A Graphical Presentation To Teach the Concept of the Fourier Transform

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Over the years, many articles on spectroscopy have focused on Fourier transform (FT) techniques, including some articles from this *Journal (1–5).* While the mathematical concepts included here have previously been presented *(1–6),* they have not been discussed in a manner suitable for clear and succinct pedagogical application. A number of other authors have used graphical aids in conjunction with mathematical representations *(7–12),* but detailed graphical presentations of the workings of the FT are scarce. In response to this need, a concise graphical approach, intended to answer common questions of "why and how does the FT work?", is presented below.

At our institution, the foundations of spectroscopy are taught in a one-semester, third-year introductory course for undergraduate students. The FT is taught towards the middle of a four-week NMR unit, and the approach described below takes approximately one hour to present, provided that the students are already familiar with basic calculus and NMR theory. The approach is characterized by repeated use of the graphical idea that an integral is a measure of the area under a curve. It begins by familiarizing students with the appearance of various harmonic functions and continues by matching the graphs to mathematical formulas and operations. A more formal generalization is presented in the context of FT-NMR. For simplicity, the functions and transformations described use real variables and integer angular frequencies, although these restrictions are relaxed in the formal generalization. Our experience is that this is an effective approach to help students understand the FT. This has been corroborated by increasing students' success in solving numerical problems.

Time-Domain Function

The simplified analytic form of a time-domain function is a superposition of sinusoidal waves

$$f(t) = \sum_j A_j \cos\left(\omega_j t\right) \tag{1}$$

where the A_j and ω_j are the amplitude and the angular frequency of each component, respectively, and t is time. For example, consider the case of the superposition of two functions with frequencies of $\omega_1 = 1$ and $\omega_2 = 3$ and respective amplitudes of $A_1 = 1$ and $A_2 = 5$ (Figure 1):

$$f(t) = \cos(t) + 5\cos(3t) \tag{2}$$

A periodic interval for this function is [0, 2π), although the graph in Figure 1 deliberately covers two periods to graphically reinforce this notion of periodicity. The vertical dashed line in Figure 1 helps to visualize this.

Often, experiments use the Fourier transform to detect the frequencies present in such functions. The following discussion will describe how the FT accomplishes this.

Graphical Integration of a Product

The next step is to construct products of the original time-domain function $f(t)$ (eq 2) with a *kernel* cosine function, for example,

$$\begin{aligned} g_1(t) &= f(t)\cos(t) \\ g_2(t) &= f(t)\cos(2t) \\ g_3(t) &= f(t)\cos(3t) \end{aligned} \tag{3}$$

The result is depicted in Figure 2. The kernel's angular frequencies are $\omega = 1$, 2, and 3. Note that for only the first and third examples do these frequencies actually coincide with the ones present in $f(t)$.

At this point the students are asked to recall that an integral is the area between a curve and the *x*-axis and can have a positive or negative magnitude. They are then asked to state *qualitatively* whether the integration of each one of the functions (eq 3) in the periodic interval will be zero or not. There are two main concepts related to the answers they must give, that is, periodicity and symmetry. Thus, in a visual and heuristic way, it becomes clear that nonzero integrations, as in the first and third examples, occur only when the kernel frequency ω coincides with frequencies present in the time-domain function. This is a crucial point, as it explains how the Fourier transform operates to detect the spectroscopic frequencies hidden in the time-domain function.

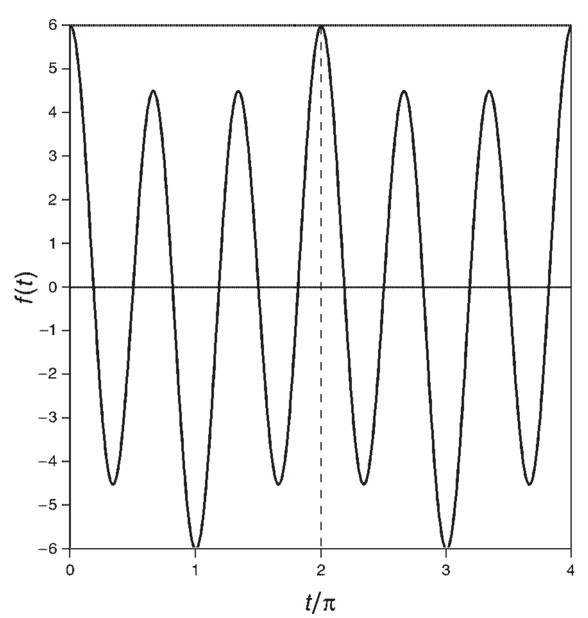

Figure 1. The time domain function $f(t)$ is the result of the interference of two functions with frequencies $\omega_1 = 1$ and $\omega_2 = 3$ and respective amplitudes of $A_1 = 1$ and $A_2 = 5$.

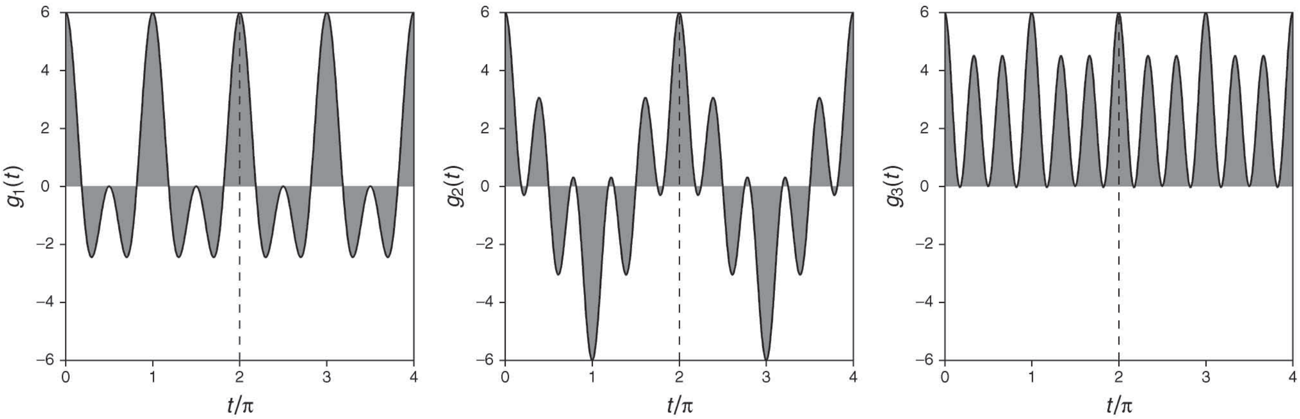

Figure 2. Graphical representation of the products of the time function $f(t)$ multiplied by the cosine Fourier kernels. Kernel frequencies are $\omega = 1$, 2, and 3, respectively. Shadings help to visualize the areas involved in the integration.

Analytical Formulation

It is now possible to obtain the frequency spectrum of the time-domain function. This is accomplished by letting the kernel frequency, ω, vary continuously. This leads to the concept of a mathematical transform: from the time function (eq 1) a new one is constructed, F, depending on the frequency variable, ω. Defining it in the interval of interest, our Fourier transform function is

$$F(\omega) = \int_0^{2\pi} f(t)\cos(\omega t)\,\mathrm{d}t; \quad \omega \in [0, +\infty) \qquad (4)$$

Explicitly,

$$F(\omega) = \sum_j A_j \int_0^{2\pi} \cos(\omega_j t)\cos(\omega t)\,\mathrm{d}t \qquad (5)$$

and following the general integration rule

$$\int_0^{2\pi} \cos(mt)\cos(nt)\,\mathrm{d}t = \begin{cases} 0 \text{ for } m \neq n \\ \pi \text{ for } m = n \end{cases} \qquad (6)$$

the integral of the product of the cosine functions is only different from zero if both frequencies are integer numbers and coincide. It follows that the frequency-domain function (eq 5) takes the following values

$$F(\omega) = \begin{cases} \pi A_j & \text{if } \omega = \omega_j \\ 0 & \text{otherwise} \end{cases} \qquad (7)$$

Namely, the transform function (eq 4) is zero for all the values of ω except for the ones coinciding with a frequency present in the time-domain function (eq 1). This was already shown graphically in the previous section. In other words, the frequency-domain variable acts as a dial and the Fourier transform is different from zero when one experimental frequency is "tuned".

Furthermore, from the result in eq 7 it can be seen how the numerical value of the transform is proportional to the amplitude of the tuned signal. For instance, the integrated area in left-side graph of Figure 2 is smaller than the right-side graph. This is visually evident because in the left-side graph there are some compensating negative contributions in the integrated area (owing to the presence of inscribed areas on both sides of the zero baseline) whereas in the last case all the integration areas contribute additively. Note that for comparison purposes the graphical scaling has been preserved in Figure 2.

Application to FT–NMR

The restrictions mentioned previously must be relaxed to reach a formal theory. The NMR free induction decay (FID) technique provides a convenient example. One way to represent the FID is to write a superposition of modulating exponential functions, specifically, in this case,

$$f(t) = \left[\sum_j A_j \cos(\omega_j t)\right] e^{\frac{-t}{T}} \qquad (8)$$

where T is the relaxation time. For example, Figure 3 depicts the case in eq 8 where T is 10. This is the function in eq 2 but modulated by the exponential decay term. The interval of representation has been enlarged to demonstrate the decay.

The Fourier transform is properly defined including the complex variable and, owing to the asymptotic decay, integrating in an infinite interval:

$$\begin{aligned} I(\omega) &= 2\,\mathrm{Re}\int_0^{\infty} f(t)\, e^{i\omega t}\,\mathrm{d}t \\ &= 2\,\mathrm{Re}\sum_j A_j \int_0^{\infty} \cos(\omega_j t)\, e^{\frac{-t}{T}}\, e^{i\omega t}\,\mathrm{d}t \end{aligned} \qquad (9)$$

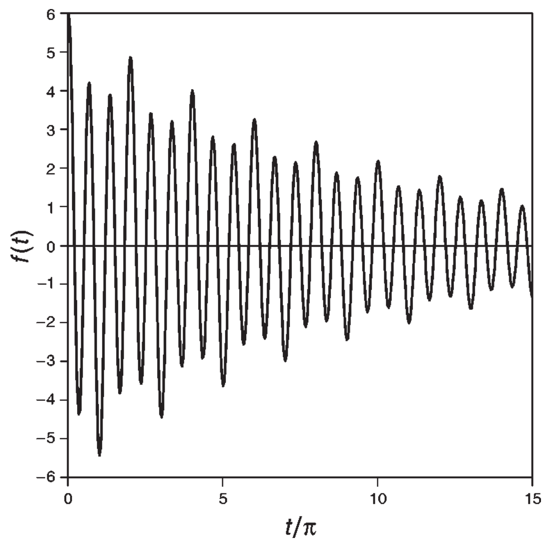

Figure 3. Representation of the FID function in the time domain.

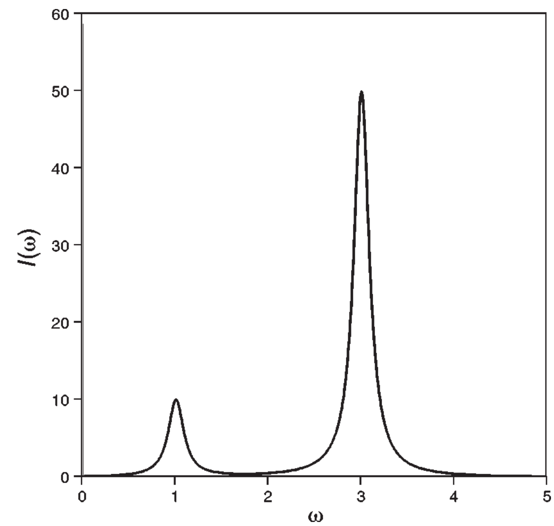

Figure 4. Fourier transform for $f(t)$, composed with two emissions having frequencies equal to 1 and 3.

As Euler's relationship states that $\cos(at) = (e^{iat} + e^{-iat})/2$, the integration in eq 9 is straightforward and the relevant remaining real terms give the well-known superposition of Lorentzian curves:

$$I(\omega) = \sum_j \frac{A_j T}{1 + \left(\omega - \omega_j\right)^2 T^2} \qquad (10)$$

Figure 4 shows the graph of this function corresponding to the transformation of the function shown in Figure 3. Clearly, the shape recalls the typical signals found in NMR spectra (albeit to avoid noise effects, a real spectrum is obtained by the superposition and averaging of hundreds of single signals). Note how the peak height is proportional to T and to the original amplitudes present in eq 2. The areas under the peaks are roughly proportional to the amplitudes as well.

The activity presented here can also be extended, as analytical or even numerical integration exercises can be proposed to reproduce the integration of the functions in eqs 2 or 9, giving the results in eqs 7 and 10, respectively. The graphical and numerical treatments can be reproduced with the aid of symbolic programs. As complements, some related Mathcad modules by Grubbs, Van Bramer, and Iannone *(13)* are available from the *Journal of Chemical Education* SymMath Collection *(14)*.

Conclusions

The reasons why the Fourier transform technique is useful to detect the originating frequencies of a complicated superposition of waves have been visualized. The FID has been also treated. The mathematics has been presented graphically and progressively, together with a subsequent analytical justification. Instructors can adapt parts of this pictorial presentation to show how the time-domain functions may be transformed into the frequency domain. Previous experience shows that students respond well to this visual approach.

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