n-Pole Approximation [nln87]

Relaxation function after n successive projections (Mori formalism [nln36]) or n iterations (recursion method [nln84]),

$$c_0(z) = \cfrac{1}{z + \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cdots \cdots + \cfrac{\Delta_{n-1}}{z + \cfrac{1}{\tau_n}}}}}, \tag{1}$$

has termination function represented by a relaxation time τ_n:

$$\Gamma_n(z) = \Delta_n \frac{c_n(z)}{c_{n-1}(z)} = \frac{1}{\tau_n}. \tag{2}$$

Consequences:

- Singularity structure of $c_0(z)$ reduced to n poles in complex z-plane.
- Frequency moments $M_{2k} = \langle \omega^{2k} \rangle$ divergent for $k \geq n$.

Limiting cases:

- $\tau_n \to \infty$:
  All poles approach ω-axis: $z = \epsilon - \imath\omega$ with $\epsilon \to 0$.
  Spectral density $\Phi_0(\omega)$ is a sum of δ-functions.

- $\tau_n \to 0$:
  Transition to $(n-1)$-pole approximation: $\dfrac{\Delta_{n-1}}{z + 1/\tau_n} \to \dfrac{1}{\tau_{n-1}}$.

Illustrations for $n = 1, 2, 3$:

- relaxation function: $c_0(z) = \dfrac{1}{z + \Sigma(z)}$,
- memory function: $\Sigma(z)$,
- spectral density: $\Phi_0(\omega) = 2 \lim_{\epsilon \to 0} \mathrm{Re}\big[c_0(\epsilon - \imath\omega)\big]$.

1-pole spectral approximation

Memory function representing white noise:

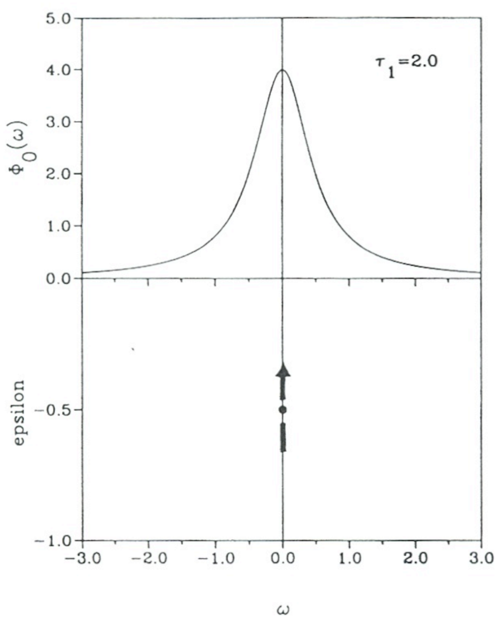
$$\Sigma(z) = \frac{1}{\tau_1} = \text{const.}$$

Relaxation function:

$$c_0(z) = \frac{1}{z + \dfrac{1}{\tau_1}} = \frac{\tau_1}{\tau_1 z + 1}.$$

Spectral density:

$$\Phi_0(\omega) = \frac{2\tau_1}{1 + \tau_1^2\omega^2}.$$



2-pole spectral approximation

Memory function representing classical relaxator:

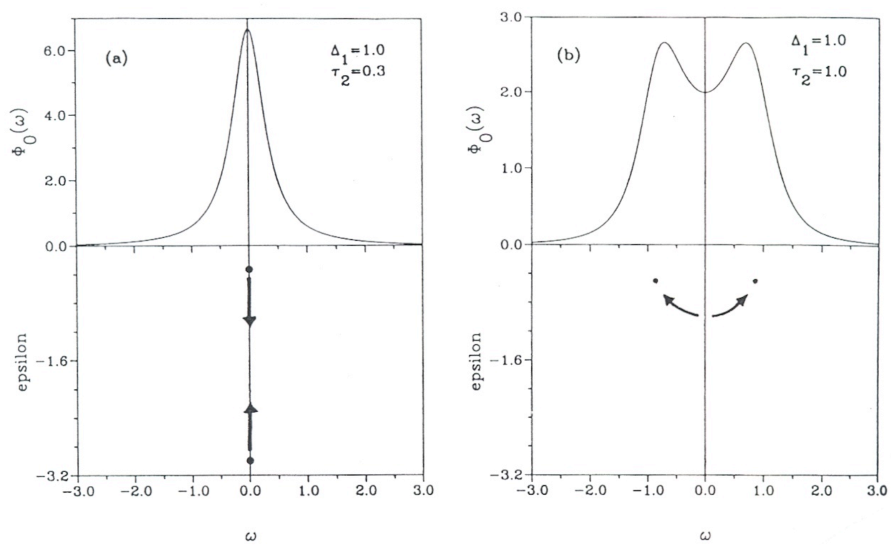
$$\Sigma(z) = \frac{\Delta_1}{z + \frac{1}{\tau_2}}.$$

Relaxation function:

$$c_0(z) = \frac{\tau_2 z + 1}{\tau_2 z^2 + z + \Delta_1 \tau_2}.$$

Spectral density:

$$\Phi_0(\omega) = \frac{2\Delta_1 \tau_2}{\tau_2^2(\Delta_1 - \omega^2)^2 + \omega^2}.$$



3-pole spectral approximation

Memory function representing damped classical oscillator:

$$\Sigma(z) = \cfrac{\Delta_1}{z + \cfrac{\Delta_2}{z + \cfrac{1}{\tau_3}}}.$$

Relaxation function:

$$c_0(z) = \frac{\tau_3 z^2 + z + \Delta_2 \tau_3}{\tau_3 z^3 + z^2 + (\Delta_1 + \Delta_2)\tau_3 z + \Delta_1}.$$

Spectral density:

$$\Phi_0(\omega) = \frac{2\Delta_1 \Delta_2 \tau_3}{[\tau_3 \omega(\omega^2 - \Delta_1 - \Delta_2)]^2 + (\omega^2 - \Delta)^2}.$$