Stochastic unraveling of positive quantum dynamics

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Stochastic unravellings represent a useful tool to describe the dynamics of open quantum systems and standard methods, such as quantum state diffusion (QSD), call for the complete positivity of the open-system dynamics. Here, we present a generalization of QSD, which also applies to positive, but not completely positive evolutions. The rate and the action of the diffusive processes involved in the unraveling are obtained by applying a proper transformation to the operators which define the master equation. The unraveling is first defined for semigroup dynamics and then extended to a definite class of time-dependent generators. We test our approach on a prototypical model for the description of exciton transfer, keeping track of relevant phenomena, which are instead disregarded within the standard, completely positive framework.

Introduction.—The investigation of open quantum systems coupled to complex and possibly structured environments has led to a renewed interest toward the description of quantum dynamics beyond the paradigm of completely positive (CP) semigroups [1–3], as fixed by the well-known Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) master equation [4, 5]. The development of more general approaches has made possible to take into account memory effects and others phenomena which are neglected within that framework; see for example the recent reviews [6, 8].

Mostly, the assumption to have a semigroup dynamics is relaxed, while one holds firm that the evolution has to be given by CP maps. If there are no initial correlations between the system and the environment and the initial state of the latter is fixed, the exact reduced dynamics, mathematically obtained via the partial trace on the environmental degrees of freedom, is indeed CP [1–3]. On the other hand, the partial trace can be hardly ever performed explicitly, even with powerful numerical techniques. The restriction to CP maps becomes then questionable, not only when initial correlations have to be considered [9,12], but also when one uses an approximated description for specific open quantum systems at hand. The weaker condition that the dynamics is positive (P) may be enough to guarantee the consistency of the predictions one is interested in. Moreover, when a master equation is derived from some underlying microscopic model, CP is usually obtained by introducing some specific approximations, which, needless to say, may overlook some relevant phenomena. As a paradigmatic example, in the weak coupling regime one imposes (on top of the Born-Markov approximation) the secular approximation. The latter is justified when the free dynamics of the system is much faster than its relaxation [1], which is not the case for several systems of interest. Non-secular non-CP evolutions, possibly still in the semigroup regime, are extensively used, e.g., to model transport phenomena in nanoscale biomolecular networks [13–16].

Certainly, CP evolutions possess several advantages, mainly due to the general mathematical results which allow for their full characterization, such as the Kraus decomposition or the GKSL theorem itself [1]. In addition, CP evolutions have been equivalently formulated in terms of unravelings in the form of stochastic trajectories, being they with jumps [17,18] or continuous [19–24]. These methods yield a very powerful tool to simulate numerically open-system dynamics, as well as a deeper understanding of the different effects induced on the system by the interaction with the environment.

Here, we prove that a proper unraveling can be generally formulated also for P, not necessarily CP dynamics. We focus in particular on a continuous form of the unraveling, the so-called quantum state diffusion (QSD) [19–23], and we show how it can be directly extended to the more general case of P dynamics. The role of the rates and Lindblad operators in the CP unraveling is replaced by the eigenvalues and eigenvectors of a rate operator [19,21,24]. Our approach includes not only semigroup dynamics, but also a more general kind of evolutions; namely, P-divisible dynamics [26–30], which has been recently taken into account within the context of the definition of quantum Markovianity. In this way, we provide a significant class of open-system dynamics with a useful tool to describe physical phenomena, which would be neglected within the usual CP framework. This is explicitly shown by taking into account a model, which is of interest for the description of energy transfer in biomolecular networks [15,16,31].

Unraveling of CP semigroups.—Let us first briefly recall the standard results about (diffusive) unravelings of CP semigroups, as well as the relevant notation.

We consider a finite dimensional quantum system, whose state $\rho$ is an element of the set $S(C^n)$ of positive trace-one operators on $C^n$. The dynamics is described by a one-parameter family of linear maps $\{A_t\}_{t\geq 0}$, where $A_t : S(C^n) \to S(C^n)$ evolves the state $\rho$ at the initial time $t_0 = 0$, into the state $\rho_t = A_t[\rho]$ at time $t$. 

\[ S(C^n) = \{ \rho \in C^n \mid \rho = \rho^* \geq 0, \text{ Tr} \rho = 1 \} \]
These maps satisfy the semigroup property whenever \( \Lambda_t \Lambda_s = \Lambda_{t+s}, \forall t, s \geq 0 \), and in this case they can be expressed as \( \Lambda_t = e^{t\hat{G}} \) for some generator \( \hat{G} \), so that \( \rho_t \) is fixed by the master equation (ME) \( d\rho_t/dt = \hat{G}[\rho_t] \). The maps \( \Lambda_t \) ensure the trace and hermiticity preservation of the system’s state \( \rho_t \) if and only if the generator \( \hat{G} \) can be written as [3]

\[
\hat{G}[\rho] := -i[H, \rho] + \frac{n^2-1}{2} \sum_{j=1}^{n^2} c_j \left[ L_j \rho L_j^\dagger - \frac{1}{2} \left( L_j^\dagger L_j, \rho \right) \right], \quad (1)
\]

for some coefficients \( c_j \in \mathbb{R} \), linear operators \( L_j \) and an hermitian operator \( H = H^\dagger \). According to the GKSL theorem [4, 5], the maps \( \Lambda_t \) generated by \( \hat{G} \) are CP if and only if \( c_j \geq 0 \) \( \forall j \).

In addition to the GKSL theorem, another crucial feature of CP semigroups, further motivating their ubiquitous use to describe open system’s dynamics, is that they can be equivalently characterized via unravelings. An unraveling consists of a stochastic dynamics for the differential Equation (SDE) in the form [19–24]

\[ d\psi(t) = A_{\psi,t} |\psi_t\rangle dt + \sum_{k=1}^{m} B_{\psi,t,k} |\psi_t\rangle d\xi_{k,t}, \quad (2) \]

where \( A_{\psi,t}, B_{\psi,t,k} \) are (possibly non-linear) operators and \( \xi_{k,t} \) are independent complex-valued Wiener processes, with \( \mathbb{E}[d\xi_{j,t} d\xi_{k,t}] = \delta_{jk} dt, \mathbb{E}[d\xi_{j,t} d\xi_{k,t}] = \mathbb{E}[d\xi_{j,t}] = 0 \), where \( \mathbb{E} \) denotes the statistical mean. The resulting trajectories in the Hilbert space are usually referred to as quantum trajectories. We always assume that the SDE preserves the norm of \( |\psi_t\rangle \).

The connection with the statistical operator \( \rho_t \) is obtained via the stochastic average \( \mathbb{E} \). Given the stochastic projector \( P_t := |\psi_t\rangle \langle \psi_t| \) and its infinitesimal change \( dP_t \) fixed by the Itô formula, \( dP_t = [d|\psi_t\rangle \langle \psi_t|] + |d\psi_t\rangle \langle d\psi_t| \), one says that Eq. (2) is an unraveling of Eq. (1) when \( \mathbb{G}[\rho_t] = \mathbb{E}[dP_t/dt] \). In general, there exist infinite unravelings for the same ME. In the case of CP semigroups the QSD unraveling is given by [19] [24].

Eq. (2), with \( m = n^2 - 1 \) and

\[
A_{\psi,t} = -iH - \frac{1}{2} \sum_{j=1}^{n^2} c_j \left( L_j^\dagger L_j - 2\ell_{\psi,j} L_j + |\ell_{\psi,j}|^2 \right), \quad (3)
\]

\[
B_{\psi,t,j} = \sqrt{c_j} \left( L_j - \ell_{\psi,j} \right), \quad (4)
\]

where \( \ell_{\psi,j} := \langle \psi | L_j | \psi \rangle \).

Unraveling of P semigroups.—The previous approach can be extended to the case of P, but not necessarily CP semigroups. In [32], the author shows that such an extension exists for two-level systems. Here we generalize the result to Hilbert spaces of arbitrary finite dimension.

As long as we assume a semigroup evolution, this is the largest class of dynamics that can have a norm-preserving unraveling: any state obtained via the statistical average, \( \rho_t = \mathbb{E}[|\psi_t\rangle \langle \psi_t|] \), is automatically positive, being the convex mixture of pure states. Later, we will see how we can replace the semigroup assumption with a more general property of the dynamics.

The unraveling of a P semigroup depends on the behaviour of a nonlinear operator, whose relevance for CP semigroups was noticed in [19, 21, 25]. Consider a generator as in Eq. (1); for any normalized vector \( \psi \in \mathbb{C}^n \), we define the generalised transition rate operator (GTRO) as the linear combination [21, 24]

\[
W_\psi := \sum_{j=1}^{n^2-1} c_j \left( L_j - \ell_{\psi,j} \right) |\psi\rangle \langle \psi| \left( L_j - \ell_{\psi,j} \right)^\dagger. \quad (5)
\]

The crucial role of this non-linear operator for the unraveling of P semigroups traces back to the following result, which is a direct consequence of a theorem by Kossakowski [33, 34] (and is proven in [35]).

**Lemma 1.** The dynamical map \( \Lambda_t = e^{t\hat{G}} \) is P if and only if, for any normalized vector \( \psi \in \mathbb{C}^n \), \( W_\psi \) is a positive semi-definite operator.

This implies that when we have a semigroup of P maps and we consider the linear operator \( W_\psi \) for any fixed \( \psi \), its eigenvalues \( \lambda_{\psi,i} \) \( (i = 0, \ldots, n-1) \) are non-negative, where \( \lambda_{\psi,0} = 0 \) corresponds to the eigenvector \( |\psi\rangle \), so that we can write the spectral decomposition as

\[
W_\psi = \sum_{i=1}^{n-1} \lambda_{\psi,i} |\phi_{\psi,i}\rangle \langle \phi_{\psi,i}| = \sum_{i=1}^{n-1} \lambda_{\psi,i} (V_{\psi,i} |\psi\rangle \langle \psi| V_{\psi,i}^\dagger), \quad (6)
\]

with \( \lambda_{\psi,i} \geq 0 \) and \( |\phi_{\psi,i}\rangle \langle \phi_{\psi,i}| \) the corresponding orthogonal projectors, satisfying \( \langle \phi_{\psi,i} |\psi\rangle = 0 \). The second equivalence in Eq. (6) is trivially justified by defining \( V_{\psi,i} = |\phi_{\psi,i}\rangle \langle \psi| \), which will also provide us with a clear physical interpretation of the unraveling.

Now, by using Itô calculus, it is readily verified that Eq. (2) yields the following SDE for \( P_t = |\psi_t\rangle \langle \psi_t| \):

\[
dP_t = \left( A_{\psi,t} P_t + P_t A_{\psi,t}^\dagger + \sum_{k=1}^{m} B_{\psi,t,k} P_t B_{\psi,t,k}^\dagger \right) dt + \sum_{k=1}^{m} (B_{\psi,t,k} P_t d\xi_{k,t} + P_t B_{\psi,t,k}^\dagger d\xi_{k,t}^\dagger). \quad (7)
\]

In addition, since we want the SDE to be an unraveling of the ME fixed by \( \mathbb{G} \) at any time \( t \), we are assuming, in particular, that this is the case at time \( t = 0 \), i.e. \( \mathbb{E}[dP_t/dt|_{t=0}] = \mathbb{G}[\rho_0] \). From this relation, along with Eq. (7), it follows that the noise term \( \sum_{k=1}^{m} B_{\psi,t,k} P_t B_{\psi,t,k}^\dagger \) is given by the component of \( \mathbb{G}[P] \) orthogonal to \( |\psi\rangle \), i.e.

\[
\sum_{k=1}^{m} B_{\psi,t,k} P_t B_{\psi,t,k}^\dagger = (I - \mathbb{P}) \mathbb{G}[P] (I - \mathbb{P}); \quad (8)
\]
this statement, which was first shown in [19], is re-derived consistently with our notation in [35]. With the help of simple algebra, Eq. (8) reduces to

$$\sum_{k=1}^{m} B_{\psi,k} P B_{\psi,k}^\dagger = W_\psi. \quad (9)$$

We can conclude that Eq. (9) has to be satisfied by all possible (norm preserving) unravelings as in Eq. (2) of the semigroup fixed by Eq. (1). Moreover, this relation implies that the action of the drift operator $A_\psi$ on the state $|\psi\rangle$ is determined by $W_\psi$ and the generator $G$ via

$$A_\psi P + PA_\psi^\dagger = G[P] - W_\psi. \quad (10)$$

This means that $A_\psi$ can be set independently from the specific solution of Eq. (9) for the $B_{\psi,k}$, and, in particular, $A_\psi$ is still fixed by $W_\psi$, which, by virtue of the positivity of the semigroup and then Lemma 1, is characterized by the non-negative eigenvalues $\lambda_{\psi,k}$. Hence, let us set $m = n - 1$ and

$$B_{\psi,k} = \sqrt{\lambda_{\psi,k}} V_{\psi,k}. \quad (11)$$

It is then easy to see that $B_{\psi,k}$ as in Eq. (11) satisfies Eq. (8) and, along with $A_\psi$ as in Eq. (4), defines a SDE as in Eq. (2), which provides us with a proper unraveling of the P semigroup generated by Eq. (1). Eqs. (3) and (11) generalize the QSD unraveling of CP semigroups to this case: one has simply to replace $c_j \rightarrow c_j(t)$, $L_j \rightarrow L_j(t)$ and $H \rightarrow H(t)$. On the other hand, if some coefficient $c_j(t)$ takes on negative values, this construction no longer applies: by defining the operators $B_{\psi,k}$ as in Eq. (11), and deriving the ME via $P_t := |\psi_t\rangle\langle\psi_t|$, one would get the positive coefficients $|c_j(t)|$.

The unraveling defined via Eqs. (3) and (11) can also be extended to ME with time-dependent coefficients, which need not be positive functions of time. Consider any ME leading to a dynamics which, instead of being CP-divisible, is $P$-divisible, which means that the decomposition in Eq. (12) still applies, but now we make the weaker requirement that the maps $\Lambda_{t,s}$ are $P$ [20]; this property, in turn, has been identified with quantum Markovianity in [21]. The construction presented before can be immediately generalized to this situation, since the equivalence in Lemma 1 still applies. The dynamical map $\Lambda_t = T \exp \left( \int_t^s G_s ds \right)$ is $P$ and can be written as in Eq. (12) in terms of positive $\Lambda_{t,s}$ for any $t \geq s \geq 0$ if and only if, for any normalized vector $\psi \in \mathbb{C}^n$, $W_\psi$ is a positive semi-definite operator (where $c_j \rightarrow c_j(t)$ and $L_j \rightarrow L_j(t)$ in the definition of $W_\psi$ in Eq. (3) is understood). Then Eqs. (4) and (11), with the proper introduction of time-dependence, define a valid unraveling of a generic $P$-divisible ME.

Of course, there are several open-system dynamics which are not $P$-divisible and, therefore, cannot be unravelled via our approach, but where other diffusive [38] or jump [39] techniques can be exploited. On the other hand, our approach can be applied to dynamics which are straightforwardly generalized to a much wider class of dynamics, which goes beyond the class that can be treated via the usual unravelings for CP maps. We consider evolutions where the coefficients, and possibly the operators, in the ME depend on time. This allows us to describe several situations of interest, where the semigroup approximation cannot be used, because time inhomogeneous and non-Markovian effects become relevant [6,8].

Consider a time-dependent generator $G_t$, which at any time $t$ has the form as in Eq. (1), with the replacements $c_j \rightarrow c_j(t)$, $L_j \rightarrow L_j(t)$ and $H \rightarrow H(t)$. The most general conditions to guarantee CP, not to mention P, of the resulting dynamical maps $\Lambda_t = T \exp \left( \int_t^s G_s ds \right)$ (with $T$ the chronological time-ordering operator) are not known. Nevertheless, the positivity in time of the coefficients, $c_j(t) \geq 0$, guarantees that the dynamics is CP and can be decomposed into intermediate CP steps [3,36]; for any $t \geq s \geq 0$, there is a CP map $\Lambda_{t,s}$ such that

$$\Lambda_t = \Lambda_{t,s} \circ \Lambda_s; \quad (12)$$

in this case the dynamics is said to be $CP$-divisible and this property has been identified with the Markovianity of the quantum dynamics in [37]. Note that the positivity of the coefficients allows to extend the QSD unraveling of CP semigroups to this case: one has simply to replace $c_j \rightarrow c_j(t)$, $L_j \rightarrow L_j(t)$ and $H \rightarrow H(t)$ in Eqs. (13) and (14). On the other hand, if some coefficient $c_j(t)$ takes on negative values, this construction no longer applies: by defining the operators $B_{\psi,k}$ as in Eq. (11), and deriving the ME via $P_t := |\psi_t\rangle\langle\psi_t|$, one would get the positive coefficients $|c_j(t)|$. The unraveling defined via Eqs. (3) and (11) can also be extended to ME with time-dependent coefficients, which need not be positive functions of time. Consider any ME leading to a dynamics which, instead of being CP-divisible, is $P$-divisible, which means that the decomposition in Eq. (12) still applies, but now we make the weaker requirement that the maps $\Lambda_{t,s}$ are $P$ [20]; this property, in turn, has been identified with quantum Markovianity in [21]. The construction presented before can be immediately generalized to this situation, since the equivalence in Lemma 1 still applies. The dynamical map $\Lambda_t = T \exp \left( \int_t^s G_s ds \right)$ is $P$ and can be written as in Eq. (12) in terms of positive $\Lambda_{t,s}$ for any $t \geq s \geq 0$ if and only if, for any normalized vector $\psi \in \mathbb{C}^n$, $W_\psi$ is a positive semi-definite operator (where $c_j \rightarrow c_j(t)$ and $L_j \rightarrow L_j(t)$ in the definition of $W_\psi$ in Eq. (3) is understood). Then Eqs. (4) and (11), with the proper introduction of time-dependence, define a valid unraveling of a generic $P$-divisible ME.

Unraveling of $P$-divisible dynamics and relation with Markovianity.—Now, we show how our approach can be
P and not CP and, more importantly, it yields a direct
generalization of the construction for the semigroup case,
without calling for hierarchical equations, nor for corre-
lations between different trajectories, which are instead
usually required by the above-mentioned techniques.

As a final remark, we note that Eqs. (2), (3) and (11)
comprise the most general (Markovian) dynamics of col-
lapse models \cite{41-45}. If we limit to a dynamics as in
Eq. (2), the requirement of getting a closed linear average
description (i.e. a closed ME for the statistical operator
\( \rho_t \), which is physically motivated by the request of no-
superluminal-signaling \cite{46, 47}) is not enough to guaran-
tee the CP. This has been shown with a counterexample
in \cite{18}, and it traces back to the possible lack of norm
preservation of the SDE extended to an arbitrary ancilla,
as explained more in detail in \cite{35}. In this context, the
CP of the ensemble dynamics is an extra assumption, not
emerging from fundamental requirements.

The Bloch-Redfield equation for a dimer system.—As
a specific example, we consider a simple description of a
dimer system, which nevertheless yields a relevant
model to investigate the exciton transfer, for example
in biomolecular complexes \cite{15-16, 31}.

The state of the excitation is associated with a three-
level system: two levels for the excitation being in one or
the other site, and one level for the absence of excitation.
The most relevant sources of noise are the pure dephas-
ing and the recombination process. Using a perturbative
approach (e.g., the projection operator techniques) up to
second order and the Born-Markov approximation, one
gets the Bloch-Redfield equation \cite{1}. This equation usu-
ally does not guarantee the positivity of the evolution
and it is then further approximated by a Lindblad equa-
tion, which even ensures that the dynamics is CP. The
Lindblad equation is obtained via the secular approxi-
amation (SA), which essentially neglects all the terms cou-
ping population and coherences of the system. However,
this approximation is not always justified from a physical
point of view, as it calls for a large difference in the time
scales of the free evolution and the dissipative relaxation
of the system. To overcome this difficulty and retain all
the relevant phenomena in the dimer evolution, yet in a
semigroup description of the dynamics, a partial SA was
introduced in \cite{15}. The latter discards only some terms
which couple population and coherences, while it pre-
serves the most relevant ones. The resulting ME implies
a P, but in general not CP evolution. Hence, it provides
us with a natural benchmark to test our method.

The ME both after the full and the partial SA can be
written as \cite{15}

\[
\dot{\rho}_{ij}(t) = \sum_{kl=1}^{3} R_{ij,kl}^{\chi} \rho_{kl}(t),
\tag{13}
\]

where \( \rho_{kl}(t) = |k\rangle \langle \rho(t) |l\rangle \). We will use the notation
\( \chi = \text{CP} \) for the full SA, while \( \chi = \text{P} \) for the partial
SA; the explicit coefficients \( R_{ij,kl}^{\chi} \) are given in \cite{35}. In
Fig.1.a and b) we report some trajectories for the evolu-
tion of the, respectively, first and second site popula-
tions, which are obtained by means of the unraveling of the
P dynamics after the partial SA. Thus, we demon-
strate the effectiveness of our approach on a physically
relevant model; the explicit form of the GTRO and the
resulting unraveling operators \( A_\psi \) and \( B_\psi,k \) are given in
\cite{35}. Let us stress that the traditional unravelings for CP
semigroups could not be applied to this dynamics, since
they require a Lindblad equation and thus, in this con-
text, a full SA. Crucially, the latter would cancel any cou-
ping between population and coherences, therefore poten-
tially disregarding some significant phenomena. This
is explicitly shown in Fig.1.c) and d) where we compare
the evolution of the populations obtained by solving the
Lindblad equation after the full SA and the populations
obtained by averaging 1000 trajectories of our unravel-
ing. The former completely neglects significant oscillations
\cite{15}, which are instead fully captured by the unravel-
ling of the P dynamics.

Conclusions.— We have introduced a continuous unrav-
eling for dynamics which are P, but not necessarily
CP. Our approach directly generalizes the QSD method:
the rates and operators extracted from the master equa-
tion have to be replaced by, respectively, the eigenval-
ues and eigenvectors of a proper rate operator. We have
taken into account the case of semigroup dynamical maps
and, additionally, we have extended our result to include
a more general class of divisible open-system dynamics.
By virtue of the unraveling of P dynamics, one can avoid
to impose approximations which could introduce signifi-

\begin{figure}[ht]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Trajectories for the evolution of the population of site one (a) and two (b); each trajectory corresponds to a different
realization of the solution of the SDE in Eq. (2), with \( A_\psi \), as in Eq. (3) and \( B_\psi \), as in Eq. (11) and derived by diag-
onalizing the GTRO at each point of the computational time
domain; the deterministic initial state is \( |\psi(0)\rangle = |2\rangle \), while
the state at time \( t \) is \( |\psi(t)\rangle = \alpha(t) |1\rangle + \beta(t) |2\rangle + \gamma(t) |3\rangle \). Evo-
lution of the population of site one (c) and site two (d) given
by the ensemble average of 1000 trajectories of our unravel-
ing (blue), and the solution of the Lindblad equation after
full SA (green); in the inset, the ensemble average (blue) and
the solution of the P ME (red dotted) are shown to agree
within the standard deviation of the mean (vertical bars) of
the trajectories; the initial state is set as \( \rho(0) = |2\rangle \langle 2| \).
}
\end{figure}
ciant errors in the system of interest. This has been shown explicitly in a case study, by investigating the population evolution in a dimer system.

Certainly, a crucial point will be to simplify the task of diagonalizing the GTRO at each time step, e.g. by looking for possible connections between its spectral decompositions at subsequent times. Also, it will be of interest to study how and to what extent the range of applicability of our method can be further extended, for example, combining it with other unraveling techniques \[38-40\], which apply to general non-Markovian dynamics.

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[42] A. Bassi, K. Lochan, S. Satin, T.P. Singh, and H. Ulbricht, Rev. Mod. Phys. 85, 471 (2013).
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Proof of Lemma 1

We prove Lemma 1 in the main text, that is,
\[(\rho \geq 0 \Rightarrow \Lambda_t[\rho] \geq 0) \Leftrightarrow (W_\psi \geq 0, \ \forall \psi).\]  \hspace{1cm} (14)

The lemma is actually equivalent to a theorem of Kossakowski [23, 34]. As noticed in [27], such a theorem can be rephrased as follows: given any orthonormal basis \(\{|u_i\}_{i=1\ldots n}\), then
\[(\rho \geq 0 \Rightarrow \Lambda_t[\rho] \geq 0) \Leftrightarrow \sum_{j=1}^{n^2-1} c_j |\langle u_i | L_j | u_\psi \rangle|^2 \geq 0,\]  \hspace{1cm} (15)

for any couple \(i \neq i'\).

Let us consider two arbitrary states \(|\psi\rangle, |\varphi\rangle\). Write
\[|\varphi\rangle = a |\psi\rangle + b |\psi_\perp\rangle,\]  \hspace{1cm} (16)

where the two vectors on the r.h.s. are the components of \(|\varphi\rangle\), which are parallel and perpendicular to \(|\psi\rangle\), respectively. Notice the relations
\[\langle \psi | (L_j - \ell_{\psi,j}) | \psi \rangle = 0,\]  \hspace{1cm} (17)
\[\langle \psi | (L_j - \ell_{\psi,j}) | \psi_\perp \rangle = \langle \psi | L_j | \psi_\perp \rangle.\]  \hspace{1cm} (18)

Then, using Eq. (17) and Eq. (18), we obtain for any \(\psi\) the equivalence
\[\langle \varphi | W_\psi | \varphi \rangle = |b|^2 \sum_{j=1}^{n^2-1} c_j |\langle \psi | L_j | \psi_\perp \rangle|^2 \geq 0, \quad \forall |\psi\rangle, |\varphi\rangle.\]  \hspace{1cm} (19)

Given the above equation, the proof of the Lemma is straightforward. On the one hand, the positivity of \(W_\psi\) for any \(|\psi\rangle\) implies the positivity of the r.h.s. of Eq. (15) for any couple of orthogonal elements of any given basis (just set \(|\psi\rangle = |u_i\rangle\) and \(|\psi_\perp\rangle = |u_{i'}\rangle\)), from which the positivity of the semigroup follows. One the other hand, if \(\Lambda_t\) is P, and hence the r.h.s. of Eq. (15) is positive, the non-negativity of the r.h.s. of Eq. (19) for any \(|\varphi\rangle\) and \(|\psi\rangle\), therefore the positive semidefiniteness of \(W_\psi\) for any \(|\psi\rangle\), directly follows from setting \(|u_i\rangle = |\psi\rangle\) and using the decomposition of \(|\psi_\perp\rangle\) on the elements of the basis \(|u_\psi\rangle\) orthogonal to \(|u_i\rangle\), i.e. with \(i \neq i'\).

The extension to the case of P-divisible dynamics directly follows from the analogous extension of the theorem by Kossakowski, pointed out in [27]. Given a ME as in Eq. (11), with \(c_j \to c_j(t)\), \(L_j \to L_j(t)\) and \(H \to H(t)\), the resulting dynamical map \(\Lambda_t\) is P and can be decomposed via Eq. (12) with \(P \Lambda_t, s\) if and only if
\[\sum_{j=1}^{n^2-1} c_j(t) |\langle u_i | L_j(t) | u_\psi \rangle|^2 \geq 0,\]  \hspace{1cm} (20)

for any couple \(i \neq i'\). But then, similarly to the proof here above one can show that the latter condition is equivalent to the positivity of \(W_\psi\), defined as in Eq. (5), with the replacements \(c_j \to c_j(t)\) and \(L_j \to L_j(t)\).

Proof of Eq. (8).

To prove Eq. (8), let us take the expectation of Eq. (7) for a deterministic initial condition, \(|\psi_0\rangle =: |\psi\rangle\) so that \(\rho_0 = P_0 =: P\); since \(\mathbb{E} [dP_t/dt|_{t=0}] = \mathcal{G}[P_0]\), we get
\[A_\psi P + PA_\psi^\dagger + \sum_{k=1}^m B_{\psi,k} P B_{\psi,k}^\dagger = \mathcal{G}[P].\]  \hspace{1cm} (21)

The SDE in Eq. (2) preserves the norm of the state vector only if
\[\langle \psi | B_{\psi,k} | \psi \rangle = 0, \quad \forall \psi,k.\]  \hspace{1cm} (22)

Then, if we denote by \(|\psi_\perp\rangle\) a vector orthogonal to \(|\psi\rangle\), the norm constraint translates into \(B_{\psi,k} |\psi_\perp\rangle = 0\). In other words, the noise operators must produce orthogonal changes to the state vector they act upon. For any fixed \(|\psi\rangle\) this condition implies
\[P \left( \sum_{k=1}^m B_{\psi,k} P B_{\psi,k}^\dagger \right) P = 0;\]  \hspace{1cm} (23)

so that by projecting Eq. (21) on the subspace orthogonal to \(|\psi\rangle\), Eq. (23) together with Eq. (24) prove the claim.

In addition, it is clear that Eq. (21), along with Eq. (9), leads to Eq. (10). Writing explicitly \(\mathcal{G}[P]\) and \(W_\psi\), respectively, Eq. (1) and Eq. (9), one can easily check that Eq. (3) gives a solution to Eq. (10). Let us emphasize that, indeed, this is not the only non-linear operator satisfying Eq. (10), but any other solution \(A_\psi\) would act on the state \(\psi\) exactly in the same way, such that
\[A_\psi \langle \psi \rangle = A_\psi \langle \psi \rangle;\]  \hspace{1cm} (25)

in other terms, it would lead exactly to the same unraveling, see Eq. (3): in this regard, the choice of \(A_\psi\), for fixed \(B_{\psi,k}\) and noise \(\xi_{k,\ell}\) (see also the next Section), is unique. To prove the validity of Eq. (25), consider two different solutions, \(A_\psi\) and \(A'_{\psi}\), to Eq. (10). Then,
\[A_\psi P + PA_\psi^\dagger = A'_{\psi} P + PA'_{\psi}^\dagger.\]  \hspace{1cm} (26)

Hence, for any state \(|\psi_\perp\rangle\) orthogonal to \(|\psi\rangle\), one has
\[\langle \psi_\perp | A_\psi | \psi \rangle = \langle \psi_\perp | A'_{\psi} | \psi \rangle\]

and, analogously for the parallel component,
\[\text{Re}[\langle \psi | A_\psi | \psi \rangle] = \text{Re}[\langle \psi | A'_{\psi} | \psi \rangle].\]

In principle, \(A_\psi\) and \(A'_{\psi}\) could differ by a purely imaginary component parallel to \(|\psi\rangle\); but it is then easy to see [45] that such a difference corresponds simply to an irrelevant global phase applied to \(|\psi\rangle\).
Unraveling of a non-CP qubit ME

In this section, we deal with the unravelling of the non-CP semigroup which was first derived in \cite{32,48}. Although the physical relevance of the model is not clear, it is the first example of an unravelling of a P, but non CP semigroup and it was thus used in \cite{48} to prove that the CP of the average dynamics is not guaranteed by the existence of a Markovian unravelling. We will show now how such a result can be straightforwardly re-derived and further clarified using our method.

Hence, consider the non-CP semigroup acting on $\mathcal{S}(C^2)$ and generated by

$$\frac{d\rho_t}{dt} = \sum_{j=1}^{3} c_j (\sigma_j \rho_t \sigma_j - \rho_t), \quad c_1 = c_2 = -c_3 = 1,$$  \hspace{1cm} (26)

where $\sigma_j$ are the usual Pauli matrices $\sigma_1 \equiv \sigma_x$, $\sigma_2 \equiv \sigma_y$ and $\sigma_3 \equiv \sigma_z$. The GTRO associated to Eq. (26) is

$$W_\psi = \sum_{j=1}^{3} c_j (\sigma_j - s_j) |\psi\rangle \langle \psi| (\sigma_j - s_j)$$ \hspace{1cm} (27)

with $s_j := |\psi\rangle \langle \sigma_j |\psi\rangle$, and it has spectral decomposition

$$W_\psi = \lambda_1 |\psi\rangle \langle \psi| + \lambda_2 |\psi\rangle_N \langle \psi_N|,$$

where the eigenvalues are $\lambda_1 = 0$ and $\lambda_2 = 2 s_3^2$, while the eigenvectors are $|\psi\rangle$ and $|\psi_N\rangle$ orthogonal to $|\psi\rangle$. The first eigenvalue and eigenvector can be easily found by noticing that $W_\psi |\psi\rangle = 0$, as Eq. (17) ensures (see also the discussion before Eq. (6)). Then, we are left with verifying that

$$(W_\psi - 2 s_3^2) |\psi\rangle_N = \sum_{j=1}^{3} c_j \left(\sigma_j P \sigma_j - s_j P \sigma_j - 2 s_3^2\right) |\psi_N\rangle = 0.$$ \hspace{1cm} (28)

To show that, we project Eq. (28) on the basis vectors $|\psi\rangle$ and $|\psi_N\rangle$, respectively. Since for any $j$

$$\langle \psi | \sigma_j P \sigma_j |\psi_N\rangle = \langle \psi | \sigma_j |\psi\rangle \langle \sigma_j |\psi_N\rangle = (\psi | s_j |\psi\rangle \langle \sigma_j |\psi\rangle |\psi_N\rangle = (\psi | s_j P \sigma_j |\psi_N\rangle, \hspace{1cm} (29)$$

we have

$$\langle \psi | (W_\psi - 2 s_3^2) |\psi\rangle_N = \sum_{j=1}^{3} c_j \langle \psi | (\sigma_j P \sigma_j - s_j P \sigma_j) |\psi_N\rangle = 0.$$ \hspace{1cm} (29)

On the other hand, since $\sum_{j=1}^{3} 1 s_j^2 = 1$ and $r_j = |\langle \psi | \sigma_j |\psi_N\rangle|^2 = 1 - s_j^2$, we have

$$\langle \psi_N | (W_\psi - 2 s_3^2) |\psi\rangle_N = \sum_{j=1}^{3} c_j \langle \psi_N | \sigma_j P \sigma_j |\psi_N\rangle - 2 s_3^2 r_j = \sum_{j=1}^{3} c_j r_j - 2 s_3^2 = 0.$$ \hspace{1cm} (30)

Eq. (29) together with Eq. (30) prove Eq. (28), which implies $W_\psi = 2 s_3^2 |\psi\rangle \langle \psi|_N$.

Then, according to Eq. (6) and (3), the noise and the drift terms which define a unraveling of Eq. (26) are given, for any $|\psi\rangle$, by

$$B_\psi = \sqrt{2} s_3 |\psi_\perp\rangle \langle \psi|$$

$$A_\psi = -i H - \frac{1}{2} \sum_{j=1}^{3} c_j (\sigma_j - s_j)^2,$$

so that

$$|d\psi\rangle = -i H - \frac{1}{2} \sum_{j=1}^{3} (\sigma_j - s_j)^2 |\psi\rangle dt + \sqrt{2} s_3 |\psi_\perp\rangle d\xi_{t}. \hspace{1cm} (31)$$

In fact, one can verify that Eq. (31) is norm preserving $\langle d\psi | d\psi \rangle + |d\psi\rangle \langle d\psi| = 0$ and generates, on average, the ME in Eq. (26).

CP and norm preservation

The requirement of getting a closed ME from a diffusive norm preserving SDE does not imply, by itself, CP. In this section we argue that the non CP character of the resulting ME can be related to the lack of norm preservation of its unraveling extended to an arbitrary ancilla.

To see this, let us recall that a linear map $\Lambda : \mathcal{S}(C^n) \rightarrow \mathcal{S}(C^n)$ is CP if and only if the map $\Lambda \otimes I : \mathcal{S}(C^n \otimes C^n) \rightarrow \mathcal{S}(C^n \otimes C^n)$ is P. Let $G$ and $G'$ be the generators of $\Lambda$ and $\Lambda \otimes \mathbb{1}$, respectively. Assume $\Lambda$ (at least) P, and call $d\psi$ the norm preserving unraveling of its generator. Moreover, we define $d\psi'$ to be a particular extension of the original SDE to an enlarged Hilbert space, such that it reproduces, on average, $G'$. Then, we are led to the following diagram

$$d\psi \rightarrow d\psi' \hspace{1cm} (32)$$

where the vertical arrows represent the operations of unraveling and taking the stochastic average, and the horizontal ones stand for tensoring with auxiliary operators, in such a way that the diagram commutes.

Now let us assume that $\Lambda$ is not CP. Then, there exist $t$ and $\rho' \in \mathcal{S}(C^n \otimes C^n)$ such that $\rho = (\Lambda_t \otimes \mathbb{1})[\rho'] = E[P'_t]$, where $P'_t = |\psi'_t\rangle \langle \psi'_t|$, is not a proper quantum state, i.e. $\rho$ is either not positive, not trace one, or both. However, any operator obtained via stochastic average is positive, being the convex combination of the positive operators $P'_t$. Then, if $\Lambda \otimes \mathbb{1}$ is not P, it must be the case that $\text{Tr}(E[P'_t]) = E[\text{Tr}(P'_t)] \neq 1$, i.e. $|d\psi'|$ does not preserve the norm of all state vectors. In summary, under the
hypothesis that diagram \([32]\) commutes, asking that the extended SDE be norm preserving is a sufficient condition for the CP of \(\Lambda\).

Unraveling operators for the dimer system of \([15]\)

Here, we show how to derive the explicit expression of the unraveling operators \(A_\psi\) and \(B_{\psi,k}\), see Eqs.\([2]\), \([3]\) and \([11]\), for the dimer system, which was investigated in \([15]\): indeed, the reader is referred to the mentioned paper for more details about the model. Hence, we first need to write the master equation \([13]\) into the Lindblad form as in Eq.\([1]\).

Before that, let us report the explicit expression of the coefficients for the master equation in Eq.\([13]\). After the partial SA, we have [see Eq.\((11)\) in \([15]\)]

\[
\begin{align*}
\mathcal{R}_{11,11}^P &= \mathcal{R}_{22,22}^P = \mathcal{R}_{33,33}^P / 2 = -4 \\
\mathcal{R}_{11,33}^P &= \mathcal{R}_{22,33}^P = \mathcal{R}_{33,22}^P = 4 \\
\mathcal{R}_{11,12}^P &= \mathcal{R}_{22,31}^P = \mathcal{R}_{31,32}^P = \mathcal{R}_{32,31}^P = -71i \\
\mathcal{R}_{22,12}^P &= \mathcal{R}_{11,21}^P = \mathcal{R}_{13,23}^P = \mathcal{R}_{23,13}^P = 71i \\
\mathcal{R}_{21,11}^P &= \mathcal{R}_{12,11}^P = -\mathcal{R}_{12,22}^P = -\mathcal{R}_{21,22}^P = -1 + 71i \\
\mathcal{R}_{12,12}^P &= \mathcal{R}_{32,21}^P = -8 - 46i \\
\mathcal{R}_{13,13}^P &= \mathcal{R}_{33,21}^P = -9 + 12210i \\
\mathcal{R}_{23,23}^P &= \mathcal{R}_{32,32}^P = -9 + 12256i, \tag{33}
\end{align*}
\]

and all the other coefficients are equal to 0; as one can directly check, this provides us with a P, but not CP evolution. On the other hand, as widely discussed in \([15]\), a CP evolution is obtained with a full SA, which means that the terms coupling populations and coherences are set to 0:

\[
\begin{align*}
\mathcal{R}_{11,12}^{\text{CP}} &= \mathcal{R}_{22,21}^{\text{CP}} = \mathcal{R}_{31,32}^{\text{CP}} = \mathcal{R}_{32,31}^{\text{CP}} = 0 \\
\mathcal{R}_{12,12}^{\text{CP}} &= \mathcal{R}_{13,23}^{\text{CP}} = \mathcal{R}_{23,13}^{\text{CP}} = 0 \\
\mathcal{R}_{21,11}^{\text{CP}} &= \mathcal{R}_{12,11}^{\text{CP}} = \mathcal{R}_{22,22}^{\text{CP}} = \mathcal{R}_{21,22}^{\text{CP}} = 0, \tag{34}
\end{align*}
\]

while all the other coefficients in Eq.\((33)\) are not changed. The Lindblad form of these two master equations is now readily obtained following \([4]\). First, note that the generator \(\mathcal{G}\) can be directly reconstructed via the coefficients in Eq.\((13)\), since

\[
\mathcal{R}_{ij,kl}^{\xi} = \langle i | \mathcal{G}^{\xi} | k \rangle \langle l | j \rangle. \tag{35}
\]

Then, consider the basis of operators on \(\mathbb{C}^3\) given by \(\{\tau_i\}_{i=0,\ldots,8}\), with \(\tau_0 = \frac{1}{\sqrt{3}}\), while the \(\tau_i\)s with \(i = 1,\ldots,8\) are the Gell-Mann matrices over \(\sqrt{2}\) (to guarantee the normalization with respect to the Hilbert-Schmidt scalar product). Hence, the so-called non-diagonal form of the generator \(\mathcal{G}\) is given by

\[
\mathcal{G}[\rho] := -i [H, \rho] + \sum_{ij=1}^8 \sum_{k=0}^8 \mathcal{R}_{ij} \tau_i \rho_j^\dagger - \frac{1}{2} \left\{ \tau_j^\dagger \tau_i, \rho \right\}, \tag{36}
\]

with

\[
H = \frac{1}{2i} (\tau_i^\dagger - \tau_i), \quad \tau = \frac{1}{3} \sum_{i=1}^8 \text{Tr} \left\{ \tau_k \tau_i \mathcal{G}[\tau_k] \right\} \tau_i \tag{37}
\]

The matrix of coefficients \(d_{ij}\) is Hermitian, as the dynamics is Hermiticity preserving; so there is a unitary matrix \(U\), with elements \(U_{ij}\), which diagonalizes it. The resulting coefficients of the diagonal matrix are just the coefficients \(c_j\) appearing in the diagonal form of \(\mathcal{G}\) in Eq.\([1]\), and the matrix \(U\) also defines the corresponding Lindblad operators \(L_j\): explicitly one has

\[
c_j = \sum_{kk'=1}^8 U_{kj}^* d_{kk'} U_{k'j}, \tag{38}
\]

For the generator \(\mathcal{G}^P\) fixed by Eq.\([33]\) we get the coefficients

\[
c_1 = 2 + \sqrt{5}, \quad c_2 = c_3 = c_4 = c_5 = 4, \quad c_6 = \frac{1}{3} \left( 4 + \sqrt{19} \right), \quad c_7 = 2 - \sqrt{5}, \quad c_8 = \frac{1}{3} \left( 4 - \sqrt{19} \right),
\]

where, note, the last two are negative, thus witnessing the non CP of the resulting semigroup dynamics. The corresponding (canonical) Lindblad operators are

\[
\begin{align*}
L_1 &= -f_{1-,\tau_1} + f_{1+,\tau_1^*} \\
L_2 &= \tau_4 \\
L_3 &= \tau_5 \\
L_4 &= \tau_6 \\
L_5 &= \tau_7 \\
L_6 &= i f_{2-,\tau_6} + f_{2+,\tau_6^*} \\
L_7 &= -i f_{2+,\tau_2} + f_{2-,\tau_2^*} \\
L_8 &= \sqrt{\frac{1}{2} \pm \frac{1}{\sqrt{5}}}.
\end{align*}
\]

finally, the Hamiltonian part of the dynamics is given by

\[
H = -71 \sqrt{2} \tau_1 - \sqrt{2} \tau_2 + 23 \sqrt{2} \tau_3 - 12233 \sqrt{\frac{2}{3} \tau_8}. \tag{41}
\]

The unraveling operator \(A_\psi\) is hence directly defined by Eq.\([3]\), while \(B_{\psi,k}\) is obtained via the evaluation of the GTRO in Eq.\([3]\) and its diagonalization, see Eqs.\([4]\) and \([11]\).

Repeating the same calculations for the generator \(\mathcal{G}^{\text{CP}}\) fixed by the full SA, i.e., Eq.\([34]\), we directly get a diagonal form of the generator, with (positive) coefficients

\[
c_1 = c_2 = c_3 = c_4 = c_5 = 4, \quad c_6 = \frac{8}{3} \tag{42}
\]

and Lindblad operators, as well as Hamiltonian, given by

\[
\begin{align*}
L_1 &= \tau_3 \\
L_2 &= \tau_4 \\
L_3 &= \tau_5 \\
L_4 &= \tau_6 \\
L_5 &= \tau_7 \\
L_6 &= \tau_8 \\
H &= 23 \sqrt{2} \tau_3 - 12233 \sqrt{\frac{2}{3} \tau_8}. \tag{43}
\end{align*}
\]
Here, since the dynamics is CP one could apply the usual formulation of the (diffusive) unraveling, which is directly fixed by Eqs. (3) and (4).