UCONN LIBRARY

University of Connecticut
DigitalCommons@UConn

Chemistry Education Materials

Department of Chemistry

10-24-2006

Fourier Series, Examples and the Fourier Integral

Carl W. David
University of Connecticut, Carl.David@uconn.edu

Follow this and additional works at: http://digitalcommons.uconn.edu/chem_educ
Part of the Chemistry Commons

Recommended Citation
David, Carl W., "Fourier Series, Examples and the Fourier Integral" (2006). *Chemistry Education Materials*. 28.
http://digitalcommons.uconn.edu/chem_educ/28

Fourier Series, Examples and the Fourier Integral

C. W. David
Department of Chemistry
University of Connecticut
Storrs, Connecticut 06269-3060

(Dated: October 24, 2006)

I. SYNOPSIS

The Fourier Integral is introduced by converting a Fourier series, in complex form, into the integral. Some examples are then given.

II. INTRODUCTION

We chose to introduce Fourier Series using the Particle in a Box solution from standard elementary quantum mechanics, but, of course, the Fourier Series antedates Quantum Mechanics by quite a few years (Joseph Fourier, 1768-1830, France).

Normal discussion of Fourier Series starts with a domain for the independent variable (here x) from $-\pi \leq x \leq \pi$ and considers replicating functions (such as sine and cosine) which map partly on this domain, and yet really extend over the domain $-\infty \leq x \leq +\infty$, replicating themselves every 2π.

So, assume we have a function f(x) in the domain $-\pi \leq x \leq \pi$ which may be replicating itself as noted above. The Fourier Series for f(x) is then given by

$$f(x) = \frac{A_0}{2} + \sum_{n=1}^{n=\infty} \left(A_n \sin nx + B_n \cos nx \right) \tag{2.1}$$

To repeat the derivation of the minimum error (above) here would require us to come to grips with the idea that $\sin x$ and $\cos x$ are orthogonal to each other. These integrals are trivial, over the domain in question, whether using 'x' or 'nx'. All one really needs is DeMoivre's Theorem and some familiarity in using it.

The coefficients are determinable (using this orthogonality) via

$$A_n = \frac{\int_{-\pi}^{\pi} f(x) \sin nx dx}{\int_{-\pi}^{\pi} \sin^2 nx dx} \tag{2.2}$$

$$B_n = \frac{\int_{-\pi}^{\pi} f(x) \cos nx dx}{\int_{-\pi}^{\pi} \cos^2 nx dx} \tag{2.3}$$

and

$$A_0 = \frac{\int_{-\pi}^{\pi} f(x) dx}{\int_{-\pi}^{\pi} dx} \tag{2.4}$$

(where the last term is often thought of as the "direct current" equivalent value, when translating the original f(x) into a language of voltage (f) versus time (x)).

Anyway, assuming that we accept the 2π domain Fourier Series, can we go on to any "even" domain Fourier Series? Yes. Consider the domain $-L/2 \leq \tau \leq +L/2$, and write

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{n=\infty} \left\{ a_n \sin\left(\frac{2n\pi x}{L}\right) + b_n \cos\left(\frac{2n\pi x}{L}\right) \right\} \tag{2.5}$$

where we use lower case letters for the constants in this case. The same argument that got us the coefficients before, works here, and we find

$$a_n = \frac{2}{L} \int_{-L/2}^{L/2} f(x) \sin\left(\frac{2n\pi x}{L}\right) dx \tag{2.6}$$

$$b_n = \frac{2}{L} \int_{-L/2}^{L/2} f(x) \cos\left(\frac{2n\pi x}{L}\right) dx \tag{2.7}$$

with

$$a_0 = \frac{2}{L} \int_{-L/2}^{L/2} f(x) \sin\left(\frac{0\pi x}{L}\right) dx = \frac{1}{L} \int_{-L/2}^{L/2} f(x) dx \tag{2.8}$$

Converting to Complex Form

We now use DeMoivre's Theorem, to re-write these equations in a form more suited to the purposes at hand, i.e., passing to the Fourier Integral.

$$a_n = \frac{1}{2L} \int_{-L/2}^{L/2} f(x) \frac{e^{\imath 2n\pi x/L} - e^{-\imath 2n\pi x/L}}{\imath} dx \tag{2.9}$$

$$b_n = \frac{1}{L} \int_{-L/2}^{L/2} f(x) \frac{e^{\imath 2n\pi x/L} + e^{-\imath 2n\pi x/L}}{2} dx \tag{2.10}$$

with

$$a_0 = \frac{1}{L} \int_{-L/2}^{L/2} f(x) dx \tag{2.11}$$

Adding, we have

$$c_n = b_n + \imath a_n = \frac{1}{2L} \int_{-L/2}^{L/2} f(x) e^{\imath 2n\pi x/L} dx \tag{2.12}$$

and, subtracting, we have

$$c_n^* = b_n - \imath a_n = \frac{1}{2L} \int_{-L/2}^{L/2} f(x) e^{-\imath 2n\pi x/L} dx \tag{2.13}$$

so that our Fourier Series can be rewritten as

Typeset by REVTEX

$$f(x) = \frac{a_0}{2} + \sum_{n=1}^{n=\infty} \left(a_n \sin \frac{2n\pi x}{L} + b_n \cos \frac{2n\pi x}{L} \right) = \sum_{n=-\infty}^{n=\infty} \left(c_n e^{\imath 2n\pi x/L} \right) \tag{2.14}$$

where we have changed the summation from running $-\infty \rightarrow -1$ and then $a_0/2$ and then $1 \rightarrow -\infty$ to $-\infty \rightarrow +\infty$. Remember,

$$c_n = \frac{1}{2L} \int_{-L/2}^{L/2} f(x) e^{-\imath 2\pi n x/L} dx \tag{2.15}$$

but this is deceptive (for future work) because of the presence of 'x' in the integral. One needs to remember that 'x' in this integral has disappeared once the integration is done! That means that 'x' is a "dummy" variable. Which in turn means that we can re-write this equation as

$$c_n = \frac{1}{2L} \int_{-L/2}^{L/2} f(\tau) e^{-\imath 2\pi n \tau/L} d\tau$$

Combining the last two equation into a single one we have

$$f(x) = \sum_{n=-\infty}^{n=\infty} \left(\left(\frac{1}{2L} \int_{-L/2}^{L/2} f(\tau) e^{\imath 2\pi n \tau/L} d\tau \right) e^{-\imath 2n\pi x/L} \right) \tag{2.16}$$

$$= \sum_{n=-\infty}^{n=\infty} \left(\left(\frac{1}{2L} \int_{-L/2}^{L/2} f(\tau) e^{\imath 2\pi n \tau/L} d\tau \right) e^{-\imath 2n\pi x/L} \right) (n+1-n) = \sum_{n=-\infty}^{n=\infty} \left(\left(\frac{1}{2L} \int_{-L/2}^{L/2} f(\tau) e^{\imath 2\pi n \tau/L} d\tau \right) e^{-\imath 2n\pi x/L} \right) \Delta n \tag{2.17}$$

which is, passing through the standard calculus procedure

$$f(x) = \int_{n=-\infty}^{n=\infty} \left(\left(\frac{1}{2L} \int_{-L/2}^{L/2} f(\tau) e^{\imath 2\pi n \tau/L} d\tau \right) e^{-\imath 2n\pi x/L} \right) dn \tag{2.18}$$

$$f(x) = \frac{1}{2L} \int_{n=-\infty}^{n=\infty} \left(\int_{-L/2}^{L/2} f(\tau) e^{\imath 2\pi n \tau/L - \imath 2n\pi x/L} \right) d\tau dn \tag{2.19}$$

Defining $\omega = 2\pi n/2L$ we have

$$d\omega = \pi/L dn \tag{2.20}$$

so, solving, we have

$$dn = \frac{1}{\pi/L} d\omega \tag{2.21}$$

so

$$f(x) = \left(\frac{1}{2L} \right) \left(\frac{1}{\pi/L} \right) \int_{\omega=-\infty}^{\omega=\infty} \left(\int_{\tau=-L}^{\tau=L} f(\tau) e^{\imath \omega(\tau - x)} \right) d\tau d\omega \tag{2.22}$$

which, in the limit, L$\rightarrow \infty$ becomes

$$f(x) = \frac{1}{4\pi} \int_{\omega=-\infty}^{\omega=\infty} \left(\int_{\tau=-\infty}^{\tau=\infty} f(\tau) e^{\imath \omega(\tau - x)} \right) d\tau d\omega \tag{2.23}$$

We can split this into symmetric "pairs":

$$f(\tau) = \frac{1}{\sqrt{2\pi}} \int_{\omega=-\infty}^{\omega=\infty} \left(g(\omega) e^{\imath \omega \tau} \right) d\omega \tag{2.24}$$

$$g(\omega) = \frac{1}{\sqrt{2\pi}} \int_{\lambda=-\infty}^{\lambda=\infty} \left(f(\tau) e^{-\imath \omega \tau} \right) d\tau \tag{2.25}$$

III. AN EXAMPLE

Consider the Fourier Transform of the function $A\cos\omega_0\tau$ in a range $-a \le \tau \le a$ and zero elsewhere. This is a truncated cosine! We have

$$g(\omega) = \int_{-a}^{a} \frac{1}{\sqrt{2\pi}} A\cos\omega_0\tau e^{-\imath\omega\tau} d\tau$$

where the limits are recognizing that f(τ) (the cosine) is zero outside the domain $|\tau| \ge a$, which is easily evaluated using DeMoivre's Theorem (smile):

$$\cos\omega_0\tau = \frac{e^{\imath\omega_0\tau} + e^{-\imath\omega_0\tau}}{2}$$

so we have

$$g(\omega) = \frac{1}{\sqrt{2\pi}} A \int_{-a}^{a} \left(\frac{e^{\imath\omega_0\tau} + e^{-\imath\omega_0\tau}}{2}\right) e^{-\imath\omega\tau} d\tau$$

which becomes, upon integration

$$g(\omega) = \frac{A}{2\sqrt{2\pi}} \int_{-a}^{a} \left(\frac{e^{\imath(\omega_0-\omega)\tau} + e^{-\imath(\omega_0+\omega)\tau}}{2}\right) d\tau$$

which becomes, upon integration

$$g(\omega) = \frac{A}{2\sqrt{2\pi}} \left(\left.\frac{e^{\imath(\omega_0-\omega)\tau}}{\imath(\omega_0-\omega)}\right|_{-a}^{a} + \left.\frac{e^{-\imath(\omega_0+\omega)\tau}}{-\imath(\omega_0+\omega)}\right|_{-a}^{a} \right)$$

$$g(\omega) = \frac{A}{2\sqrt{2\pi}} \left\{ \frac{e^{\imath(\omega_0-\omega)a}}{\imath(\omega_0-\omega)} - \frac{e^{-\imath(\omega_0-\omega)a}}{\imath(\omega_0-\omega)} + \frac{e^{-\imath(\omega_0+\omega)a}}{-\imath(\omega_0+\omega)} - \frac{e^{+\imath(\omega_0+\omega)a}}{-\imath(\omega_0+\omega)} \right\}$$

$$g(\omega) = \frac{A}{\sqrt{2\pi}} \left\{ \frac{\sin(\omega_0-\omega)a}{(\omega_0-\omega)} - \frac{\sin(\omega_0+\omega)a}{(\omega_0+\omega)} \right\}$$

IV. THE CLASSIC EXAMPLE

The classic Fourier Transform illustration is the Gaussian, since the transform of a Gaussian turns out to be a Gaussian itself. Then as one narrows one Gaussian, the other widens, illustrating the Heisenberg uncertainty principle relating 'x' to 'p' expectation values. We have

$$g(\omega) = Ae^{-B\omega^2}$$

defining a function g which is Gaussian in its dependence. We then have

$$f(\tau) = \frac{1}{\sqrt{2\pi}} \int_{\omega=-\infty}^{\omega=\infty} (g(\omega)e^{\imath\omega\tau})\, d\omega$$

which would read, substituting g(ω),

$$f(\tau) = \frac{1}{\sqrt{2\pi}} \int_{\omega=-\infty}^{\omega=\infty} \left(Ae^{-B\omega^2} e^{\imath\omega\tau}\right) d\omega$$

How do we do this integral? Recalling from high school the "completing the square" idea, we write

$$B\left(\omega^2 - \imath\frac{\omega\tau}{B}\right) = B(\omega+\alpha)^2 = B\left(\omega^2 + 2\omega\alpha + \alpha^2\right)$$

so,

$$\imath\frac{\omega\tau}{B} = 2\omega\alpha$$

must be true, identifying α in terms of problem variables.

$$\alpha = \frac{\imath\tau}{2B}$$

and, of course

$$\alpha^2 = \left(\frac{\imath\tau}{2B}\right)^2$$

This means that the integrand in question can be written as

$$e^{-B\left((\omega+\frac{\imath\tau}{2B})^2 - \frac{\tau^2}{4B^2}\right)}$$

Substituting, we have

$$f(\tau) = \frac{1}{\sqrt{2\pi}} \int_{\omega=-\infty}^{\omega=\infty} \left(Ae^{-B\left((\omega+\frac{\imath\tau}{2B})^2 - \frac{\tau^2}{4B^2}\right)}\right) d\omega$$

which allows us to move the constant factor out of the integrand, obtaining

$$f(\tau) = e^{-B\frac{\tau^2}{4B^2}} \frac{1}{\sqrt{2\pi}} \int_{\omega=-\infty}^{\omega=\infty} \left(Ae^{B\left((\omega+\frac{\imath\tau}{2B})^2\right)}\right) d\omega$$

i.e.,

$$\gamma = (\omega + \imath\tau/(2B))$$

and

$$d\gamma = d\omega$$

So

$$f(\tau) = Ae^{-B\frac{\tau^2}{4B^2}} \frac{1}{\sqrt{2\pi}} \int_{\omega=-\infty}^{\omega=\infty} e^{-B\gamma^2} d\gamma$$

Now, it is known that the Gauss integral:

$$\int_{-\infty}^{\infty} e^{-ax^2} dx = \sqrt{\frac{\pi}{a}}$$

where here x=γ and a=B, so

$$f(\tau) = \frac{A}{\imath} e^{-B\frac{\tau^2}{4B^2}} \frac{1}{\sqrt{2\pi}} \sqrt{\frac{\pi}{B}}$$

or, cleaning up,

$$f(\tau) = \frac{A}{\imath\sqrt{2B}} e^{-\frac{\tau^2}{4B}}$$