tells us that $\psi(x)$, and thus the probability density $|\psi(x)|^2$, is zero in an <u>interval</u> 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~~ 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 for $|x| \to \infty$ the fall off of ~~the~~ wave function is exponential (as we saw before). At the turning point $\psi(x)$ has an <u>inflection point</u> (i.e. a point where the curvature changes sign). ~~To the~~ Outside the region comprised ~~by~~ <u>outside</u> the inflection points the wave function cannot have zeros since ψ'' has the same sign as ψ in that region.

In the region comprised between the two inflection points, $E > U(x)$. ~~and~~ If $U(x)$ varies slowly enough it is easy to see that the wave function <u>can</u> oscillate in this region. In particular it can have zeros. If $U(x)$ is finite everywhere $\Rightarrow$ the zeros of $\psi(x)$ are isolated points.

What do the zeros of $\psi(x)$ tell us? There is an interesting <u>Oscillation Theorem</u> (which only holds in $d=1$). It states the following. Consider a set of wave functions $\psi_n(x)$ which constitute the <u>discrete</u> part of the energy spectrum with eigenvalues $\{E_n\}$. Without loss of generality we can order the e.v.'s (and the states) as $E_0 < E_1 < E_2 < \cdots$

Let ψ_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 <u>zeroes or nodes</u>.

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

$$\hat{H}\psi = E\psi \quad \text{and}$$

$$\langle\psi|\hat{H}|\psi\rangle = E \quad \text{and} \quad \int dx\, |\psi(x)|^2 = 1$$

$$\Rightarrow \quad E = \langle\psi|\hat{T}|\psi\rangle + \langle\psi|\hat{U}|\psi\rangle$$

but

$$\langle\hat{T}\rangle = \int dx\, \psi^*(x) \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\psi(x) =$$

$$= \frac{\hbar^2}{2m}\int dx \left|\frac{d\psi}{dx}\right|^2$$

and $\langle\hat{U}\rangle = \int dx\, U(x)\, |\psi(x)|^2$

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

$\Rightarrow$ in order to lower the $\langle\hat{T}\rangle$ we want wave functions with small derivatives and in order to lower $\langle\hat{U}\rangle$ we want wave functions peaked ~~at~~ where

$U(x)$ is small. These two requirements are clearly in conflict with each other. However if a wave function $\psi_n(x)$ has n nodes on average its derivative will be larger (in abs. value) than that of ψ_{n-1} which has $n-1$ nodes. Also ψ_n will be larger away from its nodes than close to them. $\Rightarrow$ wave functions with n nodes are more spread out than 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 ψ_1 and ψ_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 ψ_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 Eqn. for ψ_1 and ψ_2

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}(E_1 - U(x))\,\psi_1(x) = 0$$

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E_2 - U(x))\,\psi_2(x) = 0$$

$$W(\psi_1,\psi_2)\Big|_a^b = \left(\psi_1'(x)\,\psi_2(x) - \psi_2'(x)\,\psi_1(x)\right)\Big|_a^b =$$

$$= \int_a^b dx\,\frac{d}{dx}\left(\psi_1'(x)\,\psi_2(x) - \psi_2'(x)\,\psi_1(x)\right)$$

$$= \int_a^b dx\,\left(\psi_1''(x)\,\psi_2(x) - \psi_2''(x)\,\psi_1(x)\right)$$

$$= \int_a^b dx\,\frac{2m}{\hbar^2}\left[(\cancel{U(x)} - E_1)\,\psi_2\psi_1 - (\cancel{U(x)} - E_2)\,\psi_1\psi_2\right]$$

$$= \frac{2m}{\hbar^2}(E_2 - E_1)\int_a^b dx\,\psi_2(x)\,\psi_1(x)$$

Since $\psi_1(a) = \psi_2(b) = 0 \Rightarrow$

$$\psi_1'(x)\,\psi_2(x)\Big|_a^b = \frac{2m}{\hbar^2}(E_2 - E_1)\int_a^b dx\,\psi_2(x)\,\psi_1(x)$$

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 ψ_2 does <u>not</u> 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 ψ_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

<u>Contradiction</u> $\Rightarrow$ ~~ψ_2 must~~ if $E_2 > E_1 \Rightarrow \psi_2$ must have a zero lying between a pair of zeros of ψ_1.

$\Rightarrow$ if ψ_1 has n zeros $\Rightarrow \psi_2$ must have $n+1$ zeros.

In particular the wave function $\psi_0(x)$ for the lowest energy eigenvalue E_0, the ground state, has no <u>zeros</u> in the entire interval (except possibly at the boundaries).

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Simple $d=1$ QM problems

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 $0 \leq x < L$ the particle is free.

The solutions of the Schrödinger Equation in this region are $e^{\pm ikx}$ when $E = \frac{\hbar^2 k^2}{2m}$

$$\psi(x) = A e^{ikx} + B e^{-ikx}$$

we must impose $\Rightarrow \psi(0) = \psi(L) = 0$ (as $U \to \infty$ at $x = 0, L$)

Note that since $U = \infty$ for $x > L$ and $x < 0$

$\Rightarrow \psi'$ is <u>not</u> continuous at $x = 0, L$.

What do these BC's imply?

$\psi(0) = 0 \Rightarrow \quad A + B = 0$

$\psi(L) = 0 \Rightarrow \quad A e^{ikL} + B e^{-ikL} = 0$

$\Rightarrow A = -B \Rightarrow A \sin kL = 0$

$\Rightarrow k_n L = n\pi \quad (n \in \mathbb{N}^+) \Rightarrow$ quantization!

$k_n = \frac{n\pi}{L}$ are the <u>allowed</u> 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

$$E_1 = \frac{\pi^2 \hbar^2}{2mL^2} \qquad n=1$$

The first excited state has energy

$$E_2 = \frac{\pi^2 \hbar^2}{2mL^2} \times 4 = 4E_1$$

and $E_n = n^2 E_1$

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

$$\left(E_{n+1} - E_n = \frac{\pi^2\hbar^2}{2mL^2}(2n+1)\right)$$

wave functions must be normalized:

$$\int |\psi_n|^2 dx = 1 \Rightarrow \int_0^L dx\, A_n^2 \sin^2(k_n x) = 1$$

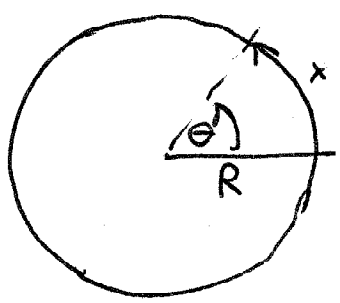
$$1 = \frac{A_n^2}{2k_n} \Rightarrow A_n = \sqrt{2k_n} = \sqrt{\frac{2n\pi}{L}}$$

$$\psi_n(x) = \sqrt{\frac{2\pi n}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad \text{with} \quad E_n = \frac{\pi^2\hbar^2 n^2}{2mL^2}$$

2) Particle on a circle

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

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



~~x~~ Same as $x = \theta R$ with $0 < \theta < 2\pi$ and

$$L = 2\pi R$$

("compactified")

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

$\psi_n \sim e^{ik_n x}$ 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 <u>any</u> integer; ~~positive~~ positive or negative.

What is the energy?

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

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

$\Rightarrow$ the solutions are <u>degenerate</u> since $E_n = E_{-n}$ corresponding to particles 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

$$\psi_n = A_n e^{i k_n x}$$

$$\int_0^L dx \, |\psi_n(x)|^2 = 1 \Rightarrow A_n^2 L = 1$$

$$\Rightarrow A_n = \frac{1}{\sqrt{L}}$$

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

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

Why do we have a degeneracy?

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Because the particle moves on a circle $\Rightarrow$ there is no preferred origin $\Rightarrow$ we have translation invariance $\Rightarrow$ $\hat{P}$ is a generator of a symmetry and $[\hat{P}, \hat{H}] = 0 \Rightarrow$ 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 $p_n = \hbar k_n = \dfrac{2\pi n \hbar}{L}$

$\Rightarrow$ states with $E_n = E_{-n}$ are labelled by the sign of their momentum. Notice that in the case of a particle ~~or~~ in an ∞ ~~potential~~ potential well translation invariance is broken by the potential $\Rightarrow$ momentum is <u>not</u> a good quantum number ~~and~~ and the eigenstates of $\hat{H}$ are <u>not</u> 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 ($L \to \infty$) and that ~~there is a potential~~ the potential energy is sharply concentrated at $x = 0$

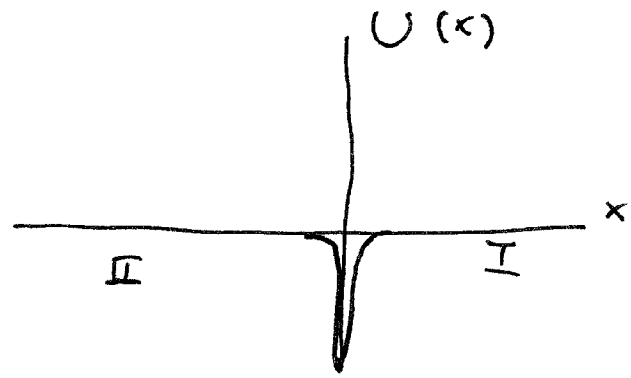
$$U(x) = -|g|\,\delta(x)$$

i.e. $U(x)$ is very large and negative for $x \sim 0$ and zero everywhere else. Note: the units of $|g|$ are energy $\times$ 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 translation invariance $\Rightarrow [\hat{P}, \hat{H}] \neq 0 \Rightarrow$ 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:

$$\int_{-\infty}^{+\infty} dx \; |\psi(x)|^2 = 1$$

$\Rightarrow$ For $x>0$ the only allowed solution is

$$\psi_I = A_I \, e^{-k_I x} \longrightarrow 0 \quad \text{as } x \to +\infty$$

and for $x<0$

$$\psi_{II} = B_{II} \, e^{k_{II} x} \longrightarrow 0 \quad \text{as } x \to -\infty$$

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

$\Rightarrow$ $k_I = k_{II} = k$ and $|E| = \frac{\hbar^2 k^2}{2m}$

Q: What is the effect of $U(x)$? $\Leftrightarrow$ What B.C.'s are satisfied at $x=0$?

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}\left(E - U(x)\right)\psi$$

$$\Rightarrow \int_{-\varepsilon}^{\varepsilon} dx \, \frac{d^2\psi}{dx^2} = \psi'(\varepsilon) - \psi'(-\varepsilon) = \text{jump in } \psi'$$

ε small

$$\int_{-\varepsilon}^{\varepsilon} dx \, \frac{d^2\psi}{dx^2} = \int_{-\varepsilon}^{\varepsilon} dx \, \frac{2m}{\hbar^2} \left(U(x) - E\right) \psi(x)$$

$$\int_{-\varepsilon}^{\varepsilon} dx \, U(x) \, \psi(x) = -|g| \int_{-\varepsilon}^{\varepsilon} dx \, \delta(\varepsilon) \, \psi(x)$$

$$= -|g| \, \psi(0)$$

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

$\Rightarrow$ $\psi(x)$ is continuous at $x = 0$ but $\psi'(x)$ is discontinuous at $x = 0$

① Continuity: $\psi_I(0) = \psi_{II}(0)$

$$\Rightarrow A_I = B_{II} \equiv A = \psi(0)$$

② $\psi_I' = -AK \, e^{-Kx} \Rightarrow \psi_I'(0) = -KA$

$\psi_{II}' = AK \, e^{Kx} \Rightarrow \psi_{II}'(0) = +KA$

$\Rightarrow$ ~~$\psi_I'(0) = \psi$~~ $\psi_I'(0) - \psi_{II}'(0) = -\dfrac{2m}{\hbar^2}|g| \psi(0)$

$$(-KA) - (KA) = -\frac{2m|g|}{\hbar^2} A$$

$\Rightarrow$ $K = \dfrac{m|g|}{\hbar^2}$ (check the units!)

Energy: $E = -\frac{\hbar^2}{2m}\frac{m^2 g^2}{\hbar^4}$

$$\Rightarrow \quad E = -\frac{m g^2}{2\hbar^2} < 0$$

Normalization:

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

$$\Rightarrow \quad 1 = 2\int_0^\infty dx\, A^2 e^{-2Kx}$$

$$1 = \frac{\cancel{2}A^2}{\cancel{2}K} \Rightarrow \quad A = \sqrt{K} = \sqrt{\frac{m|g|}{\hbar^2}}$$

$$\Rightarrow \quad \psi_0(x) = \sqrt{\frac{m|g|}{\hbar^2}}\, e^{-K|x|}$$

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

is the ground state energy

$\Rightarrow$ There is exactly one bound state with energy E_0.

<u>Positive energy states:</u> These 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

$$\left[E + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\psi(x) = g\,\delta(x)\,\psi(x)$$
$$\equiv g\,\delta(x)\,\psi(0)$$

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

$$\psi_{inc}(x) = \frac{1}{\sqrt{2\pi\hbar}}\, e^{\pm ikx} \qquad k = \frac{1}{\hbar}\sqrt{2mE}$$
$$(E>0)$$

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

Let us check that

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

① $$\left[E + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right]\psi_{inc} = \left(E - \frac{\hbar^2k^2}{2m}\right)\psi_{inc} = 0$$

since $E = \dfrac{\hbar^2k^2}{2m}$

2) $$\left(E + \frac{\hbar^2}{2m}\frac{d^2}{dx^2}\right)\int_{-\infty}^{+\infty}\frac{dp}{2\pi\hbar}\;\frac{e^{ipx/\hbar}}{E - p^2/2m}\; g\,\psi(0) =$$

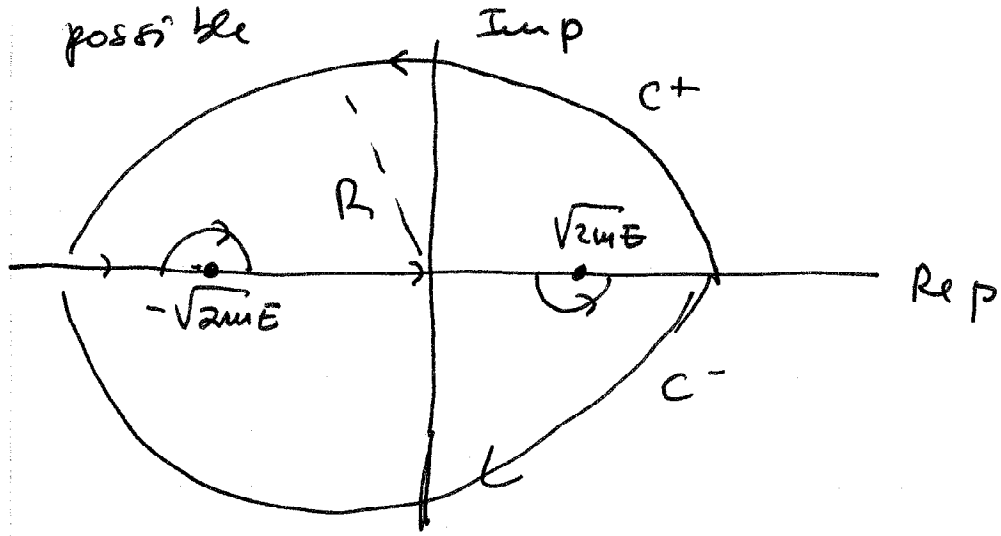
$$= \int_{-\infty}^{+\infty}\frac{dp}{2\pi\hbar}\left(\frac{E - p^2/2m}{E - p^2/2m}\right) e^{ipx/\hbar}\; g\,\psi(0)$$

$$= \delta(x)\, g\,\psi(0) \quad \checkmark$$

This is <u>almost</u> 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 <u>defining</u> an integration path on the complex $\mathbb{P}$ plane which avoids the poles. However there are different choices of paths (and hence $\neq$ integrals). These $\neq$ choices turn out to correspond to $\neq$ possible boundary conditions.

Suppose we want a solution with the B.C. that for $x > 0$ is an <u>outgoing wave</u> (i.e. right moving). This solution is obtained by

The following choices of integration paths are possible



Which one should we choose? This is the same as moving the poles up and down infinitesimally and hence to the replacement $E - \frac{p^2}{2m} \to E - \frac{p^2}{2m} + i\varepsilon$

$(\varepsilon > 0)$

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

For outgoing waves $(x > 0)$ we choose C_+ and close the path ~~out~~ on the upper ½ plane.

$\Rightarrow$ the pole enclosed by the path is at $\sqrt{2mE} + i\varepsilon$

Hence, for $x > 0$, the integral is

$$\int_{-\infty}^{+\infty} \frac{dp}{2\pi\hbar} \frac{e^{ipx/\hbar}}{E - \frac{p^2}{2m} + i\varepsilon} = \oint_{\Gamma^+} \frac{dp}{2\pi\hbar} \frac{e^{ipx/\hbar}}{E - \frac{p^2}{2m} + i\varepsilon}$$

$$= 2\pi i \, \mathrm{Res}\left[\frac{1}{2\pi\hbar} \frac{e^{ipx/\hbar}}{E - \frac{p^2}{2m} + i\varepsilon} ; \quad p = \sqrt{2mE} + i\varepsilon \right]$$

$$= 2\pi i \, \frac{1}{2\pi\hbar} \frac{e^{\frac{i}{\hbar}\sqrt{2mE}\, x}}{-\frac{1}{m}\sqrt{2mE}}$$

$$= \frac{m}{i\hbar\sqrt{2mE}} e^{\frac{i}{\hbar}\sqrt{2mE}\, x} \qquad x > 0$$

Conversely, for $x < 0$, we choose Γ^- (i.e. we close on the lower ½plane) and the ~~at~~ enclosed pole is now at $-\sqrt{2mE} - i\varepsilon \Rightarrow$

$$\int = -2\pi i \, \frac{1}{2\pi\hbar} \frac{e^{-\frac{i}{\hbar}\sqrt{2mE}\, x}}{-\frac{1}{m}(-\sqrt{2mE})}$$

$$= \frac{m}{i\hbar\sqrt{2mE}} e^{-\frac{i}{\hbar}\sqrt{2mE}\, x} \qquad x < 0$$

which is also outgoing.

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

$$\psi(x) = \psi_{inc}(x) + \frac{mg}{i\hbar\sqrt{2mE}} e^{\frac{i}{\hbar}\sqrt{2mE}|x|} \psi(0)$$

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

$$\psi(0) = \psi_{inc}(0) + \frac{mg}{i\hbar\sqrt{2mE}} \psi(0)$$

$$\Rightarrow \psi(0) = \frac{i\hbar p}{i\hbar p - mg} \psi_{inc}(0) \quad \text{where } p=\sqrt{2mE}$$

If we choose a right moving incident wave

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$$\psi_{inc}(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \Rightarrow$$

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$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \left[e^{ipx/\hbar} + \frac{mg}{ip\hbar - mg} e^{ip\frac{|x|}{\hbar}} \right]$$

For $x>0$, $\psi(x) = \psi_{transmitted}(x)$

$$\Rightarrow \psi_{trans}(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \left(1 + \frac{mg}{i\hbar p - mg} \right)$$

$$= \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \frac{i\hbar p}{i\hbar p - mg}$$

Let us write ψ_{trans} in the form

$$\psi_{trans}(x) = \frac{A(E)}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$$

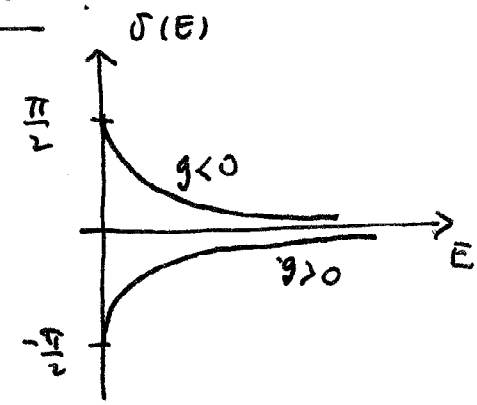
Notice that in the absence of the potential, $A(E)=1$.

The <u>complex</u> number $A(E)$ is called the transmitted amplitude. For this problem it is given by

$$S(E) \equiv A(E) = \frac{i\hbar\sqrt{2mE}}{i\hbar\sqrt{2mE} - mg} = \left(\frac{E}{E + \frac{m^2g^2}{2\hbar^2}}\right)^{1/2} e^{i\delta(E)}$$

where $\delta(E)$ is the <u>phase shift</u>:

$$\delta(E) = -\,\mathrm{sgn}(g)\,\tan^{-1}\sqrt{\frac{mg^2}{2\hbar^2 E}}$$



The transmission amplitude $S(E)$ is related to the <u>transmission coefficient</u>

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

for the δ-function potential $T(E)$ is monotonic.

Notice that $S(p) = \dfrac{i\hbar p}{i\hbar p - mg}$ has

a pole at $p = -\dfrac{img}{\hbar}$ which lies on the

imaginary axis. ~~However for~~ This (imaginary) pole

is called a <u>resonance</u>. However for attractive

interactions, as a function of <u>energy</u>, this

pole appears on the real axis as the

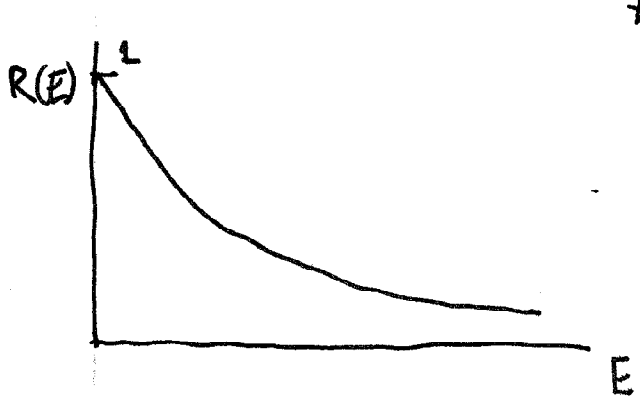
bound state discussed before.

What about the reflected amplitude $S_r(E)$

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

$$S_r(E) = \frac{mg}{ip\hbar - mg} = \frac{mg}{i\hbar\sqrt{2mE} - mg}$$

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



Notice that,

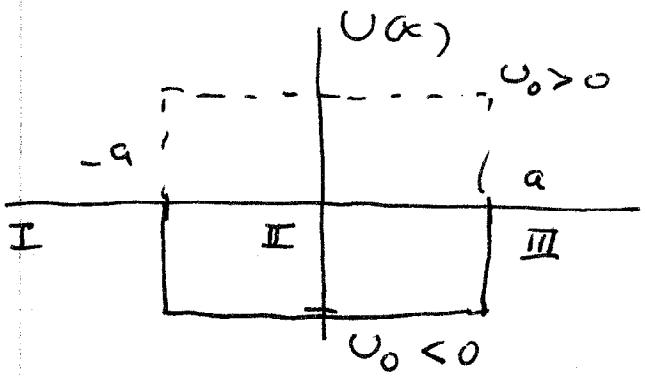
$R(E) + S(E) = 1$ conservation of probability

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.



Note that if we let $a \to 0$ and $U_0 \to \infty$ and keep $2aU_0 \equiv g$ fixed we have a δ-function potential with strength g.

Also, for $U_0 \to -\infty$ we recover the ∞ 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:

$$I = \{ x < -a \}$$

$$II = \{ |x| < a \}$$

$$III = \{ x > a \}$$

States with $E < 0$ must have wave functions which vanish as $|x| \to \infty$

Before solving these equations in their full glory we note the following general property:

<u>Parity</u> : Let $U(x) = U(-x)$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + U(x)\,\psi(x) = E\,\psi(x)$$

$$x \to -x \quad \to \quad -\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2} + U(-x)\,\psi(-x) = E\,\psi(-x)$$

but $U(-x) = U(x) \Rightarrow$

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

$$\hat{\mathcal{P}}^{+} = \hat{\mathcal{P}}^{-1} = \hat{\mathcal{P}}$$

$$\Rightarrow \quad \mathcal{P}^{+}\hat{H}\,\hat{\mathcal{P}} = \hat{H} \qquad \text{if} \quad U(x) = U(-x)$$

$\Rightarrow$ The eigenstates of $\hat{\mathcal{P}}$ are eigenstates of $\hat{H}$ since $[\hat{\mathcal{P}}, \hat{H}] = 0$

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

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

$\Rightarrow$ <u>even</u> w.f's have $\oplus$ e.v. and <u>odd</u> w.f.'s have $\ominus$ e.v. $\Rightarrow$ we can choose the solutions to be <u>even</u> or <u>odd</u>

<u>Region I</u>: The Eqn. is

$$-\frac{\hbar^2}{2m}\psi_I'' = E\,\psi_I \qquad E<0$$

$$\Rightarrow \quad \psi_I'' = \frac{2m|E|}{\hbar^2}\,\psi_I$$

$$\Rightarrow \quad \psi_I = e^{\pm K x} \qquad \text{with } K^2 = \frac{2m|E|}{\hbar^2}$$

The B.C $\Rightarrow$ $\psi_I \to 0$ as $x \to -\infty$ if

we choose the $\oplus$ root

$\Rightarrow$ for $x < -a \Rightarrow \psi_I(x) = A_I\, e^{Kx}$

<u>Region III</u> same story but now

for $x > a \Rightarrow \psi_{III}(x) = B_{III}\, e^{-Kx}$

which is the solution that vanish a $x \to +\infty$

$\Rightarrow$ even states $\Rightarrow$ $B_{III} = A_I$

odd state $\Rightarrow$ $B_{III} = -A_I$

<u>Region II</u>: the solutions are now oscillatory

with

$$\psi_{II} = A_{II}\, e^{ikx} + B_{II}\, e^{-ikx}$$

where $k^2 = -\frac{2m}{\hbar^2}\left(|E| - |U_0|\right)$ for $E<0$, $U_0<0$

even states $\Rightarrow$ $A_{II} = B_{II}$

odd states $\Rightarrow$ $A_{II} = -B_{II}$

$\Rightarrow$ even states
$$\psi(x) = \begin{cases} A_I^e\, e^{\kappa x} & x<-a \\ A_{II}^e \cos kx & |x|\le a \\ A_I^e\, e^{-\kappa x} & x>a \end{cases}$$

odd states
$$\psi(x) = \begin{cases} A_I^o\, e^{\kappa x} & x<-a \\ A_{II}^o \sin kx & |x|\le a \\ -A_I^o\, e^{-\kappa x} & x>a \end{cases}$$

B.C.'s: $x=a$
$$\psi_{II}(a) = \psi_{III}(a)$$
$$\psi_{II}'(a) = \psi_{III}'(a)$$

$$\Rightarrow \quad A_{II}^{e} \cos ka = A_I^e\, e^{-\kappa a}$$
$$-k A_{II} \sin ka = -A_I^e\, \kappa\, e^{-\kappa a}$$
for even states.

There is a non zero solution iff. the system is linearly dependent $\Rightarrow$ the determinant must vanish $\Rightarrow$ $\boxed{\tan(ka) = \frac{K}{k}}$ for even states.

The allowed states satisfy this quantization condition

and $A_{II}^{e} = A_{II}^{e} \, e^{Ka} \cos ka$

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

for odd states we have:

$$-A_I^o \, e^{-Ka} = A_{II}^o \sin ka$$

$$A_I^o \, K \, e^{-Ka} = A_{II}^o \, k \cos ka$$

$\Rightarrow$ the quantization condition now is:

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

and $A_I^o = \frac{k}{K} e^{Ka} \cos(ka) \, A_{II}^o$

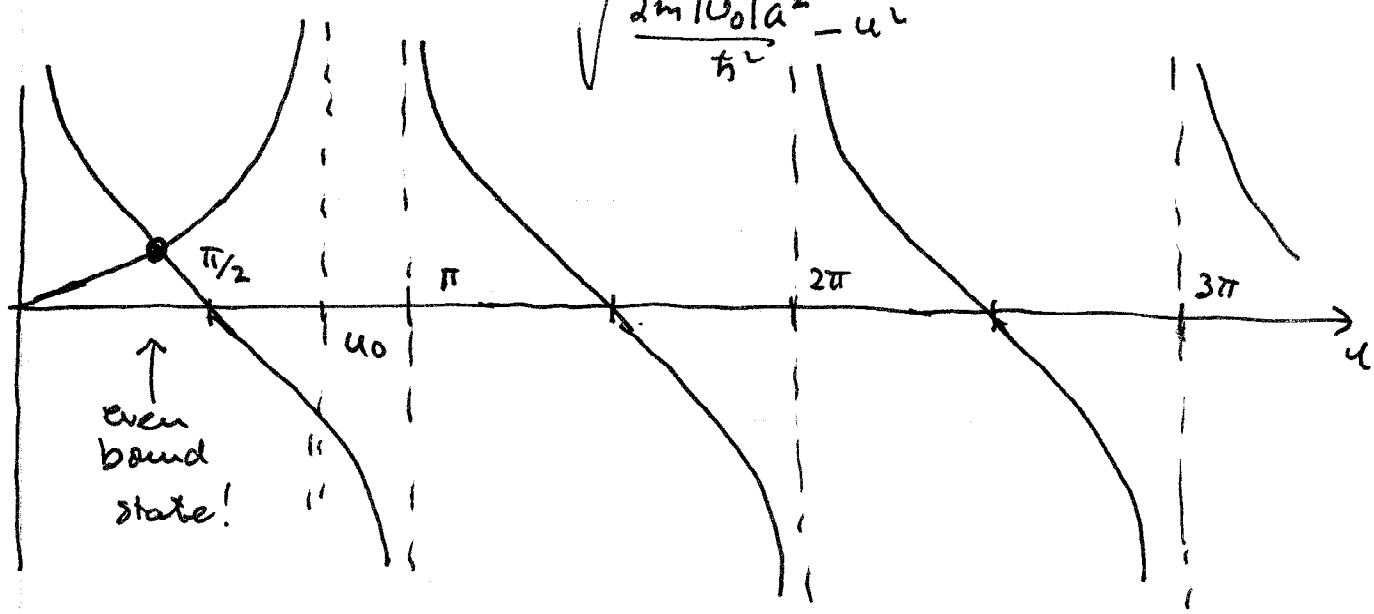
since $\quad k^2 = \dfrac{2m|U_0|}{\hbar^2} - K^2 > 0$

$$\Rightarrow \quad K^2 = \frac{2m|U_0|}{\hbar^2} - k^2 > 0$$

$$\Rightarrow \quad \tan(ka) = \frac{K}{k} = \sqrt{\frac{2m|U_0|}{\hbar^2 k^2} - 1}$$

or if $u = ka \quad \Rightarrow \qquad u_0^2 = \dfrac{2m|U_0|a^2}{\hbar^2}$

$$\cot u = \frac{k}{K} = \frac{u}{\sqrt{\dfrac{2m|U_0|a^2}{\hbar^2} - u^2}}$$



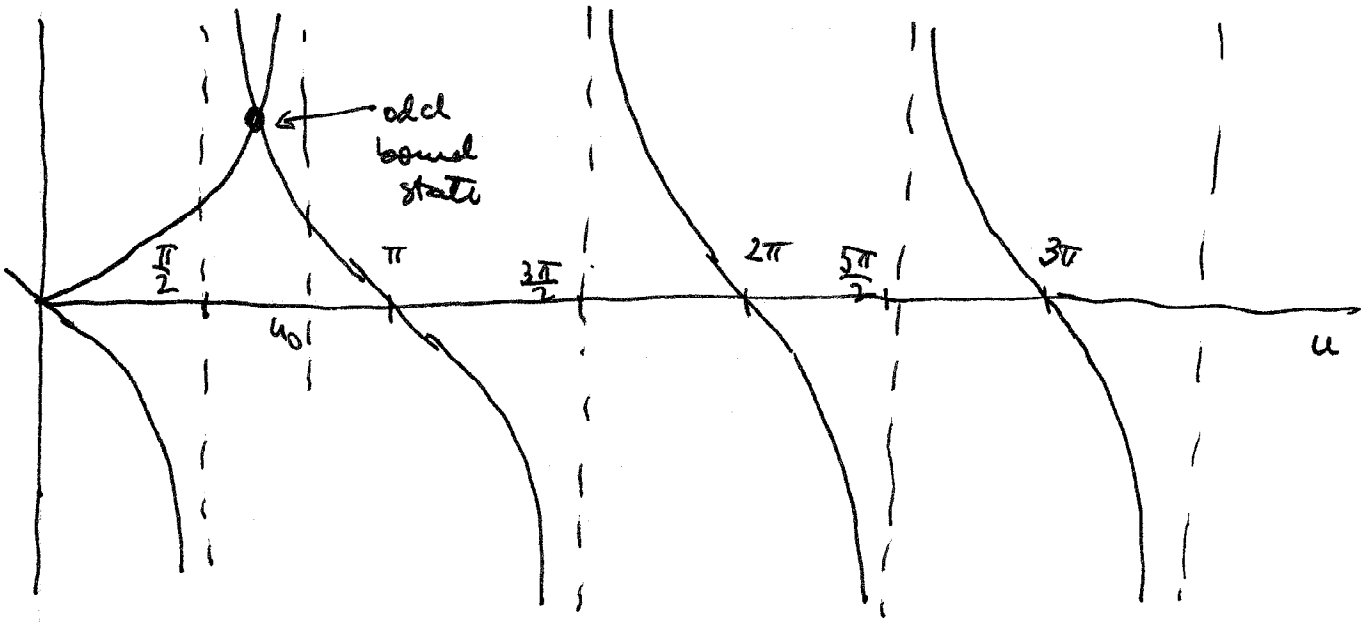
$\Rightarrow$ if $u_0 < \pi \Rightarrow$ 1 <u>even</u> bound state

if $\pi < u_0 < 2\pi \Rightarrow$ 2 <u>even</u> bound states etc.

For the odd states we have instead:

$$\tan u = -\frac{k}{K} \Rightarrow \quad -\tan u = \frac{+u}{\sqrt{u_0^2 - u^2}}$$

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 $\frac{\pi}{2} < u < \pi$, $\frac{3\pi}{2} < u < 2\pi$, etc.

while the even bound states are in the complementary regions $0 < u < \frac{\pi}{2}$, $\pi < u < \frac{3\pi}{2}$, etc.

Also there is <u>always</u> an even bound state but the first odd bound state only appears if

$$u_0 > \frac{\pi}{2} \Rightarrow \frac{2m\,|U_0|\,a^2}{\hbar^2} > \frac{\pi^2}{4}$$

$$\Rightarrow |U_0| > \frac{\pi^2\hbar^2}{8ma^2}$$ to have at least 1 odd bound state.

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<u>Scattering states</u>: It turns out that for scattering states it is not convenient to use the even-odd basis since these ~~are~~ are stationary states. We will use ~~[illegible]~~ instead <u>travelling waves</u>, as in the case of the δ-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

$$\psi_{III} = A_{III}\, e^{ikx} \qquad \frac{\hbar^2 k^2}{2m} = E > 0$$

and

$$\psi_I = A_I\, e^{ikx} + B_I\, e^{-ikx}$$ with

the same k. A_I is the <u>incident amplitude</u> B_I is the reflected (outgoing) amplitude and $A_{III} = S(E)$ is the transmitted amplitude.

In region II we have

$$\psi_{II} = A_{II}\, e^{ik'x} + B_{II}\, e^{-ik'x}$$ 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 : $x = -a$

$$A_I e^{-ika} + B_I e^{ika} = A_{II} e^{-ik'a} + B_{II} e^{ik'a}$$

$$ik\left(A_{II} e^{-ika} - B_I e^{ika}\right) = ik'\left(A_{II} e^{-ik'a} - B_{II} e^{ik'a}\right)$$

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

$$\Rightarrow \begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix} = M_L \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

$M_L =$ transfer matrix

$$\begin{pmatrix} e^{-ika} & e^{+ika} \\ ik e^{-ika} & -ik e^{ika} \end{pmatrix}\begin{pmatrix} A_I \\ B_I \end{pmatrix} = \begin{pmatrix} e^{-ik'a} & e^{ik'a} \\ ik' e^{-ik'a} & -ik' e^{ik'a} \end{pmatrix}\begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix}$$

$$\Rightarrow M_L \begin{pmatrix} e^{-ik'a} & e^{ik'a} \\ ik' e^{-ik'a} & -ik' e^{ik'a} \end{pmatrix}^{-1}\begin{pmatrix} e^{-ika} & e^{ika} \\ ik e^{-ika} & -ik e^{ika} \end{pmatrix}$$

$$\Rightarrow M_L = \begin{pmatrix} \left(\frac{k'+k}{2k'}\right) e^{i(k'-k)a} & \left(\frac{k'-k}{2k'}\right) e^{i(k'+k)a} \\ \left(\frac{k'-k}{2k'}\right) e^{-i(k+k')a} & \left(\frac{k'+k}{2k'}\right) e^{-i(k'-k)a} \end{pmatrix}$$

Notice that $\det M_L = \frac{k}{k'}$

For the B.C. at $x = a$ we do the same and find

$$\begin{pmatrix} A_{III} \\ B_{III} \end{pmatrix} = M_R \begin{pmatrix} A_{II} \\ B_{II} \end{pmatrix}$$

By symmetry M_R is the matrix obtained from M_L by replacing $k \leftrightarrow k'$ and $a \leftrightarrow -a$

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

and $\det M_R = \frac{k'}{k}$

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$$\Rightarrow \begin{pmatrix} A_{III} \\ B_{III} \end{pmatrix} = M_R M_L \begin{pmatrix} A_I \\ B_I \end{pmatrix} \equiv M \begin{pmatrix} A_I \\ B_I \end{pmatrix}$$

Note: $\det M = \det M_R \det M_L = 1$

and $M = \begin{pmatrix} \alpha & \beta \\ \beta^* & \alpha^* \end{pmatrix}$

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

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

check $\quad |\alpha|^2 - |\beta|^2 = \det M = 1$

$$\Rightarrow B_{III} = 0 = \beta^* A_I + \alpha^* B_I$$

$$\Rightarrow \frac{B_I}{A_I} = -\frac{\beta^*}{\alpha^*}$$ <u>reflected amplitude</u>

$$A_{III} = \alpha A_I + \beta B_I$$

$$\frac{A_{III}}{A_I} = \alpha + \beta\left(-\frac{\beta^*}{\alpha^*}\right) =$$ transmitted amplitude

$$\frac{A_{III}}{A_I} = \alpha - \frac{|\beta|^2}{\alpha^*} = \frac{|\alpha|^2 - |\beta|^2}{\alpha^*} = \frac{1}{\alpha^*}$$

$$\Rightarrow S(E) = \frac{A_{III}}{A_I} = \frac{1}{\alpha^*}$$ transmitted amplitude.

$$T(E) = |S(E)|^2 = \frac{1}{|\alpha|^2}$$

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

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

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

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

This solution is valid for all $E > 0$ if $U_0 < 0$ or $E > U_0$ if $U_0 > 0$. For $U_0 > E > 0$ the solution is somewhat different (see problem set)

and

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

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

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

Notice that if $2k'a = n\pi \Rightarrow \boxed{T(E_n) = 1}$

maximum transmission.

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

these are the e.v.'s of the ∞ well.

Phase shift:

$$\delta(E) = \arg S(E) = \arg \alpha$$

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

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

At perfect transmission, i.e. $2k'_n a = n\pi$

$$\Rightarrow \delta(E_n) = -n\pi$$

<u>Behavior of $S(E)$</u>

$$S(E) = \frac{1}{\alpha^*} = \frac{e^{-ika}}{\cos(2k'a) - \frac{i}{2}\left(\frac{k}{k'}+\frac{k'}{k}\right)\sin(2k'a)}$$

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

<u>Resonant Behavior</u>: near a resonance, i.e. where $\tan(2k'a) = 0$, we can approximate $(E \approx E_0)$

$$\left(\frac{k}{k'}+\frac{k'}{k}\right)\tan(2k'a) \approx 4\left(\frac{E-E_0}{\Gamma}\right)$$

where E_0 is the energy of the resonance, and

the quantity Γ is defined by

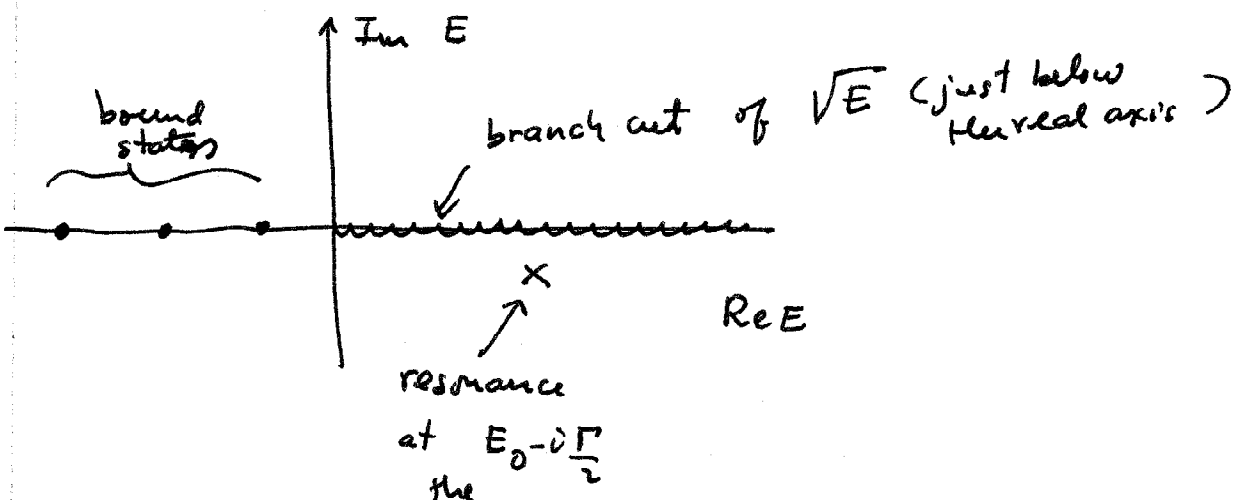
$$\frac{4}{\Gamma} = \left(\frac{k}{k'} + \frac{k'}{k}\right)\frac{1}{\hbar}\frac{dk'}{dE}\,2a\Big|_{E=E_0}$$

$\Rightarrow$ close to a resonance $S(E)$ behaves like

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

where $\cos(2ka) \simeq 1$

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



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