Causality and the Kramers-Kronig relations

Causality describes the temporal relationship between cause and effect. A bell rings after you strike it, not before you strike it. This means that the function that describes the response of a bell to being struck must be zero until the time that the bell is struck. Consider a particle of mass m moving in a viscous fluid. The differential equation that describes this system is,

$$m\,\frac{dv}{dt} + bv = F(t).$$

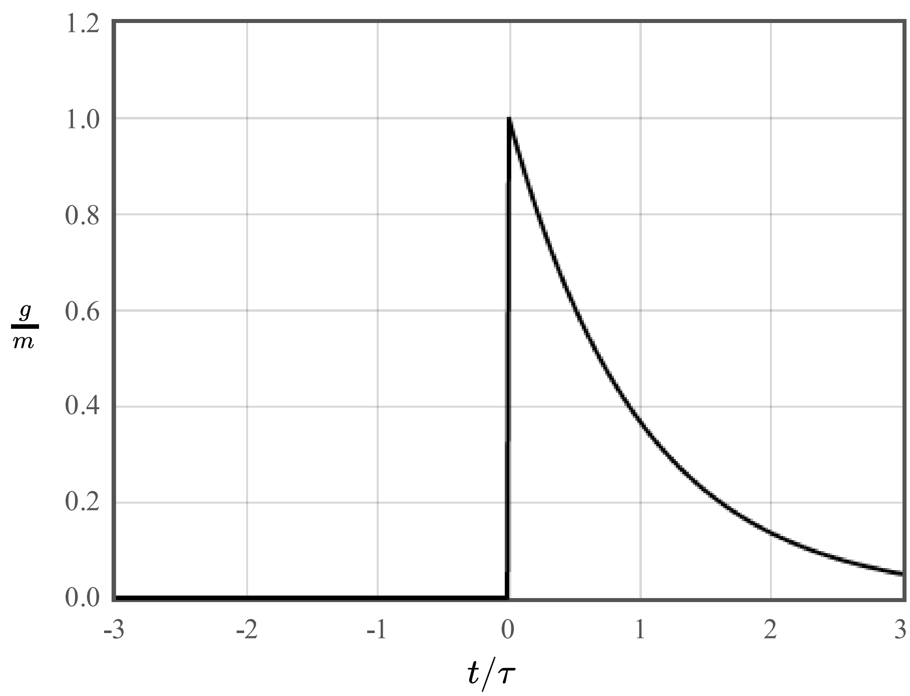
Here b is the damping constant, v is the velocity, and $F(t)$ is a driving force. A special case for the driving force is a δ-function force which strikes the system at $t = 0$. The solution to the differential equation for a δ-function drive force is called the **impulse response function** $g(t)$. The symbol g is used because the impulse response function is sometimes called the Green's function.

$$m\,\frac{dg}{dt} + bg = \delta(t).$$

The solution to this equation is,

$$g(t) = \frac{1}{m}\exp(-t/\tau),$$

Where τ is the decay time $\tau = m/b$.



The utility of the impulse response function is that any driving force can be thought of as being built up of many δ-function forces.

$$F(t) = \int_{-\infty}^{\infty} \delta(t-t')F(t')dt'$$

By superposition, the response to a driving force $F(t)$ is a sum of the impulse response functions.

$$v(t) = \int_{-\infty}^{\infty} g(t-t')F(t')dt'$$

A special driving force is a harmonic driving force, $F(t) = F(\omega)e^{i\omega t}$. The response will occur at the same frequency as the driving force, $v(t) = v(\omega)e^{i\omega t}$. To show this, insert a harmonic force into the equation above.

$$v(t) = \int_{-\infty}^{\infty} g(t-t')F(\omega)e^{i\omega t'}dt'$$

Since the integral is over t', a factor of $e^{-i\omega t}$ can be put inside the integral.

$$v(t) = e^{i\omega t}\int_{-\infty}^{\infty} g(t-t')F(\omega)e^{-i\omega(t-t')}dt'$$

Make a change of variables: $t'' = t-t'$, $dt'' = -dt'$, and reverse the limits of integration.

$$v(t) = e^{i\omega t}F(\omega)\int_{-\infty}^{\infty} g(t'')e^{-i\omega t''}dt''$$

The only time dependence of $v(t)$ is the factor of $e^{i\omega t}$ because the t'' variable gets integrated out. Thus a harmonic driving force $F(\omega)e^{i\omega t}$ produces a harmonic response $v(\omega)e^{i\omega t}$ where,

$$v(\omega) = F(\omega)\int_{-\infty}^{\infty} g(t)e^{-i\omega t}dt$$

The **generalized susceptibility** χ is the ratio of response to driving force.

$$\chi(\omega) = \frac{v(\omega)}{F(\omega)} = \int_{-\infty}^{\infty} g(t)e^{-i\omega t}dt$$

The generalized susceptibility is the Fourier transform of the impulse response function. For the case of a particle moving in a viscous fluid,

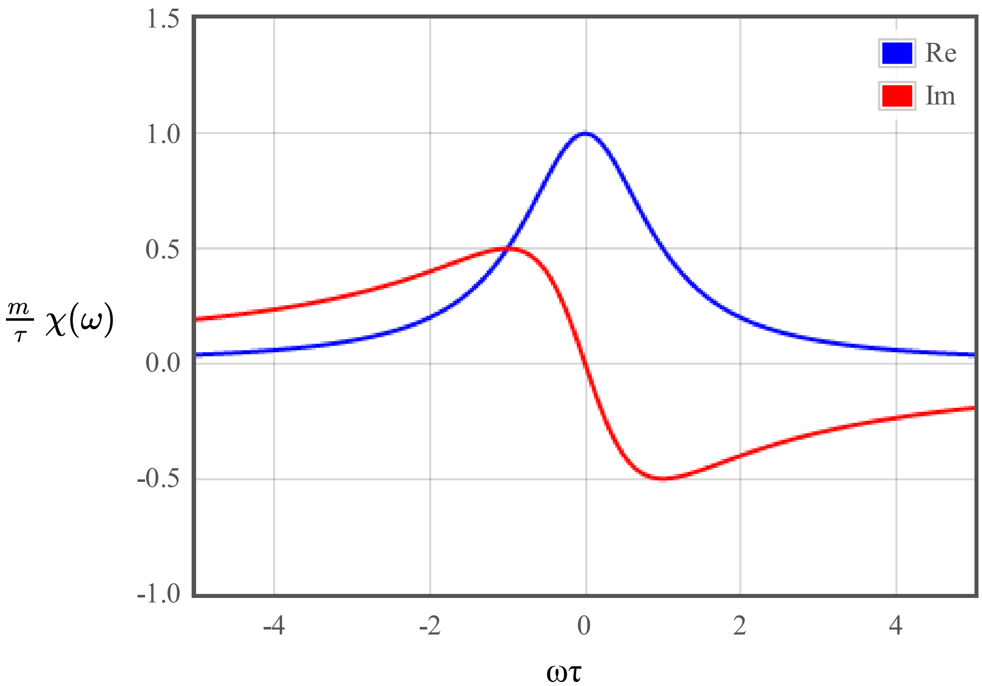
$$\chi(\omega) = \frac{\tau}{m}\,\frac{(1-i\omega\tau)}{1+\omega^2\tau^2}\,.$$

Another way to calculate the generalized susceptibility is to assume that the driving force and the response both have a harmonic time dependence $v(t) = v(\omega)e^{i\omega t}$, $F(t) = F(\omega)e^{i\omega t}$. Substituting this form into the differential equation yields,

$$i\omega m v(\omega) + b v(\omega) = F(\omega).$$

This can be solved for the generalized susceptibility.

$$\chi(\omega) = \frac{v(\omega)}{F(\omega)} = \frac{1}{i\omega m + b} = \frac{\tau}{m}\frac{1 - i\omega\tau}{1 + \omega^2\tau^2}.$$



There is a subtle issue with minus signs here. It is equally valid to assume that the harmonic dependencies of the drive and the response have the form $v(t) = v(\omega)e^{-i\omega t}$, $F(t) = F(\omega)e^{-i\omega t}$. Notice the minus sign that has appeared in the exponent. With this choice, the imaginary part of the susceptibility changes sign:

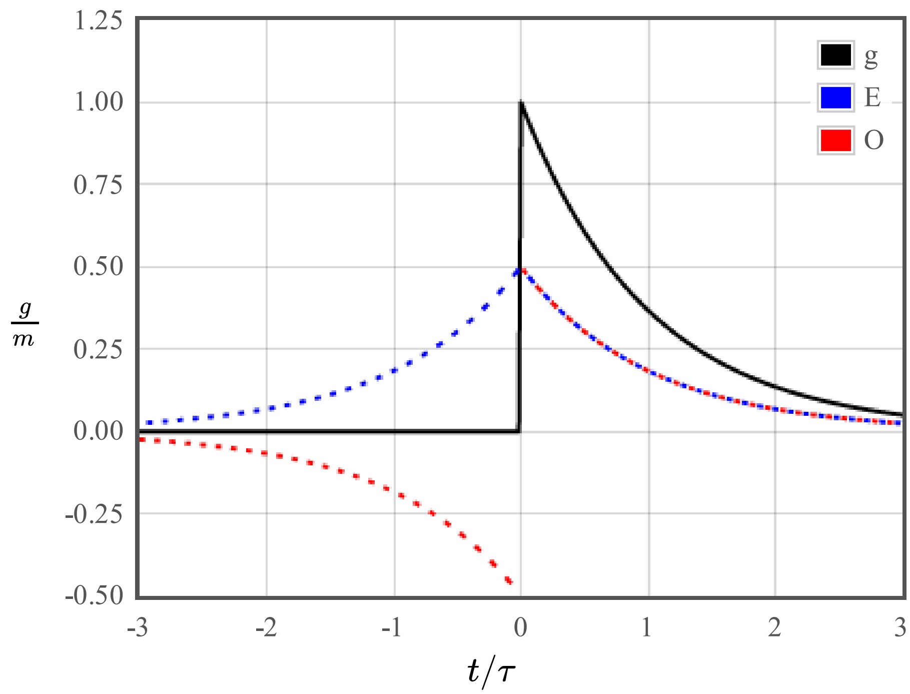
$$\chi(\omega) = \frac{1}{-i\omega m + b} = \frac{\tau}{m}\frac{1 + i\omega\tau}{1 + \omega^2\tau^2}$$

Either descriptions of the harmonic dependence $e^{i\omega t}$ or $e^{-i\omega t}$ are equally valid and there is no consistent choice made in the literature. Here we continue with assuming a harmonic dependence of $e^{i\omega t}$. Be aware that the sign of the imaginary part of the susceptibility might be different from formulas found in other sources.

The causal nature of the impulse response function (it has to be zero for $t < 0$) has consequences for the form of the susceptibility. Any function can be written in terms of an even component $E(t)$ and an odd component $O(t)$.

$$g(t) = E(t) + O(t).$$

Since the impulse response function must be zero for $t < 0$, the even and the odd components must add to zero for $t < 0$.



Note that if we know the either the even component or the odd component we construct the other.

$$E(t) = \text{sgn}(t)O(t) = \tfrac{1}{2}\left(g(-t) + g(t)\right)$$

$$O(t) = \text{sgn}(t)E(t) = \tfrac{1}{2}\left(-g(-t) + g(t)\right)$$

Repeating what was stated above, the susceptibility is the Fourier transform of the impulse response function,

$$\chi(\omega) = \int\limits_{-\infty}^{\infty} g(t)e^{-i\omega t}dt = \int\limits_{-\infty}^{\infty} (E(t) + O(t))(\cos(-\omega t) + i\sin(-\omega t))dt.$$

The integral of an odd function over an even interval $(-\infty, \infty)$ is zero so the real part of the susceptibility is the Fourier transform of the even component,

$$\text{Re}[\chi] = \chi' = \int\limits_{-\infty}^{\infty} E(t)\cos(\omega t)dt,$$

and the imaginary part is the Fourier transform of the odd component,

$$\text{Im}[\chi] = \chi'' = -\int\limits_{-\infty}^{\infty} O(t)\sin(\omega t)dt.$$

Moreover χ' is an even function $\chi'(\omega) = \chi'(-\omega)$ while χ'' is an odd function $\chi''(\omega) = -\chi''(-\omega)$.

The Kramers-Kronig relations

The Kramers-Kronig relations describe how the real and imaginary parts of the susceptibility are related to each other. If either the real part or the imaginary part of the susceptibility is known for positive frequencies $\omega > 0$, the entire susceptibility can be calculated at all frequencies. Suppose we know χ' for $\omega > 0$. Then χ' for all frequencies can be constructed because $\chi'(\omega) = \chi'(-\omega)$. The even component of the impulse response function can be found by inverse Fourier transforming χ'. The odd component of the impulse response function is related to the even component by $O(t) = \text{sgn}(t)E(t)$. The imaginary part of the susceptibility χ'' can then be constructed since it is the Fourier transform of the odd component.

$$\chi'(\omega) = \int\limits_{-\infty}^{\infty} E(t)\cos(\omega t)dt \qquad E(t) = \frac{1}{2\pi}\int\limits_{-\infty}^{\infty} \chi'(\omega)\cos(\omega t)d\omega$$

$$\boxed{O(t) = \text{sgn}(t)E(t) \qquad E(t) = \text{sgn}(t)O(t)}$$

$$\chi''(\omega) = -\int\limits_{-\infty}^{\infty} O(t)\sin(\omega t)dt \qquad O(t) = \frac{-1}{2\pi}\int\limits_{-\infty}^{\infty} \chi''(\omega)\sin(\omega t)d\omega$$

The equations in the box above are known as the Kramers-Kroning relations. This is the representation of the Kramers-Kronig relations in the time domain. Many observable quantities obey the Kramers-Kroning relations. For instance the electric susceptibility describes the electric polarization of a material responds to an applied electric field. This response must be causal so the real and imaginary parts of the electric susceptibility must be related by the Kramers-Kronig relations. This is also true for the magnetic susceptibility, the electrical conductivity, the thermal conductivity, and the dielectric constant.

A plane wave moving in the positive x-direction has the form $e^{ikx-\omega t}$. If the frequency is negative, the wave moves in the negative x-direction. Typically in an experiment, only the positive frequencies are measured where the waves move from a source to the detector. This presents no difficulty since all of the information is contained in the positive frequencies.

Sometimes it is experimentally easier to measure the real part or the imaginary part of the susceptibility. The Kramer-Kronig relations can then be used to calculate the part that is difficult to measure. If both real and imaginary parts can be measured, it is possible to check for experimental errors using the Kramers-Kronig relations. If a susceptibility is calculated theoretically, it is a good idea to check and see if it satisfies the Kramers-Kronig relations. It is considered a serious error to present a result that violates causality.

It is traditional to write the Kramers-Kronig relations in the frequency domain. This unfortunately introduces a singularity in the formula. The singularity in the integral makes the form that is given below less suitable for a numerical evaluation of the Kramers-Kronig relation. Nevertheless, it commonly appears in the literature and is given for completeness. Since the Fourier transform of $\text{sgn}(t)$ is $\frac{-i}{\pi\omega}$, we can use the convolution theorem to take the Fourier transform of the equations $O(t) = \text{sgn}(t)E(t)$ and $E(t) = \text{sgn}(t)O(t)$,

$$\chi' = \frac{-i}{\pi\omega} * (-i\chi''),$$

$$-i\chi'' = \frac{-i}{\pi\omega} * \chi'.$$

Here '*' represents convolution. Using the definition of convolution yields the Kramers-Kronig relations in the frequency domain.

$$\chi' = \frac{-1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi''(\omega')}{\omega' - \omega} d\omega',$$

$$\chi'' = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi'(\omega')}{\omega' - \omega} d\omega'.$$

Here the P before the integral indicates that one should use the Cauchy principle value of the integral. This is necessary because of the singularity that the integral contains. The advantage of this form is that one sees immediately that the real part of the susceptibility can be determined from the imaginary part and vice versa without transforming to the time domain.

The Kramers-Kronig relations are often put in another form where the integrals only involve positive frequencies. The integral for χ' is split into two parts.

$$\chi' = -\frac{1}{\pi} P \int_{-\infty}^{0} \frac{\chi''(\omega')}{\omega' - \omega} d\omega' - \frac{1}{\pi} P \int_{0}^{\infty} \frac{\chi''(\omega')}{\omega' - \omega} d\omega',$$

In the first term make a change of variables $\omega' \rightarrow -\omega''$, use the fact that χ'' is an odd function: $\chi''(-\omega) = -\chi''(\omega)$, and reverse the limits of integration.

$$\chi' = -\frac{1}{\pi} P \int_{0}^{\infty} \frac{\chi''(\omega'')}{\omega'' + \omega} d\omega'' - \frac{1}{\pi} P \int_{0}^{\infty} \frac{\chi''(\omega')}{\omega' - \omega} d\omega',$$

The integrals can be combined.

$$\chi' = -\frac{1}{\pi} P \int_{0}^{\infty} \left(\frac{1}{\omega' + \omega} + \frac{1}{\omega' - \omega} \right) \chi''(\omega') d\omega'$$

Rewriting the factor,

$$\left(\frac{1}{\omega' + \omega} + \frac{1}{\omega' - \omega} \right) = \frac{2\omega'}{(\omega')^2 - \omega^2},$$

the Kramers-Kronig relations can also be written,

$$\chi' = \frac{-2}{\pi} P \int_0^\infty \frac{\omega' \chi''(\omega')}{(\omega')^2 - \omega^2} d\omega',$$

$$\chi'' = \frac{2\omega}{\pi} P \int_0^\infty \frac{\chi'(\omega')}{(\omega')^2 - \omega^2} d\omega'.$$

Note that the singularity is stronger in this form making it less suitable for a numerical evaluation.

---

1. Classical linear response theory is described in *Response and Stability* by A. B. Pippard, Cambridge University Press (1985).
2. A discussion of causality and separating the impulse response function into even and odd parts is found in *The Fourier Transform and Its Applications* by R. N. Bracewell, McGraw-Hill (1978).