater than -4, less energy is required on the right side of the well, and thus the particle is more likely to be found there.

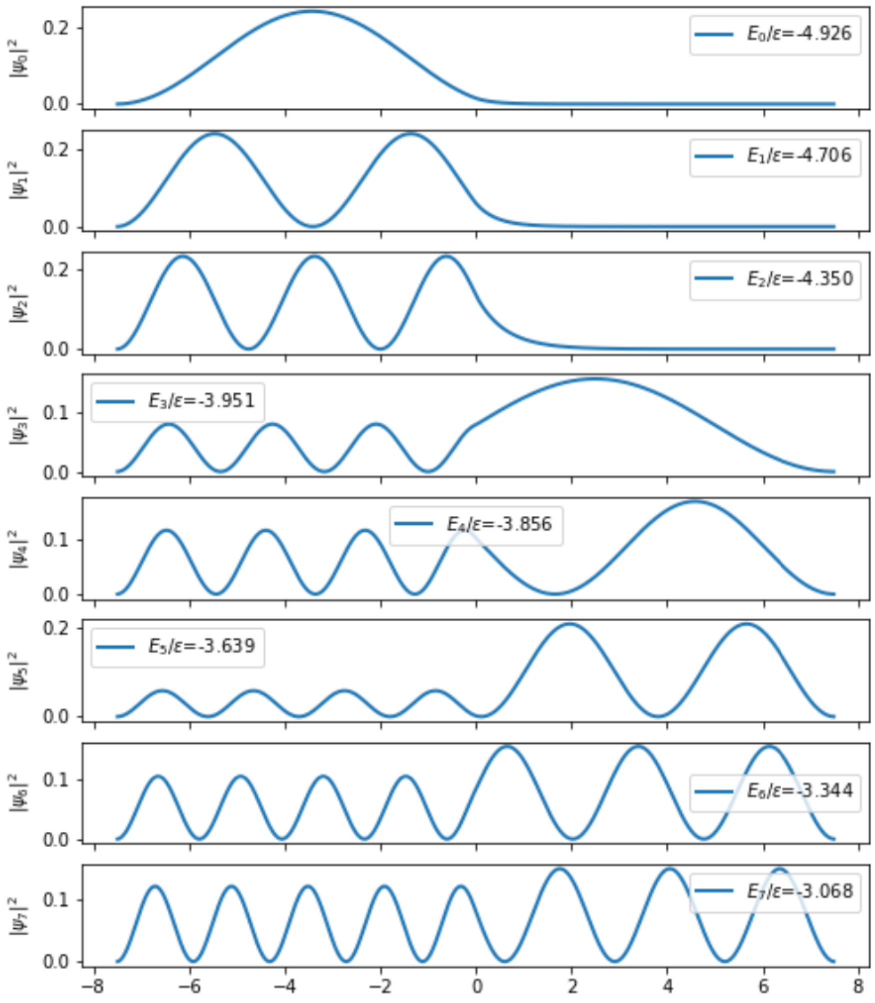


Figure 4: Wavefunctions of the potential square step for values $U_0 = 5$ and $\epsilon_s = 1$.

This aligns with case 1 that the particle is more likely to be found in regions where there is less potential. A note as the energy crosses a value of -4, there is a discontinuity from the left to the right side of the well, which can clearly be seen for the wavefunction of n = 3.

3.3 Case 3: $\epsilon_s > U_0$

In the third case, the values examined are at $\epsilon_s > U_0$. This allows the potential on the right side of the well to be greater than 0.

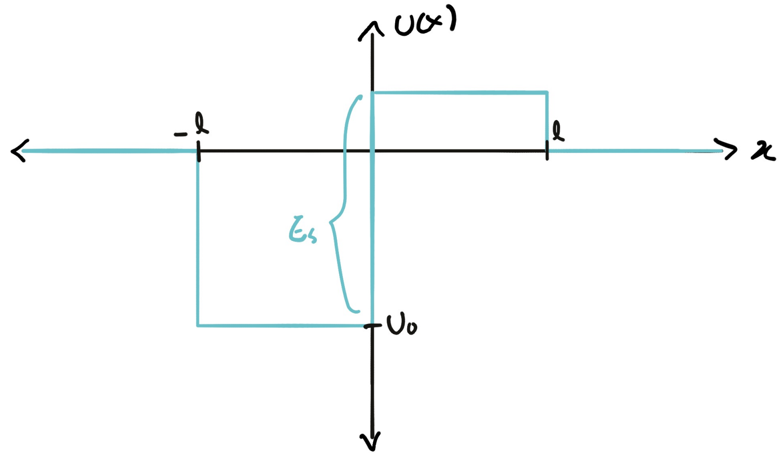


Figure 5: Potential well of square step function for $\epsilon_s > U_0$

The wavefunction for the spectrum of energies are similar to that of case 2, where for eigenenergies between $-U_0$ and $-U_0 + \epsilon_s$ the particle is more likely to be found between $-l$ and 0. For values greater than $-U_0 + \epsilon_s$ the particle was more likely to be found on the right side of the well, between 0 and l. The values of the energies used in this case are $U_0 = 1$ and $\epsilon_s = 3$. As shown, as the eigenenergy passes a value of 2, the particle is more likely to be found on the right side of the well.

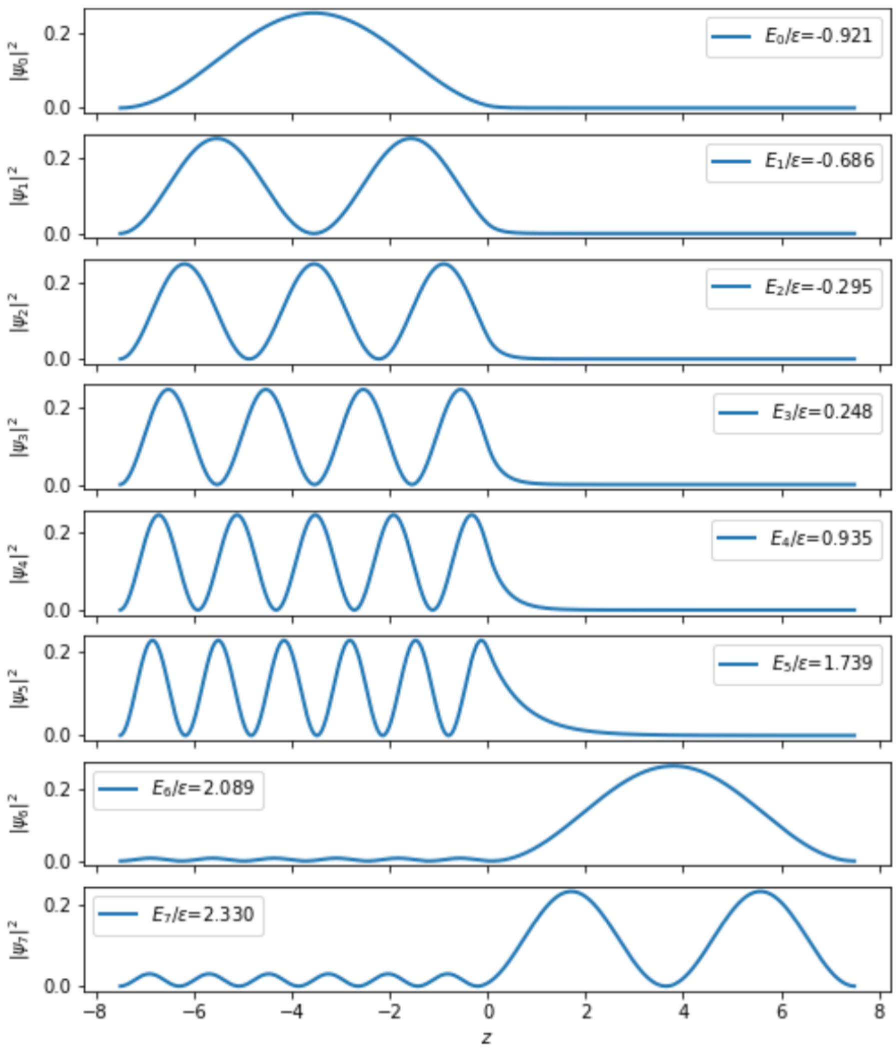
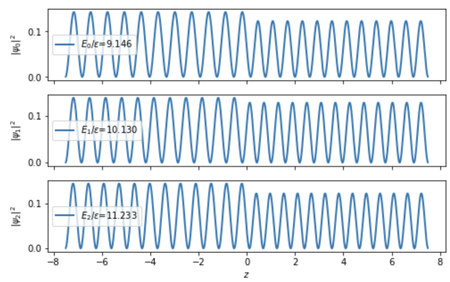


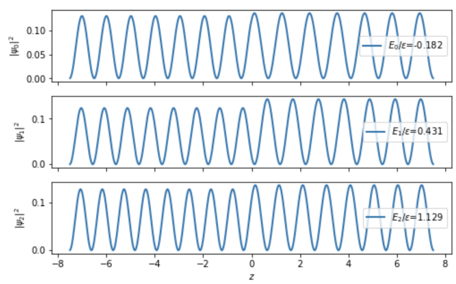
Figure 6: Wavefunctions of the potential square step for values $U_0 = 1$ and $\epsilon_s = 3$.

3.4 Further analysis

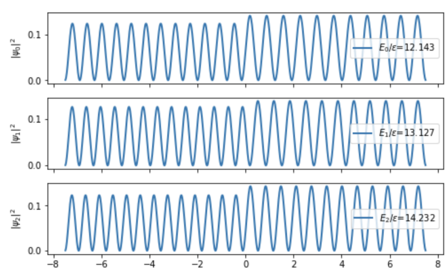
All three cases show similar wavefunctions as the energies go to values significantly greater than 0. The results are similar to the finite square well, where the wavefunctions of the energies oscillate between $-l$ and l. For the first case examined, there is a slightly higher probability that the particle is found in the left side of the well, as shown in figure 7a. In the second and third cases, there is a slightly higher probability that the particle is found in the right side of the well, as shown in figures 7b and 7c, respectively.



(a) Case 1: $U_0 = 1$, $\epsilon_s = -3$



(b) Case 2: $U_0 = 5$, $\epsilon_s = 1$



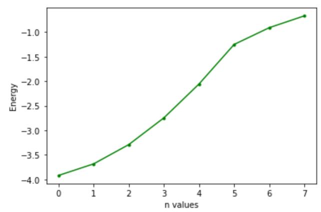
(c) Case 3: $U_0 = 1$, $\epsilon_s = 3$

Figure 7: Energies of the square step with their respective U_0 and ϵ_s values

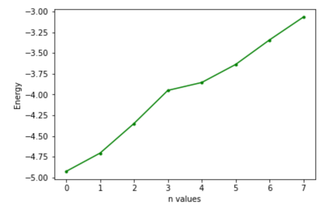
In case 1, the wavefunction tends to the left side of the well because $-U_0$ has less energy than $-U_0 + \epsilon_s$. In the second and third cases, the particle tends to the right of the well because of the lower potential energy required to be in that state.

3.5 Energies of the wavefunctions

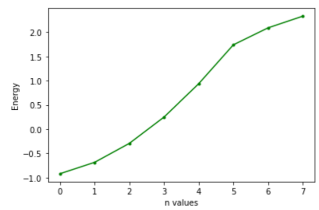
The energies for each respective case is given as follows



(a) Case 1: $U_0 = 1$, $\epsilon_s = -3$



(b) Case 2: $U_0 = 5$, $\epsilon_s = 1$



(c) Case 3: $U_0 = 1$, $\epsilon_s = 3$

Figure 8: Energies of the square step with their respective U_0 and ϵ_s values

A common result is seen in all three graphs, there is a slight discontinuity at the 'step' where the potential changes. This can be due to the difference in the energies of the particle as they go from the state of one potential energy to another.

3.6 Solving using an analytical method

To check if the outcome of the numerical method gives an expected result, we can take an analytical approach to see if the solutions give a similar result.

A square step potential of the form

$$U(x) = \begin{cases} -U_0 & -l < x < 0 \\ -U_0 + \epsilon_s & 0 < x < l \\ 0 & |x| > l \end{cases}$$

describes a medium where the potential energy of a square well changes with respect to the medium. In this case, the potential of the two mediums differs by a factor of ϵ_s and is 0 everywhere else.

Schrodingers equation takes the form

$$\frac{-\partial\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} - U_0\psi = E\psi \quad -l < x < 0 \tag{4}$$

$$\frac{-\partial\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} - (U_0 + \epsilon)\psi = E\psi \quad 0 < x < l \tag{5}$$

$$\frac{-\partial\hbar}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi \quad |x| > l \tag{6}$$

These give solutions of the form

$$\psi(x) = \begin{cases} A_- e^{k_0 x} & x < -l \\ L_- e^{ik_1 x} + L_+^{-ik_1 x} & -l < x < 0 \\ R_- e^{ik_2 x} + R_+ e^{-ik_2 x} & 0 < x < l \\ A_+ e^{-k_0 x} & x > l \end{cases}$$

Where $k_1 = \sqrt{-U_0 - k_0^2}$ and $k_2 = \sqrt{\epsilon_s - U_0 - k_0^2}$.

As seen in the solutions, the wavefunctions of the particle will oscillate between values of $-l$ and l and decay everywhere else. These results makes sense as they align with the results determined using the numerical method.

4 Conclusion

After examining 3 cases of the square step, it is determined that the wavefunctions will depend upon eigenenergies, and on the value of ϵ_s. By analysing the wavefunctions for $\epsilon_s < 0$, it is shown that between $-U_0$ and $-U_0 + \epsilon$, the particle can be found on the right of the well, between 0 and l. For energy values greater than $-U_0$, the particle can be found anywhere between $-l$ and l, with differing probabilities. Cases 2 ($0 > \epsilon_s > -U_0$) and 3 ($\epsilon_s > 0$) yield similar results, where for values between $-U_0$ and $-U_0 + \epsilon_s$, the wavefunction oscillates on the left of the well, between $-l$ and 0, and for values greater than $-U_0 + \epsilon_s$, the particle can be found anywhere in the well, with varying probabilities.

These results can be used to further study similar problems, and can be extended to other applications. In the cases examined here, we have confined the particle to a set length l in one dimension. Using these results, we can further study the effects of what would happen for the same values of U_0 and ϵ_s in a well of different l. We can extend these results to more than one dimension, to find the probabilities of the particle in, for example, a 2 dimensional plane, or in 3 dimensional space. These can, in turn, be applied to studying the energy orbitals of electrons around atoms, as we did with the hydrogen atom.