

Technische Universität Graz

Institute of Solid State Physics

17. Superconductivity/ Linear Response

Dec. 2, 2019

Vortices in Superconductors



Defects are used to pin the vortices

Superconducting Magnets





Whole body MRI

Magnets and cables





Maglev trains

ITER



Superconducting magnets



Largest superconducting magnet, CERN 21000 Amps

ac - Josephson effect



http://www.nist.gov/pml/history-volt/superconductivity_2000s.cfm

SQUID

Superconducting quantum interference device



Sensitive detectors

 $10^{-6} \Phi_0 / (Hz)^{1/2}$

10⁻²⁰ m/ (Hz)^{1/2}



Gravity wave detector



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Linear Response Theory





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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



Outline

Introduction Linear

Interpolation Numerical

Equations

Solutions Computer Measurement

Numerical Methods

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,

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

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.



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

$$F_{-1,-1}\left(ec{k}
ight) = rac{1}{\left(2\pi
ight)^d}\int f(ec{r})e^{-iec{k}\cdotec{r}}\,dec{r}\,.$$

$$fig(ec{r}ig) = \int F_{-1,-1}\left(ec{k}
ight) e^{iec{k}\cdotec{r}}dec{k}.$$

f(r) is built of plane waves

$\exp\bigl(- a x\bigr)$	$rac{ a }{\pi(a^2+k^2)}$	$rac{2 a }{a^2+k^2}$
${\mathop{\mathrm{sgn}} olimits(x) = -1 ext{ for } x < 0 ext{ and } \ {\mathop{\mathrm{sgn}} olimits(x) = 1 ext{ for } x > 0}$	$\frac{-i}{\pi\omega}$	$\frac{-2i}{\omega}$
$\mathrm{sgn}ig(x)\expig(- a xig)$	$rac{-ik}{\pi(a^2+k^2)}$	$rac{-i2k}{a^2+k^2}$
$Hig(x)\expig(- a xig)$	$rac{ a -ik}{2\pi ig(a^2+k^2ig)}$	$\frac{ a {-}ik}{a^2{+}k^2}$
$\Box(x) = H\left(x + \frac{1}{2}\right)H\left(\frac{1}{2} - x\right)$ Square pulse: height = 1, width = 1, centered at $x = 0$.	$rac{\sin(k/2)}{\pi k}$	$rac{2\sin(k/2)}{k}$
$\Box\left(\frac{x-x_0}{a}\right)$ Square pulse: height = 1, width = a, centered at x_0 .	$rac{\sin(ka/2)}{\pi k}\exp(-ikx_0)$	$rac{2\sin(ka/2)}{k}\expig(-ikx_0ig)$
$\exp\!\left(iec{k}_0\cdotec{r} ight)$ Plane wave	$\delta\!\left(ec{m k}-ec{m k}_0 ight)$	$ig(2\piig)^d\deltaig(ec k-ec k_0ig)$
1	$\delta(k)$	$2\pi\delta(k)$
$\delta(x)$	$\frac{1}{2\pi}$	1
$\delta\!\left(rac{ec{r}-ec{r}_0}{a} ight)$	$\left(rac{a}{2\pi} ight)^d \exp\!\left(-iec{k}\cdotec{r}_0 ight)$	$a^d \exp \Bigl(-i ec{k} \cdot ec{r}_0 \Bigr)$
$\exp\!\left(-rac{ert ec r - ec r_0 ert^2}{a^2} ight)$	$\left(rac{a}{2\sqrt{\pi}} ight)^d \exp\!\left(-rac{a^2k^2}{4} ight) \exp\!\left(-iec{k}\cdotec{r}_0 ight)$	$ig(a\sqrt{\pi}ig)^d \expig(-rac{a^2k^2}{4}ig) \expig(-iec{k}\cdotec{r}_0ig)$
$H(R-ert ec r-ec r_0ert))$ Disc of radius R centered at $ec r_0, ec r\in { m R}^2$	$rac{R}{2\pi ec{k}ec{l}} J_1(ec{k}ec{R}) \exp(-ec{k}\cdotec{r}_0)$	$rac{2\pi R}{ec{k}ec{ec{k}}ec{ec{k}}ec{ec{k}}ec{ec{k}}ec{ec{k}}ec{ec{r}_0})$
$H(R-ert ec r-ec r_0ert)$ Sphere of radius R centered at $ec r_0,$ $ec r\in \mathrm{R}^3$	$rac{1}{(2\pi)^3 ec k ^3}\left(\sin(ec k R)- ec k R\cos(ec k R) ight)\exp(-iec k\cdotec r_0)$	$igg rac{4\pi}{ert ec kert^3} \left(\sin(ec kert R) - ec kert R \cos(ec kert R) ight) \exp(-ec kec kert$

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

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

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

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

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

has the solution

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

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

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

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.

First order differential equation



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 $u = Ae^{i\omega t}$ $F = F_0 e^{i\omega t}$



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



Damped mass-spring system

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*.

 $\operatorname{Re}(\lambda_i) < 0$ 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



frequency

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

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

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

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

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



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) = sgn(t)E(t). Fourier transform O(t) to find χ'' .

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

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 E(t) = sgn(t)O(t)O(t) = sgn(t)E(t)

Reciprocal space

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

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



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.