Open Quantum Systems Theory behind Quantarhei Package

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(Dated: September 19, 2016)

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 gat 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.

I. BATH CORRELATION FUNCTIONS AND SPECTRAL DENSITIES

Bath correlation function

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

Fourier transform of the bath correlation function

$$\tilde{C}(\omega) = \int_0^\infty \mathrm{d}t\ C(t)e^{i\omega t} \tag{2}$$

Spectral density

$$J(\omega) = \sum_\xi |g_\xi|^2\delta(\omega - \omega_\xi) \tag{3}$$