1 Energy levels

Consider a particle of mass \( m \) in the finite square well potential

\[
V(x) = \begin{cases} 
V(x) = 0 & -\frac{a}{2} \leq x \leq \frac{a}{2} \\
V(x) = V_0 & \text{otherwise.}
\end{cases}
\]

where \( V_0 > 0 \). A general argument based on the symmetry of the potential energy about \( x = 0 \) leads to the conclusion that the energy eigenfunctions are either symmetric or antisymmetric about \( x = 0 \). The symmetric eigenfunctions are:

\[
\psi_{\text{sym}}(x) = \begin{cases} 
C_s e^{qx} + B_s e^{-qx} & x \leq -\frac{a}{2} \\
A_s \cos(kx) & -\frac{a}{2} \leq x \leq \frac{a}{2} \\
B_s e^{qx} + C_s e^{-qx} & x \geq \frac{a}{2}
\end{cases}
\]

where \( A_s, B_s \) and \( C_s \) are constants. The antisymmetric eigenfunctions are:

\[
\psi_{\text{anti}}(x) = \begin{cases} 
-C_a e^{qx} + B_a e^{-qx} & x \leq -\frac{a}{2} \\
A_a \sin(kx) & -\frac{a}{2} \leq x \leq \frac{a}{2} \\
B_a e^{qx} + C_a e^{-qx} & x \geq \frac{a}{2}
\end{cases}
\]

where \( A_a, B_a \) and \( C_a \) are constants. For both types of solution:

\[
k = \sqrt{\frac{2mE}{\hbar^2}} \\
q = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}
\]

where \( E \) is the energy of the state.

a) Verify that both the symmetric and antisymmetric eigenfunctions satisfy the time-independent Schrödinger equation.

b) (These results are crucial but you can leave the derivation to the end of this assignment.) Show that the requirement that \( \psi(x) \) and \( \frac{d\psi}{dx} \) be continuous at \( x = a/2 \) implies that

\[
B_s = \frac{A_s}{2q} e^{-qa/2} (q \cos (ka/2) - k \sin (ka/2))
\]

\[
C_s = \frac{A_s}{2q} e^{qa/2} (q \cos (ka/2) + k \sin (ka/2))
\]

for the symmetric eigenfunctions and

\[
B_a = \frac{A_a}{2q} e^{-qa/2} (k \cos (ka/2) + q \sin (ka/2))
\]

\[
C_a = \frac{A_a}{2q} e^{qa/2} (-k \cos (ka/2) + q \sin (ka/2))
\]

for the antisymmetric eigenfunctions. You should also be able to show that these guarantee that the same conditions will be satisfied at \( x = -a/2 \).
There are now four unknowns: \(a, V_0, E\) and \(A\). The first two must be supplied via external considerations; you will be given fixed values for these. The amplitude \(A\) can be used to ensure that the eigenfunctions are normalized and this will not be our concern. Most importantly \(E\) determines \(k\) and \(q\) and hence the form of the solutions. It should be no surprise that only some choices of \(E < V_0\) will result in well behaved solutions, i.e. those which can be normalized. In fact, for the infinite square well of width \(a\) the energies are

\[
E_n = n^2 \frac{\hbar^2 \pi^2}{2ma^2}
\]

where \(n = 1, 2, 3, \ldots\). It will be convenient to measure energies in units of \(\frac{\hbar^2 \pi^2}{2ma^2}\). Thus define:

\[
V_0' = V_0 / \left(\frac{\hbar^2 \pi^2}{2ma^2}\right) \quad \text{and} \quad E' = E / \left(\frac{\hbar^2 \pi^2}{2ma^2}\right)
\]

Set \(a = 1\) and \(A = 1\).

c) Determine an expression for the infinite square well energy levels in these units, \(E_n'\).

d) Show that

\[
k = \pi \sqrt{E'}
\]

\[
q = \pi \sqrt{V_0' - E'}
\]

One method of finding suitable energy values is to guess \(E\) and plot the resulting wavefunction. A well behaved wavefunction will not diverge as \(x \to \pm \infty\). For one particular value of \(E\) you may find that \(\psi(x) \to \infty\) as \(x \to \infty\) and for another value of \(E\) you may find that \(\psi(x) \to -\infty\) as \(x \to \infty\). It follows that at least one true energy value lies somewhere between these. You can use this to narrow down on energy eigenvalues.

In the following set \(V_0' = 100\) and use this graphical method to determine the energy values and eigenstates.

e) Consider symmetric eigenfunctions. Using the infinite square well energy levels and eigenfunctions as a guide, guess approximate energy values \(E_0'\) for the three lowest energy symmetric states. Will the actual energies be smaller of larger?

f) Use your guess for the lowest energy level, \(E_0'\) to plot \(\psi_s(x)\) for \(-0.75 \leq x \leq 0.75\). How does \(\psi_s(x)\) behave as \(x \to \infty\)? Find a nearby value of \(E'\) such that \(\psi_s(x)\) displays the opposite behavior as \(x \to \infty\). Switch back and forth repeatedly until you determine \(E'\) for the lowest energy level. Show me a plot of the wavefunction. Use the template finitewell.nb in my public space. Check that the wavefunctions that appear there are those given by Eqs. (1)-(8).

g) Repeat this for the next two symmetric energy eigenstates. Use your plots to comment on the probability that the particle will be located in the classical forbidden region. Does this increase or decrease with \(E'\)?

h) Find the three lowest energies for antisymmetric energy eigenstates.