Dynamics of open quantum systems with initial system-environment correlations via stochastic unravelings

Federico Settimo,[1,*] Kimmo Luoma,[1] Dariusz Chruściński,[2] Andrea Smirne,[3,4] Bassano Vacchini,[3,4] and Jyrki Piilo[1]

[1]*Department of Physics and Astronomy, University of Turku, FI-20014 Turun yliopisto, Finland*
[2]*Institute of Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University, Grudziadzka 5/7, 87-100 Toruń, Poland*
[3]*Dipartimento di Fisica "Aldo Pontremoli", Università degli Studi di Milano, Via Celoria 16, I-20133 Milan, Italy*
[4]*Istituto Nazionale di Fisica Nucleare, Sezione di Milano, Via Celoria 16, I-20133 Milan, Italy*

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In standard treatments of open quantum systems, the reduced dynamics is described starting from the assumption that the system and the environment are initially uncorrelated. This assumption, however, is not always guaranteed in realistic scenarios and several theoretical approaches to characterize initially correlated dynamics have been introduced. For the uncorrelated scenario, stochastic unravelings are a powerful tool to simulate the dynamics. So far they have not been used in the most general case in which correlations are initially present since they cannot be applied to nonpositive operators or noncompletely positive maps. In our work, we employ the bath positive (B+) or one-sided positive decomposition (OPD) formalism as a starting point to generalize stochastic unraveling in the presence of initial correlations. Noticeably, our approach does not depend on the particular unraveling technique, but holds for both piecewise deterministic and diffusive unravelings. This generalization allows not only for more powerful simulations for the reduced dynamics, but also for a deeper theoretical understanding of open system dynamics.

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I. INTRODUCTION

In standard open quantum system scenarios, one typically starts from the assumption that the system and the environment are in a product state at the initial time [1–3]

$$\rho_{SE}(0) = \rho_S(0) \otimes \rho_E, \tag{1}$$

with some fixed environmental state ρ_E. If this is the case, the global system environment evolution is fixed by a unitary $U(t)$, while for the system it is given by $\rho_S(t) = \Phi_t[\rho_S(0)]$, where [4,5]

$$\Phi_t[\cdot] = \mathrm{tr}_E[U(t)(\cdot \otimes \rho_E)U^\dagger(t)] \tag{2}$$

is a completely positive trace-preserving (CPTP) map whose domain extends to the whole set of quantum states $\mathcal{S}(\mathscr{H}_S)$. Assuming that Φ_t is invertible, one can introduce a two-parameters family of maps $\Phi_{t,s} := \Phi_t \Phi_s^{-1}$, describing the evolution from time s to time $t > s$. If $\Phi_{t,s}$ is completely positive (CP) for all t, s, we say that the dynamics is CP divisible. If $\Phi_{t,s}$ is only positive (P), then we say that it is P divisible. Violations of both P and CP divisibility have been connected to quantum non-Markovianity [6–12].

The dynamical map Φ_t can be derived as the solution of the master equation $d\rho/dt = \mathcal{L}_t[\rho]$, with the generator $\mathcal{L}_t = \dot{\Phi}_t \Phi_t^{-1}$ that can be put in Lindblad form [13,14]

$$\mathcal{L}_t[\rho] = -i[H(t), \rho] + \sum_j \gamma_j(t) L_j(t) \rho L_j^\dagger(t) - \frac{1}{2}\{\Gamma(t), \rho\}, \tag{3}$$

where $\Gamma(t) = \sum_j \gamma_j(t) L_j^\dagger(t) L_j(t)$. From the point of view of the master equation, CP divisibility corresponds to the positivity of all rates $\gamma_i(t) \geqslant 0$. P divisibility, on the other hand, corresponds to the condition [15]

$$\sum_j \gamma_j(t) |\langle \varphi_\mu | L_j(t) | \varphi_{\mu'} \rangle|^2 \geqslant 0 \tag{4}$$

for all orthonormal bases $\{\varphi_\mu\}_\mu$ and for all $\mu \neq \mu'$.

However, the assumption of a product initial state, although leading to a simple form of the master equation, cannot cover all situations of interest, for instance, when the system and environment are strongly coupled, so that it has been criticized from a fundamental and a practical perspective [16–21]. Different strategies have thus been devised both for the detection of initial correlations [22–27] and their inclusion in the dynamical description [28–31]. There is indeed no obvious and unique standpoint allowing to obtain the reduced dynamics of a system interacting with an environment if all these degrees of freedom are correlated. In all cases, at variance with what happens in the framework of an initially factorized state, not all possible system states can appear as an initial reduced system state. A recently proposed strategy [31] that takes as starting point a fixed environmental state ρ_E and a fixed correlation operator χ, admits as the domain of the possible initial reduced system states the statistical operators

*Contact author: fesett@utu.fi

ρ_S such that $\rho_S \otimes \rho_E + \chi$ is a positive operator. The size of this convex set depends on the pair ρ_E and χ, and can even be reduced to a single point if the environmental state and correlation operator are determined by a maximally entangled system-environment state. For all elements in this set, the dynamics can be described by a time-local master equation of the form (3). A different strategy [30] takes as starting point a specified correlated system-environment state, for which a suitable decomposition known as bath positive (B+) or one-sided positive decomposition (OPD) is given, which allows to obtain the time-evolved reduced system state in terms of the action of a set of CPTP maps of the form (2) whose dimensionality is bounded by the square of the dimension of the system Hilbert space. In this case the dynamics are no longer described by a single time-local master equation of the form (3), but by a set of master equations, one for each completely positive map. While the strategy works for a specified correlated system-environment state, suitable linear combinations of the maps introduced for this state allow to deal with all other initial states obtained by local transformations on the system degrees of freedom.

The master equation (3) is typically very difficult to solve or simulate, and a powerful tool to deal with it is that of stochastic unravelings. They consist of stochastic processes taking values on the system's Hilbert space, and the exact dynamics (2) is obtained by averaging over a large number of stochastic realizations

$$\rho(t) = \sum_i \frac{N_i(t)}{N} |\psi_i(t)\rangle \langle\psi_i(t)| , \tag{5}$$

where the $|\psi_i(t)\rangle$ are suitable random pure states. In different unraveling methods, the stochastic realizations can be of two major families: they can either consist of piecewise deterministic processes, interrupted by sudden jumps [32–42], or they can be diffusive [43–47]. In the following, we will consider different unraveling techniques since our results are independent of the particular unraveling scheme used. For the piecewise deterministic methods, we will consider the Monte Carlo wave function (MCWF) [33], which gives positive jump rates if and only if the dynamics is CP divisible, and the generalized rate operator (RO) [41,42], which can give positive rates also in some non-P divisible dynamics. Both methods can be equipped with the non-Markovian quantum jumps (NMQJ) technique [36,37] whenever the jump rates are temporarily negative. For the diffusive methods, we will consider the quantum state diffusion (QSD) [44], which, like the MCWF, can be applied only to CP-divisible dynamics, although extensions to non-Markovian dynamics have been proposed [45]. In Appendix A we provide an overview of these unraveling methods.

So far, these stochastic methods have only been applied to scenarios in which the system and the environment are initially in a product state since they are defined starting from the Lindblad master equation, which is guaranteed to hold only under this assumption. In this work, we will present a method to apply unraveling techniques also in the case in which the dynamics cannot be obtained from a single master equation of the form (3), so as to allow the use of stochastic methods in combination with the OPD formalism for the treatment of initially correlated states of the system and environment.

The rest of the paper proceeds as follows. In Sec. II, we recall two techniques for describing the initially correlated dynamics. Then, in Sec. III, we present our main result, a simple way to apply the stochastic unravelings to the non-positive operators that are used in the OPD, with a simple example of the usefulness of our method. In Sec. IV, we recall the adaptive projection operator (APO) technique to derive the second-order master equations corresponding to the CPTP maps of the OPD. We also provide some examples of unravelings of the initially correlated dynamics obtained via the APO technique. Finally, in Sec. V, we present the conclusions of our work.

II. INITIALLY CORRELATED SYSTEM AND ENVIRONMENT

We now present in more detail the two techniques to deal with the initially correlated system and environment states recalled in the Introduction to better clarify the difference between the approaches and the point of connection with stochastic methods for the solution of the obtained reduced equations of motion.

A. One-sided positive decomposition

One possible way to describe the reduced dynamics of the initially correlated system and environment is via the so-called OPD. This technique relies on the fact that any system side operator can be expanded in terms of frames, i.e., a possibly overcomplete basis of system side operators $\{Q_\alpha\}_\alpha \subset \mathcal{L}_2(\mathscr{H}_S)$ of self-adjoint Hilbert-Schmidt class operators [48,49]. For arbitrarily dimensional systems and environments, one can always construct frames such that any bipartite system-environment state $\rho_{SE} \in \mathcal{S}(\mathscr{H}_S \otimes \mathscr{H}_E)$ can be written as [30]

$$\rho_{SE} = \sum_\alpha w_\alpha Q_\alpha \otimes \rho_\alpha, \tag{6}$$

where w_α are positive numbers and the environmental operators ρ_α corresponding to the frame element Q_α are density matrices, i.e., environmental states. The representation of Eq. (6) is known as OPD. Such a frame $\{Q_\alpha\}_\alpha$ giving states on the environmental side is highly nonunique, see [30] for more details. In this work, we consider a special case of frame $\{Q_\alpha\}_\alpha$ such that, for $\alpha > 0$, the frame elements Q_α are proportional to the generalized Pauli matrices, while Q_0 is proportional to $\mathbb{1}_d - \sum_{\alpha>0} Q_\alpha$; see Eq. (36) for an explicit construction of the frame for the case in which the system is a qubit. The number of terms in the sum is bounded by d^2, where $d = \dim \mathscr{H}_S$ [50].

The reduced system state is obtained as

$$\rho_S = \mathrm{tr}_E\, \rho_{SE} = \sum_\alpha w_\alpha Q_\alpha, \tag{7}$$

with the weights and environmental states implicitly defined as

$$w_\alpha \rho_\alpha = \mathrm{tr}_E[(P_\alpha \otimes \mathbb{1}_E)\rho_{SE}], \tag{8}$$

where $\{P_\alpha\}_\alpha$ is the dual frame of $\{Q_\alpha\}_\alpha$, i.e., the frame such that any operator A acting on $\mathscr{H}_S$ can be written as

$$A = \sum_\alpha \mathrm{tr}[AP_\alpha]Q_\alpha = \sum_\alpha \mathrm{tr}[AQ_\alpha]P_\alpha. \tag{9}$$

Such a dual frame can be taken to be composed of positive operators such that $\mathrm{tr}[P_\alpha Q_\beta] = \delta_{\alpha\beta}$. In this case, it can be written as [30]

$$P_\alpha = \sum_\beta M_{\alpha\beta} Q_\beta, \quad M = (T^\top T)^{-1}, \tag{10}$$

where T is a $d^2 \times d^2$ matrix with coefficients $T_{\alpha\beta} = \mathrm{tr}[Q_\alpha G_\beta]$ and $\{G_\beta\}_\beta$ is an orthonormal basis of Hermitian operators on $\mathscr{H}_S$. Notice that the weights and states of Eq. (8) depend not only on the frame $\{Q_\alpha\}_\alpha$, but also on the arbitrary global state ρ_{SE}. Furthermore, if ρ_{SE} can be written using positive operators Q_α also on the system side, then it is separable [51]; if, additionally, Q_α or ρ_α (or both) are orthogonal projectors, then ρ_{SE} is zero-discord [52–54].

Equation (6) allows us to write the time evolution of ρ_S as the weighted sum of CPTP maps

$$\rho_S(t) = \sum_\alpha w_\alpha \Phi_t^\alpha[Q_\alpha], \tag{11}$$

where the dynamical maps

$$\Phi_t^\alpha[\cdot] := \mathrm{tr}_E[U(t)(\cdot \otimes \rho_\alpha)U^\dagger(t)] \tag{12}$$

are guaranteed to be CPTP since $\rho_\alpha \in \mathcal{S}(\mathscr{H}_E)$, and for each term of the sum system and environment are factorized.

With the same set of CPTP maps $\{\Phi_t^\alpha\}$, it is possible to obtain not only the dynamics of ρ_{SE}, but also the dynamics of all states obtainable from it via system-side operations. Let $\mathcal{R}$ be a completely positive operation on $\mathcal{S}(\mathscr{H}_S)$ and

$$\rho_{SE}^{\mathcal{R}} := \frac{(\mathcal{R}\otimes \mathrm{id})\rho_{SE}}{\mathrm{tr}\,[(\mathcal{R}\otimes \mathrm{id})\rho_{SE}]}, \tag{13}$$

then the time evolution of $\rho_S^{\mathcal{R}} = \mathrm{tr}_E\, \rho_{SE}^{\mathcal{R}}$ is given by

$$\rho_S^{\mathcal{R}}(t) = \frac{\sum_{\alpha,\alpha'} w_\alpha R_{\alpha,\alpha'} \Phi_t^\alpha[Q_{\alpha'}]}{\sum_\alpha w_\alpha \,\mathrm{tr}\, \mathcal{R}[Q_\alpha]}, \tag{14}$$

where $R_{\alpha,\alpha'}$ is an expansion of $\mathcal{R}$ in the basis $\{Q_\alpha\}$, i.e., $\mathcal{R}[Q_\alpha] = \sum_{\alpha,\alpha'} R_{\alpha,\alpha'} Q_{\alpha'}$. Therefore, with up to d^2 maps $\{\Phi_t^\alpha\}$, it is possible to describe the reduced dynamics starting from all system-environment states of the form (13). The set of such global states has dimension up to $(d^4 - 1)$, with the maximum obtained if ρ_{SE} is maximally entangled [30]. For instance, if the initial state is

$$|\Psi_{SE}\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} |k\rangle \otimes |k\rangle\,, \tag{15}$$

then all the maximally entangled generalized Bell states [55]

$$|\Psi_{n,m}\rangle = \frac{1}{\sqrt{d}} \sum_{k=0}^{d-1} e^{2\pi i k n/d} |k \oplus m\rangle \otimes |k\rangle\,, \tag{16}$$

with $n, m = 0, \dots, d-1$, and $k \oplus m = k + m \mod d$, can be obtained via system side repreparations

$$|k\rangle \mapsto e^{2\pi i k n/d} |k \oplus m\rangle\,. \tag{17}$$

Also, all zero discord states $\rho_S^{\mathcal{R}_0} = \sum_{k=0}^{d-1} p_k |k\rangle\langle k| \otimes |k\rangle\langle k|$ can be obtained via the repreparation $\mathcal{R}_0[\rho] = \sum_{k=0}^{d-1} p_k \langle k|\rho|k\rangle |k\rangle\langle k|$. The price one has to pay to do so is to compute the $d^2 \times d^2$ matrix $R_{\alpha,\alpha'}$. Nevertheless, computing this matrix is an arguably less complicated task than directly computing the time evolution of all states as in Eq. (13).

B. Fixed correlations approach

Another possible way to deal with initially correlated system and environment is to start by fixing the environmental state ρ_E and correlations χ, with $\chi = \chi^\dagger$, $\mathrm{tr}\,\chi = 0$ [31]. The global state reads

$$\rho_{SE} = \rho_S \otimes \rho_E + \chi, \tag{18}$$

and the reduced evolved state can then be written as

$$\rho_S(t) = \Phi_t^\chi[\rho_S] := \Phi_t[\rho_S] + I_t^\chi, \tag{19}$$

$$\begin{aligned} \Phi_t &= \mathrm{tr}_E[U(t)\rho_S \otimes \rho_E U^\dagger(t)], \\ I_t^\chi &= \mathrm{tr}_E[U(t)\chi U^\dagger(t)], \end{aligned} \tag{20}$$

where Φ_t is the CP map describing the uncorrelated evolution, with the initial correlations entirely described by I_t^χ. From here, it is possible to derive a single master equation

$$\mathcal{L}_t^\chi[X] := \dot{\Phi}_t^\chi \circ \left(\Phi_t^\chi\right)^{-1}[X] = \mathcal{L}_t[X] + \Delta_t^\chi \,\mathrm{tr}\, X, \tag{21}$$

where $\mathcal{L}_t = \dot{\Phi}_t \circ \Phi_t^{-1}$ is the generator of the uncorrelated dynamics, and

$$\Delta_t^\chi = \dot{I}_t^\chi - \mathcal{L}_t\big[I_t^\chi\big] \tag{22}$$

is the correlated part. It is always possible to put Δ_t^χ in Lindblad form

$$\Delta_t^\chi \,\mathrm{tr}\, X = \sum_i \eta_i(t)\left[J_i(t) X J_i^\dagger(t) - \frac{1}{2}\{J_i^\dagger(t) J_i(t), X\}\right], \tag{23}$$

where

$$J_i(t) = G_i(t) - \frac{1}{d}\,\mathrm{tr}[G_i(t)]\mathbb{1}_d, \tag{24}$$

$$G_i(t) = |\xi_j(t)\rangle\langle \xi_{j'}(t)|\,, \quad \eta_i(t) = b_j(t), \tag{25}$$

where $i = \{j, j'\}$ is a double index and $|\xi_j(t)\rangle$ and $b_j(t)$ are (respectively) the eigenvectors and eigenvalues of Δ_t^χ, i.e.,

$$\Delta_t^\chi = \sum_j b_j(t)\,|\xi_j(t)\rangle\langle \xi_j(t)|\,. \tag{26}$$

Since the master equation (21) can always be put in Lindblad form, then all unraveling methods can be applied in a straightforward way.

The resulting master equation (21), however, does not describe the evolution of the entire set of quantum states $\mathcal{S}(\mathscr{H})$, but only of a limited subset, depending on both ρ_E and χ and containing all states $\rho \in \mathcal{S}(\mathscr{H}_S)$ such that

$$\rho \otimes \rho_E + \chi \geqslant 0. \tag{27}$$

This subset can even contain only a single state, as happen, for example, if χ and ρ_E are the correlations and environmental state corresponding to a maximally entangled system environment state. For further details see Appendix B.

It is worth noticing that, since Δ_t^χ is traceless, then the sum of the rates of the correlated generator $\eta_i(t)$ must also equal zero

$$\sum_i \eta_i(t) = \sum_j b_j(t) = \operatorname{tr} \Delta_t^\chi = 0, \tag{28}$$

and therefore, at least one rate must be negative at all times. Therefore, even if the uncorrelated generator $\mathcal{L}_t$ has all positive rates, it might happen that the addition of the correlated term gives rise to some negative rates for $\mathcal{L}_t^\chi$, thus making the dynamics more difficult and computationally expensive to unravel.

For example, if one considers χ and ρ_E corresponding to a maximally entangled state and a global unitary evolution $U(t)$ giving a unital uncorrelated reduced evolution, i.e., $\Phi_t[\mathbb{1}] = \mathbb{1}$, then the corresponding dynamics has a negative rate already at $t = 0$. This happens because the generator at $t = 0$ is simply

$$\mathcal{L}_0^\chi[\rho_S(0)] = \Delta_0^\chi, \tag{29}$$

since $\rho_S(0) = \mathbb{1}_d/d$ and $\mathcal{L}_t[\mathbb{1}] = 0$ because of unitality of Φ_t. In this case, not only the correlated generator Δ_t^χ has some negative rates at $t = 0$, but also the total generator $\mathcal{L}_t^\chi$ does. The fact that such negativity is present since $t = 0$ not only makes the unravelings computationally more expensive, but might also cause the failure of the reverse jumps. An explicit example of such a kind of dynamics will be discussed in Sec. III B.

For these reasons, as well as the fact that unravelings can be directly applied in this formalism, in the following we will only focus on the OPD formalism, for which unravelings cannot be applied in a straightforward way since the initial condition of the master equation is not a density matrix. Notice that recently a Keldysh-contour based (two-state) unraveling that can deal with both uncorrelated and correlated initial global states was introduced [56].

III. UNRAVELINGS WITH ONE-SIDED POSITIVE DECOMPOSITION

When the system and environment are initially uncorrelated, it is possible to derive a single generator $\mathcal{L}_t$ in Lindblad form, valid for all open system initial states. Starting from such a generator, it is possible to approximate the dynamics by applying the unraveling techniques to it. So far, however, such stochastic techniques have only been applied to the uncorrelated system and environment. In this section, we provide a way to apply them also to cases in which initial correlations are present, by exploiting the OPD formalism.

A. Unravelings for nonpositive operators

For the initially uncorrelated system environment, the reduced dynamics is described by a single Lindblad master equation $d\rho/dt = \mathcal{L}_t[\rho]$, depending on the environmental state ρ_E. If, instead, the system and environment are initially correlated, it is not possible to derive a single master equation. However, the OPD (6) allows one to write the correlated state ρ_{SE} as a sum of uncorrelated terms $Q_\alpha \otimes \rho_\alpha$ with weights w_α. Since each term is uncorrelated and with a state ρ_α on the environmental side, the associated reduced operator will evolve according to a Lindblad master equation

$$\frac{d}{dt} Q_\alpha(t) = \mathcal{L}_t^\alpha[Q_\alpha(t)], \quad \mathcal{L}_t^\alpha = \dot{\Phi}_t^\alpha \circ \left(\Phi_t^\alpha\right)^{-1}, \tag{30}$$

where the generator $\mathcal{L}_t^\alpha$ depends on the corresponding environmental state ρ_α. Since Eq. (6) contains up to $d^2 - 1$ terms, then to describe the reduced dynamics one needs up to $d^2 - 1$ generators $\{\mathcal{L}_t^\alpha\}_{\alpha=1}^{d^2-1}$, see Fig. 1. The maps Φ_t^α of Eq. (12) are the solutions of the Lindblad master equations generated by $\mathcal{L}_t^\alpha$.

When applying unravelings, another crucial difference between the two scenarios is that the master equation for the initially uncorrelated case has a state $\rho(0)$ as initial condition, and therefore, its time evolution can be described as a convex mixture of pure states as in Eq. (5). When correlations are present, instead, each generator $\mathcal{L}_t^\alpha$ has a nonpositive (but self-adjoint) operator Q_α as initial condition, which cannot be written as a convex mixture of pure states. Nevertheless, it is possible to reconcile stochastic unravelings and OPD by noticing that the system-side operators Q_α can always be written as the weighted difference of two states

$$Q_\alpha = Q_\alpha^+ - Q_\alpha^- = \mu_\alpha^+ \Sigma_\alpha^+ - \mu_\alpha^- \Sigma_\alpha^-, \tag{31}$$

where $Q_\alpha^\pm \geqslant 0$ are the positive and negative parts of Q_α

$$Q_\alpha^\pm = \tfrac{1}{2}(|Q_\alpha| \pm Q_\alpha), \quad |X| = \sqrt{X^\dagger X}, \tag{32}$$

$\mu_\alpha^\pm = \operatorname{tr} Q_\alpha^\pm$, and $\Sigma_\alpha^\pm = Q_\alpha^\pm/\mu_\alpha^\pm$. It is straightforward to verify that the $\Sigma_\alpha^\pm$ defined this way are indeed self-adjoint, positive, trace-one operators, i.e., $\Sigma_\alpha^\pm \in \mathcal{S}(\mathscr{H}_S)$. Furthermore, $\Sigma_\alpha^\pm$ do not depend on ρ_{SE}, but only on the fixed operators Q_α.

Then it is possible to unravel the $\mathcal{L}_\alpha$ with $\Sigma_\alpha^\pm$ as initial conditions in the same way as for the uncorrelated case,since the states $\Sigma_\alpha^\pm$ can be written as convex mixture of pure states, thus obtaining $\Phi_t^\alpha[\Sigma_\alpha^\pm]$. The linearity and positivity of Φ_t^α ensure that this way of writing Q_α is preserved by the time evolution

$$Q_\alpha(t) = \Phi_t^\alpha[Q_\alpha] = \mu_\alpha^+ \Phi_t^\alpha[\Sigma_\alpha^+] - \mu_\alpha^- \Phi_t^\alpha[\Sigma_\alpha^-]. \tag{33}$$

Therefore, unraveling with the states $\Sigma_\alpha^\pm$ as initial conditions allows to reconstruct the time evolution of Q_α. The evolution of the system state can then be obtained as

$$\rho_S(t) = \sum_\alpha w_\alpha \mu_\alpha^+ \Phi_t^\alpha[\Sigma_\alpha^+] - w_\alpha \mu_\alpha^- \Phi_t^\alpha[\Sigma_\alpha^-]. \tag{34}$$

Therefore, it is possible to obtain the dynamics of the marginal state ρ_S of the initially correlated global state by unraveling each of the generators $\mathcal{L}_t^\alpha$, with initial states Σ_α^+ and Σ_α^-, and then recombining them with weights $\pm w_\alpha \mu_\alpha^\pm$.

In the literature, unraveling methods relying on additional degrees of freedom [57–62] or temporarily negative probabilities for the occupation of certain states [63] have been introduced. These methods can also be applied to the generators obtained via the OPD.

The use of unraveling techniques is consistent with the system-side repreparations of Eq. (14). The time evolution of any state $\rho_S^{\mathcal{R}} = \operatorname{tr}_E[(\mathcal{R} \otimes \mathrm{id})\rho_{SE}]$, obtained from ρ_{SE} via a

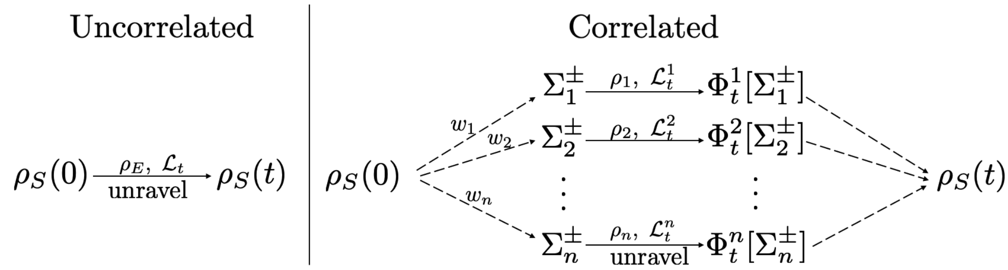

FIG. 1. For the uncorrelated case, a single Lindblad master equation, depending on ρ_E, is sufficient to describe the reduced evolution. If initial correlations are present, then one needs a set of up to d^2-1 master equations, one for each term of Eq. (6), to describe the reduced evolution. Such master equations act on non-positive operators Q_α, and therefore, cannot be directly unraveled. However, as discussed in Sec. III, they can be reconstructed from positive operators $\Sigma_\alpha^\pm$, which can be unraveled.

system-only operation $\mathcal{R}$, can be written as

$$\rho_S^{\mathcal{R}}(t) = \frac{\sum_{\alpha,\alpha'} w_\alpha R_{\alpha,\alpha'}(\mu_{\alpha'}^+ \Phi_t^\alpha[\Sigma_{\alpha'}^+] - \mu_{\alpha'}^- \Phi_t^\alpha[\Sigma_{\alpha'}^-])}{\sum_\alpha w_\alpha \,\mathrm{tr}\,\mathcal{R}[Q_\alpha]}. \tag{35}$$

Therefore, from unraveling the master equations $\mathcal{L}_t^\alpha$ with initial states $\Sigma_{\alpha'}^\pm$, one can obtain the reduced dynamics of all states obtainable via local repreparations on the system only from a reference initial system-environment state ρ_{SE}.

Notice that our method can be applied to arbitrarily dimensional systems, with the number of master equations to be considered that scales quadratically with the dimension of the system's Hilbert space, as it follows from the OPD technique of Sec. II. If one considers infinite-dimensional systems, then one must necessarily truncate the dimensionality to apply any computational method, but this fact is not peculiar to our method. Furthermore, the dimensionality of the environment does not play any role since the number of master equations and the frame $\{Q_\alpha\}$ only depend on the system. Therefore, our method can be applied in a straightforward way to infinite-dimensional or structured environments.

For the sake of example, we now provide one possible choice for a frame $\{Q_\alpha\}_\alpha$, as well as the environmental states ρ_α for the special case in which the system is a qubit $\mathscr{H}_S = \mathbb{C}^2$, without making any assumption on the dimension of $\mathscr{H}_E$. One possible choice of frame for the system is given by

$$Q_0 = \frac{\mathbb{1} - \sum_i \sigma_i}{2}, \quad Q_i = \frac{1}{2}\sigma_i, \tag{36}$$

where σ_i, $i = x, y, z$, are the Pauli matrices, leading to a positive frame for the environment

$$\rho_0 = \mathrm{tr}_S\, \rho_{SE}, \quad \rho_i = \frac{1}{w_i}\mathrm{tr}_S\,[((\mathbb{1}+\sigma_i)\otimes \mathbb{1}_E)\rho_{SE}] \tag{37}$$

with weights

$$w_0 = 1, \quad w_i = \mathrm{tr}_{SE}\,[((\mathbb{1}+\sigma_i)\otimes\mathbb{1}_E)\rho_{SE}]. \tag{38}$$

The corresponding dual frame $\{P_\alpha\}_\alpha$ of Eq. (10) reads

$$P_0 = \mathbb{1}, \quad P_i = \mathbb{1} + \sigma_i. \tag{39}$$

This choice of a system frame can be generalized in a straightforward way to higher-dimensional systems by considering the generalized Pauli matrices instead of the σ_i.

From Eq. (36), it is possible to obtain the states $\Sigma_\alpha^\pm$ and weights $\mu_\alpha^\pm$ of Eq. (31) in a straightforward way. For $\alpha = x, y, z$, one has $\mu_x^\pm = \mu_y^\pm = \mu_z^\pm = 1$ and the corresponding states are simply the positive and negative eigenstates of the Pauli matrices

$$\sigma_x = |+\rangle\langle+| - |-\rangle\langle-|,$$
$$\sigma_y = |+_y\rangle\langle+_y| - |-_y\rangle\langle-_y|, \tag{40}$$

$$\sigma_z = |1\rangle\langle1| - |0\rangle\langle0|. \tag{41}$$

For $\alpha = 0$, the expression of the states $\Sigma_0^\pm$ instead reads

$$Q_0 = \mu_0^+ |\phi_0^+\rangle\langle\phi_0^+| - \mu_0^- |\phi_0^-\rangle\langle\phi_0^-|, \quad \mu_0^\pm = \frac{\sqrt{3}\pm 1}{2}, \tag{42}$$

$$|\phi_0^\pm\rangle = \frac{\pm\sqrt{3}-1}{2\sqrt{3\mp\sqrt{3}}}(i-1)|1\rangle + \frac{1}{\sqrt{3\mp\sqrt{3}}}|0\rangle. \tag{43}$$

The explicit form of the environmental states (37), and therefore, of the generators $\mathcal{L}_t^\alpha$, will depend on the full system-environment state. Let us suppose that the initial state is entangled and of the form

$$|\Psi_{SE}\rangle = \frac{|0\rangle\otimes|\psi_0\rangle + |1\rangle\otimes|\psi_1\rangle}{\sqrt{2}}, \tag{44}$$

with $|\psi_{0,1}\rangle$ not necessarily orthogonal. Let us stress the fact that we are not making any assumptions on the dimensionality of the environment and it can even be infinite-dimensional. The environmental states of the OPD are

$$\rho_0 = \tfrac{1}{2}(|\psi_0\rangle\langle\psi_0| + |\psi_1\rangle\langle\psi_1|), \quad \rho_x = |\phi_x\rangle\langle\phi_x|, \tag{45}$$

$$\rho_y = |\phi_y\rangle\langle\phi_y|, \quad \rho_z = |\psi_1\rangle\langle\psi_1|, \tag{46}$$

with

$$|\phi_x\rangle = \frac{|\psi_0\rangle + |\psi_1\rangle}{\sqrt{N_x}}, \quad N_x = 2(1 + \mathrm{Re}\,\langle\psi_0|\psi_1\rangle), \tag{47}$$

$$|\phi_y\rangle = \frac{|\psi_0\rangle + i|\psi_1\rangle}{\sqrt{N_y}}, \quad N_y = 2(1 - \mathrm{Im}\,\langle\psi_0|\psi_1\rangle), \tag{48}$$

with weights

$$w_0 = w_z = 1, \quad w_{x,y} = \frac{N_{x,y}}{2}. \tag{49}$$

The dynamics of $\Phi_t^{0,z}$ can be unraveled by mixing the dynamics obtained from the generators obtained with $|\psi_i\rangle$ as initial states. For $\Phi_t^{x,y}$ this is indeed no longer the case and one needs to simulate the dynamics with different initial environmental states.

B. Example: Dephasing dynamics

As a first example of the application of the unravelings to the OPD, let us consider an exactly solvable dephasing dynamics for a d-dimensional system [5]. They are a class of dynamics such that the populations are preserved

$$\frac{d}{dt}\langle k|\Phi_t[\rho]|k\rangle = 0, \quad \forall k = 1, \dots, d, \tag{50}$$

while coherences are not. This is obtained by considering system-environment Hamiltonians of the form

$$H = H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E + \sum_{k=1}^{d} |k\rangle\langle k| \otimes B_k, \tag{51}$$

where $H_S = \sum_k E_k |k\rangle\langle k|$, and $B_k = B_k^\dagger$ are arbitrary environmental operators defining the coupling. For this model, both the maps Φ_t^α and the generators $\mathcal{L}_t^\alpha$ of Eqs. (12) and (30) can be analytically calculated. The master equations read

$$\mathcal{L}_t^\alpha[X] = -i[H_\alpha(t), X] + \sum_{k,\ell=1}^{d-1} K_{k\ell}^\alpha(t)\left(S_k X S_\ell - \frac{1}{2}\{S_\ell S_k, X\}\right), \tag{52}$$

where

$$S_\ell = \frac{1}{\sqrt{\ell(\ell+1)}}\left(\sum_{k=0}^{\ell-1} |k\rangle\langle k| - \ell\,|\ell\rangle\langle \ell|\right), \tag{53}$$

and $K_{k\ell}^\alpha(t)$ is a self-adjoint matrix which depends on the environmental state ρ_α. Equation (52) can be put in Lindblad form by diagonalizing the matrix $K_{k\ell}^\alpha(t)$. This class of dephasing dynamics contains as a special case the spin boson dephasing in the presence of initial correlations [64,65]. Our method, being independent of the particular system-environment, can be applied also to this special case.

We now proceed to apply stochastic unravelings for this type of dynamics. For the sake of example, we now fix $d = 4$, $\mathscr{H}_E = \mathscr{H}_S = \mathbb{C}^4$, and

$$H_S = H_E = \Omega \sum_{k=1}^{4} k\,|k\rangle\langle k|\,, \tag{54}$$

$$B_k = g(|k\rangle\langle k+1| + |k+1\rangle\langle k|), \quad k = 1, 2, 3, \tag{55}$$

and $B_4 = 0$. As initial state, let us consider the maximally entangled state

$$|\Psi_{SE}\rangle = \frac{|1,1\rangle + |2,2\rangle + |3,3\rangle + |4,4\rangle}{2}. \tag{56}$$

The system-side frame Q_α can be obtained similarly to the qubit case of Eq. (36) as

$$Q_0 = \frac{1}{4}\mathbb{1}_4 - \frac{1}{2}\sum_\alpha \sigma_\alpha, \quad Q_\alpha = \frac{1}{2}\sigma_\alpha, \tag{57}$$

where the σ_α are the generalized 4×4 Pauli matrices. The corresponding environmental states ρ_α can be found in Appendix C. The unravelings can, therefore, be applied to the generators $\mathcal{L}_t^\alpha$ with the initial conditions from the system-side states $\Sigma_\alpha^\pm$ obtained from the positive and negative part of the operators Q_α of Eq. (57) via Eq. (31). The $Q_\alpha(t)$ are then reconstructed via Eq. (33) and the reduced dynamics via Eq. (34).

With this choice, all the resulting maps Φ_t^α are CP divisible up to some time, and therefore, the unravelings can be performed using the MCWF and the QSD techniques up to that time. The unraveling of $\mathcal{L}_t^x$, in the interaction picture with respect to the free Hamiltonian $H_S + H_E$, with initial conditions the states $\Sigma_x^\pm$, corresponding to the frame element Q_x, are shown in the left and middle panels of Fig. 2. In the right panel, the dynamics of Q_x is obtained from the dynamic of Σ_x^+ and Σ_x^- by combining them with appropriate weights. The code used for obtaining the unravelings is available in [66].

If one neglects the correlations and simply considers the dynamics of $\rho_S \otimes \rho_E$, then the resulting time evolution is trivial since $\rho_S = \mathbb{1}/4$ and the dynamics is unital. However, when the initial correlations are taken into account, there is a revival in coherence $\langle 0|\rho_S(t)|1\rangle$, as can be seen in the right panel of Fig. 2.

If one performs the unravelings of all $\mathcal{L}_t^\alpha$ with initial conditions $Q_{\alpha'}$ then, via Eq. (14), it is possible to describe a subspace of initial states with dimension $d^4 - 1 = 255$. This subspace contains, for example, all the generalized Bell states of Eq. (16), as well as all zero-discord states $\rho_S^{\mathcal{R}_0} = \sum_{k=0}^{3} p_k\,|k\rangle\langle k| \otimes |k\rangle\langle k|$.

It is worth stressing that if one describes the same dynamics with the fixed correlations approach of Sec. II B, then the resulting dynamics is P indivisible since $t = 0$. This happens because the dephasing is unital, and therefore, the resulting master equation has at least one negative rate, as discussed in Sec. II B, and therefore, is CP indivisible. However, since for the dephasing P and CP divisibility coincide [5], then it is also P indivisible since $t = 0$. This fact causes not only the MCWF to fail, but also the Ψ-RO.

IV. UNRAVELINGS WITH THE ADAPTED PROJECTION OPERATOR TECHNIQUE

To apply stochastic unravelings to the initially correlated system and environment, one does not need the *a priori* knowledge of the maps Φ_t^α, but the knowledge of the generators $\mathcal{L}_t^\alpha$ is sufficient. However, the derivation of the exact generators is, in general, a difficult task. In this section, we recall the adapted projection operator (APO) technique that allows one to derive second-order master equations corresponding to the environmental states ρ_α of the OPD of Eq. (6), thus drastically simplifying the task of deriving the generators. We then apply this technique to two examples, performing the unravelings to the obtained master equations.

A. Adapted projection operator technique

The APO technique generalizes the projector operator technique [1] by introducing projection operators of the form [67]

$$\mathcal{P}_\alpha[\cdot] = \mathrm{tr}_E[\cdot] \otimes \rho_\alpha. \tag{58}$$

Then, the dynamics of the relevant part $\mathcal{P}_\alpha[\rho_{SE}(t)]$ for the system side operators $Q_\alpha(t) = \Phi_t^\alpha[Q_\alpha]$ is described by the

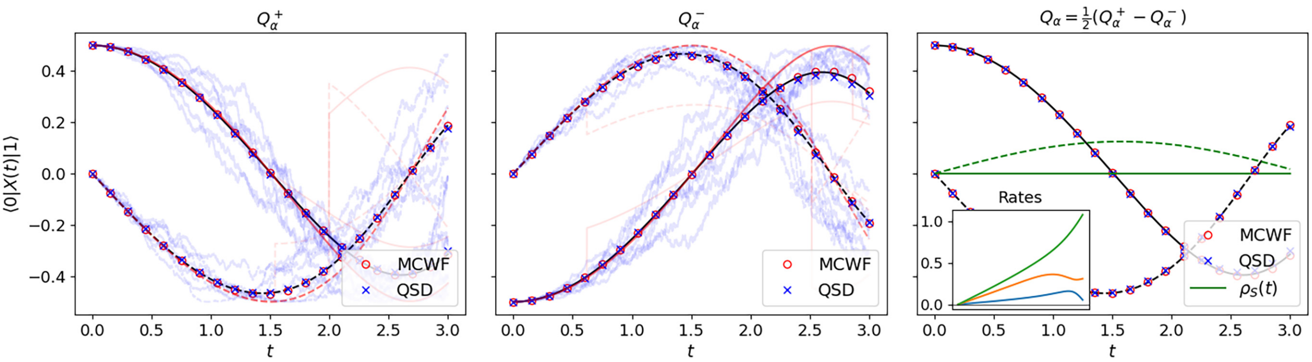

FIG. 2. Unravelings of $\Phi_t^x(Q_x)$ for the dephasing dynamics of Eqs. (54) and (55); showing the real (solid) and imaginary (dashed) components of $\langle 0|\Phi_t^x(Q_x)|1\rangle$. Left: Unraveling of the positive part Σ_x^+. Middle: Unraveling of the negative part Σ_x^-. Right: Unraveling of Q_x, obtained as the difference between the two, and dynamics of the coherence of $\rho_S(t)$ (green). Inset: dephasing rates, i.e., eigenvalues of $K_{k\ell}^x(t)$. The unravelings are done using MCWF (red lines and circles) and QSD (blue lines and crosses) and for both six stochastic trajectories (piecewise deterministic using MCWF and diffusive using QSD) are shown in lighter shades. Parameters: $g = 0.5$, 10^3 stochastic realizations are used.

master equations $dQ_\alpha(t)/dt = \mathcal{L}_t^\alpha[Q_\alpha(t)]$, with

$$\begin{aligned}\mathcal{L}_t^\alpha[X] = &-ig\sum_j [A_j(t), X]\,\langle B_j(t)\rangle_{\rho_\alpha}\\ &- g^2\sum_{j,j'}\int_0^t d\tau\,[A_j(t), A_{j'}(\tau)X]\,\mathrm{Cov}_{j,j'}^{\rho_\alpha}(t,\tau)\\ &+ g^2\sum_{j,j'}\int_0^t d\tau\,[A_j(t), XA_{j'}(\tau)]\,\mathrm{Cov}_{j',j}^{\rho_\alpha}(\tau,t),\end{aligned}\tag{59}$$

where the operators $A_j(t)$ are the system-side operators of the interaction Hamiltonian in the interaction picture with respect to the free Hamiltonian

$$H_I(t) = \sum_j A_j(t)\otimes B_j(t),\tag{60}$$

with $A_j(t) = e^{iH_St}A_je^{-iH_St}$ and $B_j(t) = e^{iH_Et}B_je^{-iH_Et}$, while

$$\mathrm{Cov}_{j,j'}^{\rho_\alpha}(t,\tau) = \langle B_j(t)B_{j'}(\tau)\rangle_{\rho_\alpha} - \langle B_j(t)\rangle_{\rho_\alpha}\langle B_{j'}(\tau)\rangle_{\rho_\alpha},\tag{61}$$

where we use the notation $\langle O\rangle_\rho = \mathrm{tr}[O\rho]$.

Therefore, by using the APO technique, it is possible to derive in a simple way a set of master equations, one for each component in the sum of Eq. (6), describing separately the time evolution of each component Q_α of the reduced state (7).

B. Example: Jaynes-Cummings

As a first example, let us consider a qubit $\mathscr{H}_S = \mathbb{C}^2$ interacting with a bosonic environment, with a Jaynes-Cummings form of the interaction

$$H = \frac{\omega_0}{2}\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sum_k (g_k\sigma_+\otimes b_k + g_k^+\sigma_-\otimes b_k^\dagger).\tag{62}$$

By applying the APO technique, the corresponding master equations read

$$\begin{aligned}\mathcal{L}_t^\alpha[X] = &\,i\beta_+^\alpha(t)[\sigma_+\sigma_-, X] + i\beta_-^\alpha(t)[\sigma_-\sigma_+, X]\\ &+ \gamma_-^\alpha(t)\big(\sigma_-X\sigma_+ - \tfrac{1}{2}\{\sigma_+\sigma_-, X\}\big)\\ &+ \gamma_+^\alpha(t)\big(\sigma_+X\sigma_- - \tfrac{1}{2}\{\sigma_-\sigma_+, X\}\big),\end{aligned}\tag{63}$$

with the rates $\gamma_\pm^\alpha$ and the driving $\beta_\pm^\alpha$ that can be found in [67].

1. Continuum limit

As a first example, let us consider an initial state of the form

$$|\Psi_{SE}\rangle = \frac{1}{\sqrt{2}}\,|0\rangle\otimes|0\rangle + \frac{1}{\sqrt{2}}\,|1\rangle\otimes|\{N_k\}_k\rangle\,,\tag{64}$$

where $|\{N_k\}_k\rangle$ is the environmental state with N_k bosons in the mode of frequency ω_k. The explicit form of the weights w_α and environmental states ρ_α can be found in [67]. Although the APO technique was already used on this example, we stress that unravelings could not be performed because of the nonpositivity of the system side operators. Here, we use the same example and use our results of Sec. III to apply unravelings to the resulting dynamics.

We consider infinitely many bath modes in the continuum limit [1] and an Ohmic spectral density

$$J(\omega) = g\omega\Theta(\omega_c - \omega),\tag{65}$$

where Θ is the Heaviside theta function and ω_c a cutoff frequency, and we assume N bosons up to ω_c

$$N(\omega) = N\Theta(\omega_c - \omega).\tag{66}$$

We find that, under a suitable choice of the parameters, the rates $\gamma_\pm^\alpha$ of the master equation (63) remain positive at all times, as shown in the inset of Fig. 3. Because of this, the unraveling methods for Markovian dynamics are sufficient for describing the dynamics. Indeed, in Fig. 3 we show the unravelings obtained using the MCWF and QSD techniques. Like in Sec. III B, we first unravel separately the positive and negative parts $\Sigma_\alpha^\pm$ of the frame element Q_α and then recombine the two to obtain the dynamics of Q_α. From these unravelings,

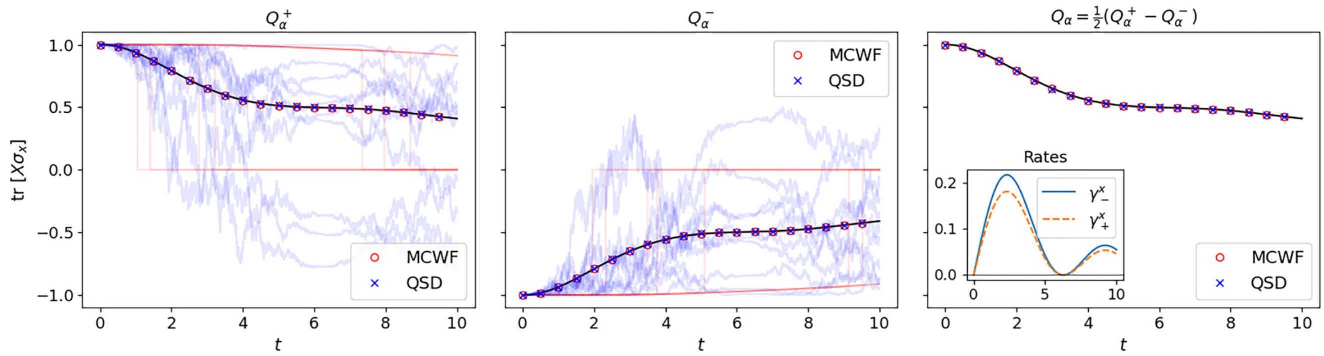

FIG. 3. Unraveling of $\Phi_t^x[Q_x]$ for the Jaynes-Cummings dynamics in the continuum limit, for the maximally initial state of Eq. (64). Left: unravelings for the positive part of Q_x; middle: for the negative part; right: Q_x is obtained as the difference between the two. The unravelings are done both with the MCWF (red circles) and QSD (blue crosses), and ten trajectories are shown. Inset: rates $\gamma_\pm^x$ for $\mathcal{L}_t^x$ of Eq. (63). Parameters: $g = 0.05$, $N = 10$. 10^4 stochastic realizations are used.

one is then able to also obtain the dynamics of all initial states obtainable via system-only repreparations according to Eq. (35).

2. Single mode

Let us now consider the case of a single mode with a maximally entangled initial state of the form

$$|\Psi_{SE}\rangle = \frac{|0\rangle \otimes |n_0\rangle + |1\rangle \otimes |n_1\rangle}{\sqrt{2}}. \tag{67}$$

For this intial state, the rates read

$$\gamma_+^\alpha(t) = |g|^2(n_\alpha + 1)\frac{\sin[(\omega_0 - \omega)t]}{\omega_0 - \omega}, \tag{68}$$

$$\gamma_-^\alpha(t) = |g|^2 n_\alpha \frac{\sin[(\omega_0 - \omega)t]}{\omega_0 - \omega}, \tag{69}$$

where $n_\alpha = \mathrm{tr}[\hat{n}\rho_\alpha]$, with ρ_α as in Eqs. (45) and (46). It is worth noticing that $\Phi_t^0 = \Phi_t^x = \Phi_t^y$ since the dynamics depends on ρ_α only via n_α and $n_0 = n_x = n_y$. It is easy to see that the rates are either both positive or both negative at the same time and correspondingly the dynamics is non-Markovian. Nevertheless, it is possible to perform the unravelings by using the NMQJ technique with an effective ensemble consisting of only three states: the deterministically evolving initial state $|\psi_{\mathrm{det}}(t)\rangle$ and the eigenstates $|0\rangle, |1\rangle$ of σ_z. The results are shown in the left panel of Fig. 4.

Additionally, if one performs the unravelings also of $\Phi_t^\alpha[Q_{\alpha'}]$, $\alpha' \neq \alpha$, then it is possible to obtain the evolution of all initial states obtainable from ρ_{SE} via system-only repreparations according to Eq. (35). This task is drastically simplified by the fact that some maps are actually the same: $\Phi_t^0 = \Phi_t^x = \Phi_t^y$. For instance, it is possible to recover the reduced dynamics corresponding to a zero discord initial state

$$\rho_{SE}^{\mathcal{R}_0^p} = p\,|0\rangle\langle 0| \otimes |n_0\rangle\langle n_0| + (1-p)\,|1\rangle\langle 1| \otimes |n_1\rangle\langle n_1| \tag{70}$$

or to the factorized initial state in which the correlations are eliminated

$$\rho_{SE}^{\mathcal{R}_\mathrm{f}} = \frac{\mathbb{1}}{2} \otimes \frac{|n_0\rangle\langle n_0| + |n_1\rangle\langle n_1|}{2}. \tag{71}$$

The dynamics corresponding to such initial states is shown in the right panel of Fig. 4. Clearly, the different kinds of correlations play nontrivial roles in modifying the resulting dynamics.

C. Example: Damped two-qubit model

As a last example, let us consider two interacting qubits, considering one of them as our system and the other as the environment, with the environmental qubit also coupled to an external harmonic oscillator. The global Hamiltonian reads

$$H = \frac{\omega_1}{2}\sigma_z \otimes \mathbb{1} \otimes \mathbb{1} + \frac{\omega_2}{2}\mathbb{1} \otimes \sigma_z \otimes \mathbb{1} + \omega\mathbb{1} \otimes \mathbb{1} \otimes b^\dagger b$$
$$+ g\sigma_x \otimes \sigma_z \otimes \mathbb{1} + \mu\mathbb{1} \otimes (\sigma_+ \otimes b + \sigma_- \otimes b^\dagger), \tag{72}$$

where $b^\dagger$ and b are (respectively) the creation and annihilation operators. As the initial state, we consider a maximally entangled state in which the entanglement is shared between the system qubit and the environmental qubit, with the harmonic

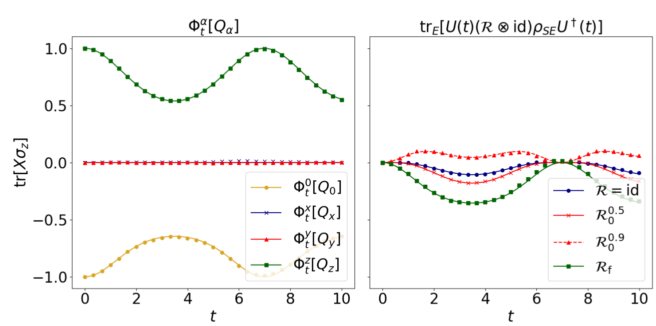

FIG. 4. Unravelings of the single-mode Jaynes-Cummings dynamics for the maximally entangled initial state of Eq. (67), obtained using NMQJ. Left panel: z component of the Bloch vector for $\Phi_t^\alpha[Q_\alpha]$. Right panel: reduced dynamics for the maximally entangled state (blue) and of states obtained via the system-side repreparations: zero discord states $\rho_{SE}^{\mathcal{R}_0^p}$ of Eq. (70) with $p = 0.5$ (red solid), $p = 0.9$ (red dashed), factorized initial state $\rho_{SE}^{\mathcal{R}_\mathrm{f}}$ of Eq. (71) (green). Parameters: $n_0 = 1, n_1 = 0, \omega_0 = 1, \omega = 0.1, g = 0.5$. 10^4 stochastic realizations are used.

oscillator in the vacuum

$$|\Psi_{SE}\rangle = \frac{|000\rangle + |110\rangle}{\sqrt{2}}. \tag{73}$$

If one calculates the master equations with the APO formalism as in Eq. (59), then the dynamics for ρ_z only adds a driving of the form

$$H_z(t) = g[\cos(\omega_1 t)\sigma_x - \sin(\omega_1 t)\sigma_y]. \tag{74}$$

This happens because the ρ_z covariance of Eq. (61) is zero, and therefore, no terms in g^2 appear in the master equation. The other master equations, instead, give nontrivial modifications to the Lindbladian

$$\mathcal{L}_t^{0,x,y}[X] = -i[H(t), X] + A(t)X\tilde{A}(t) + \tilde{A}(t)XA(t) - \tfrac{1}{2}\{\Gamma(t), X\}, \tag{75}$$

where

$$H(t) = \frac{g}{\omega_1}[1-\cos(\omega_1 t)]\sigma_z,$$

$$\Gamma(t) = 2\frac{g^2}{\omega_1}\sin(\omega_1 t)\mathbb{1}, \tag{76}$$

$$A(t) = g[\cos(\omega_1 t)\sigma_x - \sin(\omega_1 t)\sigma_y], \tag{77}$$

$$\tilde{A}(t) = \int_0^t d\tau\, A(\tau) = \frac{g}{\omega_1}\{\sin(\omega_1 t)\sigma_x - [1-\cos(\omega_1 t)]\sigma_y\}. \tag{78}$$

Notice that the master equations (75) do not depend on the coupling μ with the external bath. This happens because we assume it to be in the vacuum, and the covariances in the APO formalism all have terms proportional to $\langle 0|b|0\rangle$ or $\langle 0|b^\dagger|0\rangle$, which are both zero.

The jump term can be rewritten in the standard Lindblad form

$$\mathcal{J}_t[X] = A(t)X\tilde{A}(t) + \tilde{A}(t)XA(t) = \sum_{i=\pm}\gamma_i(t)L_i(t)XL_i^\dagger(t), \tag{79}$$

where $L_\pm(t)$ are a time-dependent combinations of σ_x and σ_y, with rates

$$\gamma_\pm(t) = \sin(\omega_1 t) \pm 2\sin\left(\frac{\omega_1 t}{2}\right), \tag{80}$$

that are shown in the inset of Fig. 5. Importantly, the resulting dynamics has a negative rate since $t = 0$, and therefore, methods such as the NMQJ fail, but it is possible to unravel the master equation (75) using the Ψ-RO formalism. Additionally, it is possible to have positive unravelings using only three states in the effective ensemble: $|\psi_{\rm det}(t)\rangle$, $|0\rangle$, and $|1\rangle$. These unravelings are shown in Fig. 5. Interestingly, in the Ψ-RO formalism, it is not necessary to explicitly compute the standard Lindblad form of Eq. (79), but the form of Eq. (75) is enough.

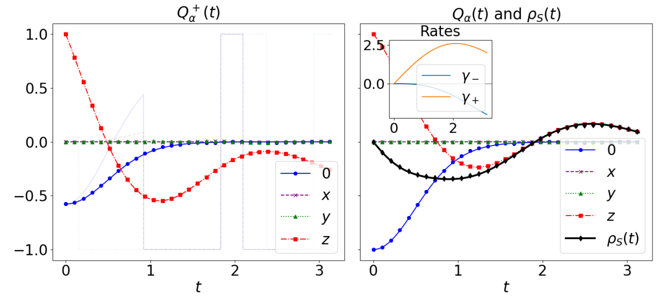

FIG. 5. Unravelings of the system qubit dynamics obtained from Eq. (72). Left: dynamics of $\Phi_t^\alpha[Q_\alpha^+]$, showing (in lighter shade) five trajectories; for $t \leqslant 1$, no reverse jumps are needed even if $\gamma_- < 0$. Right: dynamics of $\Phi_t^\alpha[Q_\alpha]$ and of $\rho_S(t)$. Inset: rates $\gamma_\pm$ of Eq. (80). Parameters: $g = \omega_1 = \omega_2 = \omega = \mu = 1$.

V. CONCLUSIONS

In this work we extended the applicability of stochastic unraveling techniques to the most general case of open systems initially correlated with their environment. As a starting point, we considered the OPD formalism for describing the reduced dynamics, where the system density matrix was described by a sum of nonpositive operators. These operators pose challenges for unravelings, as they cannot be expressed as convex mixtures of pure states. However, we addressed this limitation by decomposing each nonpositive operator as the weighted difference of two states and performing the unravelings separately for each state. Our approach enables the use of both piecewise deterministic and diffusive unravelings even in the most general case of initially correlated system and environment.

We validated our approach with examples, including dephasing and Jaynes-Cummings dynamics, with the master equations obtained either exactly or via the APO technique, generalizations of the projector operator technique in the OPD framework. Different unraveling techniques were used, depending on the presence or absence of negative rates. Our examples also demonstrated that a small number of unravelings sufficed to describe the dynamics of all states obtainable from the initially correlated state via system-only operations.

Wehave also compared our method based on the OPD with another recently introduced formalism that started from fixed correlations and allowed one to obtain a single master equation valid on a subset of the system states. We showed that, if one starts from a maximally entangled state, the fixed correlation approach describes the dynamics of only a single state, while with the OPD one was able to characterize a (d^4-1)-dimensional subspace. Furthermore, the fixed correlations master equation can present a negative rate since $t = 0$, which makes the unravelings notoriously more complicated; the OPD formalism, on the other hand, avoids such an issue, as shown explicitly in the dephasing example of Sec. III B.

Our results allow not only for the use of powerful simulation methods to the most general scenarios, but also for a deeper understanding of the reduced dynamics of the initially correlated system and environment.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [66].

APPENDIX A: STOCHASTIC UNRAVELINGS OF OPEN SYSTEM DYNAMICS

Here, we provide a small overview of some widely used unraveling methods, which are used in our work.

1. Monte-Carlo wave function

Whenever the dynamics is CP divisible [i.e., the rates $\gamma_j(t)$ in the master equation (3) are positive at all times], it is possible to unravel the dynamics via the so-called MCFW method [33]. The deterministic evolution is given by

$$|\psi(t)\rangle \mapsto |\psi(t+dt)\rangle = \frac{(\mathbb{1} - iK(t)\,dt)\,|\psi(t)\rangle}{\|(\mathbb{1} - iK(t)\,dt)\,|\psi(t)\rangle\,\|} \tag{A1}$$

with the effective non-Hermitian Hamiltonian

$$K(t) := H(t) - \frac{i}{2}\Gamma(t), \tag{A2}$$

and is interrupted by sudden jumps

$$|\psi(t)\rangle \mapsto |\psi(t+dt)\rangle = \frac{L_j(t)\,|\psi(t)\rangle}{\|L_j(t)\,|\psi(t)\rangle\,\|} \tag{A3}$$

taking place with probability

$$p^j_{\psi(t)} = \gamma_j(t)\|L_j(t)\,|\psi(t)\rangle\,\|^2 dt. \tag{A4}$$

Naturally, this method fails whenever $\gamma_j(t) < 0$ since it would give rise to negative probabilities for the jumps.

2. Non-Markovian quantum jumps

Whenever the rates $\gamma_j(t)$ become temporarily negative, it is possible to unravel open system dynamics via the non-Markovian quantum jumps (NMQJ) technique [36,37]. The deterministic evolution is as in Eq. (A1). For the jumps, if the rate $\gamma_j(t)$ is positive, they are as in Eq. (A3). If, on the other hand, $\gamma_j(t) < 0$, then the jumps will be

$$|\psi_i(t)\rangle = \frac{L_j(t)\,|\psi_{i'}(t)\rangle}{\|L_j(t)\,|\psi_{i'}(t)\rangle\|} \mapsto |\psi_{i'}(t)\rangle\,, \tag{A5}$$

with probability

$$p^j_{\psi_i(t)\to\psi_{i'}(t)} = -\frac{N_{i'}(t)}{N_i(t)}\gamma_j(t)\|L_j(t)\,|\psi_{i'}(t)\rangle\|^2\;dt, \tag{A6}$$

where $N_{i,i'}$ are the occupations of the realizations $|\psi_{i,i'}(t)\rangle$, as in Eq. (5). These jumps are known as reverse jumps and are possible only if the source state $|\psi_i(t)\rangle$ is the possible target of a jump with a positive rate. The reverse jump, therefore, has the effect of canceling a jump that had previously happened. It is worth stressing that the probability of the reverse jump depends on the target state, instead of the source, and on the ratio $N_{i'}(t)/N_i(t)$, and therefore, the different stochastic realizations are not independent, thus making the simulations more expensive.

3. Generalized rate operator

The master equation (3) can be written as the sum of a jump term

$$\mathcal{J}_t[\rho] := \sum_j \gamma_j(t)L_j(t)\rho L_j^\dagger(t) \tag{A7}$$

and a driving term

$$\mathcal{D}_t[\rho] := -i(K(t)\rho - \rho K^\dagger(t)), \tag{A8}$$

where $K(t)$ is the non-Hermitian Hamiltonian of Eq. (A2). Such a decomposition, however, is highly nonunique: any transformation [40]

$$\mathcal{J}_t[\rho] \mapsto \mathcal{J}'_t[\rho] := \mathcal{J}_t[\rho] + \tfrac{1}{2}(C(t)\rho + \rho C^\dagger(t)), \tag{A9}$$

$$K(t) \mapsto K'(t) := K(t) - \frac{i}{2}C(t) \tag{A10}$$

preserves the structure of the master equation.

From this decomposition, it is possible to define an unraveling method with the deterministic evolution as in Eq. (A1), with $K(t)$ substituted by $K'(t)$, and jumps to the eigenstates $|\varphi^i_{\psi(t)}\rangle$ of the so-called rate operator (RO) [34,39,40]

$$R_{\psi(t)} := \mathcal{J}'[|\psi(t)\rangle\,\langle\psi(t)|], \tag{A11}$$

happening with probability

$$p^i_{\psi(t)} = \lambda^i_{\psi(t)}\,dt, \tag{A12}$$

where $\lambda^i_{\psi(t)}$ is the eigenvalue corresponding to $|\varphi^i_{\psi(t)}\rangle$. Note that both the eigenvalues and the eigenvectors depend on the prejump state.

In [41], it was shown that, given that the stochastic realization is the state $|\psi(t)\rangle$, then it is possible to consider transformations $C(t)$ that depend not only on time, but also on the state of the realization $|\psi(t)\rangle$: $C(t) \mapsto C_{\psi(t)}$. This leads to the introduction of the generalized RO (Ψ-RO), defined as

$$\begin{aligned}\Psi\text{-}R_{\psi(t)} &:= \mathcal{J}_t[|\psi(t)\rangle\,\langle\psi(t)|] \\ &\quad + \tfrac{1}{2}[|\Phi_{\psi(t)}\rangle\,\langle\psi(t)| + |\psi(t)\rangle\,\langle\Phi_{\psi(t)}|],\end{aligned} \tag{A13}$$

with $|\Phi_{\psi(t)}\rangle := C_{\psi(t)}\,|\psi(t)\rangle$. The deterministic evolution is again as in Eq. (A1), but with a nonlinear effective Hamiltonian

$$K_{\psi(t)} = H(t) - \frac{i}{2}\Gamma(t) - \frac{i}{2}\,|\Phi_{\psi(t)}\rangle\,\langle\psi(t)|\,, \tag{A14}$$

and the jumps are to the eigenstates of Ψ-$R_{\psi(t)}$, with probability proportional to the corresponding eigenvalue.

With this new method, it is also possible to unravel some non-Markovian dynamics without the need to use reverse jumps. Nevertheless, when this is not possible, both the RO and the Ψ-RO can be equipped with reverse jumps as the NMQJ technique of Appendix A 2. We refer to unravelings in which only jumps with positive rates occur as positive unravelings.

4. Quantum state diffusion

Quantum state diffusion (QSD) represents a well-known and widely used diffusive unraveling of open system dynamics. In QSD, assuming that all rates are positive, the state vector $|\psi\rangle$ obeys the stochastic Schrödinger equation [44]

$$|d\psi\rangle = -iH|\psi\rangle\,dt + \sum_j \gamma_j(\langle L_j^\dagger\rangle_\psi L_j - L_j^\dagger L_j - \langle L_j^\dagger\rangle_\psi \langle L_j\rangle_\psi)|\psi\rangle\,dt + \sum_j \sqrt{\gamma_j}(L_j - \langle L_j\rangle_\psi)|\psi\rangle\,dW_j, \tag{A15}$$

where the explicit time dependence has been neglected, $\langle L_j\rangle_\psi = \langle\psi|L_j|\psi\rangle$, and dW_j are independent complex Wiener processes satisfying

$$\mathbb{E}[\mathrm{Re}(dW_j)\,\mathrm{Re}(dW_{j'})] = \mathbb{E}[\mathrm{Im}(dW_j)\,\mathrm{Im}(dW_{j'})] = \tfrac{1}{2}\delta_{j,j'}dt \tag{A16}$$

$$\mathbb{E}[dW_j] = \mathbb{E}[\mathrm{Re}(dW_j)\,\mathrm{Im}(dW_{j'})] = 0, \tag{A17}$$

where $\mathbb{E}$ is the expectation value over the trajectories.

The stochastic Schrödinger equation (A15) is readily simulated by adding to the deterministic drift (the first two lines) the stochastic term, with the Wiener processes that are sampled by simply generating random complex Gaussian numbers with zero mean and standard deviation $\sqrt{dt}$. The exact dynamics of Eq. (3) is then obtained by averaging over many realizations of the stochastic process. As it happened for the MCWF, the positivity of all rates is required. However, it is possible to generalize the QSD to master equations having also negative rates via the non-Markovian QSD [45].

APPENDIX B: COMPATIBLE SYSTEM STATES WITH THE FIXED CORRELATIONS APPROACH

We now investigate the set of compatible states in the fixed correlations approach, as in Eq. (27) for global states consisting of mixtures of the maximally entangled and the maximally mixed state. Let $\dim\mathscr{H}_S = \dim\mathscr{H}_E = n$ and

$$\rho_{SE}(\lambda) = \lambda\,|\Psi_{SE}\rangle\langle\Psi_{SE}| + (1-\lambda)\frac{\mathbb{1}_n}{n}\otimes\frac{\mathbb{1}_n}{n}, \tag{B1}$$

for $0 \leqslant \lambda \leqslant 1$, where

$$|\Psi_{SE}\rangle = \frac{1}{\sqrt{n}}\sum_{i=1}^{n}|\varphi_S^i\rangle\otimes|\varphi_E^i\rangle \tag{B2}$$

is a maximally entangled state, where $\{\varphi_S^i\}_i$ and $\{\varphi_E^i\}_i$ are orthonormal sets for (respectively) the system and the environment. The environmental marginal is the maximally mixed state, independently of λ, $\rho_E = \mathbb{1}_n/n$, while the correlations read

$$\chi(\lambda) = \lambda\left[|\Psi_{SE}\rangle\langle\Psi_{SE}| - \frac{\mathbb{1}_n}{n}\otimes\frac{\mathbb{1}_n}{n}\right]. \tag{B3}$$

Proposition B1. The set of compatible states $\rho_S(\lambda)$ such that $\rho_S(\lambda)\otimes\rho_E + \chi(\lambda) \geqslant 0$ consists of all states of the form

$$\rho_S(\lambda) = \lambda\frac{\mathbb{1}_n}{n} + (1-\lambda)\sigma_S, \tag{B4}$$

where σ_S is an arbitrary state in $\mathcal{S}(\mathscr{H}_S)$.

Proof. In the basis $\{\varphi_S^i\otimes\varphi_E^r\}_{i,r=1,\ldots,n}$, the operator $B(\lambda) := \rho_S(\lambda)\otimes\rho_E + \chi(\lambda)$ reads

$$B_{ir,js}(\lambda) = \left(\rho_S^{ij}(\lambda) - \frac{\lambda}{n}\delta_{ij}\right)\frac{1}{n}\delta_{rs} + \frac{\lambda}{n}\delta_{ir}\delta_{js}, \tag{B5}$$

and is positive iff

(1) $B_{ir,ir}(\lambda) \geqslant 0 \quad i,r = 1,\ldots,n$;

(2) $|B_{ir,js}(\lambda)|^2 \leqslant B_{ir,ir}(\lambda)B_{js,js}(\lambda) \quad i,r,j,s = 1,\ldots,n$ and $(i,r)\neq(j,s)$.

These conditions become

(1) $\forall r = 1,\ldots,n$

$$\left(\rho_S^{ii}(\lambda) - \frac{\lambda}{n}\right) + \lambda\delta_{ir} \geqslant 0, \tag{B6}$$

and therefore

$$\rho_S^{ii}(\lambda) \geqslant \frac{\lambda}{n} \quad \forall i = 1,\ldots,n. \tag{B7}$$

It is convenient to consider the notation

$$\rho_S^{ii}(\lambda) = \frac{\lambda}{n} + q_i \quad \forall i = 1,\ldots,n \tag{B8}$$

with $q_i \geqslant 0$ and $\sum_{i=1}^n q_i = (1-\lambda)$. For the initial maximally entangled state ($\lambda = 1$) the q_i all vanish, while for the initial maximally mixed and hence factorized state ($\lambda = 0$) the q_i are a probability distribution.

(2) For $(i,r)\neq(j,s)$, we have

$$\left|\left(\rho_S^{ij}(\lambda) - \frac{\lambda}{n}\delta_{ij}\right)\delta_{rs} + \lambda\delta_{ir}\delta_{js}\right|^2 \leqslant (q_i + \lambda\delta_{ir})(q_j + \lambda\delta_{js}), \tag{B9}$$

so that for $r\neq s$ the constraint is trivially satisfied

$$\lambda^2\delta_{ir}\delta_{js} \leqslant (q_i + \lambda\delta_{ir})(q_j + \lambda\delta_{js}), \tag{B10}$$

while for $r = s$ and $i\neq j$ we have the nontrivial constraint

$$\left|\rho_S^{ij}(\lambda)\right|^2 \leqslant q_iq_j + \lambda(q_j\delta_{ir} + q_i\delta_{jr}) \quad \forall r = 1,\ldots,n \tag{B11}$$

leading to

$$\left|\rho_S^{ij}(\lambda)\right|^2 \leqslant q_iq_j. \tag{B12}$$

We can thus write

$$\rho_S(\lambda) = \lambda\frac{\mathbb{1}_n}{n} + Q \tag{B13}$$

with Q a matrix with diagonal matrix elements fixed by the q_i, so that $Q_{ii} \geqslant 0$ and $\sum_{i=1}^n Q_{ii} = 1-\lambda$, $|Q_{ij}|^2 \leqslant Q_{ii}Q_{jj}$, that is a positive matrix with trace equal to $(1-\lambda)$. Apart from a multiplicative factor, such a matrix is a statistical operator $Q = (1-\lambda)\sigma_S$. ■

It is worth stressing that in the limit $\lambda = 0$, any state is compatible since the global state is factorized. For $\lambda = 1$, instead, the global state is the maximally entangled state and the only compatible reduced system state is the maximally mixed state $\rho_S = \mathbb{1}_n/n$.

APPENDIX C: OPD FOR $d = 4$

For the four-dimensional example considered in Sec. III B, we considered a system side frame that generalises the one of

Eq. (36) of $d = 2$, i.e.,

$$Q_0 = \frac{1}{4}\mathbb{1}_4 - \frac{1}{2}\sum_\alpha \sigma_\alpha, \quad Q_\alpha = \frac{1}{2}\sigma_\alpha, \tag{C1}$$

where σ_α are the generalized Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$
$$\sigma_4 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{C2}$$

$$\sigma_5 = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \sigma_6 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \sigma_7 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$
$$\sigma_8 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \tag{C3}$$

$$\sigma_9 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \sigma_{10} = \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, \quad \sigma_{11} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$
$$\sigma_{12} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}, \tag{C4}$$

$$\sigma_{13} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \sigma_{14} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix},$$
$$\sigma_{15} = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix}. \tag{C5}$$

For the initial state

$$|\Psi_{SE}\rangle = \frac{|0,0\rangle + |1,1\rangle + |2,2\rangle + |3,3\rangle}{2} \tag{C6}$$

used in Eq. (56), the weights are

$$w_\alpha = \mathrm{tr}\,[((\mathbb{1}_4 + \sigma_\alpha)\otimes \mathbb{1}_4)\rho_{SE}] = 1 \quad \forall\alpha. \tag{C7}$$

The environmental states

$$\rho_\alpha = \mathrm{tr}_S\,[((\mathbb{1}_4 + \sigma_\alpha)\otimes \mathbb{1}_4)\rho_{SE}] \tag{C8}$$

can be evaluated in a straightforward way, reading

$$\rho_0 = \tfrac{1}{4}\mathbb{1}_4, \quad \rho_\alpha = \tfrac{1}{4}\mathbb{1}_4 + \sigma_\alpha. \tag{C9}$$

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