

Graphical Solution of the Finite Square Well

This section provides a more detailed understanding of the solution of the Schrödinger equation for a one-dimensional square well of finite depth, a physically more realistic potential whose understanding will be helpful in many future discussions. Let us first shift the $V(x)$ and x axes so as to arrange the potential symmetrically about $x = 0$ with the walls at $\pm a$ as shown in Figure 6-8b. The purpose is to enable us to simplify the mathematics a bit. As above, we will only be concerned with energies inside the well; that is, $0 < E < V_0$.

Equation 6-33 is the Schrödinger equation for $-a > x > +a$ where $V(x) = V_0$ and its general solution is

$$\psi(x) = B_1 e^{\alpha x} + B_2 e^{-\alpha x} \quad \mathbf{6-36}$$

where B_1 and B_2 are constants. The condition that $\psi(x) \rightarrow 0$ as $x \rightarrow -\infty$ means that $B_2 = 0$ for $x < -a$. Similarly, $B_1 = 0$ for $x > +a$ and we conclude that

$$\psi(x) = B_1 e^{\alpha x} \quad x < -a \quad \mathbf{6-37a}$$

$$\psi(x) = B_2 e^{-\alpha x} \quad x > +a \quad \mathbf{6-37b}$$

Equation 6-26 is the Schrödinger equation for $-a < x < +a$ where $V(x) = 0$, and its general solution, we have already noted, is

$$\psi(x) = A_1 \sin kx + A_2 \cos kx \quad \mathbf{6-38}$$

where A_1 and A_2 are constants. In contrast with the infinite square well, however, we cannot eliminate either the sine or cosine functions by requiring that they be zero at the boundaries of the well because the boundaries are not infinitely high. However, because of their particular symmetry (cosine is *even*, sine is *odd*), we can consider them separately with the symmetric arrangement that was chosen for $V(x)$.

Equations 6-37 and 6-38 are all continuous functions with continuous first derivatives; therefore, the complete $\psi(x)$ and $\psi'(x)$ for the finite square well will also be continuous, as required by the acceptability conditions, if they are also continuous at $x = -a$ and $x = +a$. How do we ensure continuity at those two points? Let us consider first the even solution in the well, $\psi(x) = A_2 \cos kx$.

For $x = +a$:

$$\text{For continuity of } \psi(x) \quad A_2 \cos ka = B_2 e^{-\alpha a} \quad \mathbf{6-39a}$$

$$\text{For continuity of } \psi'(x) \quad -kA_2 \sin ka = -\alpha B_2 e^{-\alpha a} \quad \mathbf{6-39b}$$

For $x = -a$:

$$\text{For continuity of } \psi(x) \quad A_2 \cos(-ka) = A_2 \cos ka = B_1 e^{-\alpha a} \quad \mathbf{6-40a}$$

$$\text{For continuity of } \psi'(x) \quad -kA_2 \sin(-ka) = kA_2 \sin ka = \alpha B_1 e^{-\alpha a} \quad \mathbf{6-40b}$$

We note immediately that $B_1 = B_2$, which the symmetry of the potential might also have suggested to us. Combining Equation 6-39 and 6-40, we have that

$$\frac{A_2}{B_2} = \frac{e^{-\alpha a}}{\cos ka} = \frac{\alpha e^{-\alpha a}}{k \sin ka}$$

or

$$\frac{\sin ka}{\cos ka} = \tan ka = \frac{\alpha}{k} \quad \mathbf{6-41}$$

Substituting values of k and α from above, Equation 6-41 can also be written as

$$\tan\left(\frac{\sqrt{2mE}}{\hbar}a\right) = \sqrt{\frac{V_0 - E}{E}} \quad \mathbf{6-42}$$

Considering the odd solutions in the well, $\psi(x) = A_1 \sin kx$, an equivalent discussion leads to the condition that

$$-\cot ka = \frac{\alpha}{k} \quad \mathbf{6-43}$$

Though tedious to solve analytically, the solutions to these transcendental equations can be readily found graphically. The solutions are those points where the graphs of $\tan ka$ and $-\cot ka$ have values in common with α/k . Figure 6-15 illustrates the

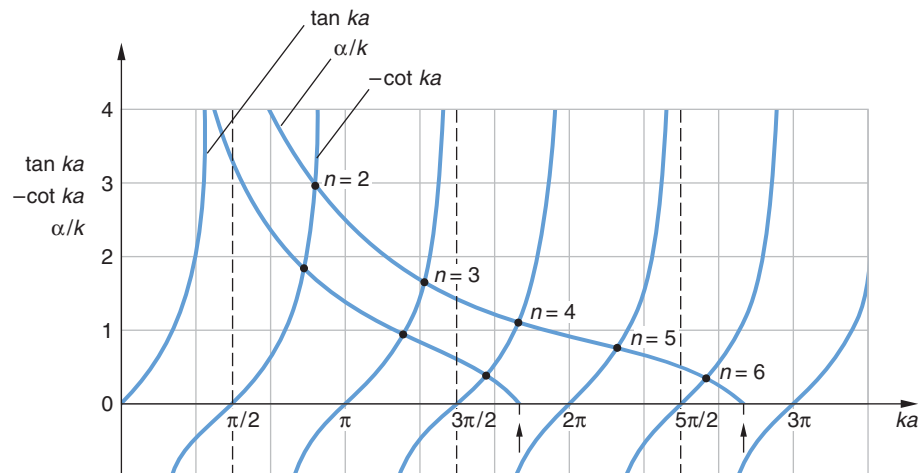


FIGURE 6-15 Graphical solutions of Equations 6-41 and 6-43. Two different curves of α/k are shown, each corresponding to a different value of V_0 . The value of V_0 in each case is given by the value of ka where $\alpha/k = 0$, indicated by the small arrows. For example, the top α/k curve has $\alpha/k = 0$ for $ka = 2.75\pi$, or $(2mV_0)^{1/2} a/\hbar = 2.75\pi$. Allowed values of E are those given by the values of ka at the intersections of the α/k and $\tan ka$ and α/k and $-\cot ka$ curves.

graphical solution. The $\tan ka$ and $-\cot ka$ are both graphed versus ka . They are, of course, just the curves of $\tan \theta$ versus θ and the negative of the curves of $\cos \theta$ versus θ that you first saw in trigonometry. The “angle” ka contains both the particle’s energy E and the half width of the well a ; thus, the ka axis is the energy axis. The value of α/k is also graphed against ka . The point where the α/k curve intersects the ka (energy) axis is the point where $E = V_0$; that is, it corresponds to the top of the well. Some features of the finite square well solutions are worth noting:

1. As the well gets deeper—that is, as the point where $\alpha/k = 0$ moves to the right in Figure 6-15—a new quantized energy and solution appear each time the point where $\alpha/k = 0$ reaches an integer multiple of $\pi/2$. The solution intersections move up the \tan and $-\cot$ curves with $ka \rightarrow n\pi/2$, as for the infinite square well.
2. As the well gets more shallow—that is, as the point where $\alpha/k = 0$ moves to the left in Figure 6-15—a solution is lost out of the top of the well each time that point passes an integer multiple of $\pi/2$. Note that there is always at least one quantized energy in the well no matter how shallow it gets, as long as $V_0 \neq 0$.

Obtaining the values of the constants in the general expressions for $V(x)$ is not particularly useful for our purposes here since we have already found the general form of the wave functions for the finite square well. (See Figure 6-12, noting that $L = 2a$ there.) Using the graphical technique outlined, you can now construct energy-level diagrams for finite square wells.