Semi-infinite square well.

1) Wave function in region I
   In region I \( x < 0 \) & \( V(x) = \infty \)
   So \( \psi_1(x) = 0 \).

2) Possible range for bound state energy \( E \)?
   - \( E > 0 \) \( \Rightarrow \) unbound state.
   - \( E < -V_0 \) is excluded.
   Bound states have energy \( E \) such that \( -V_0 < E < 0 \).

3) Schrödinger equation in region II
   \[
   -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} - V_0 \psi = E \psi \Rightarrow \frac{\partial^2 \psi}{\partial x^2} = -\frac{2m(E + V_0)}{\hbar^2} \psi
   \]
   or \( \frac{\partial^2 \psi}{\partial x^2} = -k^2 \psi \) with \( k = \sqrt{\frac{2m(E + V_0)}{\hbar^2}} \).

4) General form of the solution in region II:
   \( \psi_\Pi = A \sin kx + B \cos kx \)
   Since \( V(x) = \infty \) we must have \( \psi_\Pi(0) = 0 \) & \( B = 0 \) so
   \( \psi_\Pi(x) = A \sin kx \).

5) Schrödinger equation in region III
   \[
   -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} = E \psi \quad \text{or} \quad \frac{\partial^2 \psi}{\partial x^2} = -\frac{2mE}{\hbar^2} \psi = \alpha^2 \psi \text{ with } \alpha = \sqrt{\frac{2mE}{\hbar^2}} \]
6) General form of the solution in region III.
\[ \psi_\text{III}(x) = C e^{-\alpha x} + D e^{\alpha x}. \]

We need \[ \int_{-\infty}^{+\infty} \psi_\text{II}(x) \psi_\text{III}(x) \, dx = 1 \]
\[ \lim_{x \to +\infty} \psi_\text{II}(x) = 0 \quad \text{and} \quad \psi_\text{III}(x) = 0 \] as \( x \to 0 \).

So \[ \psi_\text{III}(x) = C e^{-\alpha x}. \]

7) Boundary conditions in \( x = a \).
Both \( \psi(x) \) and \( \frac{d\psi}{dx}(x) \) must be continuous at \( x = a \).

\[ \psi_\text{II}(a) = \psi_\text{III}(a) \quad \text{or} \quad A \sin k a = C e^{-\alpha a}. \]

\[ \frac{d\psi_\text{II}}{dx}(a) = \frac{d\psi_\text{III}}{dx}(a) \quad \text{or} \quad k A \cos k a = -\alpha C e^{-\alpha a}. \]

8) Energy quantization from the boundary conditions.
Taking the ratio \( \frac{E}{\theta^2} \), we get \( \cot k a = -\frac{\alpha}{k} \) or

\[ \cot \left[ \sqrt{\frac{2m a^2 (E + V_0)}{\hbar^2}} \right] = -\sqrt{\frac{-E}{E + V_0}}. \]

With \( \theta = k \cdot a \) and \( \theta_0 = \sqrt{2m a^2 V_0/\hbar^2} \), this is equivalent to

\[ \cot \theta = -\sqrt{-\frac{\theta_0^2 - E^2}{\theta_0^2}}. \]

9) Graphical solution for \( \theta_0 = 1 \) and \( \theta_0 = 5/2 \).
We can use the abacus used in class when solving the first square well.
Solutions correspond to intersections between \( \sqrt{\theta_0^2 - E^2/\theta_0^2} \) and \( \cot \theta \).

(The \( \tan \theta \) curves should be ignored as they correspond to even solutions.)

* For \( \theta_0 = 1 \) there are two intersections, so there are two bound states.
* For \( \theta_0 = 5/2 \) there is only one intersection, so \( \theta \approx 2.125 \) which we round down to \( \theta = 2 \).
10) Expansion & representation of \( \psi \) in the case \( E_0 = 5/2 \).

- \( \psi_\Pi(x) = A \sin kx = A \sin \frac{\theta_0}{a} \cdot \frac{2x}{a} \) (as we found \( \theta_0 = 2 \))

\[ \psi_\Pi(x) = C e^{-\frac{ax}{\alpha}} = C e^{-\sqrt{\frac{\theta_0^2 - \theta^2}{a^2}}} = C e^{-\frac{3\theta}{2a}}. \]

- The point where the probability density to find the particle is the highest is such that \( \frac{2\alpha}{a} = \frac{\pi}{2} \) or \( x = \frac{\pi}{4} a \).

- Adding the squared boundary condition equations 1 & 2 in 7)

\[ A^2 = C^2 e^{-2\alpha a} \left( 1 + \frac{\alpha^2}{\kappa^2} \right) \]

- The normalization condition is \( \int_{-\infty}^{+\infty} \psi_* \psi(x) dx = 1 \) which gives

\[ \int_{0}^{a} \psi_\Pi^2(x) dx + \int_{a}^{\infty} \psi_\Pi^2(x) dx = 1 \]

\[ A^2 \left[ \int_{0}^{a} \sin^2 \frac{\theta_0 x}{a} dx + e^{2\alpha a} \left( 1 + \frac{\alpha^2}{\kappa^2} \right) \int_{a}^{\infty} e^{-\sqrt{\frac{\theta_0^2 - \theta^2}{a^2}}} \frac{x}{a} dx \right] = 1. \]

The integrals are easy to calculate & so we could easily find \( A \) as well.

It is just not very interesting to do.

11) Compare the fundamental state with \( E_0 = 5/2 \) to the first excited state of the \( L = 2a \) finite square well with the same \( E_0 \).

The energy and wave function we obtained is just the same as the first excited state of the twice as large finite square well.

The semi infinite square well simply accepts all the odd wave function states of the twice as large finite square well as they satisfy the condition \( \psi(0) = 0 \) and the same boundary condition \( \psi(a) = 0 \).
No solution

$\text{To be ignored (Finite square will even rotate)}$

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2.125

Just one solution.