Linear response theory

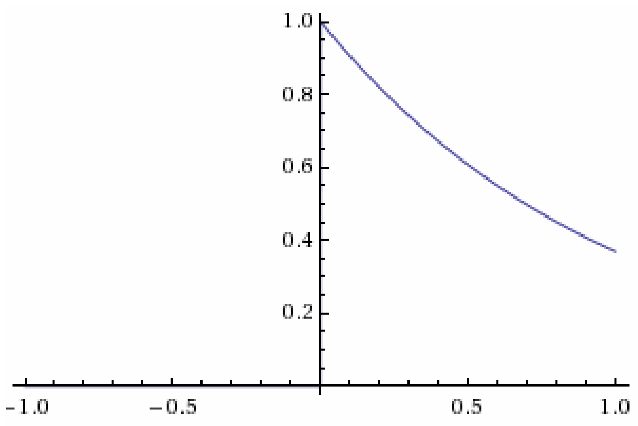
First order differential equation

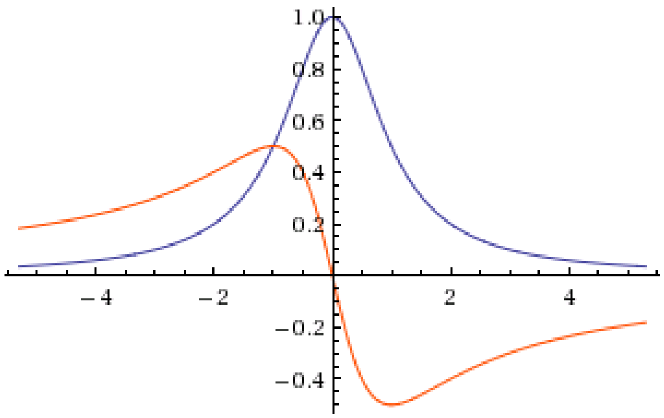
$$m\frac{dg}{dt}+bg=\delta(t)$$

$$g(t)=\frac{1}{m}H(t)\exp\left(-\frac{bt}{m}\right) \qquad \frac{b}{m}>0$$

$$\chi(\omega)=\int g(t)e^{-i\omega t}dt$$

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





The Fourier transform of a decaying exponential is a Lorentzian

Susceptibility

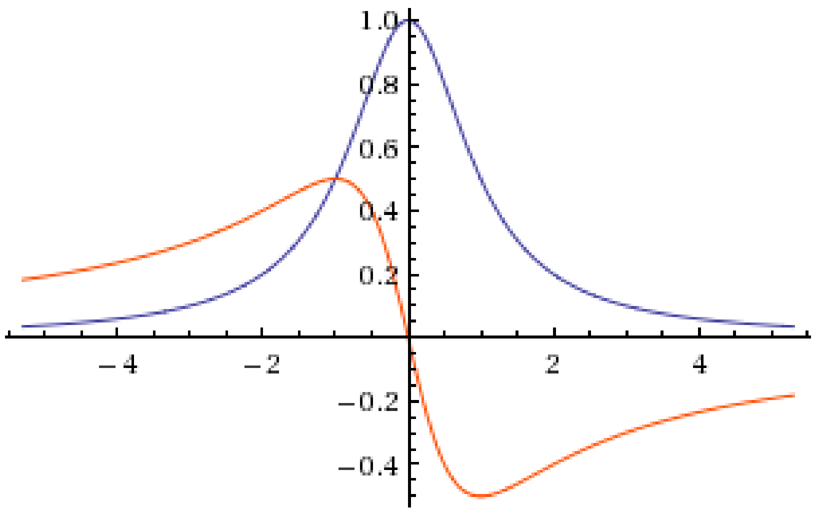
$$m\frac{du}{dt} + bu = F(t)$$

Assume that u and F are sinusoidal $\quad u = Ae^{i\omega t} \quad F = F_0 e^{i\omega t}$

$$i\omega mA + bA = F_0$$

$$A = \frac{F_0}{b + i\omega m} = F_0 \frac{b - i\omega m}{b^2 + m^2\omega^2}$$

$$\chi = \frac{u}{F} = \frac{1}{m}\frac{\frac{b}{m} - i\omega}{\left(\frac{b}{m}\right)^2 + \omega^2}$$



The sign of the imaginary part depends on whether you use $e^{i\omega t}$ or $e^{-i\omega t}$.

Susceptibility

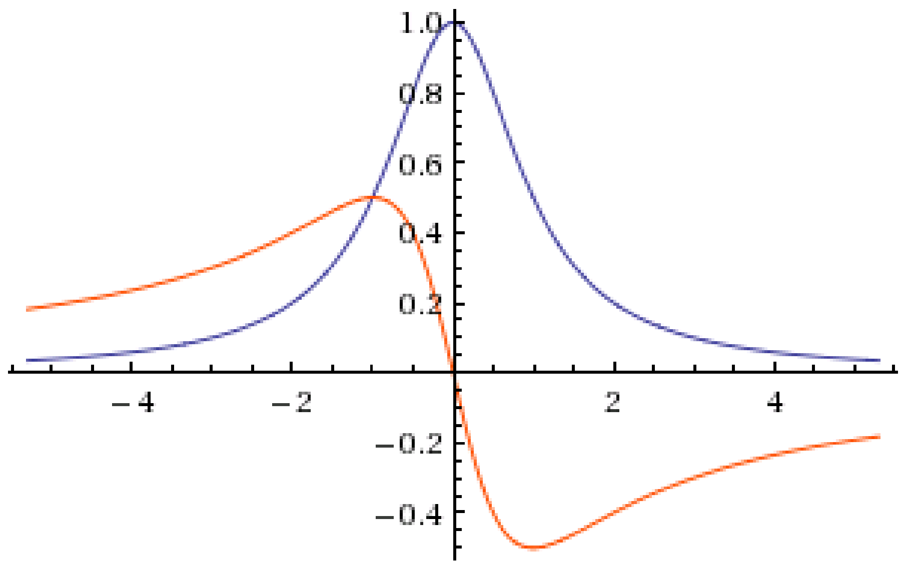
$$m\frac{dg}{dt}+bg=\delta(t)$$

Fourier transform the differential equation

$$i\omega m\chi(\omega)+b\chi(\omega)=1$$

$$\chi=\frac{1}{b+i\omega m}$$

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

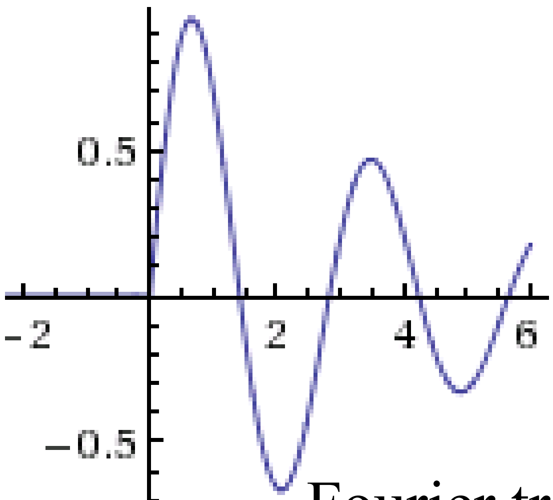


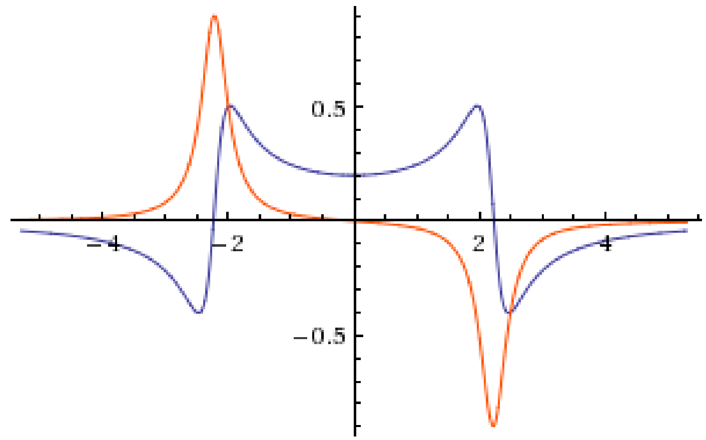
Damped mass-spring system

$$m\frac{d^2g}{dt^2} + b\frac{dg}{dt} + kg = \delta(t)$$

$$-\omega^2 m\chi + i\omega b\chi + k\chi = 1$$

$$g = e^{\lambda t} \qquad \lambda_\pm = \frac{-b \pm \sqrt{b^2 - 4mk}}{2m}$$





Fourier transform pair

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

$$g(t) = H(t)\frac{1}{m}\exp\left(\frac{-bt}{2m}\right)\sin\left(\frac{\sqrt{4mk - b^2}}{2m}t\right)$$

Table of Fourier transforms

The Fourier transforms of some functions in the four notations are given in the table below.

$f(\vec{r})$	$F_{-1,-1}(\vec{k})$	$F_{1,-1}(\vec{k})$	$F_{0,-1}(\vec{k})$
$\exp\left(-\left(\frac{x}{a}\right)^2\right)$	$\frac{a}{2\sqrt{\pi}}\exp\left(-\frac{a^2k^2}{4}\right)$	$a\sqrt{\pi}\exp\left(-\frac{a^2k^2}{4}\right)$	$\frac{a}{\sqrt{2}}\exp\left(-\frac{a^2k^2}{4}\right)$
$\exp(ik_0x)$	$\delta(k-k_0)$	$2\pi\delta(k-k_0)$	$\sqrt{2\pi}\delta(k-k_0)$
$\sin(k_0x)$	$\frac{i}{2}\left(\delta(k+k_0)-\delta(k-k_0)\right)$	$i\pi(\delta(k+k_0)-\delta(k-k_0))$	$i\sqrt{\frac{\pi}{2}}\left(\delta(k+k_0)-\delta(k-k_0)\right)$
$\cos(k_0x)$	$\frac{1}{2}\left(\delta(k+k_0)+\delta(k-k_0)\right)$	$\pi(\delta(k+k_0)+\delta(k-k_0))$	$\sqrt{\frac{\pi}{2}}\left(\delta(k+k_0)+\delta(k-k_0)\right)$
$\exp(-\lvert a\rvert x)$	$\frac{\lvert a\rvert}{\pi(a^2+k^2)}$	$\frac{2\lvert a\rvert}{a^2+k^2}$	$\frac{\sqrt{2}\lvert a\rvert}{\sqrt{\pi}(a^2+k^2)}$
$\operatorname{sgn}(x)\exp(-\lvert a\rvert x)$	$\frac{-ik}{\pi(a^2+k^2)}$	$\frac{-i2k}{a^2+k^2}$	$\frac{-i\sqrt{2}k}{\sqrt{\pi}(a^2+k^2)}$
$H(x)\exp(-\lvert a\rvert x)$	$\frac{\lvert a\rvert-ik}{2\pi(a^2+k^2)}$	$\frac{\lvert a\rvert-ik}{a^2+k^2}$	$\frac{\lvert a\rvert-ik}{\sqrt{2\pi}(a^2+k^2)}$
$H\left(x+\frac{1}{2}\right)H\left(\frac{1}{2}-x\right)$	$\frac{\sin(ka/2)}{\pi k}$	$\frac{2\sin(ka/2)}{k}$	$\frac{\sqrt{2}\sin(ka/2)}{\sqrt{\pi}k}$
$H\left(\frac{x-x_0}{a}+\frac{1}{2}\right)H\left(\frac{1}{2}-\frac{x-x_0}{a}\right)$	$\frac{\sin(ka/2)}{\pi k}\exp(-ikx_0)$	$\frac{2\sin(ka/2)}{k}\exp(-ikx_0)$	$\frac{\sqrt{2}\sin(ka/2)}{\sqrt{\pi}k}\exp(-ikx_0)$
$\exp\left(i\vec{k}_0\cdot\vec{r}\right)$	$\delta\left(\vec{k}-\vec{k}_0\right)$	$(2\pi)^d\delta\left(\vec{k}-\vec{k}_0\right)$	$(2\pi)^{d/2}\delta\left(\vec{k}-\vec{k}_0\right)$
$\delta\left(\frac{\vec{r}-\vec{r}_0}{a}\right)$	$\left(\frac{a}{2\pi}\right)^d\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$	$a^d\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$	$\left(\frac{a}{\sqrt{2\pi}}\right)^d\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$
$\exp\left(-\frac{\lvert\vec{r}-\vec{r}_0\rvert^2}{a^2}\right)$	$\left(\frac{a}{2\sqrt{\pi}}\right)^d\exp\left(-\frac{a^2k^2}{4}\right)\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$	$(a\sqrt{\pi})^d\exp\left(-\frac{a^2k^2}{4}\right)\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$	$\left(\frac{a}{\sqrt{2}}\right)^d\exp\left(-\frac{a^2k^2}{4}\right)\exp(-i\vec{k}\cdot\vec{r}_0$

Here $H(x)$ is the Heaviside step function, $\delta(x)$ is the Dirac delta function, and d is the number of dimensions $\vec{r}$ is defined in.

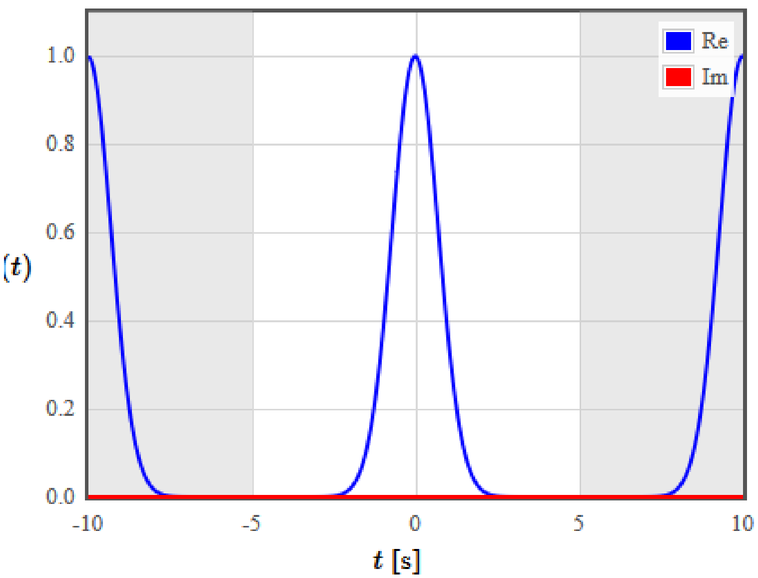
http://lamp.tu-graz.ac.at/~hadley/ss1/crystaldiffraction/ft/ft.php

Numerical Calculations of Fourier Transforms

Typically a Discrete Fourier Transform (DFT) is used to numerically calculate the Fourier transform of a function. A DFT algorithm takes a discrete sequence of N equally spaced points $(g_0, g_1, \cdots, g_{N-1})$ and returns the Fourier components of a continuous periodic that passes through all of those points. There are infinitely many periodic functions that will pass a discrete sequence of points. Here we restrict ourselves to the periodic function that can be constructed using only those complex exponentials in the first Brillouin zone.

The Fourier transform of a function $g(t)$ is $G(f)$. The values of $g(t)$ at equally spaced points can be input into the textbox in the lower left as three columns. If the data you have is not eually spaced, use linear interpolation, or a cubic spline to generate euqally spaced points. Alternatively, the functional form of $g(t)$ can be given and equally spaced points will be calculated. If is also possible to specify $G(f)$ by providing equally spaced points or by giving its functional form in the first Brillouin zone.

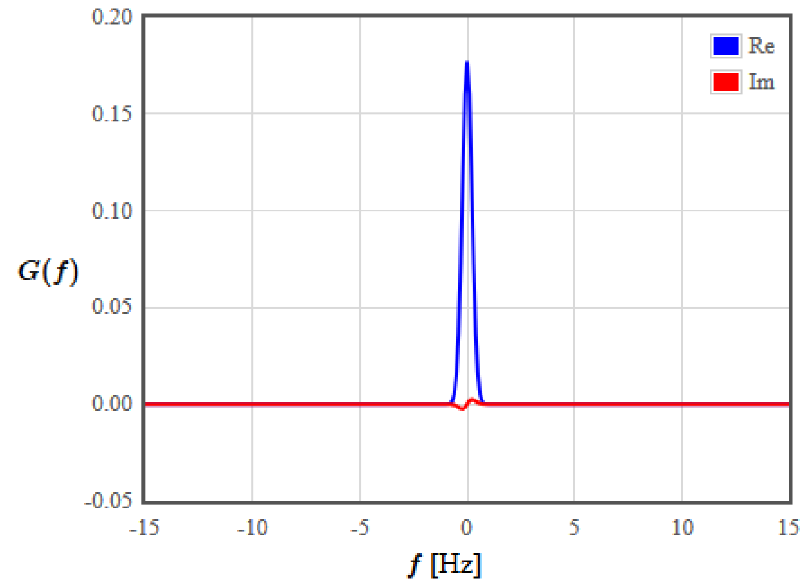
Real space



→ DFT →

← invDFT ←

Reciprocal space



t [s]	Re[$g(t)$]	Im[$g(t)$]
4.9000000	3.7375713e-11	0.0000000
4.8666667	5.1757879e-11	0.0000000
4.8333333	7.1515199e-11	0.0000000
4.8000000	9.8595056e-11	0.0000000
4.7666667	1.3562721e-10	0.0000000
4.7333333	1.8615444e-10	0.0000000
4.7000000	2.5493819e-10	0.0000000
4.6666667	3.4836241e-10	0.0000000
4.6333333	4.7496605e-10	0.0000000
4.6000000	6.4614318e-10	0.0000000
4.5666667	8.7706111e-10	0.0000000

f [Hz]	Re[$G(f)$]	Im[$G(f)$]
-15	5.076726813641739e-13	-9.719385418441837
-14.9	1.3705810894114153e-12	-8.737357111630713
-14.8	1.9410449394383604e-12	-7.438149987579592
-14.7	2.2123178251277097e-12	-6.053108453801513
-14.6	1.7449718986371344e-12	-3.713301030908255
-14.5	-4.58301578239992e-13	7.975294433261938e
-14.4	-5.258503585988779e-12	7.739262485643038e
-14.3	-1.253502856914109e-11	1.598179325432863e
-14.2	-2.0915194582514254e-11	2.351340881092470б
-14.1	-2.7885489671314272e-11	2.803110600565487б

More complex linear systems

Any coupled system of linear differential equations can be written as a set of first order equations

$$\frac{d\vec{x}}{dt} = M\vec{x}$$

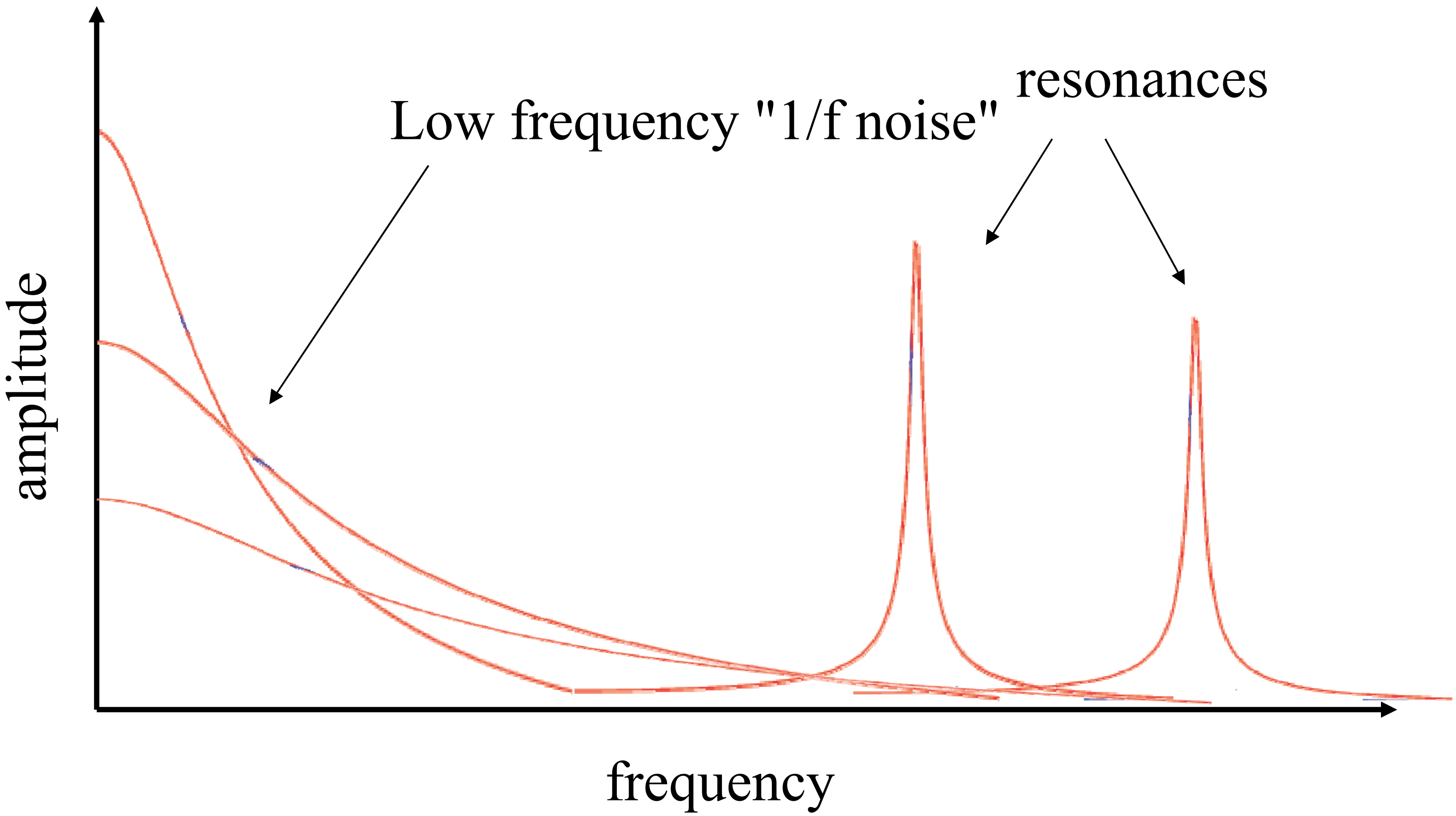
The solutions have the form $\vec{x}_i e^{\lambda t}$

where $\vec{x}_i$ are the eigenvectors and λ are the eigenvalues of matrix M.

Re(λ) < 0 for stable systems

λ is either real and negative (overdamped) or comes in complex conjugate pairs with a negative real part (underdamped).

More complex linear systems



Odd and even components

Any function $f(t)$ can be written in terms of its odd and even components

$$E(t) = \tfrac{1}{2}[f(t) + f(-t)]$$

$$O(t) = \tfrac{1}{2}[f(t) - f(-t)]$$

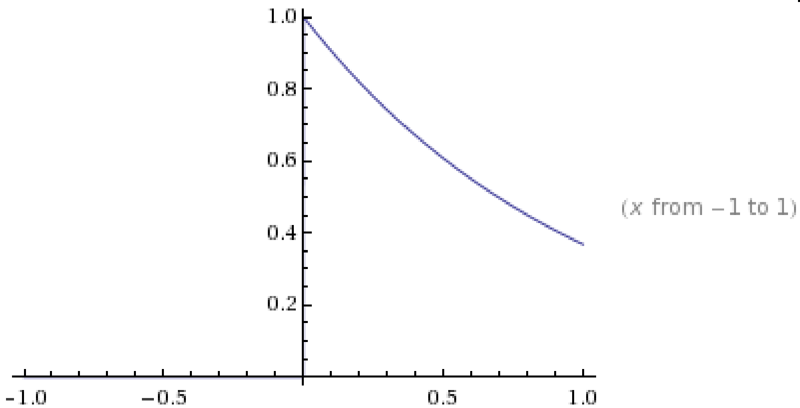
$$f(t) = \mathrm{E}(t) + O(t)$$

$$f(t) = \tfrac{1}{2}[f(t) + f(-t)] + \tfrac{1}{2}[f(t) - f(-t)]$$

$$\int_{-\infty}^{\infty} f(t)e^{-i\omega t}dt = \int_{-\infty}^{\infty} \big(E(t) + O(t)\big)\big(\cos\omega t - i\sin\omega t\big)dt$$

$$= \int_{-\infty}^{\infty} E(t)\cos\omega t dt - i\int_{-\infty}^{\infty} O(t)\sin\omega t dt$$

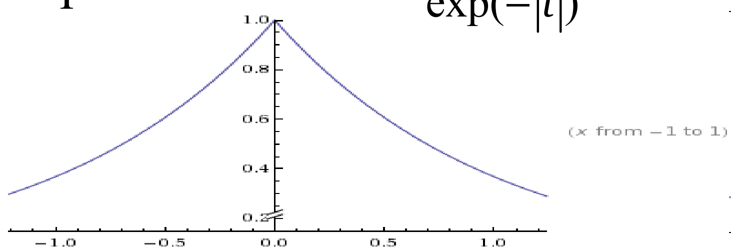
The Fourier transform of $E(t)$ is real and even
The Fourier transform of $O(t)$ is imaginary and odd

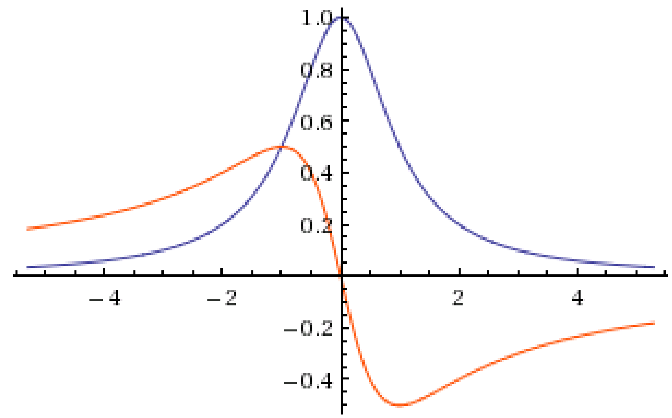


$$\chi(\omega) = \frac{1}{m}\frac{\frac{b}{m} - i\omega}{\left(\frac{b}{m}\right)^2 + \omega^2}$$

even component

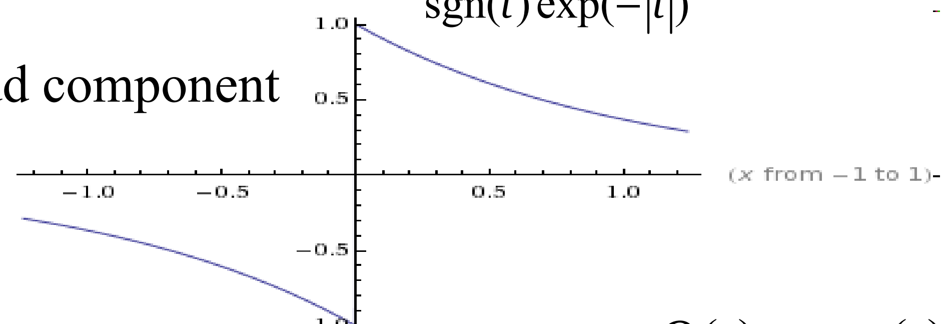
$\exp(-|t|)$





$\mathrm{sgn}(t)\exp(-|t|)$

odd component



$$O(t) = \mathrm{sgn}(t)E(t)$$

$$E(t) = \mathrm{sgn}(t)O(t)$$

Causality and the Kramers-Kronig relations (I)

$$\chi(\omega) = \int g(\tau)e^{-i\omega\tau}d\tau = \int E(\tau)\cos(\omega\tau)d\tau - i\int O(\tau)\sin(\omega\tau)d\tau = \chi'(\omega) + i\chi''(\omega)$$

The real and imaginary parts of the susceptibility are related.

If you know χ', inverse Fourier transform to find $E(t)$. Knowing $E(t)$ you can determine $O(t) = \mathrm{sgn}(t)E(t)$. Fourier transform $O(t)$ to find χ''.

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

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

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

Causality and the Kramers-Kronig relation (II)

Real space

$$E(t) = \mathrm{sgn}(t) O(t)$$

$$O(t) = \mathrm{sgn}(t) E(t)$$

Reciprocal space

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

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

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

Take the Fourier transform, use the convolution theorem.

P: Cauchy principle value (go around the singularity and take the limit as you pass by arbitrarily close)

Singularity makes a numerical evaluation more difficult.

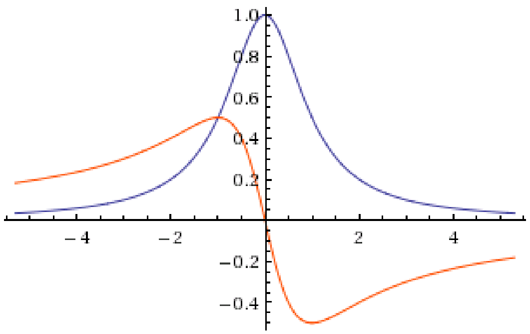
http://lamp.tu-graz.ac.at/~hadley/ss2/linearresponse/causality.php

Kramers-Kronig relations (III)

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

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

Kramers-Kronig relations II



$$\chi'(\omega) = \chi'(-\omega)$$

$$\chi''(\omega) = -\chi''(-\omega)$$

Real part is even
Imaginary part is odd

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

change variables ω'→-ω'
(4 minus signs)

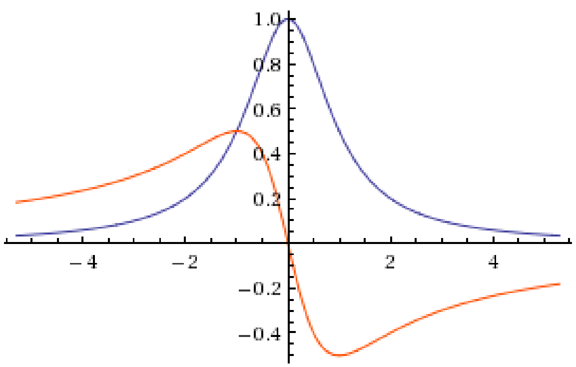
Kramers-Kronig relations (III)

$$\chi'(\omega) = -\frac{1}{\pi} P\int_0^\infty \frac{\chi''(\omega')}{\omega' + \omega} d\omega' - \frac{1}{\pi} P\int_0^\infty \frac{\chi''(\omega')}{\omega' - \omega} d\omega'$$

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

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

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



Singularity is stronger in this form.

Impulse response/generalized susceptibility

The impulse response function is the response of the system to a δ-function excitation. The response function must be zero before the excitation.

The generalized susceptibility is the Fourier transform of the impulse response function.

Any function that is zero before the excitation and nonzero afterwards must have both an odd component and an even component.

The generalized susceptibility must have a real and imaginary part. All information about the real part is contained in the imaginary part and vice versa.