# Linear response theory



### 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  $\chi'$ , 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  $\chi''$ .

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

### 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.

# 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

# Impulse response/generalized susceptibility

The impulse response function is the response of the system to a  $\delta$ -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

### Dielectric response of insulators

The electric polarization is related to the electric field

$$P_i = \varepsilon_0 \chi_{ij} E_j$$

The electric displacement vector *D* is also related to the electric field

$$D_{i} = P_{i} + \varepsilon_{0}E_{i} = \varepsilon_{0}(1 + \chi_{ij})E_{j} = \varepsilon_{0}\varepsilon_{ij}E_{j}$$

$$\mathcal{E}_{ij} = (1 + \chi_{ij})$$



*E* is decreased by a factor of the dielectric constant

### Dielectric response of insulators

In an insulator, charge is bound. The response to an electric field can be modeled as a collection of damped harmonic oscillators



The core electrons of a metal respond to an electric field like this too.

### Dielectric response of insulators

The differential equation that describes how the position of the charge changes in time is:

$$m\frac{d^{2}x}{dt^{2}} + b\frac{dx}{dt} + kx = -eE(t)$$

The impulse response function is:

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

### Electric susceptibility

$$\vec{P} = \varepsilon_0 \chi_E \vec{E} \qquad \vec{P} = nq\vec{x}$$
$$\chi_E = \frac{P}{\varepsilon_0 E} = \frac{nqx}{\varepsilon_0 E}$$

Assume a solution of the form  $x(\omega)e^{i\omega t}$ ,  $E(\omega)e^{i\omega t}$ 

$$m\frac{d^2x}{dt^2} + b\frac{dx}{dt} + kx = qE(t)$$

$$\frac{d^2x}{dt^2} + \gamma \, \frac{dx}{dt} + \omega_0^2 x = - \frac{qE}{m}$$
$$\omega_0 = \sqrt{\frac{k}{m}} \qquad \gamma = \frac{b}{m}$$

# Electric susceptibility

$$\chi_{E}(\omega) = \frac{n_{\omega_{0}}q^{2}}{\varepsilon_{0}m} \frac{1}{\omega_{0}^{2} - \omega^{2} + i\gamma\omega}$$



#### Resonance of a damped driven harmonic oscillator



http://lamp.tu-graz.ac.at/~hadley/physikm/apps/resonance.en.php

### **Dielectric function**





#### Gross and Marx

There can be more resonances.



Insulators can often be modeled as a simple resonance.

### **Dispersion relation**

In the section on photons, we derived the wave equation for light in vacuum. Here the wave equation for light in a dielectric material is derived.



The normal mode solutions are plane waves:

 $\vec{D} = \vec{D}_0 \exp(\vec{k} \cdot \vec{r} - \omega t)$ 

$$\varepsilon(\omega,k)\mu_0\varepsilon_0\omega^2 = k^2$$

### **Dispersion relation**

$$\varepsilon(\omega)\mu_0\varepsilon_0\omega^2 = k^2$$

If  $\varepsilon$  is real and positive: propagating electromagnetic waves  $\exp(i(\vec{k} \cdot \vec{r} - \omega t))$ 

If  $\epsilon_r < 0$ : decaying solutions

 $\exp(-\vec{k}\cdot\vec{r}-i\omega t)$ 

If  $\varepsilon$  is complex,  $\varepsilon_{\rm r} > 0$ : decaying electromagnetic waves  $\exp(i(\vec{k} \cdot \vec{r} - \omega t)) \exp(-\kappa r)$ 



### **Dielectric function**



Intensity  $I(x) = I(0) \exp(-\alpha x)$  J m<sup>-2</sup> s<sup>-1</sup> Beer-Lambert absorption coefficient  $\longrightarrow \alpha = \frac{2\omega K}{c}$ 

#### The index of refraction *n* and the extinction coefficient *K*



# Dispersion



Cause of chromatic aberration in lenses.

http://en.wikipedia.org/wiki/Dispersion\_%28optics%29#mediaviewer/File:Prism\_rainbow\_schema.png http://en.wikipedia.org/wiki/Refractive\_index

### Absorption coefficient $\alpha$



### Reflectance



Dielectric function of silicon  $\sqrt{\varepsilon(\omega)} = n(\omega) + iK(\omega)$ 





#### Advanced Solid State Physics

#### Optical properties of insulators and semiconductors

In an insulator, all charges are bound. By applying an electric field, the electrons and ions can be pulled out of their equilibrium positions. When this electric field is turned off, the charges oscillate as they return to their equilibrium positions. A simple model for an insulator can be constructed by describing the motion of the charge as a damped mass-spring system. The differential equation that describes the motion of a charge is,

$$m \, \frac{d^2 x}{dt^2} + b \, \frac{dx}{dt} + kx = -qE.$$

Rewriting above equation using  $\omega_0=\sqrt{rac{k}{m}}$  and the damping constant  $\gamma=rac{b}{m}$  yields,

 $rac{d^2x}{dt^2} + \gamma rac{dx}{dt} + \omega_0^2 x = - rac{qE}{m} \ .$ 

If the electric field is pulsed on, the response of the charges is described by the impulse response function g(t). The impulse response function satisfies the equation,

$$rac{d^2g}{dt^2}+\gammarac{dg}{dt}+\omega_0^2g=-rac{q}{m}\,\delta(t).$$

The solution to this equation is zero before the electric field is pulsed on and at the time of the pulse the charges suddenly start oscillating with the frequency  $\omega_1 = \sqrt{\omega_0^2 - \frac{\gamma^2}{4}}$ . The amplitude of the oscillation decays exponentially to zero in a characteristic time  $\frac{2}{\gamma}$ .

$$g(t) = -\frac{q}{m\omega_1} \exp(-\frac{\gamma}{2}t) \sin(\omega_1 t).$$



Outline Quantization Photons Electrons Magnetic effects and Fermi surfaces Linear response Transport **Crystal Physics** Electron-electron interactions Quasiparticles Structural phase transitions Landau theory of second order phase transitions Superconductivity Exam guestions Appendices Lectures Books Course notes TUG students Making presentations

### Dielectrics

Dielectrics used as electrical insulators should not conduct.

Large breakdown field.

Low AC losses.

Sometimes a low dielectric constant is desired (CMOS interconnects)

Sometimes a high dielectric constant is desired (supercapacitors).



Electrode separation in meters  $\times 10^{-2}$ 

In an ideal capacitor, current leads voltage by 90°.

Because the dielectric constant is complex, in real materials current leads voltage by  $90^{\circ}$  -  $\delta$ .

Power loss = 
$$\frac{\omega \varepsilon_1 V_0^2}{2} \tan \delta$$

Becomes more of an issue at high frequencies (microwaves)



### Loss tangent

Substance	Dielectric Constant (relative to air)	Dielectric Strength (V/mil)	Loss Tangent	Max Temp (°F)
ABS (plastic), Molded	2.0 - 3.5	400 - 1350	0.00500 - 0.0190	171 - 228
Air	1.00054	30 - 70		
Alumina - 96% - 99.5%	10.0 9.6		0.0002 @ 1 GHz 0.0002 @ 100 MHz 0.0003 @ 10 GHz	
Aluminum Silicate	5.3 - 5.5			
Bakelite	3.7			
Bakelite (mica filled)	4.7	325 - 375		
Balsa Wood	1.37 @ 1 MHz 1.22 @ 3 GHz		0.012 @ 1 MHz 0.100 @ 3 GHz	
Beeswax (yellow)	2.53 @ 1 MHz 2.39 @ 3 GHz		0.0092 @ 1 MHz 0.0075 @ 3 GHz	
Beryllium oxide	6.7		0.006 @ 10 GHz	
Butyl Rubber	2.35 @ 1 MHz 2.35 @ 3 GHz		0.001 @ 1 MHz 0.0009 @ 3 GHz	
Carbon Tetrachloride	2.17 @ 1 MHz 2.17 @ 3 GHz		<0.0004 @ 1 MHz 0.0004 @ 3 GHz	
Diamond	5.5 - 10			
Delrin (acetyl resin)	3.7	500		180
Douglas Fir	1.9 @ 1 MHz		0.023 @ 1 MHz	
Douglas Fir Plywood	1.93 @ 1 MHz 1.82 @ 3 GHz		0.026 @ 1 MHz 0.027 @ 3 GHz	
Enamel	5.1	450		
Epoxy glass PCB	5.2	700		
Ethyl Alcohol (absolute)	24.5@1MHz 6.5@3GHz		0.09 @ 1 MHz 0.25 @ 3 GHz	
Ethylene Glycol	41 @ 1 MHz 12 @ 3 GHz		-0.03 @ 1 MHz 1 @ 3 GHz	
Formica XX	4.00			
FR-4 (G-10) - low resin	4.9		0.008 @ 100 MHz	
- high resin	4.2		0.008 @ 3 GHz	
Fused quartz	3.8		0.0002 @ 100 MHz 0.00006 @ 3 GHz	
Fused silica (glass)	3.8			
Gallium Arsenide (GaAs)	13.1		0.0016 @ 10 GHz	
Germanium	16			
Glass	4 - 10			
Glass (Corning 7059)	5.75		0.0036 @ 10 GHz	
Gutta-percha	2.6			
Halowax oil	4.8			
High Density Polyethylene (HDPE), Molded	1.0 - 5.0	475 - 3810	0.0000400 - 0.00100	158 - 248
Ice (pure distilled water)	4.15 @ 1 MHz 3.2 @ 3 GHz		0.12 @ 1 MHz 0.0009 @ 3 GHz	
Kapton® Type 100 Type 150	3.9 2.9	7400 4400		500

# Polarizability

Overdamped modes

- Orientation polarizability
- Space charge polarizability

Underdamped modes

- Ionic polarizability
- Electronic polarizability

## Orientation (dipolar) Polarizability

For materials (gases, liquids, solids) with a permanent dipole moment.

The theory is very similar to paramagnetism.



$$\chi \propto \frac{1}{T}$$
 Curie law

## **Orientation Polarizability**

Ion jumps. doubly ionized