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

Plan for Lecture 22:

Read Chapter 7 & Appendices A-D

Generalization of the one dimensional wave equation ➔ various mathematical problems and techniques including:
1. Complex variables
2. Contour integrals

6	Mon, 9/10/2018	Chap. 3	Calculus of Variation	#5	9/12/2018
7	Wed, 9/12/2018	Chap. 3	Calculus of Variation	#6	9/17/2018
	Fri, 9/14/2018	No class	University closed due to weather.		
8	Mon, 9/17/2018	Chap. 3	Lagrangian Mechanics	#7	9/19/2018
9	Wed, 9/19/2018	Chap. 3 and 6	Lagrangian Mechanics and constraints	#8	9/24/2018
10	Fri, 9/21/2018	Chap. 3 and 6	Constants of the motion		
11	Mon, 9/24/2018	Chap. 3 and 6	Hamiltonian formalism	#9	9/28/2018
12	Wed, 9/26/2018	Chap. 3 and 6	Liouville theorem	#10	10/3/2018
13	Fri, 9/28/2018	Chap. 3 and 6	Canonical transformations		
14	Mon, 10/1/2018	Chap. 4	Small oscillations about equilibrium	#11	10/5/2018
15	Wed, 10/3/2018	Chap. 4	Normal modes of vibration		
16	Fri, 10/5/2018	Chap. 1-4, 6	Review		
17	Mon, 10/8/2018	Chap. 7	Strings		
18	Wed, 10/10/2018	Chap. 7	Wave equation		
	Fri, 10/12/2018	No class	Fall break		
19	Mon, 10/15/2018	Chap. 7	Wave equation		
20	Wed, 10/17/2018	Chap. 7	Fourier Transforms	#12	10/22/2018
21	Fri, 10/19/2018	Chap. 7	Laplace transforms; Contour integrals	#13	10/24/2018
22	Mon, 10/22/2018	Chap. 7	Contour integgrals		
23	Wed, 10/24/2018	Chap. 5	Rigid body motion		

Dr. Ilias Belharouak

Distinguished Scientist and Group Leader
Oak Ridge National Laboratory

"Science and Technology Drivers in Batteries for Renewables Energy & Mobility Applications"

Wednesday, October 24, 2018, at 4:00 pm

George P. Williams, Jr. Lecture Hall (Olin 101)

The worldwide growing integration of renewable energies and electric vehicles will require massive deployment of energy storage solutions. The aim of this seminar is to discuss the potential of batteries to stabilize the grid whilst storing energy, understand various types of batteries used to store energy and address battery life expectancy, and how it can be maintained for maximum efficiency. A case study centered around a 250kW/500kWh lithium-ion battery coupled with a 200kW PV-plant represents an opportunity for investigating the cycling conditions and aging behavior of a grid-connected Li-ion battery. In a second part, the application of the LNMO/LTO cell chemistry will be discussed in the light of recent results which anticipate the potential deployment of this lithium-ion battery in both grid-storage and electric vehicles.

Complex numbers

$$i \equiv \sqrt{-1} \qquad i^2 = -1$$

Define $z = x + iy$

$$|z|^2 = zz^* = (x+iy)(x-iy) = x^2 + y^2$$

Polar representation

$$z = \rho(\cos\phi + i\sin\phi) = \rho\, e^{i\phi}$$

Functions of complex variables

$$f(z) = \Re(f(z)) + i\Im(f(z)) \equiv u(x,y) + iv(x,y)$$

Derivatives: Cauchy-Riemann equations

$$\frac{\partial f(z)}{\partial x} = \frac{\partial u(z)}{\partial x} + i\frac{\partial v(z)}{\partial x} \qquad \frac{\partial f(z)}{i\partial y} = \frac{\partial u(z)}{i\partial y} + i\frac{\partial v(z)}{i\partial y} = \frac{\partial v(z)}{\partial y} - i\frac{\partial u(z)}{\partial y}$$

Argue that $\frac{df}{dz} = \frac{\partial f(z)}{\partial x} = \frac{\partial f(z)}{i\partial y} \quad \Rightarrow \frac{\partial u(z)}{\partial x} = \frac{\partial v(z)}{\partial y}$ and $\frac{\partial v(z)}{\partial x} = -\frac{\partial u(z)}{\partial y}$

Analytic function

$f(z)$ is analytic if it is:

- continuous
- single valued
- its first derivative satisfies Cauchy-Rieman conditions

Examples of analytic functions

$$e^z = e^{x+iy} = e^x\cos(y) + ie^x\sin(y)$$

$$\frac{\partial u}{\partial x} = e^x\cos(y) = \frac{\partial v}{\partial y} \qquad \frac{\partial v}{\partial x} = e^x\sin(y) = -\frac{\partial u}{\partial y}$$

$$z^2 = (x+iy)^2 = (x^2 - y^2) + 2ixy$$

$$\frac{\partial u}{\partial x} = 2x = \frac{\partial v}{\partial y} \qquad \frac{\partial v}{\partial x} = 2y = -\frac{\partial u}{\partial y}$$

Examples of non-analytic functions

Note that $z = \rho e^{i\phi} = \rho e^{i\phi + i2\pi n}$ for any integer n

$$\Rightarrow \ln z = \ln\rho + i(\phi + 2\pi n)$$

$\ln z$ is not analytic because it is multivalued

$$\Rightarrow z^\alpha = \rho^\alpha e^{i\alpha\phi} e^{i2\pi n\alpha}$$

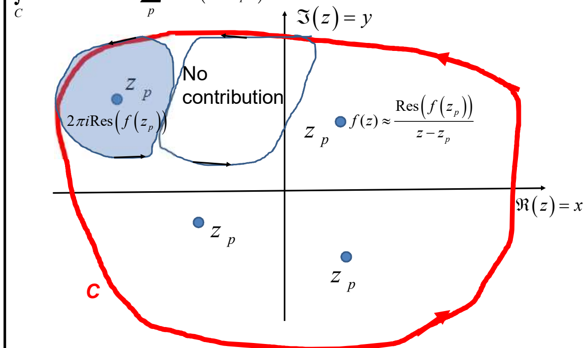
z^α is not analytic for non-integer α because it is multivalued

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

For an integer n, consider

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

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



General formula for determining residue:

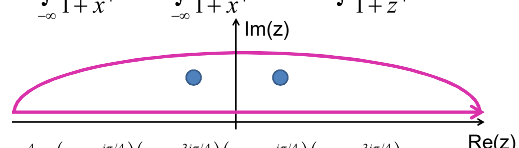
Suppose that in the neighborhood of z_p, $f(z) \approx \frac{g(z)}{(z-z_p)^m} \underset{z\to z_p}{\equiv} \frac{\text{Res}\left(f(z_p)\right)}{z-z_p}$

Since $g(z)$ is analytic near z_p, we can make a Taylor exansion about z_p :

$$g(z) \approx g(z_p) + (z-z_p)\frac{dg(z_p)}{dz} + \ldots + \frac{(z-z_p)^{m-1}}{(m-1)!}\frac{d^{m-1}g(z_p)}{dz^{m-1}} + \ldots.$$

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

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*

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

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

Some details:

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

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

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

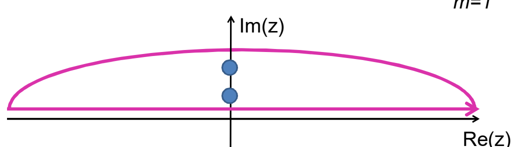
$$=\frac{e^{i\pi/4}}{2\left(i-(-i)\right)}=\frac{e^{i\pi/4}}{4i}$$

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*



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

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

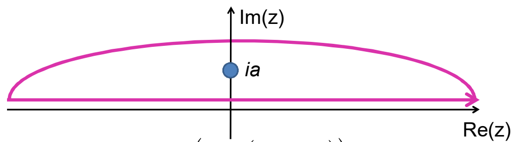
$$=2\pi i\left(\text{Res}\left(z_p=i\right)+\text{Res}\left(z_p=\tfrac{i}{2}\right)\right)$$

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

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

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

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



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

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

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

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

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

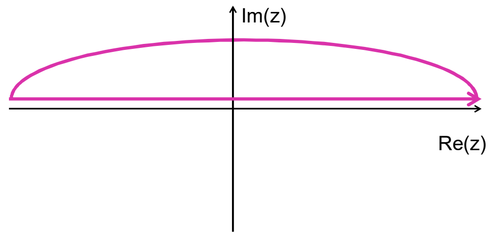
Cauchy integral theorem for analytic function *f(z)*:

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

Example

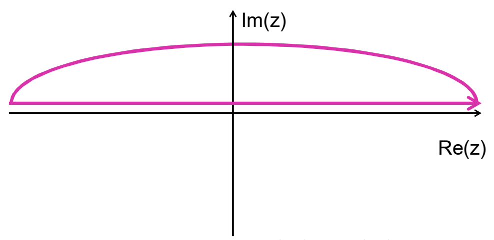
Suppose $f(|z| \to \infty) = 0$ and for $z = x$:

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



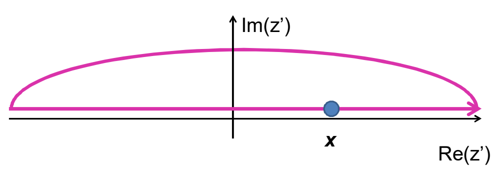
Example -- continued

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



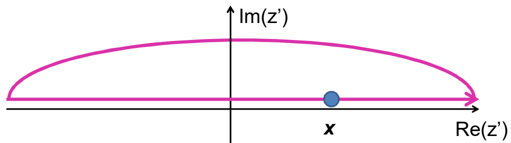
$$a(x) + ib(x) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{a(x') + ib(x')}{x'-x}dx' + 0$$

Example -- continued



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

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



let $u = x' - x$

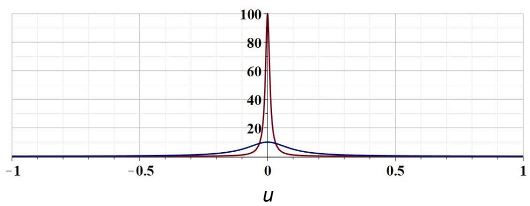
let $x \to x + i\eta$

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

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

More details --

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



Example -- continued

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

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

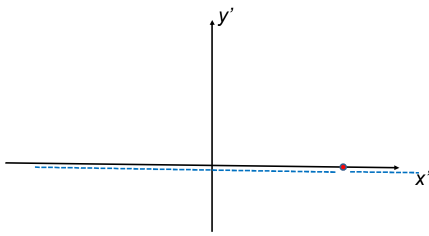
$$a(x) + ib(x) = \frac{P}{2\pi i} \int_{-\infty}^{\infty} \frac{a(x') + ib(x')}{x'-x}\,dx' + \frac{\pi i}{2\pi i}\left(a(x) + ib(x)\right)$$

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

Kramers-Kronig relationships

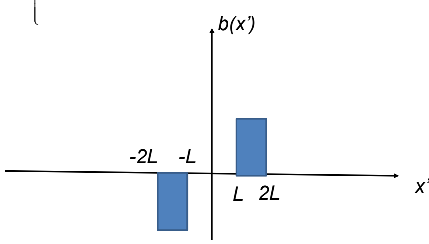
Comment on evaluating principal parts integrals

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



Example:

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



Example:

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

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

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

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

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

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

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