Response functions 9.01.2018

We would like to be able to calculate much more than the specific heat and static conductivity. In general one can think of many interesting observables

- Electric polarizability
  ↳ static + dynamic
- Magnetic polarizability
  ↳ static + dynamic
- Conductivity
  ↳ static + dynamic
- Reflectivity / Absorption (of photons)
- Compressibility / Strength / Stiffness
- ....

any Hermitian operator you think of

we are interested how a static change to the Hamiltonian changes the ground-state (static responce) i.e. $H \Rightarrow H + O$ and

$$H\phi = E\phi \rightarrow (H+O)\tilde{\phi} = \tilde{E}\tilde{\phi}$$

we want to know $\langle\tilde{\phi}|O|\tilde{\phi}\rangle$

or if I use operator O to make an excitation at time t and site x, how does this propagate.

and How does that relate to excitations in the frequency domain? i.e. $O e^{i\omega t}$

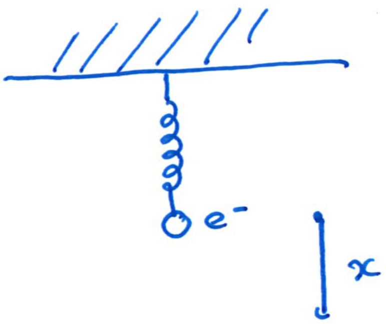
For this we can use response theory and calculate the response functions from our one particle Green's functions ...

Today define classicle response theory

on Friday the quantum equivalence

Response functions for classical systems behave the same as response functions for quantum systems so we can introduce them for classical systems.

Take as an example an Harmonic oscylator i.e. particle on a spring



$$F_{spring} = -kx$$

$$F_{ext} = F_0 \cos(\omega t)$$

we want to know what the position, velocity and accelleration is as a function of t if the system is driven with $F_{ext} = F_0 \cos(\omega t)$

note that position $\cdot$ e $\Rightarrow$ dipole moment

velocity $\cdot$ e $\Rightarrow$ current

accellration of charge $\Rightarrow$ radiation

$\Rightarrow$ diffraction

equation of motion:

$$m\, x''(t) = -k\, x(t) + F_0 \cos(\omega t)$$

Solution:

$$x(t) = -\frac{1}{m} \frac{1}{\omega^2-\omega_0^2} F_0 \cos(\omega t) + c_1 \cos(\omega_0 t) + c_2 \sin(\omega_0 t)$$

with $\omega_0 = \sqrt{\frac{k}{m}}$

we can show that this is indeed a solution by substituting it back into the equation

$$m\, x''(t) = \omega^2 \frac{1}{\omega^2-\omega_0^2} F_0 \cos(\omega t) - m\,\omega_0^2\, c_1 \cos(\omega_0 t) - m\,\omega_0^2\, c_2 \sin(\omega_0 t)$$

and

$$-k\, x(t) + F_0 \cos(\omega t) = \frac{k}{m} \frac{1}{\omega^2-\omega_0^2} F_0 \cos(\omega t) + F_0 \cos(\omega t) - k\, c_1 \cos(\omega_0 t) - k\, c_2 \sin(\omega_0 t)$$

$$\omega_0^2 \frac{1}{\omega^2-\omega_0^2} + \frac{\omega^2-\omega_0^2}{\omega^2-\omega_0^2} = \omega^2 \frac{1}{\omega^2-\omega_0^2}$$

and

$$m\omega_0^2 = k$$

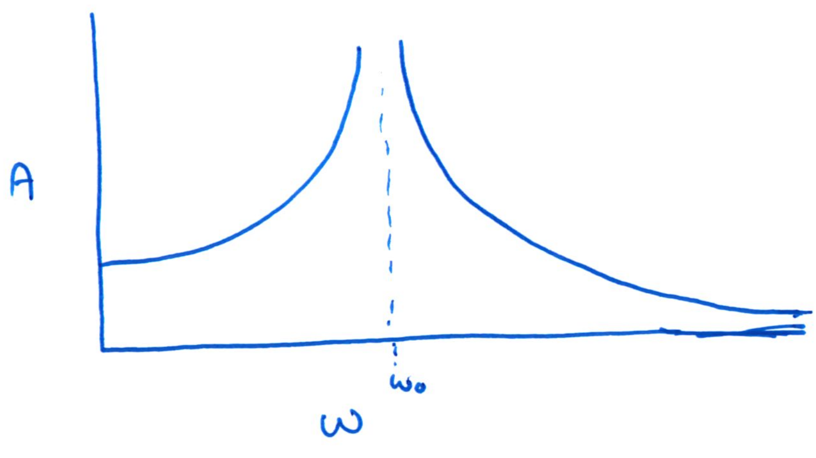
such that our proposed function is indeed a solution

the two terms with frequen cy ω_0 allow oscilatin at the eigen frequency of the system and are not related to the driving force. i.e. not a responce to our eahrnal action

The term that describes the response to the entrnal force yields

$$x(t) = -\frac{1}{m} \frac{1}{\omega^2-\omega_0^2} F_{ext}(t)$$

the amplitude of the oscilation is $\left| \frac{1}{m} \frac{1}{\omega^2-\omega_0^2} \right|$



the phase of the oscilator with respect to the driving force is 0 for $\omega < \omega_0$ and π for $\omega > \omega_0$

For a slowly oscilating force the particle follows the driving force.

For a fast oscilating force the particle can't follow and lags behind.

In order to discuss absorbtion we should look at the energy in the system

kinetic energy in the oscilator:

$$\frac{1}{2} m x'(t)^2 = \frac{F_0^2 \omega^2 \sin(\omega t)^2}{2m (\omega^2 - \omega_0^2)^2}$$

potential energy in the oscitator

$$\frac{1}{2} m x(t)^2 = \frac{F_0^2 \omega_0^2 \cos(\omega t)^2}{2m (\omega^2 - \omega_0^2)^2}$$

Total energy $= E_{pot} + E_{kin}$ oscilates between kinetic energy with prefactor ω^2 and potential energy with prefactor ω_0^2

The energy change of the oscilator is given by the field. The energy provided by the field i.e. the power of the field is:

$$P = F x'(t) = \frac{F_0^2 \omega \sin(\omega t) \cos(\omega t)}{m(\omega^2 - \omega_0^2)}$$

$$= \frac{\partial}{\partial t} \left(E_{kin} + E_{pot} \right)$$

The energy in the oscilator varies and is provided by the field, i.e. time dependent absorbtion and emission of photons; but:

$$\frac{\int_0^{2\pi/\omega} P \, dt}{\int_0^{2\pi/\omega} 1 \, dt} = 0$$

on average over one cycle there is no net absorbtion.

In order to describe friction we need to add damping which will lead to absorption

Assume force due to friction proportional to velocity. The equation of motion then becomes:

$$m x''(t) = -k x(t) - m\gamma x'(t) + F_0 \cos(\omega t)$$

The choice to call the friction constant $m\gamma$ becomes clear later once we know the solution

We will solve this equation by making the force complex and only keeping the real part of the complex solution

$$F_0 \cos(\omega t) \Rightarrow F_0 \cos(\omega t) - i F_0 \sin(\omega t) = e^{-i\omega t}$$

For the solution we have that the real part of $x(t)$ is the position

The imaginary part is neglected

We find similar to the undamped case 3 terms in the solution:

$$x(t) = \frac{1}{m(\omega_0^2 - \omega^2 - i\gamma\omega)} e^{-it\omega} F_0$$

$$+ c_1 e^{-t\gamma/2} e^{-t\sqrt{(\gamma/2)^2 - \omega_0^2}}$$

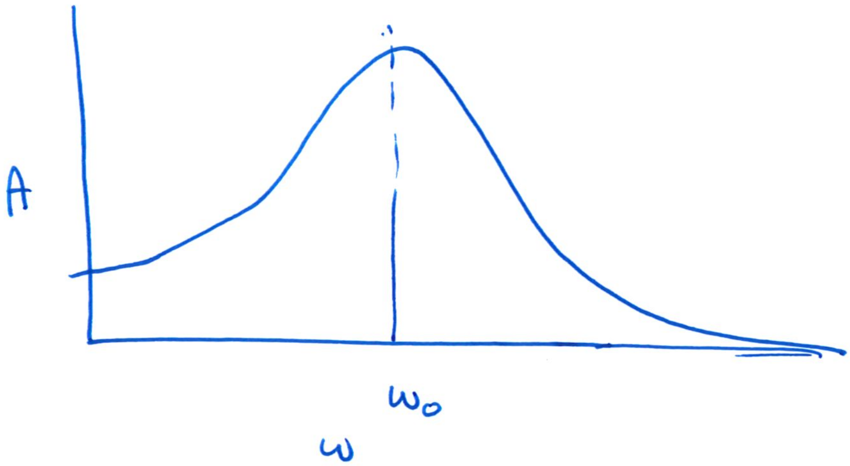
$$+ c_2 e^{-t\gamma/2} e^{t\sqrt{(\gamma/2)^2 - \omega_0^2}}$$

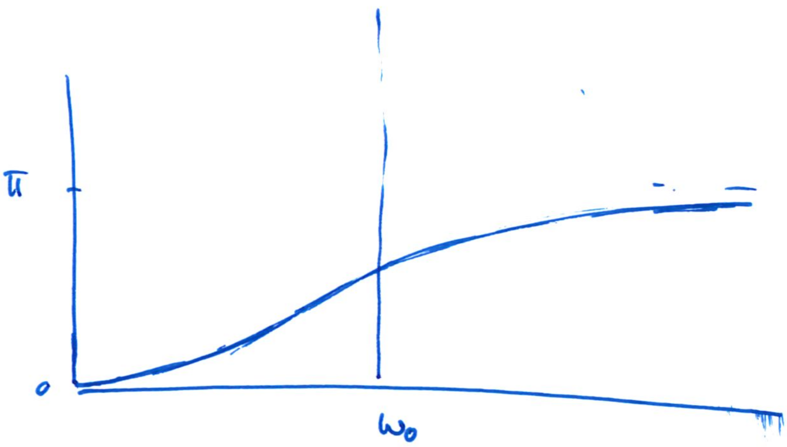
The terms with c_1 and c_2 exponentially decay. If at some point in time the system oscilates at it's eigen frequency then this oscilation is damped. These two terms are not related to the response to the external force.

The response to the force is given as:

$$x(t) = \frac{1}{m(\omega_0^2 - \omega^2 - i\gamma\omega)} F_0 e^{-i\omega t}$$

We can again look at the amplitude of the oscillator and the phase between the oscillator and the driving force.





Which now behave smooth.

In order to look at the absorbtion we can look at the energy in the oscilator:

$$E_{kin} = \frac{1}{2} m \left(\frac{\partial}{\partial t} \, Re\left[x(t) \right] \right)^2$$

$$E_{pot} = \frac{1}{2} k \left(Re\left[x(t) \right] \right)^2$$

$$E_{tot} = E_{kin} + E_{pot}$$

which oscilates, but once averaged over one period $2\pi/\omega$ is constant.

The work done by the field is

$$P = F \frac{\partial}{\partial t} Re\left[x(t) \right]$$

and the time averaged work yields

$$\frac{\int_0^{2\pi/\omega} P \, dt}{2\pi/\omega} = \frac{F_0^2 \, \gamma \omega^2}{2m\left(\gamma^2 \omega^2 + (\omega^2 - \omega_0^2)^2 \right)}$$

The intermediate results can be seen in the online notes

The energy in the system oscilates, but once averaged over one cycle is constant.

The field constantly provides energy, but this is dissipated by the term $-m\gamma x'(t)$

We now can define the response functions

we have $x = \dfrac{1}{m(\omega_0^2 - \omega^2 - i\gamma\omega)} F$

we define the susceptibility as

$$\chi(\omega) = \frac{1}{m(\omega_0^2 - \omega^2 - i\gamma\omega)}$$

such that $x = \chi(\omega)\, F$

The susceptibility relates the induced dipole moment (ex) to the external force ($\propto$ Electric field)

The conductivity relates the current $\Rightarrow$ velocity to the external force. (Field)

$$x' = \sigma(\omega)\, F$$

with $F = F_0\, e^{-i\omega t}$ and $\dfrac{\partial F}{\partial t} = -i\omega F$

we have

$$\sigma(\omega) = -i\omega\, \chi(\omega)$$

Absorbtion is given by the movement of the electron against the force.

Being careful with our complex variables introduced to make the math easier we have that the actual force is $Re[F]$

the absorbtion thus is $Re[F]\ Re[\sigma]\ Re[F]$

averaged over a full cycle

$$Re[\sigma] = -\frac{\gamma^2\omega^2}{m(\gamma^2 m^2 + (\omega_0^2-\omega^2)^2)}$$

and the field strength is

$$\frac{\int_0^{2\pi/\omega} (F_0 \cos\omega t)^2\, dt}{\int_0^{2\pi/\omega} 1\, dt} = \frac{F_0^2}{2}$$

The accelleration of electrons produces radiation with is given by the scattering length

$$X'' = f(\omega)\ F$$

and $f(\omega) = -i\omega\ \sigma(\omega) = -\omega^2\ \chi(\omega)$

Warning: these 3 response functions have about ~200 years of history in different sub-fields

(scattering Bragg / Laue)

(polarizability Maxwell)

(optics conductivity Newton)

This has lead to different phases used

$$f(\omega) = \omega\,\sigma(\omega) = \omega^2\ \chi(\omega)$$

and offsets

$$D = (1+\chi)\,E \quad \text{instead of} \quad P = \chi E$$

On Friday we'll derive the response functions for quantum systems, but lett us rewrite $\cancel{\chi}(\omega)$ slightly to get a form one might recognize

$$\chi(\omega) = \frac{1}{2m} \frac{2}{\omega_0^2 - \omega^2 - i\gamma\omega}$$

$$\approx \frac{1}{2m} \frac{1}{\omega_0} \left(\frac{1}{\omega + i\gamma/2 - \omega_0} - \frac{1}{\omega + i\gamma/2 + \omega_0} \right)$$

$$= \frac{1}{2m} \frac{2}{\omega_0^2 - \omega^2 - i\gamma\omega + (\gamma/2)^2}$$

The susceptibility has two poles. one at $\omega = \omega_0 - i\gamma/2$ and one at $\omega = -\omega_0 - i\gamma/2$ ....