tells us that $\Psi(x)$, and thus the probability density $|\Psi(x)|^2$, is zero in an interval only if $U(x) \to \infty$ in that interval, in which case $\Psi(x)$ will have a node (or zero) at the end of that interval.

Otherwise $\Psi(x)$ and $\Psi'(x)$ vary smoothly (i.e. are continuous and differentiable). In particular, in the classically forbidden region ($x > b$ or $x < a$) the wave function is monotonically decreasing (in abs. value) and as $|x| \to \infty$ the fall off of the wave function is exponential (as we saw before). At the turning point $\Psi(x)$ has an inflection point (i.e. a point where the curvature changes sign). Outside the region comprised by the inflection points the wave function cannot have zeros since $\Psi''$ has the same sign as $\Psi$ in that region.
In the region comprised between the two inflection points, \( E > U(x) \).

If \( U(x) \) varies slowly enough it is easy to see that the wave function can oscillate in this region. In particular it can have zeros. If \( U(x) \) is finite everywhere, the zeros of \( \psi(x) \) are isolated points.

What do the zeros of \( \psi(x) \) tell us?

There is an interesting Oscillation Theorem (which only holds in \( d=1 \)). It states that the following. Consider a set of wave functions \( \psi_n(x) \) which constitute the discrete part of the energy spectrum with eigenvalues \( E_n \). Without loss of generality we can order the e.v.'s (and the states) as \( E_0 < E_1 < E_2 < \ldots \).
Let \( \Psi_n \) be the wave function of the \( n+1 \)st state \( \Rightarrow \Psi_n(x) \) vanishes \( n \) times, i.e. \( \Psi_n(x) \) has \( n \) zeroes or nodes.

Let us first discuss the physical meaning of this theorem. If \( \Psi(x) \) is an eigenstate of \( \hat{\mathcal{H}} \) with eigenvalue \( E \Rightarrow \)

\[
\hat{\mathcal{H}} \Psi = E \Psi \quad \text{and} \quad \langle \Psi | \hat{\mathcal{H}} | \Psi \rangle = E \quad \text{and} \quad \int dx \psi^2(x) = 1
\]

\( \Rightarrow E = \langle \Psi | \hat{T} | \Psi \rangle + \langle \Psi | \hat{\mathcal{U}} | \Psi \rangle \)

but

\[
\langle \hat{T} \rangle = \int dx \psi^2(x) \left( -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) \psi(x) = \frac{\hbar^2}{2m} \int dx \left| \frac{d\psi}{dx} \right|^2
\]

and

\[
\langle \hat{\mathcal{U}} \rangle = \int dx \mathcal{U}(x) \left| \psi(x) \right|^2
\]

\( \Rightarrow E = \int dx \left[ \frac{\hbar^2}{2m} \left| \frac{d\psi}{dx} \right|^2 + \mathcal{U}(x) \left| \psi(x) \right|^2 \right] \)

in order to lower the \( \langle \hat{T} \rangle \) we want wave function with small derivatives and in order to lower \( \langle \hat{\mathcal{U}} \rangle \) we want wave function peaked # where
$U(x)$ is small. These two requirements are clearly in conflict with each other. However, a wave function $\Psi_n(x)$ has $n$ nodes on average; its derivative will be larger (in abs. value) than most of $\Psi_{n-1}$, which has $n-1$ nodes. Also $\Psi_n$ will be larger away from its nodes than close to them. A wave function with $n$ nodes is more spread out than a wave function with $n-1$ nodes, leading to a higher $\langle T \rangle$ and a higher $\langle U \rangle$ as well $\rightarrow$ a larger $E$.

Let us prove this theorem. Let us consider two solutions $\Psi_1$ and $\Psi_2$ with eigenvalues $E_1$ and $E_2$, with $E_2 > E_1$. Let us define the Wronskian $W[\Psi_1, \Psi_2]$

$$W[\Psi_1, \Psi_2] = \Psi_1 \Psi_2' - \Psi_2 \Psi_1'$$
Suppose that $\Psi_1$ has a zero at $x=a$ and a zero at $x=b > a$. The change in the Wronskian $W(\Psi_1, \Psi_2)$ between $x=a$ and $x=b$ can be calculated as follows. Let us write the Schrödinger equation for $\Psi_1$ and $\Psi_2$

$$\frac{d^2\Psi_1}{dx^2} + \frac{2m}{\hbar^2} (E_1 - U(x)) \Psi_1(x) = 0$$

$$\frac{d^2\Psi_2}{dx^2} + \frac{2m}{\hbar^2} (E_2 - U(x)) \Psi_2(x) = 0$$

$$W(\Psi_1, \Psi_2)|_a^b = (\Psi_1|_a^b \Psi_2|_a^b - \Psi_1|_a^b \Psi_2|_a^b)|_a^b$$

$$= \int_a^b \frac{d\xi}{dx} \left( \Psi_1' \Psi_2(x) - \Psi_1 \Psi_2' \right)$$

$$= \int_a^b dx \frac{2m}{\hbar^2} \left[ (U(x)-E_1) \Psi_1 \Psi_2 - (U(x)-E_2) \Psi_1 \Psi_2 \right]$$

$$= \frac{2m}{\hbar^2} (E_2 - E_1) \int_a^b dx \Psi_2(x) \Psi_1(x)$$

Since $\Psi_1(a) = \Psi_1(b) = 0$ implies

$$\Psi_1'(x) \Psi_2(x)|_a^b = \frac{2m}{\hbar^2} (E_2 - E_1) \int_a^b \Psi_2(x) \Psi_1(x)$$
Let us assume that $\psi_1 > 0$ for $a < x < b$.

Since $\psi_1(a) = \psi_1(b) = 0 \Rightarrow \psi_1'(a) > 0$ and $\psi_1'(b) < 0$. Suppose that $\psi_2$ does not have a zero for $a < x < b \Rightarrow \psi_2(a)$ has the same sign as $\psi_2(b)$ (say > 0) $\Rightarrow$ the L.H.S. < 0. But if $\psi_2$ does not have a zero $\Rightarrow$ it remains > 0 for the entire interval and it will have the same sign as $\psi_1 \Rightarrow$ since $E_2 > E_1 \Rightarrow$ R.H.S. > 0

Contradiction $\Rightarrow$ $\psi_2$ has not if $E_2 > E_1 \Rightarrow$ $\psi_2$ must have a zero between a pair of zeros of $\psi_1$.

$\Rightarrow$ if $\psi_1$ has n zeros $\Rightarrow$ $\psi_2$ must have $n+1$ zeros.

In particular the wave function for the lowest energy eigenvalue $E_0$, the ground state, has no zeros in the entire interval (except possibly at the boundaries).
1) **Infinite Potential Well**

Consider a particle of mass \( m \) in a potential

\[
U(x) = \begin{cases} 
0 & 0 < x < L \\
\infty & \text{otherwise}
\end{cases}
\]

\( \Rightarrow \) for \( 0 < x < L \) the particle is free.

The solutions of the Schrödinger Equation in this region are

\[
\psi(x) = e^{\pm ikx}
\]

when \( kE = \frac{n^2 \hbar^2}{2m} \)

\[\Rightarrow \psi(0) = \psi(L) = 0 \quad (n \rightarrow \infty \text{ at } x = 0, L)\]

Note that \( U = \infty \) for \( x > L \) and \( x < 0 \).

\( \Rightarrow \psi \) is not continuous at \( x = 0, L \).

What do these BC's imply?

\[
\psi(0) = 0 \Rightarrow A + B = 0
\]

\[
\psi(L) = 0 \Rightarrow Ae^{ikL} + Be^{-ikL} = 0
\]

\( \Rightarrow A = -B \Rightarrow A \sin kL = 0 \)

\( \Rightarrow kL = n\pi \quad (n \in \mathbb{N}) \Rightarrow \text{ quantization!} \)
\[ k_n = \frac{n\pi}{L} \]  on the allowed values of \( k \).

The energy of this state is
\[ E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \]

The lowest energy state has energy
\[ E_1 = \frac{\hbar^2 \pi^2}{2mL^2} \quad n=1 \]

The first excited state has energy
\[ E_2 = \frac{\hbar^2 \pi^2}{2mL^2} \times 4 = 4E_1 \]

and \[ E_n = n^2 E_1 \]

Energy spacing:
\[ E_2 - E_1 = \frac{3\hbar^2 \pi^2}{2mL^2} \xrightarrow{L \to \infty} 0 \]

\[ (E_{n+1} - E_n = \frac{\hbar^2 \pi^2}{2mL^2} (2n+1)) \]

Wave functions must be normalized:
\[ \int_0^L \Psi_n^2 \, dx = 1 \Rightarrow \int_0^L \Psi_n^2 \, dx \cdot A_n^2 \cdot \sin^2 (k_n x) = 1 \]

\[ 1 = \frac{A_n^2}{2k_n} \Rightarrow \quad A_n = \sqrt{2k_n} = \sqrt{\frac{2n\pi}{L}} \]

\[ \Psi_n (x) = \sqrt{\frac{2n\pi}{L}} \sin \left( \frac{n\pi x}{L} \right) \quad \text{with} \quad E_n = \frac{\hbar^2 \pi^2 n^2}{2mL^2} \]
2) **Particle on a circle**

Let us imagine that we have a particle moving on a segment of length $L$ wrapped on a circle so that points $x=0$ and $x=L$ are physically equivalent $\Rightarrow \Psi(x)$ must be periodic with period $L$

$$\Psi(x + L) = \Psi(x)$$

\[ x \text{ same as } x = \Theta R \]

with $0 < \Theta < 2\pi$ and

$$L = 2\pi R$$

("compactified")

If $\Psi(x)$ is periodic $\Rightarrow$ solutions are

$$\psi_n = e^{ik_n x}$$

but s.t. $e^{ik_n L} = 1$

$\Rightarrow k_n L = 2\pi n$

$$k_n = \frac{2\pi n}{L}$$

(Note the factor of 2.)

Notice that $n$ can be any integer, positive or negative.
What is the energy? 

\[ E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{4\pi^2 \hbar^2 n^2}{2mL^2} \]

\[ \Rightarrow E_n = \frac{2\pi^2 \hbar^2 n^2}{mL^2} \]

\[ \Rightarrow \text{the solutions are degenerate since } E_n = E_m \]

corresponding to partners with momenta \( p_n = \hbar k_n \)

moving to the right or to the left. There is a solution with \( n = 0 \) with energy \( E_0 = 0 \)

but \( \psi_0 \neq 0 \)

In fact 

\[ \psi_n = A_n \ e^{i k_n x} \]

\[ \int_0^L dx \ |\psi_n(x)|^2 = 1 \Rightarrow \quad A_n \ L = 1 \]

\[ \Rightarrow A_n = \frac{1}{\sqrt{L}} \]

\[ \Rightarrow \psi_n(x) = \frac{1}{\sqrt{L}} e^{i k_n x} \]

Note: \( \psi_0(x) = \frac{1}{\sqrt{L}} \)

Why do we have a degeneracy?
Because the particle moves on a circle, there is no preferred origin, so we have translational invariance. \( \hat{P} \) is a generator of a symmetry and \( [\hat{H}, \hat{P}] = 0 \) so the energy eigenstates are eigenstates of \( \hat{P} \):

\[
\hat{P} \psi_n = \frac{\hbar}{i} \frac{\partial}{\partial x} \psi_n = \hbar k_n \psi_n
\]

with \( p_n = \hbar k_n = \frac{2\pi n \hbar}{\lambda} \)

\( \Rightarrow \) states with \( E_n = E_{-n} \) are labelled by the sign of their momentum. Notice that in the case of a particle in an infinite potential well, translational invariance is broken by the potential \( \Rightarrow \) momentum is not a good quantum number and the eigenstates of \( \hat{H} \) are not eigenstates of \( \hat{P} \) (since \( [\hat{P}, \hat{H}] \neq 0 \)).
3) Bound States: The δ-function Potential

We will consider now a very simple problem. Imagine a particle on an infinite line \( x \to \infty \) and that the potential energy is sharply concentrated at \( x = 0 \)

\[ U(x) = -|q| \delta(x) \]

i.e. \( U(x) \) is very large and negative for \( x \to 0 \) and zero everywhere else. Note: the units of \( |q| \) are energy per length.

Q. What is the spectrum of

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + U(x) \]

in this case?

Since \( U(x) \neq 0 \) we don't have translational invariance \( \{ \hat{E}, \hat{H} \} \neq 0 \). In both regions \( x > 0 \) (region I) and \( x < 0 \) (region II) we may have right and left moving states.
Are there bound states? i.e. states with \( E < 0 \).

These states must be normalizable:

\[
\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1
\]

\[
\Rightarrow \quad \text{For } x > 0 \quad \text{the only allowed } \psi
\]

\[
\psi_I = A_I e^{-k_I x} \rightarrow 0 \quad \text{as } x \rightarrow +\infty
\]

and for \( x < 0 \)

\[
\psi_II = B_{II} e^{k_{II} x} \rightarrow 0 \quad \text{as } x \rightarrow -\infty
\]

Clearly,

\[
-k_I^2 = \frac{-\hbar^2}{2m} k_{II}^2 = \frac{E}{m} < 0
\]

\[
\Rightarrow \quad k_I = k_{II} = k
\]

and

\[
|E| = \frac{\hbar^2 k^2}{2m}
\]

Q. What is the effect of \( U(x) \)?

What B.C.'s are satisfied at \( x = 0 \)?

\[
\frac{d^2 \psi}{dx^2} = -\frac{2m}{\hbar^2} (E - U(x)) \psi
\]

\[
\Rightarrow \quad \int_{-\varepsilon}^{\varepsilon} dx \frac{d^2 \psi}{dx^2} = \left. \psi'(x) \right|_{-\varepsilon}^{\varepsilon} - \left. \psi(x) \right|_{-\varepsilon}^{\varepsilon} = \text{jump in } \psi'
\]

\( \varepsilon \) small
\[
\int_{-\varepsilon}^{\varepsilon} dx \, \frac{d^2\psi}{dx^2} = \int_{-\varepsilon}^{\varepsilon} dx \, \frac{2m}{\hbar^2} (U(x) - E) \psi(x)
\]

\[
\int_{-\varepsilon}^{\varepsilon} dx \, U(x) \psi(x) = -|g| \int_{-\varepsilon}^{\varepsilon} dx \, J(E) \psi(x)
\]

\[
= -|g| \psi(0)
\]

and \[
\int_{-\varepsilon}^{\varepsilon} dx \, \psi(x) = \varepsilon \psi(0) + O(\varepsilon^2) \to 0 \quad \varepsilon \to 0
\]

\[\Rightarrow \psi(x) \text{ is continuous at } x=0 \text{ but } \psi'(x) \text{ is not continuous at } x=0\]

1. Continuity: \[\psi_I(0) = \psi_{\Pi}(0)\]

\[\Rightarrow A_I = B_{\Pi} = A = \psi(0)\]

2. \[\psi_I'(0) = -AK e^{-kx} \quad \Rightarrow \psi_I'(0) = -KA\]

\[\psi_{\Pi}'(0) = AK e^{kx} \quad \Rightarrow \psi_{\Pi}'(0) = +KA\]

\[\Rightarrow \psi_{\Pi}'(0) = \psi_{\Pi}'(0)\quad \psi_{\Pi}'(0) = -\psi_{\Pi}'(0) = -2m|g|\psi(0)\]

\[-KA - (KA) = -2m|g|A \]

\[\Rightarrow K = \frac{m|g|}{\hbar^2} \quad \text{(Check the units!)}\]
Energy: \[ E = -\frac{\hbar^2}{2m} \frac{m^2 g^2}{\hbar^4} \]

\[ \Rightarrow E = -\frac{m^2 g^2}{2\hbar^2} < 0 \]

Normalization:

\[ 1 = \int_{-\infty}^{\infty} dx \, |\Psi(x)|^2 = \int_{-\infty}^{0} dx \, A^2 \, e^{2Kx} + \int_{0}^{\infty} dx \, A^2 \, e^{-2Kx} \]

\[ \Rightarrow 1 = 2 \int_{0}^{\infty} dx \, A^2 \, e^{-2Kx} \]

\[ 1 = \frac{2A^2}{K} \Rightarrow A = \sqrt{K} = \sqrt{\frac{m|\theta|}{\hbar^2}} \]

\[ \Rightarrow \Psi_0(x) = \sqrt{\frac{m|\theta|}{\hbar^2}} \, e^{-K |x|} \]

K = \frac{m|\theta|}{\hbar^2} \quad \text{and} \quad E_0 = -\frac{m^2 g^2}{2\hbar^2}

13. The ground state energy.

There is exactly one bound state with energy E_0.
Positive energy states: They are part of the continuous part of the spectrum ("the continuum"). These states are not bound. They are "scattering states".

Let us rewrite the Schrödinger Equation (for the stationary states of energy $E$) as

$$\left[ E + \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] \psi(x) = \delta(x) \psi(x)$$

$$\equiv \delta(x) \psi(0)$$

Let $\psi_{inc}(x)$ be a free particle state

$$\psi_{inc}(x) = \frac{1}{\sqrt{2\pi \hbar}} e^{\pm ikx}$$

$k = \frac{1}{\hbar} \sqrt{2mE}$

($E > 0$)

which represent states with momenta $\pm \hbar k$ (right and left moving states).

Let us check that

$$\psi(x) = \psi_{inc}(x) + \int_{-\infty}^{\infty} \frac{dp}{2\pi \hbar} e^{ipx/\hbar} \frac{e^{ipx/\hbar} \delta(x)}{E^2 - p^2/2m} \psi(0)$$

$\psi_{inc} = 0$

$$\left[ E + \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right] \psi_{inc} = \left( E - \frac{\hbar^2 k^2}{2m} \right) \psi_{inc} = 0$$

since $E = \frac{\hbar^2 k^2}{2m}$
\(2\) \( \left(E + \frac{\hbar^2}{2m} \frac{d^2}{dx^2}\right) \int_{-\infty}^{\infty} \frac{dp}{2\pi \hbar} \frac{e^{ipx/\hbar}}{E - p^2/2m} \varphi(0) = \int_{-\infty}^{\infty} \frac{dp}{2\pi \hbar} \left(\frac{E - p^2/2m}{E - p^2/2m}\right) e^{ipx/\hbar} \varphi(0) = \delta(x) \varphi(0) \bar{\nu}

This is almost correct except for a problem: the integrand has poles on the real axis, along the integration path, at \( p = \pm \sqrt{2mE} \). Thus the solution is ill-defined. We will remedy this problem by defining an integration path in the complex \( p \) plane which avoids the poles. However, there are different choices of paths (and hence \( \neq \) integrals). These choices turn out to correspond to \( \neq \) possible boundary conditions.

Suppose we want a solution with the B.C. that \( \varphi(x) \) is an outgoing wave (i.e. right moving). This solution is obtained by
The following choice of integration paths are possible:

Which one should we choose? This is the same as moving the poles up and down infinitely and hence to the replacement

$$E - \frac{p^2}{2m} \rightarrow E - \frac{p^2}{2m} + i\epsilon$$  \hspace{1cm} (E>0)$$

The integral over $C_+$ vanishes as $R \rightarrow \infty$ if $x > 0$ and over $C_-$ if $x < 0$.

For outgoing waves ($x > 0$) we choose $C_+$ and close the path in the upper $\Im p$ plane. The pole enclosed by the path is at $\sqrt{\frac{p^2}{2m} + i\epsilon}$.

Hence, for $x > 0$, the integral is
\[ \int_{-\infty}^{+\infty} \frac{dp}{2\pi i} \frac{e^{ipx}}{E - \frac{p^2}{2m} + i\varepsilon} = \int_{-\infty}^{+\infty} \frac{dp}{E - \frac{p^2}{2m} + i\varepsilon} \]

\[ = 2\pi i \text{ Res} \left[ \frac{e^{ipx}}{E - \frac{p^2}{2m} + i\varepsilon} \right] \]

\[ = 2\pi i \cdot \frac{1}{2\pi i} \frac{e^{ipx} \sqrt{2mE}}{E - \frac{p^2}{2m} + i\varepsilon} \]

\[ = \frac{m}{\sqrt{2mE}} \cdot e^{\frac{c}{\hbar} \sqrt{2mE} x} \quad x > 0 \]

Conversely, for \( x < 0 \), we choose \( E^- \) (i.e. \( x \) close on the lower \( \varepsilon \)-plane) and the enclosed pole is now at \(-\sqrt{2mE} - i\varepsilon \) \( \Rightarrow \)

\[ \int = -2\pi i \cdot \frac{1}{2\pi i} \frac{e^{-\frac{c}{\hbar} \sqrt{2mE} x}}{-\frac{1}{m} (\sqrt{2mE})} \]

\[ = \frac{m}{\sqrt{2mE}} \cdot e^{-\frac{c}{\hbar} \sqrt{2mE} x} \quad x < 0 \]

which is also outgoing.
Hence the solution with an outgoing wave for $x > 0$

is

$$\Psi(x) = \Psi_{inc}(x) + \frac{mg}{\cosh \sqrt{2mE}} e^{\frac{c}{\hbar} \sqrt{2mE} |x|} \Psi(0)$$

We now need to find $\Psi(0)$:

$$\Psi(0) = \Psi_{inc}(0) + \frac{mg}{\cosh \sqrt{2mE}} \Psi(0)$$

$$\Rightarrow \Psi(0) = \frac{\cosh p}{\cosh p - mg} \Psi_{inc}(0) \quad \text{where} \quad p = \sqrt{2mE}$$

If we choose a right moving incident wave

$$\Psi_{inc}(x) = \frac{1}{\sqrt{2\pi k}} e^{i px/\hbar}$$

$$\Psi(x) = \frac{1}{\sqrt{2\pi k}} \left[ e^{i px/\hbar} + \frac{mg}{\cosh \sqrt{2mE}} e^{i \hbar p 1/x |} \right]$$

For $x > 0$, $\Psi(x) = \Psi_{transmitted}(x)$

$$\Rightarrow \Psi_{trans}(x) = \frac{1}{\sqrt{2\pi k}} e^{i px/\hbar} \left( 1 + \frac{mg}{\cosh \sqrt{2mE}} \right)$$

$$= \frac{1}{\sqrt{2\pi k}} e^{i px/\hbar} \frac{\cosh p}{\cosh \sqrt{2mE} - mg}$$
Let us write \( \psi_{\text{trans}} \) in the form
\[
\psi_{\text{trans}}(x) = \frac{A(E)}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}
\]

Notice that in the absence of the potential, \( A(E) = 1 \).

The complex number \( A(E) \) is called the transmitted amplitude. For this problem, it is given by

\[
S(E) \equiv A(E) = \frac{c\sqrt{2\mu E}}{i\hbar \sqrt{2\mu E - mg}} = \left( \frac{E}{E + mg^2/2\hbar^2} \right)^{1/2} e^{i\delta(E)}
\]

where \( \delta(E) \) is the phase shift:

\[
\delta(E) = -sgn(\theta) \tan^{-1} \sqrt{\frac{mg^2}{2\hbar^2 E}}
\]

The transmission amplitude \( S(E) \) is related to the transmission coefficient \( T(E) \) by

\[
T(E) = |S(E)|^2 = |A(E)|^2 = \frac{E}{E + mg^2/2\hbar^2}
\]

for the \( \delta \)-function potential \( T(E) \) is monotonic.
Notice that $S(p) = \frac{ip}{ip - mg}$ has a pole at $p = -\frac{mg}{h}$ which lies on the imaginary axis. This imaginary pole is called a resonance. However, for attractive interactions, as a function of energy, this pole appears on the real axis as the bound state discussed before.

What about the reflected amplitude $S_r(E)$ and the associated reflection coefficient $R(E) = |S_r(E)|^2$?

$$S_r(E) = \frac{mg}{ip\sqrt{\omega} - mg}$$

$$\Rightarrow |S_r(E)|^2 = R(E) = \frac{mg^2}{\hbar^2 \omega + mg^2} = \frac{mg^2/2\hbar^2}{E + mg^2/2\hbar^2}$$

Notice that $R(E) + S(E) = 1$ conservation of probability.
4) The Square Well

Consider the potential \( U(x) = \begin{cases} 
U_0, & |x| \leq a \\
0, & |x| > a 
\end{cases} \)

If \( U_0 < 0 \) \( \Rightarrow \) square well
\( U_0 > 0 \) \( \Rightarrow \) square barrier.

\[
\begin{array}{c|c|c}
& I & II \\
\hline
U(x) & U_0 > 0 & -a < x < a \\
\hline
& \hline
\end{array}
\]

Note: If we let \( a \to 0 \) and \( U_0 \to \infty \)
and keep \( 2aU_0 = g \) fixed we have a \( \delta \)-function potential with strength \( g \).

Also, for \( U_0 \to -\infty \) we recover the square well.

Let us solve for the spectrum of states for this problem. As before, we will look first at the

**bound states**, i.e., states with \( E < 0 \).

There are three regions:

- \( I = \frac{1}{2} \ x < -a \)
- \( II = \frac{1}{2} \ 1x1 < a \)
- \( III = \frac{1}{2} \ x > a \)

States with \( E < 0 \) must have wave function which vanish as \( |x| \to \infty \).
Before solving these equations in their full glory we note the following general property:

**Parity:** Let \( u(x) = u(-x) \)

\[
\Rightarrow -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} + u(x) \psi(x) = E \psi(x)
\]

\( x \rightarrow -x \Rightarrow -\frac{\hbar^2}{2m} \frac{d^2 \psi(-x)}{dx^2} + u(-x) \psi(-x) = E \psi(-x) \)

But \( u(-x) = u(x) \Rightarrow \)

If \( \psi(x) \) is a solution \( \Rightarrow \psi(-x) \) is also a solution. Define \( \hat{\mathcal{P}} \psi(x) = \psi(-x) \)

\( \hat{\mathcal{P}}^+ = \hat{\mathcal{P}}^{-1} = \hat{\mathcal{P}} \)

\( \hat{\mathcal{P}}^+ \hat{\mathcal{H}} \hat{\mathcal{P}} = \hat{\mathcal{H}} \) if \( u(x) = u(-x) \)

\( \Rightarrow \) The eigenstates of \( \hat{\mathcal{P}} \) are eigenstates of \( \hat{\mathcal{H}} \) since

\( [\hat{\mathcal{P}}, \hat{\mathcal{H}}] = 0 \)

If \( \psi(x) = \psi(-x) \Rightarrow \hat{\mathcal{P}} \psi = +\psi \)

\( \psi(x) = -\psi(-x) \Rightarrow \hat{\mathcal{P}} \psi = -\psi \)

\( \Rightarrow \) even \psi's have \( \oplus \) ev. and odd \( \psi \) have \( \ominus \) ev. \( \Rightarrow \) we can choose the solutions to be \( \overset{\ominus}{\text{even}} \) or \( \overset{\oplus}{\text{odd}} \)
Region I: The Eqn. is

\[-\frac{\hbar^2}{2m} \psi''_I = E \psi_I \Rightarrow E < 0\]

\[\Rightarrow \psi''_I = \frac{2m |E|}{\hbar^2} \psi_I\]

\[\Rightarrow \psi_I = e^{\pm kx} \text{ with } k = \frac{2m |E|}{\hbar^2}\]

The B.C. \Rightarrow \psi_I \to 0 \text{ as } x \to -\infty \text{ if}

we choose the + root.

\[\text{for } x < -a \Rightarrow \psi_I(x) = A_I e^{kx}\]

Region III: Same story but now

\[\text{for } x > a \Rightarrow \psi_{III}(x) = B_{III} e^{-kx}\]

which is the solution \[\text{ that vanishes as } x \to \infty\]

\[\Rightarrow \text{ even state } \Rightarrow B_{III} = A_I\]

\[\text{odd state } \Rightarrow B_{III} = -A_I\]

Region II: The solutions are now oscillatory

with

\[\psi_{II} = A_{II} e^{i\omega x} + B_{II} e^{-i\omega x}\]
when \( k^2 = -\frac{2m}{\hbar^2} (E - V_0) \) for \( E < 0 \) \( V_0 < 0 \)

even states \( \Rightarrow \) \( A_{\Pi} = B_{\Pi} \)

odd states \( \Rightarrow \) \( A_{\Pi} = -B_{\Pi} \)

\[ \begin{align*}
\psi(x) &= \begin{cases} 
A_{\Pi}^e e^{kx} & x < -a \\
A_{\Pi}^o \cos kx & |x| \leq a \\
A_{\Pi}^o e^{-kx} & x > a 
\end{cases} 
\]

odd states \( \Rightarrow \) \( \psi(x) = \begin{cases} 
A_{\Pi}^o e^{kx} & x < -a \\
A_{\Pi}^o \sin kx & |x| \leq a \\
- A_{\Pi}^o e^{-kx} & x > a 
\end{cases} \)

\[ \begin{align*}
\psi_{\Pi}(a) &= \psi_{\Pi}(a) \\
\psi_{\Pi}'(a) &= \psi_{\Pi}'(a) \\
\end{align*} \]

\[ \Rightarrow \] \( A_{\Pi}^e \cos ka = A_{\Pi}^o e^{-ka} \) \( \text{for even states} \)

\( -k A_{\Pi}^o \sin ka = -A_{\Pi}^e k e^{-ka} \)
There is a non zero solution iff. the system is linearly dependent $\Rightarrow$ the determinant must vanish $\Rightarrow$ 

$$\tan(ka) = \frac{k}{k}$$

in even states.

The allowed states satisfy this quantization condition

$$A^e_{II} = A^e_{II} e^{ka} \cos ka$$

Notice that due to the symmetry the BC at $x = -a$ is automatically satisfied.

In odd states we have:

$$-A^o_{II} e^{-ka} = A^o_{II} \sin ka$$

$$A^o_{II} k e^{-ka} = A^o_{II} k \cos ka$$

$\Rightarrow$ the quantization condition now is:

$$\tan(ka) = -\frac{k}{k}$$

and

$$A^o_{II} = \frac{k}{k} e^{ka} \cos(ka) A^o_{II}$$
Since \[ k^2 = \frac{2mU_0}{\hbar^2} - k^2 > 0 \]

\[ \Rightarrow k^2 = \frac{2mU_0}{\hbar^2} - k^2 > 0 \]

\[ \Rightarrow \tan(k\alpha) = \frac{k}{k} = \frac{\sqrt{2mU_0}}{k^2-k^2} - 1 \]

On if \[ U = k\alpha \]

\[ u^2 = \frac{2mU_0}{\hbar^2} \]

\[ \cot \alpha = \frac{k}{k} = \frac{\alpha}{\sqrt{2mU_0\alpha^2 - u^2}} \]

If \[ U_0 < \pi \Rightarrow 1 \text{ even bound state} \]

\[ \pi < U_0 < 2\pi \Rightarrow 2 \text{ even bound states} \]

For the odd state we have instead:

\[ \tan \alpha = -\frac{k}{k} \Rightarrow -\tan \alpha = \frac{\alpha}{\sqrt{U_0^2-u^2}} \]
which now looks like

Note: there are odd bound states only if

\[ u_0 > \frac{\pi}{2} \]

the odd bound states are in the regions

\[ \frac{\pi}{2} < u < \frac{3\pi}{2}, \frac{3\pi}{2} < u < 2\pi \text{, etc.} \]

while the even bound states are in the complementary regions

\[ 0 < u < \frac{\pi}{2}, \frac{\pi}{2} < u < \frac{3\pi}{2}, \text{etc.} \]

Also there is always an even bound state

but the odd bound state only appears if

\[ u_0 > \frac{\pi}{2} \Rightarrow \frac{2m|u_0|a^2}{\hbar^2} > \frac{\pi^2}{4} \]

\[ \Rightarrow |u_0| > \frac{\pi^2 \hbar^2}{8ma^2} \text{ to have at least an odd bound state} \]
Scattering states: It turns out that for scattering states it is not convenient to use the even-odd basis since these are all stationary states. We will use instead travelling waves, as in the case of the $r$-function potential. Once again we have 3 regions: I, II and III. We will look for states with an outgoing wave to the right $\Rightarrow B_{III} = 0$ and

$$
\Psi_{III} = A_{III} e^{i k x} \quad \frac{\hbar^2 k^2}{2m} = E > 0
$$

and

$$
\Psi_{I} = A_{I} e^{i k x} + B_{I} e^{-i k x}
$$

with the same $k$. $A_{I}$ is the incident amplitude, $B_{I}$ is the reflected (outgoing) amplitude and $A_{III} = S(E)$ is the transmitted amplitude.

In region II we have

$$
\Psi_{II} = A_{II} e^{i k' x} + B_{II} e^{-i k' x}
$$

where
\[ \frac{\hbar^2 k^2}{2m} = E - U_0 > 0 \]

Note: \( U_0 < 0 \Rightarrow E - U_0 = E + |U_0| > E \)
\[ U_0 > 0 \Rightarrow E - U_0 < E \]

B.C.'s: \[ A_I e^{-ika} + B_I e^{ika} = A_{II} e^{-ike} + B_{II} e^{ike} \]
\[ ike(A_{II} e^{-ika} - B_I e^{ika}) = ike(A_{II} e^{-ike} - B_{II} e^{ike}) \]

\[ \begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1} = \frac{1}{\Delta} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}, \Delta = ad - bc \]

\[ \Rightarrow \begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix} = M_L \begin{pmatrix} A_I \\ B_I \end{pmatrix} \]
\[ M_L = \text{transfer matrix} \]

\[ \begin{pmatrix} e^{-ika} & e^{i\alpha} \\ ike & -ike \end{pmatrix} \begin{pmatrix} A_I \\ B_I \end{pmatrix} = \begin{pmatrix} e^{-i\alpha} & e^{i\alpha} \\ ike & -ike \end{pmatrix} \begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix} \]

\[ \Rightarrow M_L = \begin{pmatrix} (e^{-ika} & e^{i\alpha} \\ ike & -ike \end{pmatrix}^{-1} = \begin{pmatrix} e^{-ika} & e^{i\alpha} \\ ike & -ike \end{pmatrix} \]

\[ M_L = \begin{pmatrix} (e^{-ika} & e^{i\alpha}) \\ ike & -ike \end{pmatrix}^{-1} \begin{pmatrix} (e^{-i\alpha} & e^{i\alpha} \\ ike & -ike \end{pmatrix} \]
Notice that \( \det M_L = \frac{k}{k'} \).

For the B.C. at \( x = a \) we do the same and find:

\[
\begin{pmatrix}
A_\Pi \\
B_\Pi
\end{pmatrix} = M_R
\begin{pmatrix}
A_I \\
B_I
\end{pmatrix}
\]

By symmetry, \( M_R \) is the matrix obtained from \( M_L \) by replacing \( k \leftrightarrow k' \) and \( a \leftrightarrow -a \):

\[
M_R =
\begin{pmatrix}
\left( \frac{k+k'}{2k} \right) e^{i(k-k')a} & \left( \frac{k-k'}{2k} \right) e^{-i(k+k')a} \\
\left( \frac{k-k'}{2k} \right) e^{i(k+k')a} & \left( \frac{k+k'}{2k} \right) e^{-i(k-k')a}
\end{pmatrix}
\]

and \( \det M_R = \frac{k'}{k} \)

\[
\Rightarrow \begin{pmatrix}
A_\Pi \\
B_\Pi
\end{pmatrix} = M_R
\begin{pmatrix}
A_I \\
B_I
\end{pmatrix} = M
\begin{pmatrix}
A_I \\
B_I
\end{pmatrix}
\]

Note: \( \det M = \det M_R \det M_L = 1 \)

and \( M = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix} \)
\[ \alpha = e^{-i2ka} \left[ \cos(2k'a) + i \left( \frac{k^2 + k'^2}{2kk'} \right) \sin(2k'a) \right] \]

\[ \beta = -i e^{-i2ka} \left( \frac{k'^2 - k^2}{2kk'} \right) \sin(2k'a) \]

check \quad \| \alpha \|^2 - |\beta|^2 = \det M = 4

\Rightarrow \beta_{II} = \beta^* A_{II} + \alpha^* B_{II}

\Rightarrow \frac{B_{II}}{A_{II}} = -\frac{\beta^*}{\alpha^*} \quad \text{reflected amplitude}

\beta_{III} = \alpha A_{II} + \beta B_{II}

\frac{A_{III}}{A_{II}} = \alpha + \beta \left( -\frac{\beta^*}{\alpha^*} \right) = \frac{|\alpha|^2 - |\beta|^2}{\alpha^*} \quad \text{transmitted amplitude}

\Rightarrow S(E) = \frac{A_{III}}{A_{II}} = \frac{1}{\alpha^*} \quad \text{transmitted amplitude}
$$T(E) = \left| S(E) \right|^2 = \frac{1}{\left| k \right|^2}$$

$$\left| k \right|^2 = \cos^2 (2k'a) + \left( \frac{k^2 + k'^2}{2kk'} \right)^2 \sin^2 (2k'a)$$

$$k^2 = \frac{2mE}{\hbar^2}$$

$$k'^2 = \frac{2m}{\hbar^2} \left( E - U_0 \right)$$

$$\frac{k^2 + k'^2}{2kk'} = \frac{2E - U_0}{2\sqrt{E(E-U_0)}}$$

This solution is valid for all $E > 0$ if $U_0 < 0$ or $E > U_0$ if $U_0 > 0$.

For $U_0 > 0$ the solution is somewhat different (see problem set).

and

$$\left( \frac{k^2 + k'^2}{2kk'} \right)^2 = 1 + \frac{U_0^2}{4E(E-U_0)}$$

$$\Rightarrow \left| k \right|^2 = 1 + \frac{U_0^2}{4E(E-U_0)} \sin^2 (2k'a)$$

$$\Rightarrow T(E) = \frac{1}{1 + \frac{U_0^2}{4E(E-U_0)} \sin^2 (2k'a)}$$

Notice that if $2k'a = \pi n \Rightarrow \left| k \right| = \frac{n\pi}{2a}$

$$E_n = U_0 + \frac{n^2\pi^2}{8ma^2}$$

Then the e.v.'s of this wave function.

$$T(E_n) = 1$$

maximum transmission.
Phasor shift:

\[ \delta(E) = \arg S(E) = \arg \alpha \]

\[ \Rightarrow \delta(E) = -2ka + \tan^{-1} \left[ \frac{k^2 + k'^2}{2kk'} \tan(2ka) \right] \]

\[ \delta(E) = -2ka + \tan^{-1} \left[ \frac{E - U_0}{2\sqrt{E(E - U_0)}} \tan(2ka) \right] \]

At perfect transmission, i.e. \( 2ka = n\pi \)

\[ \Rightarrow \delta(E_n) = -2n\pi \]

Behavior of \( S(E) \)

\[ S(E) = \frac{1}{\alpha^*} = \frac{e^{-ika}}{\cos(2ka) - \frac{\zeta}{2} \left( \frac{k^2 + k'^2}{k} \right) \sin(2ka)} \]

has poles at the (negative) \( \lambda \) values of \( E \) where the square well has bound states.

Resonant Behavior: near a resonance, i.e. when \( \tan(2ka) = 0 \), we can approximate \( (E \approx E_0) \)

\[ \left( \frac{k}{k'} + \frac{k'}{k} \right) \tan(2ka) \approx 4 \left( \frac{E - E_0}{\lambda} \right) \]

where \( E_0 \) is the energy of the resonance, and
The quantity $\Gamma$ is defined by

$$\frac{\hbar}{\Gamma} = \left( \frac{k'}{k} + \frac{|k|}{k} \right) \frac{\partial}{\partial E} \frac{\hbar}{\Gamma} \frac{dE}{dE} \bigg|_{E = E_0}$$

\(\Rightarrow\) Close to a resonance, \(S(E)\) behaves like

$$S(E) = \frac{1}{\cos(2k'a)} \frac{c^2 \Gamma/2}{E - E_0 + i\frac{\Gamma}{2}}$$

when \(\cos(2k'a) \approx 1\)

\(\Rightarrow\) \(S(E)\) has a pole at \(E_0 - i\frac{\Gamma}{2}\)

bound

\[\text{Im } E\]

branch cut of \(\sqrt{E}\) (just below real axis)

\[\text{Re } E\]

resonance

at \(E_0 - i\frac{\Gamma}{2}\)

on 2nd Riemann sheet

\(\Rightarrow\) bound states are poles of \(S(E)\) on the negative real axis.

We also see that the phase shift near a resonance is

$$\delta(E) = \tan^{-1} \left[ \frac{2}{\Gamma} (E - E_0) \right]$$

and

$$\frac{d\delta}{dE} = \frac{2\Gamma}{\left(1 + \left(\frac{2(E - E_0)}{\Gamma}\right)^2\right)^{\frac{3}{2}}} \rightarrow \text{maximum at resonance}.$$