Linear Response Theory

'Linear response' is the response of a system of interest an external perturbation to the linear order in the perturbation.

Consider, for example, a damped harmonic oscillator driven by an external force :

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

where $\gamma > 0$ is the damping strength.

Fourier transforming, $x(t) = \int_\omega x(\omega)\, e^{-i\omega t}$,

$$\left[-\omega^2 + \omega_0^2 - i\gamma\omega\right] x(\omega) = \frac{f(\omega)}{m}$$

$$\Rightarrow \quad x(\omega) = \frac{f(\omega)}{m\left[-\omega^2 + \omega_0^2 - i\gamma\omega\right]}$$

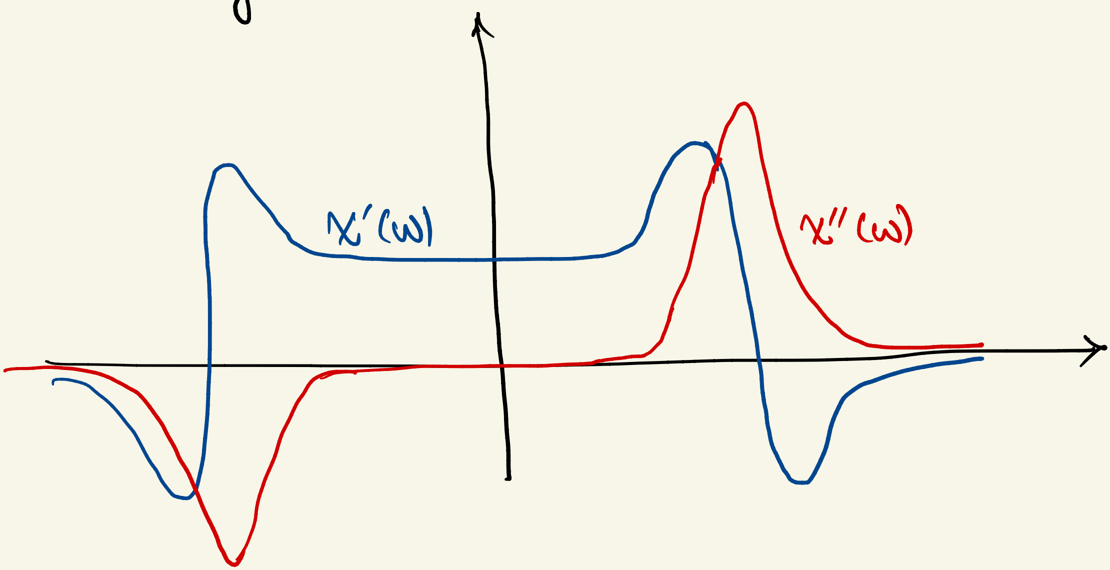
One defines susceptibility for this system as $\chi(\omega) = \dfrac{\partial x(\omega)}{\partial f(\omega)}$, so that $x(\omega) = \chi(\omega) f(\omega)$, Therefore, $\chi(\omega) = \dfrac{1}{m[-\omega^2 + \omega_0^2 - i\gamma\omega]}$

Decomposing $\chi(\omega)$ into its real and imaginary parts as $\chi(\omega) = \chi'(\omega) + i\chi''(\omega)$,

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

$$\chi''(\omega) = \frac{\omega\gamma}{m[(\omega^2 - \omega_0^2)^2 + (\omega\gamma)^2]}.$$

Qualitatively, these look like



One notices/finds several properties of $\chi(\omega)$:

1. $\chi'(\omega)$ is even in ω while $\chi''(\omega)$ is odd.

2. Poles of $\chi(\omega)$ correspond to the complex mode frequencies of the oscillator.

3. As the damping $\gamma \to 0$, $\chi''(\omega)$ has poles at $\omega = \pm \omega_0$.

4. The dissipation generated due to the external force is proportional to $\chi''(\omega)$.

To see this, one calculates the average power dissipated over a long time T:

$$P = \lim_{T\to\infty} \frac{1}{T} \int_0^T dt \; f(t) \frac{dx(t)}{dt}$$

Lets consider force applied at a single frequency ω, so that $f(t) = f_0 \cos(\omega t)$.

$$\Rightarrow \quad x(t) = \mathrm{Re}\left[x(\omega)\, e^{-i\omega t}\right]$$
$$= \mathrm{Re}\left[\chi(\omega) f_0 e^{-i\omega t}\right]$$

$$= f_0 \, \mathrm{Re}\left[\left(\chi'(\omega) + i\, \chi''(\omega) \right) \left[\cos(\omega t) - i \sin(\omega t) \right] \right]$$

$$= f_0 \left[\chi'(\omega) \cos(\omega t) + \chi''(\omega) \sin(\omega t) \right]$$

$\Rightarrow$ Power $P =$

$$\lim_{T \to \infty} \frac{f_0^2 \omega}{T} \int_0^T dt \left[-\chi'(\omega) \sin(\omega t) + \chi''(\omega) \cos(\omega t) \right] \cos(\omega t)$$

$$= f_0^2 \omega \left[\chi''(\omega) \langle \cos^2(\omega t) \rangle + \chi'(\omega) \langle \cos(\omega t) \sin(\omega t) \rangle \right]$$

$$= \frac{f_0^2 \omega \, \chi''(\omega)}{2}$$

Reference: X G Wen, Philips.

Consider a system in an eigenstate $|\varphi_0\rangle$ at $t = t_0$ and turn on a perturbation:

$$H = H_0 + f(t)\, O_1 \quad (\text{with } H_0|\varphi_0\rangle = E_0|\varphi_0\rangle)$$

We are interested in $\langle O_2\rangle(t)$ for some general operator O_2.

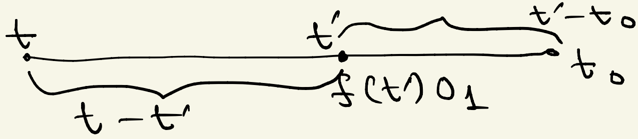
The time evolution is given by

$$|\varphi(t)\rangle = \dots e^{-iH_0 dt}\, e^{-if(t_0+dt)O_1 dt}\, e^{-iH_0 dt}\, e^{-if(t_0)O_1 dt}\, |\varphi_0\rangle$$

$$\simeq \dots e^{-iH_0 dt}\, [1 - i f(t_0+dt)\, O_1 dt]\, e^{-iH_0 dt}$$

$$[1 - i f(t_0)\, O_1\, dt]\, |\varphi_0\rangle$$

If we are only interested in 'linear response' i.e. time-evolved state only to the linear order in f, then the above expression may be written as (after taking continuum limit in the time direction):



$$|\varphi(t)\rangle =$$

$$\left[e^{-iH_0(t-t_0)} - i\int_{t_0}^{t} dt'\, f(t')\, e^{-iH_0(t-t')}\, O_1\, e^{-iH_0(t'-t_0)} \right] |\varphi_0\rangle$$

$$= \left[e^{-iH_0(t-t_0)} - i\int_{t_0}^{t} dt'\, f(t')\, e^{-iH_0(t-t_0)}\, O_1(t') \right] |\varphi_0\rangle$$

where $O_1(t') = e^{iH_0(t'-t_0)}\, O_1\, e^{-iH_0(t'-t_0)}$

This leads to the object of our interst,

$$\langle O_2\rangle(t) = \langle\varphi(t)|\, O_2\, |\varphi_2(t)\rangle$$

$$= \langle O_2\rangle(t_0) + i\int_{t_0}^{t} dt'\, f(t')\, \langle\varphi_0|\, O_1(t')\, O_2(t)\, |\varphi_0\rangle$$

$$- i\int_{t_0}^{t} dt'\, f(t')\, \langle\varphi_0|\, O_2(t)\, O_1(t')\, |\varphi_0\rangle$$

$$= \langle O_2\rangle(t_0) - i\int_{t_0}^{t} dt'\, \langle\varphi_0|\, [O_2(t), O_1(t')]\, |\varphi_0\rangle\, f(t')$$

$$\Rightarrow \delta O_2(t) \overset{\text{def}}{=} \langle O_2\rangle(t) - \langle O_2\rangle(t_0)$$

$$= \int_{-\infty}^{\infty} \chi(t-t')\, f(t')\, dt'$$

where $\chi(x-x', t-t')$

$$= -i\,\theta(t-t') \langle [O_2(x,t), O_1(x',t')] \rangle$$

where we have put back the space-coordinates x, x' as well.

Note that $\chi(x-x', t-t')$ is real by definition if O_1, O_2 are hermitian.

Consequence of Causality:

The factor of $\theta(t-t')$ in $\chi(t-t')$ is a consequence of causality: past affects future and not vice-versa. This simple fact has consequences for the Fourier transform of χ.

Let's write $\chi(x,t) = 2i\,\theta(t)\,\chi''(t)$ so that χ'' is purely imaginary $(= -2\langle [O_2(t), O_1(0)] \rangle)$

Fourier transforming this equation,

$$\chi(\omega) = \int_{-\infty}^{\infty} \chi(t)\, e^{i\omega t}\, dt$$

$$= 2\int_{-\infty}^{\infty} i\, \tilde{\chi}(t)\, \theta(t)\, e^{i\omega t}\, dt$$

Now we use the following integral form for $\theta(t)$

$$\theta(t) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{e^{i\omega' t}}{\omega' - i\varepsilon}\, d\omega' \qquad (\varepsilon > 0)$$

(Reasoning: when $t > 0$, we need to close the contour in the upper half plane, which gives 1. when $t < 0$, we close it in the lower half plane, which gives 0).

Using this,

$$\chi(\omega) = \frac{2i}{2\pi i}\int_{-\infty}^{\infty} \frac{\chi''(t)\, e^{i(\omega+\omega')t}}{\omega' - i\varepsilon}\, dt\, d\omega'$$

$$= \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{\chi''(\omega+\omega')\, d\omega'}{\omega' - i\varepsilon}$$

$$= \frac{1}{\pi}\underbrace{\int_{-\infty}^{\infty} \frac{\chi''(\omega')\, d\omega'}{\omega' - \omega - i\varepsilon}}$$

Thus, we have related $\chi(\omega)$ to $\chi''(\omega)$.

This is called a Kramers-Kronig relation.

By definition, $\chi(\omega) = \chi'(\omega) + i\,\chi''(\omega)$

where $\chi'(\omega)$ and $\chi''(\omega)$ are the real and imaginary parts of $\chi(\omega)$.

Since $\dfrac{1}{x - i\varepsilon} = P\left(\dfrac{1}{x}\right) + i\pi\,\delta(x)$

where P denotes the principal part,

$$\Rightarrow \quad \chi(\omega) = \frac{1}{\pi} P \int \frac{\chi''(\omega')\,d\omega'}{\omega' - \omega} + i\chi''(\omega')$$

Therefore, $\chi'(\omega) = \dfrac{1}{\pi} P \displaystyle\int \frac{\chi''(\omega')\,d\omega'}{\omega' - \omega}$

which is another way to write the Kramers-Kronig relation. This relation is experimentally quite useful if one has access only to (say) the imaginary part of a response function as a function of frequency. Then, one may be able to obtain the real part using above relation.

Symmetries, Spectral decomposition and Fluctuation-Dissipation relation

Symmetries :

For a classical harmonic oscillator, we saw that $\chi''(\omega)$ was odd in ω. This is true more generally, under some assumptions.

$$\chi''_{O_1O_2}(x,x',t-t') = [\,O_1(x,t)\;,\;O_2(x',t')\,]$$

Interchanging $x \leftrightarrow x'$, $t \leftrightarrow t'$ $\Rightarrow$

$$\chi''_{O_1O_2}(x',\,x\,,\,t'-t) = -\chi''_{O_2O_1}(x,x',t-t')$$

fourier transforming,

$$\chi''_{O_1O_2}(x',\,x\,,\,\omega) = -\chi''_{O_2O_1}(x,x',-\omega)\,.$$

Assuming that operators O_1, O_2 are hermitian, one can take the complex conjugation of $\chi''(x,x',t-t') = [\,O_1(x,t)\;,\;O_2(x',t')\,]$,

$$\Rightarrow \quad \chi''_{O_1O_2}(x,x',t-t')^* = \chi_{O_2O_1}(x',x,t'-t).$$

fourier transforming,

$$\left[\chi''_{O_1O_2}(x, x', \omega)\right]^* = \chi_{O_2O_1}(x', x, \omega)$$

Now lets assume that $\chi''_{O_1O_2}(x, x', \omega)$

$= \chi''_{O_2O_1}(x', x, \omega)$ i.e. it is even

under exchanging $O_1(x) \longleftrightarrow O_2(x')$.

$$\Rightarrow \left[\chi''_{O_1O_2}(x, x', \omega)\right]^* = \chi''_{O_1O_2}(x, x', \omega)$$

and

$$\chi''_{O_1O_2}(x, x', \omega) = -\chi''_{O_1O_2}(x, x', -\omega).$$

That is, $\chi''(\omega)$ is real and <u>odd</u> in ω.

Dissipation :

For the classical harmonic oscillator, we saw that the dissipation was proportional to $\chi''(\omega)$. This is also true more generally.

Work done on the system

$$= \frac{dE}{dt} = \frac{d}{dt} \mathrm{Tr}\left[\rho(t) H(t)\right]$$

$$= \mathrm{tr}\left[\frac{d\rho(t)}{dt} H(t)\right] + \mathrm{tr}\left[\rho(t)\frac{dH(t)}{dt}\right]$$

Recall that $H = H_0 + \int_x f(x,t)\, O_1(x)$.

and therefore the only time-dependence in $H(t)$ comes through $f(x,t)$.

Further, $\frac{d\rho(t)}{dt} = i[\rho(t), H(t)]$

and therefore, $\mathrm{tr}\left[\frac{d\rho(t)}{dt} H(t)\right]$

$$= i\,\mathrm{tr}\left[\rho(t) H(t) H(t)\right] - i\,\mathrm{tr}\left[H(t)\rho(t)H(t)\right]$$

$$= 0.$$

$$\Rightarrow \frac{dE}{dt} = \int_x \mathrm{tr}\left[\rho(t) \frac{df(x,t)}{dt} O_1(x)\right]$$

$$= \int_x \frac{df(x,t)}{dt} \langle O_1(x) \rangle_t$$

$$= \int_x \frac{df(x,t)}{dt} \Big[\langle O_1(x) \rangle_0 +$$

$$\int_{-\infty}^{t} dt' \, dx' \; 2i\, \theta(t-t')\, \chi''_{O_1 O_1}(x, x', t-t') f(x', t') \Big]$$

Let's restrict to the case when $f(x,t)$ $= f_0 \cos(\omega t)$ i.e. a single frequency.

The term proportional to $\langle O_1(x) \rangle_0$ averages out to zero, while the second term becomes,

$$\omega \int_{-\infty}^{t} dt' \, dx \, dx' \; f_0(x) f_0(x') \sin(\omega t) \cos(\omega t') \, \chi''_{O_1 O_1}(x, x', t-t')$$

Using $\sin(\omega t)\cos(\omega t') = \dfrac{\sin[\omega(t+t')] + \sin[\omega(t-t')]}{2}$,

the term proportional to $\sin \dfrac{\omega(t+t')}{2}$

will average out to zero. Using

$$\chi''(x,x',t-t') = \int_\omega \chi''(x,x',\omega)\, e^{i\omega(t-t')}$$

and changing the variables to $t_1 = t-t'$,

$$\Rightarrow \left\langle \frac{dE}{dt} \right\rangle$$

$$= \frac{\omega}{2} \int_0^\infty dt_1\, dx\, dx'\, \chi''(x,x',\omega) f_0(x) f_0(x')$$

where we have used $\langle \sin^2(t) \rangle = \frac{1}{2}$.