Linear Response Theory: Kramers-Kronig relations

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

Fourier analysis of real data sets

Consider a series of N measurements x_n that are made at equally spaced time intervals Δt. The total time to make the measurement series is $N\Delta t$. A discrete Fourier transform can be used to find a periodic function $x(t)$ with a fundamental period $N\Delta t$ that passes through all of the points. This function can be expressed as a Fourier series in terms of sines and cosines,

$$x(t) = \sum_{n=0}^{n<N/2}\left[a_n\cos\left(\frac{2\pi nt}{N\Delta t}\right) + b_n\sin\left(\frac{2\pi nt}{N\Delta t}\right)\right]. \quad ($$

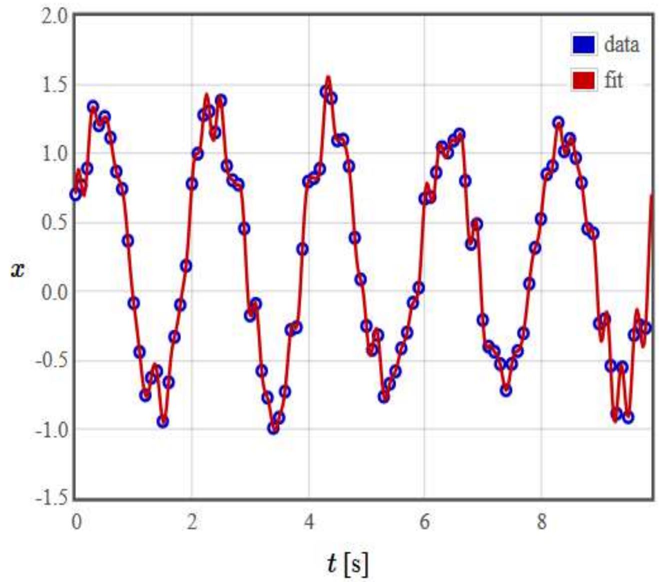
Data for x_n can be input in the textbox below. When the 'Calculate Fourier Coefficients' button is pressed, the periodic function $x(t)$ is plotted through the data points. The Fourier coefficients are tabulated and plotted as well. The fft algorithm first checks if the number of data points is a power-of-two. If so, it calculates the discrete Fourier transform using a Cooley-Tukey decimation-in-time radix-2 algorithm. If the number of data points is not a power-of-two, it uses Bluestein's chirp z-transform algorithm. The fft code was taken from Project Nayuki.

x_n

```
0.704755992151468
0.7702905111005827
0.8931618373710344
1.3406823044010674
1.2059826464418861
1.2675358230469096
1.1156175628382647
0.8703050439010842
0.7442227455673327
0.3681609224807739
-0.08539320011647894
```

$\Delta t =$ 0.1 s

Calculate Fourier Coefficients



http://lampx.tugraz.at/~hadley/num/ch3/3.3a.php

Notations for Fourier Transforms

$$F_{-1,-1}\left(\vec{k}\right) = \frac{1}{(2\pi)^d} \int f(\vec{r}) e^{-i\vec{k}\cdot\vec{r}} d\vec{r}\,.$$

$$f(\vec{r}) = \int F_{-1,-1}\left(\vec{k}\right) e^{i\vec{k}\cdot\vec{r}} d\vec{k}\,.$$

f(*r*) is built of plane waves

$\exp(-\|a\|x)$	$\frac{\|a\|}{\pi(a^2+k^2)}$	$\frac{2\|a\|}{a^2+k^2}$
$\mathrm{sgn}(x)$ $\mathrm{sgn}(x)=-1$ for $x<0$ and $\mathrm{sgn}(x)=1$ for $x>0$	$\frac{-i}{\pi\omega}$	$\frac{-2i}{\omega}$
$\mathrm{sgn}(x)\exp(-\|a\|x)$	$\frac{-ik}{\pi(a^2+k^2)}$	$\frac{-i2k}{a^2+k^2}$
$H(x)\exp(-\|a\|x)$	$\frac{\|a\|-ik}{2\pi(a^2+k^2)}$	$\frac{\|a\|-ik}{a^2+k^2}$
$\sqcap(x)=H\left(x+\frac{1}{2}\right)H\left(\frac{1}{2}-x\right)$ Square pulse: height = 1, width = 1, centered at $x=0$.	$\frac{\sin(k/2)}{\pi k}$	$\frac{2\sin(k/2)}{k}$
$\sqcap\left(\frac{x-x_0}{a}\right)$ Square pulse: height = 1, width = a, centered at x_0.	$\frac{\sin(ka/2)}{\pi k}\exp(-ikx_0)$	$\frac{2\sin(ka/2)}{k}\exp(-ikx_0)$
$\exp\left(i\vec{k}_0\cdot\vec{r}\right)$ Plane wave	$\delta\left(\vec{k}-\vec{k}_0\right)$	$(2\pi)^d\delta\left(\vec{k}-\vec{k}_0\right)$
1	$\delta(k)$	$2\pi\delta(k)$
$\delta(x)$ $\delta\left(\frac{\vec{r}-\vec{r}_0}{a}\right)$	$\frac{1}{2\pi}$ $\left(\frac{a}{2\pi}\right)^d\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$	1 $a^d\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$
$\exp\left(-\frac{\|\vec{r}-\vec{r}_0\|^2}{a^2}\right)$	$\left(\frac{a}{2\sqrt{\pi}}\right)^d\exp\left(-\frac{a^2k^2}{4}\right)\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$	$(a\sqrt{\pi})^d\exp\left(-\frac{a^2k^2}{4}\right)\exp\left(-i\vec{k}\cdot\vec{r}_0\right)$
$H(R-\|\vec{r}-\vec{r}_0\|)$ Disc of radius R centered at $\vec{r}_0$, $\vec{r}\in\mathrm{R}^2$ $H(R-\|\vec{r}-\vec{r}_0\|)$ Sphere of radius R centered at $\vec{r}_0$, $\vec{r}\in\mathrm{R}^3$	$\frac{R}{2\pi\|\vec{k}\|}J_1(\|\vec{k}\|R)\exp(-i\vec{k}\cdot\vec{r}_0)$ $\frac{1}{(2\pi)^3\|\vec{k}\|^3}\left(\sin(\|\vec{k}\|R)-\|\vec{k}\|R\cos(\|\vec{k}\|R)\right)\exp(-i\vec{k}\cdot\vec{r}_0)$	$\frac{2\pi R}{\|\vec{k}\|}J_1(\|\vec{k}\|R)\exp(-i\vec{k}\cdot\vec{r}_0)$ $\frac{4\pi}{\|\vec{k}\|^3}\left(\sin(\|\vec{k}\|R)-\|\vec{k}\|R\cos(\|\vec{k}\|R)\right)\exp(-i\vec{k}\cdot\vec{}$

Here $H(x)$ is the Heaviside step function, $\delta(x)$ is the Dirac delta function, $J_1(x)$ is the first order Bessel function of the first kind, and d is the number of dimensio

Calculate a Fourier transform numerically.

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

Properties of Fourier transforms

Linearity and superposition

$\mathcal{F}\{\alpha f(\vec{r}) + \beta g(\vec{r})\} = \alpha\mathcal{F}\{f(\vec{r})\} + \beta\mathcal{F}\{g(\vec{r})\}$ where α and β are any constants.

Similarity

$\mathcal{F}\{f\left(\frac{\vec{r}}{a}\right)\} = |a|^d\mathcal{F}\{f(\vec{r})\}.$

Shift

$\mathcal{F}\{f(\vec{r} - \vec{r}_0)\} = \mathcal{F}\{f(\vec{r})\}\exp\left(-i\vec{k}\cdot\vec{r}_0\right).$

Convolution (Faltung)

$$f(\vec{r}) * g(\vec{r}) = \int f(\vec{r}')g(\vec{r}-\vec{r}')d\vec{r}$$

Notation [-1,-1]: $\mathcal{F}\{fg\} = \mathcal{F}\{f\} * \mathcal{F}\{g\}, \quad \mathcal{F}^{-1}\{FG\} = \frac{1}{2\pi}\mathcal{F}^{-1}\{F\} * \mathcal{F}^{-1}\{G\}.$

Notation [1,-1]: $\mathcal{F}\{fg\} = \frac{1}{2\pi}\mathcal{F}\{f\} * \mathcal{F}\{g\}, \quad \mathcal{F}^{-1}\{FG\} = \mathcal{F}^{-1}\{F\} * \mathcal{F}^{-1}\{G\}.$

Notation [0,-1]: $\mathcal{F}\{fg\} = \frac{1}{\sqrt{2\pi}}\mathcal{F}\{f\} * \mathcal{F}\{g\}, \quad \mathcal{F}^{-1}\{FG\} = \frac{1}{\sqrt{2\pi}}\mathcal{F}^{-1}\{F\} * \mathcal{F}^{-1}\{G\}.$

Notation [0,-2π]: $\mathcal{F}\{fg\} = \mathcal{F}\{f\} * \mathcal{F}\{g\}, \quad \mathcal{F}^{-1}\{FG\} = \mathcal{F}^{-1}\{F\} * \mathcal{F}^{-1}\{G\}.$

Impulse response function (Green's functions)

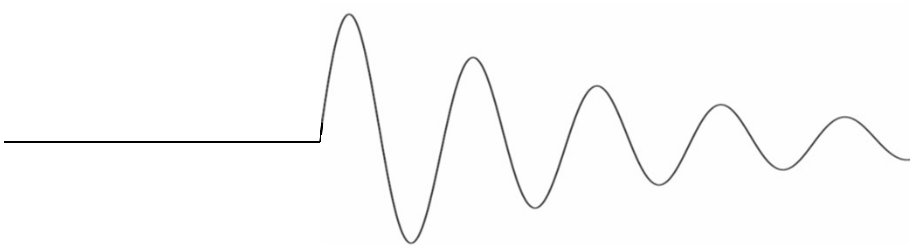
A Green's function is the solution to a linear differential equation for a δ-function driving force

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.

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

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

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

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

has the solution

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

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

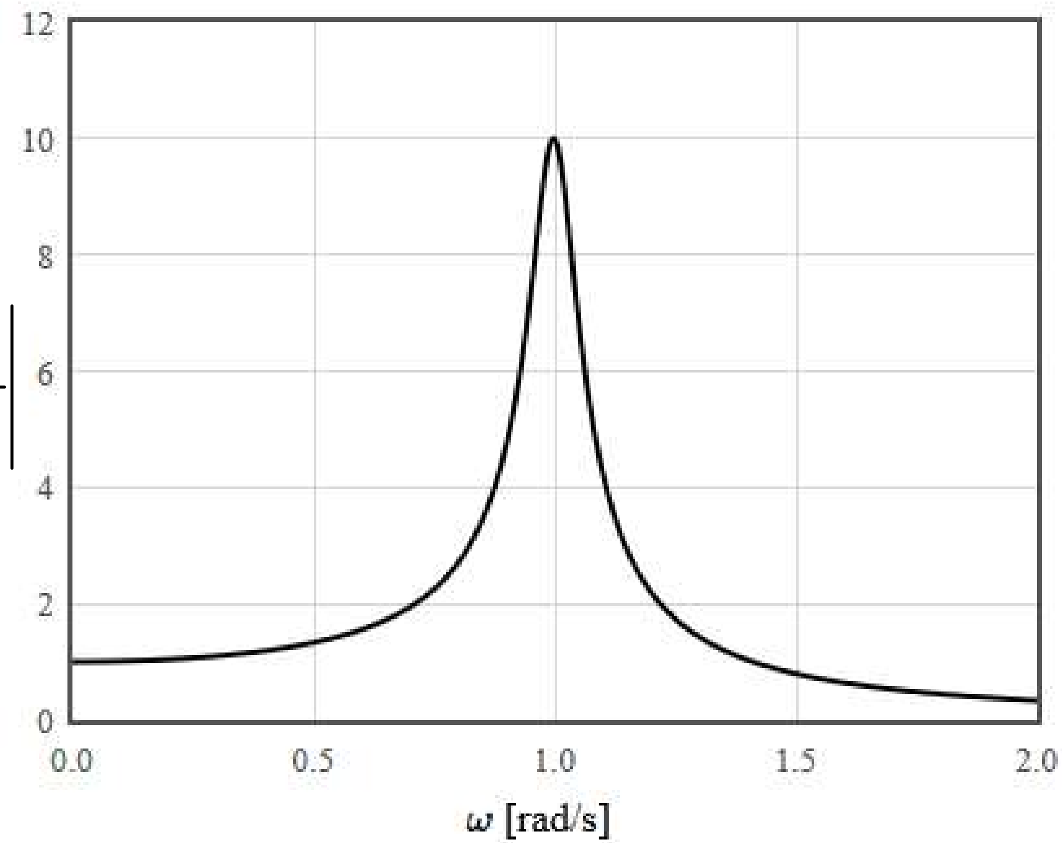
$$\chi(\omega) = \frac{u}{f} = \frac{\int g(t-t')e^{i\omega t'}dt'}{e^{i\omega t}}$$

Generalized susceptibility

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

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

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



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

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.

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

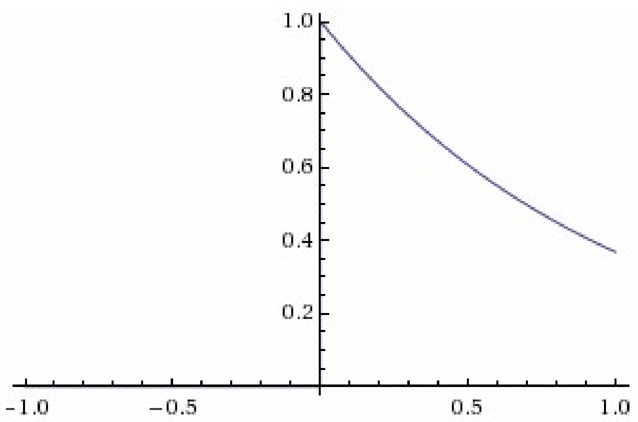
First order differential equation

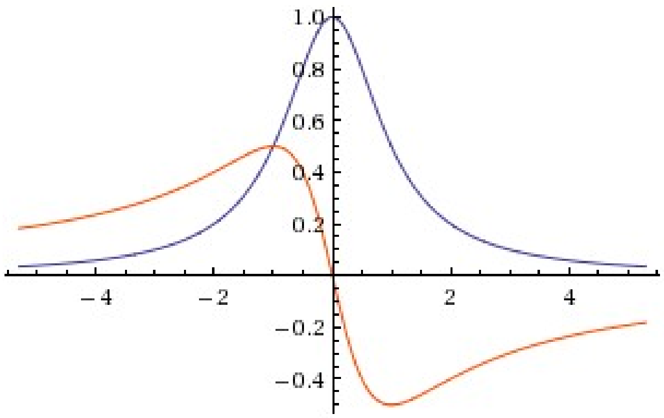
$$m\frac{dg}{dt} + bg = \delta(t)$$

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

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

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





The Fourier transform of a decaying exponential is a Lorentzian

Susceptibility

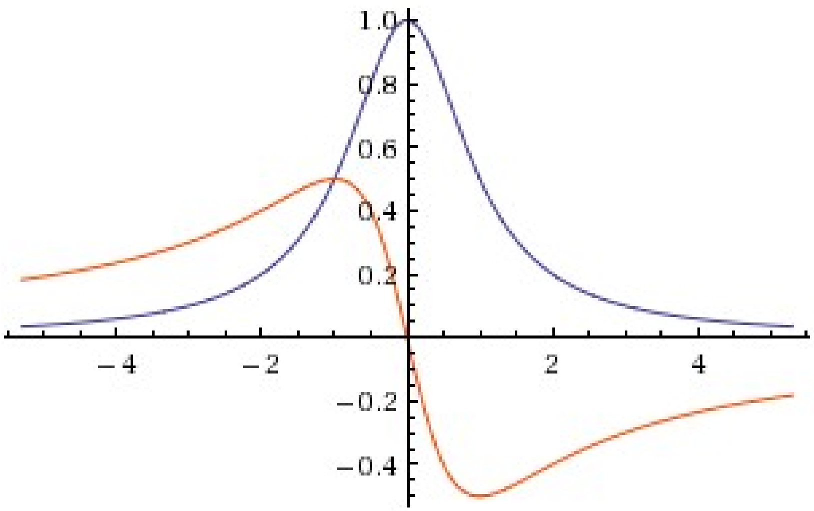
$$m\frac{du}{dt} + bu = F(t)$$

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

$$i\omega m A + bA = F_0$$

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

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



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

Susceptibility

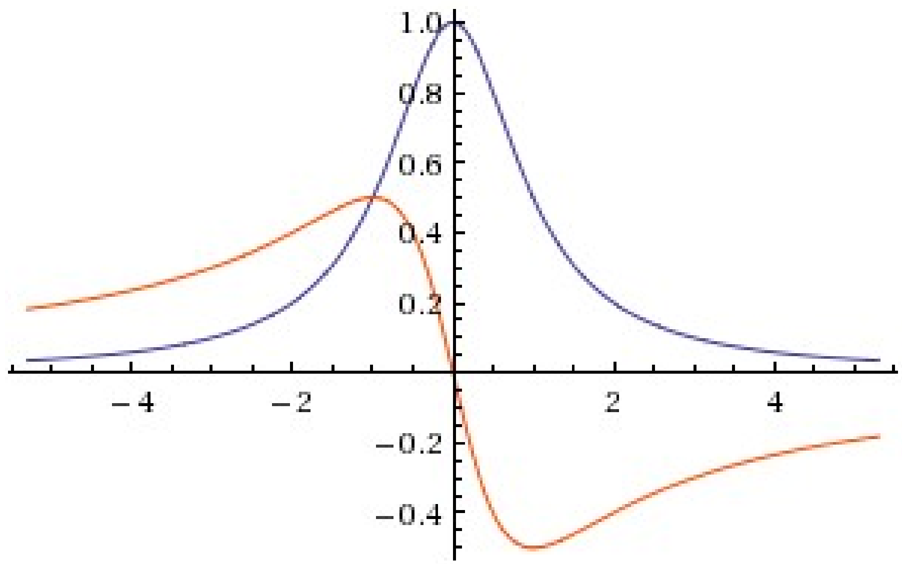
$$m\frac{dg}{dt} + bg = \delta(t)$$

Fourier transform the differential equation

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

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

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

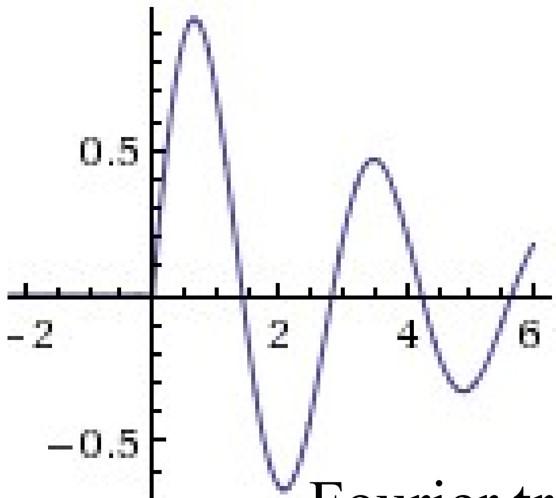


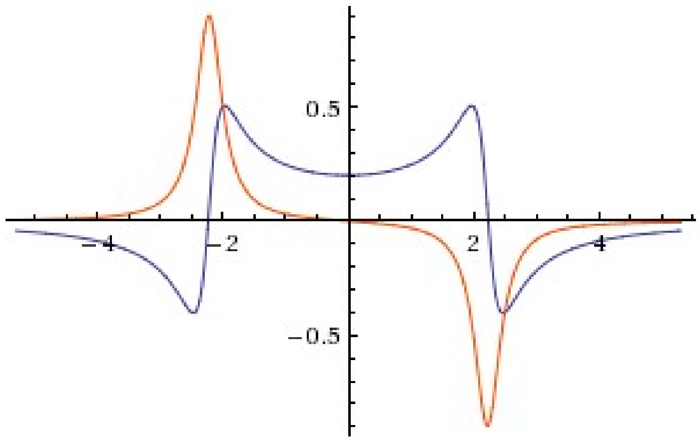
Damped mass-spring system

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

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

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





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

Fourier transform pair

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

More complex linear systems

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

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

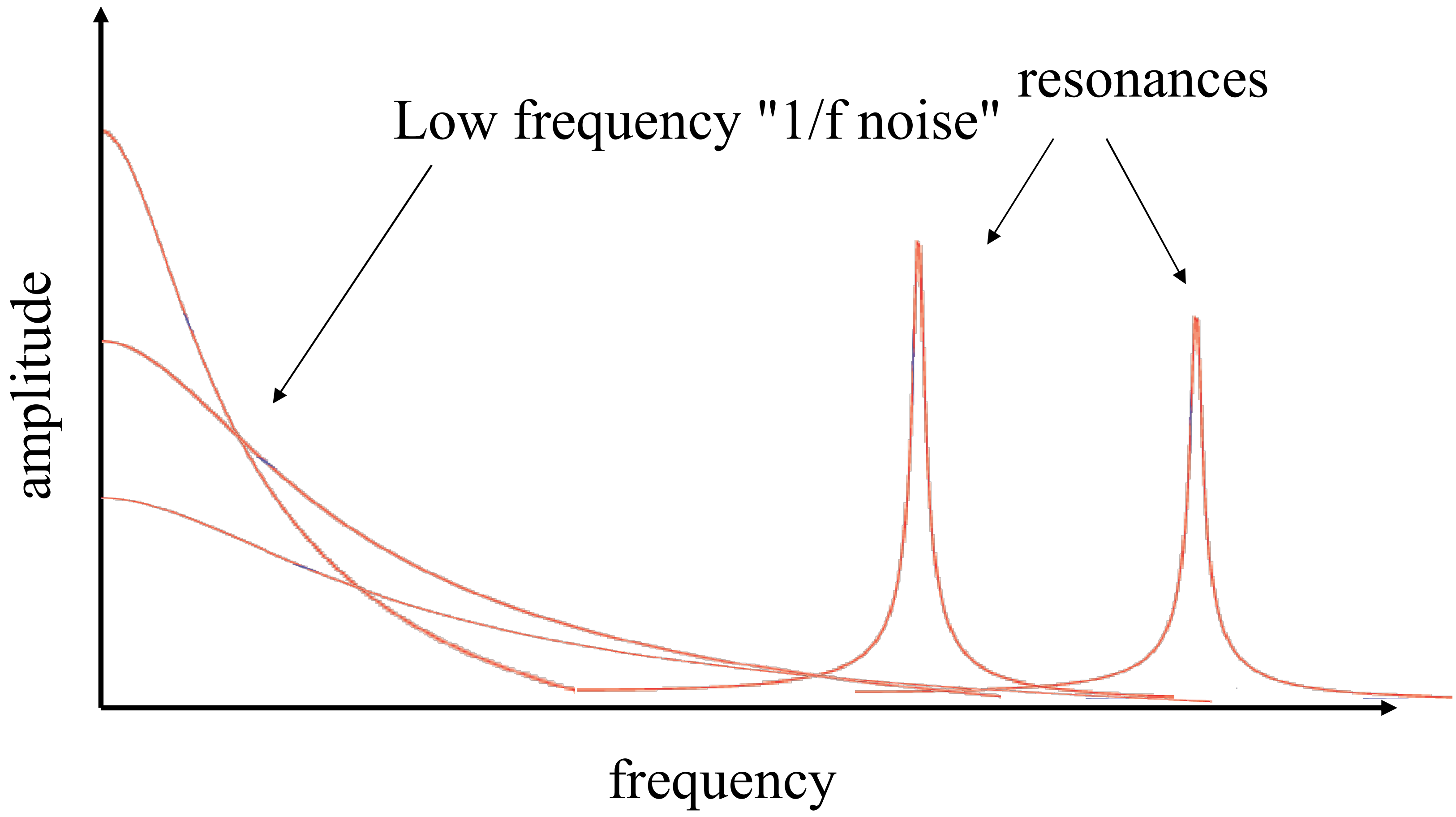
The solutions have the form $\vec{x}_i e^{\lambda_i t}$

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

$\mathrm{Re}(\lambda_i) < 0$ for stable systems

λ_i 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

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

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

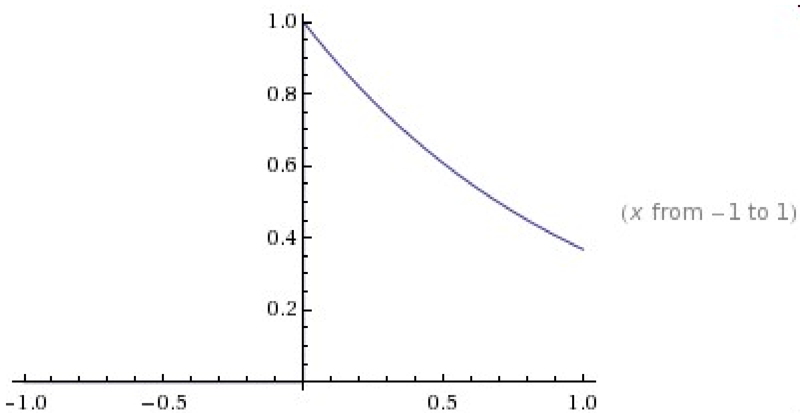
$$f(t) = \mathrm{E}(t) + O(t)$$

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

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

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

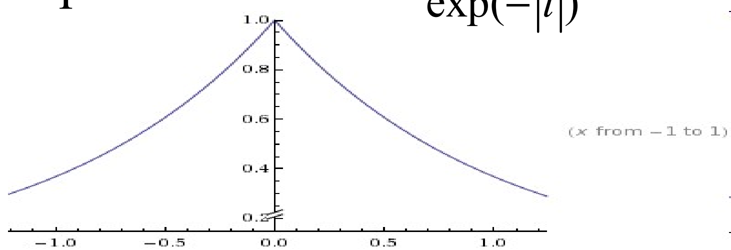
The Fourier transform of $E(t)$ is real and even
The Fourier transform of $O(t)$ is imaginary and odd

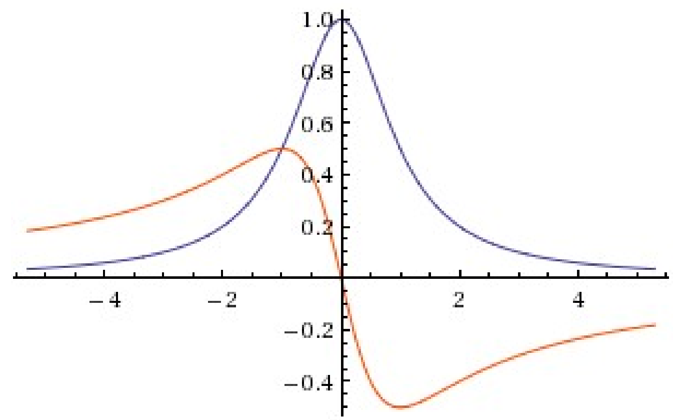


$$\chi(\omega) = \frac{1}{m}\frac{\frac{b}{m} - i\omega}{\left(\frac{b}{m}\right)^2 + \omega^2}$$

even component

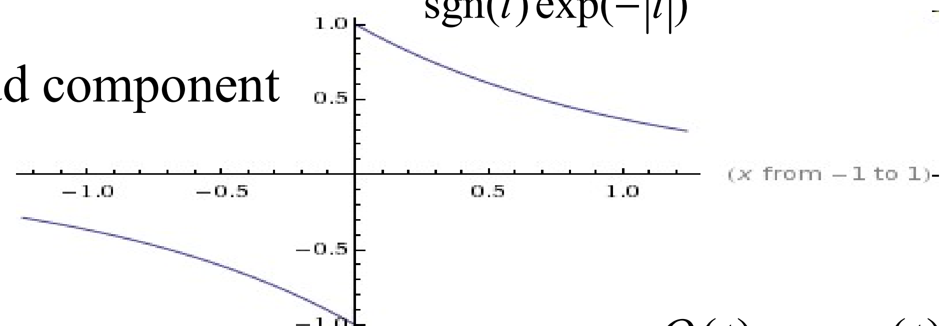
$$\exp(-|t|)$$





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

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.

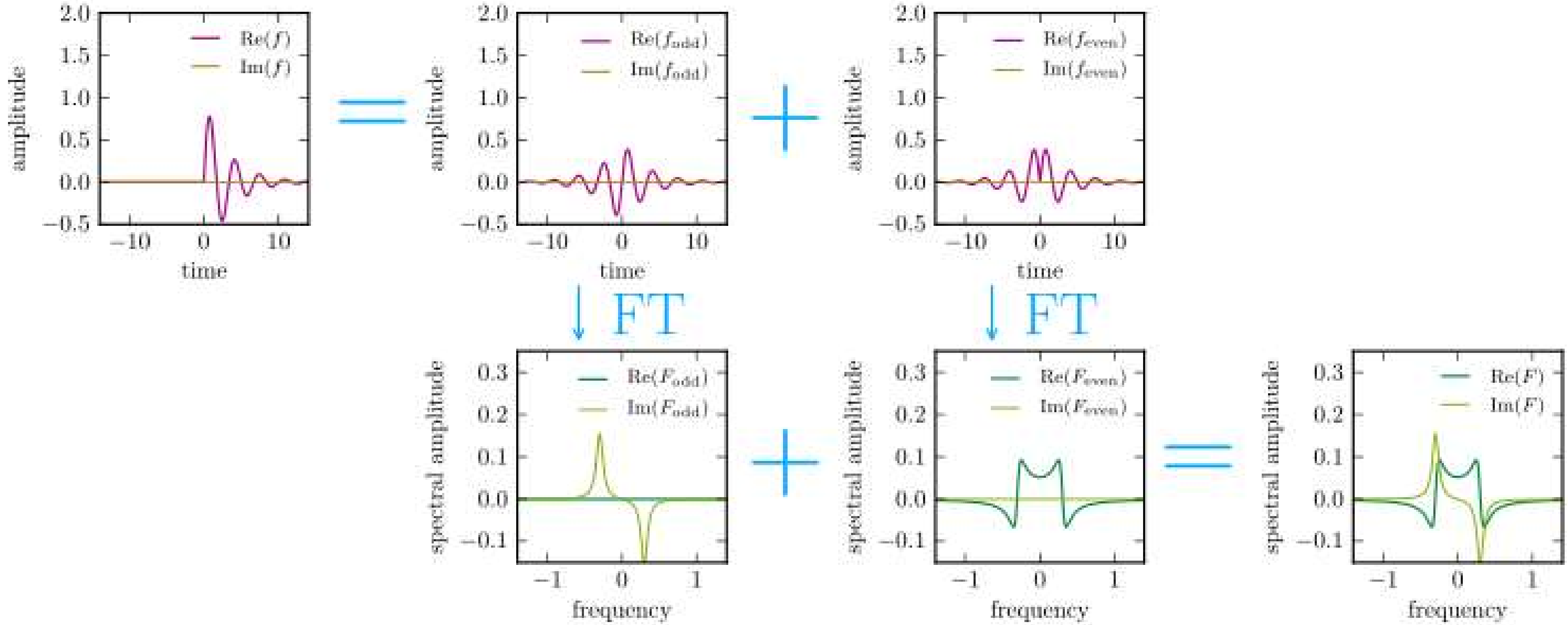
If you know χ', inverse Fourier transform to find $E(t)$. Knowing $E(t)$ you can determine $O(t) = \mathrm{sgn}(t)E(t)$. Fourier transform $O(t)$ to find χ''.

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

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

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

Kramers-Kronig relations



If you know any of these for just positive frequencies,
you can calculate all the others.

https://en.wikipedia.org/wiki/Kramers%E2%80%93Kronig_relations

Causality and the Kramers-Kronig relation (II)

Real space	Reciprocal space
$E(t) = \text{sgn}(t) O(t)$ $O(t) = \text{sgn}(t) E(t)$	$\chi'(\omega) = -\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi''(\omega')}{\omega' - \omega} d\omega'$ $\chi''(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi'(\omega')}{\omega' - \omega} d\omega'$

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

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.

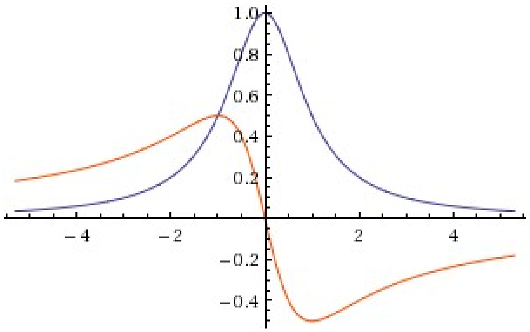
http://lamp.tu-graz.ac.at/~hadley/ss2/linearresponse/causality.php

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)

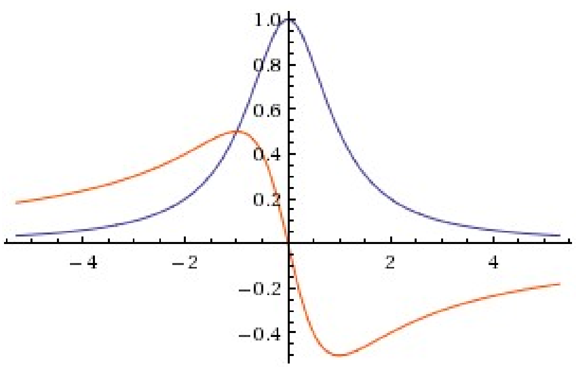
Kramers-Kronig relations (III)

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

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

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

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



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.

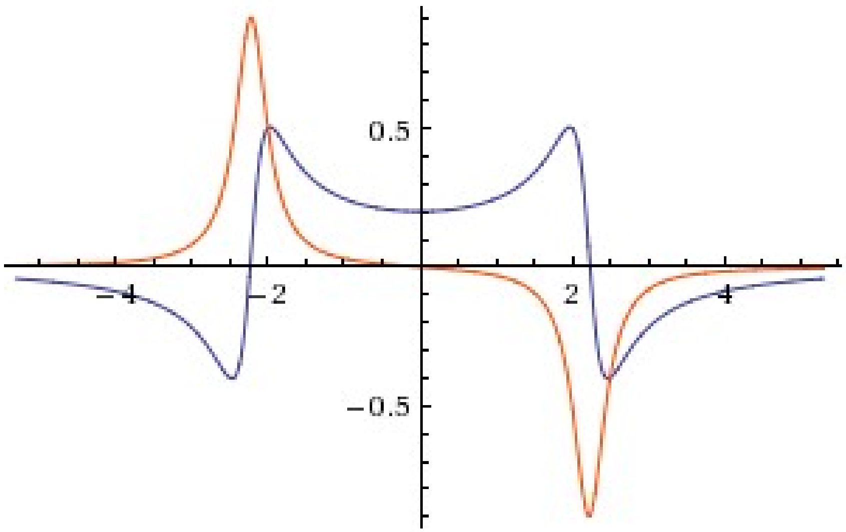
Any function that is zero before the excitation and nonzero afterwards must have both an odd component and an even component.

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.

Fluctuation-dissipation theorem

The fluctuation-dissipation theorem relates the size of the fluctuations to the dissipation in a system.

Most of the dissipation in a resonant system occurs at frequencies near the resonance.



http://en.wikipedia.org/wiki/Fluctuation_dissipation_theorem

Fluctuation-dissipation theorem

Brownian motion: The response to thermal noise is related to the viscosity.

$$m\frac{dv}{dt} = -\mu v \qquad\qquad D = \mu k_B T$$

Johnson noise: The voltage fluctuations are related to the resistance.

$$V_{rms} = \sqrt{4k_B TRB}$$

The fluctuation-dissipation theorem holds at equilibrium (where the equations are linear to a good approximation).

http://en.wikipedia.org/wiki/Fluctuation_dissipation_theorem