Bound and Unbound States of a Particle in a Finite Potential Well in One Dimension

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A one dimensional Potential of the form:

$$V(x) = \begin{cases} V_0, & \text{if } |x| \geq \frac{L}{2} \\ 0, & |x| < \frac{L}{2} \end{cases}$$

where V_0 is a positive constant is said to be a Finite Square Well.
A Finite Square Well admits Stationary States that can be either Bound ($E < V_0$) or Free ($E \geq V_0$), unlike the Infinite Square Well, which admits only Bound States.
On writing the Time Independent Schrödinger Equation for the Bound States, we get:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi, \text{ for } x < -\frac{L}{2} \tag{1}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi, \text{ for } -\frac{L}{2} < x < \frac{L}{2} \tag{2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi, \text{ for } x > \frac{L}{2} \tag{3}$$

Clearly, we must solve the Schrödinger Equation separately for these three regions of space and apply the Boundary Conditions at $x = \pm\frac{L}{2}$ to get the overall Wave Function.
The boundary conditions to be applied are:

$$\psi(-\frac{L}{2}^-) = \psi(-\frac{L}{2}^+) \tag{4}$$

$$\psi(\frac{L}{2}^-) = \psi(\frac{L}{2}^+) \tag{5}$$

These two conditions arise from the requirement that the Wave Function be continuous.

$$\frac{d\psi}{dx}(-\frac{L}{2}^-) = \frac{d\psi}{dx}(-\frac{L}{2}^+) \tag{6}$$

$$\frac{d\psi}{dx}(\frac{L}{2}^-) = \frac{d\psi}{dx}(\frac{L}{2}^+) \tag{7}$$

These two conditions arise from the requirement that the Wave Function be differentiable at all points (since the potential $V(x)$ is finite at all points). The other conditions that we need to impose are $\psi(\pm\infty) \to 0$. This is so that the Wave Function (or at least Linear Combinations containing it) is Normalizable.
On solving the Schrödinger Equation and imposing these conditions, we get the following condition on the Energies of the Bound States[1].

$$\sqrt{C^2 - v^2} = v\tan(v) \tag{8}$$

or

$$\sqrt{C^2 - v^2} = -v\cot(v) \tag{9}$$

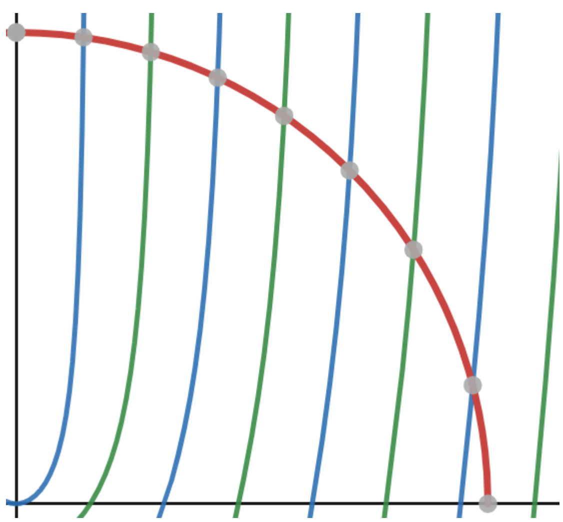
where

$$C^2 = \frac{mL^2V_0}{2\hbar^2} \tag{10}$$

and

$$v = \frac{L}{2\hbar}\sqrt{2mE} \tag{11}$$

Unfortunately, these equations are transcendental equations which do not yield any analytic solutions. Yet, we can still get information about the solutions by graphing these equations.



In this Illustration, the red curve represents the graph of $\sqrt{C^2 - v^2}$, the blue curve represents the graph of $v\tan(v)$ and the green curve represents the graph of $-v\cot(v)$. The points at which the red curve intersects the other two curves represent the allowed Energies of the Stationary States.

[1] It is guaranteed that for any stationary state, $E > V_{min}$, where V_{min} is the minimum value of the Potential. Since for a Finite Square Well, $V_{min} = 0$, $E > 0$ for all the Stationary States, including Free and Bound States.

Note that, at $v = 0$, $v \tan(v) = 0$, whereas $\sqrt{C^2 - v^2} = C > 0$. However, as $v \to \frac{\pi}{2}$, $\sqrt{C^2 - v^2}$ remains finite, whereas $v \tan(v) \to +\infty$. Since these functions are continuous, by the Intermediate Value Theorem, they intersect at atleast one point between 0 and $\frac{\pi}{2}$. This can be clearly seen from the graph also.
This means that, **no matter the value of C (the value of V_0), no matter how shallow or deep or wide the well is, there will always exist at least one Bound state.**
The number of Bound States, however, depends on the Parameters of the well (L and V_0). From the graph, it is clear that the number of solutions is given by $1 + [\frac{2C}{\pi}]$, where $[x]$ represents the greatest integer less than or equal to x.
Therefore, if there are k bound states (using $C = \sqrt{\frac{mL^2V_0}{2\hbar^2}}$, we get:

$$1 + [\frac{2}{\pi}\sqrt{\frac{mL^2V_0}{2\hbar^2}}] = k \tag{12}$$

Solving this equation, we get:

$$\boxed{\frac{(k-1)^2\pi^2\hbar^2}{2mL^2} \leq V_0 < \frac{k^2\pi^2\hbar^2}{2mL^2}} \tag{13}$$

Notice, that these limits on V_0 are exactly the Allowed Energies of the Infinite Square Well! ($E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$)
Therefore, if there are two bound states, then:

$$\boxed{\frac{\pi^2\hbar^2}{2mL^2} \leq V_0 < \frac{2\pi^2\hbar^2}{mL^2}} \tag{14}$$

and if there are three bound states, then:

$$\boxed{\frac{2\pi^2\hbar^2}{2mL^2} \leq V_0 < \frac{9\pi^2\hbar^2}{2mL^2}} \tag{15}$$