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

Plan for Lecture 21:

Summary of mathematical methods

1. **Contour integration**
2. **Fourier transforms**
3. **Fast Fourier transforms**

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8	Fri, 9/13/2013	Chap. 3	Lagrangian mechanics	#7
9	Mon, 9/16/2013	Chap. 3 & 6	Lagrangian mechanics	#8
10	Wed, 9/18/2013	Chap. 3 & 6	Lagrangian mechanics	#9
11	Fri, 9/20/2013	Chap. 3 & 6	Lagrangian & Hamiltonian mechanics	#10
12	Mon, 9/23/2013	Chap. 3 & 6	Hamiltonian formalism	#11
13	Wed, 9/25/2013	Chap. 3 & 6	Hamiltonian formalism	#12
14	Fri, 9/27/2013	Chap. 3 & 6	Hamiltonian formalism	#13
15	Mon, 9/30/2013	Chap. 4	Small Oscillations	#14
16	Wed, 10/02/2013	Chap. 4	Small Oscillations	
17	Fri, 10/04/2013	Chap. 4	Small Oscillations	#15
18	Mon, 10/07/2013	Chap. 4 & 7	Small Oscillations and waves	#16
19	Wed, 10/09/2013	Chap. 7	Wave equation	
	Fri, 10/11/2013		No class (Fall Break)	
20	Mon, 10/14/2013	Chap. 7	Wave equation (Presentation topic due)	#17
21	Wed, 10/16/2013	Chap. 7	Mathematical methods	#18
22	Fri, 10/18/2013	Chap. 5	Rigid rotations	
23	Mon, 10/21/2013	Chap. 5	Rigid rotations	
24	Wed, 10/23/2013	Chap. 5	Rigid rotations	
25	Fri, 10/25/2013	Chap. 5	Rigid rotations	
	Mon, 10/28/2013	No class	Take-home exam	
	Wed, 10/30/2013	No class	Take-home exam	
	Fri, 11/01/2013	No class	Take-home exam	
26	Mon, 11/04/2013		Take-home exam due	

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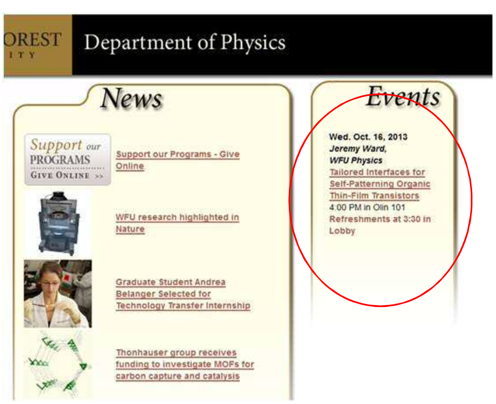

10/16/2013 PHY 711 Fall 2013 -- Lecture 21 3

WFU Physics Colloquium

TITLE: Tailored Interfaces for Self-Patterning Organic Thin-Film Transistors

SPEAKER: Jeremy W. Ward,

Department of Physics
Wake Forest University

TIME: Wednesday October 16, 2013 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

Increased demand in novel electronic devices has grown much interest in the development of organic electronics, specifically due to features including flexible applications, low-cost manufacturing and large-area fabrication. Patterning organic thin-film transistors (OTFTs) is a critical step towards achieving high electronic performance and low power consumption in these devices. In this talk, I will discuss a high-yield, low-complexity patterning method based on using the tendency of halogen-substituted organic semiconductors to crystallize along interfaces with halogenated self-assembled monolayers (SAMs). This method allows for the fabrication of self-patterned devices having small features and good insulation from neighboring devices. Particularly noteworthy is that this patterning is self-established at

PHY 711 – Contour Integration

These notes summarize some basic properties of complex functions and their integrals. An *analytic* function $f(z)$ in a certain region of the complex plane z is one which takes a single (non-infinite) value and is differentiable within that region. Cauchy's theorm states that a closed contour integral of the function within that region has the value

$$\oint_C f(z) = 0. \tag{1}$$

As an example, functions composed of integer powers of z –

$$f(z) = z^n, \quad \text{for} \quad n = 0, 1, \pm 2, \pm 3.... \tag{2}$$

fall in this catogory. Notice that non-integral powers are generally not analytic and that $n = -1$ is also special. In fact, we can show that

$$\oint_C \frac{dz}{z} = 2\pi i. \tag{3}$$

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This result follows from the fact that we can deform the contour to a unit circle about the origin so that $z = e^{i\theta}$. Then

$$\oint_C \frac{dz}{z} = \int_0^{2\pi} \frac{e^{i\theta}}{e^{i\theta}} i d\theta = 2\pi i. \tag{4}$$

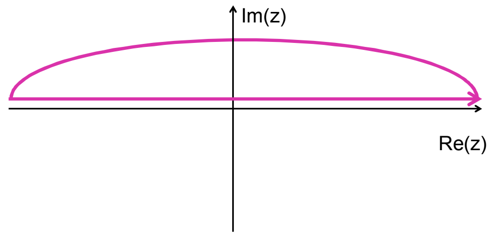
One result of this analysis is the Cauchy integral formula which states that for any analytic function $f(z)$ within a region C,

$$f(z) = \frac{1}{2\pi i} \oint_C \frac{f(z')}{z' - z} dz'. \tag{5}$$

Example

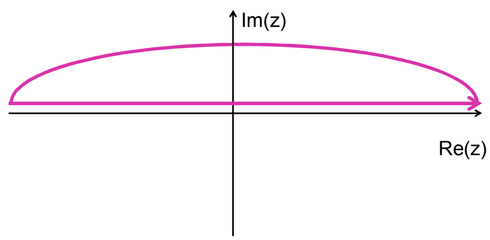
Suppose $f(|z| \to \infty) = 0$ and for $z = x$:

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



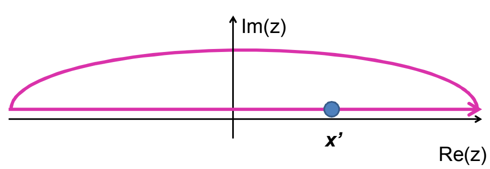
Example -- continued

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



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

Example -- continued



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

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

Example -- continued

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

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

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

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

Kramers-Kronig relationship

Another result of this analysis is the Residue Theorm which states that if the complex function $g(z)$ has poles at a finite number of points z_p within a region C but is otherwise analytic, the contour integral can be avaluated according to

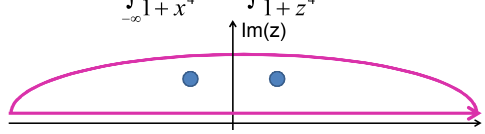
$$\oint_C g(z)dz = 2\pi i \sum_p Res(g_p), \qquad (6)$$

where the residue is given by

$$Res(g_p) \equiv \lim_{z\to z_p}\left\{\frac{1}{(m-1)!}\frac{d^{m-1}}{dz^{m-1}}\left((z-z_p)^m g(z)\right)\right\}, \qquad (7)$$

where m denotes the order of the pole.

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



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

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

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

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

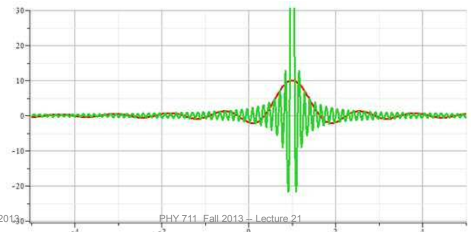
Fourier transforms

A useful identity

$$\int_{-\infty}^{\infty} dt\, e^{-i(\omega-\omega_0)t} = 2\pi\delta(\omega-\omega_0)$$

Note that

$$\int_{-T}^{T} dt\, e^{-i(\omega-\omega_0)t} = \frac{2\sin[(\omega-\omega_0)T]}{\omega-\omega_0}$$



Definition of Fourier Transform for a function $f(t)$:

$$f(t) = \int_{-\infty}^{\infty} d\omega\, F(\omega)\, e^{-i\omega t}$$

Backward transform:

$$F(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, f(t)\, e^{i\omega t}$$

Check:

$$f(t) = \int_{-\infty}^{\infty} d\omega \left(\frac{1}{2\pi}\int_{-\infty}^{\infty} dt'\, f(t')\, e^{i\omega t'}\right) e^{-i\omega t}$$

$$f(t) = \int_{-\infty}^{\infty} dt'\, f(t') \left(\frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{i\omega(t'-t)}\right) = \int_{-\infty}^{\infty} dt'\, f(t')\, \delta(t'-t)$$

Properties of Fourier transforms -- Parseval's theorem:

$$\int_{-\infty}^{\infty} dt\, (f(t))^* f(t) = \int_{-\infty}^{\infty} d\omega\, (F(\omega))^* F(\omega)$$

Fourier transform for periodic function:

Suppose $f(t+nT) = f(t)$ for and integer n

$$F(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, f(t) e^{i\omega t} = \sum_{n=-\infty}^{\infty}\left(\int_0^T dt\, f(t) e^{i\omega(t+nT)}\right)$$

Note that:

$$\sum_{n=-\infty}^{\infty} e^{in\omega T} = \Omega \sum_{\nu=-\infty}^{\infty} \delta(\omega-\nu\Omega), \quad \text{where } \Omega \equiv \frac{2\pi}{T}$$

Some details :

$$\sum_{n=-M}^{M} e^{in\omega T} = \frac{\sin\left(\left(M+\frac{1}{2}\right)\omega T\right)}{\sin\left(\frac{1}{2}\omega T\right)}$$

$$\lim_{M\to\infty}\left(\frac{\sin\left(\left(M+\frac{1}{2}\right)\omega T\right)}{\sin\left(\frac{1}{2}\omega T\right)}\right) = 2\pi\sum_{\nu}\delta(\omega T-\nu\Omega T) = \frac{2\pi}{T}\sum_{\nu}\delta(\omega-\nu\Omega)$$

$$\Rightarrow \sum_{n=-\infty}^{\infty} e^{in\omega T} = \Omega\sum_{\nu=-\infty}^{\infty}\delta(\omega-\nu\Omega), \quad \text{where} \quad \Omega \equiv \frac{2\pi}{T}$$

$$\Rightarrow F(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dt\, f(t)e^{i\omega t} = \sum_{\nu=-\infty}^{\infty}\Omega\delta(\omega-\nu\Omega)\left(\int_{0}^{T} dt\, f(t)e^{i\omega t}\right)$$

Thus, for a periodic function

$$f(t) = \sum_{\nu=-\infty}^{\infty} F(\nu\Omega)e^{-i\nu\Omega t}$$

Now suppose that the transformed function is bounded;

$|F(\nu\Omega)| \leq \varepsilon$ for $|\nu| \geq N$

Define a periodic transform function function

$$\widetilde{F}(\nu\Omega) \equiv \widetilde{F}(\nu\Omega + \nu'((2N+1)\Omega))$$

Effect on time domain :

$$f(t) = \sum_{\nu=-\infty}^{\infty}\widetilde{F}(\nu\Omega)e^{-i\nu\Omega t} = \frac{2\pi}{(2N+1)\Omega}\sum_{\nu=-N}^{N}\widetilde{F}(\nu\Omega)e^{-i\nu\Omega t}\sum_{\mu}\delta\left(t-\frac{\mu T}{2N+1}\right)$$

Doubly periodic functions

$$t \to \frac{\mu T}{2N+1}$$

$$\widetilde{f}_{\mu} = \frac{1}{2N+1}\sum_{\nu=-N}^{N}\widetilde{F}_{\nu}e^{-i2\pi\nu\mu/(2N+1)}$$

$$\widetilde{F}_{\nu} = \sum_{\mu=-N}^{N}\widetilde{f}_{\mu}e^{i2\pi\nu\mu/(2N+1)}$$

More convenient notation

$2N+1 \rightarrow M$

$$\tilde{f}_\mu = \frac{1}{M}\sum_{\nu=0}^{M-1}\tilde{F}_\nu e^{-i2\pi\nu\mu/M}$$

$$\tilde{F}_\nu = \sum_{\mu=0}^{M}\tilde{f}_\mu e^{i2\pi\nu\mu/M}$$

Note that for $W = e^{i2\pi/M}$

$$\tilde{F}_0 = \tilde{f}_0 W^0 + \tilde{f}_1 W^0 + \tilde{f}_2 W^0 + \tilde{f}_3 W^0 + \cdots$$

$$\tilde{F}_1 = \tilde{f}_0 W^0 + \tilde{f}_1 W^1 + \tilde{f}_2 W^2 + \tilde{f}_3 W^3 + \cdots$$

$$\tilde{F}_2 = \tilde{f}_0 W^0 + \tilde{f}_1 W^2 + \tilde{f}_2 W^4 + \tilde{f}_3 W^6 + \cdots$$

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$$\tilde{F}_2 = \tilde{f}_0 W^0 + \tilde{f}_1 W^2 + \tilde{f}_2 W^4 + \tilde{f}_3 W^6 + \cdots$$

However, $W^M = \left(e^{i2\pi/M}\right)^M = 1$

and $W^{M/2} = \left(e^{i2\pi/M}\right)^{M/2} = -1$

Cooley-Tukey algorithm: J. W. Cooley and J. W. Tukey, "An algorithm for machine calculation of complex Fourier series" Math. Computation 19, 297-301 (1965)

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