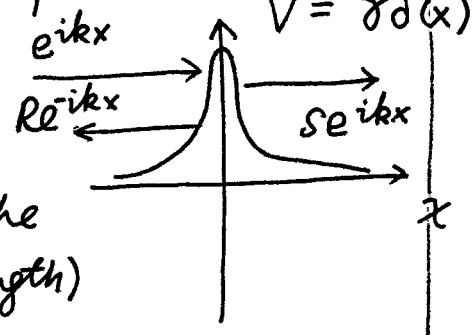


We first consider the simplest case of δ -potential $V = \gamma \delta(x)$

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



define $k = \sqrt{\frac{2mE}{\hbar^2}}$, and $a = \frac{\hbar^2}{m\gamma}$ (a carries the unit of length)

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$$\Rightarrow \frac{d^2}{dx^2} \psi + k^2 \psi = \frac{2}{a} \delta(x) \psi$$

consider the boundary condition under incident/transmission/reflection

$$\psi(x) = \begin{cases} e^{ikx} + R e^{-ikx} & x < 0 \\ S e^{ikx} & x > 0 \end{cases}$$

Q: Should $\psi(x)$ and $\psi'(x)$ be continuous at $x=0$?

A: $\psi(x)$ should be continuous but $\psi'(x)$ not

$$\int_{0^-}^{0^+} dx \frac{d^2}{dx^2} \psi + k^2 \psi = \frac{2}{a} \int_{0^-}^{0^+} dx \delta(x) \psi(x)$$

$$\psi'(0^+) - \psi'(0^-) = \frac{2\psi(0)}{a}$$

$|S|^2$ transmission coefficient

$|R|^2$ reflection coefficient!

$$\Rightarrow \begin{cases} 1 + R = S \\ ikS - ik(1-R) = \frac{2S}{a} \end{cases}$$

$$\Rightarrow \begin{cases} S = \frac{1}{1 + i/ka} \\ R = \frac{-i/ka}{1 + i/ka} \end{cases}$$

Ex: ① check that $|S|^2 + |R|^2 = 1$

② although $\psi'(x)$ is not continuous at $x=0$, but the current density

$$j_x = \frac{\hbar}{2m} \left[\psi^*(x) \frac{d}{dx} \psi(x) - \psi(x) \frac{d}{dx} \psi^*(x) \right] \text{ remains}$$

continuous at $x=0$.

Comment: (1) at low energy limit $k \rightarrow 0 \Rightarrow \begin{cases} S = \pm ika \rightarrow 0 \\ R = -1 \end{cases}$
complete reflection.

$k \rightarrow \infty$ (high energy) $\Rightarrow \begin{cases} S = 1 \\ R = \frac{-i}{ka} \rightarrow 0 \end{cases}$ complete transmission.

Analytical Continuation

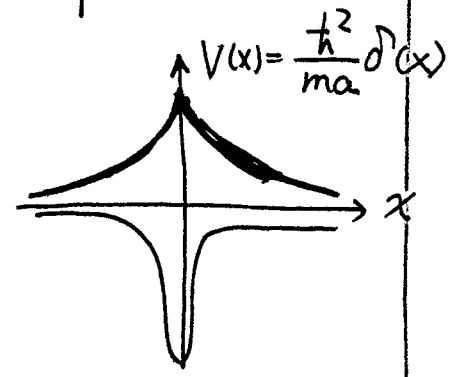
define $E_0 = \frac{\hbar^2}{2ma^2}$, we write S, R as

$$\begin{cases} S = \frac{\sqrt{E/E_0}}{\sqrt{E/E_0} \pm i} \\ R = \frac{\mp i}{\sqrt{E/E_0} \pm i} \end{cases}$$

' \pm ' refers to the case $a > 0$ and $a < 0$, respectively.

a. For the case of $a > 0$, we know that $E > 0$, there's no ambiguity for the interpretation of \sqrt{E} , and S, R are regular with respect to E .

b. For the case of $a < 0$, we know that in addition to the scattering states, which can be described by switching the sign of a , we also have bound state.



Solution for bound state:

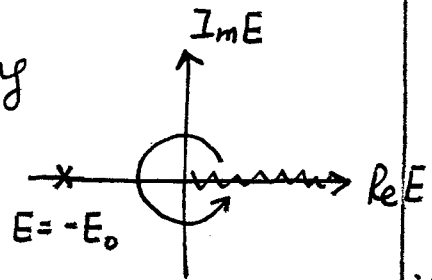
choosing $\psi = \begin{cases} e^{\beta x}, & x < 0 \\ e^{-\beta x}, & x > 0 \end{cases}$ $E = -\frac{\hbar^2 \beta^2}{2m} < 0$.

according to continuity relation, $2\beta = \frac{2}{a}$
 $\psi'(0^+) - \psi'(0^-) = \frac{2\psi(0)}{a} \Rightarrow$ or $\beta = \frac{1}{a}$.

The question is "Do we have a unified description for both scattering and bound states?"

The answer is yes! we need do analytic continuation of $S(E)$ and $R(E)$ for $E < 0$.

We need to define the branch cut of \sqrt{E} : along the positive E -axis, i.e. if we write $E = |E|e^{i\theta}$ with $0 \leq \theta < 2\pi$, we define $\sqrt{E} = \sqrt{|E|} e^{i\theta/2}$.



This Riemann sheet is the physical sheet, and the other one $\sqrt{E} = -\sqrt{|E|} e^{i\theta/2}$ is called the un-physical sheet, or the second Riemann sheet.

Now, we can see the bound state corresponds to the simple pole on the physical sheet.

$$\begin{cases} S = \frac{\sqrt{E/E_0}}{\sqrt{E/E_0} - i} \\ R = \frac{i}{\sqrt{E/E_0} - i} \end{cases}; \quad \sqrt{E/E_0} \xrightarrow{E=-E_0} i, \text{ a simple pole.}$$

Because S and R diverge, we can maintain the "reflection" and "transmission" wave amplitude, but set the incident wave to zero, i.e. no incident wave, but we can have "reflection/transmission", because $\frac{S}{R} \rightarrow \infty$.

Then at $E = -E_0$, $R = S \rightarrow \infty$, we can write $\psi(x) = e^{-\beta|x|}$, which is just what we have directly solved.

Why we can do this? Look back at the Schrödinger Eq

$$\left(\frac{d^2}{dx^2} + \frac{2mE}{\hbar^2} \right) \psi = \frac{2}{a} \delta(x) \psi, \quad "E" \text{ is a parameter.}$$

At the level of differential Eq, we can treat E as complex. Once we

have solved the scattering states for $E > 0$, by complex continuation to $E < 0$.
S and R for

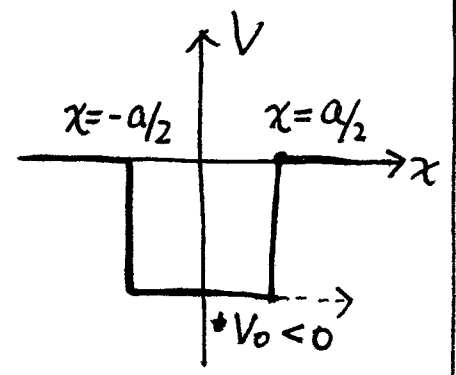
we arrive bound states.

★ Bound states correspond to poles of scattering amplitudes $S(E), R(E)$ on the physical sheet of E ! And scattering states correspond to a branch cut.

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§3. potential well with finite depth

$$V(x) = \begin{cases} 0 & \text{for } |x| > a/2 \\ V_0 \text{ (negative)} & \text{for } |x| < \frac{a}{2} \end{cases}$$



① we first look at the solution of bound states with $E < 0$.

define $k' = \sqrt{\frac{2m(E+|V_0|)}{\hbar^2}}$ and $\beta = \sqrt{\frac{2m|E|}{\hbar^2}}$.

The hamiltonian has parity symmetry, i.e. $H(x) = H(-x)$, or, $PHP^{-1} = H$.

The operation of parity transformation $P\psi(x) = \psi(-x)$. Since $[P, H] = 0$, we can find H and P common eigenstates, i.e. eigensolutions that are even or odd functions with respect to x .

② even parity solution

$$\psi(x) = \begin{cases} A \cos k'x & , |x| \leq \frac{a}{2} \\ B e^{-\beta|x|} & |x| \geq \frac{a}{2} \end{cases}$$

Ex: Based on the fact that the jumps of $V(x)$ at $x = \pm a/2$ are finite, prove that both $\psi(x)$ and $\psi'(x)$ are continuous at $x = \pm a/2$.

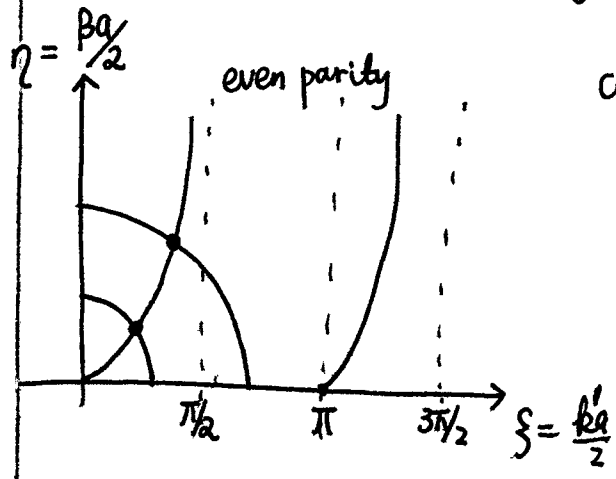
Since both ψ and ψ' are continuous, $(\ln \psi)' = \frac{\psi'}{\psi}$ should be continuous.

$$-k' \frac{\sin k'x}{\cos k'x} = \frac{-\beta e^{-\beta x}}{e^{-\beta x}} \Big|_{x=a/2} \Rightarrow k \tan ka/2 = \beta a$$

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define $\begin{cases} \frac{ka}{2} = \xi > 0 \\ \frac{\beta a}{2} = \eta > 0 \end{cases}$

$$\begin{cases} \xi^2 + \eta^2 = \frac{2m|V_0|}{\hbar^2} \cdot \frac{a^2}{4} = \frac{|V_0|}{\frac{\hbar^2}{2m(a/2)^2}} \\ \xi \tan \xi = \eta \end{cases}$$

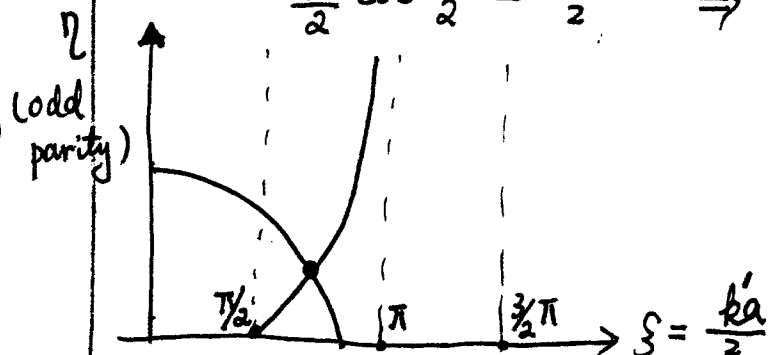


Comment:
 ① no matter how small $|V_0|$ is, there's always a bound state solution in the even parity channel.

② odd parity solution $\psi(x) = \begin{cases} A \sin k'x, & |x| \leq a/2 \\ B e^{-\beta x} & x > a/2 \\ -B e^{-\beta x} & x < -a/2 \end{cases}$

$(\ln \psi)'$ continuity at $x = a/2 \Rightarrow \frac{k' \cos k'x}{\sin k'x} = -\beta \frac{e^{-\beta x}}{e^{-\beta x}} \Big|_{x=a/2}$

$$-\frac{ka}{2} \cot \frac{ka}{2} = \frac{\beta a}{2} \Rightarrow \begin{cases} \xi^2 + \eta^2 = \frac{|V_0|}{\frac{\hbar^2}{2m(a/2)^2}} \\ \eta = -\xi \cot \xi \end{cases}$$



Comment: The odd solution only appear when $\xi^2 + \eta^2 \geq (\frac{\pi}{2})^2$, or

$$\frac{|V_0|}{\frac{\hbar^2}{2m(\frac{a}{2})^2}} \geq (\frac{\pi}{2})^2 \Rightarrow |V_0| \geq \frac{\hbar^2 \pi^2}{2ma^2}$$

② imagine that we gradually enlarge the potential depth $|V_0|$, as

$$\frac{|V_0|}{\frac{\hbar^2}{2m(\frac{a}{2})^2}} \sim (\frac{n\pi}{2})^2, \text{ i.e. } |V_0| = \frac{\hbar^2 \pi^2}{2ma^2} n^2, \text{ a new } (n+1)\text{th bound state appears at zero energy.}$$

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③ For infinite depth, i.e. $\xi^2 + \eta^2 \rightarrow \infty$,

the solutions appear at $\begin{cases} \xi = \frac{n\pi}{2}, \text{ or } k = \frac{n\pi}{a} \\ \eta = \infty \end{cases} \leftarrow \text{wavefunction only appears inside well.}$

④ the ground state is "no-node",
n-th excited states has n-nodes.

2. Now we solve the scattering problem for $E > 0$.

$$\psi(x) = \begin{cases} e^{ikx} + R e^{-ikx} & x < -\frac{a}{2} \quad (\text{incident + reflection}) \\ A e^{ik'x} + B e^{-ik'x} & -\frac{a}{2} < x < \frac{a}{2} \\ S e^{ikx} & \frac{a}{2} < x \quad (\text{transmission}) \end{cases}$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$, and $k' = \sqrt{\frac{2m(E+|V_0|)}{\hbar^2}}$.

at $x = -\frac{a}{2}$

$$\begin{cases} e^{-ik\frac{a}{2}} + R e^{ik\frac{a}{2}} = A e^{-ik'\frac{a}{2}} + B e^{ik'\frac{a}{2}} \\ ik e^{-ik\frac{a}{2}} + R(-ik) e^{ik\frac{a}{2}} = A(ik') e^{-ik'\frac{a}{2}} + B(-ik') e^{ik'\frac{a}{2}} \end{cases}$$

$$\Rightarrow \left. \begin{aligned} A e^{-ik'a/2} &= \frac{1}{2} \left(1 + \frac{k}{k'}\right) e^{-ik'a/2} + \frac{1}{2} R \left(1 - \frac{k}{k'}\right) e^{ik'a/2} \\ B e^{ik'a/2} &= \frac{1}{2} \left(1 - \frac{k}{k'}\right) e^{-ik'a/2} + \frac{1}{2} R \left(1 + \frac{k}{k'}\right) e^{ik'a/2} \end{aligned} \right\} \textcircled{1}$$

at $x = a/2$

$$\left\{ \begin{aligned} S e^{ik'a/2} &= A e^{ik'a/2} + B e^{-ik'a/2} \\ ik S e^{ik'a/2} &= A(ik') e^{ik'a/2} + B(-ik') e^{-ik'a/2} \end{aligned} \right.$$

AMPAD \Rightarrow $\textcircled{2} \left\{ \begin{aligned} A e^{ik'a/2} &= \frac{1}{2} S \left(1 + \frac{k}{k'}\right) e^{ik'a/2} \\ B e^{-ik'a/2} &= \frac{1}{2} S \left(1 - \frac{k}{k'}\right) e^{ik'a/2} \end{aligned} \right.$

compare $\textcircled{1}$ and $\textcircled{2}$

$$\left(1 + \frac{k}{k'}\right) + R \left(1 - \frac{k}{k'}\right) e^{ika} = S \left(1 + \frac{k}{k'}\right) e^{i(k-k')a}$$

$$\left(1 - \frac{k}{k'}\right) + R \left(1 + \frac{k}{k'}\right) e^{ika} = S \left(1 - \frac{k}{k'}\right) e^{i(k+k')a}$$

$$\Rightarrow \left. \begin{aligned} S &= e^{-ika} \frac{1}{\cos k'a - \frac{i}{2} \left(\frac{k}{k'} + \frac{k'}{k}\right) \sin k'a} \\ R &= e^{-ika} \frac{\frac{i}{2} \left(\frac{k'}{k} - \frac{k}{k'}\right) \sin k'a}{\cos k'a - \frac{i}{2} \left(\frac{k}{k'} + \frac{k'}{k}\right) \sin k'a} \end{aligned} \right\}$$

where $k = \sqrt{\frac{2mE}{\hbar^2}}$
and $k' = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$

\star Again let us do analytic continuation of the energy variable E . The pole is located

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

using $\cos x = \frac{1 - \tan^2 \frac{x}{2}}{1 + \tan^2 \frac{x}{2}}$ $\sin x = \frac{2 \tan \frac{x}{2}}{1 + \tan^2 \frac{x}{2}}$

$$\Rightarrow \frac{1 - \tan^2 \frac{k'a}{2}}{\tan \frac{k'a}{2}} = \left(\cot \frac{k'a}{2} - \tan \frac{k'a}{2} \right) = \frac{ik}{k'} - \frac{k'}{ik}$$

the solution is equivalent to $\cot \frac{k'a}{2} = \frac{ik}{k'}$, or $-\tan \frac{k'a}{2} = \frac{ik}{k'}$.

according to the convention of using the first Riemann sheet

$k = \sqrt{\frac{2mE}{\hbar}} = i\beta \Rightarrow$ the above Eqs become

$k' \cot \frac{k'a}{2} = -\beta$, or $k' \tan \frac{k'a}{2} = \beta$

Which are just the energies we solved before for bound states.

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a) if $k' \tan \frac{k'a}{2} = \beta$ is satisfied, then

$\sin k'a = \frac{2 \frac{\beta}{k'}}{1 + (\frac{\beta}{k'})^2} = \frac{2}{\frac{k'}{\beta} + \frac{\beta}{k'}}$

$\frac{R}{S} = \frac{i}{2} (-\frac{i\beta}{k'} + \frac{k'}{i\beta}) \sin k'a = +1$, thus it corresponds to even parity.

b) if $k' \cot \frac{k'a}{2} = -\beta \Rightarrow \tan \frac{k'a}{2} = -\frac{k'}{\beta} \Rightarrow \sin k'a = \frac{-2 \frac{k'}{\beta}}{1 + (\frac{k'}{\beta})^2} = \frac{-2}{\frac{k'}{\beta} + \frac{\beta}{k'}}$

$\Rightarrow R/S = -1$, thus it corresponds to odd parity solution.

§3: Transmission resonances

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

$$T(E) = |S(E)|^2 = \frac{1}{(\cos k'a)^2 + \frac{1}{4} \left(\frac{k'}{k} + \frac{k}{k'} \right)^2 \sin^2 k'a}$$

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

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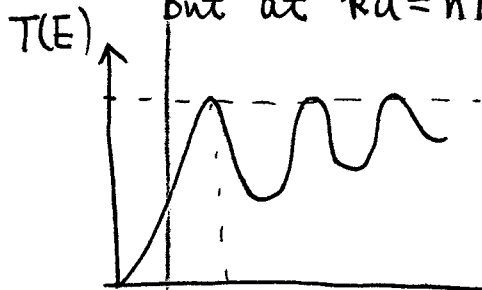
The perfect transmission occurs at $k'a = n\pi$.

$$\left(\frac{k}{k'} - \frac{k'}{k} \right)^2 = \left(\frac{k^2 - k'^2}{kk'} \right)^2 = \frac{|V_0|^2}{E(E+|V_0|)} = \frac{1}{E/|V_0|(E/|V_0|+1)}$$

$$\Rightarrow T(E) = \left[1 + \frac{\sin^2 k'a}{4 \frac{E}{|V_0|} (E/|V_0|+1)} \right]^{-1}$$

if $k'a \neq n\pi$, because V_0/E typically speaking $\gg 1$, $T(E) \sim E/V_0 \ll 1$.

but at $k'a = n\pi$, $T(E) \rightarrow 1$, we get perfect transmission.



$$E = \frac{\hbar^2 k^2}{2m}$$

$$= \frac{\hbar^2 k'^2}{2m} - V_0$$

$$S(E) \approx \frac{e^{-ika}}{\cos k'a} \frac{1}{1 - \frac{i}{2} \left(\frac{k'}{k} + \frac{k}{k'} \right) \tan k'a}$$

Next, we expand around $k'a = n\pi$

$$\left(\frac{k}{k'} + \frac{k'}{k} \right) \tan k'a \approx \frac{4}{\Gamma_n} (E - E_n)$$

$$\left\{ \begin{aligned} \frac{4}{\Gamma_n} &= \frac{d}{dE} \left[\left(\frac{k}{k'} + \frac{k'}{k} \right) \tan k'a \right] \Big|_{k'=k_n} \\ E_n &= \frac{\hbar^2 k_n^2}{2m} \end{aligned} \right.$$

$$e^{-ika} \sim 1, \quad \cos k'a \approx \pm 1$$

$$\frac{4}{\Gamma_n} = \left(\frac{k}{k'} + \frac{k'}{k} \right) \frac{d}{dE} \tan k'a \Big|_{E=E_n} = \left(\frac{k}{k'} + \frac{k'}{k} \right) \left(\sec^2 k'a \frac{dk'a}{dE} \right) \Big|_{E=E_n}$$

(∵ $\tan k'_n a = 0$)

$$= \left(\frac{k}{k'} + \frac{k'}{k} \right) \frac{dk'a}{dE} \Big|_{E=E_n}$$

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Consider the case $k' \gg k$ we have $\frac{4}{\Gamma_n} \approx \frac{ak'}{k} \frac{dk'}{dE} \Big|_{E=E_n} \approx \frac{a}{k} \frac{m}{\hbar^2}$

$$\approx \frac{ma}{\hbar^2} \sqrt{\frac{\hbar^2}{2mE_n}} = \frac{a}{\hbar} \sqrt{\frac{m}{2E_n}}$$

$$\Rightarrow \Gamma_n \approx \frac{4\hbar}{a} \sqrt{\frac{2E_n}{m}} = \left(E_n \frac{\hbar^2}{2ma^2} \right)^{1/2} \cdot 8$$

$\approx 8(E_n \cdot E_k)^{1/2}$ where $E_k = \frac{\hbar^2}{2ma^2}$. We consider $V_0 \gg E_n \gg E_k$

Then
$$S(E) \approx \frac{e^{ika}}{\cos k'a} \frac{1}{1 - \frac{i\Gamma_n}{2} \frac{2}{\Gamma_n} (E - E_n)} \approx \pm \frac{i\Gamma_n/2}{(E - E_n) + i\Gamma_n/2}$$

and
$$T(E) \approx \frac{(\Gamma_n/2)^2}{(E - E_n)^2 + (\Gamma_n/2)^2}$$
 Breit - Wigner - formula

$S(E)$ has a pole at $E = E_n - i\Gamma_n/2$, however, this pole is not on the physical sheet of E .

$$S = e^{ika} \frac{1}{\cos \sqrt{\frac{2m(E+|V_0|)}{\hbar^2}} a - \frac{i}{2} \left(\sqrt{\frac{E}{E+|V_0|}} + \sqrt{\frac{E+|V_0|}{E}} \right) \sin \sqrt{\frac{2m(E+|V_0|)}{\hbar^2}} a}$$

The pole is reached if we interperate $\sqrt{E} = \sqrt{E_n} \left(1 - \frac{i\Gamma_n}{2E_n} \right)$, thus is defined

\sqrt{E} on the second Riemann sheet!