PHY 711 Classical Mechanics and Mathematical Methods
10-10:50 AM MWF in Olin 103

Notes for Lecture 25: Chap. 7 & App. A-D (F&W)

Generalization of the one dimensional wave equation ➔ various mathematical problems and techniques including:

1. **Complex variables**
2. **Contour integrals**
3. **Kramers-Kronig relationships**

Physics Colloquium

Thursday

October 26th, 2023

Division of Labor and Mechanism of Translocation in a Ring ATPase

Many transport processes in the cell are performed by a diverse but structurally and functionally related family of proteins. These proteins, which belong to the ASCE (Additional Strand, Conserved E) superfamily of ATPases, often form mutimeric rings. Despite their importance, a number of fundamental questions remain as to the coordination of the various subunits in these rings. Bacteriophage phi29 packages its 6.6 mm long double-stranded DNA using a pentameric ring nano motor Using optical tweezers, we find that this motor can work against loads of up to ~55 picoNewtons on average, making it one of the strongest molecular motors ever reported. Interestingly, the packaging rate decreases as the prohead fills, indicating that an internal pressure builds up due to DNA compression attaining the value of ~3 MegaPascals at the end of packaging, a pressure that is used as part of the mechanism of DNA injection in the next infection cycle. We have used high-resolution optical tweezers to show that the motor packages the DNA in alternating phases of dwells and bursts. During the dwell the motor exchanges nucleotide, whereas during the burst, the motor packages 10 bps of DNA per cycle. We have also characterized the steps and intersubunit coordination of this ATPase. By using non-hydrolyzable ATP analogs and stabilizers of the ADP bound to the motor, we establish where DNA binding, hydrolysis, and phosphate and ADP release occur relative to translocation during the motor's cycle. Surprisingly, a division of labor exists among the subunits: while only 4 of the subunits translocate DNA, all 5 bind and hydrolyze ATP, suggesting that the fifth subunit fulfills a regulatory function. Furthermore, we show that the motor not

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4 pm - Olin 101

Refreshments served prior to seminar beginning at 3:30 pm

20	Wed, 10/11/2023		Review and summary	Mid term due
	Fri, 10/13/2023	Fall Break		
21	Mon, 10/16/2023	Chap. 7	The wave and other partial differential equations	#15
22	Wed, 10/18/2023	Chap. 7	Sturm-Liouville equations	#16
23	Fri, 10/20/2023	Chap. 7	Sturm-Liouville equations	#17
24	Mon, 10/23/2023	Chap. 7	Laplace transforms and complex functions	#18
25	Wed, 10/25/2023	Chap. 7	Complex integration	#19
26	Fri, 10/27/2023			
27	Mon, 10/30/2023			
28	Wed, 11/01/2023			
29	Fri, 11/03/2023			
31	Mon, 11/06/2023			
32	Wed, 11/08/2023			
33	Fri, 11/10/2023			
34	Mon, 11/13/2023			

PHY 711 – Homework # 19

Assigned: 10/25/2023 Due: 10/30/2023

Read Appendix A of **Fetter and Walecka**.

1. Assume that $a > 0$ and $b > 0$; use contour integration methods to evaluate the integral:

$$\int_{-\infty}^{\infty} \frac{e^{iax}}{x^2 + b^2} dx.$$

Note that you may use Maple, Mathematica, or other software to evaluate this integral, but full credit will be earned by using the contour integration methods.

Basic ideas of complex integration --

For an analytic function, its integral over a closed region in the complex plane vanishes:

$$\oint f(z)dz = 0$$

However, consider the integration of a function which has a pole --

Behavior of $f(z) = \dfrac{1}{z^n}$ about the point $z = 0$:

For an integer n, consider

$$\oint \frac{1}{z^n} dz = \int_0^{2\pi} \frac{\rho e^{i\phi} i d\phi}{\rho^n e^{in\phi}} = \rho^{1-n} \int_0^{2\pi} e^{i(1-n)\phi} i d\phi = \begin{cases} 0 & n \neq 1 \\ 2\pi i & n = 1 \end{cases}$$

Behavior of $f(z)=\frac{1}{z^n}$ about the point $z=0$:

For an integer n, consider

$$\oint \frac{1}{z^n}dz = \int_0^{2\pi} \frac{\rho e^{i\phi} i d\phi}{\rho^n e^{in\phi}} = \rho^{1-n}\int_0^{2\pi} e^{i(1-n)\phi} i d\phi = \begin{cases} 0 & n \neq 1 \\ 2\pi i & n = 1 \end{cases}$$

This observation helps us to focus on a special kind of singularity called a "pole"

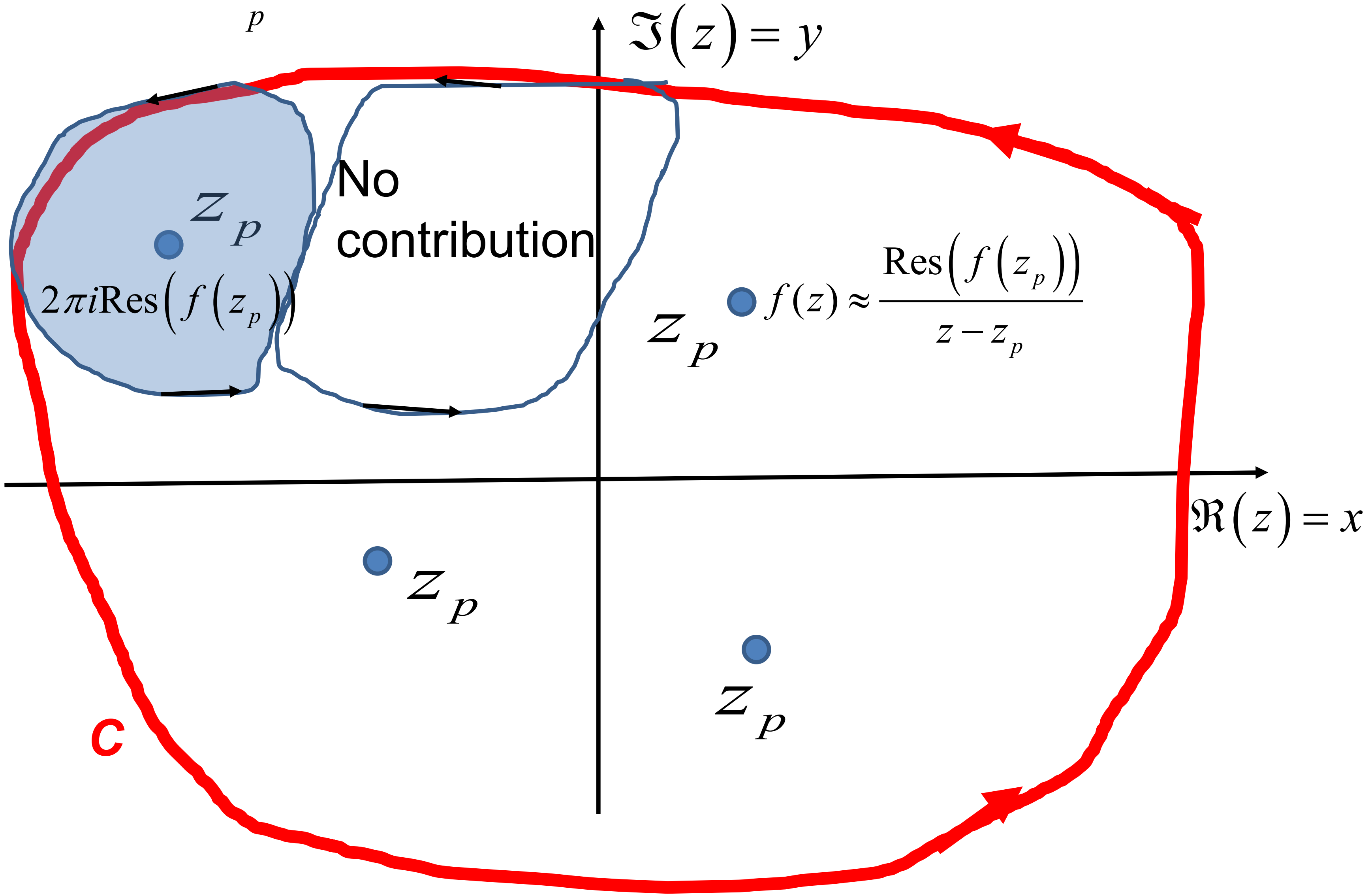
For $f(z)$ in the vicinity of $z = z_p$: $f(z) \approx \frac{g(z_p)}{z-z_p}$

Therefore: $\oint f(z)dz = 0$ or $\oint f(z)dz = g(z_p)\oint \frac{dz}{z-z_p} = 2\pi i g(z_p)$

Integration does not include z_p

Integration does include z_p

$$\oint_C f(z)dz = 2\pi i \sum_p \text{Res}\left(f(z_p)\right)$$



General formula for determining residue:

Suppose that in the neighborhood of z_p, $f(z) \approx \frac{h(z)}{\left(z-z_p\right)^m} \underset{z\to z_p}{\equiv} \frac{\text{Res}\left(f(z_p)\right)}{z-z_p}$

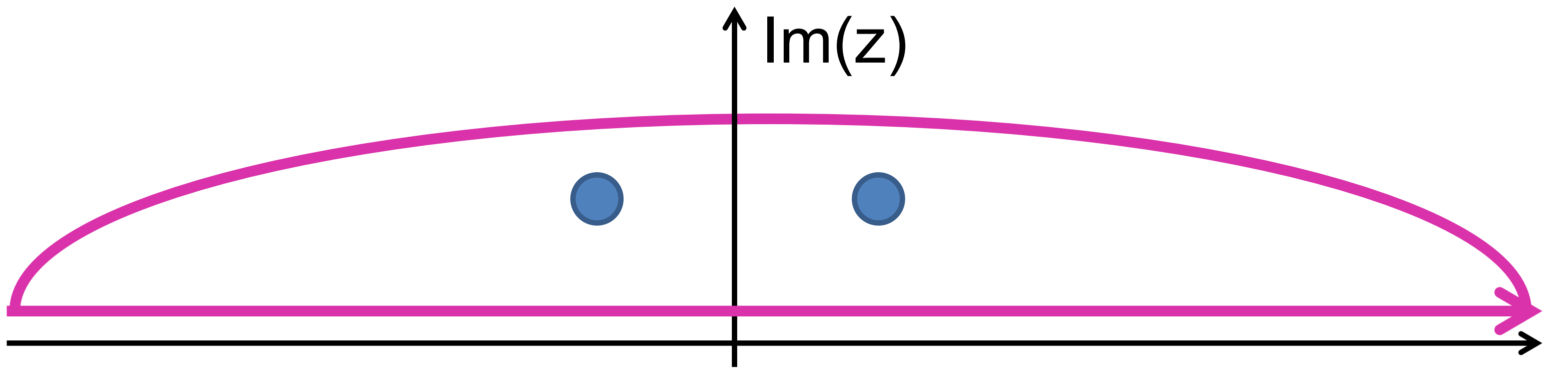
Since $h(z) \equiv \left(z-z_p\right)^m f(z)$ is analytic near z_p, we can make a Taylor exansion

about z_p: $$h(z) \approx h(z_p) + \left(z-z_p\right)\frac{dh(z_p)}{dz} + \ldots + \frac{\left(z-z_p\right)^{m-1}}{(m-1)!}\frac{d^{m-1}h(z_p)}{dz^{m-1}} + \ldots.$$

$$\Rightarrow \text{Res}\left(f(z_p)\right) = \lim_{z\to z_p}\left\{\frac{1}{(m-1)!}\frac{d^{m-1}\left(\left(z-z_p\right)^m f(z)\right)}{dz^{m-1}}\right\}$$

In the following examples *m=1*

Example: $$\int_{-\infty}^{\infty} \frac{x^2}{1+x^4}dx = \int_{-\infty}^{\infty} \frac{x^2}{1+x^4}dx + 0 = \oint \frac{z^2}{1+z^4}dz$$



$$1+z^4 = \left(z-e^{i\pi/4}\right)\left(z-e^{3i\pi/4}\right)\left(z-e^{-i\pi/4}\right)\left(z-e^{-3i\pi/4}\right)$$

$$\oint \frac{z^2}{1+z^4}dz = 2\pi i\left(\text{Res}\left(z_p = e^{i\pi/4}\right) + \text{Res}\left(z_p = e^{3i\pi/4}\right)\right)$$

Note:
m=1

$$\text{Res}\left(z_p = e^{i\pi/4}\right) = \frac{e^{i\pi/4}}{4i} \qquad \text{Res}\left(z_p = e^{3i\pi/4}\right) = -\frac{e^{3i\pi/4}}{4i}$$

$$\oint \frac{z^2}{1+z^4}dz = 2\pi i\left(\frac{e^{i\pi/4}}{4i} - \frac{e^{3i\pi/4}}{4i}\right) = \frac{\pi}{2}\left(\left(\sqrt{\frac{1}{2}} + i\sqrt{\frac{1}{2}}\right) - \left(-\sqrt{\frac{1}{2}} + i\sqrt{\frac{1}{2}}\right)\right) = \frac{\pi}{\sqrt{2}}$$

Some details:

Note that: $e^{i\pi} = -1 = e^{-i\pi}$

$$e^{-3i\pi/4} = e^{i\pi/4 - i\pi} = -e^{i\pi/4}$$

$$f(z) = \frac{z^2}{1+z^4}$$

$$\text{Res}\left(f(z = e^{i\pi/4} \right) = \frac{\left(e^{i\pi/4}\right)^2}{\left(e^{i\pi/4} - e^{3i\pi/4}\right)\left(e^{i\pi/4} - e^{-i\pi/4}\right)\left(e^{i\pi/4} - e^{-3i\pi/4}\right)}$$

$$= \frac{e^{i\pi/2}}{\left(e^{i\pi/4} + e^{-i\pi/4}\right)\left(e^{i\pi/4} - e^{-i\pi/4}\right)\left(e^{i\pi/4} + e^{i\pi/4}\right)}$$

$$= \frac{e^{i\pi/4}}{2\left(i-(-i)\right)} = \frac{e^{i\pi/4}}{4i}$$

Question – Could we have chosen the contour in the lower half plane?

a. Yes

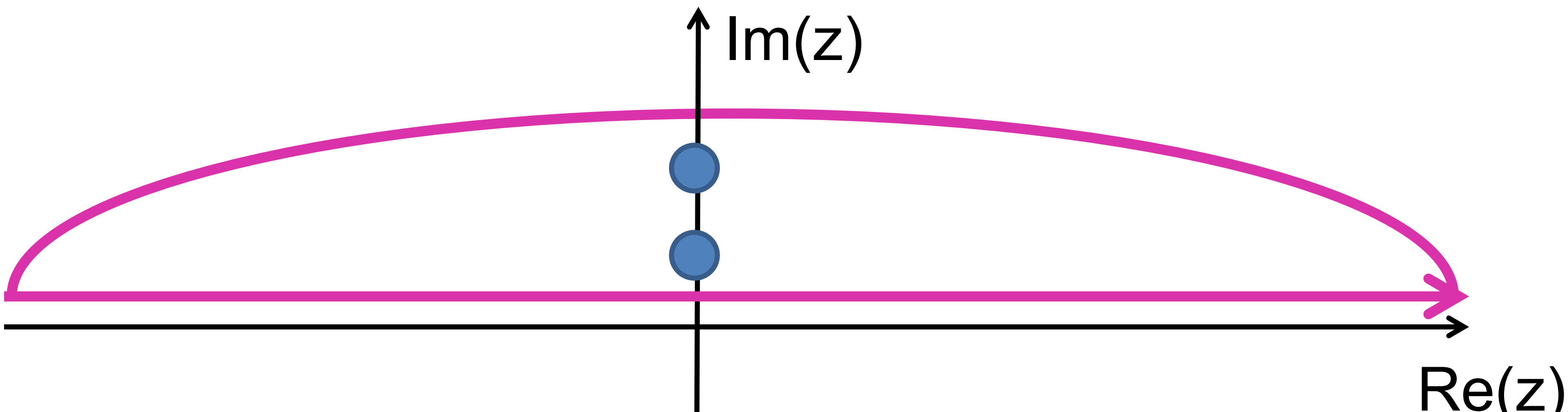
b. No

Another example: $I = \int_0^\infty \frac{\cos(ax)}{4x^4 + 5x^2 + 1} dx$

$$\int_0^\infty \frac{\cos(ax)}{4x^4+5x^2+1}dx = \frac{1}{2}\int_{-\infty}^{\infty} \frac{e^{iax}}{4x^4+5x^2+1}dx = \frac{1}{2}\oint \frac{e^{iaz}}{4z^4+5z^2+1}dz$$

$$4z^4+5z^2+1 = 4(z-i)\left(z-\tfrac{i}{2}\right)(z+i)\left(z+\tfrac{i}{2}\right)$$

Note:
m=1



$$I = 2\pi i\left(\text{Res}\left(z_p = i\right) + \text{Res}\left(z_p = \tfrac{i}{2}\right)\right)$$

$$\int_0^\infty \frac{\cos(ax)}{4x^4+5x^2+1}dx = \frac{1}{2}\oint \frac{e^{iaz}}{4z^4+5z^2+1}dz$$

$$=2\pi i\left(\mathrm{Res}\left(z_p=i\right)+\mathrm{Res}\left(z_p=\tfrac{i}{2}\right)\right)$$

$$=\frac{\pi}{6}\left(-e^{-a}+2e^{-a/2}\right)$$

Question – Could we have chosen the contour in the lower half plane?

a. Yes

b. No

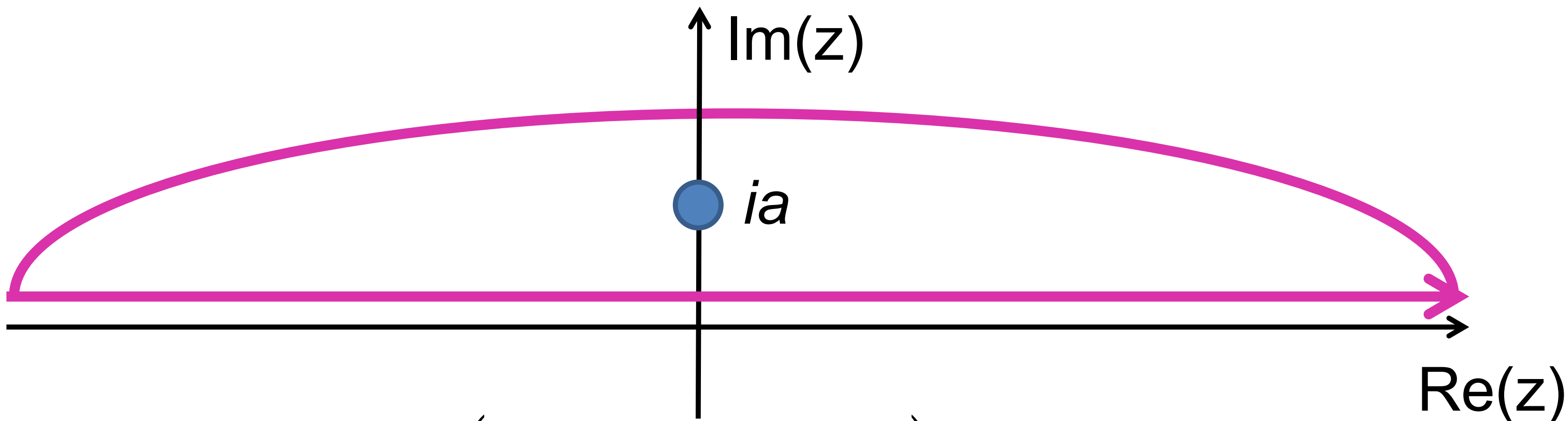
Note that for $a>0$ and $z_I>0$

in the lower half plane: $e^{iaz}=e^{iaz_R}e^{az_I}$

Another example: $I = \int_{-\infty}^{\infty} \frac{x \sin kx}{x^2 + a^2} dx \quad \text{for } k > 0 \text{ and } a > 0$

$$\int_{-\infty}^{\infty} \frac{x \sin kx}{x^2 + a^2} dx = \frac{1}{i} \int_{-\infty}^{\infty} \frac{x e^{ikx}}{x^2 + a^2} dx = \frac{1}{i} \oint \frac{z e^{ikz}}{z^2 + a^2} dz$$

$$z^2 + a^2 = (z - ia)(z + ia)$$



$$I = 2\pi i \left(\text{Res}\left(z_p = ia \right) \right) = \pi e^{-ka}$$

Some details --

$$\int_{-\infty}^{\infty} \frac{x \sin kx}{x^2 + a^2} dx = \frac{1}{i} \int_{-\infty}^{\infty} \frac{x e^{ikx}}{x^2 + a^2} dx = \frac{1}{i} \oint \frac{z e^{ikz}}{z^2 + a^2} dz$$

$$z^2 + a^2 = (z - ia)(z + ia)$$

$$\frac{1}{i} \oint \frac{z e^{ikz}}{z^2 + a^2} dz = 2\pi i \frac{1}{i} \lim_{z \to ia} \left((z - ia) \frac{z e^{ikz}}{z^2 + a^2} \right)$$

$$= 2\pi i \frac{1}{i} \frac{ia e^{-ka}}{2ia} = \pi e^{-ka}$$

From the Drude model of dielectric response --

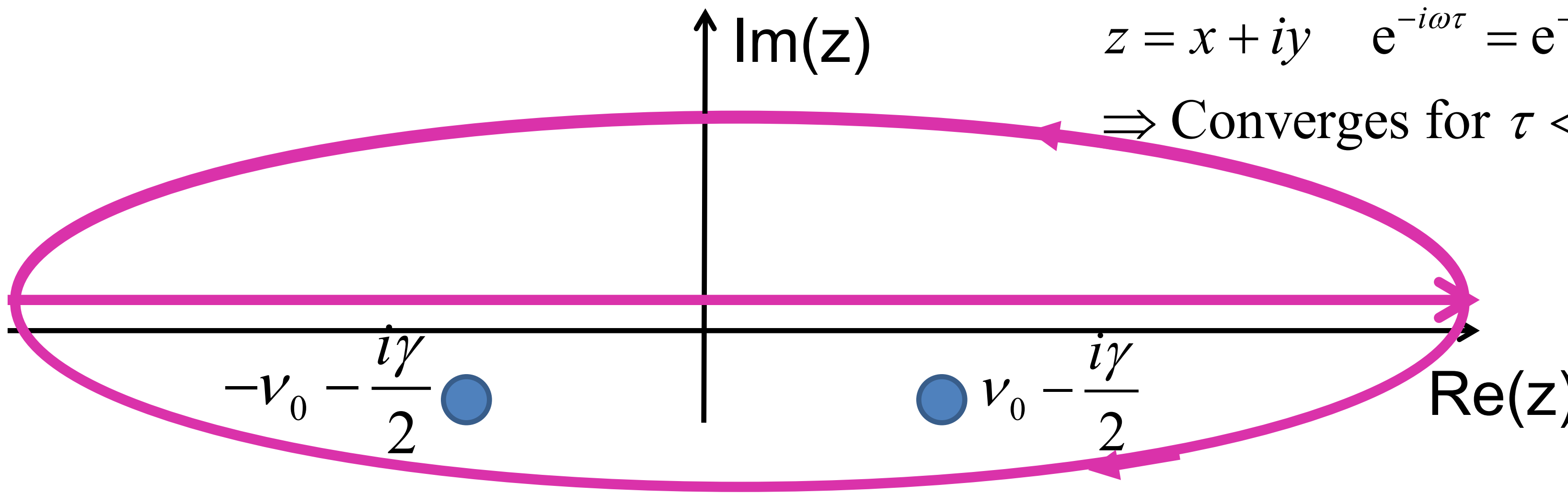
$$G(\tau) = \frac{\omega_p^2}{2\pi}\int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega\tau}}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

where ω_p, ω_0, and γ are positive constants

Upper hemisphere:

$z = x + iy \quad \mathrm{e}^{-i\omega\tau} = \mathrm{e}^{-ix\tau + y\tau}$

$\Rightarrow$ Converges for $\tau < 0$



$$\nu_0 \equiv \sqrt{\omega_0^2 - \frac{\gamma^2}{4}}$$

Lower hemisphere:

$z = x - iy \quad \mathrm{e}^{-i\omega\tau} = \mathrm{e}^{-ix\tau - y\tau}$

$\Rightarrow$ Converges for $\tau > 0$

From the Drude model of dielectric response -- continued --

$$G(\tau)=\frac{\omega_p^2}{2\pi}\int_{-\infty}^{\infty} d\omega \frac{e^{-i\omega\tau}}{\omega_0^2-\omega^2-i\gamma\omega}$$ where ω_p, ω_0, and γ are positive constants

$$G(\tau)=\omega_p^2\begin{cases} 0 & \text{for } \tau<0 \\ e^{-\gamma\tau/2}\dfrac{\sin\nu_0\tau}{\nu_0} & \text{for } \tau>0 \end{cases}$$

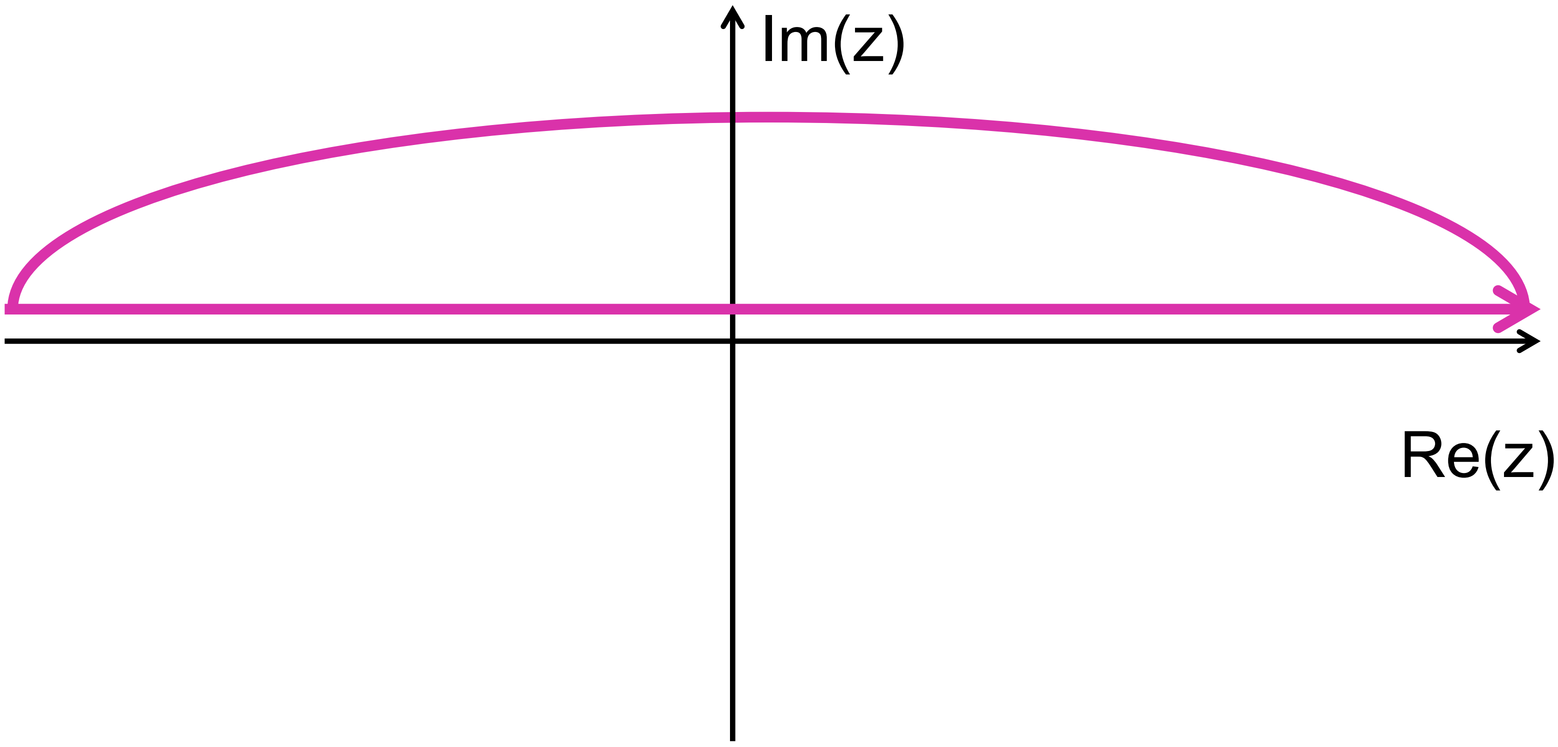
Cauchy integral theorem for analytic function *f(z)*:

$$f(z) = \frac{1}{2\pi i} \oint_C \frac{f(z')}{z' - z} dz' .$$

Example

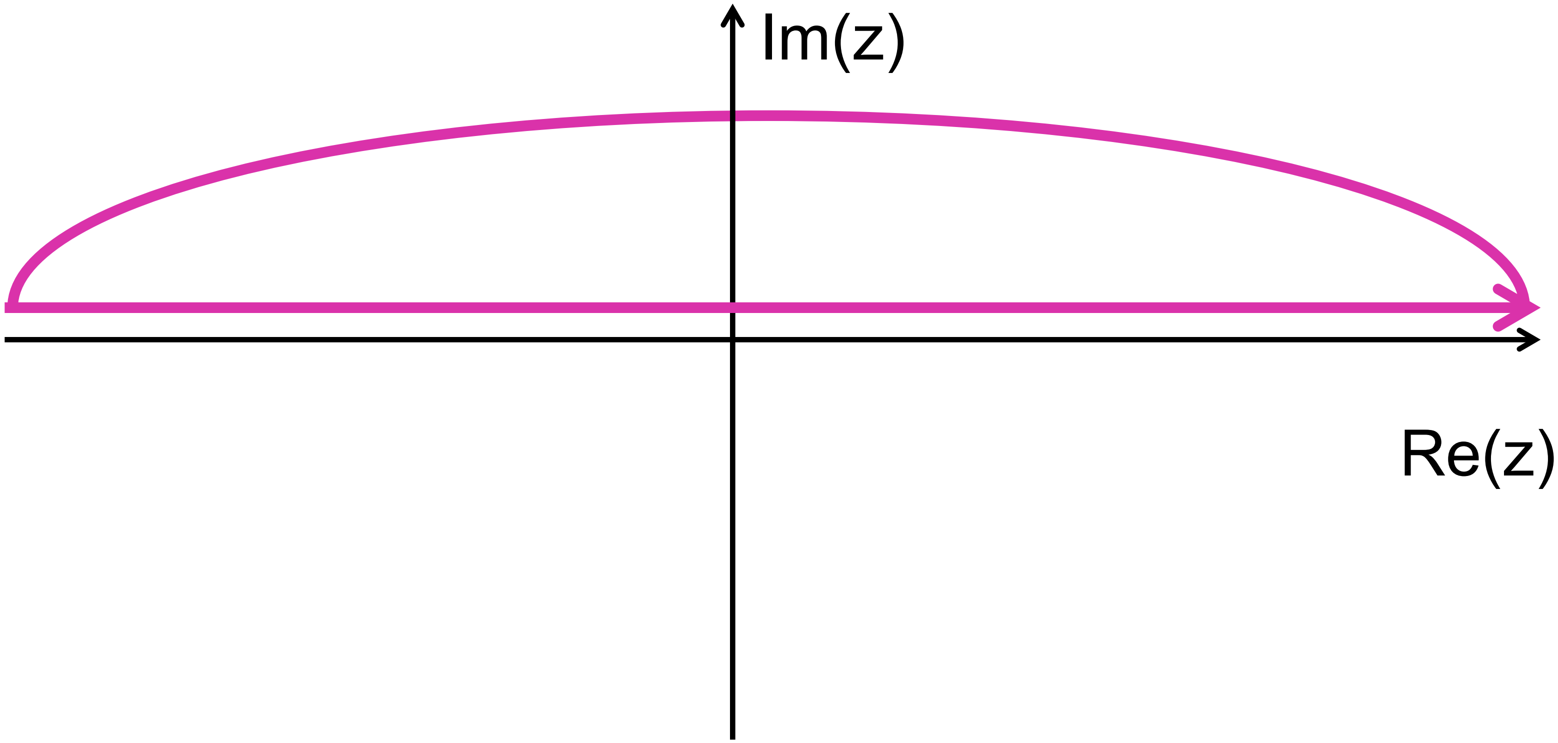
$$\text{Suppose } f\left(|z| \rightarrow \infty\right) = 0 \text{ and for } z = x:$$

$$f(x) = a(x) + ib(x)$$



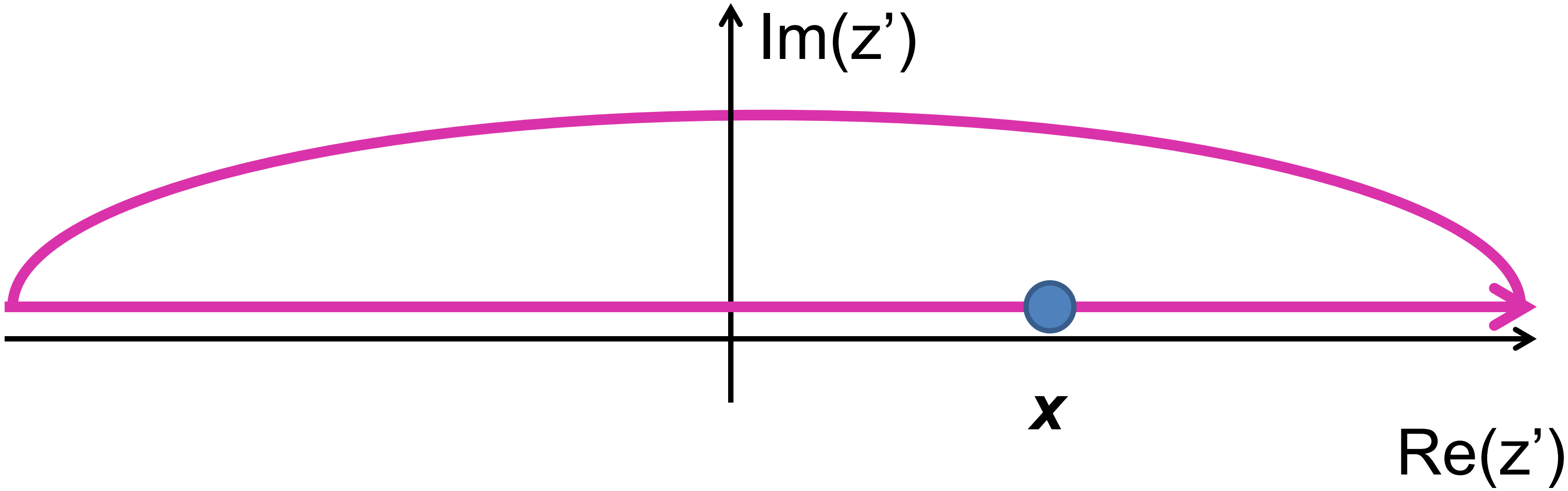
Example -- continued

$$f(z)=\frac{1}{2\pi i}\oint\frac{f(z')}{z'-z}dz' \quad \text{where} \quad f(x)=a(x)+ib(x)$$



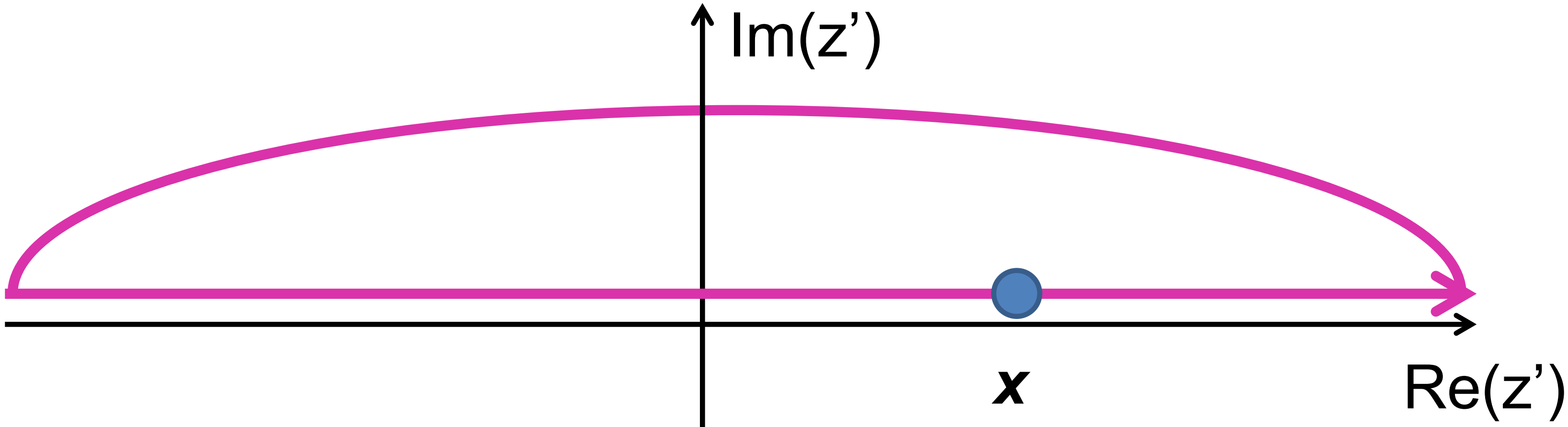
$$a(x)+ib(x)=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{a(x')+ib(x')}{x'-x}dx' + 0$$

Example -- continued



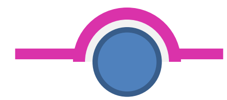
$$\int_{-\infty}^{\infty}\frac{f(x')}{x'-x}dx' = \int_{-\infty}^{x-\varepsilon}\frac{f(x')}{x'-x}dx' + \int_{x+\varepsilon}^{\infty}\frac{f(x')}{x'-x}dx' + \int_{x-\varepsilon}^{x+\varepsilon}\frac{f(x')}{x'-x}dx'$$

$$= P\int_{-\infty}^{\infty}\frac{f(x')}{x'-x}dx' + i\pi\, f(x)$$



$$\text{let} \quad u = x' - x$$

$$\text{let} \quad x \rightarrow x + i\eta$$

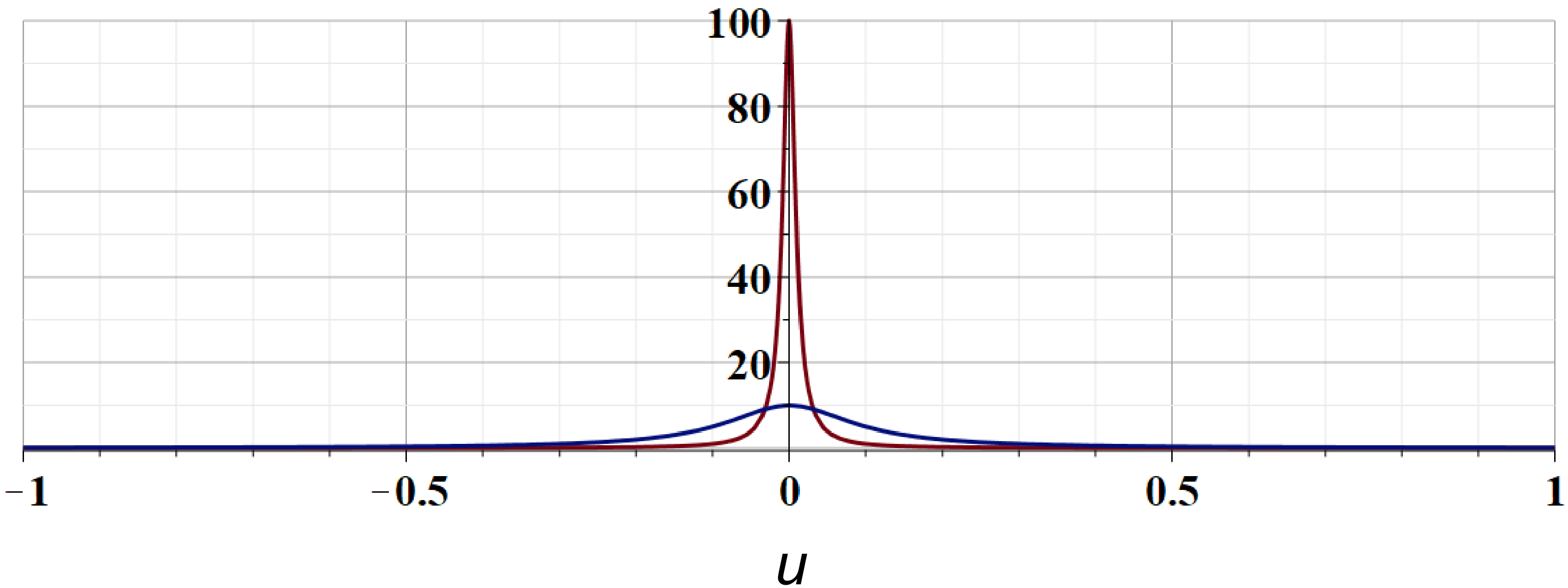


$$\int_{x-\varepsilon}^{x+\varepsilon} \frac{f\left(x'\right)}{x'-x} dx' \approx f(x) \lim_{\eta\to 0} \int_{-\varepsilon}^{\varepsilon} \frac{1}{u - i\eta} du = f(x) \lim_{\eta\to 0} \int_{-\varepsilon}^{\varepsilon} \frac{u + i\eta}{u^2 + \eta^2} du$$

$$= i\pi f\left(x\right) \qquad \text{since} \qquad \lim_{\eta\to 0} \frac{i\eta}{u^2 + \eta^2} \approx i\pi\delta(u)$$

More details --

$$\lim_{\eta\to 0}\frac{\eta}{u^2+\eta^2}\approx \pi\delta(u)$$



Example -- continued

$$\int_{-\infty}^{\infty} \frac{f(x')}{x'-x} dx' = \int_{-\infty}^{x-\varepsilon} \frac{f(x')}{x'-x} dx' + \int_{x+\varepsilon}^{\infty} \frac{f(x')}{x'-x} dx' + \int_{x-\varepsilon}^{x+\varepsilon} \frac{f(x')}{x'-x} dx'$$

$$= P\int_{-\infty}^{\infty} \frac{f(x')}{x'-x} dx' + i\pi\, f(x)$$

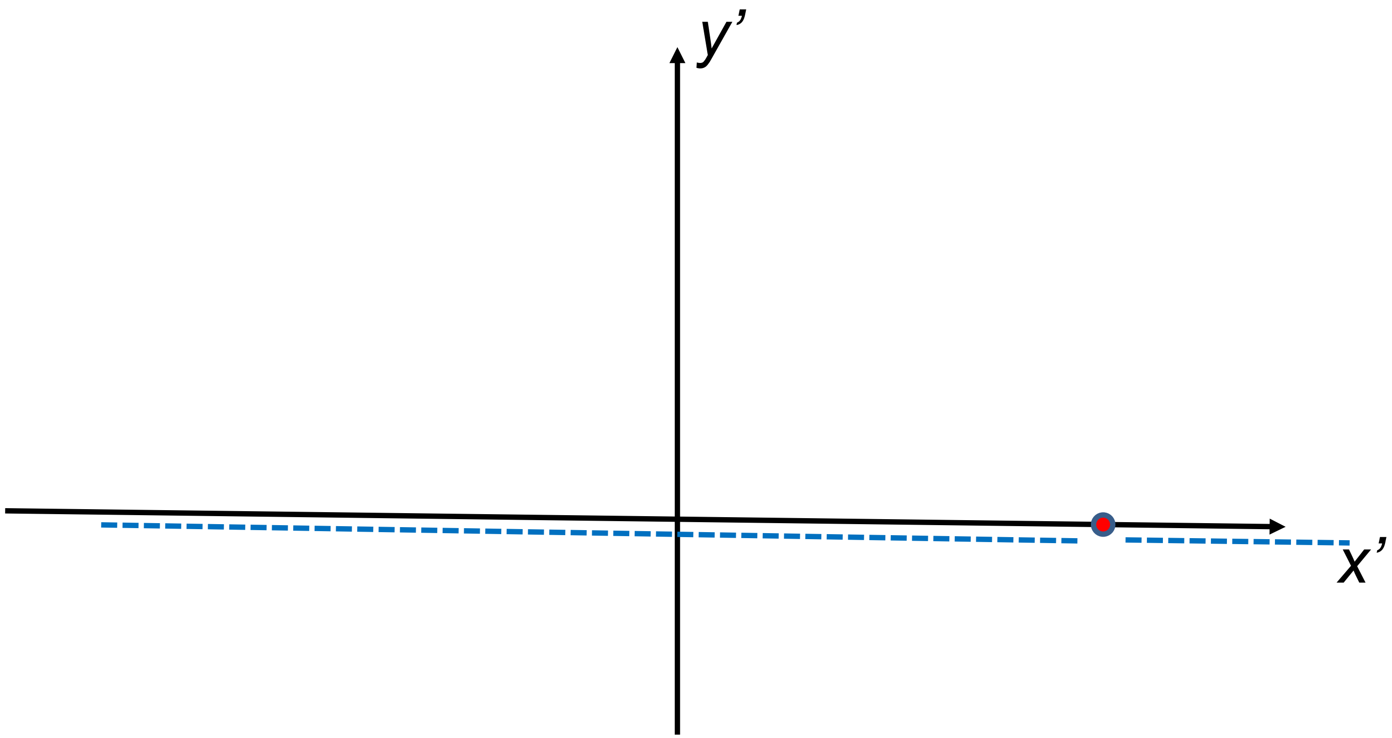
$$a(x) + ib(x) = \frac{P}{2\pi i} \int_{-\infty}^{\infty} \frac{a(x') + ib(x')}{x'-x} dx' + \frac{\pi i}{2\pi i}\left(a(x) + ib(x)\right)$$

$$\Rightarrow a(x) = \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{b(x')}{x'-x} dx' \qquad b(x) = -\frac{P}{\pi} \int_{-\infty}^{\infty} \frac{a(x')}{x'-x} dx'$$

Kramers-Kronig relationships

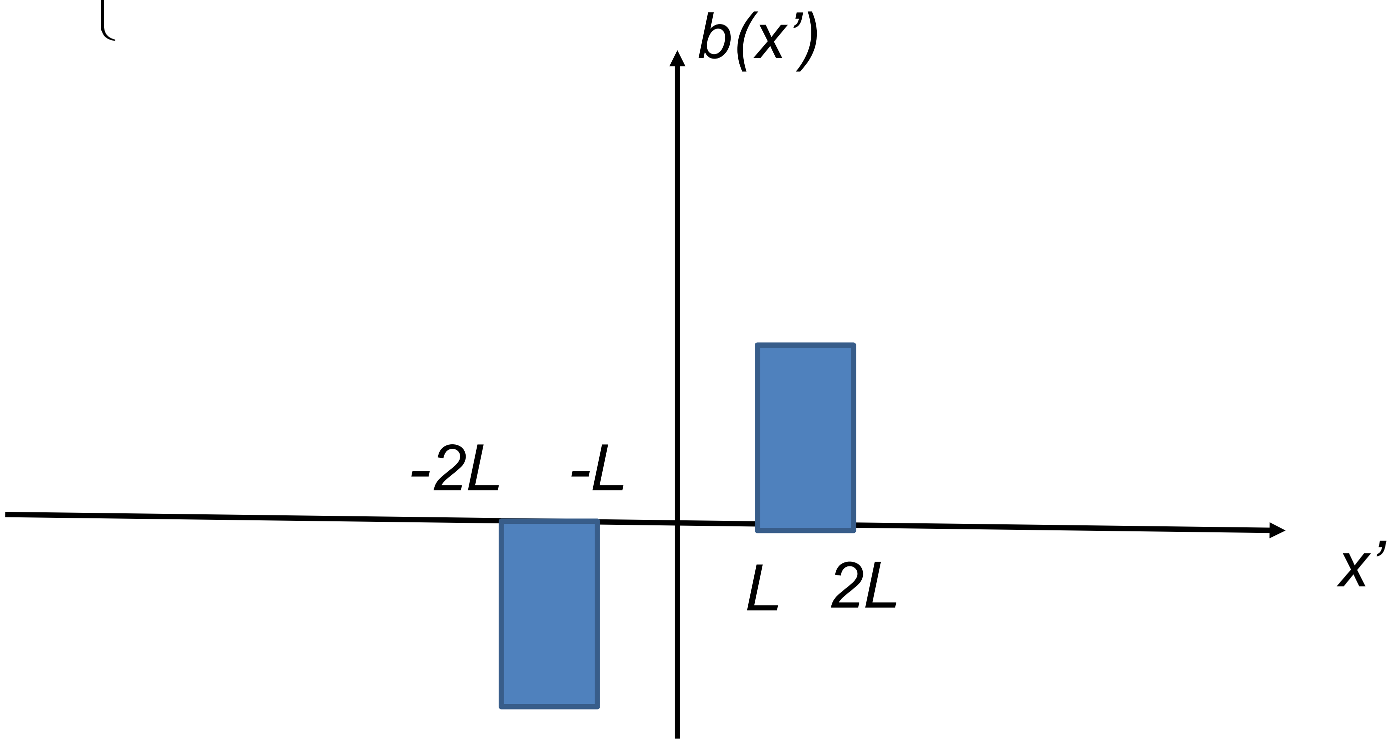
Comment on evaluating principal parts integrals

$$a(x) = \frac{P}{\pi}\int_{-\infty}^{\infty}\frac{b(x')}{x'-x}dx' = \lim_{\epsilon\to 0}\left(\frac{1}{\pi}\int_{-\infty}^{x-\epsilon}\frac{b(x')}{x'-x}dx' + \frac{1}{\pi}\int_{x+\epsilon}^{\infty}\frac{b(x')}{x'-x}dx'\right)$$



Example:

$$b(x') = \begin{cases} 0 & \text{for } x' < -2L, \quad -L < x' < L, \quad x' > 2L \\ B_0 & \text{for} \quad L < x' < 2L \\ -B_0 & \text{for} \quad -2L < x' < -L \end{cases}$$



Example:

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$$a(x) = \frac{P}{\pi}\int_{-\infty}^{\infty} \frac{b(x')}{x'-x}dx' = \lim_{\epsilon \to 0}\left(\frac{1}{\pi}\int_{-\infty}^{x-\epsilon} \frac{b(x')}{x'-x}dx' + \frac{1}{\pi}\int_{x+\epsilon}^{\infty} \frac{b(x')}{x'-x}dx' \right)$$

For $x < -2L \quad$ or $\quad x > 2L \qquad -L < x < L:$

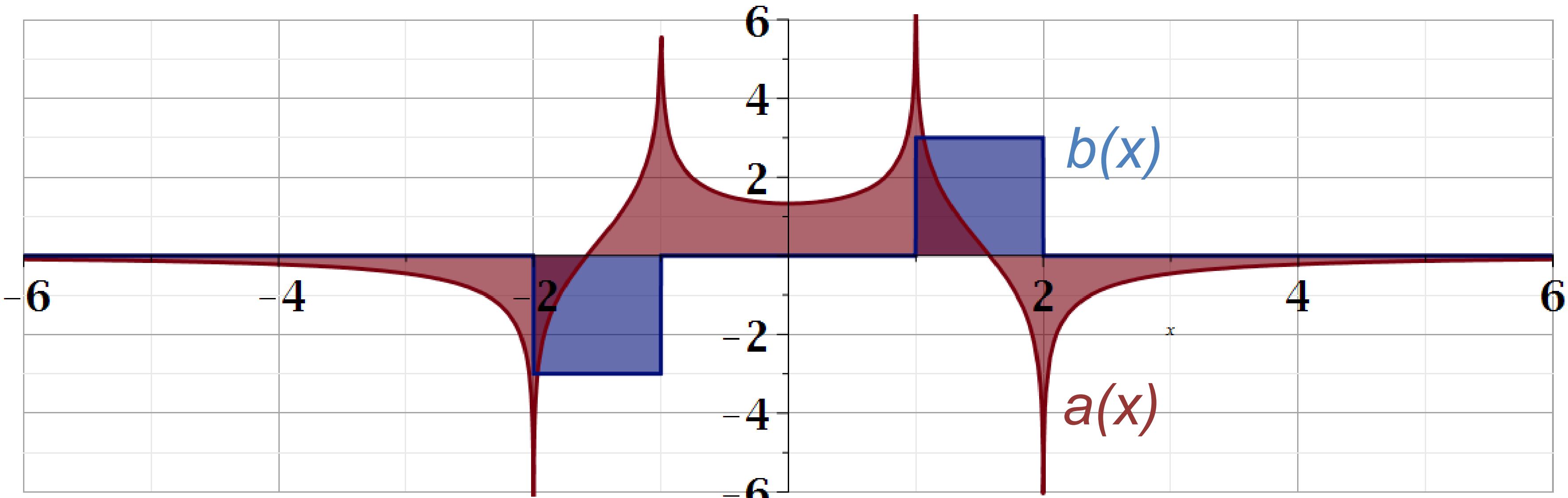
$$a(x) = \frac{-B_0}{\pi}\int_{-2L}^{-L} \frac{dx'}{x'-x} + \frac{B_0}{\pi}\int_{L}^{2L} \frac{dx'}{x'-x}$$

$$= \frac{-B_0}{\pi}\ln\left(\left| \frac{x+L}{x+2L} \right| \right) + \frac{B_0}{\pi}\ln\left(\left| \frac{x-2L}{x-L} \right| \right) = \frac{B_0}{\pi}\ln\left(\left| \frac{x^2-4L^2}{x^2-L^2} \right| \right)$$

$$a(x) = \frac{P}{\pi}\int_{-\infty}^{\infty}\frac{b(x')}{x'-x}dx' = \lim_{\epsilon \to 0}\left(\frac{1}{\pi}\int_{-\infty}^{x-\epsilon}\frac{b(x')}{x'-x}dx' + \frac{1}{\pi}\int_{x+\epsilon}^{\infty}\frac{b(x')}{x'-x}dx'\right)$$

For our example:

$$a(x) = \frac{B_0}{\pi}\ln\left(\left|\frac{4L^2 - x^2}{L^2 - x^2}\right|\right)$$



Summary

For a function $f(x)$, analytic along the real line:

$$f(x) = \Re\left(f(x)\right) + i\Im\left(f(x)\right) = a\left(x\right) + ib\left(x\right)$$

$$\Rightarrow a\left(x\right) = \frac{P}{\pi}\int_{-\infty}^{\infty} \frac{b\left(x'\right)}{x'-x}dx' \qquad b\left(x\right) = -\frac{P}{\pi}\int_{-\infty}^{\infty} \frac{a\left(x'\right)}{x'-x}dx'$$

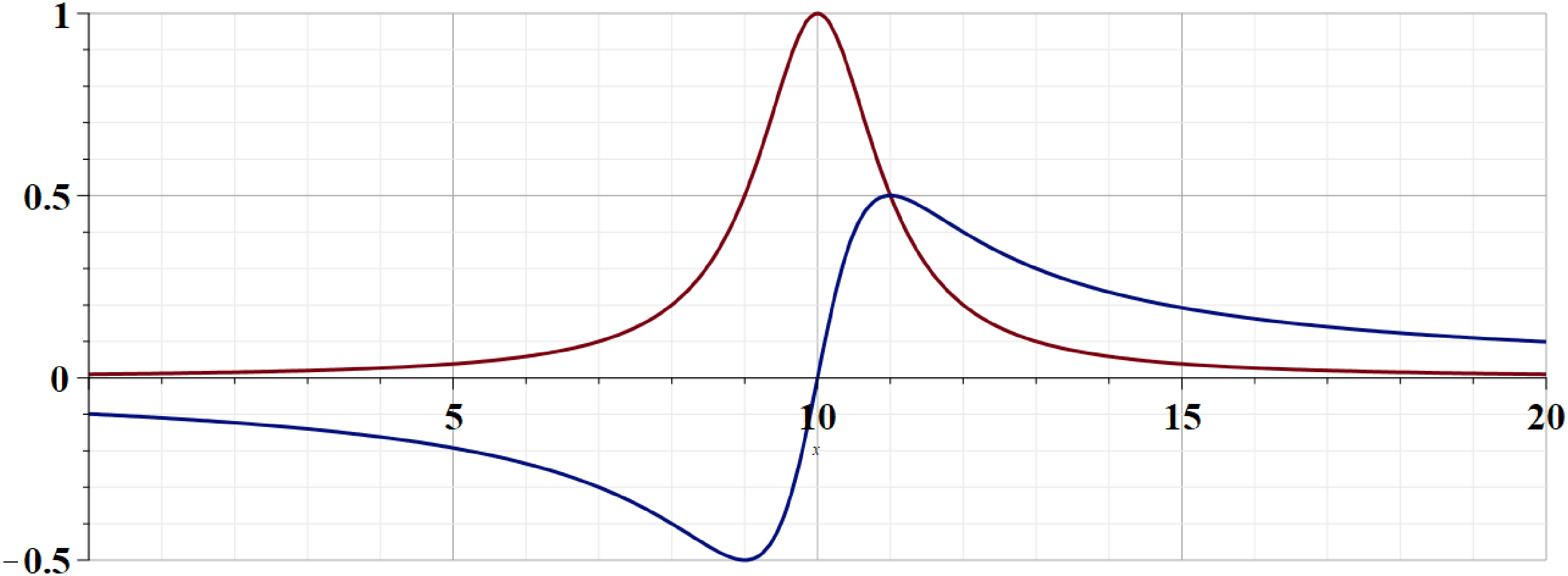
Example:

$$f(x) = \frac{1}{x+i} \qquad a(x) = \frac{x}{x^2+1} \qquad b(x) = -\frac{1}{x^2+1}$$

Check:

$$\frac{P}{\pi}\int_{-\infty}^{\infty} \frac{b\left(x'\right)}{x'-x}dx' = -\frac{P}{\pi}\int_{-\infty}^{\infty} \frac{1}{\left(x'-x\right)\left(x'^2+1\right)}dx' \overset{?}{=} \frac{x}{x^2+1} = a(x)$$

$$a(\omega) = \frac{\omega - 10}{(\omega - 10)^2 + 1} \qquad b(\omega) = \frac{1}{(\omega - 10)^2 + 1}$$



Continued:

$$\frac{P}{\pi}\int_{-\infty}^{\infty}\frac{b(x')}{x'-x}dx' = -\frac{P}{\pi}\int_{-\infty}^{\infty}\frac{1}{(x'-x)(x'^2+1)}dx'$$

$$= -\frac{P}{\pi}\int_{-\infty}^{\infty}\left(\frac{1}{(x'-x)(x'^2+1)}-\frac{1}{(x'-x)(x^2+1)}\right)dx' - \frac{1}{(x^2+1)}\frac{P}{\pi}\int_{-\infty}^{\infty}\frac{1}{x'-x}dx'$$

$$= -\frac{P}{\pi}\int_{-\infty}^{\infty}\left(\frac{x^2-x'^2}{(x'-x)(x'^2+1)(x^2+1)}\right)dx' - \frac{1}{(x^2+1)}\frac{P}{\pi}\int_{-\infty}^{\infty}\frac{1}{x'-x}dx'$$

$$= \frac{P}{\pi}\int_{-\infty}^{\infty}\left(\frac{x+x'}{(x'^2+1)(x^2+1)}\right)dx' - \frac{1}{(x^2+1)}\frac{P}{\pi}\int_{-\infty}^{\infty}\frac{1}{x'-x}dx'$$

Note that: $\displaystyle\int_{x+\epsilon}^{X}\frac{1}{x'-x}dx' = \ln(X-x)-\ln(\epsilon) = \ln\left(\frac{X-x}{\epsilon}\right)$

$$\int_{-X}^{x-\epsilon}\frac{1}{x'-x}dx' = -\ln(-X-x)+\ln(-\epsilon) = -\ln\left(\frac{X+x}{\epsilon}\right)$$

$$\frac{P}{\pi}\int_{-\infty}^{\infty}\frac{1}{x'-x}dx' = \lim_{X\to\infty}\ln\left(\frac{X-x}{X+x}\right) = 0 \qquad \frac{P}{\pi}\int_{-\infty}^{\infty}\frac{1}{x'^2+1}dx' = 1$$

$$\frac{P}{\pi}\int_{-\infty}^{\infty}\frac{b(x')}{x'-x}dx' = \frac{x}{x^2+1} = a(x)$$