Fourier Transforms of Causal Functions / Kramers Kronig

- A causal function vanishes for $t < 0$. They occur frequently and are known as response functions or memory kernels

As an example take an atom bound to a molecule. If an small external force is applied the atom is (on average) displaced

(Eq 1)
$$x(t) = \int_{-\infty}^{t} G_R(t-t')\, F(t')\, dt'$$

displacement of atom — response function also called "memory kernel" — Force

The displacement $x(t)$ depends on the past values of $F(t')$ for $t' < t$. We write

(Eq 2)
$$x(t) = \int_{-\infty}^{\infty} G_R(t-t')\, F(t')\, dt'$$

where

$G_R(t-t')$ vanishes for $t' > t$ ⇐ causality

Define $\tau \equiv t - t'$

$$G_R(\tau) = \begin{cases} 0 & \tau < 0 \\ \text{something} & \tau > 0 \end{cases}$$ ⇐ Defines a causal func

Then fourier transform (Eq 2)

(Eq 3) $$x(\omega) = G_R(\omega)\, F(\omega)$$

Take a damped harmonic oscillator for example

$$m\frac{d^2x}{dt^2} + m\eta\frac{dx}{dt} + m\omega_0^2 x = F(t)$$

Fourier transform both sides

$$x(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} x(\omega)$$

$-i\omega$ for each time deriv

$$\frac{dx(t)}{dt} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} (-i\omega)\, x(\omega)$$

Then

$$m(-i\omega)^2 x(\omega) - im\eta\omega x(\omega) + m\omega_0^2 x(\omega) = F(\omega)$$

Or

$$x(\omega) = \left[\frac{1/m}{-\omega^2 + \omega_0^2 - i\omega\eta}\right] F(\omega)$$

So camparison @ (Eq 3) shows

Response function for damped oscillator

$$\boxed{G_R(\omega) = \left[\frac{-1/m}{\omega^2 - \omega_0^2 + i\omega\eta}\right]}$$

Things to notice:

- $G_R(\omega)$ has singularities in the lower half plane:

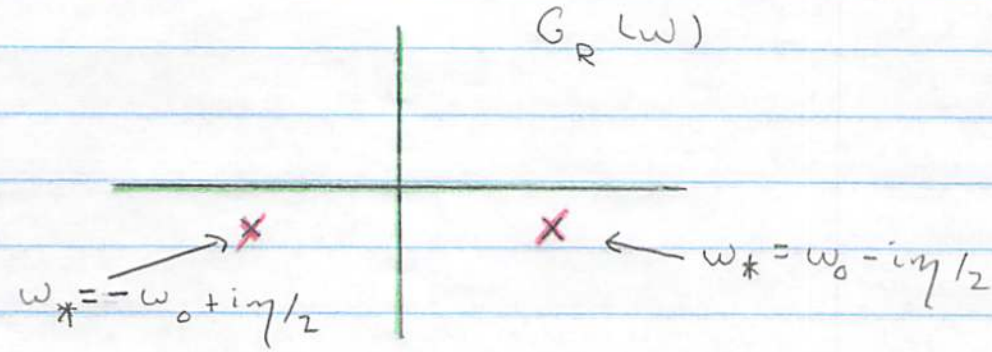
  Take small damping and solve for poles

$$\omega_*^2 - \omega_0^2 + i\underbrace{\omega_*\eta}_{\text{small}} = 0$$

Then $\omega_* = \pm\omega_0 + \underbrace{\Delta\omega}_{\text{small}}$ and then substitute keeping first order terms:

$$(\pm\omega_0 + \Delta\omega)^2 - \omega_0^2 + (\pm\omega_0 + \Delta\omega)\eta \simeq \pm 2\omega_0\Delta\omega \pm i\omega_0\eta = 0$$

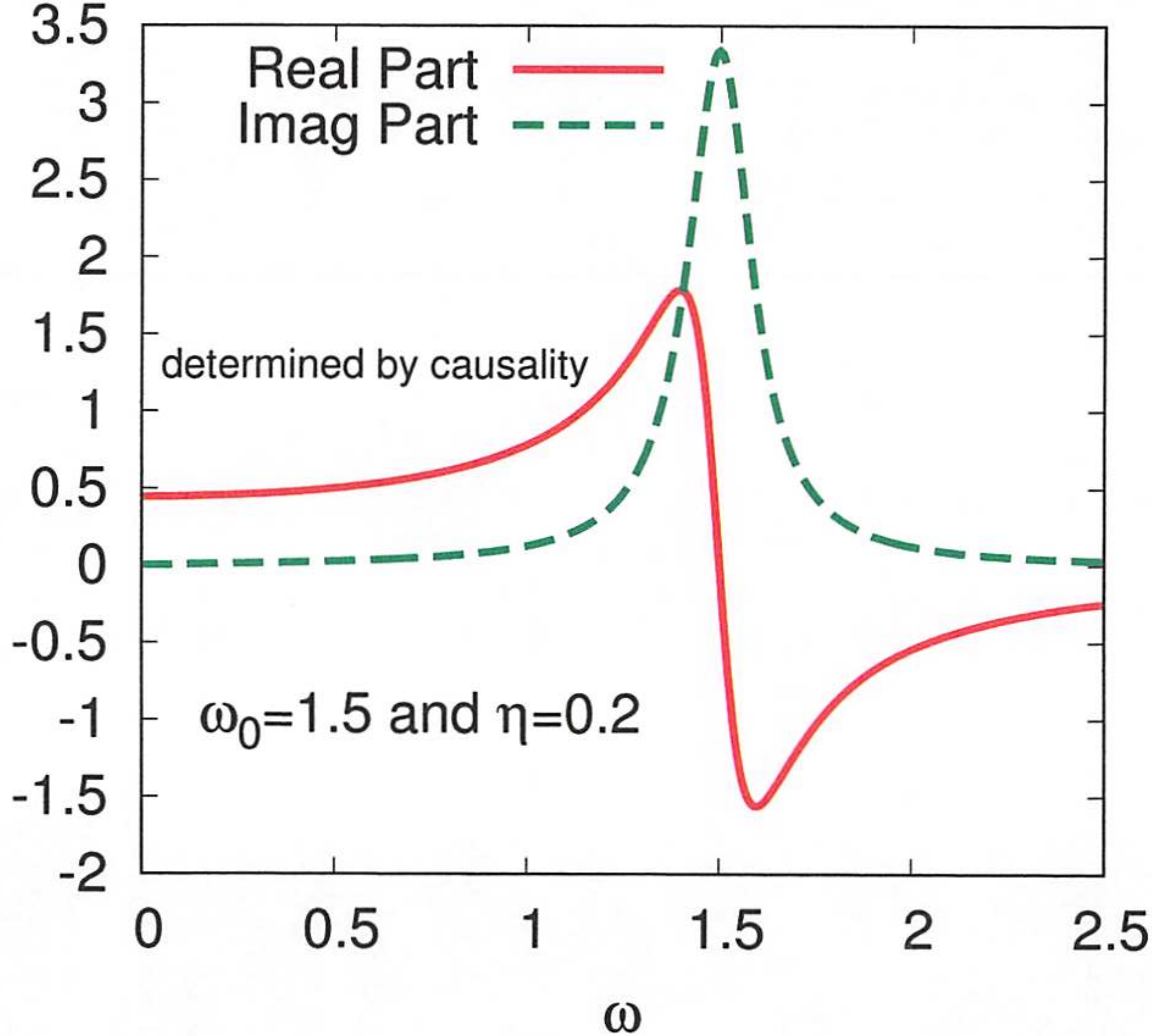
i.e. $\omega_* = \pm\omega_0 - i\eta/2$ $\qquad \Delta\omega = -i\eta/2$



- The Real and imaginary parts

$$G_R(\omega) = \frac{-(\omega^2-\omega_0^2)/m}{(\omega^2-\omega_0^2)^2 + (\omega\eta)^2} + i\,\frac{\omega\eta}{(\omega^2-\omega_0^2)^2 + (\omega\eta)^2}$$

Imaginary part $\propto$ damping



As we will see, through causality, the red curve (the real part) is determined by the green curve (imag part) and vice versa. The characteristic shape of the red ($P/\omega-\omega_0$) is a consequence of a δ-fcn like peak in green.

Causal Functions enjoy:

① The fourier transform $G_R(\omega)$ has no singularities in the upper half complex frequency plane. It is analytic there.

② The real and imaginary parts of the Fourier transform are determined by each other

Kramer's Kronig relations

$$\mathrm{Re}\, G_R(\omega) = -\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{P}{\omega-\omega'} \mathrm{Im}\, G_R(\omega')$$

$$\mathrm{Im}\, G_R(\omega) = +\int_{-\infty}^{\infty} \frac{d\omega'}{\pi} \frac{P}{\omega-\omega'} \mathrm{Re}\, G_R(\omega')$$

Can also be written (Homework)

$$\mathrm{Re}\, G_R(\omega) = -\frac{2}{\pi}\int_{0}^{\infty} d\omega' \frac{P}{\omega^2-\omega'^2} \omega' \,\mathrm{Im}\, G_R(\omega')$$

$$\mathrm{Im}\, G_R(\omega) = \frac{2\omega}{\pi}\int_{0}^{\infty} d\omega' \frac{P}{(\omega')^2-\omega^2} \mathrm{Re}\, G_R(\omega)$$

These relations imply a connection between dispersion of light (the real part of the dielectric constant) and the damping of light (the imaginary part of the dielectric constant)

Proof of (1) ≡ Analyticity in the complex plane

Then

$$G_R(\omega) = \int_{-\infty}^{\infty} G_R(\tau)\, e^{+i\omega\tau}\, d\tau = \underbrace{\int_{0}^{\infty} G_R(\tau)\, e^{i\omega\tau}\, d\tau}$$

Now consider this integral, $\tau > 0$. Now this provides an analytic continuation into the upper half plane $\mathrm{Im}\,\omega > 0$. Since for $\mathrm{Im}\,\omega > 0$

$$e^{i\omega\tau} = e^{i(\mathrm{Re}\,\omega)\tau}\, e^{-\mathrm{Im}\,\omega\,\tau}$$

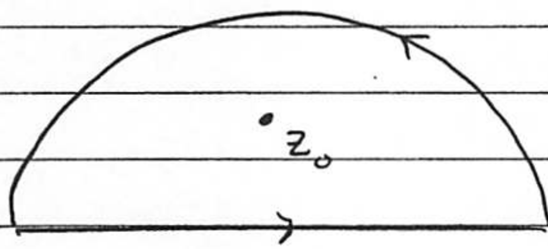
and the integral becomes more convergent. The integral can't be continued into the lower half plane

Proof of (2) ≡ Imag part determines the real part

Proof of Kramers - Kronig

Since $\chi(z)$ is analytic in the UHP we can use cauchy theorem

$$\chi(z_0) = \int_C \frac{dz}{2\pi i} \frac{\chi(z)}{z - z_0}$$



Here the only pole is at z_0, since $\chi(z)$ is analytic in UHP.

Now let $z_0 = \omega_0 + i\varepsilon$. Then, assuming that the arc at infinity gives no contribution,

$$\mathrm{Re}\,\chi(\omega_0) + i\,\mathrm{Im}\,\chi(\omega_0)$$

$$= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} \frac{\mathrm{Re}\,\chi(\omega) + i\,\mathrm{Im}\,\chi(\omega)}{(\omega - (\omega_0 + i\varepsilon))}$$

Now

$$\frac{1}{\omega - \omega_0 - i\varepsilon} = \frac{\omega - \omega_0}{[(\omega-\omega_0)^2 + \varepsilon^2]} + i\frac{\varepsilon}{[(\omega-\omega_0)^2 + \varepsilon^2]}$$

So

$$\lim_{\varepsilon \to 0} \frac{1}{\omega - \omega_0 - i\varepsilon} = \frac{P}{\omega - \omega_0} + i\pi\,\delta(\omega - \omega_0)$$

Yielding

$$\operatorname{Re} \chi(\omega_0) + i \operatorname{Im} \chi(\omega_0)$$

$$= \frac{1}{2} \operatorname{Re} \chi(\omega_0) + \frac{i}{2} \operatorname{Im} \chi(\omega_0)$$

$$+ P \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{-i \operatorname{Re} \chi(\omega) + \operatorname{Im} \chi(\omega)}{\omega - \omega_0}$$

So comparing

$$\operatorname{Im} \chi(\omega_0) = -\int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{P}{\omega - \omega_0} \operatorname{Re} \chi(\omega_0)$$

$$\operatorname{Re} \chi(\omega_0) = \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{P}{\omega - \omega_0} \operatorname{Im} \chi(\omega_0)$$

This is the same as quoted with the subs $\omega_0 \to \omega$ and $\omega \to \omega'$.

Causality And Qualitative Features of Response Functions

- Now we can understand the qualitative feautes of the damped SHO response function
- Suppose the imaginary part has a δ-fcn like peak at a frequeny ω_0

$$\operatorname{Im} G_R(\omega) = \delta_\varepsilon(\omega-\omega_0) + \text{regular part}$$

smoothed δ - fcn

Then

$$\operatorname{Re} G_R(\omega) = -\int \frac{d\omega'}{\pi} \frac{P}{\omega-\omega'} \delta_\varepsilon(\omega-\omega_0) + \text{regular}$$

So

$$\operatorname{Re} G_R(\omega) = -PV_\varepsilon \frac{1}{\omega-\omega_0} + \text{regular}$$

- This explains the $-PV(1/x)$ like shape of $G_R(\omega)$