Lecture 2

Last time: $U(x) = -g\,\delta(x)$, $g > 0$

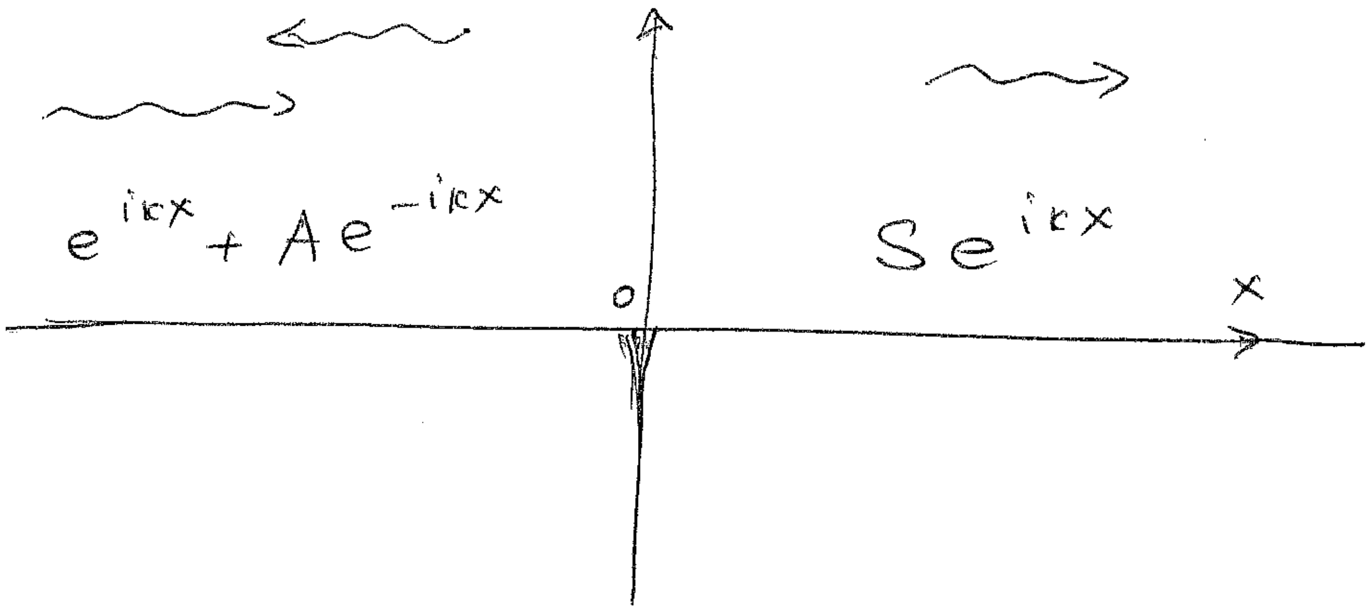
Stationary states: $\Psi(x,t) = e^{-iEt/\hbar}\,\psi(x)$

Discrete spectrum: $E < 0$

— one bound state with $E = E_* = -\dfrac{\hbar^2}{2m}\varkappa^2$,

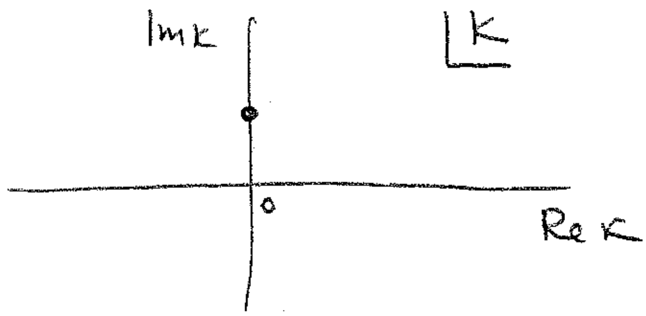
$$\varkappa \equiv mg/\hbar^2 > 0$$

Continuous spectrum: $E > 0$



$$S(k) = \frac{ik}{ik + \varkappa}$$

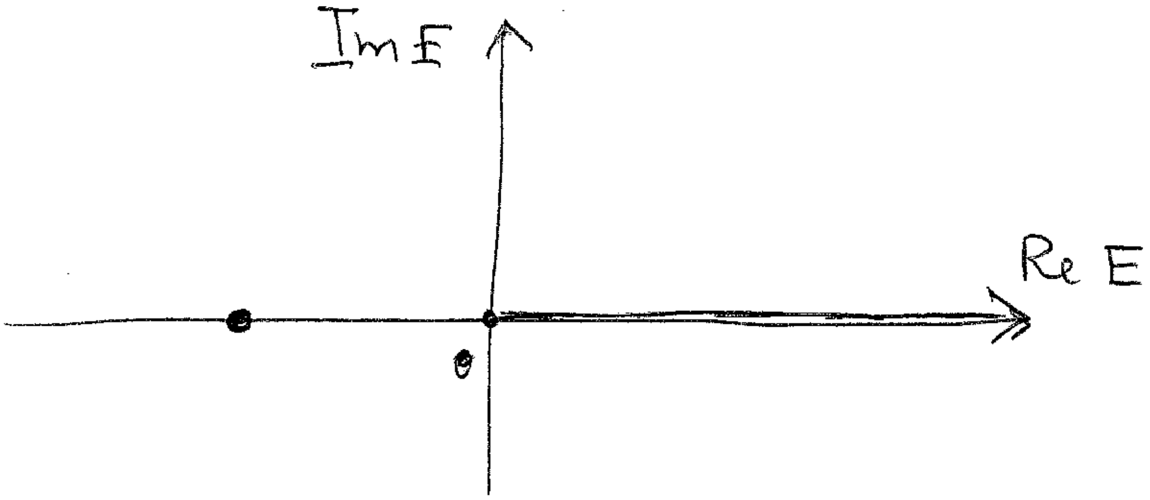
$$k^2 = 2mE/\hbar^2$$



Pole at $k = k_* = i\varkappa$,

$\varkappa > 0$

$$E = \frac{\hbar^2}{2m} k^2 \Rightarrow E = E_* = -\frac{\hbar^2}{2m} \varkappa^2$$



Treat E as complex variable:

$$E = |E| e^{i\varphi + i2\pi n}, \quad n = 0, \pm 1, \pm 2, \ldots$$

$$\sqrt{E} = |E|^{1/2} e^{\frac{i\varphi}{2} + in\pi}$$

For $E < 0$ and real, $\varphi = \pi$, so

$$\sqrt{E} = |E|^{1/2} e^{i\pi/2} = i\,|E|^{1/2} \quad \text{for } n = 0$$

$$\sqrt{E} = |E|^{1/2} e^{i\pi/2 + i\pi} = -i\,|E|^{1/2} \quad \text{for } n = 1$$

We have

$$k = \frac{\sqrt{2m}}{\hbar} \sqrt{E} = \left\{ \begin{array}{l} \frac{\sqrt{2m}}{\hbar} |E|^{1/2} i \\ -\frac{\sqrt{2m}}{\hbar} |E|^{1/2} i \end{array} \right\} = i\varkappa > 0$$

This eq. has solution for $n = 0$ value of complex E.
The pole $E = E_*$ is on the "physical sheet". The cut $[0, \infty)$.

<u>Observation</u>: poles of $S(E)$ on the negative real axis of complex $E \longleftrightarrow$ bound states of $U(x)$.

<u>Remark</u>: we expect $S(E)$ <u>to be analytic function in the upper half-plane of complex E.</u> Indeed, $\psi(t,x) \sim e^{-iEt/\hbar}$
$\Rightarrow \psi(t,x) \sim e^{(\mathrm{Im}\,E)t/\hbar}$: this increases without bound for $t \to \infty$ $\Rightarrow$ violates prob. conserv. $w \sim |\psi|^2$. We can have singularities in the lower half-plane: with $\mathrm{Im}\,E \leq 0$ $|\psi|^2 \to 0$ OK in one

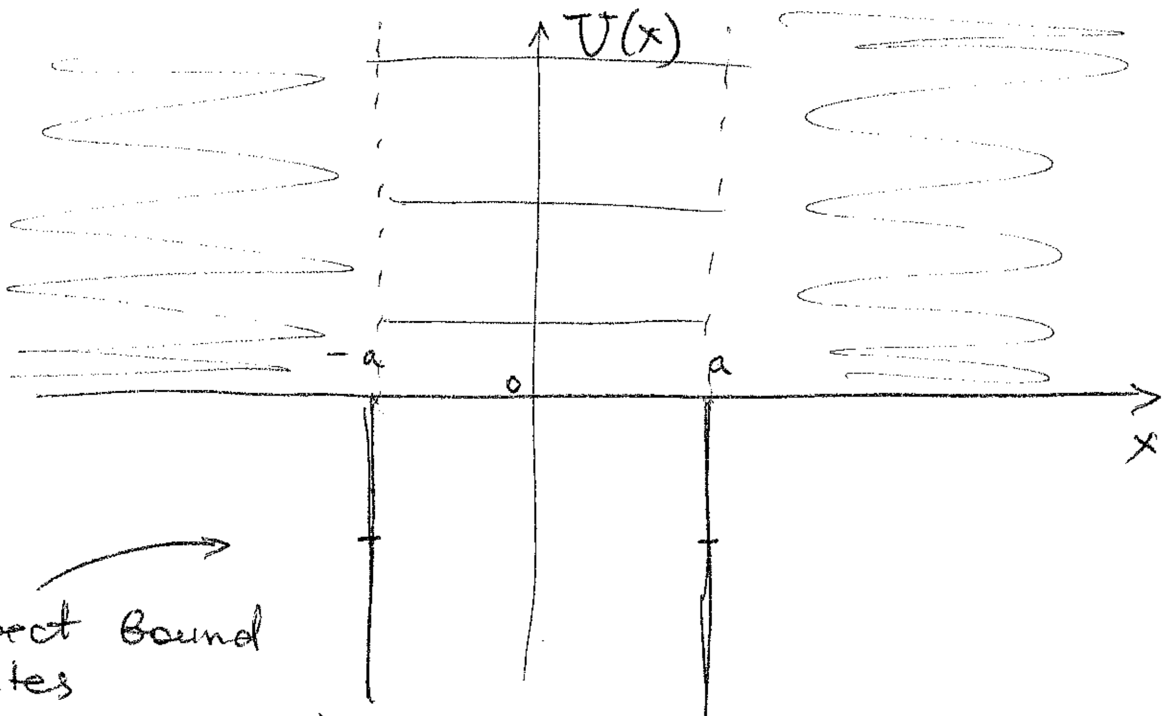
channel since $|\psi|^2$ increases in other channels and total $w = 1$.

Resonances

The pot. $U = -g\,\delta(x)$ is too simple - it has zero size. Improve this by considering

$$U(x) = -\gamma\left[\delta(x+a) + \delta(x-a)\right]$$

(or a pot. well). Here $\gamma = g/2$ to match with the prev. case.



expect bound states
(~2 for large a)

For $U = -q\,\delta(x)$, $R = \dfrac{\varkappa^2}{k^2+\varkappa^2}$,

$\varkappa = mq/\hbar^2$. $\Rightarrow$ $R \to 1$ for $\varkappa \to \infty$ (or $q \to \infty$)

$\Rightarrow$ for $q \to \infty$ expect "trapped" states for $|x| < a$ of an inf. pot. well with

$$E_n = \frac{\hbar^2 \pi^2 n^2}{8ma^2}, \quad n = 1, 2, \ldots$$

Our goal is to find $S(E)$ and $T = |S|^2$.
But first we shall learn some new tools.

Green's functions

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

Reminder : $\hat{L}(x)\,\varphi(x) = f(x)$,

where $\hat{L}$ is a diff. oper.

$$\hat{L}(x)\,G(x, x') = \delta(x-x')$$

Then $$\varphi(x) = \varphi_0(x) + \int_{-\infty}^{\infty} G(x,x')\,f(x')\,dx',$$

where $\hat{L}\varphi_0 = 0$. Proof obvious.

Green's function for the Schrödinger eq.

1) $E<0$, free particle, $G \to 0$ for $|x-x'| \to \infty$

$$\left(\hat{H} - E\right) G(x,x') = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} G - E G = \delta(x-x')$$

a) $x < x'$

$$G(x,x') = A(x')\,e^{\varkappa(x-x')} + B(x')\,e^{-\varkappa(x-x')}$$

$$\varkappa = \sqrt{2m|E|}/\hbar > 0$$

$x \in (x^{(1)} \to -\infty$ should have $G \to 0$

$\Rightarrow B(x') = 0$

b) $x > x'$: $G(x, x') = C(x')\, e^{-\varkappa(x - x')}$

c) At $x = x'$: <u>G is continuous but G' is not:</u>

$$G'(x = x' + \varepsilon, x') - G'(x = x' - \varepsilon, x') = -\frac{2m}{\hbar^2}$$

These conditions give: $A = C = m/\varkappa\hbar^2$.

$$\Rightarrow \boxed{G(x, x') = \frac{m}{\varkappa \hbar^2}\, e^{-\varkappa |x - x'|}}$$

Inhomogeneous eq:

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

Solution:

$$\psi(x) = A e^{-\varkappa x} + B e^{\varkappa x} + \int_{-\infty}^{\infty} G(x, x') f(x')\, dx'.$$

With $f = -U(x)\psi(x)$ we get

$$\psi(x) = A e^{-\varkappa x} + B e^{\varkappa x} - \int_{-\infty}^{\infty} G(x;x')\, U(x')\, \psi(x')\, dx'$$

We are interested in $\psi \to 0$ for $|x| \to \infty$,
so $A, B = 0$ and $(E < 0!)$

$$\boxed{\psi(x) = -\frac{m}{\varkappa \hbar^2} \int_{-\infty}^{\infty} e^{-\varkappa |x-x'|}\, U(x')\, \psi(x')\, dx'}$$

equiv.

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - E\psi = -U(x)\,\psi(x), \quad \psi(x) \underset{x \to \pm\infty}{\to} 0$$

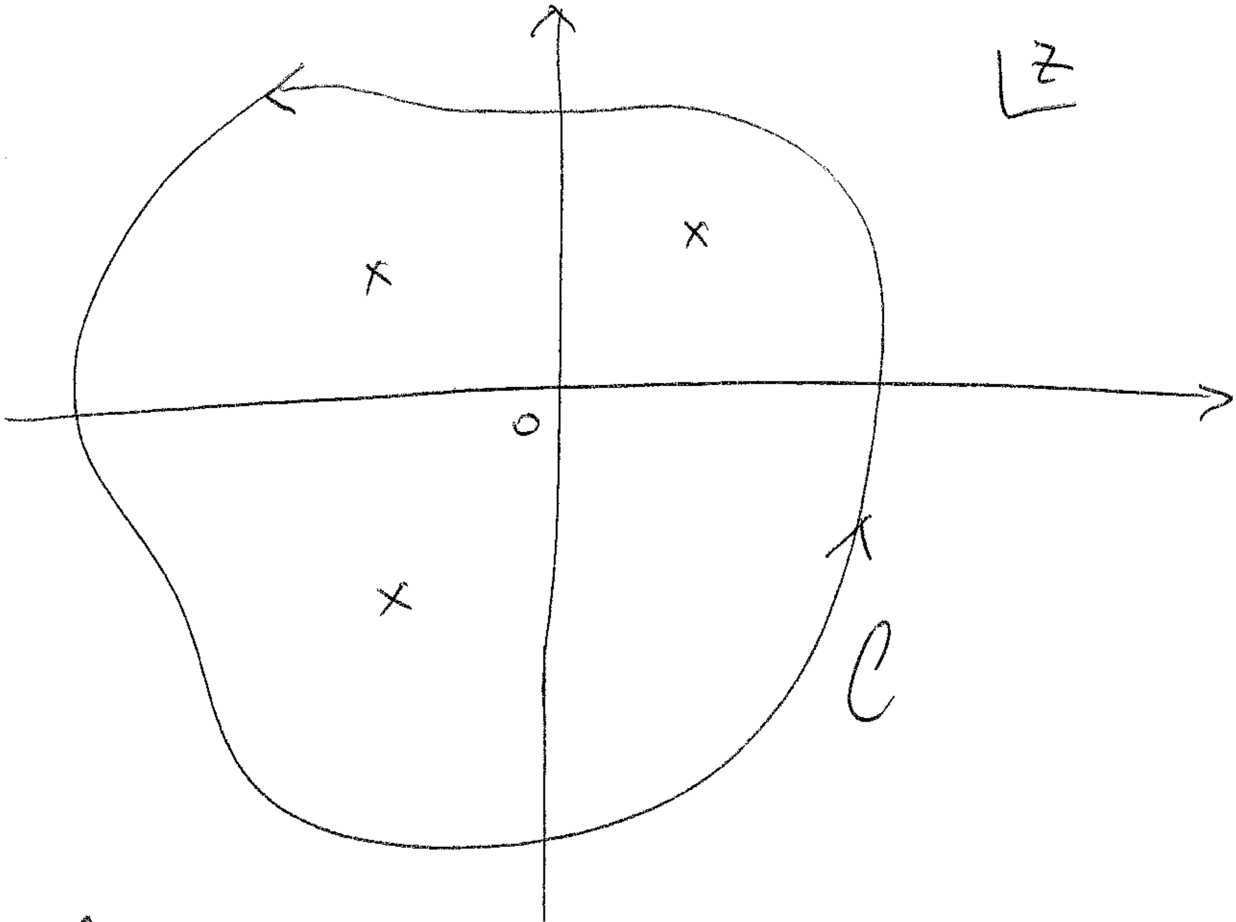
The moral: Schrödinger eq. is written as an integral eq.

Another method:

$$(\hat{H} - E)\,\hat{G} = \hat{\mathbb{1}}, \qquad \hat{H} = \hat{p}^2/2m$$

$$\hat{G} = \frac{1}{\hat{H} - E} \qquad \text{(formal solution)}$$

Cauchy theorem



$$\int_C f(z)\,dz = 2\pi i \sum_{res} \operatorname{res} f(z_k)$$

$$\left(\hat{H}-E\right)G(x,x') = -\frac{\hbar^2}{2m}\frac{\partial^2 G}{\partial x^2} - EG = \delta(x-x')$$

$$G(x,x') = \frac{1}{2\pi\hbar}\int e^{ip(x-x')/\hbar}\, G(p)\, dp$$
$$= G(x-x') =$$

$$G(p) = \int e^{-ip(x-x')/\hbar}\, G(x-x')\, dx$$

$$G(x-x') = \frac{1}{2\pi\hbar}\int e^{ip(x-x')/\hbar} dp \int e^{-ip(y-x')/\hbar}\, G(y-x')\, dy$$

$$= \frac{1}{2\pi\hbar}\iint e^{ip(x-y)/\hbar}\, G(y-x')\, dy\, dp =$$

$$= \int \delta(x-y)\, G(y-x')\, dy = G(x-x').$$

Ибо: $\boxed{\frac{1}{2\pi}\int e^{ik(x-y)}\, dk = \delta(x-y)}$.

$\Rightarrow$

$$G(p)\left(\frac{p^2}{2m}+|E|\right)=1 \qquad (E<0)$$

$$G(p)=\left(\frac{p^2}{2m}+|E|\right)^{-1}$$

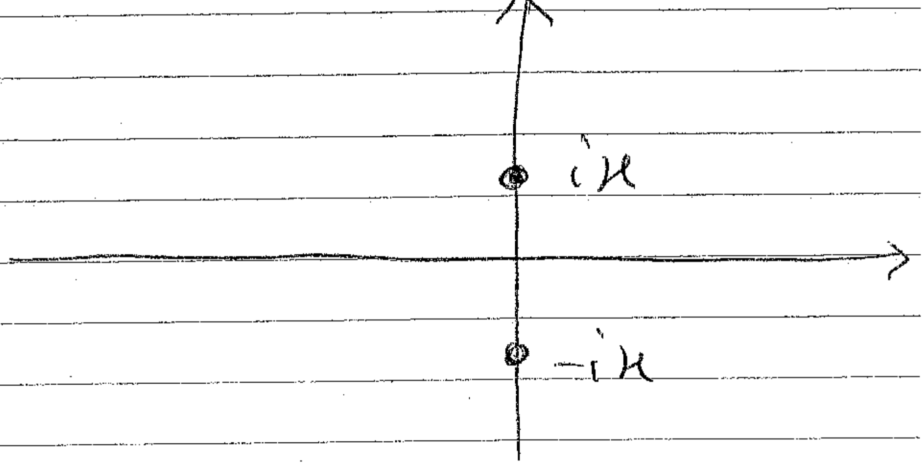
$$\boxed{G(x-x')=\frac{1}{2\pi\hbar}\int\frac{e^{ip(x-x')/\hbar}}{\frac{p^2}{2m}+|E|}\,dp}$$

$$G(x-x')=\frac{2m}{\hbar^2}\,\frac{1}{2\pi}\int\frac{e^{ik(x-x')}}{k^2+\frac{2m|E|}{\hbar^2}}\,dk$$

$$\varkappa^2=\frac{2m|E|}{\hbar^2}$$

$$G(x-x')=\frac{2m}{\hbar^2}\,\frac{1}{2\pi}\int\frac{e^{ik(x-x')}}{k^2+\varkappa^2}\,dk$$

$$k=\pm i\varkappa$$



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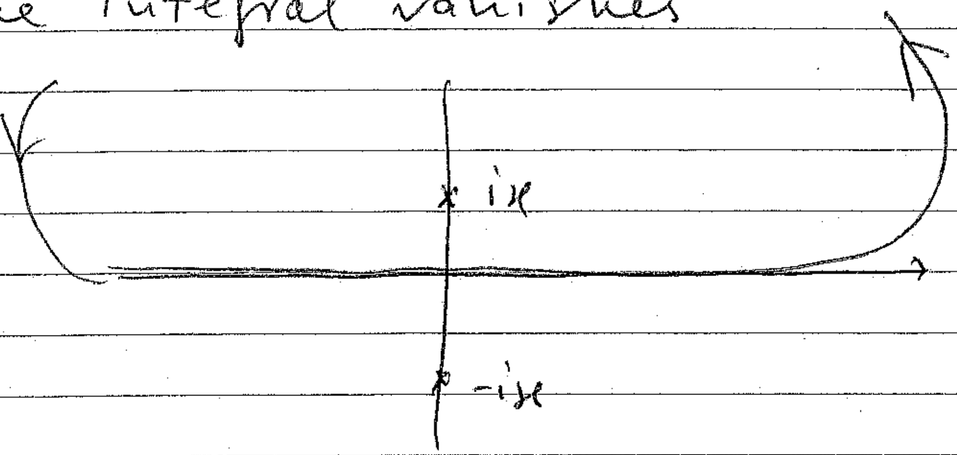
$x - x' > 0$: for $i\kappa$, $\kappa > 0$ $\kappa \to \infty$

the integral vanishes

$\Rightarrow$ 

$k^2 + \varkappa^2 = (k + i\varkappa)(k - i\varkappa)$ Cauchy theorem:

$$\int \frac{e^{ik(x-x')}}{k^2+\varkappa^2}\,dk = 2\pi i \,\frac{e^{-\varkappa(x-x')}}{2i\varkappa} = \frac{\pi}{\varkappa}\, e^{-\varkappa(x-x')}$$

$$G(x-x') = \frac{m}{\varkappa\hbar^2}\, e^{-\varkappa(x-x')}, \qquad x - x' > 0$$

Similarly (show this!):

$$G(x-x') = \frac{m}{\varkappa\hbar^2}\, e^{\varkappa(x-x')} \qquad x - x' < 0$$

$$\Rightarrow \boxed{G(x-x') = \frac{m}{\varkappa\hbar^2}\, e^{-\varkappa|x-x'|}}$$

$$G(x,x') = \int_{-\infty}^{\infty} \frac{1}{\frac{p^2}{2m}+|E|} \frac{e^{ip(x-x')/\hbar}}{2\pi\hbar} dp$$

$$= \frac{m}{\varkappa \hbar^2} \exp\left(-\varkappa |x-x'|\right).$$

<u>Exercise (optional)</u>: show this in detail.

<u>Exercise</u>: use the integral eq. to find the wave f. and energy ~~levels~~ of the bound state in the potential $U = -q\,\delta(x)$.

<u>exercise</u>*: show that the discrete energy spectrum $E_n\}$ in $U(x) \le 0$ (with $U \to 0$ for $x \to \pm\infty$) beys

$$|E_n| \le \frac{m}{2\hbar^2}\left(\int_{-\infty}^{\infty} U(x)\,dx\right)^2.$$

Hint: for the ground state $E = E_0 < 0$ $\left(|E_n| \le |E_0|\right)$ the wave function can be chosen real and positive. Show that $\psi_0(x_0) \le \frac{m}{\varkappa_0 \hbar^2} \psi_0(x_0) \int |U(x)|\,dx$, where x_0 is the point where $\psi(x)$ has maximum.

Now consider $E > 0$:

$$\varkappa = \sqrt{-2mE}/\hbar = \pm i k \,, \quad k = \sqrt{2mE}/\hbar > 0$$

$$G^{\pm}(x, x') = \pm \frac{im}{k\hbar^2} \exp\left(\pm ik|x - x'|\right)$$

$$\psi(x) = A e^{ikx} + B e^{-ikx} - \int_{-\infty}^{\infty} G^{\pm}(x, x') U(x') \psi(x') dx'$$

For $A = 1$, $B = 0$, $G = G^{+}(x, x')$:

$$\boxed{\psi(x) = e^{ikx} - \int_{-\infty}^{\infty} G^{+}(x, x') U(x') \psi(x') dx'}$$

scattering by the potential $U(x)$).

<u>exercise:</u> consider $U(x) = q\,\delta(x)$, $q > 0$, and show that $\psi(0) = (1 + imq/k\hbar^2)^{-1}$;

Free particle Green's function for $E > 0$

①. Use Fourier transform

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - E\right) G(x, x') = \delta(x - x')$$

$E > 0$, with b.c. $G \to \text{const}\, e^{ik|x|}$, $|x| \to \infty$.

$$G(x, x') = \frac{1}{2\pi\hbar}\int e^{ip(x-x')/\hbar}\, G(p)\, dp$$

$$\Rightarrow \left(\frac{p^2}{2m} - E\right) G(p) = 1, \text{ since}$$

$$\delta(x - x') = \frac{1}{2\pi\hbar}\int e^{ip(x-x')/\hbar}\, dp.$$

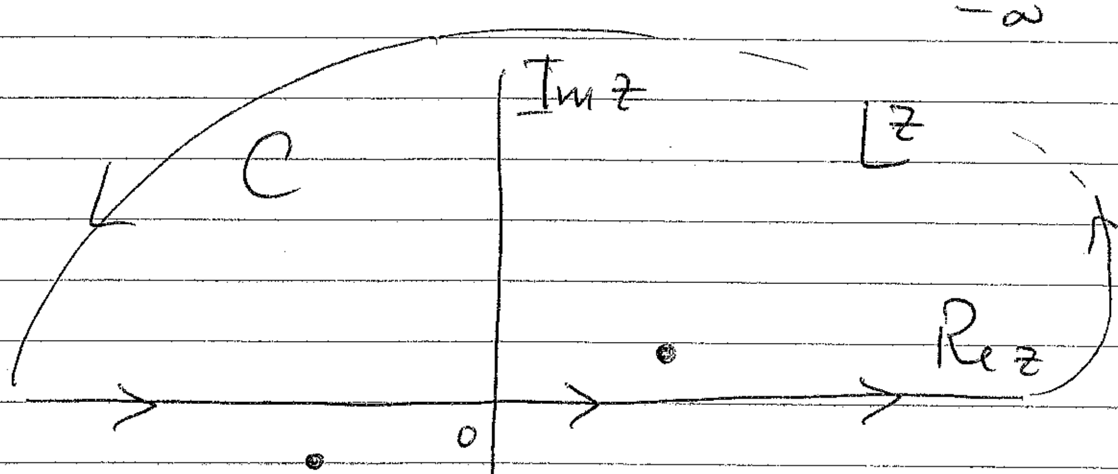
$$\Rightarrow G(p) = \frac{1}{\frac{p^2}{2m} - E}, \quad E > 0.$$

Use Cauchy th. and residues ;

$$G(x-x') = \frac{2m}{\hbar^2}\frac{1}{2\pi}\int \frac{e^{iz(x-x')}}{z^2-k^2-i\varepsilon}\,dz, \qquad 2\text{-}10''$$

$z = p/\hbar$, $k^2 = \frac{2mE}{\hbar^2} > 0$, $\varepsilon > 0$.

1) $x - x' > 0$: choose C in the upper half-plane of complex z ($\mathrm{Im}\, z > 0$, so $iz(x-x') < 0$ on the contour at ∞). Then the integral $\int_{-\infty}^{\infty} = \int_C$



Choice $\varepsilon > 0$ guarantees $G \to e^{ik|x|}$ for $|x| \to \infty$. $\quad z_* = \pm k\left(1 + \frac{i\varepsilon}{k^2}\right)^{1/2}$

$$G(x-x') = \frac{2m}{\hbar^2}\frac{1}{2\pi}\,2\pi i\,\frac{e^{ik(x-x')}}{2k} = \frac{im}{k\hbar^2}\,e^{ik(x-x')}$$

2) Same procedure for $x - x' < 0$ but C is closed in the lower half-plane (note that the direction of C now

gives minus sign in the residue theorem:

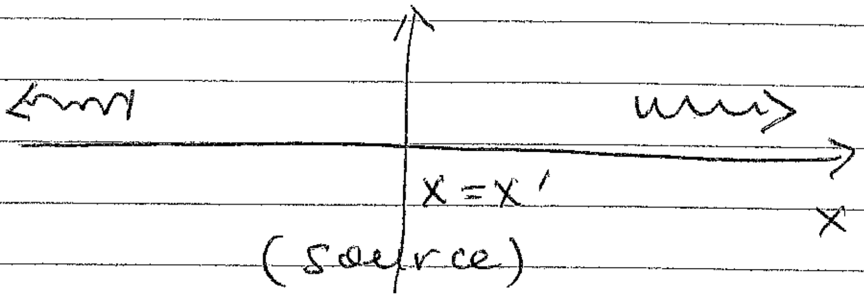
$$G(x-x') = \frac{2im}{\hbar^2}(-1)\frac{e^{-ik(x-x')}}{(-2k)} =$$

$$= \frac{im}{k\hbar^2} e^{-ik(x-x')}, \quad x-x'<0.$$

$$\Rightarrow G(x-x') = \frac{im}{k\hbar^2} e^{ik|x-x'|}, \text{ where}$$

$$k = \sqrt{2mE}, \quad E>0.$$

(2.) Solving ODE directly with the b.c. $G \to e^{ik|x|}$, $|x| \to \infty$:



We have

$$G(x,x') = \begin{cases} A e^{-ik(x-x')}, & x<x' \\ B e^{ik(x-x')}, & x>x' \end{cases}$$

Conditions $\psi(x=x'-\varepsilon) = \psi(x=x'+\varepsilon)$

and $\psi'(x=x'+\varepsilon) - \psi'(x=x'-\varepsilon) = -\frac{2m}{\hbar^2}$

give $A = B$, $A = -\frac{m}{ik\hbar^2}$ =>

$$G(x,x') = \frac{im}{k\hbar^2} e^{ik|x-x'|}$$

as before.

(3) Finally, one can first obtain $G(x,x')$ for $E<0$ using the same approach as in (1) and (2):

$$G(x,x') = \frac{m}{\varkappa \hbar^2} e^{-\varkappa|x-x'|},$$

$\varkappa = \sqrt{-2mE}/\hbar$, $E<0$.

Continuing to $E>0$, $\varkappa = \pm ik$, where $k = \sqrt{2mE}/\hbar$, $E>0$. Thus,

$$G^{\pm}(x',x) = \pm \frac{im}{k\hbar^2} e^{\pm ik|x-x'|},$$

with $G^{+}(x,x')$ corresponding to the b.c. needed.

find $T(E)$ and $R(E)$ by solving the integral equation

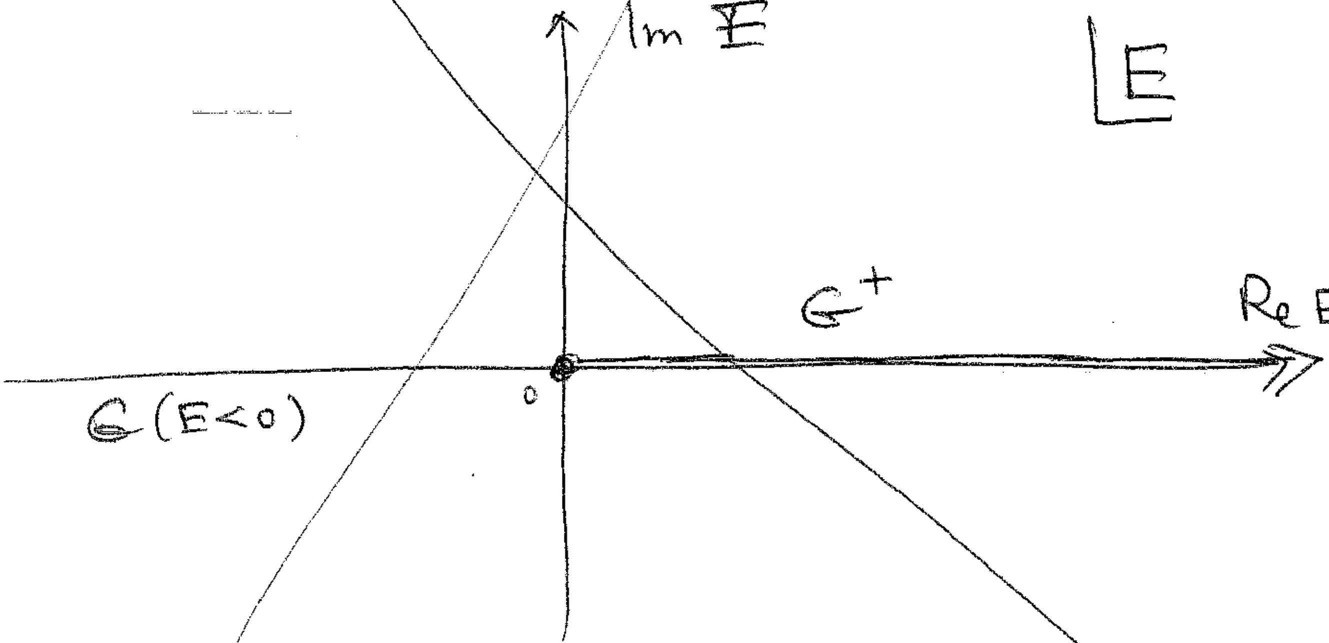
exercise**: find $T(E)$ for $U = U_0 / \cosh^2 \frac{x}{a}$

hint: see Landau-Lifshitz vol III.

Remark:

$$G(x-x') = i\sqrt{\frac{m}{2\hbar^2 E}}\, \exp\left(i\sqrt{\frac{2mE}{\hbar^2}}\,|x-x'|\right)$$

combines results for $G^{\pm}$, $G(E<0)$:



On physical sheet, $|G| \to 0$ for $|E| \to \infty$.

Return to the problem $U(x) = -\gamma\left(\delta(x+a) + \delta(x-a)\right)$

Since $[\hat{P}, \hat{H}] = 0$, where $\hat{P}$ - parity,

can choose basis of common eigenfunctions

$$\psi_\pm(x) = \frac{1}{2}\left(\psi(x) \pm \psi(-x)\right). \quad \boxed{P\psi_\pm = \pm\psi_\pm}$$

$$\boxed{\psi(x) = \psi_+(x) + \psi_-(x)} \quad \boxed{H\psi_\pm = E\psi_\pm}$$

Then:

$$\psi_+(x) = \cos kx + \gamma\left(G^+(x,-a) + G^+(x,a)\right)\psi_+(a)$$

$$\psi_-(x) = i\sin kx - \gamma\left(G^+(x,-a) - G^+(x,a)\right)\psi_-(a)$$

Should find:

$$S(k) = 1 + \frac{i\gamma}{k}\left(\frac{\cos^2 ka}{1+\gamma K_+} + \frac{\sin^2 ka}{1+\gamma K_-}\right),$$

$$K_\pm = \frac{1}{2ik}\left(1 \pm e^{2ika}\right)$$