FINITE SQUARE WELL - BOUND STATES, EVEN WAVE FUNCTIONS

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A general rule when solving the Schrödinger equation in one dimension is that in those regions where the total energy E is less than the potential V the spatial part of the wave function $\psi(x)$ decays exponentially, while if $E > V$, the wave function $\psi(x)$ oscillates in some fashion. In the case of the infinite square well, ψ is zero outside the well since the potential is infinite there, so there is zero chance of finding the particle outside the well. Within the well, the oscillation follows the pattern of a sine wave, which must be zero at the boundaries. This boundary condition is responsible for the quantization of the energy levels.

For the delta-function well, $\psi(x)$ peaks at $x = 0$ (the only place where $\delta(x) \neq 0$), and decays exponentially on either side. A kind of hybrid of these two extreme examples (the delta-function and the infinite square well) is the finite square well, in which the potential follows the rule

$$V(x) = \begin{cases} 0 & x < -a \\ -V_0 & -a \leq x \leq a \\ 0 & x > a \end{cases} \tag{1}$$

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

With such a potential, we have two main possibilities. First, $-V_0 < E < 0$, (the total energy has to be greater than the minimum value of the potential) which results in bound states in which we would expect $\psi(x)$ to oscillate within the well and decay exponentially outside the well. Second, $E > 0$, in which we would expect $\psi(x)$ to oscillate everywhere. In the first case, we also expect the energy levels to be quantized due to the boundary conditions within the well, so we can try to find the allowed states. In the second case, as with the delta-function, we can study the behaviour of an incoming beam of particles as it hits the barrier, and calculate the reflection and transmission coefficients (while keeping in mind that any real particle is composed of a combination of pure waves in the form of a wave packet, so that calculations with single energy states are at best an approximation).

The mathematics for the bound state case of the finite square well turns out to be more complicated than in the case of the delta-function, and in fact we can't get an exact formula for the allowed energies. However, the process of solving the Schrödinger equation is fairly straightforward, if a bit messy.

As usual, 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:

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

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \qquad (-a\le x\le a) \tag{3}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \qquad (x>a) \tag{4}$$

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

$$\psi(x) = \begin{cases} Ae^{-\kappa x}+Be^{\kappa x} & x<-a \\ C\sin(\mu x)+D\cos(\mu x) & -a\le x\le a \\ Fe^{-\kappa x}+Ge^{\kappa x} & x>a \end{cases} \tag{5}$$

where as usual we've introduced some convenience parameters:

$$\kappa \equiv \frac{\sqrt{-2mE}}{\hbar} \tag{6}$$

$$\mu \equiv \frac{\sqrt{2m(E+V_0)}}{\hbar} \tag{7}$$

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. Unfortunately, we need to work out these two cases separately, but in each case, it does allow us to eliminate three of the constants. We'll deal with the even solutions first, so that we require $\psi(-x) = \psi(x)$. Since the sine is an odd function, we must have $C = 0$. In the outer regions, the requirement of an even function means that $A=G$ and $B=F$.

Next, we can impose the requirement that $\psi(x)\rightarrow0$ at $\pm\infty$, so this means that $A=G=0$. We therefore get

$$\psi(x)=\begin{cases}Be^{\kappa x} & x<-a\\ D\cos(\mu x) & -a\le x\le a\\ Be^{-\kappa x} & x>a\end{cases} \tag{8}$$

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 cos is even):

$$Be^{-\kappa a} = D\cos(\mu a) \tag{9}$$

$$-\kappa Be^{-\kappa a} = -\mu D\sin(\mu a) \tag{10}$$

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

$$\kappa=\mu\tan(\mu a) \tag{11}$$

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 μ 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

$$\tan(\mu a) = \frac{\kappa}{\mu} \tag{12}$$

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

$$\kappa^2+\mu^2 = 2mV_0/\hbar^2 \tag{13}$$
$$\kappa = \sqrt{2mV_0/\hbar^2-\mu^2} \tag{14}$$
$$\frac{\kappa}{\mu} = \sqrt{2mV_0/\mu^2\hbar^2-1} \tag{15}$$
$$\tan(\mu a) = \sqrt{2mV_0/\mu^2\hbar^2-1} \tag{16}$$
$$= \sqrt{2ma^2V_0/(\mu a)^2\hbar^2-1} \tag{17}$$

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

$$\tan z = \sqrt{\frac{2ma^2V_0/\hbar^2}{z^2}-1} \tag{18}$$

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:

$$z_0^2 \equiv \frac{2ma^2V_0}{\hbar^2} \tag{19}$$

so we have the equation

$$\tan z = \sqrt{\frac{z_0^2}{z^2}-1} \tag{20}$$

and we want to find values of z for a given value of z_0.

We plot both sides of this equation on the same graph in Fig. 1 for various values of z_0 to get an idea of what happens.

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 $\sqrt{\frac{z_0^2}{z^2}-1}$. In the first graph, with $z_0=2$, we get only one intersection between the two plots, around $z=1$. Thus for $z_0=2$, there is only one bound state, with an energy that can be worked out from $z=\mu a=\frac{\sqrt{2m(E+V_0)}a}{\hbar}\approx 1$. 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.

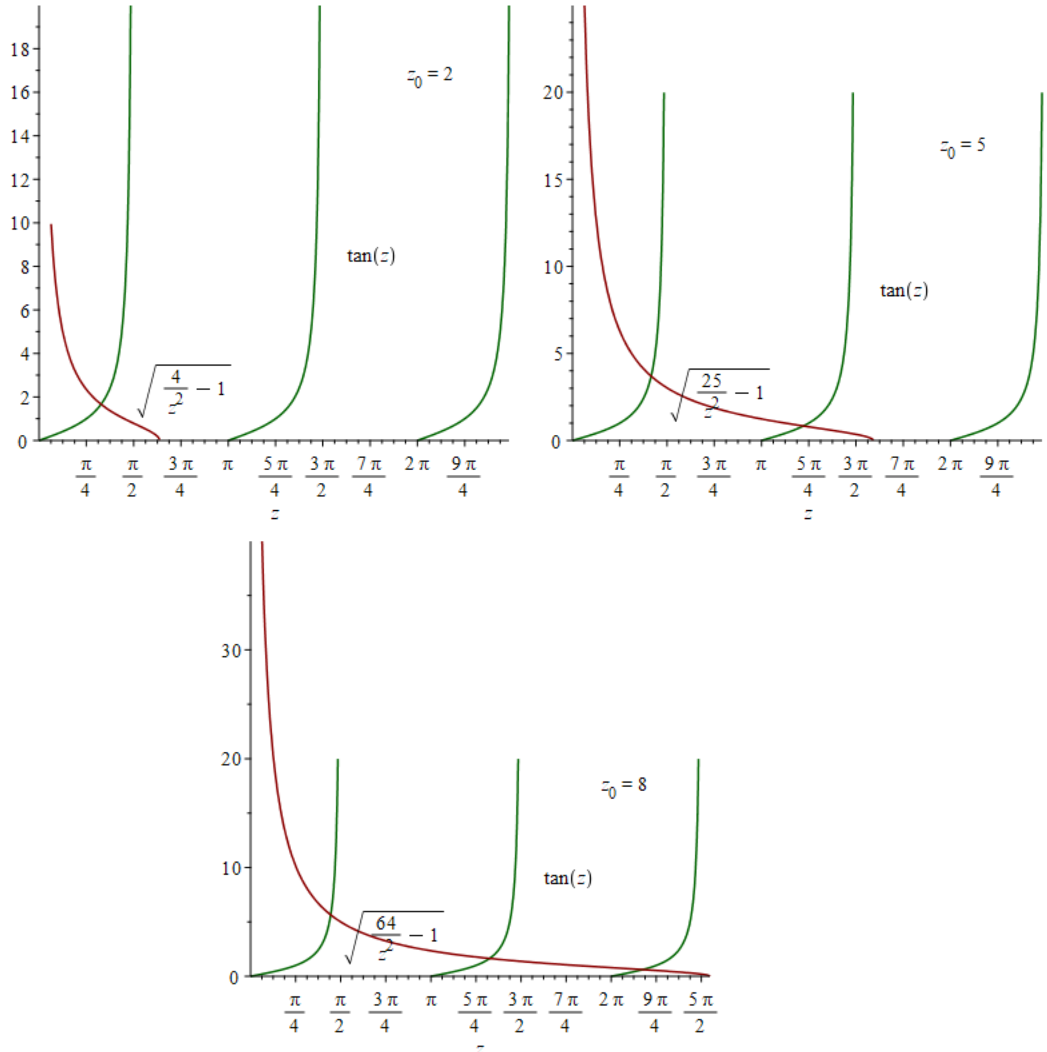

FIGURE 1. Plots of 20 for $z_0 = 2$,5, 8.

z_0	# states	z
2	1	1.030
5	2	1.306, 3.837
8	3	1.395, 4.165, 6.831

TABLE 1. Solutions of 20 for $z_0 = 2, 5, 8$.

Using Maple's fsolve command, the numerically solved values for $z_0 =$ 1,5 and 8 are given in Table 1.

In this case, we can see that no matter how small we make z_0, we will always have at least one bound state (since the $\tan z$ graph starts off from the origin). As $V_0 \to 0$, we would expect the situation to tend to that of the free particle, so the presence of this bound state might be a bit worrying. However, if $V_0 = 0$ exactly, then the quantity $\sqrt{\frac{z_0^2}{z^2} - 1}$ has no values of z which give a real value since $z_0 = 0$, so there are no intersections on the graph, thus there are no bound states. However, if there is any potential well at all, no matter how shallow, there will be at least one bound state.

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 $\sqrt{\frac{z_0^2}{z^2} - 1}$ intersects the horizontal axis at $z = z_0$, so as $V_0 \to \infty$, from 19 we see that $z_0 \to \infty$ and the intersection point 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 $\sqrt{\frac{z_0^2}{z^2} - 1}$ tends to infinity as $z_0 \to \infty$, so that means that the entire curve gets higher, so the intersections with the tangent curve will occur at higher locations. The tangent is asymptotic to the vertical lines $n\pi/2$ for odd n, so we would expect the intersection points to eventually become $z = n\pi/2$. This means that

$$z^2 = \frac{2ma^2(E+V_0)}{\hbar^2} \tag{21}$$

$$\approx \frac{n^2\pi^2}{4} \tag{22}$$

$$E + V_0 \approx \frac{n^2\pi^2\hbar^2}{2m(2a)^2} \tag{23}$$

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 $2a$, or at least those corresponding to odd n. The other ones, for even n come from a solution where we assume $\psi(x)$ is an odd function.

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