## Open Quantum Systems Theory behind Quantarhei Package

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In this document, we summarize the theory of oopen quantum systems as it is implemented in the Quantarhei package.

## I. BATH CORRELATION FUNCTIONS AND SPECTRAL DENSITIES

Bath correlation function

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

Fourier transform of the bath correlation function

$$\tilde{C}(\omega) = \int_{0}^{\infty} dt \ C(t)e^{i\omega t}$$
(2)

Spectral density

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