CHEM2024 - Week 30 Lecture 1 - Fourier transform

☐ *Chapter 15 of Steiner, "The Chemistry Maths Book", 2nd edition.*

1. Definition and meaning

The *Fourier transform* may be viewed as a connection between a signal represented as a well-behaved function of time (so-called *time domain representation*) and the same signal represented as a function of frequency (*frequency domain representation*). Both representations define a given signal completely.

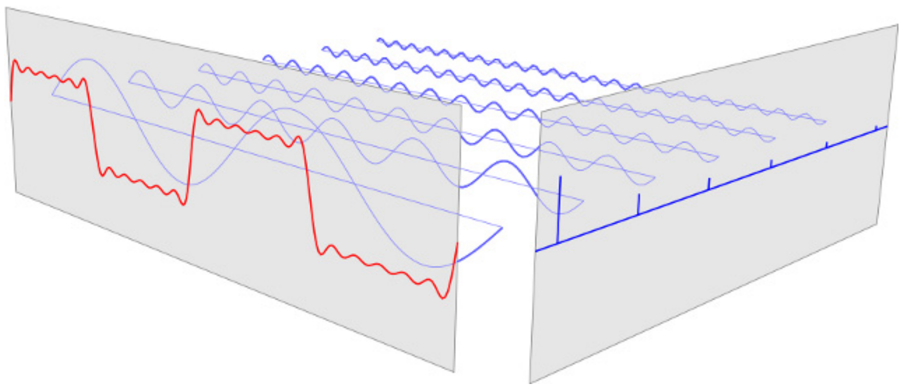

Figure 1. *A graphical illustration of the decomposition of a function into a discrete sum of sines and cosines (source: Wikipedia). The Fourier transform is the continuous version of this procedure that also works for non-periodic functions.*

This connection between the two representations may be derived formally, but in this course we would simply state it without proof:

$$f(\omega)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)e^{-i\omega t}dt \qquad f(t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(\omega)e^{+i\omega t}d\omega \tag{1}$$

The integral that produces $f(\omega)$ is called *forward Fourier transform*, and the integral that gives $f(t)$ back is called *backward Fourier transform*. Operator notation is also often used:

$$\hat{F}_{+}f(t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(t)e^{-i\omega t}dt \qquad \hat{F}_{-}f(\omega)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(\omega)e^{+i\omega t}d\omega \tag{2}$$

In situations when the time-dependent process $f(t)$ starts at time zero, the forward Fourier transform becomes *one-sided*:

$$\hat{F}_{+}f(t)=\frac{1}{\sqrt{2\pi}}\int_{0}^{\infty} f(t)e^{-i\omega t}dt \tag{3}$$

The backward transform remains two-sided because negative frequencies may be present in $f(t)$.

2. Basic properties

The most useful properties of forward and backward Fourier transforms are:

1. <u>The two transforms are each other's inverse</u>:

$$\hat{F}_{-}\hat{F}_{+}f(t)=\frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty} f(t')e^{\mathrm{i}\omega t'}dt'\right]e^{-\mathrm{i}\omega t}d\omega=f(t) \tag{4}$$

The proof is not straightforward, we shall skip it in this course.

2. Fourier transform is linear. For any two functions $f(t)$, $g(t)$ and for any two scalars α, β:

$$\hat{F}_{\pm}\left\{\alpha f(t)+\beta g(t)\right\}=\alpha\hat{F}_{\pm}\left\{f(t)\right\}+\beta\hat{F}_{\pm}\left\{g(t)\right\} \tag{5}$$

The proof is obvious and relies on the linearity of the integration operation in Equations (1).

3. Fourier transform replaces differentiation by multiplication. In the most common case (for chemical applications) of the one-sided transform:

$$\hat{F}_{+}\left\{f'(t)\right\}=i\omega\hat{F}_{+}\left\{f(t)\right\}-f(0) \tag{6}$$

This is easy to prove using integration by parts:

$$\begin{gathered}\hat{F}_{+}\left\{f'(t)\right\}=\frac{1}{\sqrt{2\pi}}\int_{0}^{\infty}f'(t)e^{-i\omega t}dt=\left\{\begin{matrix}u=e^{-i\omega t} & du=-i\omega e^{-i\omega t}dt\\ dv=f'(t)dt & v=f(t)\end{matrix}\right\}=\\ =e^{-i\omega t}f(t)\Big|_{0}^{\infty}+\frac{i\omega}{\sqrt{2\pi}}\int_{0}^{\infty}f(t)e^{-i\omega t}dt=-f(0)+\frac{i\omega}{\sqrt{2\pi}}\int_{0}^{\infty}f(t)e^{-i\omega t}dt=i\omega\hat{F}_{+}\left\{f(t)\right\}-f(0)\end{gathered} \tag{7}$$

Note that $f(0)$ refers to the original function of time, taken at time zero.

3. Applications

3.1 Differential equations

Many types of differential equations are mapped into algebraic equations by a Fourier transform. Consider a first order chemical kinetics process:

$$\frac{dA(t)}{dt}=-kA(t) \tag{8}$$

Taking the Fourier transform of both sides and using the property in Equation (7), we get:

$$\hat{F}_{+}\left[\frac{dA(t)}{dt}\right]=-k\hat{F}_{+}\left[A(t)\right]\quad\Rightarrow\quad i\omega A(\omega)-A_0=-kA(\omega) \tag{9}$$

where A_0 is the initial concentration. The equation is now algebraic and therefore easy to solve:

$$A(\omega)=\frac{A_0}{k+i\omega} \tag{10}$$

In practice, ordinary and partial differential equations are transformed into the frequency domain analytically and solved. The solutions are then numerically transformed back into the time domain.

3.2 Digital signal processing

Noise is often a problem in experimental work, but the frequencies expected in the signal may be different from the frequencies of the noise. This information may be used to "clean up" the signal, and the procedure is called *digital filtering*.

As a simple example, the following transformation performs a forward Fourier transform, multiplies the unwanted frequencies by zero and performs a backward Fourier transform:

$$f^{*}(t)=F_{-}\left\{M(\omega)F_{+}\left\{f(t)\right\}\right\},\qquad M(\omega)=\begin{cases}0\text{ for unwanted }\omega\\ 1\text{ for wanted }\omega\end{cases} \tag{11}$$

This transformation called a *bandpass filter* – it only keeps the frequencies that fall into the user-specified band. The selection function $M(\omega)$ is called *magnitude transfer function*. Similar transformations may be designed to shift, amplify and otherwise modify signal frequencies.

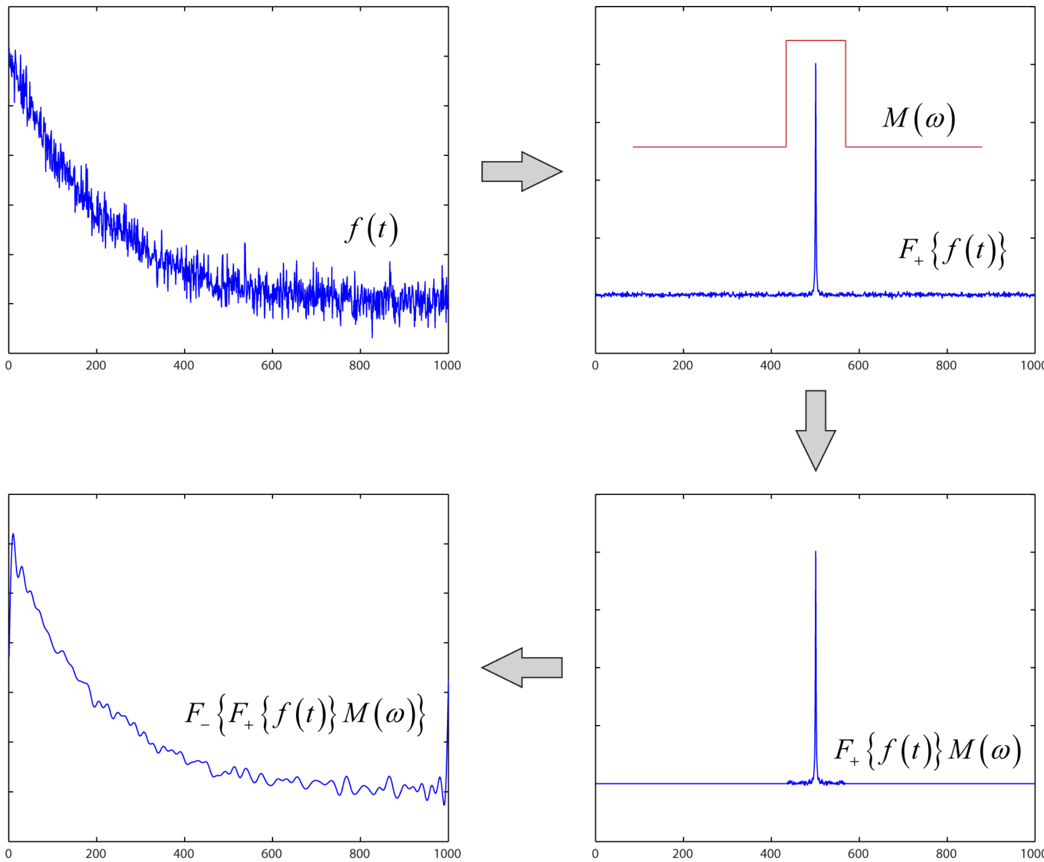

Figure 2. A bandpass filter applied to a noisy chemical kinetics decay trace.

3.3 Image compression

In its most basic form, the JPEG image compression process first separates the image into brightness and chrominance channels. This is done because human eye is more sensitive to pixel brightness than colour. Each channel is then split into blocks of 16×16 pixels, and the blocks are Fourier transformed. All frequencies above a user-specified thresholds are zeroed out and the image stored as a table of the remaining non-zero coefficients, resulting in significant reduction in the file size. When a JPEG file is opened, the reverse transformation is performed and the image is displayed. Some information is lost in the compression process, but the human eye is often unable to tell the difference.

Figure 3. Blocking and high frequency information loss at high levels of JPEG compression.

Typical JPEG artefacts are shown in Figure 3. Because high frequency information is discarded, JPEG works best on images containing smooth colour gradients.