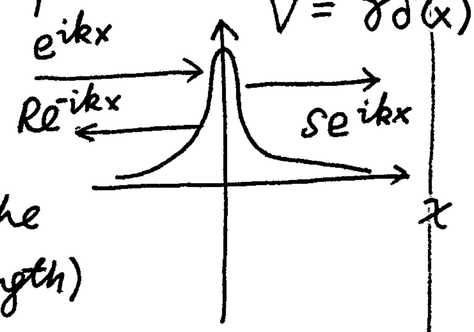
Lecture 6

1-D Scattering Problem — bound states (?)

- We first consider the simplest case of δ- potential



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

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

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

consider the boundary condition under incident/transmission/reflection

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

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

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

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

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

$|S|^2$ transmition coefficient

$|R|^2$ reflection coefficient!

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

Ex: ① check that $|S|^2 + |R^2| = 1$

- ② although $\psi'(x)$ is not continuous at $x=0$, but the current density $j_x = \frac{\hbar}{2m}\left[\psi^*(x)\frac{d}{dx}\psi(x) - \psi(x)\frac{d}{dx}\psi^*(x)\right]$ remains Continuous at $x=0$.

comment: ① at low energy limit $k \to 0$, $\Rightarrow \begin{cases} S = -ika \to 0 \\ R = -1 \end{cases}$

complete reflection.

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

§2. Analytical continuation:

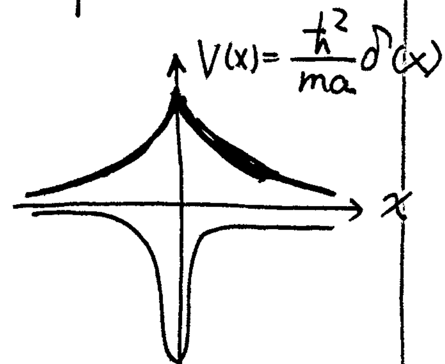
define $E_0 = \frac{\hbar^2}{2ma^2}$, we write S, R as

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

"$\pm$" 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 a bound state.



Solution for bound state: Choosing $\psi = \begin{cases} e^{\beta x}, & x < 0 \\ e^{-\beta x}, & x > 0 \end{cases}$ $\quad E_b = -\frac{\hbar^2\beta^2}{2m} < 0$.

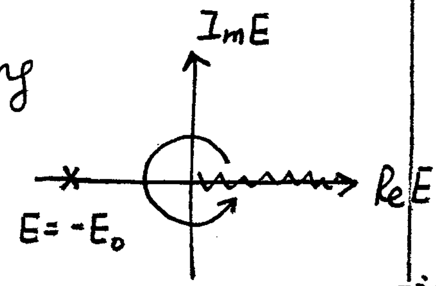
according to continuity relation,

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

or $\beta = \frac{1}{a}$.

The question is "Do we have a unified description for both scattering and bound states?" —— $\boxed{\text{The answer is yes! we need do analytic continuation of } S(E) \text{ and } R(E) \text{ for } E<0.}$

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 $0 \le \theta < 2\pi$, 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 of

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

on the physical sheet.

Because S and R diverge, we can maintain the "reflection" and "transmition" wave amplitude, but set the incident wave to zero, ie no incident wave, but we can have "reflection / transmition", because $\begin{matrix} S \\ R \end{matrix} \to \infty$.

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

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

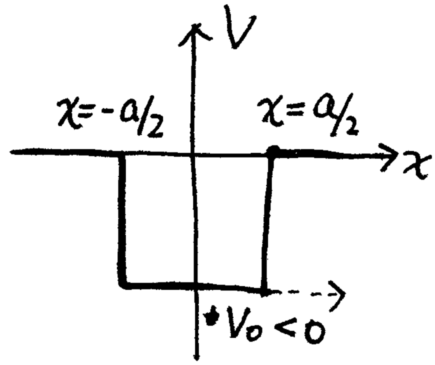
$$\left(\frac{d^2}{dx^2} + \frac{2mE}{\hbar^2}\right)\psi = \frac{2}{a}\delta(x)\psi ,$$ "E" is a parameter.

At the level of differential Eq, we can ~~treat~~ E as complex. Once we have solved S and R for the scattering states for $E>0$, by complex continuation to $E<0$.

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.

§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 hamitonian 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 respective to x.

(i) even parity solution

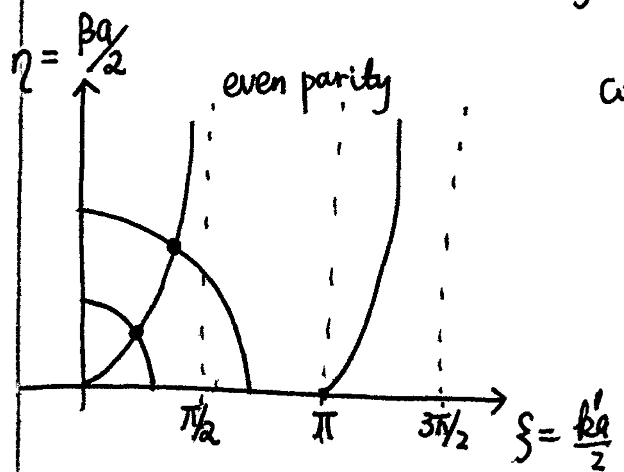
$$\psi(x) = \begin{cases} A\cos k'x, & |x| \le a/2 \\ B e^{-\beta|x|} & |x| \ge \frac{a}{2} \end{cases}$$

$\boxed{\text{Ex:}}$ 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 continous at $x = \pm a/2$.

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

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

define $\begin{cases} \frac{k'a}{2} = \xi > 0 \\ \frac{\beta a}{2} = \eta > 0 \end{cases} \Rightarrow \begin{cases} \xi^2 + \eta^2 = \frac{2m|V_0|}{\hbar^2} \cdot \frac{a^2}{4} = \frac{|V_0|}{\frac{\hbar^2}{2m(a/2)^2}} \\ \xi \tan \xi = \eta \end{cases}$



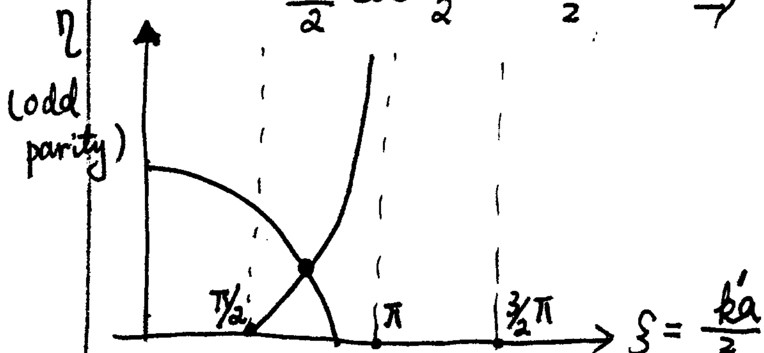
Comment:

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

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

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

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



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

①
$$\frac{|V_0|}{\frac{\hbar^2}{2m(a/2)^2}} \geq \left(\frac{\pi}{2}\right)^2 \quad \Rightarrow \quad |V_0| \geq \frac{\hbar^2\pi^2}{2ma^2}.$$

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

$$\frac{|V_0|}{\frac{\hbar^2}{2m(a/2)^2}} \sim \left(\frac{n\pi}{2}\right)^2, \quad \text{i.e} \quad \boxed{|V_0| = \frac{\hbar^2\pi^2}{2ma^2}\, n^2,}$$

a new $(n+1)$th bound state appears at zero energy!

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

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

④ the ground state is "no-node",

n-th excitated states has n-nodes.

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

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

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

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

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

at $x = a/2$

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

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

compare ① and ②

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

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

$$\Rightarrow \left.\begin{aligned} S &= e^{-ika} \frac{1}{\cos k'a - \frac{i}{2}\left(k/k' + k'/k\right)\sin k'a} \\ R &= e^{-ika} \frac{\frac{i}{2}\left(k'/k - k/k'\right)\sin k'a}{\cos k'a - \frac{i}{2}\left(k/k' + k'/k\right)\sin k'a} \end{aligned}\right\} \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}} \text{ and } k' = \sqrt{\frac{2m(E+|V_0|)}{\hbar^2}}$$

(☆) Again let us do analytic continuation of the energy variable E. The pole is located

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

using

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

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

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 became

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

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

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

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

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

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

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

§3: transmition resonances

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

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

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

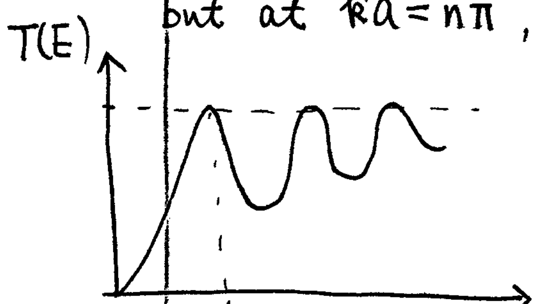
The perfect transmission occurs at $k'a = n\pi$.

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

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

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

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



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

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

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

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

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

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

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

$(\because \tan k_n' a = 0)$

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

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

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

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

$$\simeq 8\left(E_n \cdot E_K\right)^{1/2}$$ where $E_K = \frac{\hbar^2}{2ma^2}$. We consider $V_0 \gg E_n \gg E_K$.

Then $$S(E) \simeq \frac{e^{ika}}{\cos k'a} \frac{1}{1 - \frac{i2}{\Gamma_n}(E-E_n)} \simeq \pm \frac{i\Gamma_n/2}{(E-E_n)+i\Gamma_n/2}$$

and $$T(E) \simeq \frac{(\Gamma_n/2)^2}{(E-E_n)^2 + (\Gamma_n/2)^2}$$ 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.

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

The pole is reached if we interporate $\sqrt{E} \simeq \sqrt{E_n}\left(1 - \frac{i\Gamma_n}{2E_n}\right)$, thus $\sqrt{E}$ is defined on the second Riemann sheet!