Supplemental Material for "Out-of-time-order correlators in finite open systems"

Master equations for the density matrix in an open system

Off-diagonal elements. For a system with non-degenerate energy levels weakly coupled to a dissipative environment, with the Hamiltonian given by Eq. (2), the off-diagonal entries ρ_{mn} of the density matrix satisfy Bloch-Redfield master equations (see, e.g., Ref. 16)

$$\partial_t \rho_{mn} = i(E_{mn} + i\Gamma_{mn})\rho_{mn},\tag{S1}$$

where $E_{mn} = E_m - E_n$ is the frequency of coherent oscillations for an isolated system, and the complex quantity

$$\Gamma_{mn} = -i \int \frac{d\omega}{2\pi} \sum_{k} \left(\frac{S(\omega)|V_{mk}|^2}{\omega - E_{mk} - i0} + \frac{S(-\omega)|V_{nk}|^2}{\omega - E_{kn} - i0} \right) + iV_{mm}V_{nn} \int \frac{d\omega}{2\pi} \frac{S(\omega) + S(-\omega)}{\omega - i0}$$
(S2)

accounts for the effects of the environment, where $S(\omega)$ is the Fourier-transform of the correlation function $S(t-t') = \langle \hat{X}(t)\hat{X}(t')\rangle_{env} = \int \frac{d\omega}{2\pi} e^{-i\omega(t-t')}S(\omega)$ of the environment degree of freedom $\hat{X}(t)$.

The quantity Γ_{mn} , given by Eq. (S2), may be decomposed as

$$\Gamma_{mn} = \frac{1}{2} \sum_{k \neq m} \Gamma_{m \to k}^{rel} + \frac{1}{2} \sum_{k \neq n} \Gamma_{n \to k}^{rel} - i\delta E_m + i\delta E_n + \Gamma_{mn}^{deph},$$
(S3)

where

$$\Gamma_{n \to k}^{rel} = |V_{nk}|^2 S(E_n - E_k) \tag{S4}$$

is the rate of environment-induced transitions (relaxation) from level n to level k,

$$\Gamma_{mn}^{deph} = \frac{1}{2} (V_{nn} - V_{mm})^2 S(0) \tag{S5}$$

is the pure dephasing rate, and

$$\delta E_m = \sum_{k \neq m} |V_{mk}|^2 \int \frac{d\omega}{2\pi} \frac{S(\omega)}{E_m - E_k - \omega}$$
(S6)

is the shift of the energy of the *m*-th level due to the interaction with environment (Lamb shift). The relaxation rate between two levels *n* and *k*, Eq. (S4), is determined by the environment spectrum $S(\omega)$ at frequency $\omega = E_{nk}$ equal to the energy gap between these levels, while the dephasing rate (S5) is determined by the low-frequency properties of the environment.

Diagonal elements. The dynamics of the diagonal elements of the density matrix is described by the equations

$$\partial_t \rho_{nn} = -\rho_{nn} \sum_k \Gamma_{n \to k}^{rel} + \sum_k \rho_{kk} \Gamma_{k \to n}^{rel}, \tag{S7}$$

where the transition rates $\Gamma_{n\to k}$ are given by Eq. (S4).

Lindblad form. Eqs. (S1) and (S7) for the evolution of the density matrix can be rewritten in the Lindblad form

$$\partial_t \hat{\rho} = -i[\hat{\mathcal{H}}_{\text{eff}}, \hat{\rho}] - \frac{1}{2} \sum_{i,j} \left(\hat{\mathcal{L}}_{ij}^{\dagger} \hat{\mathcal{L}}_{ij} \hat{\rho} + \hat{\rho} \hat{\mathcal{L}}_{ij}^{\dagger} \hat{\mathcal{L}}_{ij} - 2 \hat{\mathcal{L}}_{ij}^{\dagger} \hat{\rho} \hat{\mathcal{L}}_{ij} \right), \tag{S8}$$

where the summation runs over all pairs of indices i = 1, ..., N and j = 1, ..., N in an N-level system; the effective Hamiltonian of coherent evolution is given by

$$\hat{\mathcal{H}}_{\text{eff}} = \sum_{i} |i\rangle \langle i| (E_i + \delta E_i), \tag{S9}$$

and the Lindblad operators

$$\hat{\mathcal{L}}_{ij} = (1 - \delta_{ij}) \sqrt{\Gamma_{j \to i}^{rel}} \left| i \right\rangle \left\langle j \right| + \delta_{ij} \sqrt{S(0)/N} \sum_{l} V_{ll} \left| l \right\rangle \left\langle l \right| \tag{S10}$$

account for the effects of dephasing and dissipation.

Master equations for OTOCs

In what follows we derive microscopically the Bloch-Redfield-type master equations for the out-of-time-order correlator (1), following a procedure similar to the derivation (see, e.g., Ref. [16]) of the master equations for the density matrix. Due to the weakness of the system-environment coupling, the OTOCs decay on long times significantly exceeding the characteristic correlation time of the environment.

It follows directly from Eq. (1) that

$$\partial_{t} K_{m_{1}m_{2},n_{1}n_{2}} = i \left\langle \left[\hat{\mathcal{H}}_{0} + \hat{\mathcal{H}}_{\text{coupl}}(t), |n_{1}\rangle \langle m_{1}|(t) \right] \hat{B}(0) |n_{2}\rangle \langle m_{2}|(t) \hat{D}(0) \right\rangle \\ + i \left\langle |n_{1}\rangle \langle m_{1}|(t) \hat{B}(0) \left[\hat{\mathcal{H}}_{0} + \hat{\mathcal{H}}_{\text{coupl}}(t), |n_{2}\rangle \langle m_{2}|(t) \right] \hat{D}(0) \right\rangle,$$
(S11)

where $\hat{\mathcal{H}}_0$ is the Hamiltonian of the system (without the environment) and $\hat{\mathcal{H}}_{\text{coupl}} = \hat{X} \sum_{n,m} V_{nm} |n\rangle \langle m|$ is the coupling between the system and the environment. By expanding all Heisenberg operators in Eq. (S11) to the first order in the perturbation $\hat{\mathcal{H}}_{\text{coupl}}$ and neglecting the change of the density matrix of the system during the characteristic correlation time of the environment, we arrive at the equations for the evolution of the elements $K_{m_1m_2,n_1n_2}$ in the form

$$\partial_{t}K_{m_{1}m_{2},n_{1}n_{2}} = i(E_{n_{1}} + E_{n_{2}} - E_{m_{1}} - E_{m_{2}})K_{m_{1}m_{2},n_{1}n_{2}} - \left\langle \int_{-\infty}^{t} \left[\hat{\mathcal{H}}_{\text{coupl}}(t'), \left[\hat{\mathcal{H}}_{\text{coupl}}(t), |n_{1}\rangle \langle m_{1}| \left(t \right) \right] \right] dt' \ \hat{B}(0) |n_{2}\rangle \langle m_{2}| \left(t \right) \ \hat{D}(0) \right\rangle - \left\langle |n_{1}\rangle \langle m_{1}| \left(t \right) \hat{B}(0) \int_{-\infty}^{t} \left[\hat{\mathcal{H}}_{\text{coupl}}(t'), \left[\hat{\mathcal{H}}_{\text{coupl}}(t), |n_{2}\rangle \langle m_{2}| \left(t \right) \right] \right] dt' \ \hat{D}(0) \right\rangle - \left\langle \left[\hat{\mathcal{H}}_{\text{coupl}}(t), |n_{1}\rangle \langle m_{1}| \left(t \right) \right] \hat{B}(0) \int_{-\infty}^{t} \left[\hat{\mathcal{H}}_{\text{coupl}}(t'), |n_{2}\rangle \langle m_{2}| \left(t \right) \right] dt' \ \hat{D}(0) \right\rangle - \left\langle \int_{-\infty}^{t} \left[\hat{\mathcal{H}}_{\text{coupl}}(t'), |n_{1}\rangle \langle m_{1}| \left(t \right) \right] dt' \ \hat{B}(0) \left[\hat{\mathcal{H}}_{\text{coupl}}(t), |n_{2}\rangle \langle m_{2}| \left(t \right) \right] \hat{D}(0) \right\rangle,$$
(S12)

where only the terms up to the second order in the system-environment coupling have been kept and the lower time integration limit has been extended to $-\infty$ in view of the short correlation time of the environment degrees of freedom, i.e. the correlation time between $\hat{\mathcal{H}}_{\text{coupl}}(t') \propto \hat{X}(t')$ and $\hat{\mathcal{H}}_{\text{coupl}}(t) \propto \hat{X}(t)$. Using Eq. (S12), we derive below the master equations for the evolution of the OTOCs in the form (4).

Due to the weakness of the system-environment coupling, the characteristic energy gaps between system levels significantly exceed the decay rates of the OTOCs, which are determined by the last four lines in Eq. (S12); the elements $K_{m_1m_2,n_1n_2}$ quickly oscillate with frequencies $E_{n_1} + E_{n_2} - E_{m_1} - E_{m_2}$ and decay with rates significantly exceeded by these frequencies. Thus, the evolution of each element $K_{m_1m_2,n_1n_2}$ depends only on other elements corresponding to the same energy splitting $E_{n_1} + E_{n_2} - E_{m_1} - E_{m_2}$. Below we consider separately the cases of finite and zero values of the splitting.

Finite energy splitting

For each combination of different m_1 , m_2 , n_1 and n_2 there are four elements K which correspond to the same energy splitting and differ from each other by permutations of indices. We assume for simplicity that there is no additional degeneracy of the quantities $E_{n_1} + E_{n_2} - E_{m_1} - E_{m_2}$ when all of the indices m_1 , m_2 , n_1 and n_2 are different. Eq. (S12) in that case gives

$$\partial_{t} K_{m_{1}m_{2},n_{1}n_{2}} = i(E_{n_{1}} + \delta E_{n_{1}} + E_{n_{2}} + \delta E_{n_{2}} - E_{m_{1}} - \delta E_{m_{1}} - E_{m_{2}} - \delta E_{m_{2}})K_{m_{1}m_{2},n_{1}n_{2}} - \frac{1}{2} \left(\sum_{k \neq m_{1}} \Gamma_{m_{1} \rightarrow k}^{rel} + \sum_{k \neq n_{1}} \Gamma_{n_{1} \rightarrow k}^{rel} + \sum_{k \neq m_{2}} \Gamma_{m_{2} \rightarrow k}^{rel} + \sum_{k \neq n_{2}} \Gamma_{n_{2} \rightarrow k}^{rel} \right) K_{m_{1}m_{2},n_{1}n_{2}} - \Gamma_{n_{2} \rightarrow n_{1}}^{rel} K_{m_{1}m_{2},n_{2}n_{1}} - \Gamma_{m_{1} \rightarrow m_{2}}^{rel} K_{m_{2}m_{1},n_{1}n_{2}} - \Gamma_{m_{1}n_{1},m_{2}n_{2}}^{\phi} K_{m_{1}m_{2},n_{1}n_{2}},$$
(S13)

where the transition rates $\Gamma_{i\to j}^{rel}$ are given by Eq. (S4); δE_i is the renormalisation of the *i*-th level by environment, given by Eq. (S6); and

$$\Gamma^{\phi}_{m_1 n_1, m_2 n_2} = \frac{1}{2} (V_{n_1 n_1} + V_{n_2 n_2} - V_{m_1 m_1} - V_{m_2 m_2})^2 S(0)$$
(S14)

is the dephasing rate in a compound system consisting of two copies of the original system coupled to the same bath.

Zero energy splitting

Elements $K_{m_1m_2,n_1n_2}$ with zero splitting $E_{n_1} + E_{n_2} - E_{m_1} - E_{m_2}$ have a greater degeneracy and require separate analyses.

"Diagonal" elements. Let us first consider the elements with $n_1 = m_1$ and $n_2 = m_2$. These elements satisfy the same equations of evolution as the diagonal elements of the density matrix of a compound system consisting of two copies of the original system. For $n_1 = n_2 = n \neq m = m_1 = m_2$ we obtain from Eq. (S12)

$$\partial_t K_{nm,nm} = -K_{nm,nm} \sum_{k \neq n} \Gamma_{n \to k}^{rel} - K_{nm,nm} \sum_{k \neq m} \Gamma_{m \to k}^{rel} + \sum_{k \neq n} \Gamma_{k \to n}^{rel} K_{km,km} + \sum_{k \neq m} \Gamma_{k \to m}^{rel} K_{nk,nk} - \Gamma_{m \to m}^{rel} K_{nm,nm} - \Gamma_{n \to m}^{rel} K_{mn,nm}.$$
(S15)

In the case n = m Eq. (S12) gives

$$\partial_t K_{nn,nn} = -2K_{nn,nn} \sum_{k \neq n} \Gamma_{n \to k}^{rel} + \sum_{k \neq n} \left(\Gamma_{k \to n}^{rel} K_{kn,kn} + \Gamma_{k \to n}^{rel} K_{nk,nk} \right) + \sum_{k \neq n} \left(\Gamma_{k \to n}^{rel} K_{nk,kn} + \Gamma_{n \to k}^{rel} K_{kn,nk} \right).$$
(S16)

From Eqs. (S15) and (S16) it follows immediately that

$$\sum_{m,n} K_{mm,nn} = \text{const},\tag{S17}$$

which is similar to the conservation of the sum of the diagonal elements of the density matrix of a compound system.

"Non-diagonal" elements. The other set of elements with zero energy splitting, different from the "diagonal" elements, correspond to $m_1 = n_2$ and $m_2 = n_1$. Their evolution is described by the equations

$$\partial_t K_{mn,nm} = -\left(\sum_{k \neq m} \Gamma_{m \to k}^{rel} + \sum_{k \neq n} \Gamma_{n \to k}^{rel}\right) K_{mn,nm} - \left(K_{mn,mn} + K_{nm,nm}\right) \Gamma_{m \to n}^{rel} + \sum_{k \neq m} K_{kn,nk} \Gamma_{m \to k}^{rel} + \sum_{k \neq n} K_{mk,km} \Gamma_{k \to n}^{rel}.$$
(S18)

Master equation for the density matrix for two copies of a system coupled to the same environment

The equations for the evolution of the elements $K_{m_1m_2,n_1n_2}$ are similar to the equations of evolution of the densitymatrix elements $\rho_{m_1m_2,n_1n_2} = \langle |n_1n_2\rangle \langle m_1m_2|(t)\rangle$ of a compound system consisting of two copies of the original system coupled to the same environment, where n_i and m_i label the states of the *i*-th subsystem; i = 1, 2. The Hamiltonian of such a compound system is given by Eq. (12). To the second order in the system-environment coupling \hat{V} the evolution of the density matrix elements is described by the equation

$$\partial_{t}\rho_{m_{1}m_{2},n_{1}n_{2}} = i(E_{n_{1}} + E_{n_{2}} - E_{m_{1}} - E_{m_{2}})\rho_{m_{1}m_{2},n_{1}n_{2}} \\ - \left\langle \int_{-\infty}^{t} \left[\hat{X}(t')\hat{V}(t') \otimes \mathbb{1} + \mathbb{1} \otimes \hat{V}(t')\hat{X}(t'), \left[\hat{X}(t)\hat{V}(t) \otimes \mathbb{1} + \mathbb{1} \otimes \hat{V}(t)\hat{X}(t), |n_{1}n_{2}\rangle \langle m_{1}m_{2}|(t) \right] \right] dt' \right\rangle,$$
(S19)

Eq. (S19) gives, for the coupling $\hat{V} = \sum_{n,m} V_{nm} |n\rangle \langle m|$ and all indices n_1, n_2, m_1 and m_2 being different,

$$\partial_{t}\rho_{m_{1}m_{2},n_{1}n_{2}} = i(E_{n_{1}} + \delta E_{n_{1}} + E_{n_{2}} + \delta E_{n_{2}} - E_{m_{1}} - \delta E_{m_{1}} - E_{m_{2}} - \delta E_{m_{2}})\rho_{m_{1}m_{2},n_{1}n_{2}} \\ - \frac{1}{2} \left(\sum_{k \neq m_{1}} \Gamma_{m_{1} \rightarrow k}^{rel} + \sum_{k \neq n_{1}} \Gamma_{n_{1} \rightarrow k}^{rel} + \sum_{k \neq m_{2}} \Gamma_{m_{2} \rightarrow k}^{rel} + \sum_{k \neq n_{2}} \Gamma_{n_{2} \rightarrow k}^{rel} \right) \rho_{m_{1}m_{2},n_{1}n_{2}} \\ - \frac{1}{2} \left(\Gamma_{n_{2} \rightarrow n_{1}}^{rel} + \Gamma_{n_{1} \rightarrow n_{2}}^{rel} + iE_{n_{1}n_{2}}^{flip} \right) \rho_{m_{1}m_{2},n_{2}n_{1}} \\ - \frac{1}{2} \left(\Gamma_{m_{2} \rightarrow m_{1}}^{rel} + \Gamma_{m_{1} \rightarrow m_{2}}^{rel} - iE_{m_{1}m_{2}}^{flip} \right) \rho_{m_{2}m_{1},n_{1}n_{2}} \\ - \Gamma_{m_{1}n_{1},m_{2}n_{2}}^{\phi} \rho_{m_{1}m_{2},n_{1}n_{2}}, \tag{S20}$$

where the quantity

$$E_{n_1n_2}^{flip} = |V_{n_1n_2}|^2 \int \frac{d\omega}{2\pi} \frac{S(\omega) - S(-\omega)}{\omega + E_{n_1n_2}}$$
(S21)

gives the rate of the flip-flop processes, i.e. the rate of the coherent interchange $n_1 \leftrightarrow n_2$, and the dephasing rate $\Gamma^{\phi}_{m_1n_1,m_2n_2}$ is defined by Eq. (S14).

Lindblad form. The master equations for the evolution of the density matrix of two systems in the same environment may may be also rewritten in the Lindblad form (S8) with the effective Hamiltonian

$$\hat{\mathcal{H}}_{\text{eff}} = \sum_{i} |i\rangle \langle i| \left[(E_i + \delta E_i) \otimes \mathbb{1} + \mathbb{1} \otimes (E_i + \delta E_i) \right] + \frac{1}{2} \sum_{i,j} E_{ij}^{flip} |i\rangle \langle j| \otimes |j\rangle \langle i|$$
(S22)

and the Lindblad operators

$$\hat{\mathcal{L}}_{ij} = (1 - \delta_{ij}) \sqrt{\Gamma_{j \to i}^{rel}} \left(\left| i \right\rangle \left\langle j \right| \otimes \mathbb{1} + \mathbb{1} \otimes \left| i \right\rangle \left\langle j \right| \right) + \delta_{ij} \sqrt{S(0)/N} \sum_{l} V_{ll} \left(\left| l \right\rangle \left\langle l \right| \otimes \mathbb{1} + \mathbb{1} \otimes \left| l \right\rangle \left\langle l \right| \right).$$
(S23)

Mapping between OTOCs and two-system density matrix. Eq. (S13), which described the evolution of OTOCs for an open system in a dissipative environment, resembles Eq. (S20), which describes the evolution of the density matrix elements for two copies of the system coupled to this environment. Indeed, both equations have the same diagonal part, i.e. the part which relates the evolution of the element $\rho_{m_1m_2,n_1n_2}$ or $K_{m_1m_2,n_1n_2}$ to itself. Both equations also have terms with interchanged indices $n_1 \leftrightarrow n_2$ or $m_1 \leftrightarrow m_2$. While two systems coupled to an environment allow for a coherent ("flip-flop") as well as inelastic interchange, the respective processes for OTOCs are purely inelastic.

As discussed in the main text, in the limit of a classical environment the evolutions of the OTOC and two systems coupled to this environment may be mapped onto each other. Classical environment corresponds to the even spectrum $S(\omega) = S(-\omega)$, which leads to the vanishing of the flip-flop rates (S21) and identical relaxation rates $\Gamma_{n_1 \to n_2}^{rel} = \Gamma_{n_2 \to n_1}^{rel}$ of the transitions $n_1 \to n_2$ and $n_2 \to n_1$ for each pair of states n_1 and n_2 . The equations (S13) and (S20) for the evolution of the OTOC and the two systems become identical in this limit.