APPPHYS383 Thursday 11 February 2010

Linear susceptibility

Consider a classical linear dynamical system,

$$\frac{d}{dt}\vec{x} = A\vec{x},$$

where $\vec{x} \in R^N$ and A is a real $N \times N$ matrix. Note that Newton's equation for a harmonic oscillator can be written in this form:

$$m\ddot{x} = F = -kx,$$
$$\vec{x} \equiv \begin{pmatrix} x \\ \dot{x} \end{pmatrix}, \qquad A = \begin{pmatrix} 0 & 1 \\ -\frac{k}{m} & 0 \end{pmatrix},$$
$$\frac{d}{dt}\vec{x} = \begin{pmatrix} \dot{x} \\ \ddot{x} \end{pmatrix} = \begin{pmatrix} \dot{x} \\ -\frac{k}{m}x \end{pmatrix} = A\vec{x}.$$

The intial value problem for the homogeneous system of equations can easily be solved,

$$\vec{x}(t) = \exp(At)\vec{x}(0),$$

which corresponds in the harmonic oscillator case to (writing $\omega_0 \equiv \sqrt{k/m}$)

$$A = \begin{pmatrix} 1 & 1 \\ i\omega_0 & -i\omega_0 \end{pmatrix}\begin{pmatrix} i\omega_0 & 0 \\ 0 & -i\omega_0 \end{pmatrix}\begin{pmatrix} \frac{1}{2} & \frac{1}{2i\omega_0} \\ \frac{1}{2} & -\frac{1}{2i\omega_0} \end{pmatrix},$$

$$\exp(At) = \begin{pmatrix} 1 & 1 \\ i\omega_0 & -i\omega_0 \end{pmatrix}\begin{pmatrix} e^{i\omega_0 t} & 0 \\ 0 & e^{-i\omega_0 t} \end{pmatrix}\begin{pmatrix} \frac{1}{2} & \frac{1}{2i\omega_0} \\ \frac{1}{2} & -\frac{1}{2i\omega_0} \end{pmatrix} = \begin{pmatrix} \cos(\omega_0 t) & \frac{1}{\omega_0}\sin(\omega_0 t) \\ -\omega_0 \sin(\omega_0 t) & \cos(\omega_0 t) \end{pmatrix},$$

$$\begin{pmatrix} x_t \\ \dot{x}_t \end{pmatrix} = \begin{pmatrix} \cos(\omega_0 t) & \frac{1}{\omega_0}\sin(\omega_0 t) \\ -\omega_0 \sin(\omega_0 t) & \cos(\omega_0 t) \end{pmatrix}\begin{pmatrix} x_0 \\ \dot{x}_0 \end{pmatrix} = \begin{pmatrix} x_0\cos(\omega_0 t) + \frac{1}{\omega_0}\dot{x}_0\sin(\omega_0 t) \\ -\omega_0 x_0 \sin(\omega_0 t) + \dot{x}_0\cos(\omega_0 t) \end{pmatrix}.$$

We recognize the solutions of course from elementary mechanics.

If we add a driving force to the model,

$$m\ddot{x} = -kx + m\alpha(t),$$
$$\frac{d}{dt}\vec{x} = A\vec{x} + \begin{pmatrix} 0 \\ \alpha(t) \end{pmatrix},$$

we can still find explicit solutions using the general formula for linear systems,

$$\vec{x}(t) = \exp(At)\vec{x}(0) + \exp(At)\int_0^t dt' \exp(-At')\begin{pmatrix} 0 \\ \alpha(t') \end{pmatrix}.$$

To begin matching up with the susceptibility notation however we now consider the Laplace domain expression,

$$x(s) = G(s)\alpha(s),$$

where s is the Laplace transform variable and $x(s)$ and $\alpha(s)$ are the transforms of $x(t)$ and $\alpha(t)$. The initial conditions are taken to be zero and we concern ourselves with steady-state response. The Laplace transfer function $G(s)$ can be written

$$
\begin{aligned}
G(s) &= \begin{pmatrix} 1 & 0 \end{pmatrix}(sI-A)^{-1}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&\to \begin{pmatrix} 1 & 0 \end{pmatrix}\begin{pmatrix} s & -1 \\ \omega_0^2 & s \end{pmatrix}^{-1}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \end{pmatrix}\frac{1}{s^2+\omega_0^2}\begin{pmatrix} s & 1 \\ -\omega_0^2 & s \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&= \frac{1}{s^2+\omega_0^2}.
\end{aligned}
$$

Considering only harmonic excitations we can set $s \to i\omega$ and note that

$$
x(i\omega) = \frac{1}{\omega_0^2-\omega^2}\alpha(i\omega),
$$

reflecting the expected divergence for $\omega = \omega_0$ (since this oscillator is completely undamped) as well as the sign change in the response above and below resonance. In these unstable (undamped cases) there are some complications with the inverse Laplace transforms, so let us temporarily consider the case of an under-damped oscillator,

$$
m\ddot{x} = -kx - \beta\dot{x} + m\alpha(t),
$$

$$
\frac{d}{dt}\begin{pmatrix} x \\ \dot{x} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\omega_0^2 & -\zeta \end{pmatrix}\begin{pmatrix} x \\ \dot{x} \end{pmatrix} + \begin{pmatrix} 0 \\ \alpha(t) \end{pmatrix},
$$

where $\zeta \equiv \beta/m.$ Then

$$
\begin{aligned}
G(s) &= \begin{pmatrix} 1 & 0 \end{pmatrix}\begin{pmatrix} s & -1 \\ \omega_0^2 & s+\zeta \end{pmatrix}^{-1}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&= \begin{pmatrix} 1 & 0 \end{pmatrix}\frac{1}{s(s+\zeta)+\omega_0^2}\begin{pmatrix} s+\zeta & 1 \\ -\omega_0^2 & s \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} \\
&= \frac{1}{s(s+\zeta)+\omega_0^2},
\end{aligned}
$$

which for a harmonic excitation gives

$$
G(i\omega) = \frac{1}{-\omega^2+i\zeta\omega+\omega_0^2} = \frac{\omega_0^2-\omega^2-i\zeta\omega}{(\omega_0^2-\omega^2)^2+\zeta^2\omega^2},
$$

from which we can easily read off the in-phase and quadrature components analogous to χ' and χ''. We note that as $\zeta \to 0$ and as long as $\omega \neq \omega_0,$ we find

$$
G(i\omega) \to \frac{1}{\omega_0^2-\omega^2}.
$$

Looking at the general equation $(\vec{x}(0) = 0)$

$$
\begin{aligned}
\vec{x}(t) &= \exp(At)\int_0^t ds\, \exp(-As)\begin{pmatrix} 0 \\ \alpha(s) \end{pmatrix} \\
&= \int_0^t ds\, \exp(A(t-s))\begin{pmatrix} 0 \\ \alpha(s) \end{pmatrix},
\end{aligned}
$$

and comparing it with Eq. (18) from the book,

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

we see that

$$
\chi(\tau) \to \theta(\tau)\exp(A\tau),
$$

and thus

$$
\begin{aligned}
\chi(\omega) &= \int_{-\infty}^{+\infty} \chi(\tau) e^{i\omega\tau} d\tau \\
&= \int_0^{+\infty} d\tau \begin{pmatrix} \cos(\omega_0\tau) & \frac{1}{\omega_0}\sin(\omega_0\tau) \\ -\omega_0 \sin(\omega_0\tau) & \cos(\omega_0\tau) \end{pmatrix} e^{i\omega\tau} \\
&= \frac{1}{2}\int_0^{+\infty} d\tau \begin{pmatrix} e^{i\omega_0\tau} + e^{-i\omega_0\tau} & -\frac{i}{\omega_0}\{e^{i\omega_0\tau} - e^{-i\omega_0\tau}\} \\ i\omega_0\{e^{i\omega_0\tau} - e^{-i\omega_0\tau}\} & e^{i\omega_0\tau} + e^{-i\omega_0\tau} \end{pmatrix} e^{i\omega\tau} \\
&= \frac{1}{2}\begin{pmatrix} \int_0^{+\infty} d\tau\, e^{i(\omega_0+\omega)\tau} + \int_0^{+\infty} d\tau\, e^{-i(\omega_0-\omega)\tau} & -\frac{i}{\omega_0}\left\{\int_0^{+\infty} d\tau\, e^{i(\omega_0+\omega)\tau} - \int_0^{+\infty} d\tau\, e^{-i(\omega_0-\omega)\tau}\right\} \\ i\omega_0\left\{\int_0^{+\infty} d\tau\, e^{i(\omega_0+\omega)\tau} - \int_0^{+\infty} d\tau\, e^{-i(\omega_0-\omega)\tau}\right\} & \int_0^{+\infty} d\tau\, e^{i(\omega_0+\omega)\tau} + \int_0^{+\infty} d\tau\, e^{-i(\omega_0-\omega)\tau} \end{pmatrix}.
\end{aligned}
$$

Using again

$$
\int_0^{\infty} d\tau \exp(i\Delta\tau) = iP\frac{1}{\Delta} + \pi\delta(\Delta),
$$

we obtain

$$
\begin{aligned}
\chi_{xa}(\omega) &= -\frac{i}{2\omega_0}\left\{\int_0^{+\infty} d\tau\, e^{i(\omega_0+\omega)\tau} - \int_0^{+\infty} d\tau\, e^{-i(\omega_0-\omega)\tau}\right\} \\
&= \frac{1}{2\omega_0}\left\{P\frac{1}{\omega+\omega_0} - i\pi\delta(\omega+\omega_0) - P\frac{1}{\omega-\omega_0} + i\pi\delta(\omega-\omega_0)\right\} \\
&= \chi'_{xa}(\omega) + i\chi''_{xa}(\omega),
\end{aligned}
$$

where

$$
\begin{aligned}
\chi'_{xa}(\omega) &= \frac{1}{2\omega_0}\left\{P\frac{1}{\omega_0+\omega} + P\frac{1}{\omega_0-\omega}\right\}, \\
\chi''_{xa}(\omega) &= -\frac{\pi}{2\omega_0}\{\pi\delta(\omega+\omega_0) - \pi\delta(\omega-\omega_0)\}.
\end{aligned}
$$

If we consider $\omega \neq \omega_0$ we find $\chi''_{xa} = 0$ and

$$
\begin{aligned}
\chi'_{xa}(\omega) &\to \frac{1}{2\omega_0}\left\{\frac{1}{\omega_0+\omega} + \frac{1}{\omega_0-\omega}\right\} \\
&= \frac{1}{2\omega_0}\left\{\frac{\omega_0-\omega}{\omega_0^2-\omega^2} + \frac{\omega_0+\omega}{\omega_0^2-\omega^2}\right\} \\
&= \frac{1}{2\omega_0}\frac{2\omega_0}{\omega_0^2-\omega^2} \\
&= \frac{1}{\omega_0^2-\omega^2},
\end{aligned}
$$

in agreement with what we found above.

Looking at the definition from the book,

$$
\langle R\rangle_t = \int_{-\infty}^{+\infty} \chi_R(\tau)\lambda(t-\tau)d\tau,
$$

where

$$
V = -R\lambda(t),
$$

is the perturbation driving the evolution of $\langle R\rangle_t$. How can we compute $\chi_R(\tau)$?

We can use the first-order perturbation theory result

$$
\tilde{U}_1(t_f,t_i) = 1 + \frac{1}{i\hbar}\int_{t_i}^{t_f} \tilde{V}(s_2)ds_2,
$$

to write

$$
\begin{aligned}
\langle R\rangle_t &\approx \mathrm{Tr}[\tilde{R}\tilde{U}\sigma_R\tilde{U}^\dagger] \\
&= \mathrm{Tr}[\tilde{R}\sigma_R] + \frac{1}{i\hbar}\int_{-\infty}^{t} \mathrm{Tr}[\tilde{R}(t)\tilde{V}(t')\sigma_R]dt' - \frac{1}{i\hbar}\int_{-\infty}^{t} \mathrm{Tr}[\tilde{R}\sigma_R\tilde{V}(t')]dt' + \frac{1}{\hbar^2}\int_{-\infty}^{t} \mathrm{Tr}[\tilde{R}\tilde{V}(t')\sigma_R\tilde{V}(t')]dt'.
\end{aligned}
$$

Using $\langle R\rangle = 0$, keeping only the first-order terms in λ, and inserting the definition of $V(t)$,

$$\begin{aligned}\langle R\rangle_t &\approx -\frac{1}{i\hbar}\int_{-\infty}^{t}\mathrm{Tr}[\tilde{R}(t)\tilde{R}(t')\lambda(t')\sigma_R]dt' + \frac{1}{i\hbar}\int_{-\infty}^{t}\mathrm{Tr}[\tilde{R}(t)\sigma_R\tilde{R}(t')\lambda(t')]\,dt' \\ &= -\frac{1}{i\hbar}\int_{-\infty}^{t}\mathrm{Tr}[\tilde{R}(t)\tilde{R}(t')\sigma_R - \tilde{R}(t')\tilde{R}(t)\sigma_R]\lambda(t')dt' \\ &= \frac{i}{\hbar}\int_{-\infty}^{t}\langle[\tilde{R}(t),\tilde{R}(t')]\rangle\lambda(t')dt'.\end{aligned}$$

If we now set $\tau \equiv t - t'$ and add a Heaviside step function to extend the upper limit of integration,

$$\begin{aligned}\langle R\rangle_t &\approx -\frac{i}{\hbar}\int_{\infty}^{0}\langle[\tilde{R}(t),\tilde{R}(t-\tau)]\rangle\lambda(t-\tau)d\tau \\ &= \frac{i}{\hbar}\int_{0}^{\infty}\langle[\tilde{R}(t),\tilde{R}(t-\tau)]\rangle\lambda(t-\tau)d\tau \\ &= \frac{i}{\hbar}\int_{-\infty}^{\infty}\theta(\tau)\langle[\tilde{R}(t),\tilde{R}(t-\tau)]\rangle\lambda(t-\tau)d\tau,\end{aligned}$$

and we see that we can at least set

$$\chi_R(t,\tau) = \frac{i}{\hbar}\theta(\tau)\langle[\tilde{R}(t),\tilde{R}(t-\tau)]\rangle.$$

But since the reservoir state is stationary the susceptibility should not depend on t, so we are free to evaluate the right-hand side at $t = \tau$:

$$\chi_R(\tau) = \frac{i}{\hbar}\theta(\tau)\langle[\tilde{R}(\tau),\tilde{R}(0)]\rangle.$$

Eq. (B.23) in the book gives

$$\begin{aligned}\langle\tilde{R}(\tau)\tilde{R}(0)\rangle &= \sum_{\mu}p_\mu\mathrm{Tr}[|\mu\rangle\langle\mu|\tilde{R}(\tau)\tilde{R}(0)] \\ &= \sum_{\mu}p_\mu\mathrm{Tr}[|\mu\rangle\langle\mu|\tilde{R}(\tau)\tilde{R}(0)|\mu\rangle\langle\mu|] \\ &= \sum_{\mu}p_\mu\langle\mu|\tilde{R}(\tau)\tilde{R}(0)|\mu\rangle\mathrm{Tr}[|\mu\rangle\langle\mu|] \\ &= \sum_{\mu}p_\mu\langle\mu|\tilde{R}(\tau)\tilde{R}(0)|\mu\rangle \\ &= \sum_{\mu,\nu}p_\mu\langle\mu|\tilde{R}(\tau)|\nu\rangle\langle\nu|\tilde{R}(0)|\mu\rangle \\ &= \sum_{\mu,\nu}p_\mu\langle\mu|e^{iH_R\tau}Re^{-iH_R\tau}|\nu\rangle\langle\nu|R|\mu\rangle \\ &= \sum_{\mu,\nu}p_\mu\langle\mu|e^{iH_R\tau/\hbar}Re^{-iH_R\tau/\hbar}|\nu\rangle\langle\nu|R|\mu\rangle \\ &= \sum_{\mu,\nu}p_\mu|R_{\mu\nu}|^2e^{i\omega_{\mu\nu}\tau},\end{aligned}$$

hence

$$\begin{aligned}\langle[\tilde{R}(\tau),\tilde{R}(0)]\rangle &= \sum_{\mu,\nu}p_\mu|R_{\mu\nu}|^2e^{i\omega_{\mu\nu}\tau} - \sum_{\mu,\nu}p_\mu|R_{\mu\nu}|^2e^{-i\omega_{\mu\nu}\tau} \\ &= \sum_{\mu,\nu}p_\mu|R_{\mu\nu}|^2 2i\sin(\omega_{\mu\nu}\tau), \\ \chi_R(\tau) &= -\frac{2}{\hbar}\sum_{\mu,\nu}p_\mu|R_{\mu\nu}|^2\theta(\tau)\sin(\omega_{\mu\nu}\tau).\end{aligned}$$

The Fourier transform can be evaluated as above,

$$
\begin{aligned}
\chi_R(\omega) &= \int_{-\infty}^{+\infty} \chi_R(\tau) e^{i\omega\tau} d\tau \\
&= -\frac{2}{\hbar} \sum_{\mu,\nu} p_\mu |R_{\mu\nu}|^2 \int_0^\infty \sin(\omega_{\mu\nu}\tau) e^{i\omega\tau} d\tau \\
&= \frac{i}{\hbar} \sum_{\mu,\nu} p_\mu |R_{\mu\nu}|^2 \int_0^\infty \{e^{i\omega_{\mu\nu}\tau} - e^{-i\omega_{\mu\nu}\tau}\} e^{i\omega\tau} d\tau \\
&= \frac{i}{\hbar} \sum_{\mu,\nu} p_\mu |R_{\mu\nu}|^2 \left\{ iP\frac{1}{\omega_{\mu\nu}+\omega} + \pi\delta(\omega_{\mu\nu}+\omega) + iP\frac{1}{\omega_{\mu\nu}-\omega} - \pi\delta(\omega_{\mu\nu}-\omega) \right\} \\
&= \frac{1}{\hbar} \sum_{\mu,\nu} p_\mu |R_{\mu\nu}|^2 \left\{ -P\frac{1}{\omega_{\mu\nu}+\omega} + i\pi\delta(\omega_{\mu\nu}+\omega) - P\frac{1}{\omega_{\mu\nu}-\omega} - i\pi\delta(\omega_{\mu\nu}-\omega) \right\} \\
&= \chi'_R(\omega) + i\chi''_R(\omega),
\end{aligned}
$$

where

$$
\begin{aligned}
\chi'_R(\omega) &= -\frac{1}{\hbar} \sum_{\mu,\nu} p_\mu |R_{\mu\nu}|^2 \left\{ P\frac{1}{\omega_{\mu\nu}+\omega} + P\frac{1}{\omega_{\mu\nu}-\omega} \right\}, \\
\chi''_R(\omega) &= \frac{\pi}{\hbar} \sum_{\mu,\nu} p_\mu |R_{\mu\nu}|^2 \{\delta(\omega_{\mu\nu}+\omega) - \delta(\omega_{\mu\nu}-\omega)\}.
\end{aligned}
$$