Finite Square Well

1 Bound States

We solve the Schrödinger equation,

\[-\frac{h^2}{2m} \frac{d^2}{dx^2} + V(x)\psi = E\psi,\]

with the potential

\[V(x) = \begin{cases} 
0, & |x| < \frac{a}{2}, \\
V_0, & |x| > \frac{a}{2}, 
\end{cases}\]

as seen in Figure 1.

This leads to having to solve the equations

\[
\psi'' = -k^2 \psi, \quad |x| < \frac{a}{2}, \\
\psi'' = q^2 \psi, \quad |x| > \frac{a}{2},
\]

where

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

Note that \(k^2 + q^2 = \frac{2mV_0}{\hbar^2}\) or \(q = \sqrt{\frac{2mV_0}{\hbar^2} - k^2}\).
The general solutions to these equations are

\begin{align*}
\psi(x) &= A \sin kx + B \cos kx, \quad |x| < \frac{a}{2}, \\
\psi(x) &= C e^{qx} + D e^{-qx}, \quad |x| > \frac{a}{2},
\end{align*}

(3)

The potential is an even function.\(^1\) If \(\psi(x)\) is an even (odd) function, then \(\psi''(x)\) will be even (odd). So, every term in the Schrödinger equation is an even (odd) function. Therefore, the solutions are either even functions or odd functions.

We will consider the even solution case leaving the odd function case to the reader. We need to impose boundary conditions on the functions in Equations (3). For \(x > \frac{a}{2}\), we set \(C = 0\), otherwise \(\psi(x)\) would grow exponentially as \(x\) increases. Since \(\psi(x)\) is an even function for \(|x| < \frac{a}{2}\), we set \(A = 0\). Thus, even solutions which decay for \(|x| > \frac{a}{2}\), are given by

\[
\psi(x) = \begin{cases} 
D e^{-qx}, & x > \frac{a}{2}, \\
B \cos kx, & -\frac{a}{2} < x < \frac{a}{2}, \\
\psi(-x), & x < -\frac{a}{2} 
\end{cases}
\]

We now impose the boundary conditions at \(x = \frac{a}{2}\). Due to symmetry, the conditions at \(x = -\frac{a}{2}\) will be automatically satisfied. We require that \(\psi(x)\) and \(\psi'(x)\) are continuous at \(x = \frac{a}{2}\). Therefore,

\[
D e^{-qa/2} = B \cos \frac{ka}{2},
\]

\[
-qDe^{-qa/2} = -kB \sin \frac{ka}{2}.
\]

(4)

Dividing the second equation by the first equation, we have

\[
q = k \tan \frac{ka}{2}.
\]

(5)

Since \(k\) and \(q\) depend on the energy, \(E\), this is an equation for the energy eigenvalues.

To solve this transcendental equation for \(E\), we introduce the variable \(z = \frac{ka}{2}\) and multiply Equation (5) by \(\frac{a}{2}\) to obtain

\[
z \tan z = \frac{aq}{2} = \frac{a}{2} \sqrt{\frac{2mV_0}{h^2} - k^2} = \sqrt{\frac{ma^2V_0}{2h^2} - z^2} = \sqrt{z_0^2 - z^2}.
\]

(6)

\(^1\)Recall, if \(f(-x) = f(x)\), it is an even function. If \(f(-x) = -f(x)\), it is an odd function.
Dividing by \( z \), we reduce Equation (5) to an equation for \( z \):

\[
\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}.
\]  

(7)

Here \( z_0 = \frac{a}{\hbar} \sqrt{\frac{mV_0}{2}} \).

Solutions are found by plotting the functions

\[
y = \tan z \quad \text{and} \quad y = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}.
\]

In Figure 2 we show this plot. The second function vanishes at \( z = z_0 \). So, there can only be a finite number of intersections. No matter how small \( z_0 \) becomes, there is always at least one intersection.

Figure 2: Solutions of the transcendental Equation (7) as intersections of the two curves \( y = \tan z \) and \( y = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \) resulting in \( m \) points of intersection.

Let the points of intersection be \( z_n = \frac{kn\pi}{2} \) for \( n = 1, 2, \ldots, m \). Since \( k_n = \frac{\sqrt{2mE_n}}{\hbar} \), then we can solve for the bound state energies,

\[
E_n = \frac{2z_n^2\hbar}{ma^2}, \quad n = 1, 2, \ldots, m.
\]

As an example, consider an electron in a 20 eV high square well of width \( a = 2a_0 \), where \( a_0 = 0.529 \times 10^{-10} \) m is the Bohr radius. The graphical solution of the transcendental equation is shown in Figure 3. In this case we obtain \( z_1 = .8234757193 \). This gives \( k_1 = 1.56 \times 10^{10} \) m\(^{-1} \) and \( E_1 = 9.24 \) eV. then, we can obtain \( q_1 = 1.68 \times 10^{10} \) m\(^{-1} \).

For the wavefunction, one solves the first equation in Equation (4) for \( D \) in terms of \( B \). Then, normalizing the wavefunction, we obtain \( B = 94300 \). Using these results, we can then obtain \( \psi(x) \). The wavefunction is shown in Figure 4.
Figure 3: Intersection of the two curves $y = \tan z$ and $y = \sqrt{\left(\frac{5a}{z}\right)^2 - 1}$ for the example of an electron in a square well. There is only one bound state.

Figure 4: The wavefunction for the example of an electron in a square well and the square well potential.

If one were to increase the width of the potential well to $a = 6a_0$, then there would be two bound states. The graphical solution of transcendental equation is shown in Figure 5. The solutions are $z = 1.226577100, 3.456253958$. From these, one finds energies $E = 2.278, 18.084$ eV. The corresponding wavefunctions are shown in Figure 6.

For completeness, one should consider the odd solutions which are given by

$$
\psi(x) = \begin{cases} 
  De^{-qx}, & x > \frac{a}{2}, \\
  A \sin kx, & -\frac{a}{2} < x < \frac{a}{2}, \\
  -\psi(-x), & x < -\frac{a}{2}.
\end{cases}
$$

As before, we only need to impose the boundary conditions at $x = \frac{a}{2}$. We require that $\psi(x)$ and $\psi'(x)$
Figure 5: Intersection of the two curves $y = \tan z$ and $y = \sqrt{\left(\frac{5a_0}{2}\right)^2 - 1}$ for the example of an electron in a square well for $a = 6a_0$. There are now two bound states.

Figure 6: The two even bound state wavefunctions for the electron in a square well of width $a = 6a_0$. 


Figure 7: Solutions of the transcendental Equation (10) as intersections of the two curves $y = -\cot z$ and $y = \sqrt{\left(\frac{z_0}{\pi}\right)^2 - 1}$ resulting in $m$ points of intersection.

be continuous at $x = \frac{a}{2}$. Therefore,

\[
De^{-qa/2} = A\sin\frac{ka}{2},
\]

\[
-qDe^{-qa/2} = kA\cos\frac{ka}{2},
\]

(8)

Dividing the second equation by the first equation, we have

\[
q = -k \cot \frac{ka}{2}.
\]

(9)

Letting $z = \frac{ka}{2}$ and multiplying Equation (9) by $\frac{a}{2}$, we obtain

\[-z \cot z = \sqrt{z_0^2 - z^2},
\]

or

\[-\cot z = \sqrt{\left(\frac{z_0}{\pi}\right)^2 - 1},
\]

(10)

where $z_0 = \frac{a}{\hbar}\sqrt{\frac{mV_0}{2}}$. Solving this transcendental equation proceeds as before. The graphical solution can be seen in Figure 7. Note that there are no odd solutions for $z < \pi/2$.

Returning to the electron example, we find that for $a = 2a_0$, there are no odd function bound states. However, for $a = 6a_0$, there is one. In Figure 8 we show the intersection of the two curves $y = -\cot z$ and $y = \sqrt{\left(\frac{z_0}{\pi}\right)^2 - 1}$ and the odd bound state wavefunction for the electron in a square well of width $a = 6a_0$. 6
Figure 8: On the left is the graph showing the intersection of the two curves \( y = -\cot z \) and \( y = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1} \) for the square well of width \( a = 6a_0 \). On the right is the odd bound state wavefunction for the electron in a square well of width \( a = 6a_0 \).

This corresponds to a bound state energy of \( E = 8.829 \text{ eV} \), which is in between the energies of the two even states found earlier.

Figure 9: The four bound state wavefunctions for a potential well of width \( a = 6a_0 \) and \( V_0 = 40 \text{ eV} \).

In Figure 9 we show the results for a potential well of width \( a = 6a_0 \) and \( V_0 = 40 \text{ eV} \). There are four bound states with energies \( E = 2.608, 10.306, 22.583, 37.398 \text{ eV} \). There are two odd bound state wavefunctions and two even ones.