Projection operator method [nln31]

Goal: Determination of symmetrized time-correlation function (fluctuation function) for a dynamical variable $A(t)$ of a quantum or classical many-body Hamiltonian system $\mathcal{H}$ in thermal equilibrium.

Fluctuation function (real, symmetric, normalized):

$$C_0(t) \doteq \frac{\langle A(t)|A\rangle}{\langle A|A\rangle} = \frac{\langle A|A(-t)\rangle}{\langle A|A\rangle} = \frac{\langle A|e^{-\imath Lt}|A\rangle}{\langle A|A\rangle}.$$

Dirac notation symbolizes inner product of choice as explained in [nln32]. Some properties of dynamic quantities depend on choice of inner product.

Relaxation function (via Laplace transform):[1]

$$c_0(z) = \int_0^\infty dt\, e^{-zt} \frac{\langle A|e^{-\imath Lt}|A\rangle}{\langle A|A\rangle} = \frac{1}{\langle A|A\rangle} \left\langle A \left| \frac{1}{z+\imath L} \right| A \right\rangle.$$

Projection operator method determines relaxation function via systematic approximation.

Inverse Laplace transform,

$$C_0(t) = \frac{1}{2\pi\imath} \int_{\mathcal{C}} dz\, e^{zt} c_0(z),$$

involves integral along straight path from $\epsilon - \imath\infty$ to $\epsilon + \imath\infty$ for $\epsilon > 0$.

In practical applications, the (real, symmetric) spectral density is inferred from the relaxation function as limit process,

$$\Phi_0(\omega) = 2 \lim_{\epsilon\to 0} \Re\{c_0(\epsilon - \imath\omega)\},$$

and the fluctuation function via inverse Fourier transform,

$$C_0(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-\imath\omega t} \Phi_0(\omega).$$

[1] The last bracket is also known as a Green's function.