







Stochastic unravelings for Heisenberg picture and trace-nonpreserving dynamics

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Stochastic unravelings allow one to efficiently simulate open system dynamics, yet their application has traditionally been restricted to master equations in the Schrödinger picture, which preserve both Hermiticity and trace. In this work we introduce a general framework that extends piecewise-deterministic unravelings to the Heisenberg picture and arbitrary trace-nonpreserving master equations, requiring only positivity and Hermiticity of the dynamics. Our approach includes, as special cases, unravelings of arbitrary dynamics in the Heisenberg picture, evolutions interpolating between fully Lindblad and non-Hermitian Hamiltonian generators, and equations employed in the derivation of full counting statistics, for which we show it can be used to obtain the moments of the associated probability distribution. The framework is suitable for both trace-decreasing and trace-increasing processes through stochastic disappearance and replication of the stochastic realizations, and it is compatible with different unraveling schemes and with reverse jumps in the non-Markovian regime.

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I. INTRODUCTION

Stochastic unravelings are a powerful tool to simulate open quantum system dynamics, in which the time evolution of the system state is reconstructed by averaging over different realizations of a stochastic process on the set of pure states. Unravelings can be divided into two major families: either they can consist of piecewise-deterministic processes interrupted by random jumps [1–14] or they can be diffusive [15–19]. Several different schemes of stochastic unravelings have been proposed in the literature, including methods that allow one to describe non-Markovian dynamics [8,9,13,16].

So far, stochastic unravelings have been mostly used to simulate open system dynamics represented in the Schrödinger picture, due to the fact that the relevant master equations (MEs) are trace-preserving (TP) [20,21] and therefore naturally allow for an interpretation as average over pure states. However, open systems can be also described in the Heisenberg picture, for which the dynamics is described by a unital but not necessarily TP map [22,23]. Methods to extend unravelings to the Heisenberg picture have been proposed only in the special case of Gaussian systems [24] or by mimicking unravelings for computing two-time correlations [25]. In this work we provide a general method to extend them to general MEs in the Heisenberg picture.

Our method does not apply only to Heisenberg picture MEs, but also to arbitrary trace-nonpreserving (TNP) MEs preserving positivity and Hermiticity. Dynamics of this form are widely used in the literature. For instance, they are employed in the study of dynamics generated by non-Hermitian

Hamiltonians featuring exceptional points, in which TNP MEs allow to interpolate between purely non-Hermitian and Lindblad dynamics [26,27]. TNP MEs also appear naturally in the context of counting fields and full counting statistics [28–31], allowing one to derive the moments and cumulants of the probability distribution of the investigated quantity. Our unraveling method will therefore extend the domain of applicability of stochastic methods including in particular dynamics in the Heisenberg picture.

The rest of the paper proceeds as follows. In Sec. II we briefly review open system dynamics, both in the Schrödinger and in the Heisenberg picture, considering general TNP MEs and some unraveling techniques widely used to solve TP Schrödinger picture MEs. In Sec. III we present our method for extending unravelings to Heisenberg picture and arbitrary TNP MEs. In Sec. IV we provide implementations and examples of our method by applying them to physically relevant TNP MEs. Lastly, in Sec. V we present the conclusions of our work.

II. OPEN SYSTEM DYNAMICS

In this section we provide a brief overview of open quantum system dynamics, both in the Schrödinger and in the Heisenberg picture. We further mention physically relevant scenarios in which TNP MEs are used, with particular emphasis on tilted Lindbadians and full counting statistics. We finally provide an overview of some commonly used unraveling schemes for Schrödinger picture MEs.

A. Schrödinger and Heisenberg pictures

Under the assumption that the system and the environment are initially uncorrelated, the reduced dynamics of the system

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in the Schrödinger picture is described by a completely positive (CP) trace-preserving (TP) map Λ_t such that [20,21]

$$\rho(t) = \Lambda_t[\rho]. \quad (1)$$

Alternatively, the dynamics can be described also in the Heisenberg picture, in which operators evolve in time instead of states [22], i.e.,

$$X(t) = \Lambda_t^*[X] \quad (2)$$

and is such that for any state ρ and operator X , it holds

$$\text{tr}[X \Lambda_t[\rho]] = \text{tr}[\Lambda_t^*[X] \rho]. \quad (3)$$

The dynamical map Λ_t^* is the adjoint of Λ_t and is a CP unital map, $\Lambda_t^*(\mathbb{I}) = \mathbb{I}$, but is not TP unless also Λ_t is unital.

The Schrödinger picture dynamics of Eq. (1) is the solution of a so-called time-convolutionless or time-local ME [32,33]

$$\frac{d\rho}{dt} = \mathcal{L}_t^S[\rho] = -i[H, \rho] + \sum_j \gamma_j L_j \rho L_j^\dagger - \frac{1}{2}\{\Gamma_S, \rho\}, \quad (4)$$

with the same structure as the Lindblad ME [34,35], but where $\Gamma_S = \sum_j \gamma_j L_j^\dagger L_j$, and all operators H , L_j and rates γ_j can depend explicitly on time. Note that the dynamical map in the Schrödinger picture Λ_t also satisfies

$$\frac{d}{dt} \Lambda_t = \mathcal{L}_t^S \circ \Lambda_t. \quad (5)$$

Passing to the Heisenberg picture one obviously gets

$$\frac{d}{dt} \Lambda_t^* = \Lambda_t^* \circ \mathcal{L}_t^{S*}. \quad (6)$$

Translating this equation for the master equation for $X(t) = \Lambda_t^*[X]$ one finds

$$\frac{d}{dt} X(t) = \Lambda_t^* \circ \mathcal{L}_t^{S*}[X] = \mathcal{L}_t^H[X(t)], \quad (7)$$

where we introduced the Heisenberg generator

$$\mathcal{L}_t^H := \Lambda_t^* \circ \mathcal{L}_t^{S*} \circ (\Lambda_t^*)^{-1}. \quad (8)$$

We stress that in general the Heisenberg generator \mathcal{L}_t^H is not the same as the adjoint of the Schrödinger one \mathcal{L}_t^S , and it can always be represented as follows [23]:

$$\mathcal{L}_t^H[X] = i[\tilde{H}, X] + \sum_j \xi_j R_j X R_j^\dagger - \frac{1}{2}\{\Gamma_H, X\}, \quad (9)$$

where $\Gamma_H = \sum_j \xi_j R_j R_j^\dagger$, with all rates and operators that can depend on time. Note, however, that in general the Hamiltonians H , \tilde{H} , the jump operators L_j , R_j , and the rates γ_j , ξ_j are different. Only in the special case of commutative dynamical maps, i.e., when $\Lambda_t \circ \Lambda_s = \Lambda_s \circ \Lambda_t$ for any pair of t and s does one have $\mathcal{L}^H = \mathcal{L}^{S*}$, which implies $\tilde{H} = H$, $R_j = L_j^\dagger$, and $\xi_j = \gamma_j$.

A key concept for open system dynamics is that of divisibility [36]: the dynamics is said to be Schrödinger (C)P-divisible if the map

$$\Lambda_{t,s}^S := \Lambda_t \circ \Lambda_s^{-1} \quad (10)$$

describing the time evolution from time s to time $t > s$ in the Schrödinger picture is (completely) positive. Similarly, it is

Heisenberg (C)P-divisible if the map

$$\Lambda_{t,s}^H := \Lambda_t^* \circ (\Lambda_s^*)^{-1} = \Lambda_t^* \circ (\Lambda_{t,s}^S)^* \circ (\Lambda_t^*)^{-1}. \quad (11)$$

is (completely) positive. Divisibility has been widely studied in open systems and connected to memory effects and quantum non-Markovianity [37–42] and is not equivalent in the two pictures [23]. From the point of view of the MEs, CP divisibility corresponds to positivity of the rates $\gamma_\alpha \geq 0$ or $\xi_\alpha \geq 0$, while P divisibility is equivalent to the weaker condition [43]

$$\sum_\alpha \gamma_\alpha |\langle \varphi_\mu | L_\alpha | \varphi_{\mu'} \rangle|^2 \geq 0 \quad (12)$$

for all orthonormal bases $\{\varphi_\mu\}_\mu$ and for all $\mu \neq \mu'$, and similarly for Heisenberg P divisibility.

B. Trace-non-preserving MEs

In many physically relevant scenarios, one is interested in MEs which preserve positivity but in general not the trace. A generic ME with these properties can be written in a similar form as Eq. (4) but with an arbitrary self-adjoint operator in the anticommutator, i.e.,

$$\frac{d\rho}{dt} = \mathcal{L}[\rho] = -i[H, \rho] + \sum_j \gamma_j L_j \rho L_j^\dagger - \frac{1}{2}\{\Gamma, \rho\}, \quad (13)$$

for any $\Gamma = \Gamma^\dagger \geq 0$. Such ME preserves the trace iff $\Gamma = \sum_j \gamma_j L_j^\dagger L_j = \Gamma_S$, corresponding to the Schrödinger picture ME (4). In the general case, the time evolution of the trace reads

$$\frac{d}{dt} \text{tr}[\rho] = \text{tr}[\mathcal{L}[\rho]] = \text{tr}[(\Gamma_S - \Gamma)\rho]. \quad (14)$$

MEs of this form are widely used in many physically relevant scenarios. They encompass the case of non-Hermitian Hamiltonians, which have been widely studied both theoretically [44–51] and experimentally [52–54]. TNP MEs allow one to interpolate between non-Hermitian and Lindblad dynamics, and schemes to experimentally obtain such dynamics have been proposed both in the trace-decreasing [26] and in the trace-increasing [27] case, via suitable postselection schemes. Unraveling schemes for the trace-decreasing case have been proposed by dealing with nonlinear MEs [55], or with stochastic equations that do not preserve the norm of the state vectors [2,15]. However, such unravelings cannot be directly used for arbitrary TNP MEs.

Other examples in which TNP MEs naturally appear encompass situations in which the loss of particles is taken into account [56,57], in energy transfer scenarios [58,59] as well as in connection to non-Markovianity in the presence of indefinite causal order [60,61]. A special class of TNP MEs are generated by the so-called tilted Lindbladians [62], i.e., TNP MEs of the form

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_j e^{-s_j} \gamma_j L_j \rho L_j^\dagger - \frac{1}{2}\{\Gamma, \rho\}, \quad (15)$$

with $\Gamma = \sum_j \gamma_j L_j^\dagger L_j$. MEs of this form are widely used to derive the full counting statistics [28–31,63,64] of a suitable observable or first-passage times [65].

C. Stochastic unravelings for trace-preserving MEs

We now provide a brief overview of some commonly used unraveling techniques, which allow for efficient numerical solution of TP MEs in the Schrödinger picture. Such methods rely on the fact that the exact solution of the ME (4) can always be written as the average over pure states

$$\rho(t) = \sum_i \frac{N_i(t)}{N} |\psi_i(t)\rangle \langle \psi_i(t)|, \quad (16)$$

where $N_i(t)$ is the number of realizations in the state $|\psi_i(t)\rangle$ and $N = \sum_i N_i(0)$. Different stochastic methods correspond to different ways of evolving the stochastic vectors $|\psi_i(t)\rangle$.

1. Monte carlo wave function

A first and widely used unraveling technique is the so-called Monte Carlo wave function (MCWF) unraveling [1–4]. Let $|\psi\rangle$ denote the current state of the stochastic realization; the MCWF method is a PDP in which the jumps are of the form

$$|\psi\rangle \mapsto \frac{L_j |\psi\rangle}{\|L_j |\psi\rangle\|} =: |\psi_j\rangle \quad (17)$$

happening between time t and $t + dt$ with probability

$$p_j = \gamma_j \|L_j |\psi\rangle\|^2 dt. \quad (18)$$

The deterministic evolution is given by

$$|\psi\rangle \mapsto \frac{(\mathbb{1} - iK dt) |\psi\rangle}{\|(\mathbb{1} - iK dt) |\psi\rangle\|} =: |\psi_{\text{det}}\rangle, \quad (19)$$

happening with probability

$$p_{\text{det}} = \|(\mathbb{1} - iK dt) |\psi\rangle\|^2, \quad (20)$$

where we introduced the non-Hermitian effective Hamiltonian

$$K = H - \frac{i}{2} \Gamma_S. \quad (21)$$

Notice that the MCWF method can be applied only when all rates γ_j are non-negative at all times, otherwise it would lead to unphysical negative probabilities. Such a condition is equivalent to CP divisibility of the dynamical map.

Nevertheless, it is possible to extend the method to temporarily negative rates via the non-Markovian Quantum Jumps (NMQJ) method [8,9], in which the reverse jump $|\psi_i\rangle = L_j |\psi_{i'}\rangle \mapsto |\psi_{i'}\rangle$ happens with probability

$$p_j^{\text{rev}} = -\frac{N_{i'}}{N_i} \gamma_j \|L_j |\psi_{i'}\rangle\|^2 dt. \quad (22)$$

Notice, however, that these reverse jumps impose mutual dependence among the different stochastic realizations, thus making the simulations less efficient since one needs to store and evolve all trajectories simultaneously.

2. Rate operator

Another unraveling scheme is the so-called Rate Operator (RO) unravelings [13,14], which, unlike the MCWF, can deal with non-(C)P-divisible dynamics without requiring mutual dependence among the stochastic realization, thus improving the numerical efficiency of the unravelings.

In order to derive the corresponding PDP, one needs to introduce the RO [10,11,66]

$$\begin{aligned} \mathcal{R}_\psi &:= \sum_i \gamma_j L_j |\psi\rangle \langle \psi| L_j^\dagger + \frac{1}{2} (|\phi_\psi\rangle \langle \psi| + |\psi\rangle \langle \phi_\psi|) \\ &= \sum_\alpha \lambda_\alpha^\psi |\chi_\alpha^\psi\rangle \langle \chi_\alpha^\psi|, \end{aligned} \quad (23)$$

where $|\psi\rangle$ is the current state of the realization and $|\phi_\psi\rangle$ is an arbitrary and possibly unnormalized state vector depending on $|\psi\rangle$; the last equality is the spectral decomposition of \mathcal{R}_ψ . The jumps are defined as $|\psi\rangle \mapsto |\chi_\alpha^\psi\rangle$, where $|\chi_\alpha^\psi\rangle$ are the eigenstates of \mathcal{R}_ψ , and happen with probability

$$p_\alpha^R = \lambda_\alpha^\psi dt, \quad (24)$$

where λ_α^ψ is the corresponding eigenvalue. In [13] it was shown that it is always possible to find a transformation $|\phi_\psi\rangle$ such that the eigenvalues are always positive (and therefore the jump process is well defined) whenever the dynamics is P-divisible and also in some cases in which P divisibility is violated. The deterministic evolution is given by

$$|\psi\rangle \mapsto \frac{(\mathbb{1} - iK_\psi dt) |\psi\rangle}{\|(\mathbb{1} - iK_\psi dt) |\psi\rangle\|} =: |\psi_{\text{det}}^R\rangle, \quad (25)$$

happening with probability

$$p_{\text{det}}^R = \|(\mathbb{1} - iK_\psi dt) |\psi\rangle\|^2, \quad (26)$$

with the nonlinear effective Hamiltonian

$$K_\psi = H - \frac{i}{2} \Gamma_L - \frac{i}{2} |\phi_\psi\rangle \langle \psi|. \quad (27)$$

In the case of negative eigenvalues, the RO unraveling technique can also be equipped with reverse jumps in a similar way as the MCWF.

III. STOCHASTIC UNRAVELINGS IN THE HEISENBERG PICTURE

In this section we provide a simple way to extend the stochastic unravelings of Sec. II C from the Schrödinger picture to the Heisenberg picture. Such a method can also be generalized to arbitrary forms of TNP MEs, and it coincides with the so-called cloning algorithm when applied to tilted Lindbladians [67–69].

In the Schrödinger picture unravelings, trace preservation via the averaging of Eq. (16) holds since the total number of stochastic realizations is preserved $\sum_i N_i(t) = N$. Therefore, in order to generalize the unravelings to TNP MEs such as the Heisenberg picture ME (9) while keeping the normalization of the state vector, one needs to allow for the total number of realizations to vary in time. The evolution of the trace is then given by the ratio between the number of realizations at time t and the number at the initial time: $\text{tr}X(t) = \sum_i N_i(t)/N \neq 1$.

Another issue of unraveling MEs in the Heisenberg picture is that they act on arbitrary operators which don't need to be positive or self-adjoint, and therefore cannot be written as an average as in Eq. (16). This issue is easily tackled in a similar manner as done in [70] for the extension of unravelings to an initially correlated system and environment: an arbitrary operator X can first be separated in Hermitian

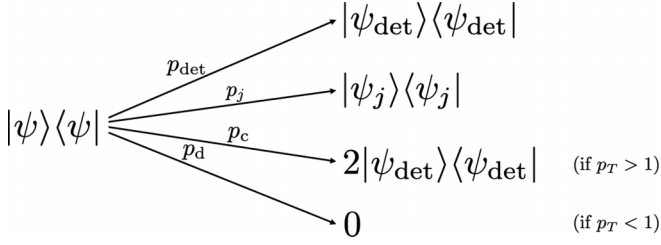


FIG. 1. At any given moment of time, there are four possibilities for the evolution of the realization, as given in Eqs. (39)–(41). It can either evolve deterministically, jump, create a copy of itself, or vanish.

and anti-Hermitian part $X = X_h + iX_a$, $X_{h,a}^\dagger = X_{h,a}$, each of which can be written as the difference between two positive operators $X_{h,a} = X_{h,a}^+ - X_{h,a}^-$, where each $X_{h,a}^\pm$ is positive and therefore proportional to a density matrix $X_{h,a}^\pm = \mu_{h,a}^\pm \rho_{h,a}^\pm$. This way of separating X into the sum of positive operators is preserved by the evolution, since it preserves positivity and Hermiticity. Therefore, each $\rho_{h,a}^\pm$ is unraveled separately, and the solution of the Heisenberg picture ME $X(t)$ is obtained as the weighted sum of the different terms

$$X(t) = \mu_h^+ \rho_h^+(t) - \mu_h^- \rho_h^-(t) + i\mu_a^+ \rho_a^+(t) - i\mu_a^- \rho_a^-(t). \quad (28)$$

We now show how to generalize unraveling to the Heisenberg picture with a nonconstant number of realizations first with the MCWF and then with the RO, with an illustration of our method presented in Fig. 1. However, our method can be generalized in a straightforward way also to different stochastic methods. Notice that the jumps and deterministic evolution are now defined via the operators \tilde{H} , R_j , and Γ_H of the Heisenberg picture ME (9).

A. Heisenberg unravelings with MCWF

When considering the MCWF unraveling applied to the operators \tilde{H} , R_j^\dagger , and Γ_H and rates ξ_j of the Heisenberg picture ME (9), then the jump and deterministic probabilities no longer sum to 1, and therefore do not form a proper probability distributions. Instead,

$$p_T = p_{\text{det}} + p_J = 1 + dt \langle \Gamma_{\text{tp}} - \Gamma_H \rangle_\psi \neq 1, \quad (29)$$

where $\langle X \rangle_\psi = \langle \psi | X | \psi \rangle$, $p_J := \sum_j p_j$ denote the total jump probability, and

$$\Gamma_{\text{tp}} := \sum_\alpha \xi_\alpha R_\alpha^\dagger R_\alpha \quad (30)$$

is the operator that would make the ME (9) TP.

The parameter p_T , depending on the ME, can generally be smaller or greater than 1, with the difference corresponding to the change in trace for the particular realization

$$p_T - 1 = dt \frac{d}{dt} \text{tr}[|\psi\rangle \langle \psi|]. \quad (31)$$

Notice that if one particular realization gives $p_T < 1$ ($p_T > 1$), it does not imply that the same holds also for other trajectories, nor a decrease (increase) of trace for the average state ρ .

Let us first consider the case $p_T < 1$. Since the sum of jump and deterministic probability is smaller than one, we can think of adding an extra process happening with the remaining probability. Since the trace is decreasing, it is natural for this process to be the disappearance of the stochastic realization $|\psi\rangle \mapsto 0$ with probability

$$p_d = 1 - p_T = \langle \Gamma_H - \Gamma_{\text{tp}} \rangle_\psi dt \geq 0. \quad (32)$$

Therefore, the realization ψ can either jump, evolve deterministically, or disappear and therefore not counting anymore in the average of Eq. (16). The corresponding probabilities are positive and correctly normalized to 1.

Indeed, with this extra process, the stochastic unravelings do match the exact solution on average

$$\begin{aligned} |\psi\rangle \langle \psi| &\mapsto \sum_j p_j \frac{R_j |\psi\rangle \langle \psi| R_j^\dagger}{\|R_j |\psi\rangle\|^2} dt + p_{\text{det}} |\psi_{\text{det}}\rangle \langle \psi_{\text{det}}| + p_d \times 0 \\ &= \sum_j \xi_j R_j |\psi\rangle \langle \psi| R_j^\dagger dt \\ &\quad + (\mathbb{1} - iK dt) |\psi\rangle \langle \psi| (\mathbb{1} + iK^\dagger dt) \\ &= |\psi\rangle \langle \psi| + \mathcal{L}_t^H [|\psi\rangle \langle \psi|] dt. \end{aligned} \quad (33)$$

For the case $p_T > 1$, one cannot indeed add an extra event, since $p_{\text{det}} + p_J$ larger than 1, and therefore they do not correspond to a proper probability distribution. Instead, we introduce a process, corresponding to the creation of a new copy in the same state ψ . Such process happens with probability

$$p_c = p_T - 1 = \langle \Gamma_{\text{tp}} - \Gamma_H \rangle_\psi dt \geq 0 \quad (34)$$

and is statistically independent of the jump or deterministic evolution. Accordingly, the probability of not creating a copy is $p_n = 1 - p_c$. Once one has evaluated whether a copy is created or not, the original realization ψ can evolve either via a jump or deterministically, but the corresponding probabilities must be renormalized in order to sum to 1 as

$$p'_j = p_j, \quad p'_{\text{det}} = 1 - p_J. \quad (35)$$

Notice that the two copies evolve independently and that the event in which the creation of a copy is followed by a jump happens with probability $O(dt^2)$ and, as it is usually the case for stochastic unravelings, we compute terms only up to dt , so one can assume that new copy is created in the state ψ_{det} . Therefore, the three possible evolutions for ψ are

(1) No copy and deterministic: $|\psi\rangle \mapsto |\psi_{\text{det}}\rangle$ with probability $p_n^{\text{det}} = p_n p'_{\text{det}} = 1 - p_J - \langle \Gamma_{\text{tp}} - \Gamma_H \rangle_\psi dt + O(dt^2)$

(2) No copy and jump: $|\psi\rangle \mapsto |\psi_j\rangle$ with probability $p_n^j = p_n p_j = p_j + O(dt^2)$

(3) Copy and deterministic: the original copy evolves deterministically and a new copy is created in the ensemble

$$|\psi\rangle \langle \psi| \mapsto 2 |\psi_{\text{det}}\rangle \langle \psi_{\text{det}}| \quad (36)$$

with probability $p_c^{\text{det}} = p_c p'_{\text{det}} = \langle \Gamma_{\text{tp}} - \Gamma_H \rangle_\psi dt + O(dt^2)$.

Indeed, also in this case the average evolution matches the solution of the ME (9):

$$|\psi\rangle\langle\psi| \mapsto \sum_j p_j \frac{R_j |\psi\rangle\langle\psi| R_j^\dagger}{\|R_j |\psi\rangle\|^2} dt + p_c^{\text{det}} |\psi\rangle\langle\psi| + (p_n^{\text{det}} + p_c^{\text{det}}) |\psi_{\text{det}}\rangle\langle\psi_{\text{det}}|. \quad (37)$$

Using $p_n^{\text{det}} + p_c^{\text{det}} = p'_{\text{det}} = 1 - \langle\Gamma_{\text{tp}}\rangle_\psi dt$ and expanding the normalization factor of the deterministic term $1/\|(\mathbb{1} - iK dt)|\psi\rangle\|^2$ to the first order in dt , it is straightforward to show that

$$|\psi\rangle\langle\psi| \mapsto |\psi\rangle\langle\psi| + \mathcal{L}_t^H[|\psi\rangle\langle\psi|] dt \quad (38)$$

also in the case in which the trace increases $p_T > 1$. Therefore, by taking the continuous time limit $dt \rightarrow 0$, it follows that the evolution of an arbitrary operator $X(t)$ does indeed correspond to the Heisenberg picture ME (9).

The correct behavior of the trace on average follows from the linearity of the trace and the fact that each realization evolves on average as prescribed by the ME.

It is possible to merge the two cases $p_T < 1$ and $p_T > 1$ as

$$p_{\text{det}} = 1 - p_j - |\langle\Gamma_{\text{tp}} - \Gamma_H\rangle_\psi| dt, \quad (39)$$

$$p_d = \max\{0, \langle\Gamma_H - \Gamma_{\text{tp}}\rangle_\psi dt\}, \quad (40)$$

$$p_c = \max\{0, \langle\Gamma_{\text{tp}} - \Gamma_H\rangle_\psi dt\}, \quad (41)$$

and p_j as in Eq. (18); p_j and p_{det} correspond to no creation or disappearance of any trajectory, p_d describes the disappearance, and p_c the creation of a copy plus deterministic evolution for the original copy. Notice that one of p_d and p_c is always zero and

$$\sum_j p_j + p_{\text{det}} + p_d + p_c = 1. \quad (42)$$

A schematic illustration of the different possibilities is described in Fig. 1, and a specific example is worked out in Sec. IV A 1.

Notice that it is possible to keep under control the numerical requirements by maintaining a fixed number of realizations in a similar way as done in [69]. This is done by first evolving all trajectories from t to $t + dt$ and then randomly sampling $N(0)$ of the $N(t + dt)$ resulting trajectories and discarding the others. The change in trace is then simply given by keeping track of the variation $N(t + dt) - N(t)$ but without the need to store more than $N(0)$ trajectories. In particular, for $N(0) \rightarrow \infty$, the fact that only the difference needs to be stored at each time ensures the exact convergence in the asymptotic limit.

So far, we have assumed that the dynamics is CP-divisible, and therefore all rates ξ_j are positive, and so p_j are indeed probabilities. However, our unraveling method for TNP MEs can be equipped with reverse jumps of Eq. (22). The probabilities for deterministic evolution and for the creation or destruction of a copy are left unchanged and computed using the (possibly negative) p_j . The jump probabilities, instead, are computed using the reverse jumps of Eq. (22). The proof that the unravelings agree with the ME on average is presented in Appendix A.

B. Heisenberg unravelings with RO

The unravelings in the Heisenberg picture can be applied in a simple way also to the RO method of Sec. II C 2. To do so, we first notice that although both the jump p_α^R and deterministic p_{det}^R probabilities depend on the transformation ϕ_ψ , their sum does not,

$$p_{\text{det}}^R + \sum_\alpha p_\alpha^R = 1 + dt \langle\Gamma_{\text{tp}} - \Gamma_H\rangle_\psi = p_T, \quad (43)$$

and is the same as for the MCWF. Therefore, it is possible to apply the same ideas also for the RO: the probabilities of creation or destruction of a copy are as in Eqs. (39)–(41), but using $p_j^R = \sum_\alpha p_\alpha^R$ instead of p_j and p_α^R as jump probabilities. Notice that, since p_T is independent of ϕ_ψ , then also p_n^R, p_c^R do not depend on it.

For $p_T < 1$, the average evolution reads

$$|\psi\rangle\langle\psi| \mapsto \sum_\alpha p_\alpha^R |\chi_\alpha^\psi\rangle\langle\chi_\alpha^\psi| + p_{\text{det}}^R |\psi_{\text{det}}^R\rangle\langle\psi_{\text{det}}^R| + p_d^R \times 0, \quad (44)$$

while for $p_T > 1$ it reads

$$|\psi\rangle\langle\psi| \mapsto \sum_\alpha p_\alpha^R |\chi_\alpha^\psi\rangle\langle\chi_\alpha^\psi| + p_c^{\text{det},R} |\psi\rangle\langle\psi| + (p_n^{\text{det},R} + p_c^{\text{det},R}) |\psi_{\text{det}}^R\rangle\langle\psi_{\text{det}}^R|. \quad (45)$$

By direct calculation, it is easy to show that in both cases

$$|\psi\rangle\langle\psi| \mapsto |\psi\rangle\langle\psi| + \mathcal{L}_t^H[|\psi\rangle\langle\psi|] dt, \quad (46)$$

and indeed the Heisenberg picture RO unravelings match the ME (9). This situation is considered in Sec. IV A 2.

If the RO has negative eigenvalues, then it is possible to equip the unravelings with the reverse jumps of Eq. (22) in a similar way as for the MCQF; see Appendix A for further details.

C. Generic TNP MEs

Our method for extending stochastic unravelings to the Heisenberg picture can be applied in a straightforward way to arbitrary TNP MEs (13). This is done by substituting Γ_H with Γ of Eq. (13) in Eqs. (39)–(41). The jump probabilities can be then computed with either the MCWF or the RO formalism. This allows one to extend the powerful simulation method that is stochastic unravelings not only beyond the Schrödinger picture, but also to arbitrary TNP MEs. An example in this direction is given in Sec. IV B.

When considering MEs corresponding to the statistics of time-integrated observables, our method with the MCWF coincides with the cloning method [67–69]. Such a method was devised for the characterization of trajectory-dependent observables of the form [69]

$$O[\omega_t] = \sum_{k=0}^{n-1} \alpha(|\psi_k\rangle, |\psi_{k+1}\rangle), \quad (47)$$

where $\omega_t = \{|\psi_0\rangle, |\psi_1\rangle, \dots, |\psi_n\rangle\}$ is a (discretized) stochastic trajectory and α is an observable-dependent function. For the special case of α being nonzero if and only if $|\psi_{k+1}\rangle = L_j |\psi_k\rangle$, the resulting dynamics is the tilted Lindbladian of

Eq. (15) and the resulting observable is the number of jumps for the trajectory ω_t .

IV. IMPLEMENTATIONS AND EXAMPLES OF TNP UNRAVELINGS

In this section we apply our method of stochastic unravelings in the Heisenberg picture described in Sec. III to two examples, one CP-divisible and one non-CP-divisible. In Sec. IV B we apply a variation of the same method to tilted Lindbladians applied to photon counting statistics.

A. Heisenberg picture ME

In order to exemplify the Heisenberg picture stochastic unravelings we consider two examples. First, we consider a dynamics which is CP-divisible in the Heisenberg picture but not in the Schrödinger picture, for which the MCWF method can be applied. Second, we consider a dynamics nondivisible in both pictures, for which one needs to either use the RO or reverse jumps.

1. Heisenberg CP-divisible

As a first example, we consider a Heisenberg picture ME of the form

$$\begin{aligned} \frac{dX}{dt} = & i\omega[\sigma_x, X] + \xi_- \left(\sigma_+ X \sigma_- - \frac{1}{2} \{ \sigma_+ \sigma_-, X \} \right) \\ & + \xi_+ \left(\sigma_- X \sigma_+ - \frac{1}{2} \{ \sigma_- \sigma_+, X \} \right), \end{aligned} \quad (48)$$

where $\sigma_+ = |1\rangle\langle 0| = \sigma_-^\dagger$, and ω and $\xi_{\pm,z}$ are time-dependent functions. We consider the strongly driven regime $|\omega| \gg \xi_{\pm} > 0$. For various choices of time-dependent rates, this corresponds to a dynamics that is CP-divisible in the Heisenberg picture ($\xi_{\pm} \geq 0$) but P-indivisible in the Schrödinger picture, as shown in Appendix B. In particular, in the strongly driven regime, the dynamics is not Schrödinger P- or CP-divisible since the initial time, thus making the reverse jumps fail. Because of divisibility, the unravelings in the Heisenberg picture can be performed using the MCWF and do not require reverse jumps, while if one unraveled the same dynamics in the Schrödinger picture they would be necessary. This makes the simulations noticeably more efficient in the Heisenberg picture.

In Fig. 2 we show the agreement between the MCWF unravelings and the exact solution of the Heisenberg picture ME. In particular, in the upper right panel, we show that the trace of the observable $\text{tr}X(t)$ oscillates between values greater and smaller than its initial value $\text{tr}X(0) = 1$. This shows that our method not only gives the correct expectation values for any measurement of the form $\text{tr}[\rho X(t)]$, but it also correctly captures the time evolution of the trace via the nonconstant number of stochastic realizations. The code used for the simulation is available at [71].

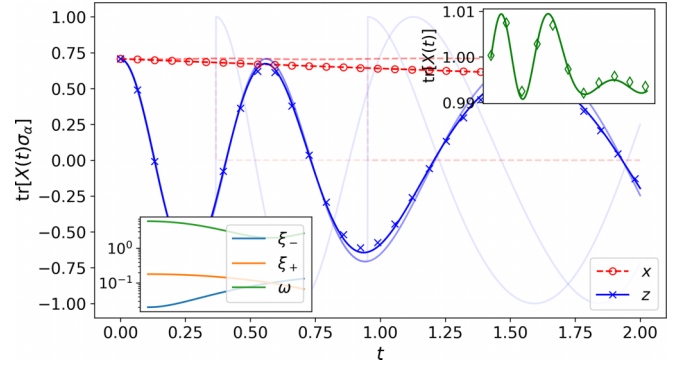


FIG. 2. Dynamics of the Heisenberg picture ME (48), x and z components of the Bloch vector. The MCWF unravelings match the exact solution (dark lines); in lighter shade seven stochastic trajectories are also shown. Lower left inset: Rates ξ_{\pm} and ϵ (logarithmic scale). Upper right inset: Dynamics of the trace $\text{tr}[X(t)]$, obtained as the ratio $\sum_i N_i(t)/N$. The time step used in the simulations is $dt = 10^{-3}$; $N = 2 \times 10^4$ stochastic realizations are present at $t = 0$, the number at time t follows the same dynamics as $\text{tr}[X(t)]$ (upper right inset). Initial value $X(0) = |\psi_0\rangle\langle\psi_0|$, with $|\psi_0\rangle = \cos(\pi/8)|+\rangle + \sin(\pi/8)|-\rangle$.

2. Heisenberg non-CP-divisible

As a second example, we consider a Heisenberg picture ME of the form

$$\frac{dX}{dt} = \sum_{\alpha=\pm,z} \xi_{\alpha} \left(\sigma_{\alpha} X \sigma_{\alpha}^{\dagger} - \frac{1}{2} \{ \sigma_{\alpha} \sigma_{\alpha}^{\dagger}, X \} \right), \quad (49)$$

where $\xi_{\pm,z}$ are time-dependent functions. Such a ME describes the phase covariant dynamics [72–74] in the Heisenberg picture [23]. The resulting dynamics is Heisenberg CP-divisible if all rates ξ_j are positive, while P divisibility corresponds to [75,76]

$$\xi_{\pm} \geq 0, \quad \text{and} \quad \xi_z \geq -\frac{1}{2}\sqrt{\xi_+ \xi_-}. \quad (50)$$

We choose the rates in such a way that CP divisibility is violated at all times, while P divisibility is preserved, in a similar manner to the eternally-non-Markovian dynamics [77,78]. The violation of divisibility arises from the negativity of ξ_z , while ξ_{\pm} are positive at all times; see Fig. 3. Because of the form of the ME and $\xi_z < 0$, the dynamics is non-CP-divisible also in the Schrödinger picture [23].

Using the RO to perform the Heisenberg picture unravelings, it is possible to obtain the evolution of any operator $X(t)$ without the need of reverse jumps despite $\xi_z < 0$ at all times. Furthermore, it is possible to perform the unravelings with a small effective ensemble: only the eigenstates $|0\rangle, |1\rangle$ of σ_z and the state conditioned to no jumps happening are needed to describe the reduced dynamics. These facts are possible due to the flexibility of the RO with a trajectory-dependent transformation ϕ_{ψ} and they drastically improve the efficiency of the simulation technique.

The resulting unravelings are presented in Fig. 3, and, unlike the previous example, here the trace $\text{tr}X(t)$ is monotonically increasing in time.

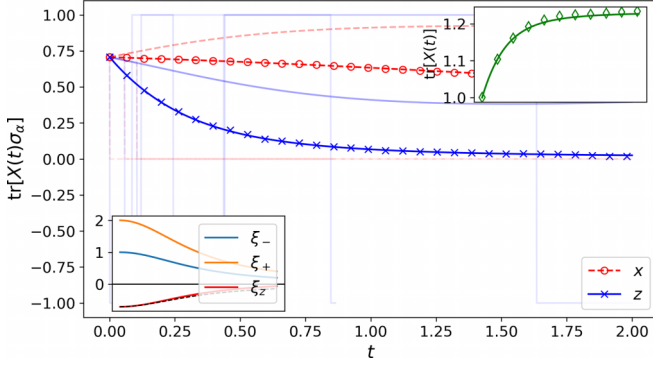


FIG. 3. Dynamics of the non-CP-divisible Heisenberg picture ME (49), x and z components of the Bloch vector. The RO unravelings match the exact solution (dark lines), with no reverse jumps required; in lighter shade seven stochastic trajectories are also shown. Lower left inset: rates ξ_α ; The dashed line is the condition for P-divisibility for γ_ζ (50). Upper right inset: Dynamics of the trace $\text{tr}[X(t)]$. The other parameters and initial value are the same as in Fig. 2.

B. Photon counting

As a last example, we apply our method to a special case of tilted Lindbladian (15), in which the TNP ME reads [64]

$$\frac{d}{dt}\rho_\zeta = \mathcal{L}[\rho_\zeta] + \zeta \mathcal{J}[\rho_\zeta], \quad (51)$$

where \mathcal{L} is a TP Lindbladian

$$\mathcal{L}[\rho] = -i[H, \rho] + \gamma(\bar{n} + 1)a\rho a^\dagger + \gamma\bar{n}a^\dagger\rho a - \frac{1}{2}\{\Gamma_S, \rho\}, \quad (52)$$

with a^\dagger , a bosonic creation and annihilation operators, ζ , γ , \bar{n} positive real numbers, and Hamiltonian

$$H = \frac{\Omega}{2}(ae^{2i\phi} + a^\dagger e^{-2i\phi}), \quad (53)$$

where ϕ and Ω are real parameters, while $\mathcal{J}[\rho] = \gamma(\bar{n} + 1)a\rho a^\dagger$. MEs of this form are typically used to describe the photon-counting statistics [63]. In particular, the trace of ρ_ζ allows one to compute the factorial moments of the probability distribution $P(n, t)$ of observing n photons at time t as

$$\mu_k = \frac{d^k}{d\zeta^k} \text{tr}[\rho_\zeta]|_{\zeta=0}. \quad (54)$$

In principle, one can directly apply the derivative to the estimate of $\text{tr}\rho_\zeta$ obtained by unraveling the TNP ME (51) for values of ζ around 0, but the obtained results are too noisy, since the derivative increases the fluctuations due to the creation or destruction of extra copies. An alternative approach is that of defining $\tau_k := d^k \rho_\zeta / d\zeta^k|_{\zeta=0}$, which are the solution of the TNP ME [62,79]

$$\frac{d}{dt}\tau_k = \mathcal{L}[\tau_k] + k \mathcal{J}[\tau_{k-1}], \quad (55)$$

and the moments can be obtained as $\mu_k = \text{tr}[\tau_k]$. This system of MEs can be simulated iteratively, with $\tau_0 = \rho$ and using the solution of the k th operator τ_{k-1} in the ME for τ_k . Notice that this does not impact drastically the numerical requirements, since at each time only the trajectories for τ_k need to be stored, as well as the average τ_{k-1} . Typically only

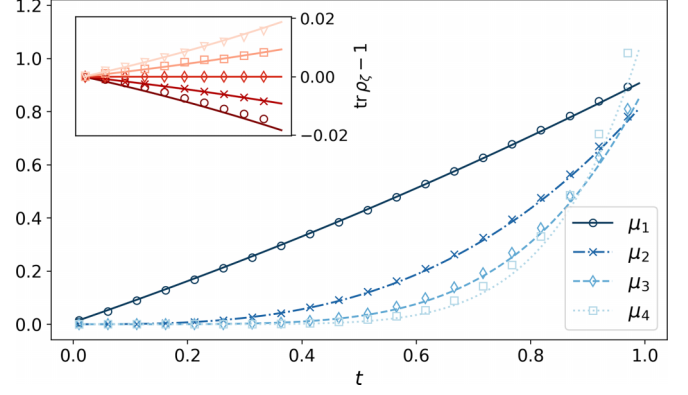


FIG. 4. Moments of $P(n, t)$. The exact solution is obtained by solving Eq. (51) and taking the derivative of the trace; the unravelings are performed on Eq. (55). Inset: $\text{tr}\rho_\zeta - 1$, for $\zeta = -0.02$ (bottom) to $\zeta = 0.02$ (top). Parameters: $\gamma = \Omega = 1$, $\bar{n} = 0.5$, $\phi = 0.2$, $dt = 10^{-2}$, initial number of trajectories: $N = 10^4$, initial state: $|\psi_0\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$. Notice that the final time is chosen to be comparable to the typical timescale $1/\gamma$ of the dynamics.

the first few moments are of interest, which are sufficient, for example, to determine whether the distribution is Poissonian or not [80]. The resulting MEs are inhomogeneous due to the term $k \mathcal{J}[\tau_{k-1}]$, which does not depend on τ_k . By using its spectral decomposition $k \mathcal{J}[\tau_{k-1}] = \sum_i \eta_i^k |\xi_i^k\rangle \langle \xi_i^k|$, our method can be extended to deal with it by adding an extra event, corresponding to the creations of copies in the eigenstates $|\xi_i^k\rangle$ of the inhomogeneous term, with rate equal to the corresponding eigenvalue η_i^k , which are positive since \mathcal{J} is CP. Such extra copies and the rate of creation do not depend on the state ψ of the realization. The initial value for $k \geq 1$ is $\tau_k(0) = 0$, and thus initially only the inhomogeneous term is relevant for the unravelings. In Fig. 4 we present the first four moments obtained by unraveling the TNP ME (55) with the RO formalism. This shows that indeed our method can be applied even beyond MEs in the Heisenberg picture.

V. CONCLUSIONS

In this work we have introduced a general framework to extend stochastic unravelings beyond the commonly used Schrödinger picture. We first extended them to the Heisenberg picture, in which, by employing the fact that the property of divisibility might be different in the two pictures, the simulations can become more efficient.

We have then showed that our method can be trivially extended to generic TNP MEs that preserve positivity and Hermiticity, thus significantly broadening the scope of stochastic unravelings beyond the standard Lindblad ME in the Schrödinger picture, enabling simulations of a wide variety of physically relevant dynamics. This includes, for instance, dynamics interpolating between non-Hermitian and Lindblad regimes, and MEs used to extract photon-counting statistics.

While we developed the method within the MCWF and RO formalism, our method can be easily applied to other piecewise-deterministic schemes, even in the presence of reverse jumps, thus providing a versatile tool for simulating fully general open quantum systems dynamics.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [71].

APPENDIX A: PROOF OF THE REVERSE JUMPS

The jump rates ξ_j of the Heisenberg picture unravelings can be decomposed into a positive and negative part $\xi_j^\pm = \frac{1}{2}(|\xi_j| \pm \xi_j)$. The presence of negative rates does not alter the deterministic nor the creation or disappearance of copies, therefore it is sufficient to show that the jump process reproduces on average the jump term of the ME (9). The average jump process reads [81]

$$\begin{aligned} |\psi\rangle\langle\psi| \mapsto dt \sum_j \xi_j^+ R_j |\psi\rangle\langle\psi| R_j^\dagger \\ - dt \sum_j \int d\psi' \xi_j^- \frac{N_{\psi'}}{N_\psi} |\psi\rangle\langle\psi| \\ \times \delta\left(|\psi\rangle - \frac{R_j |\psi'\rangle}{\|R_j |\psi'\rangle\|}\right) \|R_j |\psi'\rangle\|^2. \end{aligned} \quad (\text{A1})$$

The first term on the right-hand side is the jump term of the ME for positive rates. In order to show the agreement on average with the ME, one needs to compute the average jump evolution of the unnormalized state

$$\rho = \int d\psi \frac{N_\psi}{N} |\psi\rangle\langle\psi|, \quad (\text{A2})$$

where, unlike for the TP case, N_ψ/N is not a probability distribution since it is not normalized to 1. The average jump evolution then reads

$$\begin{aligned} \rho \mapsto \sum_j \xi_j^+ R_j \rho R_j^\dagger - dt \sum_j \int d\psi \int d\psi' \xi_j^- \frac{N_{\psi'}}{N} |\psi\rangle\langle\psi| \\ \times \delta\left(|\psi\rangle - \frac{R_j |\psi'\rangle}{\|R_j |\psi'\rangle\|}\right) \|R_j |\psi'\rangle\|^2. \end{aligned} \quad (\text{A3})$$

For the second term, the integral in ψ is readily evaluated due to the Dirac delta, and therefore the average evolution due only to the jumps is

$$\rho \mapsto \sum_j \xi_j R_j \rho R_j^\dagger. \quad (\text{A4})$$

Therefore, since deterministic evolution, creation, and destruction of a copy are not modified by the presence of negative rates, it follows that the unravelings with NMQJ match with the Heisenberg picture ME also when reverse jumps are taken into account.

In a similar manner, it is possible to show that also the Heisenberg picture RO unravelings can be equipped with the NMQJ. The RO unravelings can be equipped with NMQJ also for TNP MEs. If $\lambda_j^\psi < 0$, then the reverse jump $|\psi\rangle \mapsto |\psi'\rangle$, where $|\psi\rangle$ is an eigenstate of $R_{\psi'}$, can happen with probability

$$p_\alpha^{\text{rev},R} = -\lambda_\alpha^\psi \frac{N_\psi}{N_{\psi'}} dt. \quad (\text{A5})$$

The rest of the process is left unchanged: p_{det}^R , p_c^R , and p_d^R are computed using the (possibly negative) rates λ_j^ψ . The RO can be written as $\mathcal{R}_\psi = \mathcal{R}_\psi^+ - \mathcal{R}_\psi^-$, with

$$\mathcal{R}_\psi^\pm = \sum_\alpha \lambda_{\alpha,\psi}^\pm |\chi_\alpha^\psi\rangle\langle\chi_\alpha^\psi| \geq 0, \quad \lambda_{\alpha,\psi}^\pm = \frac{1}{2}(|\lambda_\alpha^\psi| \pm \lambda_\alpha^\psi) \geq 0. \quad (\text{A6})$$

Similarly to the MCWF, it is sufficient to show that the jump process reproduces on average the RO, with average jump process reading [14]

$$\begin{aligned} |\psi\rangle\langle\psi| \mapsto dt \sum_\alpha \lambda_{\alpha,\psi}^+ |\chi_\alpha^\psi\rangle\langle\chi_\alpha^\psi| \\ - \int d\psi' \lambda_{\alpha,\psi'}^- \frac{N_{\psi'}}{N_\psi} |\psi\rangle\langle\psi| \delta(|\psi\rangle - |\chi_\alpha^{\psi'}\rangle). \end{aligned} \quad (\text{A7})$$

Upon considering the average state as in Eq. (A2) and using the Dirac delta to compute the integral of the second term, one finds that the average jump evolution reads

$$\begin{aligned} \rho \mapsto \int d\psi \frac{N_\psi}{N} \mathcal{R}_\psi^+ dt - \sum_\alpha \int d\psi' \lambda_{\alpha,\psi'}^- \frac{N_{\psi'}}{N} |\chi_\alpha^{\psi'}\rangle\langle\chi_\alpha^{\psi'}| dt \\ = \int d\psi \frac{N_\psi}{N} (\mathcal{R}_\psi^+ - \mathcal{R}_\psi^-) dt = \int d\psi \frac{N_\psi}{N} \mathcal{R}_\psi dt \\ = \sum_j \xi_j R_j \rho R_j^\dagger dt + \frac{1}{2} \int d\psi \frac{N_\psi}{N} (|\phi_\psi\rangle\langle\psi| + |\psi\rangle\langle\phi_\psi|) dt. \end{aligned} \quad (\text{A8})$$

From here, it is straightforward to notice that the last term cancels out with the same term with opposite sign from the deterministic evolution, thus canceling all terms depending on ϕ_ψ in the average evolution. Therefore, $\rho \mapsto \rho + \mathcal{L}_t^H[\rho] dt$ and for the RO the unravelings match with the Heisenberg picture ME also when reverse jumps are taken into account.

APPENDIX B: DIVISIBILITY OF THE DYNAMICS OF EQ. (48)

We proceed to show that the solution of the TNP ME (48) gives a dynamical map which is CP-divisible in the Heisenberg picture and P- and CP-indivisible in the Schrödinger picture.

CP divisibility in the Heisenberg picture follows trivially from the positivity of the rates $\xi_\pm(t)$ of the ME. Let Λ_t^* be the solution of the ME (48), then the dynamics in the Schrödinger

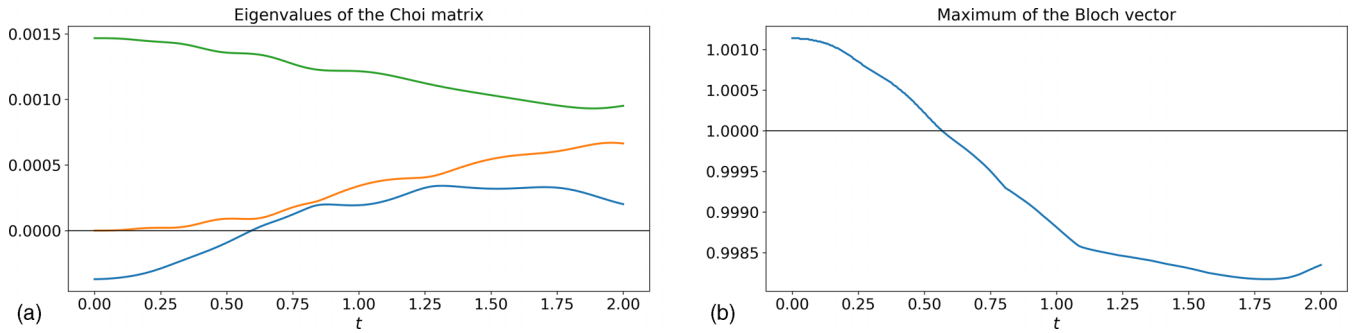


FIG. 5. (a) The three smallest eigenvalues of the Choi state of Eq. (B1), the fourth eigenvalue is such that $\text{tr}J_t = 1$. Negativity of one eigenvalue implies violations of CP divisibility. (b) Maximal norm of the Bloch vector under the action of $\Lambda_{t+dt,t}$. The fact that such norm is greater than one implies that the dynamics is not P-divisible.

picture is described by its adjoint Λ_t , which is a CPTP map. (C)P divisibility in the Schrödinger picture is equivalent to the (complete) positivity of the map $\Lambda_{t+dt,t} = \Lambda_{t+dt}\Lambda_t^{-1}$ for all times t . Complete positivity can be evaluated by checking the positivity of the corresponding Choi state

$$J_t := \sum_{i,j=0}^1 \Lambda_{t+dt,t}[|i\rangle\langle j|] \otimes |i\rangle\langle j|. \quad (\text{B1})$$

Positivity, on the other hand, is equivalent to $\Lambda_{t+dt,t}$, when considered in its Bloch representation, mapping the Bloch sphere into itself, i.e., every vector on the unit sphere must be mapped to vectors with norm smaller than 1. In Fig. 5 we show that both these conditions are not satisfied. In particular, they are violated since $t = 0$, thus making most unraveling methods fail, even in the presence of reverse jumps.

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