

University of Washington
Department of Chemistry
Chemistry 553
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Lecture 19: Causal Functions

Text Reading: Ch 21,22

A. Causal Functions

- The linear response or after-effect function is an example of a causal function.

The after effect function has the property that $\phi_{BA}(\tau) \begin{cases} = 0 & \text{if } \tau < 0 \\ \neq 0 & \text{if } \tau > 0 \end{cases}$. This

simply states that the linear response of the system cannot precede the application of the field that elicits the response.

- Now the complex susceptibility is the one-sided Fourier transform of the after-effect function according to

$$\chi_{BA}(\omega) = \chi'_{BA}(\omega) - i\chi''_{BA}(\omega) = \int_0^{\infty} d\tau \phi_{BA}(\tau) e^{-i\omega\tau} \quad (19.1)$$

- We will show that the causal nature of $\phi_{BA}(\tau)$ imposes a constraint upon the real part of the susceptibility $\chi'_{BA}(\omega)$ and the imaginary part of the susceptibility $\chi''_{BA}(\omega)$, which we know to be related to the energy absorption and dissipation of energy from the applied field by the system, respectively. To simplify discussion we will drop the subscripts BA in future equations.
- To start we must explore how to construct a function such that it is causal. This is not easy because most functions that we use to express time dependence (i.e. sine, cosine) are not causal. Functions like $\cos \omega t$ and $\sin \omega t$ exist for all t.
- To proceed we consider the properties of even and odd functions. Any function can be expressed as a sum of even and odd parts:

$$f(t) = f_e(t) + f_o(t) \quad (19.2)$$

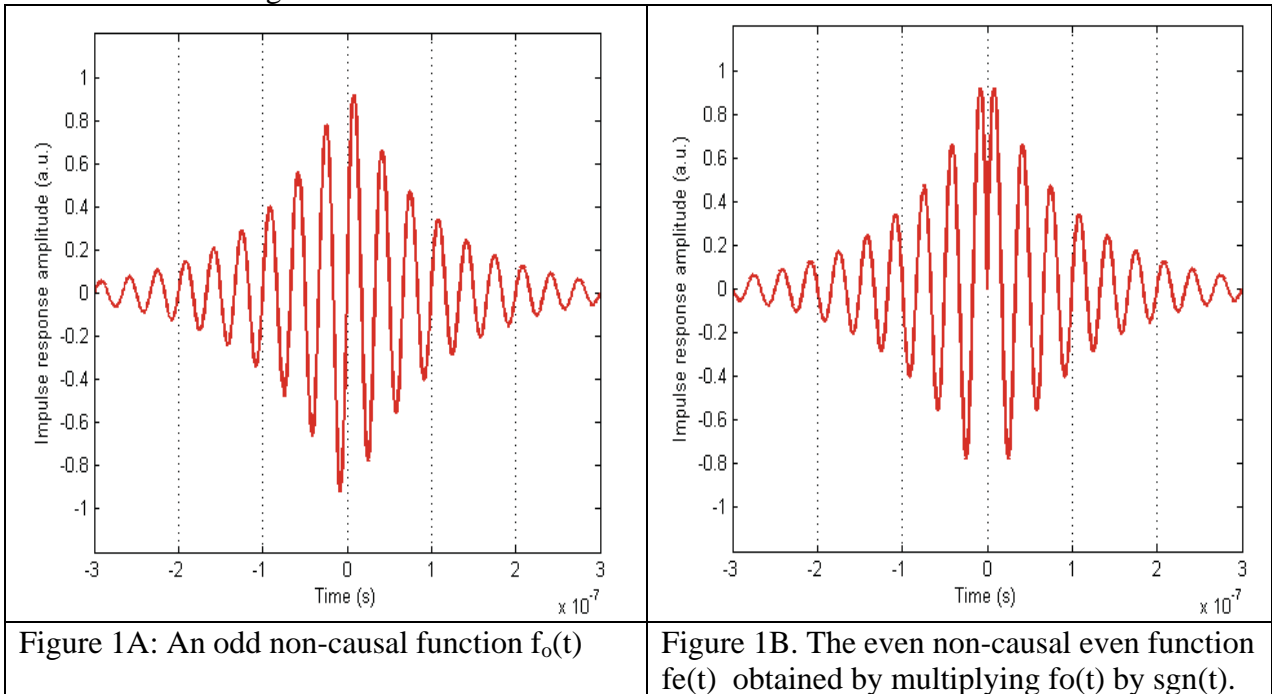
where $f_e(t) = f_e(-t)$ and $f_o(t) = -f_o(-t)$.

- Apply (19.2) to a Fourier transform:

$$\begin{aligned}
 F(\omega) &= F'(\omega) - iF''(\omega) = \int_{-\infty}^{+\infty} f(t) e^{-i\omega t} dt \\
 \therefore F'(\omega) &= \int_{-\infty}^{+\infty} f(t) \cos \omega t dt = \int_{-\infty}^{+\infty} f_e(t) \cos \omega t dt = 2 \int_0^{+\infty} f_e(t) \cos \omega t dt \\
 F''(\omega) &= \int_{-\infty}^{+\infty} f(t) \sin \omega t dt = \int_{-\infty}^{+\infty} f_o(t) \sin \omega t dt = 2 \int_0^{+\infty} f_o(t) \sin \omega t dt
 \end{aligned} \quad (19.3)$$

- From (19.3) $F'(\omega)$ is even while $F''(\omega)$ is odd.

- Equations (19.3) are altered somewhat if a function is causal.
- First define the signum function: $\text{sgn}(t) = \begin{cases} 1 & \text{if } t \geq 0 \\ 0 & \text{if } t < 0 \end{cases}$. Given an odd function $f_o(t)$, the function produced by multiplying $\text{sgn}(t)$ and $f_o(t)$ is even, i.e. $f_e(t) = \text{sgn}(t) f_o(t)$. This is because the signum function reverses the sign of $f_o(t)$ for $t < 0$, making $f_e(t) = \text{sgn}(t) f_o(t)$ for $t < 0$ the mirror image of $f_e(t) = \text{sgn}(t) f_o(t)$ for $t > 0$.
- Consider the odd function in Figure 1A. The even function $f_e(t) = \text{sgn}(t) f_o(t)$ is shown in Figure 1B



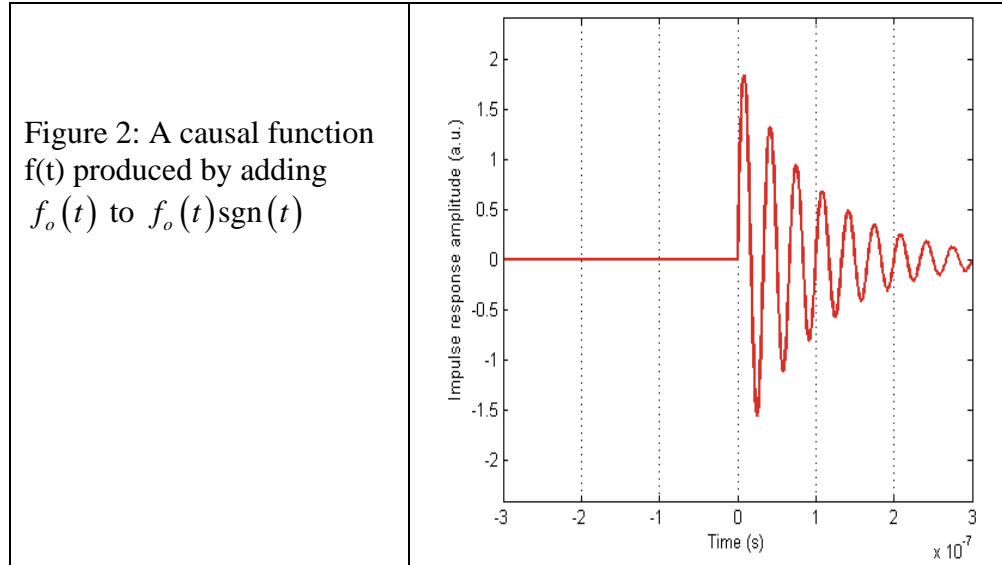
- Suppose we now construct the function
$$f(t) = f_e(t) + f_o(t) = f_o(t) \text{sgn}(t) + f_o(t) \quad (19.4)$$

From Figure 1 for $t < 0$ $f_e(t)$ will cancel $f_o(t)$ producing the causal function $f(t)$ shown in figure 2

- The question is: what happens when we Fourier transform a causal function like $f(t)$? To explore this insert (19.4) into (19.3):

$$\begin{aligned}
 F(\omega) &= F'(\omega) - iF''(\omega) = \int_{-\infty}^{+\infty} f(t) e^{-i\omega t} dt \\
 &= \int_{-\infty}^{+\infty} (\text{sgn}(t) f_o(t) + f_o(t)) e^{-i\omega t} dt
 \end{aligned} \quad (19.5)$$

- Now we have already established that $F'(\omega)$ is even and we expect it to be equal to the Fourier transform of an even function:



$$F'(\omega) = \int_{-\infty}^{+\infty} (\text{sgn}(t) f_o(t)) e^{-i\omega t} dt \quad (19.6)$$

- (19.6) is the Fourier transform of a product $\text{sgn}(t) f_o(t)$. It is therefore equal to the convolution of the Fourier transforms of $\text{sgn}(t)$ and $f_o(t)$

$$F'(\omega) = \int_{-\infty}^{+\infty} (\text{sgn}(t) f_o(t)) e^{-i\omega t} dt = FT(\text{sgn}(t); \omega) \otimes FT(f_o(t); \omega) \quad (19.7)$$

Where

$$FT(\text{sgn}(t); \omega) = \int_{-\infty}^{+\infty} \text{sgn}(t) e^{-i\omega t} dt = \frac{2}{i\omega} \quad (19.8)$$

$$FT(f_o(t); \omega) = \int_{-\infty}^{+\infty} f_o(t) e^{-i\omega t} dt = -iF''(\omega)$$

- Use the integral form for the convolution:

$$\begin{aligned} F'(\omega) &= FT(\text{sgn}(t); \omega) \otimes FT(f_o(t); \omega) \\ &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} (-iF''(y)) \left(\frac{2}{i(\omega - y)} \right) dy = -\frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{F''(y)}{(\omega - y)} dy \end{aligned} \quad (19.9)$$

- Equation (19.9) means that as a result of the causality of $f(t)$, the real and imaginary components of the Fourier transform of $f(t)$ are not independent. Knowledge of $F'(\omega)$ results in knowledge of $F''(\omega)$.