Finite Square Well

1 Bound States

We solve the Schrödinger equation,

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

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.

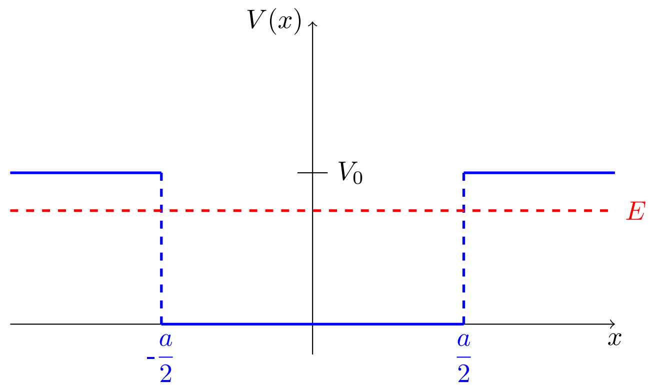

Figure 1: Finite potential well with $E < V_0$.

This leads to having to solve the equations

$$\begin{aligned} \psi'' &= -k^2\psi, \quad |x| < \frac{a}{2}, \\ \psi'' &= q^2\psi, \quad |x| > \frac{a}{2}, \end{aligned} \tag{2}$$

where

$$k^2 = \frac{2mE}{\hbar^2}, \qquad q^2 = \frac{2m(V_0 - E)}{\hbar^2}.$$

Note that $k^2 + q^2 = \dfrac{2mV_0}{\hbar^2}$ or $q = \sqrt{\dfrac{2mV_0}{\hbar^2} - k^2}$.

The **general solutions** to these equations are

$$\begin{aligned} \psi(x) &= A\sin kx + B\cos kx, \quad |x| < \frac{a}{2}, \\ \psi(x) &= Ce^{qx} + De^{-qx}, \quad |x| > \frac{a}{2}, \end{aligned} \tag{3}$$

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

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

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,

$$\begin{aligned} De^{-qa/2} &= B\cos\frac{ka}{2}, \\ -qDe^{-qa/2} &= -kB\sin\frac{ka}{2}. \end{aligned} \tag{4}$$

Dividing the second equation by the first equation, we have

$$q = k\tan\frac{ka}{2}. \tag{5}$$

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

$$\begin{aligned} z\tan z &= \frac{aq}{2} \\ &= \frac{a}{2}\sqrt{\frac{2mV_0}{\hbar^2} - k^2} \\ &= \sqrt{\frac{ma^2V_0}{2\hbar^2} - z^2} \\ &\equiv \sqrt{z_0^2 - z^2}. \end{aligned} \tag{6}$$

[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 :

$$\tan z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}. \tag{7}$$

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.

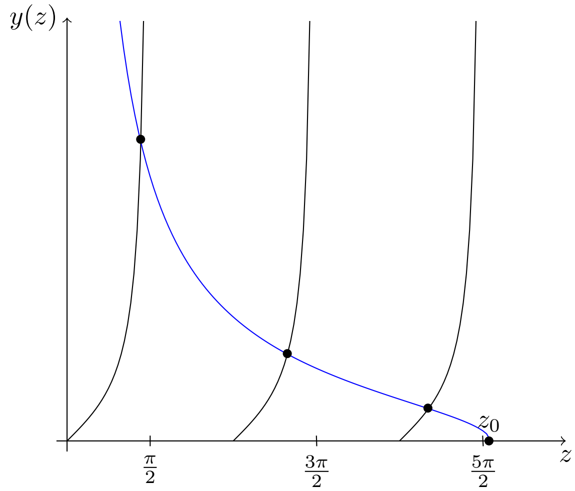

Figure 2: Solutions of the transcendental Equation (7) as intersections of the two curves $y = \tan z$ and $y = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ resulting in m points of intersection.

Let the points of intersection be $z_n = \frac{k_n a}{2}$ 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.

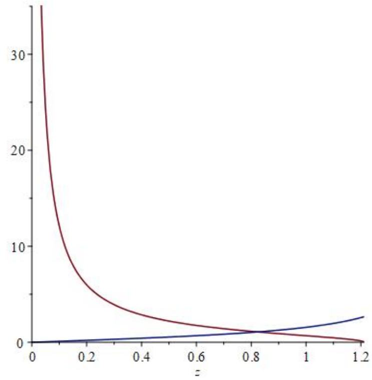

Figure 3: Intersection of the two curves $y = \tan z$ and $y = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ for the example of an electron in a square well. There is only one bound state.

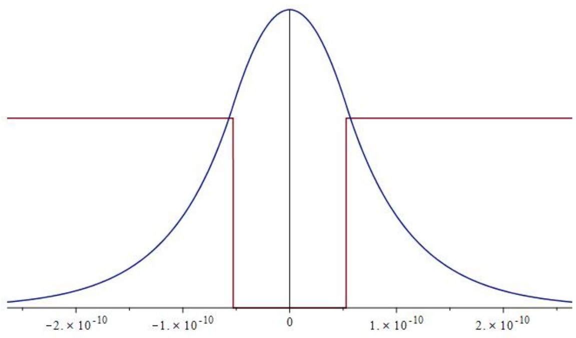

Figure 4: The wavefunction for the example of an electron in a square well and the square well potential.

If one were to increase the with 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 $\psi'(x)$

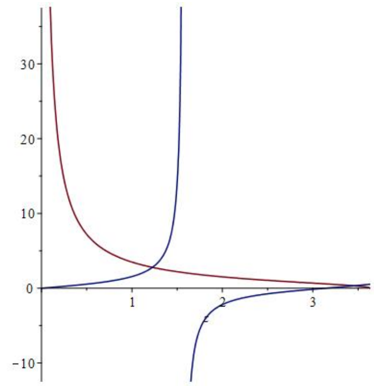

Figure 5: Intersection of the two curves $y = \tan z$ and $y = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ for the example of an electron in a square well for $a = 6a_0$. There are now two bound states.

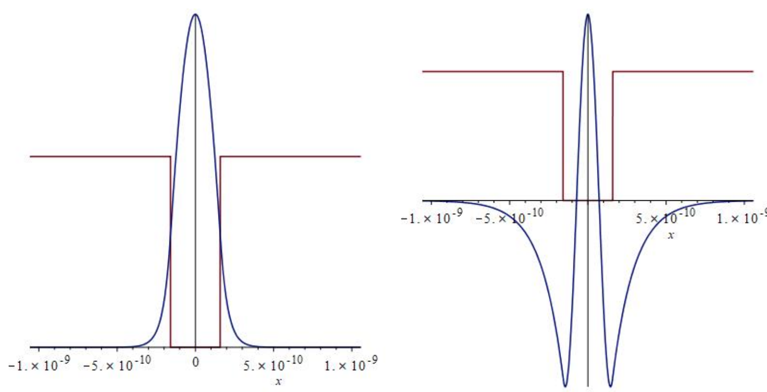

Figure 6: The two even bound state wavefunctions for the electron in a square well of width $a = 6a_0$.

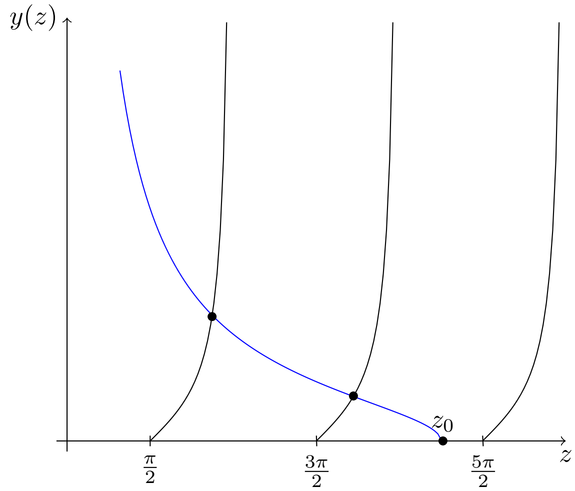

Figure 7: Solutions of the transcendental Equation (10) as intersections of the two curves $y = -\cot z$ and $y = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ resulting in m points of intersection.

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

$$De^{-qa/2} = A \sin \frac{ka}{2},$$
$$-qDe^{-qa/2} = kA \cos \frac{ka}{2}. \tag{8}$$

Dividing the second equation by the first equation, we have

$$q = -k \cot \frac{ka}{2}. \tag{9}$$

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

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

or

$$-\cot z = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}, \tag{10}$$

where $z_0 = \dfrac{a}{\hbar}\sqrt{\dfrac{mV_0}{2}}$. 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 $y = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ and the odd bound state wavefunction for the electron in a square well of width $a = 6a_0$.

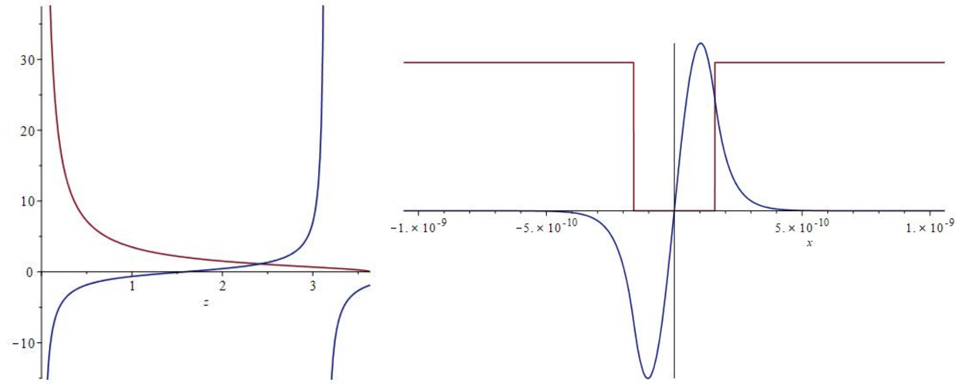

Figure 8: On the left is the graph showing the intersection of the two curves $y = -\cot z$ and $y = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}$ for the square well of width $a = 6a_0$. On the right is the odd bound state wavefunction for the electron in a square well of width $a = 6a_0$.

This corresponds to a bound state energy of $E = 8.829$ eV, which is in between the energies of the two even states found earlier.

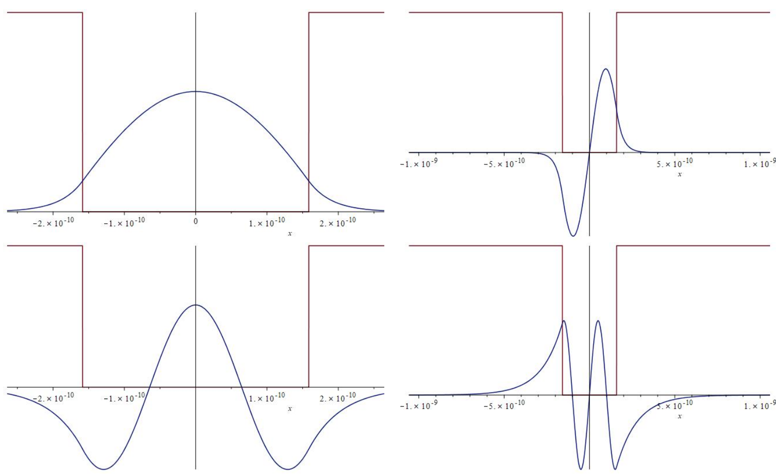

Figure 9: The four bound state wavefunctions for a potential well of width $a = 6a_0$ and $V_0 = 40$ eV.

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