Finite Square Well

If the infinite square well was an artificial potential function, then the finite square well is a step towards a more realistic potential.

\[ V(x) = \begin{cases} -V_0 & \text{for } -a < x < a \\ 0 & \text{for } |x| > a \end{cases} \]

Case 1. \( E > 0 \) \( \Rightarrow \) Everywhere is classically allowed.

We call these solutions \((E>0)\) "scattering states", since for \( E > 0 \), no bound state will exist. Again we imagine a beam of particles approaching from \( x = -\infty \) (moving to the right.)

In terms of DeBroglie wavelength, the solution will look like:

\[ \cos(\frac{2\pi x}{\lambda}) \]

But the relative amplitudes are determined by the TDSE and the boundary conditions:

1. The wave is continuous
2. \( \psi \) is continuous
In terms of probability current we have:

\[ J_{\text{transmitted}} \quad \rightarrow \quad J_{\text{reflected}} \]

The finite square well is a good 1st model to use for:

- electron scattering on an atom (at least the 1-D repulsive)
- electrons in a metal scattering on an impurity atom
- a neutron scattering on a proton or other nucler.

Solution:

\[ Q_{\text{I}}(x) = A e^{ikx} + B e^{-ikx} \quad \text{as \ } x \to 0 \quad \Rightarrow \quad x^2 = \frac{2m}{\hbar^2} (E + \text{Vol}) \]
\[ Q_{\text{II}}(x) = C e^{ikx} + D e^{-ikx} \quad \text{as \ } x \to \infty \quad \Rightarrow \quad e^{-ikx} \]
\[ Q_{\text{III}}(x) = F e^{ikx} + \phi \quad \text{no left-moving beam in Region III} \]

Boundary Conditions:

\[ Q_{\text{I}}(x=-a) = Q_{\text{III}}(x=-a) \]
\[ Q_{\text{II}}(x=a) = Q_{\text{III}}(x=a) \]
\[ Q_{1}'(x=-a) = Q_{1}'(x=a) \]
\[ Q_{2}'(x=-a) = Q_{2}'(x=a) \]

Applying these 4 boundary conditions, we can find \( B, C, D, F \) in terms of \( A \).
Again, \( T = \frac{1}{\frac{J_{\text{trans}}}{\sin \alpha}} \) & \( R = \frac{\sin^2 \alpha}{\sin \alpha} \) & \( T + R = 1 \).

Result (from Griffiths)

\[
T = \frac{1}{1 + \frac{V_0^2}{E(E+V_0)}} \sin^2 \left[ \frac{2a}{h} \sqrt{2m(E+V_0)} \right]
\]

When the \( \sin^2 \) term \( \to 0 \), then \( T = 1 \) \( \Rightarrow \) Complete transmission no reflection.

This happens when

\[
\frac{2a}{h} \sqrt{2m(E+V_0)} = \frac{n\pi}{m}
\]

or when \( E + |V_0| = \frac{n^2\pi^2 h^2}{2m(2a)^2} \) \( \Leftarrow \) Condition for full transmission

If we measure energy with respect to the bottom of the well (\( E' = E + |V_0| \)) we see that these energies are exactly those of the infinite square well. Why?

\( \Rightarrow \) Answer: at these energies, an integral of half-wavelengths fit inside the well:

Ex: \( \gamma(x) \)

2 half-wavelengths.
At other energies, the wavefunction crosses the boundary of the wrong moment.

ψ should be continuous here.
Bound State of the Finite Well

\[ V(x) = \begin{cases} -|V_0| & \text{for } -a < x < a \\ 0 & \text{for } |x| > a \end{cases} \]

We've looked at the scattering state (we found the transmission coefficient, for example). Now let's look for bound states.

**Case 1:** \( E < 0 \) but \( E > -|V_0| \)

Region I: \( \kappa^2 = k^2 \alpha \), \( k = \sqrt{-2mE + |V_0|} \)  \( (E < 0, \text{ so } k \text{ real}) \)

Region II: \( \kappa^2 = -k^2 \alpha \), \( k = \sqrt{2mE + |V_0|} \)  \( (E > 0, k \text{ real}) \)

Region III: \( \kappa^2 = k^2 \alpha \) again

Classically Forbidden  Roughly speaking, \( \Psi(x) \) will be something like
Theorem: If \( V(x) \) is an even function, then the energy eigenstates will be even and/or odd functions.

(Homework #10)

Even Solutions: Solution with positive Parity:

\[
\psi(x) = \begin{cases} 
F e^{-kx} + G e^{ikx} & x > a \\
D \cos(kx) & -a < x < a \\
F e^{ikx} & x < -a
\end{cases}
\]

Continuity of \( \psi \) at \( x = a \):

\[ F e^{-ka} = D \cos(ka) \]  

Continuity of \( \psi' \) at \( x = a \):

\[ -kF e^{-ka} = -D k \sin(ka) \]

Divide (2) by (1):

\[ k = k \tan(ka) \]

This equation determines the energy eigenvalues, \( k \) & \( E \) or both, as functions of \( E \).

This is a transcendental Eq. for \( E \), it cannot be solved algebraically. Must use a numerical technique.

Some properties:

- There is always at least one solution

\[ \Rightarrow \text{ there is always at least one bound state with even parity} \]
If the well is deep and/or wide (or large and or \(|V_0|\) large), there will be many solutions. The higher solutions correspond to "fitting more wiggles" in the the car.

For any finite \(a\) and finite \(|V_0|\), there are a finite number of bound states. Odd Solution: "Solution with negative parity."

Result: \(\psi(x) = \begin{cases} -Fe^{ikx} & x < -a \\ D\sin(kx) & -a < x < a \\ Fe^{-ikx} & x > a \end{cases} \)

Eigenvalue Eq: \(k\cot(ka) = -i\eta \).  
1st odd state (if it exists)

Since the 1st odd state has an "extra wiggle" compared to the ground state, it has higher energy. Draw diagram on x & y-axis.
Square Barrier

\[ V(x) \]

\[ +|V_0| \]

\[ E \]

I -a II a III \[ x \]

Suppose \( 0 < E < |V_0| \).

Thus Region I & III are Classically Allowed, But Region II is Classically Forbidden.

Scattering states; the particle is not bound. Solution will look like (for a beam travelling to the right):

\[ \psi(x) \]

amplitude is smaller on output side due to exponential decay in Region II.

- Classically, no particles should penetrate the barrier. But QM allows some penetration. This is another example of QM tunneling. (Alpha-decay is similar).

- The exact amplitude in each region are constrained by require \( \psi \) & \( \psi' \) to be continuous at \( x = a \) & \( x = -a \).

- A similar phenomena happens in optics. When light reflects off a barrier when there should be 100% reflection, such as \( V(x) \), when total internal reflection should occur. If the barrier thickness is small...
Summary of "Rules" for 1D wave mechanics

- Where $E > V(x)$ ($KE$ is positive), $\psi$ oscillates.
- Where $E < V(x)$ ($KE$ is negative), $\psi$ decays.
- Where $KE$ is large, wavelength is short.
- Where $KE$ is small, wavelength is long.
- $\psi$ & $\psi'$ are continuous where $V(x)$ is finite.
- $\psi''$ will be discontinuous where $V(x)$ changes suddenly.
- The amplitudes of $\psi$ in various regions are constrained by the requirement of continuity of $\psi$ & $\psi'$.
- For bound states we look for normalizable wavefunctions.
- For free-particle states we "accept" un-normalizable wavefunctions. Usually, we calculate beam currents using the $J$ vector.
- For bound states, the ground state has the minimum number of wiggles. Excited states have more wiggles.
- If $V(x)$ is an even function of $x$, we look for $\psi_n(x)$ to be even & odd functions of $x$. 
Double square well

\[ V(x) \uparrow \]

\[ V(x) \text{ is even, so } \psi \text{ will be even or odd} \]

- Bound state energy

1st excited: odd function

\[ \psi_1 \]

[Graph of odd function]

\[ \text{sinh function} \]

2nd excited: even function

\[ \psi_2 \]

[Graph of even function]

Ground state function

\[ \phi_0(x) \uparrow \]

\[ e^{-kx} \]

\[ \text{Should decay here, but } \phi \text{ should be even} \]

Use a \( \cosh(x) \) function:

\[ \cosh(x) = \frac{1}{2} (e^{kx} + e^{-kx}) \]

\[ \rightarrow \text{Remember, } \psi_i \text{ might not exist at all if } |V_0| \text{ is small or if the wells are very narrow.} \]
Harmonic Oscillator

$V(x) \propto \text{Even}$

$Q(x) \propto \text{Even}$

$a_1(x) \propto \text{Odd}$

$c_2 \propto \text{Even}$

$a_3 \propto \text{Odd}$

$Q(x) \propto \text{Even}$

$x$ continuously changes because $V(x)$ continuously changes (since KE continuously...