**WKB Approximation for an Infinite Square Well**

- $\hbar c := 197$  
  h-bar times speed of light in units of eV*nm

- $mc^2 := 511000$  
  electron rest energy in eV

- $a := 10$  
  size of the infinite square well in nm

- $b := \frac{1}{a} = 0.1$  
  parameter for the strength of the potential energy function inside the well

- $V(x) := \begin{cases} \frac{a}{2}, & x \leq \frac{a}{2} \\ 0, & \text{otherwise} \end{cases}$  
  Potential energy function inside of the well. See problem 8.1.

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**Potential Energy Function**

The potential energy goes to infinite at both boundaries.

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**Do the WKB integral numerically:**

$$f(E) := \frac{1}{\hbar c} \int_0^a \sqrt{2mc^2(E - V(x))} \, dx$$

Integral of the WKB phase across the entire well.

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**Integral of the WKB phase across the well**

The boundary condition at $x=a$ is met if the phase integral equals an integer times pi. See Eqn. 8.16.

Note that $E$ must be greater than the peak of $V(x)$. That is $E > b^2a/2$. Only values satisfying that condition are plotted.
**Find and plot the nth WKB solution**

\[ n := 6 \quad \text{Choose here what solution to plot.} \]

\[ E := 0.05 \quad \text{Just an initial guess for the energy.} \]

\[ E_{\text{wkb}} := \text{root}(f(E) - n \pi, E) \quad \text{Using MathCad to solve for the energy.} \]

\[ E_{\text{wkb}} = 0.19 \]

\[ \varphi(x) := \frac{1}{\hbar c} \left[ \int_{0}^{x} \sqrt{2mc^2(E_{\text{wkb}} - V(x))} \, dx \right] \]

\[ \psi(x) := \frac{1}{\sqrt{2mc^2(E_{\text{wkb}} - V(x))}} \cdot \sin(\varphi(x)) \]

The WKB wave function, un-normalized.

\[ A_{\text{wkb}} := \int_{0}^{a} (|\psi(x)|^2) \, dx \quad A_{\text{wkb}} = 3.981 \times 10^{-5} \]

Calculate the normalization factor.

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**WKB Solution and the Potential Energy Function**

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**First-order perturbation theory solution for the energy eigenvalue**

\[ \psi_0(x) := \frac{2}{a} \cdot \sin \left( \frac{n \cdot \pi \cdot x}{a} \right) \]

\[ E_0 := \frac{n^2 \cdot \pi^2 \cdot \hbar c^2}{2mc^2 \cdot a^2} \quad E_0 = 0.135 \]

\[ E_1 := \int_{0}^{a} (|\psi_0(x)|^2) \cdot V(x) \, dx \quad E_1 = 0.05 \]

\[ E_p := E_0 + E_1 \quad E_p = 0.185 \quad E_{\text{wkb}} = 0.19 \]

\[ E_0 + \frac{b}{2} + \frac{b^2}{16 \cdot E_0} = 0.19 \quad \text{Analytic solution} \]
WKB Approximation for an Infinite Square Well

\( hbarc := 197 \)  
\( h-bar \) times speed of light in units of eV*nm

\( mc^2 := 511000 \)  
electron rest energy in eV

\( a := 10 \)  
size of the infinite square well in nm

\( b := \frac{0.1}{a} = 0.01 \)  
parameter for the strength of the potential energy function inside the well

\[ V(x) := \begin{cases} x \leq \frac{a}{2}, & b \cdot x, b \cdot (a - x) \end{cases} \]

Potential energy function inside of the well

Do the WKB integral numerically:

\[ f(E) := \frac{1}{hbarc} \left[ \int_0^a \sqrt{2mc^2 \cdot (E - V(x))} \, dx \right] \]

Integral of the WKB phase across the entire well. This could be done analytically, but still one would not be able then to solve for the energies in closed form.

The potential energy goes to infinite at both boundaries

Integral of the WKB phase across the well

The boundary condition at \( x=a \) is met if the phase integral equals an integer times pi. See Eqn. 8.16.

Note that \( E \) must be greater than the peak of \( V(x) \). That is \( E > b^*a/2 \). Only values satisfying that condition are plotted.
Find and plot the nth WKB solution

\( n := 4 \) Choose here what solution to plot.

\( E := 0.05 \) Just an initial guess for the energy.

\( E_{\text{wkb}} := \text{root}(f(E) - n \pi, E) \) Using MathCad to solve for the energy.

\( E_{\text{wkb}} = 0.086 \)

\( \varphi(x) := \frac{1}{\hbar c} \int_0^x \sqrt{2mc^2(E_{\text{wkb}} - V(x))} \, dx \)

\( \psi(x) := \frac{1}{\sqrt{2mc^2(E_{\text{wkb}} - V(x))}} \sin(\varphi(x)) \) The WKB wave function, un-normalized.

\( A_{\text{wkb}} := \int_0^a |\psi(x)|^2 \, dx \quad A_{\text{wkb}} = 8.313 \times 10^{-5} \) Calculate the normalization factor.

First-order perturbation theory solution for the energy eigenvalue

\( \psi_0(x) := \frac{2}{a} \cdot \sin \left( \frac{n \pi}{a} \cdot x \right) \quad E_0 := \frac{n^2 \cdot \pi^2 \cdot \hbar c^2}{2mc^2 a^2} \quad E_0 = 0.06 \) Note that this generally doesn't work very well!

\( E_1 := \int_0^a (|\psi(x)|^2 \cdot V(x)) \, dx \quad E_1 = 2.272 \times 10^{-6} \)

\( E_p := E_0 + E_1 \quad E_p = 0.06 \quad E_{\text{wkb}} = 0.086 \)
**Find a solution by numerical integration of the PDE ("shooting method")**

\[ E_s := E_{\text{wkb}} \]

Use the WKB energy as a "guess" for the numerical integration

Given

\[ \frac{d^2}{dx^2} \psi(x) + \frac{2mc^2}{\hbar c^2} (E_s - V(x)) \psi(x) = 0 \]

Time independent S.E. in 1D

Conditions for starting the integration. The potential is even, so the ground state solution must be even and therefore have zero derivative at the origin. The first excited state is odd, so in that case the wave function is zero at the origin.

\[ \psi_s\left(\frac{a}{2}\right) = 0 \quad \psi_s\left(\frac{a}{2}\right) = 1 \]

Solve the differential equation numerically. By default the Adams/BDF algorithm is used, but by right clicking on Odesolve you can choose other methods, such as 4th order Runge-Kutta with fixed or adaptive step size.

\[ A_s := 2 \int_0^a \left( |\psi(x)| \right)^2 dx \]

Calculate a normalization factor.

\[ A_s = 4.036 \]

Comparing the WKB solution with numerical integration
WKB Approximation for an Infinite Square Well

\[ \hbar c = 197 \text{ eV*nm} \]

\[ mc^2 = 511000 \text{ eV} \]

\[ a = 10 \text{ nm} \]

\[ b = \frac{0.01}{a} = 1 \times 10^{-3} \text{ parameter for the strength of the potential energy function inside the well} \]

\[ V(x) := -b \left( x - \frac{a}{2} \right)^2 \]

Potential energy function inside of the well

Do the WKB integral numerically:

\[ f(E) := \frac{1}{\hbar c} \left[ \int_0^a \sqrt{2mc^2(E - V(x))} \, dx \right] \]

Integral of the WKB phase across the entire well

The boundary condition at \( x=a \) is met if the phase integral equals an integer times \( \pi \). See Eqn. 8.16.

Note that \( E \) must be greater than the peak of \( V(x) \). That is \( E > b*a/2 \). Only values satisfying that condition are plotted.
**Find and plot the nth WKB solution**

\[ n := 3 \quad \text{Choose here what solution to plot.} \]

\[ E := 0.05 \quad \text{This is just an initial guess at the energy. The value is not critical.} \]

\[ E_{\text{wkb}} := \text{root}(f(E) - n \pi, E) \quad \text{Using MathCad to solve for the energy.} \]

\[ E_{\text{wkb}} = 0.026 \]

\[ \varphi(x) := \frac{1}{\hbar c} \int_{0}^{x} \sqrt{2}mc2(E_{\text{wkb}} - V(x)) \, dx \]

\[ \psi(x) := \frac{1}{\sqrt{2mc2(E_{\text{wkb}} - V(x))}} \cdot \sin(\varphi(x)) \quad \text{The WKB wave function, un-normalized.} \]

\[ A_{\text{wkb}} := \int_{0}^{a} \left( |\psi(x)| \right)^2 \, dx \quad A_{\text{wkb}} = 1.512 \times 10^{-4} \quad \text{Calculate the normalization factor.} \]

**WKB Solution and the Potential Energy Function**

**First-order perturbation theory solution**

\[ \psi_0(x) := \frac{2}{a} \cdot \sin \left( \frac{n \pi}{a} \cdot x \right) \]

\[ E_0 := \frac{n^2 \cdot \pi^2 \cdot \hbar c^2}{2mc^2 \cdot a^2} \quad E_0 = 0.034 \quad \text{Note that this generally doesn't work very well!} \]

\[ E_1 := \int_{0}^{a} (|\psi(x)|)^2 \cdot V(x) \, dx \quad E_1 = -1.013 \times 10^{-6} \]

\[ E_p := E_0 + E_1 \quad E_p = 0.034 \quad E_{\text{wkb}} = 0.026 \]
**Find a solution by numerical integration of the PDE ("shooting method")**

\[ E_s := E_{wkb} \]

Use the WKB energy as a "guess" for the numerical integration

Given

\[
\frac{d^2}{dx^2} \psi_s(x) + \frac{2mc^2}{\hbar c^2} \left( E_s - V(x) \right) \psi_s(x) = 0
\]

Time independent S.E. in 1D

Conditions for starting the integration. The potential is even, so the ground state solution must be even and therefore have zero derivative at the origin. The first excited state is odd, so in that case the wave function is zero at the origin.

\[
\psi_s \left( \frac{a}{2} \right) = -1 \quad \psi_s \left( \frac{a}{2} \right) = 0
\]

\[ \psi_s := \text{Odesolve}(x, a) \]

Solve the differential equation numerically. By default the Adams/BDF algorithm is used, but by right clicking on Odesolve you can choose other methods, such as 4th order Runge-Kutta with fixed or adaptive step size.

\[
A_s := 2 \int_{a/2}^a \left( \frac{\psi_s(x)}{\sqrt{A_s}} \right)^2 dx
\]

\[ A_s = 4.425 \]

Calculate a normalization factor.

Comparing the WKB solution with numerical integration