Finite Square Well Potential

- For $V=\text{finite “outside” the well. Solutions to S.E. inside the well the same. Have different outside. The boundary conditions (wavefunction and its derivative continuous) give quantization for } E<V_0$
- longer wavelength, lower Energy. Finite number of energy levels
- Outside:

$$k_1 = \frac{\sqrt{2mE}}{\hbar}$$

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

$$E > V \Rightarrow \sin k_0 x, \cos k_0 \text{ and}$$

$$\frac{(\hbar k_0)^2}{2m} = (E - V)\ k_0 = \frac{\sqrt{2m(E-V)}}{\hbar}$$

$$E < V \Rightarrow e^{\pm k_2 x}\ k_2 = \frac{\sqrt{2m(V-E)}}{\hbar}$$
Boundary Condition

• Want wavefunction and its derivative to be continuous
• Often a symmetry such that solution at +a also gives one at -a
• Often can do the ratio (see book) and that can simplify the algebra

\[
\psi_-(boundary) = \psi_+(boundary)
\]

\[
\frac{\partial \psi_-(boundary)}{\partial x} = \frac{\partial \psi_+(boundary)}{\partial x}
\]

\[
\frac{1}{\psi_-} \frac{\partial \psi_-(boundary)}{\partial x} = \frac{1}{\psi_+} \frac{\partial \psi_+(boundary)}{\partial x}
\]
Finite Square Well Potential

inside : $\psi(x) = A \sin k_1 x + B \cos k_1 x$

$x < \frac{a}{2} : \psi(x) = Ce^{k_2 x} + De^{-k_2 x}$

$x > \frac{a}{2} : \psi(x) = Fe^{k_2 x} + Ge^{-k_2 x}$

as $\psi \to 0$ as $x \to \pm \infty \implies D, F = 0$

Equate wave function at boundaries

$$A \sin \frac{k_1 a}{2} + B \cos \frac{k_1 a}{2} = Ge^{-k_2 a/2}$$

$$-A \sin \frac{k_1 a}{2} + B \cos \frac{k_1 a}{2} = Ce^{-k_2 a/2}$$

And derivative

$$Ak_1 \cos \frac{k_1 a}{2} + Bk_1 \sin \frac{k_1 a}{2} = Ck_2 e^{-k_2 a/2}$$

$$Ak_1 \cos \frac{k_1 a}{2} - Bk_1 \sin \frac{k_1 a}{2} = -Gk_2 e^{-k_2 a/2}$$
Finite Square Well Potential

E+R does algebra. 2 classes. Solve numerically

\[ I : \psi(x) = A \sin k_1 x \text{ in well} \]

\[ \psi(x) = A \sin\left(\frac{k_1 a}{2}\right)e^{k_2 a/2}e^{-k_2 x} \quad x > \frac{a}{2} \]

\[ k_1 \cot \frac{k_1 a}{2} = -k_2 \text{ quantization} \]

\[ II : \psi(x) = B \cos k_1 x \text{ in well} \]

\[ \psi(x) = B \cos\left(\frac{k_1 a}{2}\right)e^{k_2 a/2}e^{-k_2 x} \quad x > \frac{a}{2} \]

\[ k_1 \tan \frac{k_1 a}{2} = k_2 \text{ quantization} \]

\[ k_1 \text{ and } k_2 \text{ both depend on } E. \text{ Quantization sets allowed energy levels} \]

\[ E_n \approx \frac{\hbar^2 \pi^2 n^2}{2ma^2} \leq V_0 \]
Finite Square Well Potential

Number of bound states is finite. Calculate assuming “infinite” well energies. Get \( n \). Add 1

\[
E_n \approx \frac{\hbar^2 \pi^2 n^2}{2ma^2} \leq V_0 \implies n^2 \leq \frac{2ma^2 V_0}{\hbar^2 \pi^2}
\]

Electron \( V=100 \text{ eV} \)
width=0.2 nm

\[
n^2 \leq \frac{2 \times 51 \text{ MeV} \times (0.2 \text{ nm})^2 \times 100 \text{ eV}}{(197 \text{ ev} \times \text{ nm})^2 \times (3.14)^2} = 10.7
\]

\[\implies N = 4 (\text{number of levels})\]

Deuteron p-n bound state. Binding energy 2.2 MeV
radius = 2.1 F (really need 3D S.E………..)

\[
n^2 \leq \frac{2 \times 940 \text{ MeV} \times (2.1F)^2 \times 2.2 \text{ MeV}}{(197 \text{ MeV} \times F)^2 \times (3.14)^2} = 0.1
\]

\[\implies N = 1 \text{ only 1 bound state}\]
Finite Square Well Potential

Can do an approximation by guessing at the penetration distance into the “forbidden” region. Use to estimate wavelength

\[ \delta = \frac{1}{b} = \frac{\hbar}{\sqrt{2m(V-E)}} \quad \psi \approx e^{-bx} \]

\[ E_n \cong \frac{n^2 \pi^2 \hbar^2}{2m(a+2\delta)^2} \text{ slightly wider} \]

Electron V=100 eV width=0.2 nm

\[ \delta = \frac{197 eV nm}{\sqrt{2*.5 MeV*100 eV}} = .02 nm \]

\[ E_1 \cong \frac{\pi^2 (197 eV nm)^2}{2.5 MeV (.2 nm+.04 nm)^2} = 5.5 eV \]

Electron V=100 eV width=0.2 nm
Delta Function Potential

- \( \delta \)-function can be used to describe potential.

\[
\delta(0) = \infty \quad \delta(x \neq 0) = 0
\]

\[
\int \delta(x) \, dx = 1 \quad \text{if} \quad 0 \quad \text{in range}
\]

- Assume attractive potential \( V \) and \( E < V \) bound state. Potential has strength \( \lambda/a \). Rewrite Schrödinger Eq

\[
V(x) = 0 \quad \text{except} \quad x = 0 \Rightarrow -\alpha" \infty"
\]

or \( V(x) = -\frac{\hbar^2 \lambda}{2ma} \delta(0) \)

S.E. \( \Rightarrow \frac{d^2 u(x)}{dx^2} + \frac{\lambda}{a} \delta(0) u(x) = k^2 u(x) \)
Delta Function Potential II

- Except for x=0 have exponential solutions.

\[ u(x) = e^{-kx} \quad x > 0 \]
\[ u(x) = e^{kx} \quad x < 0 \]

- Continuity condition at x=0 is (in some sense) on the derivative. See by integrating S.E in small region about x=0

\[
\frac{d^2 u(x)}{dx^2} = -\frac{\lambda}{a} \delta(x)u(x) + k^2 u(x)
\]

\[
\int_{-\varepsilon}^{\varepsilon} dx \frac{d^2 u(x)}{dx^2} = \int_{-\varepsilon}^{\varepsilon} dx \left[-\frac{\lambda}{a} \delta(x)u(x) + k^2 u(x)\right]
\]

\[
\frac{du}{dx} (x = \varepsilon) - \frac{du}{dx} (x = -\varepsilon) = -\frac{\lambda}{a} u(0) + O
\]

\[
-k e^{-k\varepsilon} - k e^{k(-\varepsilon)} = -\frac{\lambda}{a}
\]

\[ k = \frac{\lambda}{2a} \Rightarrow \text{quantized} \]
1D Barriers (Square)

- Start with simplest potential (same as square well)

\[
V(x) = V_0 \quad x > 0 \\
V(x) = 0 \quad x < 0
\]

\[
\psi(x) = A e^{ik_1x} + B e^{-ik_1x} \quad x < 0
\]

\[
\psi(x) = C e^{k_2x} + D e^{-k_2x} \quad x > 0, \quad E < V
\]

or \[
\psi(x) = E e^{ik_0x} + F e^{-ik_0x} \quad x > 0, \quad E > V
\]

with \[
k_1 = \frac{\sqrt{2mE}}{h} \quad k_2 = \frac{\sqrt{2m(V-E)}}{h} \quad k_0 = \frac{\sqrt{2m(E-V)}}{h}
\]
1D Barriers E<V

- Solve by having wave function and derivative continuous at x=0

\[ \psi_-(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad x < 0 \]
\[ \psi_+(x) = Ce^{k_2x} + De^{-k_2x} \quad x > 0, \quad E < V \]
\[ \psi(x \to \infty) = 0 \Rightarrow C = 0 \]
\[ \psi_-(0) = \psi_+(0) \Rightarrow A + B = D \]
\[ \frac{\partial \psi_-(0)}{\partial x} = \frac{\partial \psi_+(0)}{\partial x} \Rightarrow A - B = \frac{ik_2}{k_1} D \]

solve for A, B. As \(|\psi|^2\) gives probability or intensity

\[ |B|^2 = \text{intensity of plane wave in } -x \text{ direction} \]
\[ |A|^2 = \text{intensity of plane wave in } +x \text{ direction} \]

\[ 2A = (1 + \frac{ik_2}{k_1}) D \quad 2B = (1 - \frac{ik_2}{k_1}) D \]

\[ R = \text{Re} flection = \frac{|B|^2}{|A|^2} = 1 \]
1D Barriers \( E < V \)

- While \( R=1 \) still have non-zero probability to be in region with \( E < V \)

\[
|\psi|^2 = |D|^2 e^{-2k_2 x} \quad x > 0
\]

\[
d = \frac{1}{k_2} = \text{penetration distance}
\]

Electron with barrier \( V-E=4 \text{ eV} \).

What is approximate distance it “tunnels” into barrier?

\[
d = \frac{1}{k_2} = \frac{c\hbar}{c \sqrt{2m(V-E)}} = \frac{197 \text{ eV} \text{ nm}}{\sqrt{2 \times 0.5 \text{ MeV} \times 4 \text{ eV}}} = 0.1 \text{ nm}
\]
1D Barriers $E>V$

- X<0 region same. X>0 now “plane” wave
  \[
  \psi = Ce^{ik_0x} + De^{-ik_0x} \quad x > 0
  \]

  \[
  k_0 = \frac{\sqrt{2m(E-V)}}{h} = \frac{p(x>0)}{h}
  \]

  Will have reflection and transmission at x=0. But

  “D” term unphysical and so D=0

  \[
  B = \frac{k_1-k_0}{k_1+k_0} A \quad C = \frac{2k_1}{k_1+k_0} A
  \]
1D Barriers $E > V$

- Calculate Reflection and Transmission probabilities. Note flux is particle/second which is $|\psi|^2 \times \text{velocity}$

$$R = \frac{|B|^2}{|A|^2} = \frac{(k_1 - k_0)^2}{(k_1 + k_0)^2}$$

$$T = \frac{4k_1^2}{(k_1 + k_0)^2} \frac{k_0}{k_1}$$

$$\int |\psi|^2 \, dx \neq 1$$

$$\frac{\nu_+}{\nu_-} = \frac{k_0}{k_1}$$

“same” if $E > V$. different $k$

Note $R + T = 1$
1D Barriers: Example

- 5 MeV neutron strikes a heavy nucleus with $V = -50$ MeV. What fraction are reflected? Ignore 3D and use simplest step potential.

$$R \approx \frac{(k_1 - k_0)^2}{(k_1 + k_0)^2} = \left( \frac{1 - \sqrt{E - V}}{1 + \sqrt{E - V}} \right)^2$$

$$R \approx \left( \frac{1 - \sqrt{55/5}}{1 + \sqrt{55/5}} \right)^2 = .29$$

$$k = \frac{\sqrt{2mE}}{\hbar}$$
1D Barriers Step E<V

• Different if E>V or E<V. We’ll do E<V. again solve by continuity of wavefunction and derivative

\[ \psi_-(x) = Ae^{ik_1x} + Be^{-ik_1x} \quad x < 0 \]
\[ \psi_+(x) = Ce^{ik_1x} + De^{-ik_1x} \quad x > a \]
\[ \psi_{in}(x) = Fe^{-k_2x} + Ge^{k_2x} \quad 0 < x < a \]
\[ D = 0 \]

No “left” travelling wave

Incoming \quad falling \quad transmitted

\[ \psi_-(0) = \psi_{in}(0) \quad a \]
\[ \frac{\partial \psi_-(0)}{\partial x} = \frac{\partial \psi_{in}(0)}{\partial x} \quad , \quad \frac{\partial \psi_{in}(a)}{\partial x} = \frac{\partial \psi_+(a)}{\partial x} \]
1D Barriers Step E<V

\[ A + B = F + G \]
\[ ik_1 A - ik_1 B = -k_2 F + k_2 G \]

\[ Fe^{-k_2a} + Ge^{k_2a} = Ce^{ik_1a} \]
\[- k_2 Fe^{-k_2a} + k_2 Ge^{k_2a} = -ik_1 e^{-ik_1a} \]

4 equations \( \rightarrow \) A,B,C,F,G (which can be complex)

A related to incident flux and is arbitrary. Physics in:

\[ R = \frac{v|B|^2}{v|A|^2} \quad T = \frac{v|C|^2}{v|A|^2} \]

Eliminate F,G,B

\[ T = \left[ 1 + \frac{(e^{k_2a} - e^{-k_2a})^2}{16\frac{E}{V}(1 - \frac{E}{V})} \right]^{-1} \]

if \( k_2a \gg 1 \)

\[ T = 16e^{-2k_2a} \frac{E}{V} \left( 1 - \frac{E}{V} \right) \]
Example: 1D Barriers Step

- 2 eV electron incident on 4 eV barrier with thickness: .1 fm or 1 fm

\[ k_2 = \frac{c\sqrt{2m(V-E)}}{\hbar c} = \sqrt{\frac{2 \times 51 \text{MeV} \times 2 \text{eV}}{197 \text{eV} \times \text{nm}}} = 7.3 \text{ fm}^{-1} \]

for 1 fm  \( k_2a = 0.73 \)

\[ \sinh(0.73) = \frac{e^{0.73} - e^{-0.73}}{2} = 0.80 \]

\[ T = \left[ 1 + \frac{.8^2}{4 \times 2/4 \times (1 - 2/4)} \right]^{-1} = 0.6 \quad \text{or with} \]

approx  \( T \approx 16e^{-2 \times 0.73} \frac{2}{4} \left( 1 - \frac{2}{4} \right) = 0.81 \)

With thicker barrier:

\[ for \ 1 \ fm \quad k_2a = 7.3 \]

\[ T_{\text{exact}} = \left[ 1 + 740^2 \right]^{-1} = 1.8 \times 10^{-6} \]

\[ T_{\text{approx}} \approx 16e^{-2 \times 7.3} \frac{2}{4} \left( 1 - \frac{2}{4} \right) = 1.8 \times 10^{-6} \]
Example: 1D Barriers Step

- Even simpler

\[ T \approx O(1) \times e^{-2k_2a} \quad (\psi \propto e^{-k_2x}) \]

\[ a = \text{barrier thickness} \]

\[ k_2 = \frac{1}{\text{wavelength}} = \frac{\sqrt{2m(V-E)}}{\hbar} \]

related to how far from barrier top

For larger V-E

larger k

More rapid decrease in wave function through
classically forbidden region
Bound States and Tunneling

- State A will be bound with infinite lifetime. State B is bound but can decay to $B \rightarrow B' + X$ (unbound) with lifetime which depends on barrier height and thickness.
- Also reaction $B' + X \rightarrow B \rightarrow A$ can be analyzed using tunneling.
- Tunneling is \( \approx \) probability for wavefunction to be outside well.

![Diagram of a square well with states A and B, and transition B' to A]
Alpha Decay

• Example: \( \text{Th}^{90} \rightarrow \text{Ra}^{88} + \text{alpha} \)
• Kinetic energy of the alpha = mass difference
• have \( V(r) \) be Coulomb repulsion outside of nucleus. But attractive (strong) force inside the nucleus. Model alpha decay as alpha particle “trapped” in nucleus which then tunnels its way through the Coulomb barrier
• super quick - assume square potential
• more accurate - \( 1/r \) and integrate

\[
T_\alpha \approx e^{-2ka} \quad a = \text{barrier thickness}
\]
\[
= r'' = \frac{zZe^2}{4\pi\varepsilon_0 K_\alpha} \quad (z = 2 \text{ and } K_\alpha = V)
\]

guess \( <V> = V\left(\frac{r''}{2}\right) = 2K_\alpha \) (square)

\[
e^{\frac{-2\sqrt{2m(2K_\alpha-K_\alpha)\times2Ze^2}}{\hbar^2 \pi eK_\alpha}} = e^{-8Z\sqrt{E_0/K}} \quad E_0 = 13.6\text{eV} \frac{m_\alpha}{m_e}
\]
Alpha Decay

• Do better. Use tunneling probability for each dx from square well. Then integrate

\[ T_{ABC} = T_A T_B T_C \]

\[ -2 \int_{r''}^{r'} \sqrt{2m/\hbar^2 (V(r) - K)} \, dr \]

\[ T_\alpha \approx e \]

• as V(r) is known, integral can be calculated. See E+R and Griffiths 8.2

\[ T_\alpha (E) \approx \exp\left( -4\pi Z \sqrt{E_0 / K} + 8 \sqrt{Z R / r_0} \right) \]

\[ r_0 = \frac{4\pi \varepsilon_0 \hbar^2}{m_\alpha e^2} = 7.24 \, fm \]

\[ E_0 = 13.6 \, eV \frac{m_\alpha}{m_e} = 0.99 \, MeV \]

4\pi Z=large number
Alpha Decay

• T is the transmission probability per “incident” alpha
• \( f = \text{no. of alphas “striking” the barrier (inside the nucleus) per second} = \frac{v}{2R} \), If \( v = 0.1c \) \( f = 10^{21} \text{ Hz} \)

\[
Th^{90} \rightarrow Ra^{88} + \alpha \quad Po^{84} \rightarrow Pb^{82} + \alpha
\]

\( K_\alpha = 4 \text{ MeV} \quad 8.95 \text{ MeV} \)

\( R = 9 \text{ fm} \quad 9 \text{ fm} \)

\( T = 1.3 \times 10^{-39} \quad 8.2 \times 10^{-13} \)

\[
\frac{\text{rate/ sec}}{\text{sec}} = T \times 10^{21} \text{ Hz}
\]

\( \tau = \frac{1}{\text{rate/ sec}} = 2 \times 10^{10} \text{ yrs} \quad 5 \times 10^{-7} \text{ sec} \)

Depends strongly on alpha kinetic energy