

# Open Quantum Systems Theory behind Quantarhei Package

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In this document, we summarize the theory of open quantum systems as it is implemented in the Quantarhei package. Before it grows into a self-contained text, the following books should be consulted to get a full picture: Volkhard May and Oliver Kühn, *Charge and Energy Transfer in Molecular Systems*, Wiley-VCH, Berlin, 2000 (and later editions), Shaul Mukamel, *Principles of Nonlinear Spectroscopy*, Oxford University Press, Oxford, 1995 and Leonas Valkunas, Darius Abramavicius and Tomáš Mančal, *Molecular Excitation Dynamics and Relaxation*, Wiley-VCH, Weinheim, 2013.

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## I. BATH CORRELATION FUNCTIONS AND SPECTRAL DENSITIES

### A. Bath Correlation Function

Bath correlation function is defined as a two point correlation function of the bath part  $\Delta V$  of the system-bath interaction operator, i.e. as

$$C(t) = \frac{1}{\hbar^2} \text{Tr}_B \{ U_B^\dagger(t) \Delta V U_B(t) \Delta V w_{\text{eq}} \} \quad (1)$$

where  $w_{\text{eq}}$  is the equilibrium bath density operator,  $U_B(t)$  is the bath evolution operator and the trace is taken over the bath degrees of freedom. The bath correlation function is a complex quantity and as such it has a real part

$$C'(t) = \frac{1}{2} [C(t) + C^*(t)] \quad (2)$$

and an imaginary part

$$C''(t) = -\frac{i}{2} [C(t) - C^*(t)] \quad (3)$$

so that

$$C(t) = C'(t) + iC''(t) \quad (4)$$

### B. Spectral Density

A very important quantity is the Fourier transform of the bath correlation function

$$\tilde{C}(\omega) = \int_0^\infty dt C(t) e^{i\omega t} = 2\text{Re} \int_0^\infty dt C(t) e^{i\omega t} \quad (5)$$

It is sometimes referred to as *spectral density*, but we will reserve this name for a different quantity. We will follow Ref. [Mukamel1995]. The Fourier transform  $\tilde{C}(\omega)$  can be split into even and odd parts defined as

$$\tilde{C}'(\omega) = \int_{-\infty}^\infty dt C'(t) e^{i\omega t}, \quad \tilde{C}''(\omega) = i \int_{-\infty}^\infty dt C''(t) e^{i\omega t} \quad (6)$$

so that

$$\tilde{C}(\omega) = \tilde{C}'(\omega) + \tilde{C}''(\omega) \quad (7)$$

It can be shown (see [Mukamel1995]) that

$$\tilde{C}(-\omega) = e^{-\frac{\hbar\omega}{k_B T}} \tilde{C}(\omega) \quad (8)$$

and

$$\tilde{C}(\omega) = [1 + \coth(\hbar\omega/2k_B T)] \tilde{C}''(\omega) \quad (9)$$

Due to the relation between positive and negative frequency values of the Fourier transform of the bath correlation function, we can define it completely through the odd function  $\tilde{C}''(\omega)$  which is a Fourier transform of the imaginary part of the correlation function.

Spectral density

$$J(\omega) = \sum_{\xi} |g_{\xi}|^2 \delta(\omega - \omega_{\xi}) \quad (10)$$

### Appendix A: Microscopic Derivation of Spectral Density Symmetries

Here we will derive the Eqs. (8) and (9).