# 17. Superconductivity / Linear Response 

Dec. 2, 2019

## Vortices in Superconductors

Lorentz force

$$
\begin{gathered}
\vec{F}=q(\vec{E}+\vec{v} \times \vec{B}) \\
\vec{j}=n q \vec{v}
\end{gathered}
$$

Faraday's law

$$
\vec{F}=\frac{1}{n} \vec{j} \times \vec{B}
$$

$$
\frac{\uparrow \quad \vec{j}}{\text { exysing }}
$$

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




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10 V standard

## SQUID

Superconducting quantum interference device

$10^{-6} \Phi_{0} /(\mathrm{Hz})^{1 / 2}$
$10^{-20} \mathrm{~m} /(\mathrm{Hz})^{1 / 2}$


Sensitive detectors
Gravity wave detector

[^0]
## 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

## Numerical Methods

Outline
Introduction
Linear
Equations
Interpolation
Numerical
Solutions
Computer Measurement

## Fourier analysis of real data sets

Consider a series of $N$ measurements $x_{n}$ that are made at equally spaced time intervals $\Delta t$. 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,

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

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

## Notations for Fourier Transforms

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

$f(r)$ is built of plane waves

| $\exp (-\|a\| x)$ | $\frac{\|a\|}{\pi\left(a^{2}+k^{2}\right)}$ | $\frac{2\|a\|}{a^{2}+k^{2}}$ |
| :---: | :---: | :---: |
| $\begin{gathered} \operatorname{sgn}(x) \\ \operatorname{sgn}(x)=-1 \text { for } x<0 \text { and } \\ \operatorname{sgn}(x)=1 \text { for } x>0 \end{gathered}$ | $\frac{-i}{\pi \omega}$ | $\frac{-2 i}{\omega}$ |
| $\operatorname{sgn}(x) \exp (-\|a\| x)$ | $\frac{-i k}{\pi\left(a^{2}+k^{2}\right)}$ | $\frac{-i 2 k}{a^{2}+k^{2}}$ |
| $H(x) \exp (-\|a\| x)$ | $\frac{\|a\|-i k}{2 \pi\left(a^{2}+k^{2}\right)}$ | $\frac{\|a\|-i k}{a^{2}+k^{2}}$ |
| $\sqcap(x)=H\left(x+\frac{1}{2}\right) H\left(\frac{1}{2}-x\right)$ <br> Square pulse: height $=1$, width $=1$, centered at $\boldsymbol{x}=\mathbf{0}$. | $\frac{\sin (k / 2)}{\pi k}$ | $\frac{2 \sin (k / 2)}{k}$ |
| $\begin{gathered} \quad \sqcap\left(\frac{x-x_{0}}{a}\right) \\ \text { Square pulse: height }=1, \text { width }=a, \\ \text { centered at } x_{0} . \end{gathered}$ | $\frac{\sin (k a / 2)}{\pi k} \exp \left(-i k x_{0}\right)$ | $\frac{2 \sin (k a / 2)}{k} \exp \left(-i k x_{0}\right)$ |
| $\underset{\text { Plane wave }}{\exp \left(i \vec{k}_{0} \cdot \vec{r}\right)}$ | $\delta\left(\vec{k}-\vec{k}_{0}\right)$ | $(2 \pi)^{d} \delta\left(\vec{k}-\vec{k}_{0}\right)$ |
| 1 | $\delta(k)$ | $2 \pi \delta(k)$ |
| $\begin{gathered} \delta(x) \\ \delta\left(\frac{\vec{r}-\vec{r}_{0}}{a}\right) \end{gathered}$ | $\left(\frac{a}{2 \pi}\right)^{d} \exp \left(-i \vec{k} \cdot \vec{r}_{0}\right)$ | $\begin{gathered} 1 \\ a^{d} \exp \left(-i \vec{k} \cdot \vec{r}_{0}\right) \end{gathered}$ |
| $\exp \left(-\frac{\left\|\vec{r}-\vec{r}_{0}\right\|^{2}}{a^{2}}\right)$ | $\left(\frac{a}{2 \sqrt{\pi}}\right)^{d} \exp \left(-\frac{a^{2} k^{2}}{4}\right) \exp \left(-i \vec{k} \cdot \vec{r}_{0}\right)$ | $(a \sqrt{\pi})^{d} \exp \left(-\frac{a^{2} k^{2}}{4}\right) \exp \left(-i \vec{k} \cdot \vec{r}_{0}\right)$ |
| $H\left(R-\left\|\vec{r}-\vec{r}_{0}\right\|\right)$ Disc of radius $R$ centered at $\vec{r}_{0}, \vec{r} \in \mathrm{R}^{2}$ $H\left(R-\left\|\vec{r}-\vec{r}_{0}\right\|\right)$ Sphere of radius $R$ centered at $\vec{r}_{0}$, $\vec{r} \in \mathrm{R}^{3}$ | $\begin{gathered} \frac{R}{2 \pi\|\vec{k}\|} J_{1}(\|\vec{k}\| R) \exp \left(-i \vec{k} \cdot \vec{r}_{0}\right) \\ \frac{1}{(2 \pi)^{3}\|\vec{k}\|^{3}}(\sin (\|\vec{k}\| R)-\|\vec{k}\| R \cos (\|\vec{k}\| R)) \exp \left(-i \vec{k} \cdot \vec{r}_{0}\right) \end{gathered}$ | $\begin{gathered} \frac{2 \pi R}{\|\vec{k}\|} J_{1}(\|\vec{k}\| R) \exp \left(-i \vec{k} \cdot \vec{r}_{0}\right) \\ \frac{4 \pi}{\|\vec{k}\|^{3}}(\sin (\|\vec{k}\| R)-\|\vec{k}\| R \cos (\|\vec{k}\| R)) \exp (-i \vec{k} \cdot i \end{gathered}$ |

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 $\alpha$ and $\beta$ are any constants.

Similarity
$\mathcal{F}\left\{f\left(\frac{\vec{r}}{a}\right)\right\}=|a|^{d} \mathcal{F}\{f(\vec{r})\}$.
Shift
$\mathcal{F}\left\{f\left(\vec{r}-\vec{r}_{0}\right)\right\}=\mathcal{F}\{f(\vec{r})\} \exp \left(-i \vec{k} \cdot \vec{r}_{0}\right)$.

## Convolution (Faltung)

$$
f(\vec{r}) * g(\vec{r})=\int f\left(\vec{r}^{\prime}\right) g\left(\vec{r}-\vec{r}^{\prime}\right) d \vec{r}
$$

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

## Impulse response function (Green's functions)

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

For instance,

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

has the solution

$$
\begin{gathered}
g(t)=\frac{1}{m} \exp \left(\frac{-b t}{2 m}\right) \sin \left(\frac{\sqrt{4 m k-b^{2}}}{2 m} t\right) t>0
\end{gathered}
$$

## Green's functions

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

$$
f(t)=\int \delta\left(t-t^{\prime}\right) f\left(t^{\prime}\right) d t^{\prime}
$$

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

$$
u(t)=\int g\left(t-t^{\prime}\right) f\left(t^{\prime}\right) d t^{\prime}
$$

For instance, $\quad m \frac{d^{2} u}{d t^{2}}+b \frac{d u}{d t}+k u=f(t)$
has the solution

$$
u(t)=\int_{-\infty}^{\infty} \frac{1}{m} \exp \left(\frac{-b\left(t-t^{\prime}\right)}{2 m}\right) \sin \left(\frac{\sqrt{4 m k-b^{2}}}{2 m}\left(t-t^{\prime}\right)\right) f\left(t^{\prime}\right) d t^{\prime}
$$

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.

$$
u(t)=\int g\left(t-t^{\prime}\right) f\left(t^{\prime}\right) d t^{\prime}=\int g\left(t-t^{\prime}\right) F_{0} e^{i \omega t^{\prime}} d t^{\prime}
$$

The generalized susceptibility at frequency $\omega$ is

$$
\chi(\omega)=\frac{u}{f}=\frac{\int g\left(t-t^{\prime}\right) e^{i \omega t^{\prime}} d t^{\prime}}{e^{i \omega t}}
$$

## Generalized susceptibility

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

$$
\begin{aligned}
& m=1 {[\mathrm{~kg}] \quad b=} \\
&\left.\begin{array}{ll}
0.1 & {[\mathrm{~N} \mathrm{~s} / \mathrm{m}] \quad k=1} \\
& Q=\frac{\sqrt{m k}}{b}=10
\end{array}\right][\mathrm{N} / \mathrm{m}] \\
&
\end{aligned}
$$



## Generalized susceptibility

$$
\chi(\omega)=\frac{u}{f}=\frac{\int g\left(t-t^{\prime}\right) e^{i \omega t^{\prime}} d t^{\prime}}{e^{i \omega t}}
$$

Since the integral is over $t^{\prime}$, the factor with $t$ can be put in the integral.

$$
\chi(\omega)=\int g\left(t-t^{\prime}\right) e^{-i \omega\left(t-t^{\prime}\right)} d t^{\prime}
$$

Change variables to $\tau=t-t^{\prime}, d \tau=-d t^{\prime}$, 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.

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

## First order differential equation

$$
\begin{gathered}
m \frac{d g}{d t}+b g=\delta(t) \\
g(t)=\frac{1}{m} H(t) \exp \left(-\frac{b t}{m}\right) \quad \frac{b}{m}>0
\end{gathered}
$$

$$
\begin{gathered}
\chi(\omega)=\int g(t) e^{-i \omega t} d t \\
\chi(\omega)=\frac{1}{m} \frac{\frac{b}{m}-i \omega}{\left(\frac{b}{m}\right)^{2}+\omega^{2}}
\end{gathered}
$$




The Fourier transform of a decaying exponential is a Lorentzian

## Susceptibility

$$
m \frac{d u}{d t}+b u=F(t)
$$

Assume that $u$ and $F$ are sinusoidal $\quad u=A e^{i \omega t} \quad F=F_{0} e^{i o t}$

$$
\begin{gathered}
i \omega m A+b A=F_{0} \\
A=\frac{F_{0}}{b+i \omega m}=F_{0} \frac{b-i \omega m}{b^{2}+m^{2} \omega^{2}} \\
\chi=\frac{u}{F}=\frac{1}{m} \frac{\frac{b}{m}-i \omega}{\left(\frac{b}{m}\right)^{2}+\omega^{2}}
\end{gathered}
$$



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

## Susceptibility

$$
m \frac{d g}{d t}+b g=\delta(t)
$$

Fourier transform the differential equation

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



## Damped mass-spring system

$$
\begin{gathered}
m \frac{d^{2} g}{d t^{2}}+b \frac{d g}{d t}+k g=\delta(t) \quad-\omega^{2} m \chi+i \omega b \chi+k \chi=1 \\
g=e^{\lambda t} \quad \lambda_{ \pm}=\frac{-b \pm \sqrt{b^{2}-4 m k}}{2 m} \\
g(t)=H(t) \frac{1}{m} \exp \left(\frac{-b t}{2 m}\right) \sin \left(\frac{\sqrt{4 m k-b^{2}}}{2 m} t\right)
\end{gathered}
$$

## More complex linear systems

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

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

The solutions have the form $\vec{x}_{i} e^{\lambda_{i} t}$
where $\vec{x}_{i}$ are the eigenvectors and $\lambda_{i}$ are the eigenvalues of matrix $M$.
$\operatorname{Re}\left(\lambda_{i}\right)<0$ for stable systems
$\lambda_{i}$ 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

$$
\begin{gathered}
E(t)=1 / 2[f(t)+f(-t)] \\
O(t)=1 / 2[f(t)-f(-t)] \\
f(t)=\mathrm{E}(t)+O(t) \\
f(t)=1 / 2[f(t)+f(-t)]+1 / 2[f(t)-f(-t)] \\
\int_{-\infty}^{\infty} f(t) e^{-i \omega t} d t=\int_{-\infty}^{\infty}(E(t)+O(t))(\cos \omega t-i \sin \omega t) d t \\
=\int_{-\infty}^{\infty} E(t) \cos \omega t d t-i \int_{-\infty}^{\infty} O(t) \sin \omega t d t
\end{gathered}
$$

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

( $x$ from -1 to 1 )
even component


$$
\begin{aligned}
& \text { odd component } \\
& \hdashline O(t)=\operatorname{sgn}(t) E(t) \\
& E(t)=\operatorname{sgn}(t) O(t)
\end{aligned}
$$

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

## Causality and the Kramers-Kronig relations (I)

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

The real and imaginary parts of the susceptibility are related.
If you know $\chi^{\prime}$, inverse Fourier transform to find $E(t)$. Knowing $E(t)$ you can determine $O(t)=\operatorname{sgn}(t) E(t)$. Fourier transform $O(t)$ to find $\chi^{\prime \prime}$.

$$
\begin{array}{r}
\chi^{\prime}(\omega)=\int_{-\infty}^{\infty} E(t) \cos (\omega t) d t \quad E(t)=\frac{1}{2 \pi} \int_{-\infty}^{\infty} \chi^{\prime}(\omega) \cos (\omega t) d \omega \\
O(t)=\operatorname{sgn}(t) E(t) \quad E(t)=\operatorname{sgn}(t) O(t) \\
\chi^{\prime \prime}(\omega)=-\int_{-\infty}^{\infty} O(t) \sin (\omega t) d t \quad O(t)=\frac{-1}{2 \pi} \int_{-\infty}^{\infty} \chi^{\prime \prime}(\omega) \sin (\omega t) d \omega
\end{array}
$$

## 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\�\�\�Kronig_relations

## Causality and the Kramers-Kronig relation (II)

Real space

| $E(t)=\operatorname{sgn}(t) O(t)$ |
| :---: |
| $O(t)=\operatorname{sgn}(t) E(t)$ |

$$
\xrightarrow{\square} \chi^{\prime}=\frac{-i}{\pi \omega} * i \chi^{\prime \prime}, \quad i \chi^{\prime \prime}=\frac{-i}{\pi \omega} * \chi^{\prime}
$$

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)

$$
\begin{gathered}
\chi^{\prime \prime}(\omega)=\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi^{\prime}\left(\omega^{\prime}\right)}{\omega^{\prime}-\omega} d \omega^{\prime} \\
\chi^{\prime}(\omega)=-\frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\chi^{\prime \prime}\left(\omega^{\prime}\right)}{\omega^{\prime}-\omega} d \omega^{\prime}
\end{gathered}
$$

Kramers-Kronig relations II


$$
\begin{aligned}
& \chi^{\prime}(\omega)=\chi^{\prime}(-\omega) \\
& \chi^{\prime \prime}(\omega)=-\chi^{\prime \prime}(-\omega)
\end{aligned}
$$

Real part is even Imaginary part is odd

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

change variables $\omega^{\prime} \rightarrow-\omega^{\prime}$
(4 minus signs)

## Kramers-Kronig relations (III)

$$
\begin{gathered}
\chi^{\prime}(\omega)=-\frac{1}{\pi} P \int_{0}^{\infty} \frac{\chi^{\prime \prime}\left(\omega^{\prime}\right)}{\omega^{\prime}+\omega} d \omega^{\prime}-\frac{1}{\pi} P \int_{0}^{\infty} \frac{\chi^{\prime \prime}\left(\omega^{\prime}\right)}{\omega^{\prime}-\omega} d \omega^{\prime} \\
\frac{1}{\omega^{\prime}+\omega}+\frac{1}{\omega^{\prime}-\omega}=\frac{2 \omega^{\prime}}{\left(\omega^{\prime}\right)^{2}-\omega^{2}} \\
\chi^{\prime}(\omega)=\frac{2}{\pi} P \int_{0}^{\infty} \frac{\omega^{\prime} \chi^{\prime \prime}\left(\omega^{\prime}\right)}{\left(\omega^{\prime}\right)^{2}-\omega^{2}} d \omega^{\prime} \\
\chi^{\prime \prime}(\omega)=-\frac{2}{\pi} P \int_{0}^{\infty} \frac{\omega^{\prime}\left(\chi^{\prime}\right)}{\left(\omega^{\prime}\right)^{2}-\omega^{2}} d \omega^{\prime} \\
\text { Singularity is stronger in this form. }
\end{gathered}
$$


[^0]:    Technische Universität Graz

