FINITE SQUARE WELL: BOUND STATES & ODD WAVE FUNCTIONS

Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 2.29.

Shankar, R. (1994), *Principles of Quantum Mechanics*, Plenum Press. Section 5.2, Exercise 5.2.6.

To complete our analysis of the finite square well, we'll have a look at the solutions where the spatial wave function $\psi(x)$ is an odd function. In our analysis of the problem where $\psi(x)$ was even, we began with the potential:

$$V(x)=\begin{cases}0 & x<-a\\ -V_0 & -a\le x\le a\\ 0 & x>a\end{cases} \tag{0.1}$$

where V_0 is a positive constant energy, and a is a constant location on the x axis.

For bound states, we have $-V_0<E<0$, (the total energy has to be greater than the minimum value of the potential, as we proved before) which results in bound states in which we would expect $\psi(x)$ to oscillate within the well and decay exponentially outside the well.

Following the same procedure as in the even function case, we divide the solution into separate regions and try to solve for the various constants that pop up by applying boundary conditions. The equation to be solved can be split into three regions:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad (x<-a) \tag{0.2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}-V_0\psi = E\psi \qquad (-a\le x\le a) \tag{0.3}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad (x>a) \tag{0.4}$$

The general solutions in these three regions are easy enough to write down. We get

$$\psi(x)=\begin{cases}Ae^{-\kappa x}+Be^{\kappa x} & x<-a\\ C\sin(\mu x)+D\cos(\mu x) & -a\le x\le a\\ Fe^{-\kappa x}+Ge^{\kappa x} & x>a\end{cases} \tag{0.5}$$

where as usual we've introduced some convenience parameters:

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \tag{0.6}$$

$$\mu \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar} \tag{0.7}$$

Note that both these parameters are real and can be taken as positive, since $-V_0<E<0$ for bound states. Note that we've also expressed the solution in the middle section in terms of sin and cos rather than in terms of $e^{i\mu x}$ and $e^{-i\mu x}$. The latter is also valid, but as we'll see in the next paragraph, using sin and cos is easier.

So now we have six constants to deal with. First, we can use the theorem that says that if the potential function is even (as this one is: $V(-x)=V(x)$), then $\psi(x)$ is even or odd. We now require $\psi(x)$ to be odd, so that $\psi(-x)=-\psi(x)$. Since the cosine is an even function, we must have $D=0$. In the outer regions, the requirement of an odd function means that $A=-G$ and $B=-F$.

Next, we can impose the requirement that $\psi(x)\to 0$ at $\pm\infty$, so this means that $A=G=0$. We therefore get

$$\psi(x)=\begin{cases}Be^{\kappa x} & x<-a\\ C\sin(\mu x) & -a\le x\le a\\ -Be^{-\kappa x} & x>a\end{cases} \tag{0.8}$$

Now we can apply the boundary conditions. Since there are no infinite energies involved (the potential is finite everywhere), we apply Born's conditions and require that both ψ and ψ' are continuous at both boundaries. Because of the symmetry of the wave function, we can consider only one boundary; the other one won't give us anything new. Therefore these two conditions give us (using the fact that sine is odd and cosine is even):

$$Be^{-\kappa a} = -C\sin(\mu a) \tag{0.9}$$

$$\kappa Be^{-\kappa a} = \mu C\cos(\mu a) \tag{0.10}$$

Dividing these two equations together, we can get rid of B and C:

$$\frac{1}{\kappa} = -\frac{1}{\mu}\tan(\mu a) \tag{0.11}$$

This is actually a condition that will give us the allowed energies, since both κ and μ are functions of E. Unfortunately, this equation cannot be solved explicitly for E (it's what is known as *transcendental*, which means that the variable we're trying to solve for occurs both inside and outside of a function such as the tan). The only way such equations can be solved is numerically, but we can get an idea of the solutions by plotting the two sides of the equation on the same graph and seeing where these plots intersect.

We can rewrite this equation as

$$\tan(\mu a) = -\frac{\mu}{\kappa} \tag{0.12}$$

From the definitions of κ and μwe can eliminate κ as follows:

$$\begin{aligned}
\kappa^2+\mu^2 &= 2mV_0/\hbar^2 && (0.13)\\
\kappa &= \sqrt{2mV_0/\hbar^2-\mu^2} && (0.14)\\
\frac{\mu}{\kappa} &= \frac{1}{\sqrt{2mV_0/\mu^2\hbar^2-1}} && (0.15)\\
\tan(\mu a) &= -\frac{1}{\sqrt{2mV_0/\mu^2\hbar^2-1}} && (0.16)\\
&= -\frac{1}{\sqrt{2ma^2V_0/(\mu a)^2\hbar^2-1}} && (0.17)
\end{aligned}$$

Defining the variable $z \equiv \mu a$, we can now write this equation as a transcendental equation in the single variable z:

$$\tan z = -\left(\frac{2ma^2V_0/\hbar^2}{z^2}-1\right)^{-1/2} \tag{0.18}$$

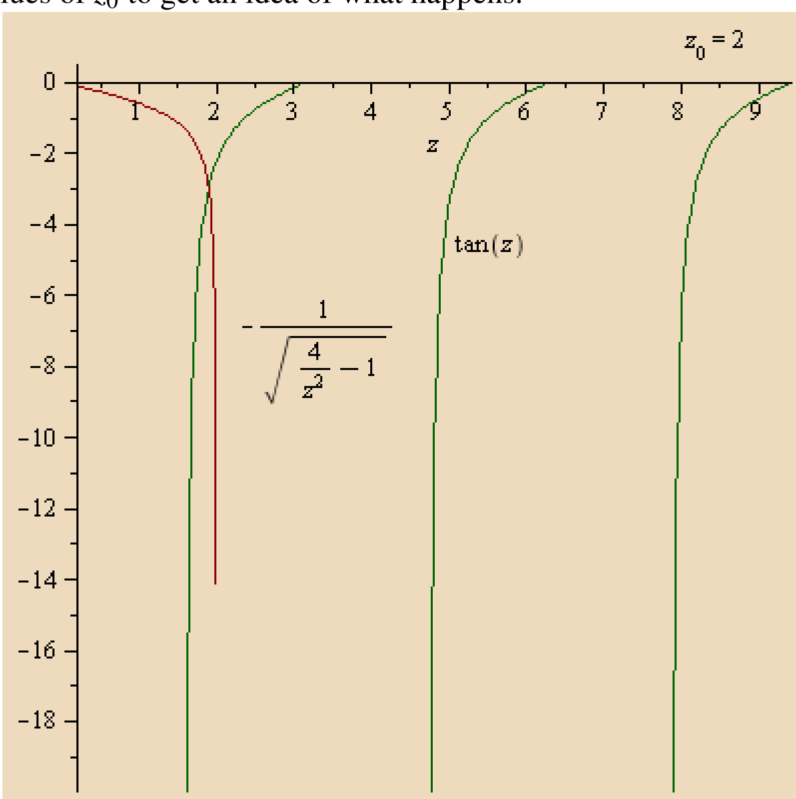
To solve this equation graphically or numerically for a given particle, we clearly need to specify values for a and V_0. However, we can treat the combination of parameters as a single parameter z_0:

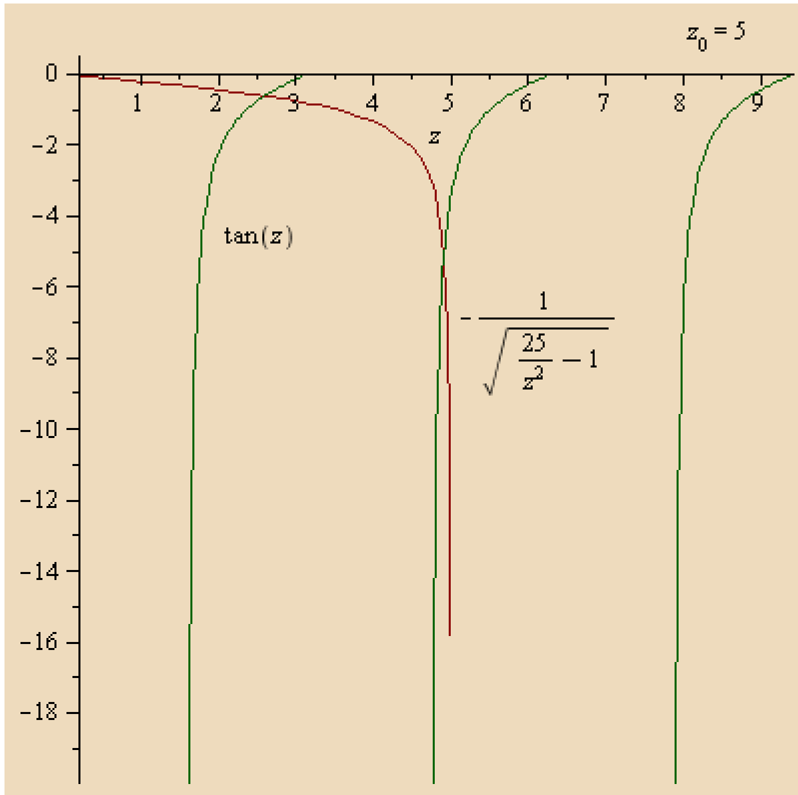
$$z_0^2 \equiv \frac{2ma^2V_0}{\hbar^2} \tag{0.19}$$

so we have the equation

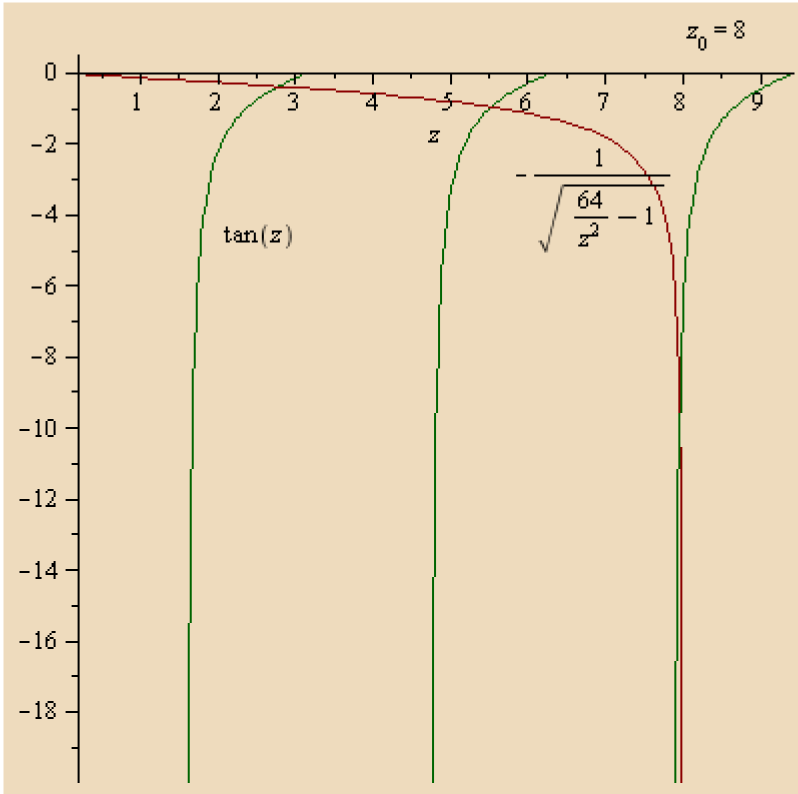
$$\tan z = -\left(\frac{z_0^2}{z^2} - 1\right)^{-1/2} \tag{0.20}$$

We can plot both sides of this equation on the same graph for various values of z_0 to get an idea of what happens.





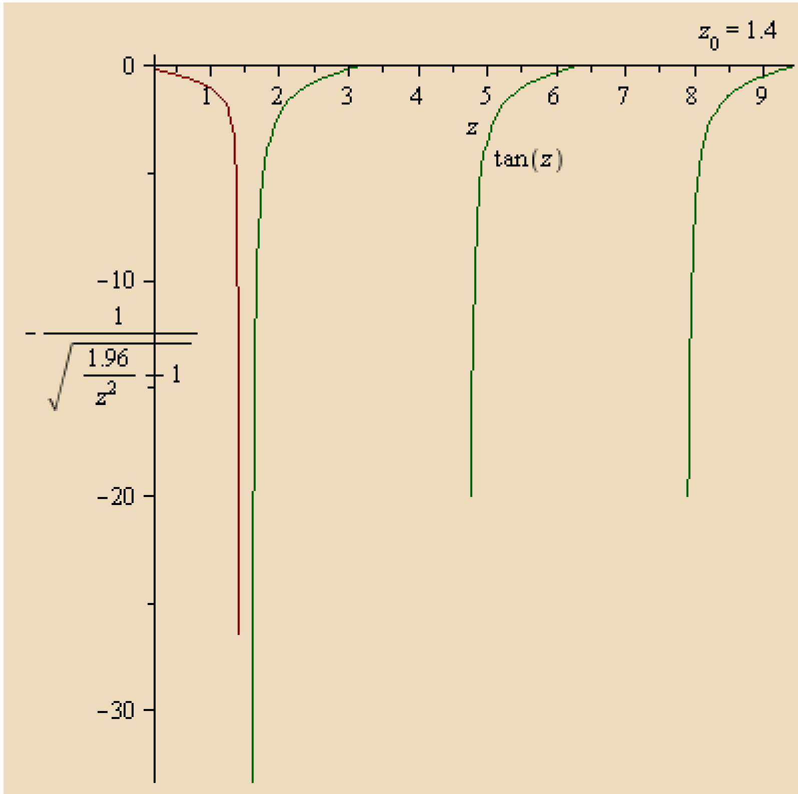
$z_0 = 5$
0
1
2
3
4
5
6
7
8
9
−2
−4
−6
−8
−10
−12
−14
−16
−18
z
tan(z)
$-\frac{1}{\sqrt{\frac{25}{z^2}-1}}$



In these plots, we show what happens for three different values of z_0. The green curves show the plot of $\tan z$; the red curves that of $-\left(\frac{z_0^2}{z^2}-1\right)^{-1/2}$. In the first graph, with $z_0 = 2$, we get only one intersection between the two plots, around $z = 2$. Thus for $z_0 = 2$, there is only one bound state, with an energy that can be worked out from $z = \mu a = \frac{\sqrt{2m(E+V_0)}a}{\hbar} \approx 2$. A more accurate value can be obtained by numerical solution of the equation, but this requires a computer (well, actually, the graphs were drawn on a computer too, but never mind).

The second and third graphs show what happens as we increase z_0 to 5 and then 8. In each case we pick up an extra intersection between the two graphs, so we add an extra bound state.

In this case, we see that if we reduce z_0 to a value less than $\pi/2$, there will be no bound states, since the tangent is asymptotic to the line $z = \pi/2$. We can see the situation in the following plot, in which $z_0 = 1.4 < \pi/2$:



The curve $-\left(\frac{z_0^2}{z^2}-1\right)^{-1/2}$ is here asymptotic to the line $z = 1.4$, so it will never intersect the tangent curve.

At the other extreme, as $V_0 \to \infty$, we would expect to get the infinite square well states. To see this, note that the graph of $-\left(\frac{z_0^2}{z^2}-1\right)^{-1/2}$ is asymptotic to the line $z = z_0$, so as $V_0 \to \infty$, $z_0 \to \infty$ and the asymptote gets further and further along the axis, so the number of intersections with branches of the tangent gets larger. Thus the *number* of energy states gets larger and larger, eventually becoming infinite. As to the locations of these intersections, we can notice that for any fixed, finite value of z, the quantity $-\left(\frac{z_0^2}{z^2}-1\right)^{-1/2}$ tends to zero as $z_0 \to \infty$, so that means that the entire curve approaches the horizontal axis, so the intersections with the tangent curve will occur very near those locations where the tangent curve meets the horizontal axis, that is, where $\tan z = 0$. These points are at $z = n\pi$. This means that

$$z^2 = \frac{2ma^2(E+V_0)}{\hbar^2} \tag{0.21}$$

$$\approx n^2\pi^2 \tag{0.22}$$

$$E+V_0 \approx \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{0.23}$$

$$= \frac{(2n)^2\pi^2\hbar^2}{2m(2a)^2} \tag{0.24}$$

Since $E+V_0$ is the height of the bound state above the bottom of the well, we can see that this formula does indeed give us the expected energy levels for an infinite square well of width $2a$, for even quantum numbers $2n$. The other ones, for odd n came from a solution where we assume $\psi(x)$ is an even function.