Fluctuation-dissipation theorem [nln39]

Three dynamical quantities in time domain:[1]

- ▷ $\tilde{\chi}''_{AA}(t) \doteq \frac{1}{2\hbar}\langle[A(t),A]_-\rangle$ response function (dissipative part),
- ▷ $\tilde{\Phi}_{AA}(t) \doteq \frac{1}{2}\langle[A(t),A]_+\rangle - \langle A\rangle^2$ fluctuation function,
- ▷ $\tilde{S}_{AA}(t) \doteq \langle A(t)A\rangle - \langle A\rangle^2$ correlation function.

Relations:

$$\tilde{\chi}''_{AA}(t) = \frac{1}{2\hbar}\Big[\tilde{S}_{AA}(t) - \tilde{S}_{AA}(-t)\Big], \qquad \tilde{\Phi}_{AA}(t) = \frac{1}{2}\Big[\tilde{S}_{AA}(t) + \tilde{S}_{AA}(-t)\Big].$$

Transformation properties under time reversal (for real t):

- $\tilde{\chi}''_{AA}(-t) = -\tilde{\chi}''_{AA}(t) = \big[\tilde{\chi}''_{AA}(t)\big]^*$ imaginary and antisymmetric,
- $\tilde{\Phi}_{AA}(-t) = \tilde{\Phi}_{AA}(t) = \big[\tilde{\Phi}_{AA}(t)\big]^*$ real and symmetric,
- $\tilde{S}_{AA}(-t) = \tilde{S}_{AA}(t - \imath\hbar\beta) = \big[\tilde{S}_{AA}(t)\big]^*$ complex.[2]

To make the last symmetry relation more transparent we write

$$\begin{aligned}\langle A(-t)A\rangle &= \mathrm{Tr}\left[e^{-\beta\mathcal{H}_0}e^{-\imath\mathcal{H}_0 t/\hbar}Ae^{\imath\mathcal{H}_0 t/\hbar}A\right] \\ &= \mathrm{Tr}\left[e^{-\beta\mathcal{H}_0}e^{\imath\mathcal{H}_0(t-\imath\hbar\beta)/\hbar}Ae^{-\imath\mathcal{H}_0(t-\imath\hbar\beta)/\hbar}A\right] = \langle A(t-\imath\beta\hbar)A\rangle.\end{aligned}$$

The imaginary part of the correlation function vanishes if

- if $\beta = 0$ i.e. at infinite temperature,
- if $\hbar = 0$ i.e. for classical systems.

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[1] using $[,]_-$ for commutators and $[,]_+$ for anti-commutators.

[2] with symmetric real part and antisymmetric imaginary part.

Three dynamical quantities in frequency domain:

- ▷ $\chi''_{AA}(\omega) \doteq \int_{-\infty}^{+\infty} dt\, e^{\imath\omega t}\tilde{\chi}''_{AA}(t)$ dissipation function,
- ▷ $\Phi_{AA}(\omega) \doteq \int_{-\infty}^{+\infty} dt\, e^{\imath\omega t}\tilde{\Phi}_{AA}(t)$ spectral density,
- ▷ $S_{AA}(\omega) \doteq \int_{-\infty}^{+\infty} dt\, e^{\imath\omega t}\tilde{S}_{AA}(t)$ structure function.

Symmetry properties:

- $\chi''_{AA}(-\omega) = -\chi''_{AA}(\omega)$ real and antisymmetric,
- $\Phi_{AA}(-\omega) = \Phi_{AA}(\omega)$ real and symmetric,
- $S_{AA}(-\omega) = e^{-\beta\hbar\omega}S_{AA}(\omega)$ real and satisfying detailed balance.

Relations:

$$\chi''_{AA}(\omega) = \frac{1}{2\hbar}\left(1 - e^{-\beta\hbar\omega}\right)S_{AA}(\omega), \quad \Phi_{AA}(\omega) = \frac{1}{2}\left(1 + e^{-\beta\hbar\omega}\right)S_{AA}(\omega).$$

Fluctuation-dissipation relation (general quantum version):

$$\Phi_{AA}(\omega) = \hbar\coth\left(\frac{1}{2}\beta\hbar\omega\right)\chi''_{AA}(\omega).$$

Dissipation effects from an interaction with a weak external force as encoded in $\chi''_{AA}(\omega)$ are determined by natural fluctuations existing in thermal equilibrium as encoded in $\Phi_{AA}(\omega)$.

Classical limit (no zero-point fluctuations):

$$\Phi_{AA}(\omega)_{cl} \stackrel{\hbar\to 0}{\longrightarrow} \frac{2k_BT}{\omega}\chi''_{AA}(\omega).$$

Classical fluctuations of any frequency related to static susceptibility:

$$\begin{aligned}\langle(A - \langle A\rangle)^2\rangle &= \tilde{\phi}_{AA}(t=0) = \lim_{t\to 0}\int_{-\infty}^{+\infty}\frac{d\omega}{2\pi}e^{-\imath\omega t}\Phi_{AA}(\omega) \\ &= k_BT\int_{-\infty}^{+\infty}\frac{d\omega}{\pi}\omega^{-1}\chi''_{AA}(\omega) = k_BT\lim_{\omega'\to 0}\frac{1}{\pi}\int_{-\infty}^{+\infty}d\omega\frac{\chi''_{AA}(\omega)}{\omega - \omega'} \\ &= k_BT\chi'_{AA}(\omega'=0) = k_BT\chi_{AA}(\omega'=0) \doteq k_BT\chi_{AA}.\end{aligned}$$