I. PARTICLE IN THE FINITE POTENTIAL WELL

A. Convenient mathematical definition

It is convenient to define so-called *step function*

$$\theta(x) = 1 \qquad x \geq 0 \tag{1}$$

$$\theta(x) = 0 \qquad x < 0 \tag{2}$$

Finite potential well: $V = 0$ if $a > x > -a$ and $V = V_0$ otherwise can be written as

$$V(x) = V_0\, \theta(|x| - a) \tag{3}$$

1. Method of soluton of stationary Schrödinger equation

Stationary Schrödinger equation

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

We will consider the case $V_0 > E$ (the case $E > V_0$ will be considered later).

$$\begin{aligned} -\tfrac{\hbar^2}{2m}\tfrac{d^2\psi(x)}{dx^2} &= E\psi(x) & a > x > -a \\ -\tfrac{\hbar^2}{2m}\tfrac{d^2\psi(x)}{dx^2} &= -(V_0 - E)\psi(x) & |x| > a \end{aligned} \tag{5}$$

Method of solution: solve in three separate regions and use matching condition: $\phi(x)$ and $\psi'(x)$ must be continuous at $x = \pm a$

Helpful trick: use the symmetry. The potential in the Eq. (5) is symmetric under replacement $x \leftrightarrow -x$ so the solution can be symmetric $\psi(x) = \psi(-x)$ or antisymmetric $\psi(x) = -\psi(-x)$. Let us consider them in turn.

B. Symmetric case

The equation (5) in the region $|x| < a$ can be rewritten as

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} = E\psi(x) \quad \Leftrightarrow \quad \frac{d^2\psi(x)}{dx^2} = -\frac{2mE}{\hbar^2}\psi(x) = -k^2\psi(x) \tag{6}$$

(since $k = \frac{p}{\hbar}$). The general solution is

$$A \cos kx + B \sin kx \tag{7}$$

so the symmetric solution is

$$\psi_1(x) \;=\; A_1 \cos kx, \qquad\qquad (|x| < a) \tag{8}$$

where the constant A_1 is to be determined later.

In the second region $|x| > a$ the equation (5) reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} \;=\; -(V_0 - E)\psi(x) \quad\Leftrightarrow\quad \frac{d^2\psi(x)}{dx^2} \;=\; \frac{2m(V_0 - E)}{\hbar^2}\psi(x) \;=\; \kappa^2\psi(x) \tag{9}$$

where $\kappa = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$. The general solution reads

$$Ae^{\kappa x} + Be^{-\kappa x} \tag{10}$$

so the symmetric solution looks like

$$A_2[e^{-\kappa x}\theta(x-a) + e^{\kappa x}\theta(-x-a)] \tag{11}$$

or

$$A_3[e^{\kappa x}\theta(x-a) + e^{-\kappa x}\theta(-x-a)] \tag{12}$$

The second solution is not acceptable since the function (20) is increasing as $x \pm \infty$ so the integral $\int_{-\infty}^{\infty} |\psi(x)|^2$ diverges and cannot be normalized.

Thus, we obtain

$$\psi_{\rm sym}(x) \;=\; A_1(\cos kx)\theta(a - |x|) + A_2[e^{-\kappa x}\theta(x-a) + e^{\kappa x}\theta(-x-a)] \tag{13}$$

Now we will use two conditions, i.e. that the function (21) and its derivative are continuous at $x = a$ (by symmetry, these statements will be also true at $x = -a$).

$$\left.\begin{array}{ccc} \psi_{\rm sym}(x) & \stackrel{x\to a-0}{\equiv} & A_1 \cos ka \\ \psi_{\rm sym}(x) & \stackrel{x\to a+0}{\equiv} & A_2 e^{-\kappa a} \end{array}\right\} \;\Rightarrow\; A_2 \;=\; A_1(\cos ka)e^{\kappa a} \tag{14}$$

Here we used convenient mathematical notation $x \to a \pm 0 \equiv x = \lim_{\epsilon\to 0} a \pm \epsilon$ (x approaches a from the left or from the right). Similarly,

$$\left.\begin{array}{ccc} \psi'_{\rm sym}(x) & \stackrel{x\to a-0}{\equiv} & -A_1 k \sin ka \\ \psi'_{\rm sym}(x) & \stackrel{x\to a+0}{\equiv} & -A_2 \kappa e^{-\kappa a} \end{array}\right\} \;\Rightarrow\; A_2 \;=\; A_1(\sin ka)\frac{k}{\kappa}e^{\kappa a} \tag{15}$$

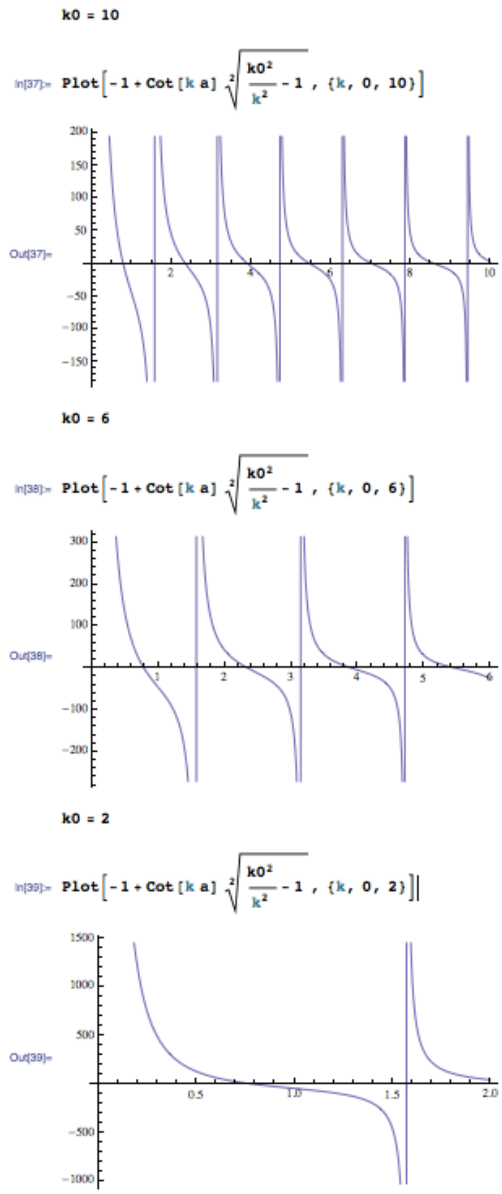
We get the equation

$$A_1(\sin ka)\frac{k}{\kappa}e^{\kappa a} \;=\; A_1(\cos ka)e^{\kappa a} \qquad \Leftrightarrow \qquad \cot ka \;=\; \frac{k}{\kappa} \;=\; \frac{k}{\sqrt{k_0^2 - k^2}} \tag{16}$$

where $k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$. Thus, we have a transcendental equation for k

$$\cot ka\sqrt{\frac{k_0^2}{k^2} - 1} - 1 \;=\; 0 \tag{17}$$

This equation may have a finite number of solutions or no solutions at all if k_0 ($\Leftrightarrow V_0$) is smaller than some critica



The constant A_1 is obtained from the normalization condition $\int_{-\infty}^{\infty} |\psi(x)|^2 \;=\; 1$

C. Antisymmetric case

The antisymmetric solution of Eq. (6) is

$$\psi_1(x) \;=\; B_1 \sin kx, \qquad (|x| < a) \tag{18}$$

where the constant B_1 is to be determined later.

The antisymmetric solution of Eq. (6) at $|x| > a$ looks like

$$B_2[e^{-\kappa x}\theta(x-a) - e^{\kappa x}\theta(-x-a)] \tag{19}$$

or

$$B_3[e^{\kappa x}\theta(x-a) - e^{-\kappa x}\theta(-x-a)] \tag{20}$$

Again, the latter solution is not acceptable since the integral $\int_{-\infty}^{\infty} |\psi(x)|^2$ diverges and cannot be normalized.

Thus, the antisymmetric solutions have the form

$$\psi_{\text{asym}}(x) \;=\; B_1(\sin kx)\theta(a-|x|) + B_2[e^{-\kappa x}\theta(x-a) - e^{\kappa x}\theta(-x-a)] \tag{21}$$

The two matching conditions are

$$\left.\begin{array}{lcl} \psi_{\text{asym}}(x) & \overset{x\to a-0}{=} & B_1 \sin ka \\ \psi_{\text{asym}}(x) & \overset{x\to a+0}{=} & B_2 e^{-\kappa a} \end{array}\right\} \;\Rightarrow\; B_2 \;=\; B_1(\sin ka)e^{\kappa a} \tag{22}$$

and

$$\left.\begin{array}{lcl} \psi'_{\text{asym}}(x) & \overset{x\to a-0}{=} & B_1 k \cos ka \\ \psi'_{\text{asym}}(x) & \overset{x\to a+0}{=} & -B_2 \kappa e^{-\kappa a} \end{array}\right\} \;\Rightarrow\; B_2 \;=\; -\,B_1(\cos ka)\frac{k}{\kappa}e^{\kappa a} \tag{23}$$

We get the equation

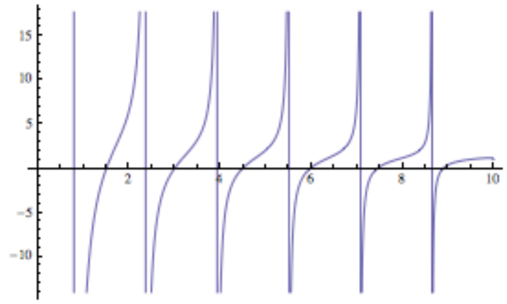
$$B_1(\cos ka)\frac{k}{\kappa}e^{\kappa a} \;=\; -\,B_1(\sin ka)e^{\kappa a} \quad\Leftrightarrow\quad -\tan ka \;=\; \frac{k}{\kappa} \;=\; \frac{k}{\sqrt{k_0^2 - k^2}} \tag{24}$$

or

$$1 + (\tan ka)\sqrt{\frac{k_0^2}{k^2} - 1} \;=\; 0 \tag{25}$$

In[43]:= $\text{Plot}\left[1+\text{Tan}[k\,a]\sqrt{\frac{k0^2}{k^2}-1},\ \{k,0,10\}\right]$

Out[43]=

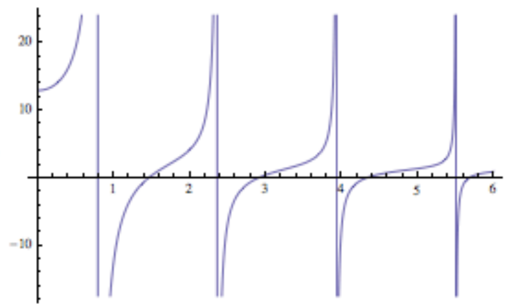


In[44]:= k0 = 6

Out[44]= 6

In[45]:= $\text{Plot}\left[1+\text{Tan}[k\,a]\sqrt{\frac{k0^2}{k^2}-1},\ \{k,0,6\}\right]$

Out[45]=

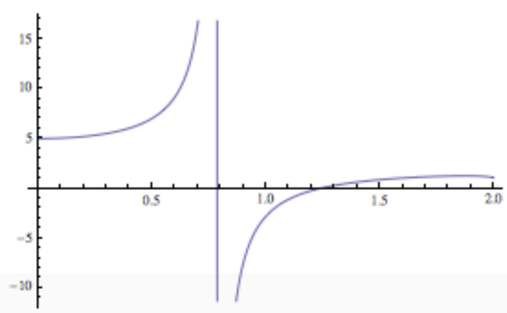


In[46]:= k0 = 2

Out[46]= 2

In[47]:= $\text{Plot}\left[1+\text{Tan}[k\,a]\sqrt{\frac{k0^2}{k^2}-1},\ \{k,0,2\}\right]$

Out[47]=



Again, the constant B_1 is obtained from the normalization condition $\int_{-\infty}^{\infty} |\psi(x)|^2 \;=\; 1$

The form of the obtained functions ϕ_{sym} and ψ_{asym} is shown in the following diagram

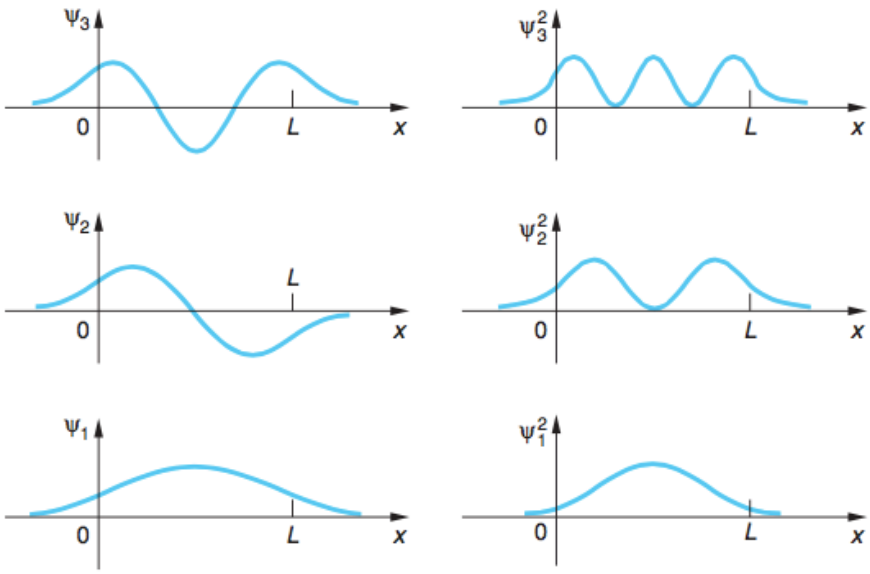


Figure 6-12 Wave functions $\psi_n(x)$ and probability distributions $\psi_n^2(x)$ for $n = 1$, 2, and 3 for the finite square well. Compare these with Figure 6-4 for the infinite square well, where the wave functions are zero at $x = 0$ and $x = L$. The wavelengths are slightly longer than the corresponding ones for the infinite well, so the allowed energies are somewhat smaller.