Lecture 29

Last time, started on Born Approx.

Integral version of Sch. Eqn:

$$\psi(\vec{r}) = \frac{2m}{\hbar^2} \int G(\vec{r}-\vec{r}_0)\, V(\vec{r}_0)\, \psi(\vec{r}_0)\, d^3\vec{r}_0$$

where $G(\vec{r})$ is Green's function, satifies

$$(\nabla^2 + k^2)\, G = \delta^3(\vec{r})$$

Last time, worked out

$$G(\vec{r}) = \frac{1}{(2\pi)^3} \int e^{i\vec{s}\cdot\vec{r}} \frac{1}{k^2-s^2}\, d^3s$$

$$= \frac{1}{(2\pi)^3} \cdot \underbrace{\int_0^{2\pi} d\phi}_{2\pi} \int_0^{\pi} \sin\theta\, d\theta \int_0^{\infty} s^2 ds\, \frac{e^{isr\cos\theta}}{k^2-s^2}$$

$u = \cos\theta$

$$= \frac{1}{(2\pi)^2} \int_0^{\infty} \frac{s^2}{k^2-s^2} \underbrace{\int_{-1}^{1} e^{isru}\, du}_{\frac{1}{isr}\left[e^{isr} - e^{-isr}\right]} ds$$

$$= \frac{1}{(2\pi)^2} \frac{2}{r} \int_0^{\infty} \frac{s \sin sr}{k^2-s^2}\, ds$$

Note integrand is even in s.
Can write

$$= \frac{1}{(2\pi)^2} \frac{1}{r} \int_{-\infty}^{\infty} \frac{s \sin sr}{k^2-s^2}\, ds$$

But actually, go back to exp form now

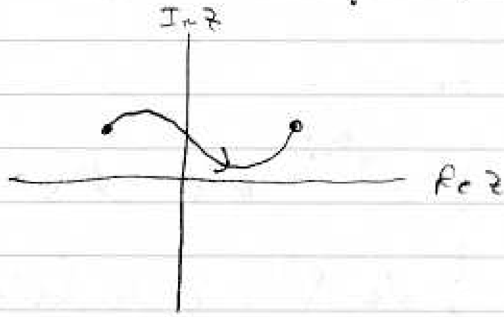
$$G = \frac{1}{(2\pi)^2}\frac{1}{2ir}\left[\int_{-\infty}^{\infty}\frac{s\,e^{isr}}{k^2-s^2}\,ds - \int_{-\infty}^{\infty}\frac{s\,e^{-isr}}{k^2-s^2}\,ds\right]$$

Do these with contour integration

Generalization of integrals to complex plane

$$\int f(z)\,dz \quad \text{for } z \text{ complex}$$

Now need to specify path in complex plane:



Much like a 2D line integral

But not exactly the same: if $\frac{\partial f}{\partial z}$ is to be well defined, need some relationship between Re z & Im z.

Most important result: Cauchy's formula

$$\oint \frac{f(z)}{z-z_0}\,dz = \begin{cases} 0 & \text{if } z_0 \text{ outside loop} \\ 2\pi i f(z_0) & \text{if } z_0 \text{ inside loop} \end{cases}$$

closed integral
= loop
= contour

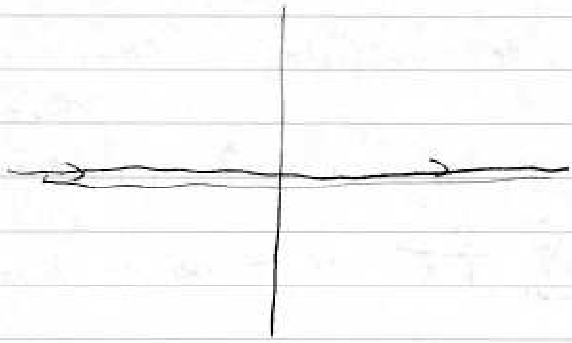
(Assuming $f(z)$ itself has no discontinuities inside the contour)

Call z_0 a pole = place where integrand $\to\infty$ like $\frac{1}{z}$

* Need to traverse contour in counter-clockwise sense. Otherwise, get − sign

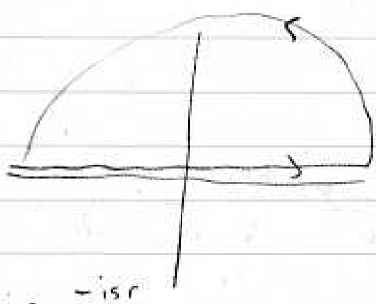
How do we apply it here?

One problem: integration path isn't a closed loop:



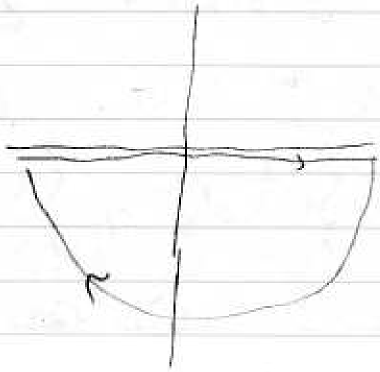
That's ok, we can close it at ∞, as long as integrand $\to 0$ for large $|z|$

For $\int \frac{s e^{isr}}{k^2-s^2}\, ds$, close with $\operatorname{Im} s > 0$:



Then $e^{isr} \to e^{ir \operatorname{Re} s}\, e^{-r \operatorname{Im} s}$ $\to 0$ for large $|s|$

For $\int \frac{s e^{-isr}}{k^2-s^2}\, ds$, need to close with $\operatorname{Im} s < 0$



In either case, can show that $\int_{\text{semi circle}} ds \to 0$

since integrand gets exponentially small

Second problem: $\dfrac{1}{k^2-s^2} = \dfrac{1}{(k-s)(k+s)}$

poles at $s = \pm k$

Neither inside nor outside contour: Cauchy's theorem doesn't apply:

Makes sense: $\displaystyle\int_{-\infty}^{\infty} \frac{e^{isr}}{k-s}\, ds = \infty$, diverges like $\frac{1}{s}$

But really, total integral is finite:

$$G(\vec{r}) = \frac{1}{4\pi^2}\frac{1}{r}\int_{-\infty}^{\infty} \frac{s \sin sr}{(k-s)(k+s)}\, ds$$

$$= B + \frac{1}{4\pi^2 r}\int_{k-\varepsilon}^{k+\varepsilon} \frac{s \sin sr}{(k-s)\underset{\substack{\downarrow \\ 2k}}{(k+s)}}\, ds + \frac{1}{4\pi^2 r}\int_{-k-\varepsilon}^{-k+\varepsilon} \frac{s \sin sr}{\underset{\substack{\downarrow \\ 2k}}{(k-s)}(k+s)}\, ds$$

Something finite

$$= B + \frac{1}{4\pi^2 r}\left[\frac{k \sin kr}{2k}\int_{k-\varepsilon}^{k+\varepsilon} \frac{1}{k-s}\, ds + \frac{(-k)\sin(-kr)}{(2k)}\int_{-k-\varepsilon}^{-k+\varepsilon} \frac{1}{k+s}\, ds\right]$$

$$= B + \frac{1}{4\pi^2 r}\frac{\sin kr}{2}\left[-\int_{k-\varepsilon}^{k+\varepsilon} \frac{1}{s-k}\, ds + \int_{-k-\varepsilon}^{-k+\varepsilon} \frac{1}{s+k}\, ds\right]$$

$u = s-k$ $\qquad\qquad$ $u = s+k$

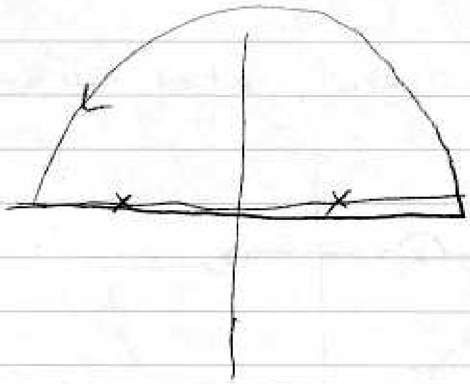
$$\left[-\int_{-\varepsilon}^{\varepsilon} \frac{1}{u}\, du + \int_{-\varepsilon}^{\varepsilon} \frac{1}{u}\, du\right]$$

$$= 0 \text{ for any } \varepsilon$$

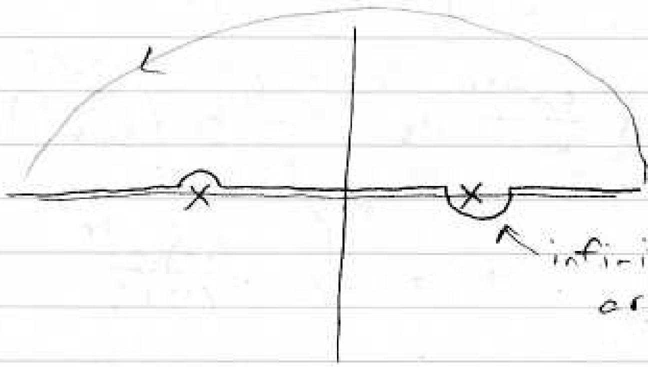
So divergent parts cancel out, get finite answer

That means that in contour integral, what happens right near the poles is not so important

Instead of



use



Easiest to include just one pole

infinitesimal "bump" around pole

Could deform contour differently... still get a valid solution.

$$\text{If} \quad G'(\vec{r}) = G(\vec{r}) + H(\vec{r})$$

with $(\nabla^2 + k^2)H = 0$,

then G' is a valid Green's func.

Shifting contour near poles just changes H

Choice shown is simplest.

So we can finally apply Cauchy's formula

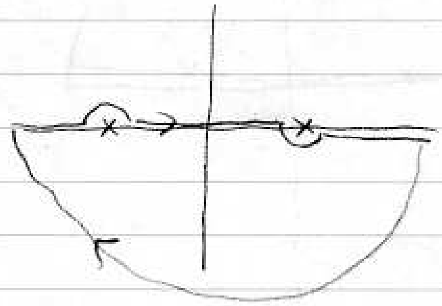
$$\int_{-\infty}^{\infty} \frac{s e^{isr}}{k^2 - s^2}\, ds = -\oint \left(\frac{s e^{isr}}{s+k} \right) \frac{1}{s-k}\, ds$$

pole at $s = k$

$$= -2\pi i \frac{k e^{ikr}}{2k}$$

$$= -\pi i e^{ikr}$$

For other integral, need to use some deformation



[Note, contour has clockwise sense

Then $\int_{-\infty}^{\infty} \frac{se^{-isr}}{k^2-s^2}\,ds = -\oint \left(\frac{se^{-isr}}{s-k}\right) \frac{1}{s+k}\,ds$

sense; pole at $s=-k$

$= +2\pi i \frac{(-k)e^{ikr}}{(-2k)} = +\pi i e^{ikr}$

And have

$$G(r) = \frac{1}{(2\pi)^2} \frac{1}{2ir}\left[\int_{-\infty}^{\infty} \frac{se^{isr}}{k^2-s^2}\,ds - \int_{-\infty}^{\infty} \frac{se^{-isr}}{k^2-s^2}\,ds\right]$$

$$= \frac{1}{4\pi^2} \frac{1}{2ir}\left[-i\pi e^{ikr} - i\pi e^{ikr}\right]$$

$$\boxed{G(\vec{r}) = -\frac{1}{4\pi r} e^{ikr}}$$

As Matt showed us last time, this is correct answer.