Generalized Langevin Equation [nln72]

The Langevin equation,

$$m\frac{dv}{dt} = -\gamma v + f_{\mathrm{w}}(t), \tag{1}$$

was designed to describe Brownian motion [nln71]. The two forces on the rhs represent an instantaneous attenuation, specified by a damping constant γ and a white-noise random force $f_{\mathrm{w}}(t)$.

The generalized Langevin equation,

$$m\frac{dv}{dt} = -\int_{-\infty}^{t} dt'\alpha(t-t')v(t') + f_{\mathrm{c}}(t), \tag{2}$$

is constructed to describe fluctuations of any mode in a many-body system. A consistent generalization requires synchronized modifications of both forces:

- The instantaneous attenuation is replaced by attenuation with memory (retarded attenuation) represented by some attenuation function $\alpha(t)$.
- The white-noise random force is replaced by a random force $f_{\mathrm{c}}(t)$ representing correlated noise.

Fluctuation-dissipation relation:

- Instantaneous attenuation:

$$\langle f_{\mathrm{w}}(t) f_{\mathrm{w}}(t')\rangle = 2k_{\mathrm{B}}T\gamma\delta(t-t'). \tag{3}$$

- Retarded attenuation:

$$\langle f_{\mathrm{c}}(t) f_{\mathrm{c}}(t')\rangle = k_{\mathrm{B}}T\alpha_{\mathrm{s}}(t-t') \tag{4}$$

  where $\alpha_{\mathrm{s}}(t) \doteq \alpha(t)\theta(t) + \alpha(-t)\theta(-t)$ is the symmetrized attenuation function.

A justification of relations (3) and (4) is based on the fluctuation-dissipation theorem derived from microscopic dynamics [nln39]. The special case (3) of instantaneous attenuation is a consequence of Einstein's relation [nln67].

The width of the (symmetrized) attenuation function $\alpha_{\mathrm{s}}(t)$ is a measure for the memory that governs the time evolution of the stochastic variable. In the limit of short memory (instantaneous attenuation) we have

$$\alpha_{\mathrm{s}}(t-t') \to 2\gamma\,\delta(t-t').$$

Fourier analysis:

Definitions:

$$\tilde{v}(\omega) \doteq \int_{-\infty}^{+\infty} dt\, e^{i\omega t} v(t), \quad \tilde{f}_{\rm c}(\omega) \doteq \int_{-\infty}^{+\infty} dt\, e^{i\omega t} f_{\rm c}(t), \quad \hat{\alpha}(\omega) \doteq \int_{0}^{\infty} dt\, e^{i\omega t} \alpha(t).$$

$$\Rightarrow \; v(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, \tilde{v}(\omega), \quad f_{\rm c}(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, \tilde{f}_{\rm c}(\omega).$$

Substitution of definitions in (2) yields (with $t'' = -t', \tau = t + t''$)

$$m \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t} (-i\omega) \tilde{v}(\omega) = \underbrace{-\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{t} dt' \alpha(t-t')\, e^{-i\omega t'}\, \tilde{v}(\omega)}_{\rm (a)}$$

$$+ \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi}\, e^{-i\omega t}\, \tilde{f}_{\rm c}(\omega).$$

$$\overbrace{-\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \int_{-t}^{\infty} dt'' \alpha(t+t'')\, e^{i\omega t''}\, \tilde{v}(\omega)}^{\rm (a)} = -\int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \underbrace{\int_{0}^{\infty} d\tau\, \alpha(\tau)\, e^{i\omega\tau}}_{\hat{\alpha}(\omega)}\, e^{-i\omega t} \tilde{v}(\omega).$$

$$\Rightarrow \quad -i\omega m \tilde{v}(\omega) = -\hat{\alpha}(\omega)\tilde{v}(\omega) + \tilde{f}_{\rm c}(\omega).$$

Relation between Fourier amplitudes:

$$\tilde{v}(\omega) = \frac{\tilde{f}_{\rm c}(\omega)}{\hat{\alpha}(\omega) - i\omega m}.$$

Spectral densities:

$$S_{vv}(\omega) \doteq \int_{-\infty}^{+\infty} d\tau\, e^{i\omega\tau} \langle v(t) v(t+\tau)\rangle, \quad S_{ff}(\omega) \doteq \int_{-\infty}^{+\infty} d\tau\, e^{i\omega\tau} \langle f_{\rm c}(t) f_{\rm c}(t+\tau)\rangle.$$

Correlations of Fourier amplitudes [nex119]:

$$\langle \tilde{v}(\omega) \tilde{v}^*(\omega')\rangle = 2\pi S_{vv}(\omega) \delta(\omega - \omega'), \quad \langle \tilde{f}_{\rm c}(\omega) \tilde{f}_{\rm c}^*(\omega')\rangle = 2\pi S_{ff}(\omega) \delta(\omega - \omega').$$

Relation between spectral densities:

$$S_{vv}(\omega) = \frac{S_{ff}(\omega)}{|\hat{\alpha}(\omega) - i\omega m|^2}. \tag{5}$$

Fluctuation-dissipation relation (4) in frequency domain:

$$\begin{aligned}\langle \tilde{f}_{\mathrm{c}}(\omega)\tilde{f}_{\mathrm{c}}^*(\omega')\rangle = 2\pi k_{\mathrm{B}}T \overbrace{\int_{-\infty}^{+\infty} d\tau\, e^{i\omega\tau}\alpha_{\mathrm{s}}(\tau)}^{\tilde{\alpha}_{\mathrm{s}}(\omega)=\hat{\alpha}(\omega)+\hat{\alpha}^*(\omega)}\,\delta(\omega-\omega') \\ = 4\pi k_{\mathrm{B}}T\mathrm{Re}\{\hat{\alpha}(\omega)\}\delta(\omega-\omega').\end{aligned}$$

$$\Rightarrow\ S_{ff}(\omega) = 2k_{\mathrm{B}}T\mathrm{Re}\{\hat{\alpha}(\omega)\}. \tag{6}$$

Note: If $S_{ff}(\omega) \geq 0$ then $\alpha(t)$ has a global maximum at $t = 0$.

Solution of generalized Langevin equation (2) expressed by the spectral density of the stochastic variable assembled from (5) and (6):

$$S_{vv}(\omega) = \frac{2k_{\mathrm{B}}T\mathrm{Re}\{\hat{\alpha}(\omega)\}}{|\hat{\alpha}(\omega) - i\omega m|^2}. \tag{7}$$

Limit of instantaneous attenuation: $\hat{\alpha}(\omega) \to \gamma$

$$S_{vv}(\omega) \to \frac{2k_{\mathrm{B}}T\gamma}{\gamma^2 + \omega^2 m^2}. \tag{8}$$

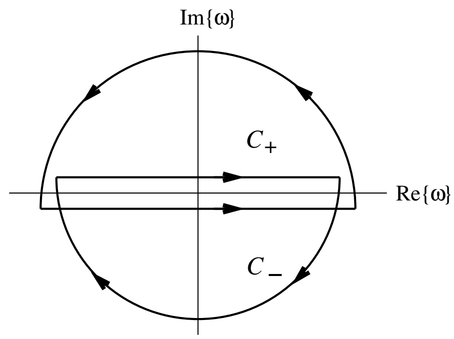
Velocity autocorrelation function:

Stationary state. Use $\hat{\alpha}(-\omega) = \hat{\alpha}^*(\omega)$.

$$
\begin{aligned}
\langle v(t)v(0)\rangle &= k_BT \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{\pm i\omega t} \overbrace{\frac{2\mathrm{Re}\{\hat{\alpha}(\omega)\}}{|\hat{\alpha}(\omega) - i\omega m|^2}}^{\text{symmetric in } \omega} \\
&= \frac{k_BT}{2\pi} \int_{-\infty}^{+\infty} d\omega e^{\pm i\omega t} \frac{\hat{\alpha}(\omega) + \hat{\alpha}^*(\omega)}{[\hat{\alpha}(\omega) - i\omega m][\hat{\alpha}^*(\omega) + i\omega m]} \\
&= \frac{k_BT}{2\pi} \int_{-\infty}^{+\infty} d\omega e^{\pm i\omega t} \Bigg[\underbrace{\frac{1}{\hat{\alpha}(\omega) - i\omega m}}_{\text{(a)}} + \underbrace{\frac{1}{\hat{\alpha}^*(\omega) + i\omega m}}_{\text{(b)}} \Bigg].
\end{aligned}
$$

(a) analytic for $\mathrm{Im}\{\omega\} > 0$,

(b) analytic for $\mathrm{Im}\{\omega\} < 0$.



$$
\langle v(t)v(0)\rangle = \frac{k_BT}{2\pi} \oint_{\mathcal{C}_-} d\omega \frac{e^{-i\omega t}}{\hat{\alpha}(\omega) - i\omega m} = \frac{k_BT}{2\pi} \oint_{\mathcal{C}_+} d\omega \frac{e^{i\omega t}}{\hat{\alpha}^*(\omega) + i\omega m}.
$$

Limit of instantaneous attenuation: $\hat{\alpha}(\omega) \to \gamma$ [nex120]

$$
\langle v(t)v(0)\rangle = \frac{k_BT}{2\pi} \oint_{\mathcal{C}_-} d\omega \frac{e^{-i\omega t}}{\gamma - i\omega m} = \frac{k_BT}{2\pi} \oint_{\mathcal{C}_+} d\omega \frac{e^{i\omega t}}{\gamma + i\omega m} = \frac{k_BT}{m} e^{-\gamma t/m}.
$$