Linear response theory

Classical linear response theory

Fourier transforms
Impulse response functions (Green's functions)
Generalized susceptibility
Causality
Kramers-Kronig relations
Fluctuation - dissipation theorem
Dielectric function
Optical properties of solids

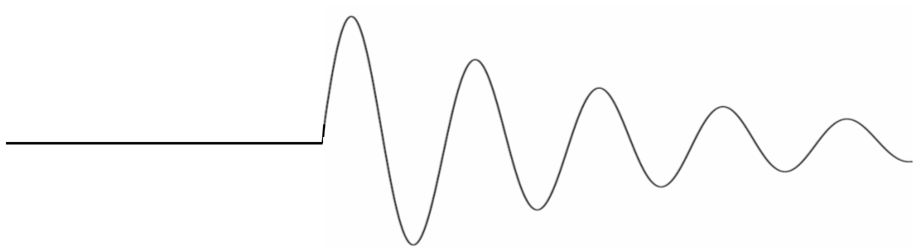
Impulse response function (Green's functions)

A Green's function is the solution to a linear differential equation for a δ-function driving force

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

has the solution

$$g(t) = \frac{1}{m}\exp\left(\frac{-bt}{2m}\right)\sin\left(\frac{\sqrt{4mk-b^2}}{2m}t\right) \qquad t > 0$$



Green's functions

A driving force *f* can be thought of a being built up of many delta functions after each other.

$$f(t) = \int \delta\left(t - t'\right) f\left(t'\right) dt'$$

By superposition, the response to this driving function is superposition,

$$u(t) = \int g(t - t') f(t') dt'$$

For instance, $$m\frac{d^2u}{dt^2} + b\frac{du}{dt} + ku = f(t)$$

has the solution

$$u(t) = \int_{-\infty}^{\infty} \frac{1}{m} \exp\left(\frac{-b\left(t - t'\right)}{2m}\right) \sin\left(\frac{\sqrt{4mk - b^2}}{2m}\left(t - t'\right)\right) f(t') dt'$$

Green's function converts a differential equation into an integral equation

Generalized susceptibility

A driving function f causes a response u

If the driving force is sinusoidal,

$$f(t) = F_0 e^{i\omega t}$$

The response will also be sinusoidal.

$$u(t) = \int g(t-t') f(t') dt' = \int g(t-t') F_0 e^{i\omega t'} dt'$$

The generalized susceptibility at frequency ω is

$$\chi(\omega) = \frac{u}{f} = \frac{\int g(t-t') e^{i\omega t'} dt'}{e^{i\omega t}}$$

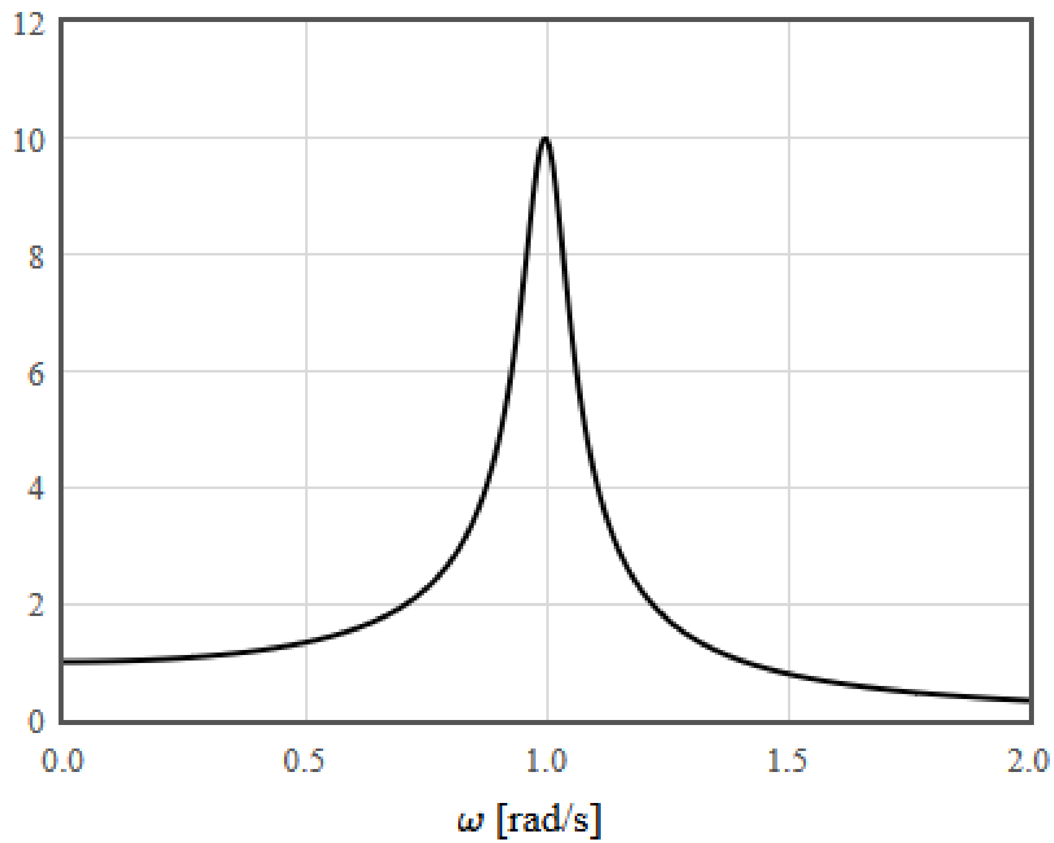
Generalized susceptibility

http://lampx.tugraz.at/~hadley/physikm/apps/resonance.en.php

$m =$ 1 [kg] $b =$ 0.1 [N s/m] $k =$ 1 [N/m] Plot

$Q = \frac{\sqrt{mk}}{b} =$ 10

$$\chi(\omega) = \frac{|u|}{f}$$



Generalized susceptibility

$$\chi(\omega) = \frac{u}{f} = \frac{\int g(t-t')e^{i\omega t'}dt'}{e^{i\omega t}}$$

Since the integral is over t', the factor with t can be put in the integral.

$$\chi(\omega) = \int g(t-t')e^{-i\omega(t-t')}dt'$$

Change variables to $\tau = t - t'$, $d\tau = -dt'$, reverse the limits of integration

$$\chi(\omega) = \int g(\tau)e^{i\omega\tau}d\tau$$

The susceptibility is the Fourier transform of the Green's function.

$$g(t) = \frac{1}{2\pi}\int \chi(\omega)e^{-i\omega t}d\omega$$

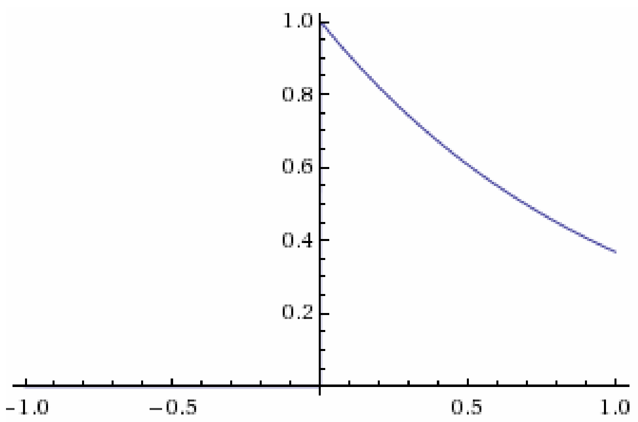
First order differential equation

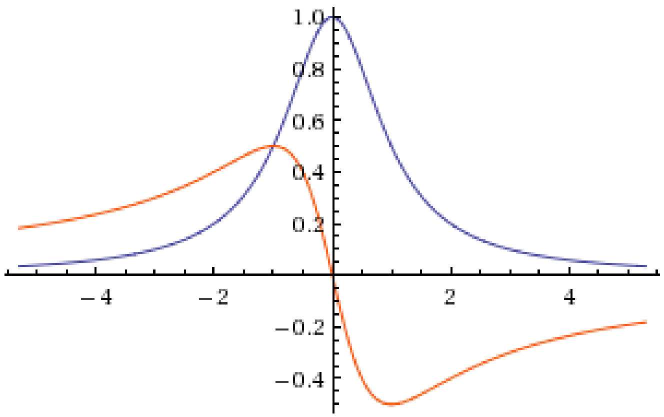
$$m\frac{dg}{dt} + bg = \delta(t)$$

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

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

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





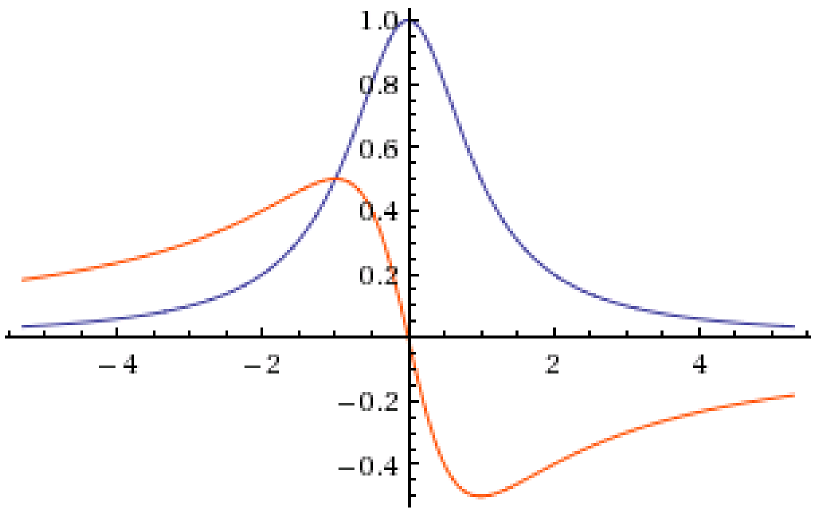
The Fourier transform of a decaying exponential is a Lorentzian

Susceptibility

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

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

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



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

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

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

Susceptibility

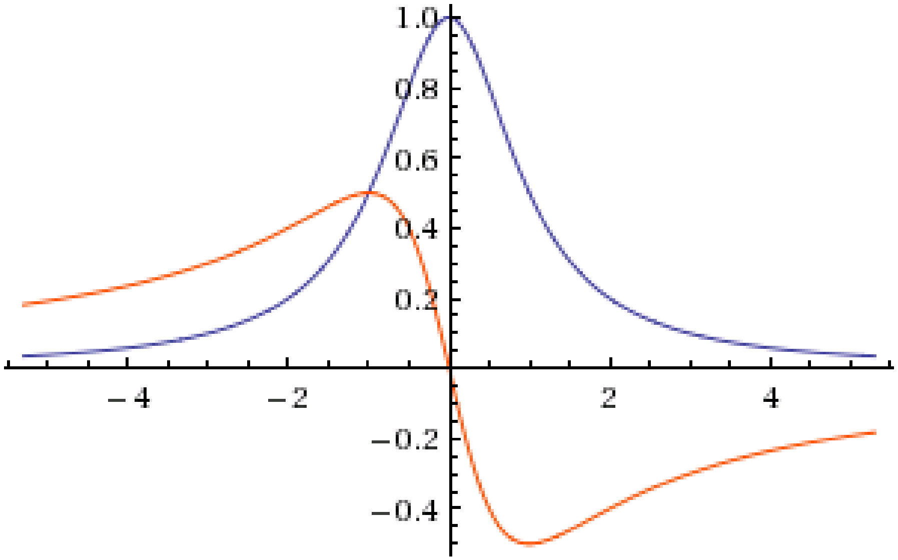
$$m\frac{dg}{dt} + bg = \delta(t)$$

Fourier transform the differential equation

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

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

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

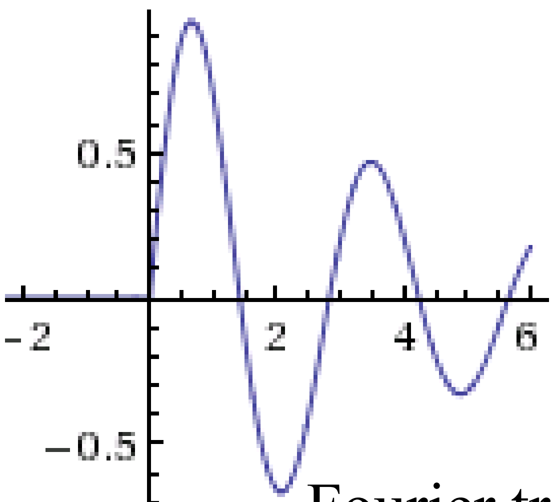


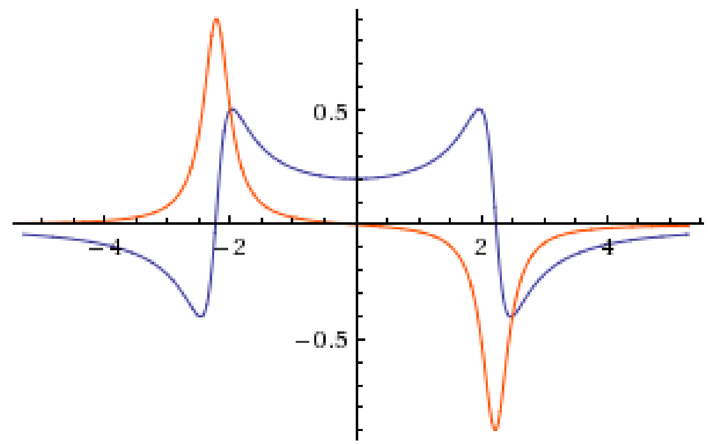
Damped mass-spring system

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

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

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





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

Fourier transform pair

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

Table of Fourier transforms

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

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

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.

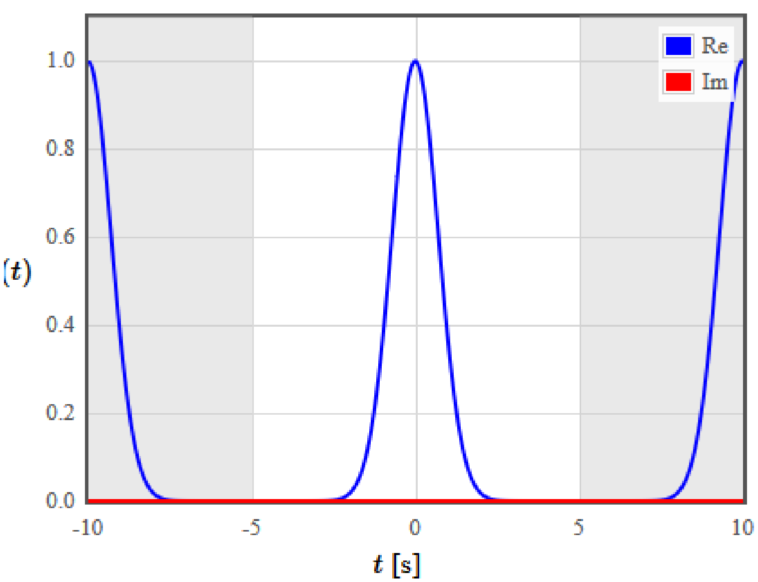
http://lamp.tu-graz.ac.at/~hadley/ss1/crystaldiffraction/ft/ft.php

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.

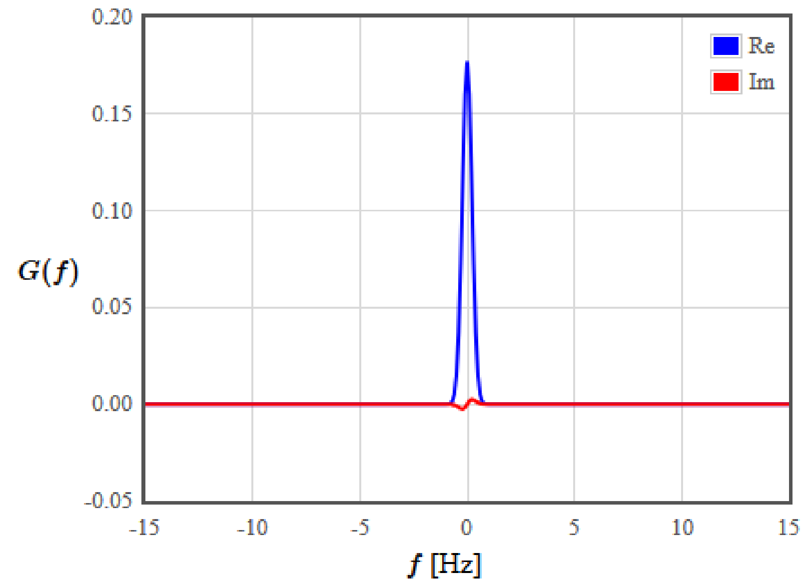
Real space



→ 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	2.3513408810924706
-14.1	-2.7885489671314272e-11	2.8031106005654876

More complex linear systems

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

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

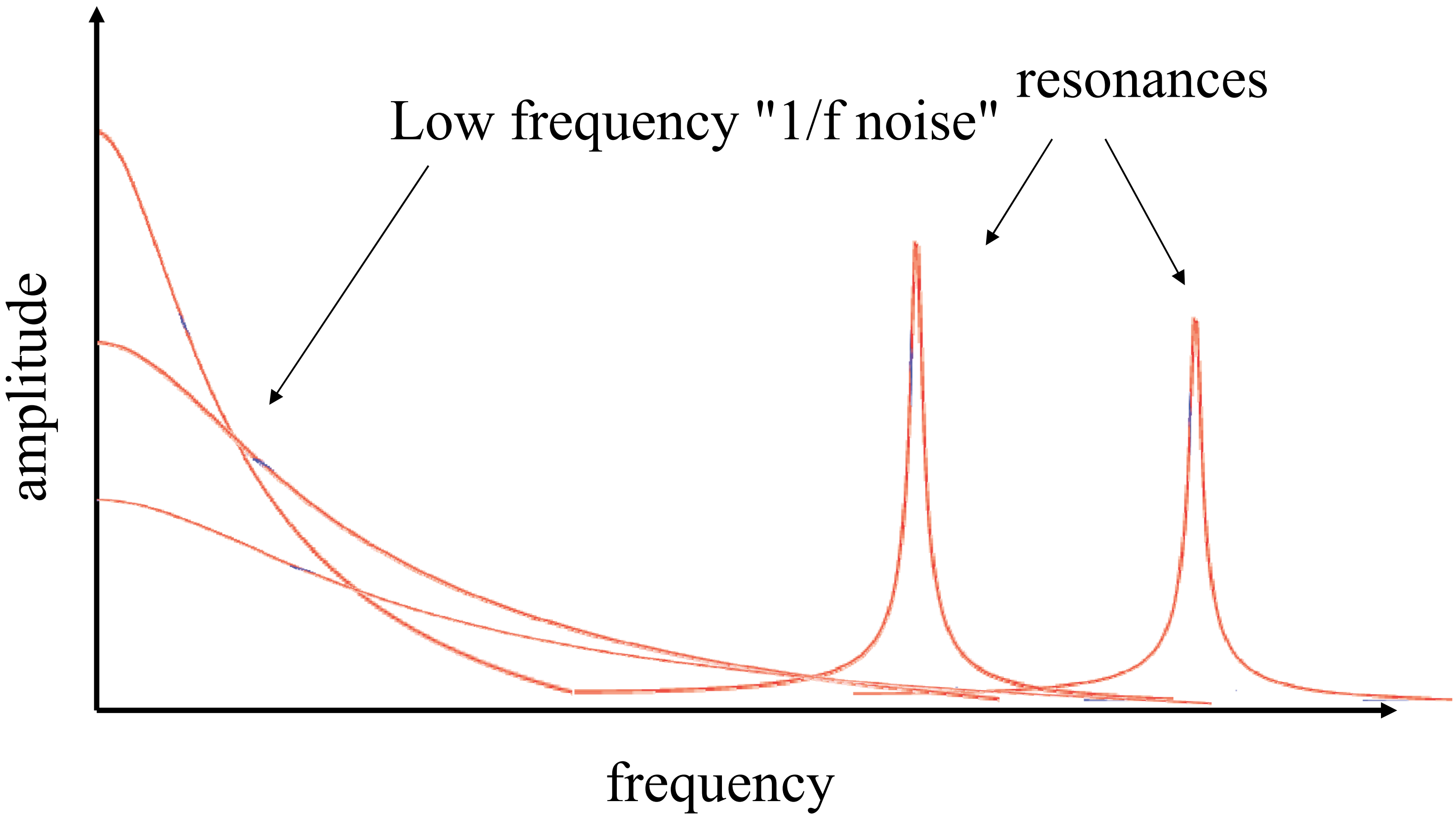
The solutions have the form $\vec{x}_i e^{\lambda t}$

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

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

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

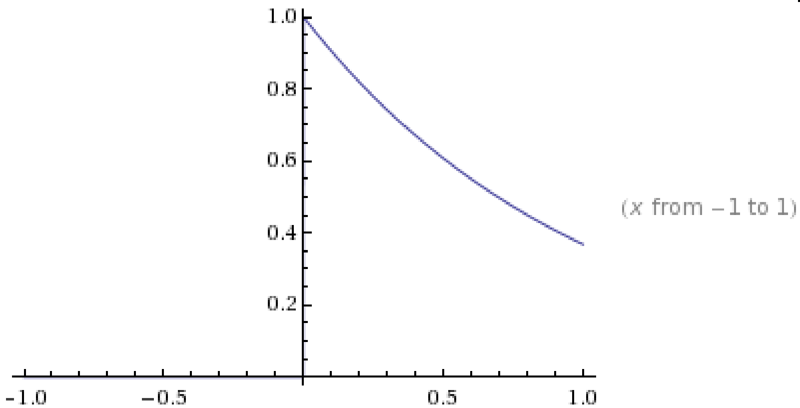
$$f(t) = E(t) + O(t)$$

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

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

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

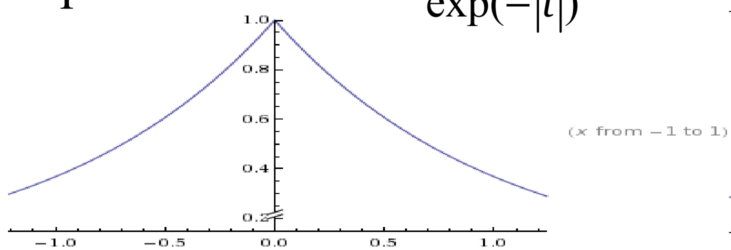
The Fourier transform of $E(t)$ is real and even
The Fourier transform of $O(t)$ is imaginary and odd

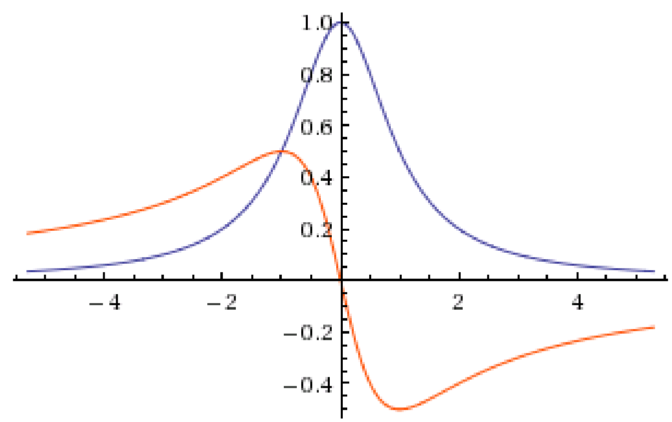


$$\chi(\omega) = \frac{1}{m}\frac{\frac{b}{m} - i\omega}{\left(\frac{b}{m}\right)^2 + \omega^2}$$

even component

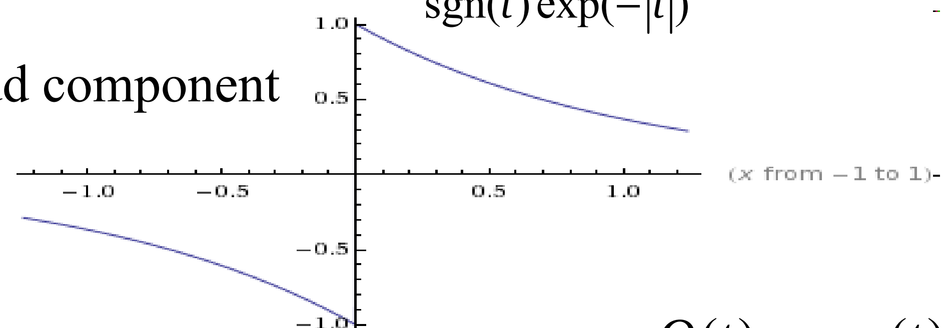
$\exp(-|t|)$





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

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

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

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

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