# The Structure of Decoherence-free Subsystems

Ji Guan, Yuan Feng and Mingsheng Ying

Abstract—Decoherence-free subsystems have been successfully developed as a tool to preserve fragile quantum information against noises. In this work, we develop a structure theory for decoherence-free subsystems. Consequently, under perfect initialization of quantum states, we propose an effective algorithm to find an optimal set of decoherence-free subsystems for any given quantum super-operator such that any other such subsystem is a subspace of one of them. Furthermore, we give an easy way to pick up faulty-tolerant ones from them. Using these mathematical techniques, we obtain a simple numerical method to obtain a basis for any tensor, generating a family of matrix product states.

Index Terms—decoherence-free subsystems, continuous coherences, faulty-tolerance, matrix product states, structure theory.

#### I. INTRODUCTION

O build large scale quantum computers, the obstacles, such as decoherences and noises, must be managed and overcome [1]. One of the effective methods for this purpose is through decoherence-free subspaces proposed by Daniel A. Lidar in [2]. A subspace of the system Hilbert space is said to be decoherence-free if the effect of the noise on it is simply unitary, and thus easily correctable. For this sake, decoherencefree subspaces are important subjects in quantum computing, where coherent control of quantum systems is often the desired goal [3]. On the other hand, decoherence-free subspaces can also be characterized as a special case of quantum error correcting codes to preserve quantum information against noises [3]. However, we do not need to restrict the decoherencefree dynamics to a subspace. E. Knill, R. Laflamme, and L. Viola introduced the concept of noiseless subsystems, by extending higher-dimensional irreducible representations of the algebra generating the dynamical symmetry in the systemenvironment interaction [4]. A subsystem is a factor in a tensor product decomposition of a subspace and the noiseless subsystem requires the evolution on it to be strict identity. Such noiseless subsystems have been fully characterized and intensely studied in [5], [6], [7], [8], [9]. Remarkably, the structure theory of noiseless subsystems was proposed in [5], leading to an algorithm which finds all noiseless subsystems for a given quantum super-operator [10], [11]. In the meanwhile, the general case of decoherence-free subspaces and noiseless subsystems, called decoherence-free subsystems, was examined and the conditions for their existence were found in [12], and subsystems with significantly reduced noises were considered in [13]. However, a clear picture of the structure of decoherence-free subsystems (subspaces) is still lacking,

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and it is hard to compute all decoherence-free subsystems (subspaces) or the highest-dimensional ones for any given quantum super-operator.

In this paper, we develop a structure theory that shows precisely how a super-operator, the evolution of a quantum system, determines its decoherence-free subsystems, generating the existing results for noiseless subsystems. As an application, under perfect initialization of quantum states, we develop an algorithm (Algorithm 1) to generate an optimal set of decoherence-free subsystems for any given super-operator such that any other decoherence-free subsystem is a subspace of one of them. We then consider decoherence-free subsystems with imperfect initialization, and obtain a very simple method to find them. We further use this mathematical tool in the quantum many-body system described by a family of matrix product states generated by a tensor and propose a feasible way to numerically derive a basis for the tensor. The basis plays an important role in fundamental theorems of Matrix product states [14], [15].

This paper is organized as follows. We recall some basic notions of quantum information theory and introduce one central concept, continuous coherences in Section II. In Section III, we review the structure theory of noiseless subsystems by studying the fixed points of super-operators. We then show a similar structure theory of decoherence-free subsystems in Section IV, which leads to an algorithm of constructing an optimal set of such subsystems with the assumption perfect initialization, for a given super-operator. In Section V, we present a procedure for checking whether or not a subsystem with a cosubsystem is decoherence-free under imperfect initialization. Furthermore, we apply previous results to find a basis for any tensor, generating a set of matrix product states to represent a quantum many-body system in Section VI. A brief conclusion is drawn in the last section.

#### II. PRELIMINARIES

In this section, for convenience of the reader, we review some basic notions and results from quantum information theory; for details we refer to [1]. Recall that given a quantum system S with the associated (finite-dimensional) state Hilbert space  $\mathcal{H}$ , the evolution of the system can be mathematically modeled by a super-operator, i.e., a completely positive and trace-preserving (CPTP) map  $\mathcal{E}$  on  $\mathcal{H}$ . We say that a quantum system A is a subsystem of S if  $\mathcal{H} = (\mathcal{H}_A \otimes \mathcal{H}_B) \bigoplus \mathcal{K}$  for some co-subsystem B, where  $\mathcal{K} = (\mathcal{H}_A \otimes \mathcal{H}_B)^{\perp}$ ,  $\mathcal{H}_A$  and  $\mathcal{H}_B$  are the state spaces of A and B, respectively. For any two Hilbert spaces  $\mathcal{H}$  and  $\mathcal{H}'$ , let  $\mathcal{L}(\mathcal{H},\mathcal{H}')$  be the set of all operators from  $\mathcal{H}$  to  $\mathcal{H}'$ . Simply, we define that  $\mathcal{L}(\mathcal{H}) = \mathcal{L}(\mathcal{H},\mathcal{H})$  and  $\mathcal{D}(\mathcal{H})$  is the set of all quantum states, i.e. density operators with unit trace, on  $\mathcal{H}$ . The support of a

quantum state  $\rho$ , denoted by supp $(\rho)$ , is the linear span of the eigenvectors corresponding to non-zero eigenvalues of  $\rho$ .

Definition 1: Given a super-operator  $\mathcal{E}$  on  $\mathcal{H}$ ,

- (1) a quantum state  $\rho$  is said to be stationary if it is a fixed point of  $\mathcal{E}$ , i.e.  $\mathcal{E}(\rho) = \rho$ . Furthermore,  $\rho$  is minimal if there is no other stationary state  $\sigma$  such that  $supp(\sigma) \subseteq supp(\rho)$ ;
- (2) a subspace  $\mathcal{H}_1 \subseteq \mathcal{H}$  is minimal if it is a support of some minimal stationary state. Furthermore, if the whole space  $\mathcal{H}$  is minimal, then we call it irreducible; otherwise it is reducible.
- (3) a subspace  $\mathcal{K}$  is called transient if for any state  $\rho \in \mathcal{D}(\mathcal{H})$ ,

$$\lim_{n\to\infty} \operatorname{tr}(P_{\mathcal{K}}\mathcal{E}^n(\rho)) = 0,$$

where  $P_{\mathcal{K}}$  is the projector onto  $\mathcal{K}$ .

Note that if two minimal states  $\rho$  and  $\sigma$  have the same support, then  $\rho = \sigma$ . Thus  $\mathcal{H}$  is irreducible if and only if there is only one stationary state.

Applying the techniques developed in [16], [17], we can decompose  $\mathcal{H}$  into mutually orthogonal minimal subspaces and the largest transient subspace:

$$\mathcal{H} = \bigoplus_{p=1}^{m} \mathcal{H}_p \bigoplus \mathcal{K}. \tag{1}$$

Furthermore, the Kraus operators  $\{E_k\}$  of  $\mathcal{E}$  have the corresponding block form:

$$E_{k} = \begin{bmatrix} E_{k,1} & & & & \\ & E_{k,2} & & & \\ & & \ddots & & \\ & & & E_{k,m} & \\ \hline & & & & K_{k} \end{bmatrix}$$

for some operators  $E_{k,p} \in \mathcal{L}(\mathcal{H}_p)$ ,  $K_k \in \mathcal{L}(\mathcal{K})$ , and  $T_k \in \mathcal{L}(\mathcal{K}, \mathcal{K}^{\perp})$ . We then define a set of associated maps  $\{\mathcal{E}_{p,q}: p, q=1,\ldots,m\}$  of  $\mathcal{E}$ :

$$\mathcal{E}_{p,q}(\cdot) = \sum_{k} E_{k,p} \cdot E_{k,q}^{\dagger}. \tag{2}$$

Obviously, for any p and q,  $\mathcal{E}_{p,q}$  is a linear map from  $\mathcal{L}(\mathcal{H}_q,\mathcal{H}_p)$  to itself. If  $p \neq q$ ,  $\mathcal{L}(\mathcal{H}_q,\mathcal{H}_p)$  can be viewed as (outer) coherences from  $\mathcal{H}_q$  to  $\mathcal{H}_p$ , i.e. upper off-diagonal blocks of all matrices restricted in the decomposition  $\mathcal{H}_p \bigoplus \mathcal{H}_q$ . Thus the coherence between  $\mathcal{H}_p$  and  $\mathcal{H}_q$  is  $\mathcal{L}(\mathcal{H}_q,\mathcal{H}_p) \bigoplus \mathcal{L}(\mathcal{H}_p,\mathcal{H}_q)$  and  $\mathcal{L}(\mathcal{H}_q)$  can be regarded as inner coherences.

For all p and q, the following two properties are easy to observe:

- (1)  $\mathcal{L}(\mathcal{H}_p, \mathcal{H}_q)$  is invariant under  $\mathcal{E}$ ; that is, for all  $A \in \mathcal{L}(\mathcal{H}_p, \mathcal{H}_q)$ ,  $\mathcal{E}(A) \in \mathcal{L}(\mathcal{H}_p, \mathcal{H}_q)$ .
- (2)  $\lambda(\mathcal{E}_{p,q}) \subseteq \lambda(\mathcal{E})$ , where  $\lambda(\cdot)$  is the set of eigenvalues of a linear map.

Furthermore, the coherence  $\mathcal{L}(\mathcal{H}_p, \mathcal{H}_q)$  is said to be continuous if there exists  $A \in \mathcal{L}(\mathcal{H}_p, \mathcal{H}_q)$  such that  $\mathcal{E}(A) = e^{i\theta}A$  for some real number  $\theta$ ; that is,  $\lambda(\mathcal{E}_{p,q})$  has an element with magnitude one. Specially, if  $\theta = 0$ , then  $\mathcal{L}(\mathcal{H}_p, \mathcal{H}_q)$  is

stationary. Obviously,  $\mathcal{L}(\mathcal{H}_p, \mathcal{H}_p)$  is always stationary because a super-operator has at least one stationary state. Stationary coherences have been intensely studied in [17], where a nice structure of  $fix(\mathcal{E})$ , the set of fixed points of super-operator  $\mathcal{E}$ , is discovered. We will restate this result in the next section.

Definition 2: Let  $\mathcal{E}$  be a super-operator on  $\mathcal{H} = \mathcal{H}_A \bigotimes \mathcal{H}_B \bigoplus \mathcal{K}$ .  $\mathcal{H}_A$  is a decoherence-free subsystem if there is a unitary matrix  $U_A$  on  $\mathcal{H}_A$  such that for any initial state  $\rho$ ,

$$\operatorname{tr}_{B}[\mathcal{E}(P_{AB}\rho P_{AB})] = U_{A}\operatorname{tr}_{B}[(P_{AB}\rho P_{AB})]U_{A}^{\dagger},\tag{3}$$

where  $P_{AB}$  is the projector onto  $\mathcal{H}_A \otimes \mathcal{H}_B$ . Furthermore, if  $U_A = I_A$ , the identity operator on  $\mathcal{H}_A$ , then we say that  $\mathcal{H}_A$  is noiseless.

Given a decomposition of  $\mathcal{H} = \mathcal{H}_A \bigotimes \mathcal{H}_B \bigoplus \mathcal{K}$  and a initial state  $\rho \in D(\mathcal{H})$ ,  $\rho$  has the following block form:

$$\rho = \begin{bmatrix} \rho_{AB} & \rho' \\ \rho'^{\dagger} & \rho_{\mathcal{K}} \end{bmatrix} \tag{4}$$

If  $\mathcal{H}_A$  is decoherence-free, then the quantum information  $\operatorname{tr}_B(\rho_{AB})$  can be preserved in it, even though  $\operatorname{tr}_B(\rho_{AB})$  is not a valid quantum state as its trace might be less than one. Ideally, we hope that  $\rho$  is initialized in  $\mathcal{H}_A \bigotimes \mathcal{H}_B$ , i.e.  $\rho' = 0$  and  $\rho_K = 0$ ; this situation is called perfect initialization. But in many cases, specially experiments, such initialization might be challenging, so we will face imperfect initialization, i.e.  $\rho' \neq 0$  or  $\rho_K \neq 0$ .

The results of [12] have shown that in perfect initialization,  $\mathcal{H}_A$  is decoherence-free if and only if the Kraus operators  $\{E_k\}_k$  of  $\mathcal{E}$  have the matrix representation:

$$E_k = \begin{bmatrix} U \otimes E_k' & T_k \\ 0 & K_k \end{bmatrix} \quad \forall k \tag{5}$$

; in imperfect initialization, we have that

$$E_k = \begin{bmatrix} U \otimes E_k' & 0\\ 0 & K_k \end{bmatrix} \quad \forall k \tag{6}$$

Obviously, co-subsystem  $\mathcal{H}_B$  is important in later case, but is inessential in former case as the initial state is prepared in  $\mathcal{H}_A \bigotimes \mathcal{H}_B$  and  $\mathcal{H}_B$  can be traced over. A decoherence-free subsystem  $\mathcal{H}_A$  under imperfect initialization is always decoherence-free under perfect initialization, but the converse part is not true in all cases.

In the following two sections, we assume perfect initialization, i.e. initial states can be prepared exactly in any subspace. In Section V, we will deal with imperfect initialization.

# III. FIXED POINTS AND NOISELESS SUBSYSTEMS

Noiseless subsystems are a special case of decoherencefree subsystems and have been intensely studied in quantum error correction [18], [7] and quantum memory [19]. As we are going to show a structure theory of decoherencefree subsystems in the upcoming section, we first review the counterpart in noiseless subsystems which is inspired by the structure of fixed points of super-operators.

To characterize  $fix(\mathcal{E})$ , the main step is to identify stationary coherences of minimal subspaces in the decomposition of Eq.(1) and this can be achieved by the following lemma.

Lemma 1 ([17]): Let  $\mathcal E$  be a super-operator on  $\mathcal H$  with the orthogonal decomposition presented in Eq.(1). For any  $1 \leq p,q \leq m, \ \mathcal L(\mathcal H_p,\mathcal H_q)$  is stationary if and only if there is a unitary matrix U such that  $E_{k,p} = U E_{k,q} U^\dagger$  for all k. Furthermore,  $\mathcal H_p \simeq \mathcal H_q$ .

From Lemma 1,  $\mathcal{L}(\mathcal{H}_p, \mathcal{H}_q)$  is stationary if and only if so is  $\mathcal{L}(\mathcal{H}_q, \mathcal{H}_p)$ . Thus in the following, we simply say that there is a stationary coherence between  $\mathcal{H}_p$  and  $\mathcal{H}_q$  without referring to the direction. Furthermore, we group together minimal subspaces by stationary coherences and obtain a structure of  $fix(\mathcal{E})$  as follows.

Theorem 1 ([17]): Let  $\mathcal{E}$  be a super-operator on  $\mathcal{H}$ . There is a unique orthogonal decomposition of  $\mathcal{H}$ 

$$\mathcal{H} = \bigoplus_{l=1}^{L} \mathcal{X}_l \bigoplus \mathcal{K} \tag{7}$$

where

- (1) K is the largest transient subspace;
- (2) each  $\mathcal{X}_l$  is either a minimal subspace or can be further decomposed into mutually orthogonal minimal subspaces with stationary coherences between any two of them:

$$\mathcal{X}_l = \bigoplus_{p=1}^{m_l} \mathcal{B}_{l,p} \simeq \mathbb{C}^{m_l} \bigotimes \mathcal{B}_l, \quad \mathcal{B}_l \simeq \mathcal{B}_{l,p} \ \forall p$$
 (8)

so that the Kraus operators  $\{E_k\}$  of  $\mathcal{E}$  have a unitarily equivalent block form:

$$E_k \simeq \begin{bmatrix} I_1 \otimes E_{k,1} & & & & \\ & \ddots & & & \\ & & I_L \otimes E_{k,L} & \\ \hline & & 0 & & K_k \end{bmatrix}$$
(9)

for some operators  $E_{k,l} \in \mathcal{L}(\mathcal{B}_l)$ ,  $K_k \in \mathcal{L}(\mathcal{K})$ , and  $T_k \in \mathcal{L}(\mathcal{K}, \mathcal{K}^{\perp})$ . Here  $I_l$  is the identity operator on  $\mathbb{C}^{m_l}$  and  $\mathcal{B}_l$  is irreducible under  $\mathcal{E}_l(\cdot) = \sum_k E_{k,l} \cdot E_{k,l}^{\dagger}$ . Furthermore,

$$fix(\mathcal{E}) \simeq \bigoplus_{l} [\mathcal{L}(\mathbb{C}^{m_l}) \otimes \rho_l] \bigoplus 0_{\mathcal{K}}$$

where  $\rho_l$  is the unique stationary state of  $\mathcal{E}_l$ , and  $0_{\mathcal{K}}$  is the zero operator on  $\mathcal{K}$ .

(3) there is no stationary coherence between any minimal subspaces  $\mathcal{B}_{l,p}$  and  $\mathcal{B}_{l',p'}$  whenever  $l \neq l'$ .

In the following parts of this paper we will, with slight abuse of formulation, write all the formulas related to splitting  $\mathcal{H}$  as in Eq.(8) or Kraus operators as in Eq.(9) with "=" instead of " $\simeq$ ".

Actually, as the following theorem shows, all noiseless subsystems have been captured by the above decomposition.

Theorem 2 ([6]): Let  $\mathcal E$  be a super-operator on  $\mathcal H$  with its unique orthogonal decomposition

$$\mathcal{H} = \bigoplus_{l=1}^{m} \left[ \mathbb{C}^{m_l} \bigotimes \mathcal{B}_l \right] \bigoplus \mathcal{K},$$

presented in Theorem 1. Then a subsystem  $\mathcal{H}_A$  is noiseless if and only if  $\mathcal{H}_A \subseteq \mathbb{C}^{m_l}$  for some l.

The decomposition in Theorem 1 can also be obtained by applying the structure of  $C^*$ -algebra generated by the Kraus operators of  $\mathcal{E}$ ; see [5] for details. Subsequently, some algorithms for implementing the above decompositions in Eqs. (7-9) were developed from the structure of the  $C^*$ -algebra or  $fix(\mathcal{E})$  [20], [10], [11]. Such algorithms will be referred as NSDecompose( $\mathcal{H}, \mathcal{E}$ ) in this paper and the time complexity is  $O(n^8)$ , where  $\dim(\mathcal{H}) = n$ .

*Example 1:* Given  $\mathcal{H} = \mathcal{H}_A \bigotimes \mathcal{H}_B$ , and  $\{|k\rangle_A\}_{k=0}^3$  and  $\{|k\rangle_B\}_{k=0}^2$  are orthonormal bases of  $\mathcal{H}_A$  and  $\mathcal{H}_B$ , respectively, let  $\mathcal{E}$  be a super-operator on  $\mathcal{H}$  with the Kraus operators:

$$\begin{array}{lcl} E_1 & = & |00\rangle\langle01| + |10\rangle\langle11| - |20\rangle\langle21| - |30\rangle\langle31| \\ E_2 & = & |01\rangle\langle00| + |11\rangle\langle10| - |21\rangle\langle20| - |31\rangle\langle30| \\ E_3 & = & |00\rangle\langle02| + |10\rangle\langle12| - |20\rangle\langle22| - |30\rangle\langle32| \end{array}$$

where  $|kl\rangle = |k\rangle_A \otimes |l\rangle_B$ . It is easy to calculate the unique decomposition of  $\mathcal{H}$  in Theorem 1 as

$$\mathcal{H} = \bigoplus_{l=1}^{2} \left[ \mathcal{H}_{l} \bigotimes \mathcal{H}' \right] \bigoplus \mathcal{K}$$

where  $\mathcal{H}_1 = \text{lin.span}\{|0\rangle_A, |1\rangle_A\}$ ,  $\mathcal{H}_2 = \text{lin.span}\{|2\rangle_A, |3\rangle_A\}$ ,  $\mathcal{H}' = \text{lin.span}\{|0\rangle_B, |1\rangle_B\}$ , and  $\mathcal{K} = \mathcal{H}_A \otimes \text{lin.span}\{|2\rangle_B\}$ . Then we can store 2-qubit quantum information in  $\mathcal{H}_1$  or  $\mathcal{H}_2$ .

# IV. DECOHERENCE-FREE SUBSYSTEMS WITH PERFECT INITIALIZATION

In this section, a similar orthogonal decomposition as that in Theorem 1 is proposed for decoherence-free subsystems. Employing it, we then develop an efficient algorithm to find all such subsystems for any given super-operator.

By the definition, a decoherence-free subsystem  $\mathcal{H}_A$  is a small place of Hilbert space  $\mathcal{H}$  with a unitary evolution under the quantum noise, modeled by a super-operator  $\mathcal{E}$ . From Eq.(5), the restriction of  $\mathcal{E}$  onto  $\mathcal{H}_A \otimes \mathcal{H}_B$ , where  $\mathcal{H}_B$  is the co-subsystem of  $\mathcal{H}_A$ , can be written as

$$\mathcal{E}_{AB} = \mathcal{U}_A \otimes \mathcal{E}_B \tag{10}$$

where  $\mathcal{U}_A$  is a unitary super-operator on  $\mathcal{H}_A$  and  $\mathcal{E}_B$  is a super-operator on  $\mathcal{H}_B$ . By the decomposition Eq.(1),  $\mathcal{H}_B$  can be chosen to be irreducible. In this section, we assume that the co-subsystem of a decoherence-free subsystem is always irreducible.

First, we observe that the joint systems of decoherence-free subsystems and irreducible co-subsystems consist of minimal subspaces with continuous coherences.

Theorem 3: Given a super-operator  $\mathcal{E}$  on

$$\mathcal{H} = \mathcal{H}_A \bigotimes \mathcal{H}_B \bigoplus \mathcal{K},$$

let  $\mathcal{H}_A$  is a decoherence-free subsystem and  $U_A$  the corresponding unitary matrix in Eq.(3). Let  $\{|p\rangle\}_{p=1}^m$  be a set of mutually orthogonal eigenvectors of  $U_A$  and  $\mathcal{H}_p = \text{lin.span}\{|p\rangle\} \otimes \mathcal{H}_B$ . Then for all  $1 \leq p,q \leq m$ ,  $\mathcal{H}_p$  is a minimal subspace and  $\mathcal{L}(\mathcal{H}_p,\mathcal{H}_q)$  is continuous.

*Proof.* Note that we assume  $\mathcal{H}_B$  is irreducible. Let  $\rho$  be the unique stationary state of  $\mathcal{E}_B$ . Then for any p,  $|p\rangle\langle p|\otimes\rho$  is a minimal stationary state of  $\mathcal{E}$ , and hence  $\mathcal{H}_p$  is minimal.

Theorem 3 indicates that minimal subspaces with continuous coherences play an important role in determining decoherence-free subsystems. To check if two orthogonal minimal subspaces have continuous coherence, we present the following lemma which is similar to Lemma 1 for stationary coherences.

Lemma 2: Let  $\mathcal{E}$  be a super-operator on  $\mathcal{H}$  with the orthogonal decomposition presented in Eq.(1). For any  $1 \leq p, q \leq m$ ,  $\mathcal{L}(\mathcal{H}_p, \mathcal{H}_q)$  is continuous if and only if there is a unitary matrix U and a real number  $\theta$  such that  $E_{k,p} = e^{i\theta}UE_{k,q}U^{\dagger}$  for all k. Furthermore,  $\mathcal{H}_n \simeq \mathcal{H}_q$ .

k. Furthermore,  $\mathcal{H}_p \simeq \mathcal{H}_q$ . Proof. Assume that  $\mathcal{L}(\mathcal{H}_p,\mathcal{H}_q)$  is continuous; that is, there is a matrix  $A \in \mathcal{L}(\mathcal{H}_p,\mathcal{H}_q)$  such that  $\mathcal{E}(A) = e^{i\theta}A$  for some real number  $\theta$ . Let  $V = e^{-i\theta}P_q + I - P_q$ , where  $P_p$  is the projector onto  $\mathcal{H}_p$ , and  $\mathcal{V} \circ \mathcal{E}(A) = A$  with  $\mathcal{V}(\cdot) = V \cdot V^{\dagger}$ . Moreover, it is obvious that  $\mathcal{H}_p$  and  $\mathcal{H}_q$  are also orthogonal minimal subspaces under  $\mathcal{V} \circ \mathcal{E}$  by the decomposition Eq.(1). Therefore, there is a stationary coherence from  $\mathcal{H}_q$  to  $\mathcal{H}_p$  under  $\mathcal{V} \circ \mathcal{E}$ . From Lemma 1 and the minimal decomposition of  $\mathcal{V} \circ \mathcal{E}$ , we have  $\mathcal{H}_p \simeq \mathcal{H}_q$ , and there exists some unitary matrix U such that that for any k,

$$E_{k,p} = e^{i\theta} U E_{k,q} U^{\dagger}.$$

Conversely, for any p and q let

$$\mathcal{E}_{p,q}(\cdot) = \sum_{k} E_{k,p} \cdot E_{k,q}^{\dagger} = \sum_{k} e^{i\theta} U E_{k,q} U^{\dagger} \cdot E_{k,q}^{\dagger}.$$

Its matrix representation [20] reads

$$M_{p,q} = \sum_{k} e^{i\theta} U E_{k,q} U^{\dagger} \otimes E_{k,q}^{*}$$
$$= e^{i\theta} (U \otimes I) \left( \sum_{k} E_{k,q} \otimes E_{k,q}^{*} \right) (U^{\dagger} \otimes I)$$

As  $\lambda(M_{p,q}) = \lambda(\mathcal{E}_{p,q})$  and  $\sum_k E_{k,q} \otimes E_{k,q}^*$  is the matrix presentation of  $\mathcal{E}_{q,q}$  which is a super-operator and has 1 as one of its eigenvalues, we have  $e^{i\theta} \in \lambda(\mathcal{E}_{p,q})$ .

Corollary 1: Let  $\mathcal E$  be a super-operator on  $\mathcal H$  with the orthogonal decomposition presented in Eq.(1). Then the relation

$$\{(p,q): 1 \leq p, q \leq m, \mathcal{L}(\mathcal{H}_p, \mathcal{H}_q) \text{ is continuous}\}$$

is an equivalence relation. That is, for any p, q, and r,

- (1) (reflexivity)  $\mathcal{L}(\mathcal{H}_p, \mathcal{H}_p)$  is continuous;
- (2) (symmetry) if  $\mathcal{L}(\mathcal{H}_p, \mathcal{H}_q)$  is continuous, then so is  $\mathcal{L}(\mathcal{H}_q, \mathcal{H}_p)$ ;
- (3) (transitivity) if  $\mathcal{L}(\mathcal{H}_p, \mathcal{H}_q)$  and  $\mathcal{L}(\mathcal{H}_q, \mathcal{H}_r)$  are both continuous, then so is  $\mathcal{L}(\mathcal{H}_p, \mathcal{H}_r)$ .

With Corollary 1, we can group together minimal subspaces by continuous coherences and obtain a structure of  $fix(\mathcal{E})$ , in a similar way to Theorem 1 for stationary coherences.

Theorem 4: Let  $\mathcal{E}$  be a super-operator on  $\mathcal{H}$ . There is a unique orthogonal decomposition of  $\mathcal{H}$ 

$$\mathcal{H} = \bigoplus_{l=1}^{L} \mathcal{X}_l \bigoplus \mathcal{K}.$$
 (11)

where

- (1) K is the largest transient subspace;
- (2) each  $\mathcal{X}_l$  is either a minimal subspace or can be further decomposed into mutually orthogonal minimal subspaces with continuous coherences between any two of them:

$$\mathcal{X}_{l} = \bigoplus_{p=1}^{m_{l}} \mathcal{B}_{l,p} = \mathbb{C}^{m_{l}} \bigotimes \mathcal{B}_{l}, \quad \mathcal{B}_{l} \simeq \mathcal{B}_{l,p} \quad \forall p$$
 (12)

such that the Kraus operators  $\{E_k\}$  of  $\mathcal{E}$  have a corresponding block form:

$$E_{k} = \begin{bmatrix} U_{1} \otimes E_{k,1} & & & & \\ & \ddots & & & \\ & & U_{L} \otimes E_{k,L} & \\ \hline & & & & K_{k} \end{bmatrix}$$
(13)

for some operators  $E_{k,l} \in \mathcal{L}(\mathcal{B}_l)$ ,  $K_k \in \mathcal{L}(\mathcal{K})$ ,  $T_k \in \mathcal{L}(\mathcal{K}, \mathcal{K}^\perp)$ , and unitary matrix  $U_l = diag(e^{i\theta_{l,1}}, \cdots, e^{i\theta_{l,m_l}})$  for some real numbers  $\{\theta_{l,p}\}_{p=1}^{m_l}$  on  $\mathbb{C}^{m_l}$ . Moreover,  $\mathcal{B}_l$  is irreducible under  $\mathcal{E}_l = \sum_k E_{k,l} \cdot E_{k,l}^{\dagger}$ . Furthermore,

$$fix(\mathcal{E}) = \bigoplus_{l} [fix(\mathcal{U}_l) \otimes \rho_l] \bigoplus_{l} 0_{\mathcal{K}}$$

where  $\mathcal{U}_l(\cdot) = U_l \cdot U_l^{\dagger}$ .

(3) there is no continuous coherence between any minimal subspaces  $\mathcal{B}_{l,p}$  and  $\mathcal{B}_{l',p'}$  whenever  $l \neq l'$ .

*Proof.* By Theorem 1, there is a unique orthogonal decomposition of  $\mathcal{H}$  as

$$\mathcal{H} = \bigoplus_{l=1}^{L'} \mathcal{X}'_l \bigoplus \mathcal{K}$$

such that for any orthogonal minimal subspaces  $\mathcal{H}_1$  and  $\mathcal{H}_2$ , they have stationary coherences if and only if  $\mathcal{H}_1 \bigoplus \mathcal{H}_2 \in \mathcal{X}'_l$  for some l. Then we divide  $\{\mathcal{X}'_l\}$  into finite disjoint subsets by continuous coherences; that is for any  $l_1 \neq l_2$ , if there is a continuous coherence between any minimal subspaces in  $\mathcal{X}'_{l_1}$  and  $\mathcal{X}'_{l_2}$ , then they are in the same subset. This can be done as the existence of continuous coherences is an equivalence relation by Corollary 1. Then we define  $\{\mathcal{X}_l\}_{l=1}^L$  be the set of the direct sum of all elements in each subset. Therefore,  $\mathcal{H}$  can be uniquely decomposed as  $\mathcal{H} = \bigoplus_l \mathcal{X}_l \bigoplus_l \mathcal{K}$ . Obviously, for any two orthogonal minimal subspaces  $\mathcal{B}_{l_1} \in \mathcal{X}_{l_1}$  and  $\mathcal{B}_{l_2} \in \mathcal{X}_{l_2}$ ,  $\mathcal{L}(\mathcal{B}_{l_1}, \mathcal{B}_{l_2})$  is continuous if and only if  $l_1 = l_2$ .

Furthermore, for each l,  $\mathcal{X}_l$  can be further decomposed to mutually orthogonal minimal subspaces:

$$\mathcal{X}_l = \bigoplus_{p=1}^{m_l} \mathcal{B}_{l,p}$$

By Lemma 2, in an appropriate decomposition of  $\mathcal{X}_l = \bigoplus_{p=1}^{m_l} \mathcal{B}_{l,p} = \mathbb{C}^{m_l} \bigotimes \mathcal{B}_l$  and  $\mathcal{B}_l \simeq \mathcal{B}_{l,p}$  for all p:

(11) 
$$E_k = \begin{bmatrix} U_1 \otimes E_{k,1} & & & & \\ & \ddots & & & T_k \\ & & U_L \otimes E_{k,L} & \\ \hline & 0 & & K_k \end{bmatrix}$$
 (14)

and  $\mathcal{B}_l$  is irreducible under  $\mathcal{E}_l := \sum_k E_{k,l} \cdot E_{k,l}^{\dagger}$  for all l, where  $U_l = diag(e^{i\theta_{l,1}}, \cdots, e^{i\theta_{l,m_l}})$  for a set of real numbers  $\{\theta_{l,p}\}_{p=1}^{m_l}$ . From Theorem 1 and noting that stationary coherences is continuous, we have that

$$fix(\mathcal{E}) = \bigoplus_{l} [fix(\mathcal{U}_l) \otimes \rho_l] \bigoplus 0_{\mathcal{K}}.$$

where  $\rho_l$  is the unique stationary state of  $\mathcal{E}_l$ .

Corollary 2: Let  $\mathcal{E}$  be a super-operator on  $\mathcal{H}$ . In a decomposition of  $\mathcal{H}$  in Eq.(12):

$$\mathcal{H} = \bigoplus_{l} (\mathbb{C}^{m_l} \bigotimes \mathcal{B}_l) \bigoplus \mathcal{K},$$

for any minimal subspace  $\mathcal{H}'$ , there is a pure state  $|\psi\rangle \in \mathbb{C}^{m_l}$ for some l such that  $\mathcal{H}' = \text{supp}(|\psi\rangle\langle\psi|) \otimes \mathcal{B}_l$ .

The above theorem shows minimal subspaces with continuous coherences can construct decoherence-free subsystem  $\mathbb{C}^{m_l}$ . Fortunately, we can further show that others are subspaces of the decoherence-free subsystems constructed in Eq.(12).

Theorem 5: Let  $\mathcal{E}$  be a super-operator on  $\mathcal{H}$  with the unique decomposition:

$$\mathcal{H} = \bigoplus_{l} (\mathbb{C}^{m_l} \bigotimes \mathcal{B}_l) \bigoplus \mathcal{K},$$

presented in Theorem 4. Then subsystem  $\mathcal{H}_A$  is decoherencefree if and only if

- (1)  $\mathcal{H}_A \subseteq \mathbb{C}^{m_l}$  for some l; (2)  $\mathcal{H}_A$  is a support of some stationary state of  $\mathcal{U}_l(\cdot) = U_l \cdot$

where  $U_l$  is the corresponding unitary matrix on  $\mathbb{C}^{m_l}$  in the decomposition Eq.(13).

*Proof.* Assume that  $\mathcal{H}_A$  is decoherence-free. By Theorem 4 and Corollary 2,  $\mathcal{H}_A \subseteq \mathbb{C}^{m_l}$  for some l. From the definition of decoherence-free subsystems and the restriction of  ${\mathcal E}$  onto  $\mathbb{C}^{m_l}$  being  $\mathcal{U}_l$ ,  $\mathcal{H}_A$  is a decoherence-free subspace under  $\mathcal{U}_l$ and  $\mathcal{U}(P_A) = P_A$ , where  $P_A$  be the projector onto  $\mathcal{H}_A$ .

To prove the other direction, we observe that if  $\mathcal{H}_A$  is a support of some stationary state of  $U_l$ , then  $P_A U_l P_A =$  $P_A U_l = U_l P_A$ . Thus  $\mathcal{H}_A$  is a decoherence-free subspace under  $U_l$ . The rest of the proof is direct from Theorem 4.

This theorem confirms that the set of decoherence-free subsystems  $\{\mathbb{C}^{m_l}\}_l$  identified in Theorem 4 is optimal; that is any other decoherence-free subsystem is a subspace of one of them. So we only need to implement the decompositions in Theorem 4 and all decoherence-free subsystems can be easily found by Theorem 5.

One easy way of achieving this is to first transform all continuous coherences to stationary ones, and then use NSDecompose( $\mathcal{H}, \mathcal{E}$ ) proposed already in the literature.

For any two operators  $E_{k,p}$  and  $E_{k,q}$  in Eq.(13) of Theorem 4, if they are unitarily equivalent with a phase  $\theta$ , i.e.  $E_{k,p} \simeq e^{i\theta} E_{k,q}$ , then let  $E'_{k,q} = e^{i\theta} E_{k,q}$  and  $E'_{k,p} = E_{k,p}$ . Then  $E'_{k,p}$  is unitarily equivalent to  $E'_{k,q}$ ; a continuous coherence is transformed to be stationary. Using this method, we develop Algorithm 1 to implement decompositions in Theorem 4 and the time complexity is  $O(n^8)$ , where dim $(\mathcal{H}) = n$ .

```
Algorithm 1 Decompose(\mathcal{H}, \mathcal{E})
```

```
Input: A Hilbert space \mathcal{H} and a super-operator \mathcal{E} with Kraus
      operators \{E_k\}_{k=1}^d on it
Output: The two-level decomposition of \mathcal{H} in the form of
       Eqs.(11) and (12).
      \begin{split} \{\mathbb{C}^{m_l}\}_{l=1}^{L}, \{\mathcal{B}_l\}_{l=1}^{L}, \mathcal{K} \leftarrow \text{NSDecompose}(\mathcal{H}, \mathcal{E}) \\ \left\{ \begin{bmatrix} \oplus_{l=1}^{L} I_l \otimes E_{k,l} & T_k \\ 0 & K_k \end{bmatrix} \right\}_{k=1}^{d} \leftarrow \text{NSDecompose}(\mathcal{H}, \mathcal{E}) \end{split}
      for each p \leftarrow 1 to L do
            if p \in \mathcal{L} then
                   for each q \leftarrow p+1 to L with q \in \mathcal{L} do
                          M\leftarrow \bar{\sum}_k \bar{E}_{k,p}\otimes E_{k,q}^* if \lambda(M) has one element with magnitude one then
                                \begin{array}{l} \theta \leftarrow \operatorname{tr}(E_{k,p})/\operatorname{tr}(E_{k,q}) \\ E_{k,q} \leftarrow e^{i\theta}E_{k,q} \\ \mathcal{L} \leftarrow \mathcal{L} \setminus \{q\} \end{array}
                   end for
            end if
      end for
      \begin{array}{c} \mathbf{for} \ \ \mathrm{each} \ \underset{}{k \leftarrow 1} \ \underset{l=1}{\text{to}} \ \underset{l}{d} \mathbf{do} \\ E_k \leftarrow \begin{bmatrix} \oplus_{l=1}^L I_l \otimes E_{k,l} & T_k \\ 0 & K_k \end{bmatrix} \\ \end{array} 
      end for
```

Now we back to see Example 1. By Algorithm 1, we can confirm that the first subsystem  $\mathcal{H}_A \simeq \mathbb{C}^4$  is decoherencefree and further compute that the evolution on it is  $|0\rangle\langle 0|$  +  $|1\rangle\langle 1|-|2\rangle\langle 2|-|3\rangle\langle 3|$ . Thus we can store 4-qubit information in this subsystem, which doubles the capacity of noiseless subsystems.

**return** NSDecompose( $\mathcal{H}, \{E_k\}_{k=1}^d$ )

#### V. IMPERFECT INITIALIZATION

In the last section, we have developed techniques to find all decoherence-free subsystems under perfect initialization. In this section, we plan to find counterparts under imperfect initialization. These subsystems are more useful in experiments.

In perfect initialization, the co-subsystem of a decoherencefree subsystem is not important, but it plays an essential role when we allow imperfect initialization. Choosing an appropriate co-subsystem for a candidate of decoherence-free subsystems is an natural problem.

Theorem 6: Assume imperfect initialization. Let  $\mathcal{E}$  be a super-operator on  ${\cal H}$  with unique decomposition

$$\mathcal{H} = \bigoplus_{l} (\mathbb{C}^{m_l} \bigotimes \mathcal{B}_l) \bigoplus \mathcal{K},$$

presented in Eq.(12). For any l and  $\mathcal{H}_A \subseteq \mathbb{C}^{m_l}$ , if  $\mathcal{H}_A$  with co-subsystem  $\mathcal{B}_l$  is not decoherence-free, then there are no non-trial co-subsystems for  $\mathcal{H}_A$  such that  $\mathcal{H}_A$  is decoherencefree, where  $\mathcal{H}_B$  a trial co-subsystem if  $\mathcal{H} = \mathcal{H}_A \bigotimes \mathcal{H}_B$ .

*Proof.* It is easy to observe that any co-subsystem  $\mathcal{H}_B$  (can not to be irreducible) of  $\mathcal{H}_A$  must satisfy  $\mathcal{B}_l \subseteq \mathcal{H}_B$  from Corollary 2.

Obviously, if  $\mathcal{H}_A$  is decoherence-free in  $\mathcal{H}=\mathcal{H}_A \bigotimes \mathcal{H}_B \bigoplus \mathcal{Y}$  with  $\mathcal{Y}=(\mathcal{H}_A \bigotimes \mathcal{H}_B)^{\perp} \neq \emptyset$ , then  $\mathcal{H}_A$  is also decoherence-free in  $\mathcal{H}=\mathcal{H}_A \bigotimes \mathcal{B}_l \bigoplus \mathcal{K}'$ , as  $\mathcal{H}_A \bigotimes \mathcal{B}_l \subseteq \mathcal{H}_A \bigotimes \mathcal{H}_B$ .

The above theorem tells us a fact that the co-subsystems identified in Eq.(12) are sufficient to determine whether a subsystem is decoherence-free or not under imperfect initialization. For example, in Example 1, we can get a decoherence-free subsystem  $\mathcal{H}_A$  and the co-subsystem  $\mathcal{H}'$  under perfect initialization from Algorithm 1. Then through Theorem 6, we can use the co-subsystem  $\mathcal{H}'$  to verify that  $\mathcal{H}_A$  is decoherence-free with trial co-subsystem  $\mathcal{H}_B$  under imperfect initialization.

# VI. AN APPLICATION TO BASIS OF MATRIX PRODUCT STATES

Describing quantum many body systems is not scalable due to the exponential growth of the Hilbert space dimension with the number of subsystems. Matrix Product States (MPS), a special case of tensor networks (a theoretical and numerical tool describing quantum many-body systems), have proven to be a useful family of quantum states for the description of ground states of one-dimensional quantum many-body systems [14].

Given a tensor  $\mathcal{A} = \{A_k \in \mathcal{M}_D\}_{k=1}^d$  with a Hilbert space  $\mathcal{H}_d = \text{lin.span}\{|k\rangle\}_{k=1}^d$ , where  $\mathcal{M}_D$  denotes  $D \times D$  complex matrices, it generates a family of translationally invariant MPS, namely

$$V(\mathcal{A}) = \{ |V_n(\mathcal{A})\rangle \}_{n \in \mathbb{N}^+},$$

where

$$|V_n(\mathcal{A})\rangle = \sum_{k_1, \dots, k_n = 1}^d \operatorname{tr}(A_{k_1} \dots A_{k_n}) |k_1 \dots k_n\rangle \in \mathcal{H}_d^{\otimes n}$$

Here, each  $|V_n(\mathcal{A})\rangle$  corresponds to a state of n spins of physical dimension d. Then we can define an associated completely positive map  $\mathcal{E}_{\mathcal{A}}(\cdot) = \sum_{k=1}^d A_k \cdot A_k^{\dagger}$ .

By [15], we can always find a set of irreducible tensors  $\{A_j\}_{j=1}^m$  with the same Hilbert space  $\mathcal{H}_d$ , and a set of complex number  $\{\mu_j\}_{j=1}^m$  such that for any  $n \in \mathbb{N}^+$ 

$$|V_n(\mathcal{A})\rangle = \sum_{j=1}^m \mu_j^n |V_n(\mathcal{A}_j)\rangle$$
 (15)

where a tenor is called irreducible if the associated map is CPTP and irreducible. That is for any tensor  $\mathcal{A}$ , the generated MPS can be linearly represented by MPS of a set of irreducible tensors. Therefore, studying irreducible tensors is an interesting problem, especially the conditions allowing two tensors describing the same family of MPS. First, we can group irreducible tensors that are essentially the same in the following sense.

Definition 3 ([15]): We say that two irreducible tensors with the same Hilbert space  $\mathcal{H}_d$ , say  $\mathcal{A} = \{A_k\}_{k=1}^d$  and  $\mathcal{B} = \{B_k\}_{k=1}^d$ , are repeated if there exist a phase  $\theta$  and a unitary matrix U so that

$$A_k = e^{i\theta} U B_k U^{\dagger} \ \forall k$$

By the definition,  $\mathcal{A}$  and  $\mathcal{B}$  are repeated, then  $|\mathcal{A}\rangle_n = e^{in\theta}|\mathcal{B}\rangle_n$  for all  $n \in \mathbb{N}^+$ . Therefore, for any tensor  $\mathcal{A}$ , we can reduce the set of irreducible tensors in Eq.(15) to be non-repeated. Such a simplified set is called a basis of  $\mathcal{A}$ .

Many results obtained for MPS rely on the basis. The fundamental problem of MPS is to relate different tensors rising the same MPS: for any two different tensors  $\mathcal{A}$  and  $\mathcal{B}$ , they can generate the same MPS, i.e.  $V(\mathcal{A}) = V(\mathcal{B})$ , which introduces an ambiguity for analyzing many-body states by MPS generated by tensors. This problem can be answered by the basis. That is, if  $\mathcal{A}$  and  $\mathcal{B}$  have the same MPS, then their basis must be related by a unitary transform [15]. Therefore, determining whether two irreducible tensors are repeated or not is a key problem. Even though such repeatability relation can be verified by Jordan decomposition of matrices by the definition, Jordan decomposition is sensitive to errors and should be avoided in numerical analysis. Here we propose a feasible method to achieve this by the results of continuous coherences in previous sections.

Theorem 7: Given two irreducible tensors with the same Hilbert space  $\mathcal{H}_d$ ,  $\mathcal{A} = \{A_k\}_{k=1}^d$  and  $\mathcal{B} = \{B_k\}_{k=1}^d$ , they are repeated if and only if  $\lambda(\mathcal{E}_{\mathcal{A},\mathcal{B}})$  has an element with magnitude one, where  $\mathcal{E}_{\mathcal{A},\mathcal{B}} = \sum_{k=1}^d A_k \cdot B_k^{\dagger}$ .

*Proof.* Let  $\mathcal{H}_{\mathcal{A}}$  and  $\overline{\mathcal{H}_{\mathcal{B}}}$  be the corresponding Hilbert spaces of tensors  $\mathcal{A}$  and  $\mathcal{B}$ , respectively; that is  $A_k \in \mathcal{L}(\mathcal{H}_{\mathcal{A}})$  and  $B_k \in \mathcal{L}(\mathcal{H}_{\mathcal{B}})$  for all k. Then the Hilbert space of  $\mathcal{E}$  is  $\mathcal{H}_{\mathcal{A}} \bigoplus \mathcal{H}_{\mathcal{B}}$ , where  $\mathcal{E}$  is a super-operator with Kraus operators  $\{diag(A_k, B_k)\}_{k=1}^d$ . Obviously,  $\mathcal{H}_{\mathcal{A}}$  and  $\mathcal{H}_{\mathcal{B}}$  are both minimal subspaces under  $\mathcal{E}$ . Then the result is direct from Lemma 2.

By the above theorem, repeatability can be easily checked by computing eigenvalues of a linear map, which is a linear algebra exercise.

# VII. CONCLUSION

In this paper, we established a structure theory for decoherence-free subsystems. Consequently, an algorithm for finding an optimal set of decoherence-free subsystems under perfect initialization has been developed. Then we gave a simple way to pick up the faulty-tolerant decoherence-free subsystems. After that, these results helped us find a basis for any tensor by computing the eigenvalues of some constructed linear maps.

For future studies, an immediate topic is to generalize our results to continuous-time quantum systems. In [21], authors studied this in quantum control setting and expected to obtain a linear-algebraic approach for finding all decoherence-free subsystems for a given generator, describing the system.

# ACKNOWLEDGMENT

The authors would like to thank...

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