



The centered box has wavefunctions that vary between cosine (the ground state and subsequent higher states) and sine, and are in a region with no potential energy. Thus, they have the form (for example), $\psi_{II} = A \cdot \cos(k_2 \cdot x)$, where $k_2 = \sqrt{2mE}/\hbar$. The wavefunction in Region III is $\psi_{III} = B \cdot \exp(i \cdot k_1 \cdot x)$, however, since we are only interested in wavefunctions with energies less than V , $k_1 = i\sqrt{2m(V - E)}/\hbar$. As a result, $\psi_{III} = B \cdot \exp(-k_1 \cdot x)$.

Note that Region I is basically identical to Region III, and thus $\psi_I = B \cdot \exp(k_1 \cdot x)$, where the argument of the exponential is positive because the x 's are negative in Region I.

For the ground \sim cosine state, starting with the stipulation of smooth and continuous:

Region II&III: Wavefunctions are equal: $A \cdot \cos\left(k_2 \left(\frac{L}{2}\right)\right) = B \cdot \exp\left(-k_1 \left(\frac{L}{2}\right)\right)$

Region II&III: Derivatives are equal: $-A \cdot k_2 \cdot \sin\left(k_2 \left(\frac{L}{2}\right)\right) = -B \cdot k_1 \cdot \exp\left(-k_1 \left(\frac{L}{2}\right)\right)$

Divide the two:
$$\frac{A \cdot \cos\left(k_2 \left(\frac{L}{2}\right)\right)}{-A \cdot k_2 \cdot \sin\left(k_2 \left(\frac{L}{2}\right)\right)} = \frac{B \cdot \exp\left(-k_1 \left(\frac{L}{2}\right)\right)}{-B \cdot k_1 \cdot \exp\left(-k_1 \left(\frac{L}{2}\right)\right)}$$

Therefore: $\frac{-1}{k_2} \cotan\left(k_2 \left(\frac{L}{2}\right)\right) = \frac{1}{k_1}$; insert the definitions of k 's:

$$\cotan\left(\frac{\sqrt{2mE}}{\hbar} \left(\frac{L}{2}\right)\right) = \frac{\sqrt{2mE}/\hbar}{\sqrt{2m(V-E)}/\hbar} = \frac{\sqrt{E}}{\sqrt{(V-E)}} \quad (1)$$

For the first excited ~sine state(s), starting with the stipulation of smooth and continuous:

Region II&III: Wavefunctions are equal: $A \cdot \sin\left(k_2 \left(\frac{L}{2}\right)\right) = B \cdot \exp\left(-k_1 \left(\frac{L}{2}\right)\right)$

Region II&III: Derivatives are equal: $A \cdot k_2 \cdot \cos\left(k_2 \left(\frac{L}{2}\right)\right) = -B \cdot k_1 \cdot \exp\left(-k_1 \left(\frac{L}{2}\right)\right)$

Divide the two:
$$\frac{A \cdot \sin\left(k_2 \left(\frac{L}{2}\right)\right)}{A \cdot k_2 \cdot \cos\left(k_2 \left(\frac{L}{2}\right)\right)} = \frac{B \cdot \exp\left(-k_1 \left(\frac{L}{2}\right)\right)}{-B \cdot k_1 \cdot \exp\left(-k_1 \left(\frac{L}{2}\right)\right)}$$

Therefore: $\frac{1}{k_2} \tan\left(k_2 \left(\frac{L}{2}\right)\right) = \frac{-1}{k_1}$; insert the definitions of k's:

$$\tan\left(\frac{\sqrt{2mE}}{\hbar} \left(\frac{L}{2}\right)\right) = \frac{-\sqrt{2mE}/\hbar}{\sqrt{2m(V-E)}/\hbar} = \frac{-\sqrt{E}}{\sqrt{(V-E)}} \quad (2)$$

The same operations can be performed between Regions I&II, but these lead to the exact same results in terms of eqs. (1) & (2).

Now we can define energy by finding the E that satisfies equations (1) and (2), which has to be done using some computer program like Matlab or Origin.