Theory of initialization-free decoherence-free subspaces and subsystems

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We introduce a generalized theory of decoherence-free subspaces and subsystems (DFSs), which do not require accurate initialization. We derive a set of conditions for the existence of DFSs within this generalized framework. By relaxing the initialization requirement we show that a DFS can tolerate arbitrarily large preparation errors. This has potentially significant implications for experiments involving DFSs, in particular for the experimental implementation, over DFSs, of the large class of quantum algorithms which can function with arbitrary input states.

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I. INTRODUCTION

In recent years much effort has been expended to develop methods for tackling the deleterious interaction of controlled quantum systems with their environment. This effort has been motivated in large part by the need to overcome decoherence in quantum-information processing tasks, a goal which was thought to be unattainable at first [1–3]. Decoherence-free (or noiseless) subspaces [4–7] and subsystems [8–11] (DFSs) are among the methods which have been proposed to this end, and also experimentally realized in a variety of systems [12–15]. In this manner of passive quantum error correction, one uses symmetries in the form of the interaction between system and environment to find a "quiet corner" in the system Hilbert space not experiencing this interaction. Of the various methods of quantum error correction, so far only DFSs have been combined with quantum algorithms in the presence of decoherence [16,17]. For a review of DFSs and a comprehensive list of references see Ref. [18].

We have reexamined the theoretical foundation of DFSs and have found that the conditions for their existence can be generalized. It is our purpose in this paper to present these generalized conditions. Our most significant result is a drastic relaxation of the initialization condition for DFSs: whereas it was previously believed that one must be able to perfectly initialize a state inside a DFS, here we show that this does in fact need not be so. Instead one can tolerate an arbitrarily large preparation error, which in turn means significantly relaxed experimental preparation conditions. In contrast, only a small preparation error can be tolerated when quantum error-correcting codes (QECCs) are used to overcome decoherence [19]. Whether a similar generalization is possible in the case of QECCs is an interesting open question, which it may be possible to address by developing a suitable generalization of the results of Ref. [20], where the DFS-QECC connection [8,21] has been strengthened.

The relaxation of the initialization requirement is perhaps most significant in light of a series of results showing that a class of important quantum algorithms (Shor [22], Grover [23], and Deutsch-Josza [24] included) can be successfully executed under imperfect initialization conditions [25–33]. This means that imperfectly initialized DFSs can be used as a "substrate" for running these algorithms.

To present our results we first review and reexamine the previous results on DFSs, in Sec. II. We do so both for general completely positive (CP) maps and for Markovian dynamics. The definitions we give for DFSs in these two cases are slightly different, reflecting the continuous-time nature of Markovian dynamics, whereas we use CP maps to describe discrete-time evolution. In Sec. III, we present our generalized DFS conditions for CP maps and for Markovian dynamics. We illustrate these conditions for Markovian dynamics with an example that reveals some of the new features. In Sec. IV we discuss the implications of our relaxed initialization condition in the context of quantum algorithms. Section V is devoted to a case study of non-Markovian dynamics, intermediate between (formally exact) CP maps and (approximate) Markovian dynamics. A unique formulation does not exist in this case, and we consider the master equation introduced in Ref. [34]. The analytical solvability of this equation permits a rigorous derivation of the conditions for a DFS. For clarity of presentation we defer most supporting calculations to the Appendix.

II. REVIEW OF PREVIOUS CONDITIONS FOR DECOHERENCE-FREE SUBSPACES AND SUBSYSTEMS

We refer the reader to Ref. [18] for a detailed review, including many references and historical context. Here we focus on aspects of direct relevance to our results.

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A. Decoherence-free subspaces

Consider a system with Hilbert space $\mathcal{H}_S$. In Refs. [5–7,35,36] a subspace $\mathcal{H}_{\mathrm{DFS}} \subset \mathcal{H}_S$ was called decoherence-free if any state $\rho_S(0)$ of the system initially prepared in this subspace is unitarily related to the final state $\rho_S(t)$ of the system, i.e.,

$$\rho_S(0) = \mathcal{P}_d \rho_S(0) \mathcal{P}_d \Rightarrow \rho_S(t) = \mathbf{U} \rho_S(0) \mathbf{U}^{\dagger}. \tag{1}$$

Here $\mathbf{U}$ is unitary and $\mathcal{P}_d$ is the projection operator onto $\mathcal{H}_{\mathrm{DFS}}$. Important and motivating early examples of DFSs were given in [4,37–39]. An alternative definition of a DFS is as a subspace in which the state purity is always 1 [40]; here we will not pursue this approach.

To exploit DF states for quantum-information preservation one needs a method to experimentally verify these states [41], but from a theoretical standpoint one needs to first formulate the effect of the environment. In the following, we consider general CP maps and Markovian dynamics.

1. Completely positive maps

The modeling of environmental effects on an open quantum system has been a challenging problem since at least the 1950s [42,43], but under certain simplifying assumptions one can obtain a simple form for the dynamical equations of open systems [44]. For example, the assumption of an initially decoupled state of system and bath, $\rho_{SB}(0) = \rho_S(0) \otimes \rho_B$, results in a CP map known as the Kraus operator sum representation [45]:

$$\rho_S(t) = \mathrm{Tr}_B\{\mathbf{\Lambda}(t)[\rho_S(0) \otimes \rho_B]\mathbf{\Lambda}(t)^{\dagger}\} = \sum_{\alpha} \mathbf{E}_{\alpha}(t)\rho_S(0)\mathbf{E}_{\alpha}^{\dagger}(t). \tag{2}$$

Here

$$\mathbf{\Lambda}(t) = \mathcal{T} \exp\left(-i\int_0^t \mathbf{H}(s)ds\right) \tag{3}$$

is the unitary propagator for the joint evolution of system and bath governed by total Hamiltonian $\mathbf{H}$ ($\mathcal{T}$ denotes time ordering and we work in units such that $\hbar = 1$); the "Kraus operators" $\{\mathbf{E}_{\alpha}\}$ are given by

$$\mathbf{E}_{\alpha} = \sqrt{\lambda_{\nu}}\langle \mu|\mathbf{\Lambda}|\nu\rangle, \quad \alpha = (\mu,\nu), \tag{4}$$

where $|\mu\rangle$ and $|\nu\rangle$ are bath states in the spectral decomposition $\rho_B = \sum_{\nu}\lambda_{\nu}|\nu\rangle\langle\nu|$. Trace preservation of $\rho_S(t)$ implies the sum rule

$$\sum_{\alpha} \mathbf{E}_{\alpha}^{\dagger}\mathbf{E}_{\alpha} = \mathbf{I}_S, \tag{5}$$

where $\mathbf{I}_S$ is the identity operator on the system.

In [36] a DFS condition was derived for general CP maps of this type. We denote the subspace of states orthogonal to $\mathcal{H}_{\mathrm{DFS}}$ by $\mathcal{H}_{\mathrm{DFS}^{\perp}}$, so that $\mathcal{H}_S = \mathcal{H}_{\mathrm{DFS}} \oplus \mathcal{H}_{\mathrm{DFS}^{\perp}}$. According to Eq. (4) in [36] the Kraus operators take the block-diagonal form

$$\mathbf{E}_{\alpha} = \begin{pmatrix} c_{\alpha}\mathbf{U}_{\mathrm{DFS}} & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_{\alpha} \end{pmatrix}, \tag{6}$$

where the upper (lower) nonzero block acts entirely inside $\mathcal{H}_{\mathrm{DFS}}$ ($\mathcal{H}_{\mathrm{DFS}^{\perp}}$); $\mathbf{U}_{\mathrm{DFS}}$ is a unitary matrix that is independent of the Kraus operator label α; c_{α} is a scalar ($\sum_{\alpha}|c_{\alpha}|^2 = 1$); and $\mathbf{B}_{\alpha}$ is arbitrary, except that $\sum_{\alpha}\mathbf{B}_{\alpha}^{\dagger}\mathbf{B}_{\alpha} = \mathbf{I}_{\mathrm{DFS}^{\perp}}$. It is simple to verify that the DFS definition (1) is satisfied in this case, with $\mathbf{U} = \mathbf{U}_{\mathrm{DFS}}$.

Theorem 1 in [36] reads: "A subspace $\mathcal{H}_{\mathrm{DFS}}$ is a DFS if and only if all Kraus operators have an identical unitary representation upon restriction to it, up to a multiplicative constant." This theorem is actually compatible with a more general form for the Kraus operators than Eq. (6), since "upon restriction to it" concerns only the upper left block of $\mathbf{E}_{\alpha}$. We derive the most general form of $\mathbf{E}_{\alpha}$ in Sec. III below, and find that, indeed, a more general form than Eq. (6) is possible: one of the off-diagonal blocks need not vanish. In other words, leakage from $\mathcal{H}_{\mathrm{DFS}^{\perp}}$ into $\mathcal{H}_{\mathrm{DFS}}$ is permitted. As we further show in Sec. III, the form (6) in fact appears in the context of unital channels.

2. Markovian dynamics

The most general form of CP Markovian dynamics is given by the Lindblad equation [46–48]

$$\frac{\partial \rho_S}{\partial t} = -i[\mathbf{H}_S, \rho_S] + \mathcal{L}[\rho_S],$$

$$\mathcal{L}\cdot = \sum_{\alpha} \mathbf{F}_{\alpha}\cdot\mathbf{F}_{\alpha}^{\dagger} - \frac{1}{2}\mathbf{F}_{\alpha}^{\dagger}\mathbf{F}_{\alpha}\cdot - \frac{1}{2}\cdot\mathbf{F}_{\alpha}^{\dagger}\mathbf{F}_{\alpha}, \tag{7}$$

where $\mathbf{F}_{\alpha}$ are bounded (or unbounded, if subject to appropriate domain restrictions [49,50]) operators acting on $\mathcal{H}_S$, and where $\mathbf{H}_S$ may include a Lamb shift [51]. Given such dynamics, one restores unitarity [i.e., the DFS definition (1) with $\mathbf{U}$ generated by the Hamiltonian $\mathbf{H}_S$] if the Lindblad term $\mathcal{L}[\rho_S]$ can be eliminated. According to Refs. [6,52], a necessary and sufficient condition for this to be the case is

$$\mathbf{F}_{\alpha}|i\rangle = c_{\alpha}|i\rangle, \tag{8}$$

where $\mathcal{H}_{\mathrm{DFS}} = \mathrm{Span}\{|i\rangle\}$ and $\{c_{\alpha}\}$ are arbitrary complex scalars. Thus the Lindblad operators can be written in block form as follows:

$$\mathbf{F}_{\alpha} = \begin{pmatrix} c_{\alpha}\mathbf{I} & \mathbf{A}_{\alpha} \\ \mathbf{0} & \mathbf{B}_{\alpha} \end{pmatrix}, \tag{9}$$

with the blocks on the diagonal corresponding once again to operators restricted to $\mathcal{H}_{\mathrm{DFS}}$ and $\mathcal{H}_{\mathrm{DFS}^{\perp}}$. Note the appearance of the off-diagonal block $\mathbf{A}_{\alpha}$ mixing $\mathcal{H}_{\mathrm{DFS}}$ and $\mathcal{H}_{\mathrm{DFS}^{\perp}}$; its presence is permitted since the DFS condition (8) gives no information about matrix elements of the form $\langle i|\mathbf{F}_{\alpha}|j^{\perp}\rangle$, with $|i\rangle \in \mathcal{H}_{\mathrm{DFS}}$ and $|j^{\perp}\rangle \in \mathcal{H}_{\mathrm{DFS}^{\perp}}$.

As observed in Refs. [6,36], one should in addition require that $\mathbf{H}_S$ does not mix DF states with non-DF ones, i.e., mixed matrix elements of the type $\langle j^{\perp}|\mathbf{H}_S|i\rangle$, with $|i\rangle \in \mathcal{H}_{\mathrm{DFS}}$ and $|j^{\perp}\rangle \in \mathcal{H}_{\mathrm{DFS}^{\perp}}$, should vanish. We show below that this condition must be made more stringent.

B. Noiseless subsystems

An important observation made in Ref. [8] is that there is no need to restrict the decoherence-free dynamics to a subspace. A more general situation is when the DF dynamics is a "subsystem," or a factor in a tensor product decomposition of a subspace. Following Ref. [8], this comes about as follows. Consider the dynamics of a system S coupled to a bath B via the Hamiltonian

$$\mathbf{H} = \mathbf{H}_S \otimes \mathbf{I}_B + \mathbf{I}_S \otimes \mathbf{H}_B + \mathbf{H}_I, \tag{10}$$

where $\mathbf{H}_S$ ($\mathbf{H}_B$), the system (bath) Hamiltonian, acts on the system (bath) Hilbert space $\mathcal{H}_S$ ($\mathcal{H}_B$); $\mathbf{I}_S$ ($\mathbf{I}_B$) is the identity operator on the system (bath) Hilbert space; $\mathbf{H}_I$ is the interaction term of the Hamiltonian which can be written in general as $\Sigma_\alpha \mathbf{S}_\alpha \otimes \mathbf{B}_\alpha$. If the system Hamiltonian $\mathbf{H}_S$ and the system components of the interaction Hamiltonian, the $\mathbf{S}_\alpha$'s, form an algebra $\mathcal{S}$, it must be †-closed to preserve the unitarity of system-bath dynamics. Now, if $\mathcal{A}$ is a †-closed operator algebra which includes the identity operator, then a fundamental theorem of C^* algebras states that $\mathcal{A}$ is a reducible subalgebra of the full algebra of operators [53]. This theorem implies that the algebra is isomorphic to a direct sum of $d_J \times d_J$ complex matrix algebras, each with multiplicity n_J:

$$\mathcal{S} \cong \bigoplus_{J \in \mathcal{J}} \mathbf{I}_{n_J} \otimes \mathcal{M}(d_J, \mathbb{C}). \tag{11}$$

Here $\mathcal{J}$ is a finite set labeling the irreducible components of $\mathcal{S}$, and $\mathcal{M}(d_J, \mathbb{C})$ denotes a $d_J \times d_J$ complex matrix algebra. Associated with this decomposition of the algebra $\mathcal{S}$ is a decomposition of the system Hilbert space:

$$\mathcal{H}_S = \bigoplus_{J \in \mathcal{J}} \mathbb{C}^{n_J} \otimes \mathbb{C}^{d_J}. \tag{12}$$

If we encode quantum information into a subsystem (factor) $\mathbb{C}^{n_J}$ it is preserved, since the noise algebra $\mathcal{S}$ acts trivially (as $\mathbf{I}_{n_J}$). In such a case $\mathbb{C}^{n_J}$ is called a decoherence-free or noiseless subsystem (NS) [8]. Examples of this construction were given independently in Refs. [9,11].

1. Completely positive maps

As the Kraus operators are given by Eq. (4), they take the form of the decomposition (11):

$$\mathbf{E}_\alpha = \bigoplus_{J \in \mathcal{J}} \mathbf{I}_{n_J} \otimes \mathbf{M}_\alpha(d_J), \tag{13}$$

where $\mathbf{M}_\alpha(d_J)$ is an arbitrary d_J-dimensional complex matrix. Therefore the factor $\mathbb{C}^{n_J}$ is a NS if the Kraus operators have the representation (13).

2. Markovian dynamics

The aforementioned reducibility theorem [53] does not apply directly in the Markovian case, since the set of Lindblad operators $\{\mathbf{F}_\alpha\}$ need not be closed under conjugation. Nevertheless, as shown in [10], the concept of a subsystem applies in the Markovian case as well: the condition for a NS was found to be

$$\mathbf{F}_\alpha \mathcal{P}_d = \mathbf{I}_{n_J} \otimes \mathbf{M}_\alpha(d_J) \mathcal{P}_d, \tag{14}$$

with the $\mathbf{M}_\alpha$ again being arbitrary complex matrices and $\mathcal{P}_d$ being the projection operator onto a given subspace $\mathbb{C}^{n_J} \otimes \mathbb{C}^{d_J}$. The NS is then a factor $\mathbb{C}^{n_J}$ as in Eq. (12), with the same tensor product structure as in Eq. (14).

III. GENERALIZED CONDITIONS FOR DECOHERENCE-FREE SUBSPACES AND SUBSYSTEMS

We now proceed to reexamine the conditions for the existence of decoherence-free subspaces and subsystems. We will show that the conditions presented in the papers laying the general theoretical foundation [5,6,8,10,35,36,52] can be generalized and sharpened, both for CP maps and for Markovian dynamics. Our main finding is that the preparation step can tolerate arbitrarily large errors. Related to this, we consider the possibility of leakage from outside of the protected subspace or subsystem into it. Previous studies did not allow for this possibility, but we will show that it can be permitted under appropriate restrictions. In doing so we generalize the definition of a NS with respect to the original definition that relied on the algebraic isomorphism (11) (see Ref. [20] for a related recent result). In the case of Markovian dynamics, our main additional finding is that if one demands perfect initialization into a DFS then the condition on the Hamiltonian component of the evolution is modified compared to previous studies.

The derivation of these results is somewhat tedious. Hence, for clarity of presentation we focus on presenting our generalized conditions in this section. Mathematical proofs are deferred to the Appendix. We begin with the simpler case of decoherence-free subspaces and consider the case of CP maps and Markovian dynamics. We then move on to the case of decoherence-free (noiseless) subsystems. The case of non-Markovian continuous-time dynamics is treated later, in Sec. V.

A. Decoherence-free subspaces

The system density matrix ρ_S is an operator on the entire system Hilbert space $\mathcal{H}_S$, which we assume to be decomposable into a direct sum as $\mathcal{H} = \mathcal{H}_{\mathrm{DFS}} \oplus \mathcal{H}_{\mathrm{DFS}^\perp}$. It is convenient for our purposes to represent the system state (and later on the Kraus and Lindblad operators) in a matrix form whose block structure corresponds to this decomposition of the Hilbert space. Thus the system density matrix takes the form

$$\rho_S = \begin{pmatrix} \rho_{\mathrm{DFS}} & \rho_2 \\ \rho_2^\dagger & \rho_3 \end{pmatrix}, \tag{15}$$

We also define a projector

$$\mathcal{P}_{\mathrm{DFS}} = \begin{pmatrix} \mathbf{I}_{\mathrm{DFS}} & \mathbf{0} \end{pmatrix}, \tag{16}$$

so that $\rho_{\mathrm{DFS}} = \mathcal{P}_{\mathrm{DFS}} \rho_S \mathcal{P}_{\mathrm{DFS}}^\dagger$. Finally,

$$\mathcal{P}_d = \begin{pmatrix} \mathbf{I}_{\mathrm{DFS}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \mathcal{P}_{d^\perp} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{\mathrm{DFS}} \end{pmatrix} \tag{17}$$

are projection operators onto $\mathcal{H}_{\mathrm{DFS}}$ and $\mathcal{H}_{\mathrm{DFS}^\perp}$, respectively.

1. Completely positive maps

The original concept of a DFS, Eq. (1), poses a practical problem: the perfect initialization of a quantum system inside a DFS might be challenging in many cases. Therefore we introduce a generalized definition to relax this constraint.

Definition 1. Let the system Hilbert space $\mathcal{H}_S$ decompose into a direct sum as $\mathcal{H}=\mathcal{H}_{\mathrm{DFS}}\oplus\mathcal{H}_{\mathrm{DFS}^\perp}$, and partition the system state ρ_S accordingly into blocks, as in Eq. (15). Assume $\rho_{\mathrm{DFS}}(0)=\mathcal{P}_{\mathrm{DFS}}\rho_S(0)\mathcal{P}_{\mathrm{DFS}}^\dagger\neq\mathbf{0}$. Then $\mathcal{H}_{\mathrm{DFS}}$ is called decoherence-free if and only if the initial and final DFS blocks of ρ_S are unitarily related:

$$\rho_{\mathrm{DFS}}(t)=\mathbf{U}_{\mathrm{DFS}}\rho_{\mathrm{DFS}}(0)\mathbf{U}_{\mathrm{DFS}}^\dagger, \tag{18}$$

where $\mathbf{U}_{\mathrm{DFS}}$ is a unitary matrix acting on $\mathcal{H}_{\mathrm{DFS}}$.

Definition 2. Perfect initialization (DF subspaces) occurs when $\rho_2=\mathbf{0}$ and $\rho_3=\mathbf{0}$ in Eq. (15).

Definition 3. Imperfect initialization (DF subspaces) occurs when ρ_2 and/or ρ_3 in Eq. (15) are nonvanishing.

We prove in Appendix A 1 the following theorem.

Theorem 1. Assume imperfect initialization. Let $\mathbf{U}$ be unitary, c_α scalars satisfying $\Sigma_\alpha|c_\alpha|^2=1$, and $\mathbf{B}_\alpha$ arbitrary operators on $\mathcal{H}_{\mathrm{DFS}^\perp}$ satisfying $\Sigma_\alpha\mathbf{B}_\alpha^\dagger\mathbf{B}_\alpha=\mathbf{I}_{\mathrm{DFS}^\perp}$. A necessary and sufficient condition for the existence of a DFS with respect to CP maps is that the Kraus operators have a matrix representation of the form

$$\mathbf{E}_\alpha=\begin{pmatrix} c_\alpha\mathbf{U} & \mathbf{0}\\ \mathbf{0} & \mathbf{B}_\alpha\end{pmatrix}. \tag{19}$$

This form is identical to the previous result (6), with the important distinction that due to the definition of a DFS, Eq. (18), the theorem holds not just for states initialized perfectly into $\mathcal{H}_{\mathrm{DFS}}$, but for arbitrary initial states. Note that unlike fault-tolerant QECCs, where the initial state must be sufficiently close to a valid code state [19], here the initial state can be arbitrarily far from a DFS code state, as long as the initial projection into the DFS is nonvanishing.

These observations lead us to reconsider the original definition, wherein the system *is* initialized inside the DFS. This situation admits more general Kraus operators. Specifically, we prove in Appendix A 1 the following corollary.

Corollary 1. Assume perfect initialization. Then the DFS condition is

$$\mathbf{E}_\alpha=\begin{pmatrix} c_\alpha\mathbf{U} & \mathbf{A}_\alpha\\ \mathbf{0} & \mathbf{B}_\alpha\end{pmatrix}, \tag{20}$$

where $\mathbf{U}$ is unitary.

Note that due to the sum rule $\Sigma_\alpha\mathbf{E}_\alpha^\dagger\mathbf{E}_\alpha=\mathbf{I}$ the otherwise arbitrary operators $\mathbf{A}_\alpha$ and $\mathbf{B}_\alpha$ satisfy the constraints (i) $\Sigma_\alpha\mathbf{A}_\alpha^\dagger\mathbf{A}_\alpha+\mathbf{B}_\alpha^\dagger\mathbf{B}_\alpha=\mathbf{I}_{\mathrm{DFS}^\perp}$ and (ii) $\Sigma_\alpha c_\alpha^*\mathbf{A}_\alpha=\mathbf{0}$, and where additionally the scalars c_α satisfy (iii) $\Sigma_\alpha|c_\alpha|^2=1$.

In contrast to the diagonal form in the previous conditions (6) and (19), Eq. (20) allows for the existence of the off-diagonal term $\mathbf{A}_\alpha$, which permits leakage from $\mathcal{H}_{\mathrm{DFS}^\perp}$ into $\mathcal{H}_{\mathrm{DFS}}$. This more general form of the Kraus operators implies that a larger class of noise processes allow for the existence of DFSs, as compared to the previous condition (6).[1]

2. Unital maps

A unital (sometimes called bi-stochastic) channel is a CP map $\mathbf{\Phi}(\rho)=\Sigma_\alpha\mathbf{E}_\alpha\rho\mathbf{E}_\alpha^\dagger$ that preserves the identity operator: $\mathbf{\Phi}(\mathbf{I})=\Sigma_\alpha\mathbf{E}_\alpha\mathbf{E}_\alpha^\dagger=\mathbf{I}$. Consider the fixed points of $\mathbf{\Phi}$, i.e., $\mathcal{F}(\mathbf{\Phi})\equiv\{\rho:\mathbf{\Phi}(\rho)=\rho\}$. Such states, which are invariant under $\mathbf{\Phi}$, are clearly examples of DF-states of the corresponding channel.

Recently it has been shown that the fixed point set of unital CP maps is the commutant of the algebra generated by Kraus operators [54]. In other words, if $\mathcal{E}$ is the set of all polynomials in $\{\mathbf{E}_\alpha\}$, or $\mathcal{E}=\mathcal{A}\{\mathbf{E}_\alpha\}$, then

$$\mathcal{F}(\mathbf{\Phi})=\{\mathbf{T}\in\mathcal{B}(\mathcal{H}):[\mathbf{T},\mathcal{E}]=\mathbf{0}\}, \tag{21}$$

where $\mathcal{B}(\mathcal{H})$ is the (Banach) space of all bounded operators on the Hilbert space $\mathcal{H}$. In other words, the fixed points of a unital CP map, which are DF states, can alternatively be characterized as the commutant of $\mathcal{A}\{\mathbf{E}_\alpha\}$, i.e., the set $\{\mathbf{T}\}$. It is our purpose in this subsection to show that, under our generalized definition of DFSs, this characterization of DF states is sufficient but not necessary.

Consider the generalized DFS condition (20) applied to unital maps. We have

$$\mathbf{\Phi}(\rho)=\sum_\alpha\begin{pmatrix} c_\alpha\mathbf{I}_{\mathrm{DFS}} & \mathbf{A}_\alpha\\ \mathbf{0} & \mathbf{B}_\alpha\end{pmatrix}\rho\begin{pmatrix} c_\alpha^*\mathbf{I}_{\mathrm{DFS}} & \mathbf{0}\\ \mathbf{A}_\alpha^\dagger & \mathbf{B}_\alpha^\dagger\end{pmatrix}. \tag{22}$$

Unitality, $\mathbf{\Phi}(\mathbf{I})=\mathbf{I}$, together with $\Sigma_\alpha|c_\alpha|^2=1$, implies

$$\begin{pmatrix} \mathbf{I}_{\mathrm{DFS}}+\sum_\alpha\mathbf{A}_\alpha\mathbf{A}_\alpha^\dagger & \sum_\alpha\mathbf{A}_\alpha\mathbf{B}_\alpha^\dagger\\ \sum_\alpha\mathbf{B}_\alpha\mathbf{A}_\alpha^\dagger & \sum_\alpha\mathbf{B}_\alpha\mathbf{B}_\alpha^\dagger\end{pmatrix}=\mathbf{I}. \tag{23}$$

This implies the vanishing of the matrices $\mathbf{A}_\alpha$, so that we are left with the Kraus operators in the simple block-diagonal form

$$\mathbf{E}_\alpha=\begin{pmatrix} c_\alpha\mathbf{I} & \mathbf{0}\\ \mathbf{0} & \mathbf{B}_\alpha\end{pmatrix}, \tag{24}$$

together with the additional constraint $\Sigma_\alpha\mathbf{B}_\alpha\mathbf{B}_\alpha^\dagger=\mathbf{I}_{\mathrm{DFS}^\perp}$ (which, in the present unital case, naturally supplements the previously derived normalization constraint $\Sigma_\alpha\mathbf{B}_\alpha^\dagger\mathbf{B}_\alpha=\mathbf{I}_{\mathrm{DFS}^\perp}$). Thus, unitality restricts the class of Kraus operators, so that in fact we must assume the DFS condition (19) rather than (20). This then means that we may consider the generalized DFS definition Eq. (18).

Next, let us find the commutant of this class of Kraus operators. First,

[1]We reemphasize that Theorem 1 in [36] is compatible with Eq. (20); the latter generalizes the explicit matrix representation Eq. (4) given in that paper [condition (6) in the present paper], but does not invalidate Theorem 1 in [36].

$$\mathcal{A}\{\mathbf{E}_\alpha\} = \left\{ \begin{pmatrix} \text{poly}(c_\alpha)\mathbf{I} & \mathbf{0} \\ \mathbf{0} & \text{poly}(\mathbf{B}_\alpha) \end{pmatrix} \right\}, \tag{25}$$

where poly(x) denotes all possible polynomials in x. Representing an arbitrary operator $\mathbf{T} \in \mathcal{B}(\mathcal{H})$ in the form

$$\mathbf{T} = \begin{pmatrix} \mathbf{L} & \mathbf{M} \\ \mathbf{N} & \mathbf{P} \end{pmatrix}, \tag{26}$$

it is simple to derive that the commutant of $\mathcal{A}\{\mathbf{E}_\alpha\}$ is the space of matrices $\mathbf{T}$ of the form

$$\mathbf{T} = \begin{pmatrix} \mathbf{L} & \mathbf{0} \\ \mathbf{0} & c\mathbf{I} \end{pmatrix}, \tag{27}$$

where $\mathbf{L}$ and c are arbitrary. The aforementioned theorem [54] states that the fixed-point set of the channel, i.e., the DF states, coincides with this commutant. Of course, for $\mathbf{T}$ to be a proper quantum state it must be Hermitian and have unit trace, whence $c \geqslant 0$ and $\mathbf{L}$ is Hermitian. Subject to these constraints we see that the aforementioned theorem [54] gives a sufficient but not necessary characterization of the allowed DF states. Indeed, the form (27) arises as a special case of our considerations, where we allow for $\mathbf{T}$ to be a state with support in $\mathcal{H}_{\text{DFS}^\perp}$, but not of the most general form allowed by Eq. (18), which includes off-diagonal blocks.

3. Markovian dynamics

In the case of CP maps we are only interested in the output state and the intermediate-time states are ignored. Since, as is well known, Markovian dynamics is a special case of CP maps (e.g., [48,51]), one may of course apply the results we have obtained above for general CP maps in the Markovian case as well, provided one is only interested in the state at the end of the Markovian channel. However, one may instead be interested in a different notion of decoherence-freeness, wherein the system remains DF throughout the entire evolution. Such a notion is more suited to experiments in which the final time is not *a priori* known. This is the notion we will pursue here in our treatment of continuous-time dynamics, in both the Markovian and non-Markovian cases. Thus, while we allow that the system not be fully initialized into the DFS, we require that the component that is, undergoes unitary dynamics *at all times*. Correspondingly, we define a DFS in the Markovian case as follows.

Definition 4. Let the system Hilbert space $\mathcal{H}_S$ decompose into a direct sum as $\mathcal{H}_S = \mathcal{H}_{\text{DFS}} \oplus \mathcal{H}_{\text{DFS}^\perp}$, and partition the system state ρ_S accordingly into blocks. Let $\mathcal{P}_{\text{DFS}}$ be a projector onto $\mathcal{H}_{\text{DFS}}$ and assume $\rho_{\text{DFS}}(0) \equiv \mathcal{P}_{\text{DFS}}\rho_S(0)\mathcal{P}_{\text{DFS}}^\dagger \neq \mathbf{0}$. Then $\mathcal{H}_{\text{DFS}}$ is called decoherence-free if and only if ρ_{DFS} undergoes Schrödinger-like dynamics,

$$\frac{\partial \rho_{\text{DFS}}}{\partial t} = -i[\mathbf{H}_{\text{DFS}}, \rho_{\text{DFS}}], \tag{28}$$

where $\mathbf{H}_{\text{DFS}}$ is a Hermitian operator.

Before presenting the DFS conditions, let us recall the quantum trajectory interpretation of Markovian dynamics [55–57]. Expanding Eq. (7) to first order in the short time interval τ yields the CP map

$$\rho_S(t+\tau) = \sum_{\beta=0} \mathbf{W}_\beta \rho(t) \mathbf{W}_\beta^\dagger, \tag{29}$$

where

$$\mathbf{W}_0 = \mathbf{I} - i\tau\mathbf{H}_S - \frac{\tau}{2}\sum_\alpha \mathbf{F}_\alpha^\dagger \mathbf{F}_\alpha, \tag{30}$$

$$\mathbf{W}_{\beta>0} = \sqrt{\tau}\mathbf{F}_\beta, \tag{31}$$

and to the same order we also have the normalization condition

$$\sum_{\beta=0} \mathbf{W}_\beta^\dagger \mathbf{W}_\beta = \mathbf{I}. \tag{32}$$

Thus the Lindblad equation has been recast as a Kraus operator sum (2), but only to first order in τ, the coarse-graining time scale for which the Markovian approximation is valid [51]. This implies a measurement interpretation, wherein the system state is $\rho_S(t+\tau) = \mathbf{W}_\beta \rho(t) \mathbf{W}_\beta^\dagger / p_\beta$ (to first order in τ) with probability $p_\beta = \text{Tr}[\mathbf{W}_\beta \rho(t) \mathbf{W}_\beta^\dagger]$. This happens because the bath functions as a probe coupled to the system while being subjected to a quasicontinuous series of measurements at each infinitesimal time interval τ [34]. The result is the well-known quantum jump process [55–57], wherein the measurement operators are $\mathbf{W}_0 \approx \exp(-i\tau\mathbf{H}_\text{c})$, the "conditional" evolution, generated by the non-Hermitian "Hamiltonian"

$$\mathbf{H}_\text{c} \equiv \mathbf{H}_S - \frac{i}{2}\sum_\alpha \mathbf{F}_\alpha^\dagger \mathbf{F}_\alpha, \tag{33}$$

and $\sqrt{\tau}\mathbf{F}_\beta$ (the "jump"). Note that $\mathbf{H}_S$ is here meant to include all renormalization effects due to the system-bath interaction, e.g., a possible Lamb shift (see, e.g., Ref. [51]). By a simple algebraic rearrangement one can rewrite the Lindblad equation in the following form:

$$\dot{\rho}_S = -i(\mathbf{H}_\text{c}\rho_S - \rho_S \mathbf{H}_\text{c}^\dagger) + \sum_\alpha \mathbf{F}_\alpha \rho_S \mathbf{F}_\alpha^\dagger, \tag{34}$$

where according to the above interpretation the first term generates nonunitary dynamics, while the second is responsible for the quantum jumps.

Now recall the Markovian DFS condition derived in Refs. [6,52]: the Lindblad operators should have trivial action on DF states, as in Eq. (8), i.e., $\mathbf{F}_\alpha|i\rangle = c_\alpha|i\rangle$. Viewed from the perspective of the quantum-jump picture of Markovian dynamics, this implies that the jump operators do not alter a DF state, i.e., the term $\Sigma_\alpha \mathbf{F}_\alpha \rho_S \mathbf{F}_\alpha^\dagger$ in Eq. (34) transforms ρ_S to $\Sigma_\alpha |c_\alpha|^2 \rho_S$ and thus has trivial action.

Given Eq. (8), the Lindblad operators can be written in block form as follows [Eq. (9)]:

$$\mathbf{F}_\alpha = \begin{pmatrix} c_\alpha \mathbf{I} & \mathbf{A}_\alpha \\ \mathbf{0} & \mathbf{B}_\alpha \end{pmatrix}, \tag{35}$$

with the blocks on the diagonal corresponding once again to operators restricted to $\mathcal{H}_{\text{DFS}}$ and $\mathcal{H}_{\text{DFS}^\perp}$. Note the appearance of the off-diagonal block $\mathbf{A}_\alpha$ mixing $\mathcal{H}_{\text{DFS}}$ and $\mathcal{H}_{\text{DFS}^\perp}$; its presence is permitted since the DFS condition (8) gives no information about matrix elements of the form $\langle i|\mathbf{F}_\alpha|j^\perp\rangle$, with $|i\rangle \in \mathcal{H}_{\mathrm{DFS}}$ and $|j^\perp\rangle \in \mathcal{H}_{\mathrm{DFS}^\perp}$.

As observed in [6], one should in addition require that $\mathbf{H}_S$ does not mix DF states with non-DF ones. It turns out that this condition is compatible with the case that the DF state is imperfectly initialized (Definition 3). In this case, as shown in Appendix A 1, the following theorem holds.

Theorem 2. Assume imperfect initialization. Then a subspace $\mathcal{H}_{\mathrm{DFS}}$ of the total Hilbert space $\mathcal{H}$ is decoherence-free with respect to Markovian dynamics if and only if the Lindblad operators $\mathbf{F}_\alpha$ and the system Hamiltonian $\mathbf{H}_S$ assume the block-diagonal form

$$\mathbf{H}_S = \begin{pmatrix} \mathbf{H}_{\mathrm{DFS}} & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_{\mathrm{DFS}^\perp} \end{pmatrix}, \quad \mathbf{F}_\alpha = \begin{pmatrix} c_\alpha \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_\alpha \end{pmatrix}, \tag{36}$$

where $\mathbf{H}_{\mathrm{DFS}}$ and $\mathbf{H}_{\mathrm{DFS}^\perp}$ are Hermitian, c_α are scalars, and $\mathbf{B}_\alpha$ are arbitrary operators on $\mathcal{H}_{\mathrm{DFS}^\perp}$.

But, as is clear from the quantum-jump picture, in particular Eqs. (33) and (34), there also exists a non-Hermitian term, which appears not to be addressed properly by merely restricting $\mathbf{H}_S$. Indeed, this is the case if one demands that the system state is perfectly initialized into the DFS (Definition 2). As shown in Appendix A 2, the full condition on the Hamiltonian term then is

$$\langle i|\left(-i\mathbf{H}_S + \frac{1}{2}\sum_\alpha \mathbf{F}_\alpha^\dagger \mathbf{F}_\alpha\right)|k^\perp\rangle = 0, \quad \forall\ i,k^\perp, \tag{37}$$

where $|i\rangle \in \mathcal{H}_{\mathrm{DFS}}$, $|k^\perp\rangle \in \mathcal{H}_{\mathrm{DFS}^\perp}$. Applying the DFS conditions (9) and (37), the Lindblad equation (7) reduces to the Schrödinger-like equation (28). Combining these results, we have the following theorem.

Theorem 3. Assume perfect initialization. Then a subspace $\mathcal{H}_{\mathrm{DFS}}$ of the total Hilbert space $\mathcal{H}$ is decoherence-free with respect to Markovian dynamics if and only if the Lindblad operators $\mathbf{F}_\alpha$ and Hamiltonian $\mathbf{H}_S$ satisfy

$$\mathbf{F}_\alpha = \begin{pmatrix} c_\alpha \mathbf{I} & \mathbf{A}_\alpha \\ \mathbf{0} & \mathbf{B}_\alpha \end{pmatrix}, \tag{38}$$

$$\mathcal{P}_{\mathrm{DFS}} \mathbf{H}_S \mathcal{P}_{\mathrm{DFS}}^\dagger = -\frac{i}{2}\sum_\alpha c_\alpha^* \mathbf{A}_\alpha. \tag{39}$$

Note that $\mathbf{H}_S$ (which, again, includes the Lamb shift) must satisfy a more stringent constraint than previously noted due to the extra condition on its off-diagonal block. This has implications in examples of practical interest, as we next illustrate.

4. Example (significance of the additional condition on the off-diagonal blocks of $\mathbf{H}_S$)

We present an example meant to demonstrate how the additional constraint, Eq. (37) [or, equivalently, Eq. (39)] may lead to a different prediction than the old constraint, that matrix elements of the type $\langle j^\perp|\mathbf{H}_S|i\rangle$, with $|i\rangle \in \mathcal{H}_{\mathrm{DFS}}$ and $|j^\perp\rangle \in \mathcal{H}_{\mathrm{DFS}^\perp}$, should vanish.

Consider a system of three qubits interacting with a common bath. The system is under influence of the bath via (1) spontaneous emission from the highest level $|111\rangle$ to the lower levels and (2) dephasing of the first and the second qubits. For simplicity we set the system and bath Hamiltonians $\mathbf{H}_S$ and $\mathbf{H}_B$ to zero. The total Hamiltonian then contains only the system-bath interaction:

$$\mathbf{H}_I = \lambda_1(\sigma_1^z + \sigma_2^z) \otimes \mathbf{B} + \lambda_2[(\sigma_1^- + \sigma_2^- + \sigma_3^-) \otimes \mathbf{b}^\dagger + (\sigma_1^+ + \sigma_2^+ + \sigma_3^+) \otimes \mathbf{b}], \tag{40}$$

where

$$\sigma_1^- = |001\rangle\langle 111|, \quad \sigma_2^- = |010\rangle\langle 111|, \quad \sigma_3^- = |100\rangle\langle 111|, \tag{41}$$

and $\mathbf{b}$ is a bosonic annihilation operator.

The corresponding Lindblad equation may be derived, e.g., using the method developed in Ref. [51]. It may then be shown that

$$\mathcal{L}[\rho_S] = \frac{1}{2}\sum_{i=1}^{2} [\mathbf{F}_i, \rho_S \mathbf{F}_i^\dagger] + [\mathbf{F}_i \rho_S, \mathbf{F}_i^\dagger], \tag{42}$$

where the Lindblad operators are

$$\mathbf{F}_1 = \sqrt{d_1}(u_{11}\mathbf{K}_1 + u_{12}\mathbf{K}_2),$$

$$\mathbf{F}_2 = \sqrt{d_2}(u_{21}\mathbf{K}_1 + u_{22}\mathbf{K}_2). \tag{43}$$

Here $\mathbf{K}_1 = \sigma_1^z + \sigma_2^z$, $\mathbf{K}_2 = \sigma_1^- + \sigma_2^- + \sigma_3^-$, and $\{d_1, d_2\}$ are the eigenvalues of the Hermitian matrix $\mathbf{A} = [a_{ij}]$ of coefficients in the prediagonalized Lindblad equation, with the diagonalizing matrix denoted $\mathbf{U} = [u_{ij}]$.

Now let us find the DFS conditions under the assumption of perfect initialization. The previously derived Eq. (8) yields that $\{|000\rangle, |001\rangle\}$ is a DFS, since $\mathbf{K}_2$ annihilates these states, and they are both eigenstates of $\mathbf{K}_1$ with an eigenvalue of +2:

$$\mathbf{F}_1|000\rangle = 2\sqrt{d_1}u_{11}|000\rangle, \quad \mathbf{F}_2|000\rangle = 2\sqrt{d_2}u_{21}|000\rangle,$$

$$\mathbf{F}_1|001\rangle = 2\sqrt{d_1}u_{11}|001\rangle, \quad \mathbf{F}_2|001\rangle = 2\sqrt{d_2}u_{21}|001\rangle F_2. \tag{44}$$

However, the condition (37) tightens the situation. Choosing as representatives the states $|001\rangle \in \mathcal{H}_{\mathrm{DFS}}$ and $|111\rangle \in \mathcal{H}_{\mathrm{DFS}^\perp}$, we find from Eq. (37)

$$\langle 001|\sum_{\alpha=1}^{2} \mathbf{F}_\alpha^\dagger \mathbf{F}_\alpha|111\rangle = 2d_1 u_{11}^* u_{12} + 2d_2 u_{21}^* u_{22} = 0. \tag{45}$$

Since $u_{11}^* u_{12} + u_{21}^* u_{22} = 0$ (from unitarity of $\mathbf{U}$), we see that the additional condition imposes the extra symmetry constraint $d_1 = d_2$. This example illustrate the importance of the condition Eq. (37).

B. Noiseless subsystems

We now consider again the more general setting of subsystems, rather than subspaces.

1. Completely positive maps

Suppose the system Hilbert space can be decomposed as $\mathcal{H}_S = \mathcal{H}_{\mathrm{NS}} \otimes \mathcal{H}_{\mathrm{in}} \oplus \mathcal{H}_{\mathrm{out}}$, where $\mathcal{H}_{\mathrm{NS}}$ is the factor in which quantum information will be stored. The subspace $\mathcal{H}_{\text{out}}$ may itself have a tensor product structure, i.e., additional factors similar to $\mathcal{H}_{\text{NS}}$ may be contained in it [as in Eq. (12)], but we shall not be interested in those other factors since the direct sum structure implies that different noiseless factors cannot be used simultaneously in a coherent manner. As in the DF subspace case considered above, we allow for the most general situation of a system that is *not* necessarily initially DF. To make this notion precise, let us generalize the definitions of the projector $\mathcal{P}_{\text{DFS}}$ and projection operators $\mathcal{P}_d, \mathcal{P}_{d^\perp}$ given in the DFS case, as follows:

$$\mathcal{P}_{\text{NS-in}} = (\mathbf{I}_{\text{NS}} \otimes \mathbf{I}_{\text{in}} \quad \mathbf{0}), \tag{46}$$

$$\mathcal{P}_d = \begin{pmatrix} \mathbf{I}_{\text{NS}} \otimes \mathbf{I}_{\text{in}} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}, \quad \mathcal{P}_{\text{d}^\perp} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{I}_{\text{NS}} \otimes \mathbf{I}_{\text{in}} \end{pmatrix}. \tag{47}$$

There is no risk of confusion in using the DFS notation $\mathcal{P}_d$ for the NS case, as the DFS case is obtained when $\mathbf{I}_{\text{in}}$ is a scalar.

The system density matrix takes the corresponding block form

$$\rho_S = \begin{pmatrix} \rho_{\text{NS-in}} & \rho' \\ \rho'^{\dagger} & \rho_{\text{out}} \end{pmatrix}. \tag{48}$$

Definition 5. Let the system Hilbert space $\mathcal{H}_S$ decompose as $\mathcal{H}_S = \mathcal{H}_{\text{NS}} \otimes \mathcal{H}_{\text{in}} \oplus \mathcal{H}_{\text{out}}$, and partition the system state ρ_S accordingly into blocks, as in Eq. (48). Assume $\rho_{\text{NS-in}}(0) = \mathcal{P}_{\text{NS-in}} \rho_S(0) \mathcal{P}_{\text{NS-in}}^{\dagger} \neq \mathbf{0}$. Then the factor $\mathcal{H}_{\text{NS}}$ is called a decoherence-free (or noiseless) subsystem if the following condition holds:

$$\text{Tr}_{\text{in}}\{\rho_{\text{NS-in}}(t)\} = \mathbf{U}_{\text{NS}} \text{Tr}_{\text{in}}\{\rho_{\text{NS-in}}(0)\} \mathbf{U}_{\text{NS}}^{\dagger}, \tag{49}$$

where $\mathbf{U}_{\text{NS}}$ *is a unitary matrix acting on* $\mathcal{H}_{\text{NS}}$.

Definition 6. Perfect initialization (DF subsystems) occurs when $\rho' = \mathbf{0}$ and $\rho_{\text{out}} = \mathbf{0}$ in Eq. (48).

Definition 7. Imperfect initialization (DF subsystems) occurs when ρ' and/or ρ_{out} in Eq. (48) are nonvanishing.

According to Definition 5, a quantum state encoded into the $\mathcal{H}_{\text{NS}}$ factor at some time t is unitarily related to the $t=0$ state. The factor $\mathcal{H}_{\text{in}}$ is unimportant, and hence is traced over. Clearly, a NS reduces to a DF subspace when $\mathcal{H}_{\text{in}}$ is one-dimensional, i.e., when $\mathcal{H}_{\text{in}} = \mathbb{C}$.

We now present the necessary and sufficient conditions for a NS and later we show that the algebra-dependent definition Eq. (11) is a special case of this generalized form. In stating constraints on the form of the Kraus operators, below, it is understood that in addition they must satisfy the sum rule $\Sigma_\alpha \mathbf{E}_\alpha^{\dagger} \mathbf{E}_\alpha = \mathbf{I}$, which we do not specify explicitly.

Theorem 4. Assume imperfect initialization. Then a subsystem $\mathcal{H}_{\text{NS}}$ in the decomposition $\mathcal{H}_S = \mathcal{H}_{\text{NS}} \otimes \mathcal{H}_{\text{in}} \oplus \mathcal{H}_{\text{out}}$ is decoherence-free (or noiseless) with respect to CP maps if and only if the Kraus operators have the matrix representation

$$\mathbf{E}_\alpha = \begin{pmatrix} \mathbf{U} \otimes \mathbf{C}_\alpha & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_\alpha \end{pmatrix}. \tag{50}$$

Corollary 2. Assume perfect initialization. Then the Kraus operators have the relaxed form

$$\mathbf{E}_\alpha = \begin{pmatrix} \mathbf{U} \otimes \mathbf{C}_\alpha & \mathbf{A}_\alpha \\ \mathbf{0} & \mathbf{B}_\alpha \end{pmatrix}. \tag{51}$$

We note that this result has been recently derived from an operator quantum error correction perspective in Ref. [20]. Note again that there is a trade-off between the quality of preparation and the amount of leakage that can be tolerated, a fact that was not noted previously for subsystems, and has important experimental implications.

As discussed above, the original definition of a NS was based on representation theory of the error algebra. Here we have argued in favor of a more comprehensive definition, based on the quantum channel picture. Let us now state explicitly why our result is more general. Indeed, in the algebraic approach one arrives at the representation (13) of the Kraus operators, namely, $\mathbf{E}_\alpha = \oplus_{J \in \mathcal{J}} \mathbf{I}_{n_J} \otimes \mathbf{G}_{\alpha,J}$. However, it is clear from Eq. (51) that our channel-based approach leads to a form for the Kraus operators that includes this latter form as a special case, since it allows for the off-diagonal block $\mathbf{A}_\alpha$. The representation (13) of the Kraus operators does agree with Eq. (50), but in that case we do not need to assume initialization inside the NS, so that again, our result is more general than the algebraic one.

2. Markovian dynamics

As in the CP-map-based definition of a NS, we need to trace out the $\mathcal{H}_{\text{in}}$ factor, here in order to obtain the dynamical equation for the subsystem factor:

$$\begin{aligned}
\frac{\partial \rho_{\text{NS}}}{\partial t} &= \frac{\partial\, \text{Tr}_{\text{in}}(\mathcal{P}_{\text{NS-in}} \rho_S \mathcal{P}_{\text{NS-in}}^{\dagger})}{\partial t} \\
&= \text{Tr}_{\text{in}}\left(\frac{\partial \mathcal{P}_{\text{NS-in}} \rho_S \mathcal{P}_{\text{NS-in}}^{\dagger}}{\partial t} \right) \\
&= \text{Tr}_{\text{in}}\Bigg\{ \mathcal{P}_{\text{NS-in}} \Bigg(-\frac{i}{\hbar}[\mathbf{H}_S, \rho_S] + \frac{1}{2}\sum_\alpha 2\mathbf{F}_\alpha \rho_S \mathbf{F}_\alpha^{\dagger} - \mathbf{F}_\alpha^{\dagger} \mathbf{F}_\alpha \rho_S \\
&\quad - \rho_S \mathbf{F}_\alpha^{\dagger} \mathbf{F}_\alpha \Bigg) \mathcal{P}_{\text{NS-in}}^{\dagger} \Bigg\}.
\end{aligned} \tag{52}$$

Definition 8. The factor $\mathcal{H}_{\text{NS}}$ is called a decoherence-free (or noiseless) subsystem under Markovian dynamics if a state subject to Eq. (52), undergoes continuous unitary evolution:

$$\dot{\rho}_{\text{NS}} = i[\mathbf{M}, \rho_{\text{NS}}], \tag{53}$$

where $\mathbf{M}$ is Hermitian.

Clearly, again, a NS reduces to a DF subspace when $\mathcal{H}_{\text{in}}$ is one dimensional, i.e., when $\mathcal{H}_{\text{in}} = \mathbb{C}$.

Our goal is to find necessary and sufficient conditions such that Eq. (52) leads to Eq. (53). In the case of perfect initialization, since it does not involve $\mathcal{H}_{\text{out}}$, Eq. (52) is meaningful only if the system remains in the subspace $\mathcal{H}_{\text{NS}} \otimes \mathcal{H}_{\text{in}}$. An analysis of Eq. (52) reveals that this leakage-prevention goal is achieved by imposing the constraints stated in the following theorem, proven in Appendix A 2:

Theorem 5. Assume perfect initialization. Then a subsystem $\mathcal{H}_{\text{NS}}$ in the decomposition $\mathcal{H}_S = \mathcal{H}_{\text{NS}} \otimes \mathcal{H}_{\text{in}} \oplus \mathcal{H}_{\text{out}}$ is decoherence-free (or noiseless) with respect to Markovian dynamics if and only if the Lindblad operators have the matrix representation

$$\mathbf{F}_\alpha = \begin{pmatrix} \mathbf{I}_{\mathrm{NS}} \otimes \mathbf{C}_\alpha & \mathbf{A}_\alpha \\ \mathbf{0} & \mathbf{B}_\alpha \end{pmatrix} \tag{54}$$

and the system Hamiltonian (including a possible Lamb shift) has the matrix representation

$$\mathbf{H}_S = \begin{pmatrix} \mathbf{H}_{\mathrm{NS}} \otimes \mathbf{I}_{\mathrm{in}} + \mathbf{I}_{\mathrm{NS}} \otimes \mathbf{H}_{\mathrm{in}} & \mathbf{H}_2 \\ \mathbf{H}_2^\dagger & \mathbf{H}_3 \end{pmatrix} \tag{55}$$

where $\mathbf{H}_{\mathrm{in}}$ is constant along its diagonal, and where

$$\mathbf{H}_2 = -\frac{i}{2}\sum_\alpha (\mathbf{I}_{\mathrm{NS}} \otimes \mathbf{C}_\alpha^\dagger)\mathbf{A}_\alpha. \tag{56}$$

Equations (55) and (56) are additional constraints on the Lindblad operators (compared to Ref. [10]) which must be satisfied in order to find a NS.

If, on the other hand, we allow for imperfect initialization, we find a different set of conditions.

Theorem 6. Assume imperfect initialization. Then a subsystem $\mathcal{H}_{\mathrm{NS}}$ in the decomposition $\mathcal{H}_S = \mathcal{H}_{\mathrm{NS}} \otimes \mathcal{H}_{\mathrm{in}} \oplus \mathcal{H}_{\mathrm{out}}$ is decoherence-free (or noiseless) with respect to Markovian dynamics if and only if the Lindblad operators have the matrix representation

$$\mathbf{F}_\alpha = \begin{pmatrix} \mathbf{I}_{\mathrm{NS}} \otimes \mathbf{C}_{\mathrm{in}}^\alpha & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_\alpha \end{pmatrix}, \tag{57}$$

and the system Hamiltonian (including a possible Lamb shift) has the matrix representation

$$\mathbf{H} = \begin{pmatrix} \mathbf{H}_{\mathrm{NS}} \otimes \mathbf{I}_{\mathrm{in}} + \mathbf{I}_{\mathrm{NS}} \otimes \mathbf{H}_{\mathrm{in}} & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_{\mathrm{out}} \end{pmatrix}. \tag{58}$$

IV. PERFORMANCE OF QUANTUM ALGORITHMS OVER IMPERFECTLY INITIALIZED DFSs

In this section we discuss applications of our generalized formulation of DFSs to quantum algorithms. As mentioned above, a major obstacle to exploiting decoherence-free methods is the unrealistic assumption of perfect initialization inside a DFS. Removing this constraint enables us to perform algorithms without perfect initialization, while not suffering from information loss. We separate the role of an initialization error in the algorithm (i.e., starting from an imperfect input state), from the effect of noise in the output due to environment-induced decoherence. Thus we first quantify an error entirely due to incorrect initialization (Δ_{leak} below), then compare the DFS situations prior to and post this work, by relating them to Δ_{leak}.

(1) Initialization error in the absence of decoherence: Assume no decoherence at all, that the initial state is

$$\rho^{\mathrm{actual}}(0) = \begin{pmatrix} \rho_1 & \rho_2 \\ \rho_2^\dagger & \rho_3 \end{pmatrix}, \tag{59}$$

while the ideal input state is fully in the DFS:

$$\rho^{\mathrm{ideal}}(0) = \begin{pmatrix} \rho & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}. \tag{60}$$

Further assume that the algorithm is implemented via unitary transformations $\mathbf{U} = \mathbf{U}_{\mathrm{DFS}} \oplus \mathbf{I}_{\mathrm{DFS}^\perp}$, applied to $\mathcal{H}_{\mathrm{DFS}}$. In general this will lead to an output error in the algorithm, which can be quantified as

$$\begin{aligned}\Delta_{\mathrm{leak}} &\equiv \|\mathbf{U}\rho^{\mathrm{actual}}(0)\mathbf{U}^\dagger - \mathbf{U}\rho^{\mathrm{ideal}}(0)\mathbf{U}^\dagger\| \\ &= \left\| \begin{pmatrix} \mathbf{U}_{\mathrm{DFS}}(\rho_1 - \rho)\mathbf{U}_{\mathrm{DFS}}^\dagger & \mathbf{U}_{\mathrm{DFS}}\rho_2 \\ \rho_2^\dagger \mathbf{U}_{\mathrm{DFS}}^\dagger & \rho_3 \end{pmatrix} \right\|,\end{aligned} \tag{61}$$

where $\|\cdot\|$ denotes an appropriate operator norm. This error appears not because of decoherence but because of an erroneous initial state. This is a generic situation in quantum algorithms, which is not special to the DFS case: Equation (59) is generic in the sense that one can view the DFS block as the computational subspace, with the other blocks representing additional levels (e.g., a qubit which is embedded in a larger Hilbert space). Methods for correcting such deviations from the ideal result exist (leakage elimination [58,59]), but are beyond the scope of this paper.

(2) Initialization error in the presence of decoherence: Assume that the input state is imperfectly initialized, as in Eq. (59), and in addition there is decoherence, i.e.,

$$\rho^{\mathrm{actual}}(t) = \sum_\alpha \mathbf{E}_\alpha(t)\rho^{\mathrm{actual}}(0)\mathbf{E}_\alpha^\dagger(t), \tag{62}$$

with the Kraus operators given by Eq. (19) [the form compatible with decoherence-free evolution starting from $\rho^{\mathrm{actual}}(0)$]. Prior to our work it was believed that for an imperfect initial state of the form $\rho^{\mathrm{actual}}(0)$, leakage due to the components ρ_2 and ρ_3 would cause nonunitary evolution of the DFS component. Thus instead of an error $\mathbf{U}_{\mathrm{DFS}}(\rho_1 - \rho)\mathbf{U}_{\mathrm{DFS}}^\dagger$ in the DFS block of Eq. (61), it was believed that one had $\mathcal{E}(\rho_1) - \mathbf{U}_{\mathrm{DFS}}\rho\mathbf{U}_{\mathrm{DFS}}^\dagger$ where $\mathcal{E}$ is an appropriate superoperator component. This would have led to a reduced algorithmic fidelity, $\Delta'_{\mathrm{leak}} < \Delta_{\mathrm{leak}}$. However, we now know that even for an initial state of the form $\rho^{\mathrm{actual}}(0)$, when the Kraus operators are given by Eq. (19) the actual algorithmic fidelity is still given by Δ_{leak}, since in fact the evolution of the DFS block is still unitary.

The above arguments apply when imperfect initialization is unavoidable *but one knows the component* ρ_1. A worse (though perhaps more typical) scenario is one where not only is imperfect initialization unavoidable, but one does not even know the component ρ_1. In this case the above arguments apply in the context of algorithms that allow arbitrary input states. Almost all the important examples of quantum algorithms are now known to have a flexibility of this type: Grover's algorithm [23] was the first to be generalized to allow for arbitrary input states, first pure [25–27], then mixed [28]; Shor's algorithm [22] can run efficiently with a single pure qubit and all other qubits in an arbitrary mixed state [29]; a similar result applies to a class of interesting physics problems, such as finding the spectrum of a Hamiltonian [30]; the Deutsch-Josza [24] algorithm was generalized to allow for arbitrary input states [31], and a similar result holds for an algorithm that performs the functional phase rotation (a generalized form of the conventional conditional phase transform) [32]. Most recently it was shown that Simon's problem and the period-finding problem can be solved quantumly without initializing the auxiliary qubits [33].

For algorithms that do not allow arbitrary input states, one could still make use of the flexibility we have introduced into DFS state initialization, provided it is possible to apply post-selection: one modifies the output error of algorithm by observing whether the measurement outcome came from the DFS block or not (this could be done, e.g., via frequency-selective measurements, similar to the cycling transition method used in trapped-ion quantum computing [60]).

V. DECOHERENCE-FREE SUBSPACES AND SUBSYSTEMS IN NON-MARKOVIAN DYNAMICS

A. Decoherence-free subspaces

In Ref. [34] a new class of non-Markovian master equations was introduced. The following equation was derived as an analytically solvable example of this class:

$$\frac{\partial \rho_S}{\partial t} = - i[\mathbf{H}_S,\rho_S] + \mathcal{L}\int_0^t dt' k(t')\exp(\mathcal{L}t')\rho_S(t-t') \quad (63)$$

where $\mathcal{L}$ is a Lindblad superoperator and $k(t)$ represents the memory effects of the bath. The Markovian limit is clearly recovered when $k(t)\propto\delta(t)$.[2]

Some examples of physical systems that can be described by this master equation are (i) a two-level atom coupled to a single cavity mode, wherein the memory function is exponentially decaying, $k(t)=e^{-\lambda t}$ [44], and (ii) a single qubit subject to telegraph noise in the particular case that $\|\mathcal{L}\|\ll 1/t$, whence Eq. (63) reduces to $\dot{\rho}_S=\mathcal{L}\int_0^t dt' k(t')\rho(t-t')$ [61]. It is interesting to investigate the conditions for a DFS in the case of dynamics governed by Eq. (63), and to compare the results with the Markovian limit, $k(t)\propto\delta(t)$. We defer proofs to Appendix A 3 and here present only the DFS condition, stated in the following theorem (note that, similarly to the Markovian case, we consider here a continuous-time DFS).

Theorem 7. Assume imperfect initialization. Then a subspace $\mathcal{H}_{\mathrm{DFS}}$ is decoherence-free if and only if the system Hamiltonian $\mathbf{H}_S$ and Lindblad operators $\mathbf{F}_\alpha$ *have the matrix representation*

$$\mathbf{H}_S = \begin{pmatrix} \mathbf{H}_{\mathrm{DFS}} & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_{\mathrm{DFS}^\perp} \end{pmatrix}, \quad \mathbf{F}_\alpha = \begin{pmatrix} c_\alpha \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_\alpha \end{pmatrix}. \quad (64)$$

These conditions are identical to those we found in the case of Markovian dynamics with imperfect initialization—cf. Theorem 2. This fact provides evidence for the robustness of decoherence-free states against variations in the nature of the decoherence process.

Interestingly, the conditions under the assumption of perfect initialization differ somewhat when comparing the Markovian and non-Markovian cases.

[2]We note that Ref. [34] contains a small error: the Markovian limit is recovered for $k(t)=\delta(t)$ only if the lower limit in Eq. (63) is $-t$. This change can easily be applied to the derivation of Ref. [34].

Corollary 3. Assume perfect initialization. Then a subspace $\mathcal{H}_{\mathrm{DFS}}$ is decoherence-free if and only if the system Hamiltonian $\mathbf{H}_S$ and Lindblad operators $\mathbf{F}_\alpha$ have the matrix representation

$$\mathbf{H}_S = \begin{pmatrix} \mathbf{H}_{\mathrm{DFS}} & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_{\mathrm{DFS}^\perp} \end{pmatrix}, \quad (65)$$

$$\mathbf{F}_\alpha = \begin{pmatrix} c_\alpha \mathbf{I} & \mathbf{A}_\alpha \\ \mathbf{0} & \mathbf{B}_\alpha \end{pmatrix} \quad \text{and} \quad \sum_\alpha c_\alpha^* \mathbf{A}_\alpha = \mathbf{0}. \quad (66)$$

Compared to the Markovian case (Theorem 3), the difference is that now the off-diagonal blocks of the Hamiltonian must vanish, whereas in the Markovian case we had the constraint [Eq. (39)] $\mathcal{P}_{\mathrm{DFS}}\mathbf{H}_S\mathcal{P}_{\mathrm{DFS}}^\dagger=-(i/2)\Sigma_\alpha c_\alpha^* \mathbf{A}_\alpha$.

B. Decoherence-free subsystems

We now consider the NS case. The dynamics governing a NS is derived by tracing out $\mathcal{H}_{\mathrm{in}}$:

$$\begin{aligned}\frac{\partial \rho_{\mathrm{NS}}}{\partial t} &= \frac{\partial\, \mathrm{Tr}_{\mathrm{in}}(\rho_S)}{\partial t} \\ &= \mathrm{Tr}_{\mathrm{in}}\left(\frac{\partial \rho_S}{\partial t}\right) \\ &= \mathrm{Tr}_{\mathrm{in}}\Bigg(- i[\mathbf{H}_S,\rho_S] + \mathcal{L}\int_0^t dt' k(t') \\ &\qquad \times \exp(\mathcal{L}t')\rho_S(t-t')\Bigg). \end{aligned} \quad (67)$$

Theorem 8. Assume imperfect initialization. Then a subsystem $\mathcal{H}_{\mathrm{NS}}$ in the decomposition $\mathcal{H}_S=\mathcal{H}_{\mathrm{NS}}\otimes\mathcal{H}_{\mathrm{in}}\oplus\mathcal{H}_{\mathrm{out}}$ is decoherence-free (or noiseless) with respect to non-Markovian dynamics [Eq. (63)] if and only if the Lindblad operators and the system Hamiltonian have the matrix representation

$$\mathbf{F}_\alpha = \begin{pmatrix} \mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_\alpha & \mathbf{0} \\ \mathbf{0} & \mathbf{B}_\alpha \end{pmatrix}, \quad (68)$$

$$\mathbf{H}_S = \begin{pmatrix} \mathbf{H}_{\mathrm{NS}}\otimes\mathbf{I}_{\mathrm{in}} + \mathbf{I}_{\mathrm{NS}}\otimes\mathbf{H}_{\mathrm{in}} & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_{\mathrm{out}} \end{pmatrix}. \quad (69)$$

Note that this form is, once again, identical to the Markovian case with imperfect initialization (cf. Theorem 6).

However, as in the DFS case, the conditions are slightly different between Markovian and non-Markovian dynamics if we demand perfect initialization.

Corollary 4. Assume perfect initialization. Then a subsystem $\mathcal{H}_{\mathrm{NS}}$ in the decomposition $\mathcal{H}_S=\mathcal{H}_{\mathrm{NS}}\otimes\mathcal{H}_{\mathrm{in}}\oplus\mathcal{H}_{\mathrm{out}}$ is decoherence-free (or noiseless) with respect to non-Markovian dynamics [Eq. (63)] if and only if the Lindblad operators and the system Hamiltonian have the matrix representation

$$\mathbf{F}_\alpha = \begin{pmatrix} \mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_\alpha & \mathbf{A}_\alpha \\ \mathbf{0} & \mathbf{B}_\alpha \end{pmatrix}, \quad (70)$$

$$\sum_{\alpha} (\mathbf{I}_{\mathrm{NS}} \otimes \mathbf{C}_{\alpha}^{\dagger})\mathbf{A}_{\alpha} = \mathbf{0}, \tag{71}$$

$$\mathbf{H} = \begin{pmatrix} \mathbf{H}_{\mathrm{NS}} \otimes \mathbf{I}_{\mathrm{in}} + \mathbf{I}_{\mathrm{NS}} \otimes \mathbf{H}_{\mathrm{in}} & \mathbf{0} \\ \mathbf{0} & \mathbf{H}_{\mathrm{out}} \end{pmatrix}. \tag{72}$$

VI. SUMMARY AND CONCLUSIONS

We have reconsidered the concepts of decoherence-free subspaces and (noiseless) subsystems (DFSs), and introduced definitions of DFSs that generalize previous work. We have analyzed the conditions for the existence of DFSs in the case of CP maps, Markovian dynamics, and non-Markovian continuous-time dynamics. Our main finding implies significantly relaxed demands on the preparation of decoherence-free states: the initial state can be arbitrarily noisy. If, on the other hand, the initial state is perfectly prepared, then almost arbitrary leakage from outside the DFS into the DFS can be tolerated.

In the case of Markovian dynamics, if one demands perfect initialization, our findings are of an opposite nature: we have shown that then an additional constraint must be imposed on the system Hamiltonian, which implies more stringent conditions for the possibility of manipulating a DFS than previously believed. We have presented an example to illustrate this fact.

We have also shown that the notion of noiseless subsystems, as originally developed using an algebraic approach, admits a generalization when it is instead developed from a quantum channel approach.

Our results have implications for experimental work on DFSs, and in particular on quantum algorithms over DFSs [16,17]. It is now known that a large class of quantum algorithms can tolerate almost arbitrary preparation errors and still provide an advantage over their classical counterparts [25–33]. The relaxed preparation conditions for DFSs presented here are naturally compatible with this approach to quantum computation in noisy systems. This should provide further impetus for the experimental exploration of quantum computation over DFSs.

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APPENDIX A: PROOFS OF THEOREMS AND COROLLARIES

Here we present proofs of all our results above. We shorten the calculations by starting from the NS case and obtain the DFS conditions as a special case.

1. CP maps

a. Arbitrary initial state

Assume the system evolution due to its interaction with a bath is described by a CP map with Kraus operators $\{\mathbf{E}_{\alpha}\}$:

$$\rho_S(t) = \sum_{\alpha} \mathbf{E}_{\alpha}\rho_S(0)\mathbf{E}_{\alpha}^{\dagger}. \tag{A1}$$

Note that here ρ_S is an operator on the entire system Hilbert space $\mathcal{H}_S$, which we assume to be decomposable as $\mathcal{H}_{\mathrm{NS}} \otimes \mathcal{H}_{\mathrm{in}} \oplus \mathcal{H}_{\mathrm{out}}$. From the NS definition Eq. (49), we have

$$\begin{aligned} &\mathrm{Tr}_{\mathrm{in}}[\mathbf{U} \otimes \mathbf{I}(\mathcal{P}_{\text{NS-in}}\rho_S(0)\mathcal{P}_{\text{NS-in}}^{\dagger})\mathbf{U}^{\dagger} \otimes \mathbf{I}] \\ &\quad = \mathrm{Tr}_{\mathrm{in}}\left(\sum_{\alpha} (\mathcal{P}_{\text{NS-in}}\mathbf{E}_{\alpha})\rho_S(0)(\mathbf{E}_{\alpha}^{\dagger}\mathcal{P}_{\text{NS-in}}^{\dagger})\right). \end{aligned} \tag{A2}$$

Let us represent the Kraus operators in the same block-structure matrix form as that of the system state, i.e., corresponding to the decomposition $\mathcal{H}_S = \mathcal{H}_{\mathrm{NS}} \otimes \mathcal{H}_{\mathrm{in}} \oplus \mathcal{H}_{\mathrm{out}}$, where the blocks correspond to the subspaces $\mathcal{H}_{\mathrm{NS}} \otimes \mathcal{H}_{\mathrm{in}}$ (upper left block) and $\mathcal{H}_{\mathrm{out}}$ (lower right block). Then

$$\rho_S = \begin{pmatrix} \rho_1 & \rho_2 \\ \rho_2^{\dagger} & \rho_3 \end{pmatrix}, \tag{A3}$$

$$\mathbf{E}_{\alpha} = \begin{pmatrix} \mathbf{P}_{\alpha} & \mathbf{A}_{\alpha} \\ \mathbf{D}_{\alpha} & \mathbf{B}_{\alpha} \end{pmatrix}, \tag{A4}$$

with appropriate normalization constraints, considered below. Equation (A2) simplifies in this matrix form as

$$\begin{aligned} \mathrm{Tr}_{\mathrm{in}}(\mathbf{U} \otimes \mathbf{I}\rho_1\mathbf{U}^{\dagger} \otimes \mathbf{I}) = \mathrm{Tr}_{\mathrm{in}}\bigg(\sum_{\alpha} &\mathbf{P}_{\alpha}\rho_1\mathbf{P}_{\alpha}^{\dagger} + \mathbf{P}_{\alpha}\rho_2\mathbf{A}_{\alpha}^{\dagger} \\ &+ \mathbf{A}_{\alpha}\rho_2^{\dagger}\mathbf{P}_{\alpha}^{\dagger} + \mathbf{A}_{\alpha}\rho_3\mathbf{A}_{\alpha}^{\dagger}\bigg), \end{aligned} \tag{A5}$$

which must hold for arbitrary $\rho_S(0)$. To derive constraints on the various terms we therefore consider special cases, which yield necessary conditions. First, consider an initial state $\rho_S(0)$ such that $\rho_2 = \mathbf{0}$. Then, as the left-hand side of Eq. (A5) is independent of ρ_3, the last term must vanish:

$$\sum_{\alpha} \mathbf{A}_{\alpha}\rho_3\mathbf{A}_{\alpha}^{\dagger} = \mathbf{0} \Rightarrow \mathbf{A}_{\alpha} = \mathbf{0}. \tag{A6}$$

Further assume $\rho_1 = |i\rangle\langle i| \otimes |i'\rangle\langle i'|$. Note that the partial matrix element $\langle j'|\mathbf{P}_{\alpha}|i'\rangle$ is an operator on the $\mathcal{H}_{\mathrm{NS}}$ factor, $|i\rangle\langle i|$. Then Eq. (A5) reduces to

$$|i\rangle\langle i| = \sum_{\alpha,j'} (\mathbf{U}^\dagger\langle j'|\mathbf{P}_\alpha|i'\rangle)|i\rangle\langle i|(\langle i'|\mathbf{P}_\alpha^\dagger|j'\rangle\mathbf{U}). \tag{A7}$$

Taking matrix elements with respect to $|i^\perp\rangle$, a state orthogonal to $|i\rangle$, yields

$$0 = \sum_{\alpha,j'} |\langle i^\perp|[\mathbf{U}^\dagger\langle j'|\mathbf{P}_\alpha|i'\rangle)|i\rangle|^2 \Rightarrow \langle i^\perp|(\mathbf{U}^\dagger\langle j'|\mathbf{P}_\alpha|i'\rangle)|i\rangle = \mathbf{0}, \tag{A8}$$

which, in turn implies that $(\mathbf{U}^\dagger\langle j'|\mathbf{P}_\alpha|i'\rangle)|i\rangle$ is proportional to $|i\rangle$, i.e.,

$$(\langle j'|\mathbf{P}_\alpha|i'\rangle)|i\rangle \propto \mathbf{U}|i\rangle. \tag{A9}$$

Since $|i'\rangle,|j'\rangle$ are arbitrary this condition implies that the submatrix $\mathbf{P}_\alpha$ must be of the form $\mathbf{P}_\alpha=\mathbf{U}\otimes\mathbf{C}_\alpha$. Substituting $\mathbf{P}_\alpha=\mathbf{U}\otimes\mathbf{C}_\alpha$ into Eq. (A5) we have $\mathrm{Tr}_{\mathrm{in}}(\mathbf{U}\otimes\mathbf{I}\rho_1\mathbf{U}^\dagger\otimes\mathbf{I}) = \mathrm{Tr}_{\mathrm{in}}(\Sigma_\alpha\mathbf{U}\otimes\mathbf{C}_\alpha\rho_1\mathbf{U}^\dagger\otimes\mathbf{C}_\alpha^\dagger\}$, so that

$$\mathrm{Tr}_{\mathrm{in}}(\rho_1) = \mathrm{Tr}_{\mathrm{in}}\left(\sum_\alpha \mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_\alpha\rho_1\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_\alpha^\dagger\right). \tag{A10}$$

Now suppose $\rho_1=\Sigma_{iji'j'}\lambda_{iji'j'}|i\rangle\langle j|\otimes|i'\rangle\langle j'|$; then from Eq. (A10) we find

$$\sum_{iji'}\lambda_{iji'i'}|i\rangle\langle j| = \sum_{iji'j'k'\alpha}\lambda_{iji'j'}|i\rangle\langle j|\langle k'|\mathbf{C}_\alpha|i'\rangle\langle j'|\mathbf{C}_\alpha^\dagger|k'\rangle. \tag{A11}$$

Using $\Sigma_{k'}|k'\rangle\langle k'|=\mathbf{I}_{\mathrm{in}}$, Eq. (A11) becomes

$$\sum_{iji'}\lambda_{iji'i'}|i\rangle\langle j| = \sum_{iji'j'}\lambda_{iji'j'}|i\rangle\langle j|\langle j'|\sum_\alpha\mathbf{C}_\alpha^\dagger\mathbf{C}_\alpha|i'\rangle. \tag{A12}$$

It follows that

$$\sum_\alpha \mathbf{C}_\alpha^\dagger\mathbf{C}_\alpha = \mathbf{I}_{\mathrm{in}}. \tag{A13}$$

Next consider the normalization constraint $\Sigma_\alpha\mathbf{E}_\alpha^\dagger\mathbf{E}_\alpha=\mathbf{I}$ for the Kraus operators, together with the additional constraints we have derived $(\mathbf{A}_\alpha=\mathbf{0},\mathbf{P}_\alpha=\mathbf{U}\otimes\mathbf{C}_\alpha)$:

$$\sum_\alpha \mathbf{P}_\alpha^\dagger\mathbf{P}_\alpha + \mathbf{D}_\alpha^\dagger\mathbf{D}_\alpha = \mathbf{I}_{\mathrm{NS}}\otimes\mathbf{I}_{\mathrm{in}}$$

$$\Rightarrow \mathbf{I}_{\mathrm{NS}}\otimes\sum_\alpha\mathbf{C}_\alpha^\dagger\mathbf{C}_\alpha + \sum_\alpha\mathbf{D}_\alpha^\dagger\mathbf{D}_\alpha=\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{I}_{\mathrm{in}}. \tag{A14}$$

But from Eq. (A13) we have $\Sigma_\alpha\mathbf{P}_\alpha^\dagger\mathbf{P}_\alpha=\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{I}_{\mathrm{in}}$. Therefore $\mathbf{D}_\alpha=\mathbf{0}$.

Taking all these conditions together finalizes the matrix representation of the Kraus operators as

$$\mathbf{E}_\alpha = \begin{pmatrix}\mathbf{U}\otimes\mathbf{C}_\alpha & \mathbf{0}\\ \mathbf{0} & \mathbf{B}_\alpha\end{pmatrix}. \tag{A15}$$

For a scalar $\mathbf{C}_\alpha$ we recover the DFS condition (19). These considerations establish the necessity of the representation (A15); it is simple to show that this representation is also sufficient, by substitution and checking that the NS and DFS conditions are satisfied. Therefore we have proved Theorems 1 and 4.

b. Perfect initialization

We now prove Corollaries 1 and 2 for DF-initialized states of the form $\rho_S(0)=\mathcal{P}_d\rho_S(0)\mathcal{P}_d$. Thus, we have to prove that $\mathbf{D}_\alpha=\mathbf{0}$ in Eq. (A4).

When $\rho_S(0)=\mathcal{P}_d\rho_S(0)\mathcal{P}_d$ we have that $\rho_2=\mathbf{0}$ and $\rho_3=\mathbf{0}$ and Eq. (A5) reduces to

$$\mathrm{Tr}_{\mathrm{in}}(\mathbf{U}\otimes\mathbf{I}\rho_1\mathbf{U}^\dagger\otimes\mathbf{I}) = \mathrm{Tr}_{\mathrm{in}}\left(\sum_\alpha\mathbf{P}_\alpha\rho_1\mathbf{P}_\alpha^\dagger\right). \tag{A16}$$

The argument leading to the vanishing of the $\mathbf{A}_\alpha$ [Eq. (A6)] then does not apply, and indeed the $\mathbf{A}_\alpha$ need not vanish. However, the arguments leading to $\mathbf{P}_\alpha=\mathbf{U}\otimes\mathbf{C}_\alpha$ and $\Sigma_\alpha\mathbf{P}_\alpha^\dagger\mathbf{P}_\alpha=\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{I}_{\mathrm{in}}$ do apply. Hence $\mathbf{D}_\alpha=\mathbf{0}$.

2. Markovian dynamics

a. Arbitrary initial state

Consider Markovian dynamics

$$\frac{\partial\rho_S}{\partial t} = -i[\mathbf{H}_S,\rho_S] + \sum_\alpha \mathbf{F}_\alpha\rho_S\mathbf{F}_\alpha^\dagger - \frac{1}{2}\mathbf{F}_\alpha^\dagger\mathbf{F}_\alpha\rho_S - \frac{1}{2}\rho_S\mathbf{F}_\alpha^\dagger\mathbf{F}_\alpha, \tag{A17}$$

with the following matrix representation of the various operators:

$$\rho_S = \begin{pmatrix}\rho_1 & \rho_2\\ \rho_2^\dagger & \rho_3\end{pmatrix},$$

$$\mathbf{H}_S = \begin{pmatrix}\mathbf{H}_1 & \mathbf{H}_2\\ \mathbf{H}_2^\dagger & \mathbf{H}_3\end{pmatrix}, \quad \mathbf{F}_\alpha = \begin{pmatrix}\mathbf{P}_\alpha & \mathbf{A}_\alpha\\ \mathbf{D}_\alpha & \mathbf{B}_\alpha\end{pmatrix}. \tag{A18}$$

Then we find the dynamics of the NS block to be

$$\begin{aligned}\frac{\partial\rho_{\mathrm{NS}}}{\partial t} &= \frac{\partial\,\mathrm{Tr}_{\mathrm{in}}(\rho_1)}{\partial t}\\ &= -i\,\mathrm{Tr}_{\mathrm{in}}([\mathbf{H}_1,\rho_1]) - i\,\mathrm{Tr}_{\mathrm{in}}[(\mathbf{H}_2\rho_2^\dagger - \rho_2\mathbf{H}_2^\dagger)]\\ &\quad + \mathrm{Tr}_{\mathrm{in}}\Bigg(\sum_\alpha \mathbf{P}_\alpha\rho_1\mathbf{P}_\alpha^\dagger + \mathbf{A}_\alpha\rho_2^\dagger\mathbf{P}_\alpha^\dagger + \mathbf{P}_\alpha\rho_2\mathbf{A}_\alpha^\dagger + \mathbf{A}_\alpha\rho_3\mathbf{A}_\alpha^\dagger\\ &\quad - \frac{1}{2}\sum_\alpha(\mathbf{P}_\alpha^\dagger\mathbf{P}_\alpha + \mathbf{D}_\alpha^\dagger\mathbf{D}_\alpha)\rho_1 + (\mathbf{P}_\alpha^\dagger\mathbf{A}_\alpha + \mathbf{D}_\alpha^\dagger\mathbf{B}_\alpha)\rho_2^\dagger\\ &\quad - \frac{1}{2}\sum_\alpha \rho_1(\mathbf{P}_\alpha^\dagger\mathbf{P}_\alpha + \mathbf{D}_\alpha^\dagger\mathbf{D}_\alpha) + \rho_2(\mathbf{A}_\alpha^\dagger\mathbf{P}_\alpha + \mathbf{B}_\alpha^\dagger\mathbf{D}_\alpha)\Bigg)\end{aligned} \tag{A19}$$

The right-hand side of this equation must be independent of ρ_2 and ρ_3, for any matrices ρ_2 and ρ_3. Therefore the term

$\mathbf{A}_\alpha\rho_3\mathbf{A}_\alpha^\dagger$ implies $\mathbf{A}_\alpha=\mathbf{0}$. Collecting the remaining terms acting on $\rho_2^\dagger$ from the left yields $\mathrm{Tr}_{\mathrm{in}}[(-i\mathbf{H}_2-\Sigma_\alpha\mathbf{P}_\alpha^\dagger\mathbf{D}_\alpha^\dagger\mathbf{B}_\alpha)\rho_2^\dagger)=\mathbf{0}$. Together we have

$$\mathbf{A}_\alpha=\mathbf{0},\quad i\mathbf{H}_2+\sum_\alpha\mathbf{D}_\alpha^\dagger\mathbf{B}_\alpha=\mathbf{0}. \tag{A20}$$

This reduces Eq. (A19) to

$$\frac{\partial\rho_{\mathrm{NS}}}{\partial t}=\frac{\partial\,\mathrm{Tr}_{\mathrm{in}}(\rho_1)}{\partial t}=-i\,\mathrm{Tr}_{\mathrm{in}}[\mathbf{H}_1,\rho_1]+\mathrm{Tr}_{\mathrm{in}}\sum_\alpha\mathbf{P}_\alpha\rho_1\mathbf{P}_\alpha^\dagger-\frac{1}{2}\mathrm{Tr}_{\mathrm{in}}\sum_\alpha[(\mathbf{P}_\alpha^\dagger\mathbf{P}_\alpha+\mathbf{D}_\alpha^\dagger\mathbf{D}_\alpha),\rho_1] \tag{A21}$$

Consider the initial state $\rho_1=\rho_{\mathrm{NS}}\otimes|i'\rangle\langle i'|$, with $|i'\rangle\in\mathcal{H}_{\mathrm{in}}$:

$$\frac{\partial\rho_{\mathrm{NS}}}{\partial t}=-i(\langle i'|\mathbf{H}_1|i'\rangle,\rho_{\mathrm{NS}})+\sum_\alpha\langle j'|\mathbf{P}_\alpha|i'\rangle\rho_{\mathrm{NS}}\langle i'|\mathbf{P}_\alpha^\dagger|j'\rangle-\frac{1}{2}\sum_\alpha[\rho_{\mathrm{NS}},(\langle i'|\mathbf{P}_\alpha^\dagger|j'\rangle\langle j'|\mathbf{P}_\alpha|i'\rangle+\langle i'|\mathbf{D}_\alpha^\dagger|j'\rangle\langle j'|\mathbf{D}_\alpha|i'\rangle)]. \tag{A22}$$

Let $\rho_{\mathrm{NS}}=|\psi\rangle\langle\psi|$ with ψ arbitrary and apply $\langle\psi^\perp|\cdots|\psi^\perp\rangle$, such that $\langle\psi^\perp|\psi\rangle=0$, to Eq. (A22), denoting $\mathbf{P}_{\alpha,i',j'}\equiv\langle j'|\mathbf{P}_\alpha|i'\rangle$:

$$\sum_\alpha|\langle\psi^\perp|\mathbf{P}_{\alpha,i',j'}|\psi\rangle|^2=0. \tag{A23}$$

Since this identity must hold for all ψ and $\psi^\perp$, we find that $\mathbf{P}_{\alpha,i',j'}=c_{\alpha,i',j'}\mathbf{I}_{\mathrm{NS}}$, which implies that $\mathbf{P}_\alpha=\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_{\mathrm{in}}^\alpha$. Moreover, by definition of a NS, there exists a Hermitian matrix $\mathbf{H}_{\mathrm{NS}}$ such that ρ_{NS} obeys a Schrödinger equation $\partial\rho_{\mathrm{NS}}/\partial t=-i[\mathbf{H}_{\mathrm{NS}},\rho_{\mathrm{NS}}]$. Therefore the non-Hermitian term $\Sigma_\alpha\mathbf{D}_\alpha^\dagger\mathbf{D}_\alpha$ in Eq. (A21) must vanish, implying that $\mathbf{D}_\alpha=\mathbf{0}$.

Combining these results with Eq. (A20) yields

$$\frac{\partial\,\mathrm{Tr}_{\mathrm{in}}(\rho_1)}{\partial t}=-i\,\mathrm{Tr}_{\mathrm{in}}([\mathbf{H}_1,\rho_1])\equiv-i[\mathbf{H}_{\mathrm{NS}},\rho_{\mathrm{NS}}]. \tag{A24}$$

This identity can be realized if and only if $\mathbf{H}_1=\mathbf{H}_{\mathrm{NS}}\otimes\mathbf{I}_{\mathrm{in}}+\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{H}_{\mathrm{in}}$. Therefore the NS conditions are obtained as

$$\mathbf{H}=\begin{pmatrix}\mathbf{H}_{\mathrm{NS}}\otimes\mathbf{I}_{\mathrm{in}}+\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{H}_{\mathrm{in}} & \mathbf{0}\\ \mathbf{0} & \mathbf{H}_3\end{pmatrix}, \tag{A25}$$

$$\mathbf{F}_\alpha=\begin{pmatrix}\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_{\mathrm{in}}^\alpha & \mathbf{0}\\ \mathbf{0} & \mathbf{B}_\alpha\end{pmatrix}.$$

The DFS condition is a special case of (A22), with $\dim(\mathcal{H}_{\mathrm{in}})=1$. This concludes the proof of Theorems 2 and 6.

b. Perfect initialization

Now consider perfect initialization:

$$\rho_S=\begin{pmatrix}\rho_1 & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}. \tag{A26}$$

This is just the case of an arbitrary initial state considered above, with $\rho_2=\mathbf{0}$ and $\rho_3=\mathbf{0}$ in Eq. (A19). This then yields the dynamics of ρ_{NS} as being given by Eq. (A21). Repeating the derivation following Eq. (A21) we conclude again that $\mathbf{D}_\alpha=\mathbf{0}$, $\mathbf{P}_\alpha=\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_{\mathrm{in}}^\alpha$, and $\mathbf{H}_1=\mathbf{H}_{\mathrm{NS}}\otimes\mathbf{I}_{\mathrm{in}}+\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{H}_{\mathrm{in}}$.

Note that Eq. (A20) now does not apply (it was obtained assuming nonzero ρ_2,ρ_3), i.e., we cannot conclude that $\mathbf{A}_\alpha$ and $\mathbf{H}_2$ vanish. This implies that $\partial\rho_S/\partial t$ has nonzero off-diagonal elements, which, using the master equation (A17), we calculate to be

$$i\rho_1\mathbf{H}_2+\sum_\alpha\mathbf{P}_\alpha\rho_1\mathbf{D}_\alpha^\dagger-\frac{1}{2}\rho_1(\mathbf{P}_\alpha^\dagger\mathbf{A}_\alpha+\mathbf{D}_\alpha^\dagger\mathbf{B}_\alpha)$$

$$=i\rho_1\mathbf{H}_2-\frac{1}{2}\rho_1\sum_\alpha(\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_{\mathrm{in}}^{\alpha\dagger})\mathbf{A}_\alpha\quad(\text{upper right block}),$$

$$\sum_\alpha\mathbf{D}_\alpha\rho_1\mathbf{D}_\alpha^\dagger=\mathbf{0}\quad(\text{bottom right block}).$$

To prevent the appearance of corresponding off-diagonal blocks in ρ_S, we must therefore demand

$$\mathbf{H}_2+\frac{i}{2}\sum_\alpha(\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_{\mathrm{in}}^{\alpha\dagger})\mathbf{A}_\alpha=\mathbf{0}, \tag{A27}$$

which is Eq. (56). The DFS case is obtained with $\dim(\mathcal{H}_{\mathrm{in}})=1$. This concludes the proof of Theorems 3 and 5.

3. Non-Markovian dynamics

The derivation of the conditions for decoherence-freeness in the case of non-Markovian dynamics is somewhat different from the other two cases we have considered, because of the appearance of the nonlocal-in-time integral in the master equation:

$$\frac{\partial\rho_S}{\partial t}=-i[\mathbf{H}_S,\rho_S]+\mathcal{L}\int_0^t dt'k(t')\exp(\mathcal{L}t')\rho_S(t-t'). \tag{A28}$$

In order to find necessary conditions on the structure of $\mathbf{H}_S$ and $\mathcal{L}$ we consider the case of small t and expand

$$\rho_S(t)=\sum_{n=0}t^n\rho_S^{(n)}(0),\quad k(t)=\sum_{m=0}t^mk^{(m)}(0), \tag{A29}$$

and substitute into Eq. (A28). The constant (t^0) term yields

$$\rho_S^{(1)}(0)=-i[\mathbf{H}_S,\rho_S(0)]. \tag{A30}$$

The terms involving t^1 yield, after Taylor-expanding $\exp(\mathcal{L}t')$,

$$2\rho_S^{(2)}(0)=-i[\mathbf{H}_S,\rho_S^{(1)}(0)]+k(0)\mathcal{L}\rho_S(0). \tag{A31}$$

Thus the solution of Eq. (A28) up to first and second order in time is

$$\rho_S(t) = \rho_S(0) - it[\mathbf{H}_S,\rho_S(0)] + O(t^2), \tag{A32}$$

$$\rho_S(t) = \rho_S(0) - it[\mathbf{H}_S,\rho_S(0)] - \frac{t^2}{2}\{-[\mathbf{H}_S,[\mathbf{H}_S,\rho_S(0)]] + k(0)\mathcal{L}\rho_S(0)\} + O(t^3). \tag{A33}$$

a. Arbitrary initial state

Consider once again the matrix representations as in Eq. (A18). Substituting these expressions into the first order equation (A32), the $\rho_1(t)$ block yields

$$\begin{aligned}\rho_{\mathrm{NS}}(t) &= \rho_{\mathrm{NS}}(0) - it\,\mathrm{Tr}_{\mathrm{in}}\{[\mathbf{H}_1,\rho_1(0)]\} \\ &\quad - it\,\mathrm{Tr}_{\mathrm{in}}[\mathbf{H}_2\rho_2^{\dagger}(0) - \rho_2(0)\mathbf{H}_2^{\dagger}] \\ &\Rightarrow \mathbf{H}_2 = \mathbf{0}, \\ \mathbf{H}_1 &= \mathbf{H}_{\mathrm{NS}}\otimes\mathbf{I}_{\mathrm{in}} + \mathbf{I}_{\mathrm{NS}}\otimes\mathbf{H}_{\mathrm{in}}.\end{aligned} \tag{A34}$$

Continuing to second order, Eq. (A33), the NS block is found to be

$$\begin{aligned}\rho_{\mathrm{NS}}(t) &= \rho_{\mathrm{NS}}(0) - it[\mathbf{H}_{\mathrm{NS}},\rho_{\mathrm{NS}}(0)] - \frac{t^2}{2}[\mathbf{H}_{\mathrm{NS}},[\mathbf{H}_{\mathrm{NS}},\rho_{\mathrm{NS}}(0)]] \\ &\quad + \mathrm{Tr}_{\mathrm{in}}\Bigg(2k(0)\sum_{\alpha}\mathbf{P}_{\alpha}\rho_1\mathbf{P}_{\alpha}^{\dagger} + \mathbf{A}_{\alpha}\rho_2^{\dagger}\mathbf{P}_{\alpha}^{\dagger} + \mathbf{P}_{\alpha}\rho_2\mathbf{A}_{\alpha}^{\dagger} \\ &\quad + \mathbf{A}_{\alpha}\rho_3\mathbf{A}_{\alpha}^{\dagger} - k(0)\sum_{\alpha}(\mathbf{P}_{\alpha}^{\dagger}\mathbf{P}_{\alpha} + \mathbf{D}_{\alpha}^{\dagger}\mathbf{D}_{\alpha})\rho_1 \\ &\quad + (\mathbf{P}_{\alpha}^{\dagger}\mathbf{A}_{\alpha} + \mathbf{D}_{\alpha}^{\dagger}\mathbf{B}_{\alpha})\rho_2^{\dagger} - k(0)\sum_{\alpha}\rho_1(\mathbf{P}_{\alpha}^{\dagger}\mathbf{P}_{\alpha} + \mathbf{D}_{\alpha}^{\dagger}\mathbf{D}_{\alpha}) \\ &\quad + \rho_2(\mathbf{A}_{\alpha}^{\dagger}\mathbf{P}_{\alpha} + \mathbf{B}_{\alpha}^{\dagger}\mathbf{D}_{\alpha})\Bigg).\end{aligned} \tag{A35}$$

The first three terms correspond to unitary evolution, but the remaining terms are essentially identical to the case of Markovian dynamics and must be made to vanish, just as in Eq. (A19). The same arguments used there apply and consequently

$$\mathbf{F}_{\alpha} = \begin{pmatrix}\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_{\mathrm{in}}^{\alpha} & \mathbf{0}\\ \mathbf{0} & \mathbf{B}_{\alpha}\end{pmatrix}. \tag{A36}$$

The conditions (A34) and (A36) are necessary and sufficient for unitary evolution of the NS block under our non-Markovian master equation. The DFS case is obtained with $\dim(\mathcal{H}_{\mathrm{in}})=1$. This concludes the proof of Theorems 7 and 8.

b. Perfect initialization

Assume

$$\rho_S(0) = \begin{pmatrix}\rho_1 & \mathbf{0}\\ \mathbf{0} & \mathbf{0}\end{pmatrix}; \tag{A37}$$

then from the first order equation (A32), the NS block is found to satisfy

$$\begin{aligned}\rho_{\mathrm{NS}}(t) &= \rho_{\mathrm{NS}}(0) - it\,\mathrm{Tr}_{\mathrm{in}}\{[\mathbf{H}_1,\rho_1]\} \\ &\Rightarrow \mathbf{H}_1 = \mathbf{H}_{\mathrm{NS}}\otimes\mathbf{I}_{\mathrm{in}} + \mathbf{I}_{\mathrm{NS}}\otimes\mathbf{H}_{\mathrm{in}}.\end{aligned} \tag{A38}$$

To second order in time [Eq. (A33)],

$$\begin{aligned}\rho_{\mathrm{NS}}(t) &= \rho_{\mathrm{NS}}(0) - it[\mathbf{H}_{\mathrm{NS}},\rho_{\mathrm{NS}}(0)] - \frac{t^2}{2}[\mathbf{H}_{\mathrm{NS}},[\mathbf{H}_{\mathrm{NS}},\rho_{\mathrm{NS}}(0)]] \\ &\quad + \frac{t^2}{2}\mathrm{Tr}_{\mathrm{in}}\Bigg(-\mathbf{H}_2\mathbf{H}_2^{\dagger}\rho_1 - \rho_1\mathbf{H}_2\mathbf{H}_2^{\dagger} \\ &\quad + 2k(0)\sum_{\alpha}\mathbf{P}_{\alpha}\rho_1\mathbf{P}_{\alpha}^{\dagger} - (\mathbf{P}_{\alpha}^{\dagger}\mathbf{P}_{\alpha} + \mathbf{D}_{\alpha}^{\dagger}\mathbf{D}_{\alpha})\rho_1 \\ &\quad - \rho_1(\mathbf{P}_{\alpha}^{\dagger}\mathbf{P}_{\alpha} + \mathbf{D}_{\alpha}^{\dagger}\mathbf{D}_{\alpha})\Bigg),\end{aligned} \tag{A39}$$

which is again similar to the Markovian case. Similar logic therefore yields $\mathbf{H}_2=\mathbf{D}_{\alpha}=\mathbf{0}$, and hence

$$\mathbf{F}_{\alpha} = \begin{pmatrix}\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_{\alpha} & \mathbf{A}_{\alpha}\\ \mathbf{0} & \mathbf{B}_{\alpha}\end{pmatrix}. \tag{A40}$$

Here we should notice that the density matrix $\rho_S(0)$ has an off-diagonal element $\rho_1\Sigma_{\alpha}(\mathbf{P}_{\alpha}^{\dagger}\mathbf{A}_{\alpha}+\mathbf{D}_{\alpha}^{\dagger}\mathbf{B}_{\alpha})=\rho_1\Sigma_{\alpha}\mathbf{P}_{\alpha}^{\dagger}\mathbf{A}_{\alpha}$. This term must vanish, for otherwise $\rho_S(t)$ has nonzero off-diagonal elements. Summarizing, we have

$$\mathbf{F}_{\alpha} = \begin{pmatrix}\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_{\alpha} & \mathbf{A}_{\alpha}\\ \mathbf{0} & \mathbf{B}_{\alpha}\end{pmatrix}, \quad \sum_{\alpha}(\mathbf{I}_{\mathrm{NS}}\otimes\mathbf{C}_{\alpha}^{\dagger})\mathbf{A}_{\alpha} = 0,$$

$$\mathbf{H} = \begin{pmatrix}\mathbf{H}_{\mathrm{NS}}\otimes\mathbf{I}_{\mathrm{in}} + \mathbf{I}_{\mathrm{NS}}\otimes\mathbf{H}_{\mathrm{in}} & \mathbf{0}\\ \mathbf{0} & \mathbf{H}_{\mathrm{out}}\end{pmatrix}. \tag{A41}$$

The DFS case is obtained with $\dim(\mathcal{H}_{\mathrm{in}})=1$. This concludes the proof of Corollaries 3 and 4.

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