Decoherence-free subspaces for multiple-qubit errors. I. Characterization

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Coherence in an open quantum system is degraded through its interaction with a bath. This decoherence can be avoided by restricting the dynamics of the system to special decoherence-free subspaces. These subspaces are usually constructed under the assumption of spatially symmetric system-bath coupling. Here we show that decoherence-free subspaces may appear without spatial symmetry. Instead, we consider a model of system-bath interactions in which to first order only multiple-qubit coupling to the bath is present, with single-qubit system-bath coupling absent. We derive necessary and sufficient conditions for the appearance of decoherence-free states in this model, and give a number of examples. In a sequel paper we show how to perform universal and fault tolerant quantum computation on the decoherence-free subspaces considered in this paper.

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I. INTRODUCTION

Quantum information must be protected against the detrimental effects of decoherence [1,2]. To this end decoherence-free subspaces (DFSs) [3–10] have recently been proposed, alongside quantum error correcting codes (QECCs) [11–14] and “dynamical decoupling” and symmetrization schemes [15–18]. A DFS is a “quiet corner” of the system’s Hilbert space, where the evolution is decoupled from the bath and thus is entirely unitary. DFSs are a special class of (fully degenerate) QECCs [9], so in order to properly distinguish between DFSs and all other QECCs we note that DFSs are passive codes, in that the information encoded in them may not require any active stabilization procedures [19,20]. All other QECCs, in contrast, always involve an active error detection/correction process. Examples of DFSs have so far focused almost exclusively on the presence of a permutation symmetry of some sort in the system-bath coupling. The most often used example is that of “collective decoherence” [3–5,8,21], where the bath couples in an identical fashion to all qubits, implying that all qubits undergo the same error. In this case four physical qubits suffice to encode a logical qubit against any collective error, and the code efficiency (number of encoded per physical qubits) approaches unity asymptotically [5]. It has been shown that the requirement of an exact symmetry can be lifted by allowing for a symmetry-breaking perturbation, without spoiling the DFS property significantly [8,10]. Moreover, by concatenation with an active QECC, a symmetry-broken DFS can be stabilized completely [9]. While these results indicate that a small departure from the exact symmetry condition for the system-bath coupling is admissible, they leave unanswered the question of whether a DFS may exist when no assumptions are made regarding the spatial symmetry of this coupling.

In this paper, the first of two, it will be shown that under conditions that do not relate to a spatially symmetric system-bath coupling DFSs may still exist. This result is exact, i.e., it is not of a perturbative nature as in Refs. [8–10]. Instead, it relies on the assumption that errors affecting single qubits are absent, and to lowest order only multiple-qubit errors are possible instead. Formally, the condition is that the qubit register is not affected by the full Pauli group of errors, but only by a subgroup thereof. One may then proceed to find DFSs with respect to this subgroup. The interesting class of system-bath interaction Hamiltonians that allow for such processes generally involve only multiple-qubit operators. Relevant physical systems are therefore those where the bath can couple only to multiple system excitations as is the case for decoherence due to dipolar coupling, e.g., in NMR [22]. Another interesting class of examples are composite particles, such as biexcitons in quantum dots/wells [23], or Cooper pairs in superconductors [24].

The structure of this paper is as follows. In Sec. II we briefly review the structure of Hamiltonians pertinent to systems that may function as quantum computers, coupled to a decohering environment. Using these Hamiltonians, we recall in Sec. III the derivation of the operator sum representation evolution equation for the system density matrix. We show in particular that for a qubit system the evolution can be expressed entirely in terms of linear combinations of tensor products of Pauli matrices. We then use this in Sec. IV to derive the DFS condition under the assumption that decoherence is the result of a subgroup of the Pauli group. In Sec. V we illustrate our general analysis with some examples, and find decoherence-free states for a number of subgroups. We derive the dimension of these DFSs in Sec. VI. Conclusions and a summary are presented in Sec. VII. Finally, some important properties of the Pauli group are summarized in Appendix A, and some examples of “nongeneric” DFSs are presented in Appendix B. We show in a following paper [25] how to perform universal fault tolerant quantum computation using at most two-body Hamiltonians on the DFSs derived here.

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II. STRUCTURE OF THE HAMILTONIAN FOR A UNIVERSAL QUANTUM COMPUTER COUPLED TO A BATH

This section provides a brief review of the structure of Hamiltonians relevant for a qubit system allowing for universal quantum computation and coupled to a decohering bath.

The dynamics of a quantum system $S$ coupled to a bath $B$ (which together form a closed system) evolves unitarily under the combined Hamiltonian

$$H = H_S \otimes I_B + I_S \otimes H_B + H_J,$$

where $H_S$, $H_B$, and $H_J$ are the system, bath, and interaction Hamiltonians, respectively; $I$ is the identity operator. Let $\sigma^\alpha_i$ denote the $\alpha$th Pauli matrix, $\alpha = \{0, x, y, z\}$, acting on qubit $i$. The $2 \times 2$ identity matrix is denoted $\sigma^I_i$. For $K$ qubits the components of $H$ can often be written as follows:

$$H_S = \sum_{i=1}^{K} \sum_{\alpha=x, y, z} \epsilon_i^\alpha \sigma_i^\alpha + \sum_{i < j} J_{ij} \sigma_i^x \sigma_j^x + \text{H.c.},$$

where $\sigma^\pm_i = (\sigma^x_i \mp i \sigma^y_i)/2$. The first sum contains the qubit energies ($\epsilon_i^\alpha$) and tunneling elements ($\epsilon_{ij}^\alpha$) [26], and the second sum expresses tunneling between sites $i$ and $j$. Other forms are also possible, e.g., in an anisotropic dipolar medium such as solid state NMR [22], where one would typically encounter an Ising $J_{ij} \sigma_i^x \sigma_j^x$ term. A Hamiltonian of the form above is sufficiently general to allow for universal quantum computation by satisfying the following two requirements [27–29]. (i) Arbitrary single-qubit operations are made possible by the presence of $\sigma^z_i$, which allows for the implementation of a continuous SU(2) rotation in the $i$th qubit Hilbert space, while the $\sigma^x_i$ term allows for the introduction of an arbitrary phase shift between the $|0\rangle$ and $|1\rangle$ states. When $\sigma^z_i$ and $\sigma^x_i$ are exponentiated, they can be combined, using the Lie sum and product formulas [30]

$$\lim_{n \to \infty} (e^{i\alpha A/n} e^{i\beta B/n})^n = e^{i(\alpha A + \beta B)},$$

$$\lim_{n \to \infty} (e^{i\alpha A} e^{i\beta B} e^{-i\alpha A} e^{-i\beta B})^n = e^{i[A,B]},$$

(2.3)

to close the Lie algebra su(2), and thus to construct any evolution in the Lie group SU(2) of all possible operations on a single qubit [28]. (ii) The second ingredient needed for universal quantum computation is the controlled-not (CNOT) gate, which is made possible through the ability to implement each of the (nearest neighbor) $(J_{ij} \sigma_i^x \sigma_j^x + \text{H.c.})$ terms. When exponentiated, such a term yields

$$U_J = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos \theta & i \sin \theta & 0 \\ 0 & i \sin \theta & \cos \theta & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

with $\theta \propto J_{ij}t$. For $\theta = \pi/4$ this is (up to a phase) the ‘‘square-root-swap’’ operation, which when combined with single-qubit rotations allows for the implementation of CNOT. Alternatively, a $J_{ij} \sigma_i^x \sigma_j^x$ term alone is sufficient, since it can be used to implement a controlled phase shift, as is done routinely in NMR [31]. It is important to emphasize that the universal gate construction just described is but one of many different ways to achieve universal quantum computation. In fact, universal gates implementing logic operations directly on physical qubits (as above) are generally inappropriate for the purpose of fault tolerant computation [32]. We consider a different gate construction in the sequel paper [25], operating instead on ‘‘encoded’’ qubits, which can be used to implement universal fault tolerant quantum computation. For a useful survey of different universal and fault tolerant sets of gates, see Ref. [33].

The bath Hamiltonian can be written as

$$H_B = \sum_k \omega_k B_k,$$

where, e.g., for the spin-boson Hamiltonian, $B_k = b_k^\dagger b_k^\alpha$ [26], and $b_k^\dagger$ and $b_k$ are, respectively, creation and annihilation operators of bath mode $k$.

Finally, the system-bath interaction Hamiltonian is

$$H_J = \sum_{i=1}^{K} \sum_{\alpha=+, c} \sum_{\lambda=1}^{K} g_{ik}^\alpha \sigma_i^\alpha \otimes B_k^\lambda,$$

(2.5)

where $g_{ik}^\alpha$ is a coupling coefficient. In the spin-boson model one would have $B_k^\alpha = b_k^\dagger b_k$, $B_k^i = b_k^i$, and $B_k^\lambda = b_k^\dagger + b_k$. Thus $\sigma_i^\alpha \otimes B_k^\lambda$ expresses a dissipative coupling (in which energy is exchanged between system and environment), and $\sigma_i^\alpha \otimes B_k^\lambda$ corresponds to a phase damping process (in which the environment randomizes the system phases, e.g., through elastic collisions).

An interesting limiting case arises when the coupling constants are independent of the qubit index: $g_{ik}^\alpha = g_{ik}$. This situation, known as ‘‘collective decoherence,’’ arises when there is full permutational symmetry of qubit positions, and implies the existence of a large DFS [5,21]. Defining collective system operators $S_i^\alpha = \sum_{i=1}^{K} \sigma_i^\alpha$, one can then express the interaction Hamiltonian in greatly simplified form as

$$H_J^{\text{coll}} = \sum_{\alpha=+, c} \sum_{\lambda=1}^{K} S_i^\alpha \otimes \left( \sum_k g_{ik}^\alpha B_k^\lambda \right).$$

(2.6)

A case of intermediate symmetry arises when the coupling constants are equal not over the entire qubit register but rather only over finite clusters $j = 1–C$. One can then define cluster system operators $S_i^\alpha = \sum_{i=1}^{K_j} \sigma_i^\alpha$, where $K_j$ is the number of qubits in cluster $j$. The interaction Hamiltonian becomes

$$H_J^{\text{clus}} = \frac{C}{\sum_{i=1}^{C} \sum_{\alpha=+, c} \sum_{\lambda=1}^{K_j} S_i^\alpha \otimes \left( \sum_k g_{ijk}^\alpha B_k^\lambda \right).$$

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In this case too DFSs can be found. The point we wish to emphasize presently is that the underlying assumption in cluster decoherence is that of spatial symmetry in the system-bath coupling. This is to be contrasted with the decoherence models studied in this paper, where DFSs will be shown to arise without the need for spatial symmetry.

Returning to the general case, \( H_f \) can be rewritten as

\[
H_f = \sum_{i=1}^{K} \sum_{a=x,y,z} \sum_{k} \sigma_i^a \otimes B_{ik}^a,
\]

where \( B_{ik}^x = B_{ik}^+ \) and \( B_{ik}^y, B_{ik}^z \) are appropriate linear combinations of \( B_{ik}^+ \) and \( B_{ik}^- \):

\[
B_{ik}^x = \frac{1}{2} (g_{ik}^x B_k^x + g_{ik}^y B_k^y),
\]

\[
B_{ik}^y = \frac{i}{2} (g_{ik}^x B_k^x - g_{ik}^y B_k^y).
\]

The qubit-coupling term in \( H_f \) can also be expressed entirely in terms of \( \sigma_i^a \), where \( a = x, y, \) or \( z \). Thus all system components of the Hamiltonian \( H \) can be expressed in terms of tensor products of the single-qubit Pauli matrices.

III. TIME EVOLUTION OF THE DENSITY MATRIX

The purpose of this section is to show that the evolution of the density matrix of an open system can be expanded in terms of tensor products of the Pauli matrices (the Pauli group), and that this follows from the structure of the Hamiltonians assumed above for a qubit register. This result is obvious from a formal mathematical point of view (since the elements of the Pauli group of order \( K \) form a complete orthogonal set for the \( 2^K \times 2^K \) matrices) [34], so that the reader for whom this type of argument is satisfactory may safely skip ahead to the next section. We present the derivation of this result here in order to motivate the appearance of the multiple-qubit errors that are the subject of this paper.

We first transform to the interaction picture [35] defined by the system and bath Hamiltonians:

\[
H \rightarrow H(t) = U_{SB}(t)H U_{SB}^\dagger(t) = H_S \otimes I_B + I_S \otimes H_B + H_f(t),
\]

where

\[
U_{SB}(t) = \exp[-(H_S \otimes I_B + I_S \otimes H_B)it/\hbar] = \exp[-itH_S/\hbar] \otimes \exp[-itH_B/\hbar] = U_S(t) \otimes U_B(t).
\]

Because the system and bath operators commute, the interaction picture interaction Hamiltonian can be written as

\[
H_i(t) = U_{SB}(t)H_f U_{SB}^\dagger(t) = \sum_{i=1}^{K} \sum_{a=x,y,z} \sum_{k} \sigma_i^a(t) \otimes B_{ik}^a(t),
\]

where

\[
\sigma_i^a(t) = U_S(t)\sigma_i^a U_S^\dagger(t) = \sum_{j,B} \lambda_{ij}^{aB}(t)\sigma_j^B,
\]

\[
B_{ik}^a(t) = U_B(t)B_{ik}^a U_B^\dagger(t)
\]

[see, e.g., Ref. [35] for an explicit calculation of the \( \lambda_{ij}^{aB}(t) \) for some examples]. The system-bath density matrix is transformed accordingly from the Schrödinger into the interaction picture (denoted by a prime):

\[
\rho_{SB}(t) \rightarrow \rho_{SB}^{'}(t) = U_{SB}^\dagger(t)\rho_{SB}(t)U_{SB}(t),
\]

and the full dynamics is

\[
\rho_{SB}^{'}(t) = U(t) \rho_{SB}^{'}(0) U(t)^\dagger,
\]

where

\[
U(t) = \mathcal{T} \exp \left[-\frac{i}{\hbar} \int_0^t H_i(\tau)d\tau \right]
\]

and \( \mathcal{T} \) is the Dyson time-ordering operator (defined explicitly below). From now on we work in the interaction picture only, so for notational simplicity the prime is dropped from the density matrices. At \( t = 0 \) the Schrödinger and interaction pictures coincide. Thus, assuming that system and bath are initially decoupled so that \( \rho_{SB}(0) = \rho_S(0) \otimes \rho_B(0) \), where \( \rho \) and \( \rho_B \) are, respectively, the system and bath density matrices, the system dynamics is described by the reduced density matrix

\[
\rho(t) = Tr_B\{U(t)[\rho(0) \otimes \rho_B(0)]U^\dagger(t)\}.
\]

Here \( Tr_B \) is the partial trace over the bath. By using a spectral decomposition for the bath, \( \rho_B(0) = \sum_n p_n |n\rangle \langle n| \), this can be rewritten in the “operator sum representation” [10,36–38]:

\[
\rho(t) = \sum_d A_d(t)\rho(0)A_d^\dagger(t)
\]

where

\[
A_d(t) = \sqrt{p_d} \mu |U(t)| \nu, \quad d = (\mu, \nu).
\]

Also, by unitarity of \( U \), one derives the normalization condition,

\[
\sum_d A_d^\dagger A_d = I_S,
\]

which guarantees preservation of the trace of \( \rho \):

\[\text{Tr}\{U(t)[\rho(0) \otimes \rho_B(0)]U^\dagger(t)\} = \text{Tr}\{\rho_S(t)\} \geq 1 \]

1For a bath in thermal equilibrium, \( |\nu\rangle \) would be an energy eigenstate with energy \( E_\nu \), and \( p_\nu = \exp(-\beta E_\nu)Z \), where \( \beta \) is the inverse temperature and \( Z = \text{Tr}\{\exp(-\beta H_B)\} \) is the canonical partition function.
qubits. The integration and time-ordering operation will not

\[ \text{Tr}[\rho(t)] = \text{Tr} \left[ \sum_d A_d \rho(0) A_d^\dagger \right] \]

\[ = \text{Tr} \left[ \rho(0) \sum_d A_d^\dagger A_d \right] \]

\[ = \text{Tr}[\rho(0)]. \quad (3.10) \]

The \( \{A_d\} \), called the Kraus operators, belong to the (Banach
or Hilbert-Schmidt) space \( \mathcal{B}(\mathcal{H}) \) of bounded operators acting
on the system Hilbert space, and for \( K \) qubits are represented by \( 2^K \times 2^K \) matrices, just like \( \rho \).

Consider now a formal Taylor expansion of the propagator:

\[ U(t) = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} T \left( \int_0^t H_j(\tau) d\tau \right)^n \]

\[ = I + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_0^t dt_n \int_0^t dt_{n-1} \cdots \int_0^t dt_1 \]

\[ \times T\{H_i(t_1) \cdots H_i(t_n)\} \]

\[ = I + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} U_n(t). \quad (3.11) \]

The Dyson time-ordered product is defined with respect to
any set of operators \( O_i(t_i) \) as [39]

\[ T\{O_i(t_1) \cdots O_n(t_n)\} = O_{t_1}(t_1) \cdots O_{t_n}(t_n) \]

\[ (t_1 > t_2 > \cdots > t_n). \]

Using Eq. (2.6) we have for the terms in the above sum

\[ \prod_{j=1}^n H_j(t_j) = \sum_{i=1}^K \sum_{\alpha=x,y,z} \sum_{k} \otimes_{j=1}^n \alpha_{ij}(t_j) \otimes_{j=1}^n B_{ij}(t_j), \]

where \( i = \{i_1, i_2, \ldots, i_n\} \), \( \alpha = \{\alpha_1, \alpha_2, \ldots, \alpha_n\} \), and \( k \)
\( = \{k_1, k_2, \ldots, k_n\} \). The important point to notice in this
complicated expression is that, after taking the bath matrix
elements \( \langle \mu| \cdots |\nu \rangle \) [because of Eq. (3.8)], one is left with
all possible tensor products \( \otimes_{j=1}^n \alpha_{ij}(t_j) \) over \( n \) out of \( K \)
qubits. The integration and time-ordering operation will not
change this conclusion. Thus, using the expansion of \( \alpha_i(t) \)
in Eq. (3.3), after a time \( O(t^K) \) one finds the tensor product
\( \otimes_{j=1}^n \alpha_{ij}(t_j) \), i.e., \( n \) qubits are involved (here \( \alpha_j = 0 \),
corresponding to the identity matrix, is allowed). At this point the
entire Pauli group \( P_K \) appears (all possible \( 4^{K+1} \) tensor
products of the three Pauli matrices and the identity matrix, and
the four roots of unity \( \{\pm, \pm i\} \)--see Appendix A), and one
has “complete decoherence,” i.e., multiple-qubit errors over
the entire system Hilbert space. In the usual approach to

\[ \text{QEC} \] one does not consider such high orders in time since one assumes that error correction can be done quickly
enough. Instead the error analysis is usually confined to time
evolution to \( O(t) \) only, which leads to “independent decoherence,” i.e., single-qubit errors affecting only one qubit at a time.\(^3\) It is possible to use multiple-error-correcting quantum
codes for \( O(t^n) \) with arbitrary \( n \), but these codes are rather unwieldy (i.e., the number of encoding qubits becomes
large). In the case of “burst errors” (a spatially contiguous cluster of errors such as \( 1 \cdots IX \cdots XI \cdots I \)) some particularly efficient codes are known [41].

On the other hand, a DFS that exists by virtue of a spatially
symmetric system-bath coupling is not affected by this
proliferation of errors, which all occur in the subspace
orthogonal to the DFS [9]. The assumption of spatial symmetry
manifests itself in restrictions on the coefficients \( g_{ik} \) appearing
in the interaction Hamiltonian [Eq. (2.5)]. For example, as
mentioned above, collective decoherence corresponds to the
condition \( g_{ik} = g_{ik}^* \forall i \), i.e., the bath cannot distinguish
between the qubits [5]. In this paper no such spatial symmetry
assumptions will be made. Instead, only multiple-qubit errors
will be allowed to lowest order instead of single-qubit errors.
This condition will be defined more precisely in the next
section.

As for the Kraus operators, it can be seen from the calcula-
tions above that they may be expanded as sums over tensor
products of the Pauli matrices:

\[ A_{d}(t) = \sum_{n=1}^{4^{K+1}} a_{d,n}(t) p_n, \quad (3.12) \]

where \( p_n \in P_K \). The Kraus operators thus belong to the
\text{group algebra} (the space of linear combinations of group
elements) of \( P_K \) [42]. As alluded to in the beginning of this
section, that this expansion is possible actually follows simply
from the fact that the Pauli group forms a complete orthog-
onal set (with respect to the trace inner product) for the
expansion (with complex coefficients) of arbitrary \( 2^K \times 2^K \)
mats. However, here we have seen how the expansion in
terms of the Pauli group (rather than some other basis) is
physically motivated by virtue of the structure of the Hamil-
tonian.

A simple example will now serve to illustrate the point
made above about multiple-qubit errors. Consider an interac-
tion Hamiltonian of the form \( H_i = \sum_{j=1}^4 \sigma_j^i \otimes B_j \) (on two
qubits). Some algebra suffices to show that then \( A_d(t) =
\sum_{\tau} \sigma_j^i (t) \otimes B_j \) (on two qubits). In this case
the single-qubit errors \( \sigma_j^i, \sigma_j^z \) appear, as well as the
multiple-qubit error \( \sigma_j^x \sigma_j^z \). This situation does not allow for
the appearance of DFSs (unless spatial symmetry is present).
Alternatively, consider the interaction Hamiltonian \( H_i = \sum_{j=1}^4 \sigma_j^i \)
(on four qubits). In this case one finds \( A_d(t) = \sum_{\tau} \sigma_j^i (t) \otimes B_j \) (on four qubits). In this case
one finds \( A_d(t) = \sum_{\tau} \sigma_j^i (t) \otimes B_j \) (on four qubits). Thus only multiple-qubit terms

\(^3\)In fact, spatially correlated errors can also be dealt with by

QECCs [40].
appear, and, as will be shown below, this allows for the existence of nontrivial DFSs, even though no spatial symmetry assumptions were made.

An important example of this correlated type of system-bath interaction is the dipolar-coupling Hamiltonian, relevant, e.g., to decoherence resulting from spin-rotation coupling in NMR [22]. The dipolar Hamiltonian for a system of spins interacting with a bath of rotations is

\[ H_j = \sum_{j,k} \frac{\gamma_j \gamma_k}{r_{jk}} \left[ \mathbf{\mathbf{\sigma}_j \cdot \mathbf{\mathbf{\sigma}_k} - 3(\mathbf{\mathbf{\sigma}_j \cdot \mathbf{\mathbf{r}_{jk}}})(\mathbf{\mathbf{\sigma}_k \cdot \mathbf{\mathbf{r}_{jk}})} \right]. \tag{3.13} \]

where \( \gamma_j \) denotes the gyromagnetic ratio of spin \( j \), \( r_{jk} \) is the distance between spins \( j \) and \( k \), and \( \mathbf{\mathbf{\sigma}} \) is the vector of Pauli matrices. Introducing an anisotropy tensor \( g_{jk}^{ab} \), this can be rewritten as

\[ H_j = \sum_{j,k} \frac{\gamma_j \gamma_k}{r_{jk}} \sum_{a,\beta=1}^{1} g_{jk}^{ab} (\sigma_j^a \otimes \sigma_k^\beta) Y_2^{-a - \beta}, \tag{3.14} \]

where \( Y_2^m \) are the spherical harmonics, and \( \sigma^0 = \sigma^z \). Even though only multiple-qubit terms appear here it is necessary to further impose anisotropy in order to obtain an example with a nontrivial DFS, as we discuss in more detail in Sec. V A 4. This is the case, e.g., when only \( \sigma_j^z \otimes \sigma_k^z \) terms remain (i.e., \( g_{jk}^{ab} = \delta_{a0} \delta_{b0} \delta_{0j0k} \)), coupled to \( Y_2^2 \) rotations.

With these observations, we are now ready to study the question of DFSs in open systems without spatial symmetry in the system-bath couplings.

IV. DECOHERENCE-FREE SUBSPACES FROM SUBGROUPS OF THE PAULI GROUP

We begin this section by recalling the condition for DFSs within the framework of the Kraus operator-sum representation, derived in Ref. [9]. We then analyze the conditions for the appearance of DFSs when the errors are spanned by a subgroup of the Pauli group. The result is summarized by a theorem presented at the end of the section.

A. Condition for decoherence-free subspaces

A DFS is a subspace \( \mathcal{R} = \text{Span}\{|j\rangle\} \) of the full system Hilbert space \( \mathcal{H}_S \) over which the evolution of the density matrix is unitary. Necessary and sufficient conditions for a DFS were derived in the Markovian case in Ref. [8] and in the exact (non-Markovian) case in Ref. [6]. A formulation of the exact DFS condition was given in terms of the operator-sum representation in Ref. [9], and will be briefly reviewed.

Let \( \{ |j\rangle \} \) be a set of system states satisfying

\[ \mathbf{A}_d |j\rangle = c_d |j\rangle \quad \forall d, \tag{4.1} \]

where \( \mathbf{\tilde{U}} \) is an arbitrary, \( d \)-independent but possibly time-dependent unitary transformation, and \( c_d \) a complex constant. Under this condition, an initially pure state belonging to \( \text{Span}\{ |j\rangle \} \),

\[ |\psi_{in}\rangle = \sum_{j} \gamma_j |j\rangle, \]

will be decoherence-free, since

\[ |\phi_d\rangle = \mathbf{A}_d |\psi_{in}\rangle = \sum_{j} \gamma_j c_d \mathbf{\tilde{U}} |j\rangle = c_d \mathbf{\tilde{U}} |\psi_{in}\rangle \]

so

\[ \rho_{out} = \sum_d \mathbf{A}_d \rho_{in} \mathbf{A}_d^\dagger = \sum_d c_d \mathbf{\tilde{U}} |\psi_{in}\rangle \langle \psi_{in}| \mathbf{\tilde{U}}^\dagger c_d^{\ast} \]

where we used the normalization of the Kraus operators [Eq. (3.9)] to set \( \Sigma_d |c_d|^2 = 1 \). This means that the time-evolved state \( \rho_{out} \) is pure, and its evolution is governed by \( \mathbf{\tilde{U}} \). This argument is easily generalized to an initial mixed state \( \tilde{\rho}_{in} = \sum_{j,j'} \rho_{jj'} |j\rangle \langle j'| \), in which case \( \rho_{out} = \mathbf{\tilde{U}} \tilde{\rho}_{in} \mathbf{\tilde{U}}^\dagger \). The unitary transformation \( \mathbf{\tilde{U}} \) is a gauge freedom which can be exploited in choosing a driving system Hamiltonian that implements a useful evolution on the DFS. In the interaction picture used in the previous section, \( \mathbf{\tilde{U}} \) can be made to disappear by redefining all Kraus operators as \( \mathbf{\tilde{U}}^\dagger \mathbf{A}_d \). The calculation above shows that Eq. (4.1) is a sufficient condition for a DFS. It follows from the results of Refs. [6,43] that it is also a necessary condition for a DFS (under ‘‘generic’’ conditions—to be explained below).

Equation (4.1), however, does not seem to be a very useful characterization of a DFS if one does not know the explicit form of the Kraus operators (in general, this cannot be found in closed analytical form, although they can be determined experimentally [34]). When the Kraus operators derive from a Hamiltonian, as in Eq. (3.8), an equivalent DFS condition is [9]

\[ \mathbf{S}_a |j\rangle = a_{d} |j\rangle \quad \forall a, \tag{4.2} \]

where the system-bath interaction Hamiltonian is written as

\[ \mathbf{H}_J = \sum_a \mathbf{S}_a \otimes \mathbf{B}_a \quad \text{[compare to Eq. (2.6)]}, \]

with \( \{ \mathbf{S}_a \} \) being the system operators. To make use of this last DFS condition, one needs to introduce assumptions about the structure of system-bath coupling, and this is how one is led to spatial symmetry considerations [8]. Here, however, the DFS condition of Eq. (4.1) will be considered directly, based purely on the expansion of the Kraus operators in terms of the Pauli group elements, and without resorting to an explicit form for these operators.

\[ \text{022306-5} \]
B. Representation theory construction of decoherence-free states

When the Kraus operators are viewed as operators in the algebra of the Pauli group, the DFS condition [Eq. (4.1)] has a natural interpretation: the decoherence-free states \{ |j⟩ \} belong to the one-dimensional irreducible representations (irreps) of the Pauli group. Motivated by this observation we now consider a group representation theory construction of decoherence-free states.

The general criterion for the reducibility of a representation \{ Γ(G_n) \}_{n=1}^N of a finite group \( G = \{ G_n \} \) of order \( N \) is [44]

\[
\sum_{n=1}^{N} |\chi[Γ(G_n)]|^2 > N,
\]

where \( \chi \) is the character of the representation \( Γ \) [trace of the matrix \( Γ(G_n) \)]. If equality holds, then the representation is irreducible.

The full Pauli group \( P_K \) is irreducible over the Hilbert space \( \mathcal{H}_K \) of \( K \) qubits: since all Pauli matrices are traceless, only the four elements proportional to the identity matrix contribute (see also Appendix A):

\[
4^{K+1} \sum_{n=1}^{N} |\chi[Γ(G_n)]|^2 = |2^K|^2 + |−2^K|^2 + |i2^K|^2 + |−i2^K|^2 = 4^{K+1},
\]

which is just the order of \( P_K \) (generally the direct product representation of irreps of any direct product group is itself an irrep of that group [44]).

Now we come to the central assumption setting the stage for the DFSs considered in this paper: what if the Kraus operators belong to the group algebra of a subgroup \( Q \) of \( P_K \)? The motivation for this situation could be the case in which either (i) only higher order errors occur, such that first-order terms of the form \( I \otimes \cdots \otimes I \otimes \sigma_i^a \otimes I \otimes \cdots \otimes I \) are absent in the Pauli group expansion of the Kraus operators, or (ii) only errors of one kind, either \( \sigma^x \), \( \sigma^y \), or \( \sigma^z \) take place. Case (i) would imply one of the following. (a) There are certain cancellations involving bath matrix element terms such that first-order system operators are absent in the expansion of Eq. (3.11). This would be a rather nongeneric situation, involving a very special “friendly” bath. (b) The system-bath Hamiltonian is in fact not of the form in Eq. (2.6), but rather involves second-order terms such as \( \sigma^a \otimes \sigma^b \) (identity on all the rest). Case (ii) is applicable in, e.g., the case of pure phase damping (relevant to NMR [22]) and optical lattices using cold controlled collisions [45], where \( \sigma^z \) errors are dominant.

In the subgroup case under consideration, we may find nontrivial irreducible representations of \( Q \) over \( \mathcal{H}_K \) (a so-called “subduced” representation [42]). This situation can be interesting especially if there exist one-dimensional irreps, as known from the general theory of DFSs [6,8]. As will be shown next, the recipe for finding these DFSs uses the standard projection operators from elementary group representation theory. The projection is onto the subspace transforming according to a particular irrep.

First, recall the multiplicity formula for unitary irreps (which we can always assume in this case since the Pauli group is finite):

\[
m_k = \frac{1}{N} \sum_{n=1}^{N} \chi[Γ^k(G_n)]^* \chi[Γ(G_n)].
\]

where \( m_k \) is the number of times irrep \( Γ^k \) appears in the given reducible representation; \( \chi[Γ^k(G_n)] \) is the character of the \( Γ^k \) irrep on the group element \( G_n \); and \( \chi[Γ(G_n)] \) is the character of \( G_n \) in the given reducible representation \( Γ \).

We denote a set of (orthonormal) basis states transforming according to an irrep \( Γ^k \) by \{ |ψ_{μ}^{k}\rangle \}. These states span the invariant subspace of the irrep \( Γ^k \) and transform according to

\[
G_n|ψ_{μ}^{k}\rangle = \sum_{ν=1}^{d_k} Γ^k(G_n)_{νμ}|ψ_{ν}^{k}\rangle.
\]

Furthermore, they obey the orthogonality relation

\[
⟨ψ_{μ}^{k}|ψ_{ν}^{k}\rangle = δ_{μν} \delta_{k}. \tag{4.6}
\]

Next, a projection operator onto the subspace belonging to the \( d_k \)-dimensional irrep \( k \) is given by the appropriate sum over group elements [44]

\[
P_{μν}^{k} = \frac{1}{N} \sum_{n=1}^{N} Γ^k(G_n)_{νμ}^{*} G_n, \quad μ, ν = 1, \ldots, d_k, \tag{4.7}
\]

and has the following properties:

\[
P_{μν}^{k} P_{νλ}^{l} = δ_{kl} δ_{νμ} P_{μλ}^{k}, \quad P_{μν}^{k} |ψ_{ν}^{k}\rangle = δ_{νμ} |ψ_{μ}^{k}\rangle. \tag{4.8}
\]

To obtain a set of (orthonormal) basis states \{ |ψ_{μ}^{k}\rangle, \ldots, |ψ_{d_k}^{k}\rangle \} transforming as a set of partners in the basis for \( Γ^k \) from an arbitrary state \( |φ⟩ \), one can apply the set of operators \{ \( P_{μν}^{k} \) \} for a fixed \( ν \) (such that \( P_{νν}^{k}|φ⟩ \neq 0 \)) and renormalize the states thus obtained. Every state \( |φ⟩ \) can be expanded in terms of basis states for the constituting irreps \( Γ^k \) as

\[
|φ⟩ = \sum_{k} \sum_{ν=1}^{d_k} θ_{ν}^{k} |ψ_{ν}^{k}\rangle, \tag{4.9}
\]

where \( P_{νν}^{k}|φ⟩ = θ_{ν}^{k} |ψ_{ν}^{k}\rangle \) and the summation over \( k \) is over inequivalent irreps [44].

Let us now consider the effect of applying the operators \( A_d = \sum_{a,d,n} G_n \) from the group algebra to an arbitrary state \( |φ⟩ \):

\[
022306-6
Thus for \( u \)\textsuperscript{k} At this point it is useful to introduce another index \( z \):

\[
\Gamma^k(G_n)_{\mu\nu} = \gamma^k_{\mu\nu}, \quad \mu, \nu = 1. \tag{4.11}
\]

In this case the indices \( \mu, \nu \) are irrelevant and we will omit them. Then,

\[
A_d|\phi\rangle = \sum_{n=1}^{N} a_{d,n} \sum_{k} c^k_{d,n} |\psi^k_n\rangle. \tag{4.12}
\]

For \( |\phi\rangle \) to be a decoherence-free state, one would like to have this proportional to \( |\phi\rangle = \sum_{k} c^k |\psi^k\rangle \) [as in the original expansion of Eq. (4.9)]. However, this does not work because of the presence of \( \gamma^k_{\mu\nu} \) in the sum. We thus see that the initial function \( |\phi\rangle \) must be restricted to be one of the basis states \( |\psi^k\rangle \). Then, with

\[
c^k_{d,n} = \sum_{n=1}^{N} a_{d,n} \gamma^k_{\mu\nu}. \tag{4.13}
\]

we have finally

\[
A_d|\phi\rangle = c^k_{d,n} |\psi^k\rangle. \tag{4.14}
\]

At this point it is useful to introduce another index \( z \) for the multiplicity of the irrep \( k \), i.e., \( z = 1, \ldots, m_k \). The Hilbert space of \( K \)-qubit states splits into invariant one-dimensional subspaces \( V^k_z \) that are spanned by (fixed) basis states \( |\psi^k_z\rangle \). Each of the \( |\psi^k\rangle \) in Eq. (4.9) is a linear combination of the \( z \):

\[
|\psi^k\rangle = \sum_{z=1}^{m_k} \theta^k_{z} |\psi^k_z\rangle. \tag{4.15}
\]

[Because of Eq. (4.9), the \( \theta^k_z \) depend on the initial state \( |\phi\rangle \).] Therefore for \( |\phi\rangle \) to be a decoherence-free state, it is allowed to be an arbitrary superposition inside copies of a given irrep (different \( z \)'s), but not to be a superposition between different irreps (different \( k \)'s). In particular we have within each copy of the irrep \( \Gamma^k \)

\[
A_d|\psi^k_z\rangle = c^k_{d,n} |\psi^k_z\rangle, \quad z = 1, \ldots, m_k. \tag{4.16}
\]

This is just the DFS condition, Eq. (4.1), with the \( \{ |\psi^k_z\rangle \} \) being the basis states for the DFS. Therefore Eq. (4.11) is a sufficient condition for a DFS, provided that our initial state satisfies the condition that it is a superposition of states within a fixed irrep, Eq. (4.15).

It will now be shown that Eq. (4.11) is also a necessary condition for a DFS under the “generic” assumption that the error coefficients \( \{ a_{d,n} \} \) are arbitrary. In other words, it will be shown under these conditions that, if a set of basis states \( \{ |\tilde{j}\rangle \} \) satisfies the DFS condition Eq. (4.1), then the \( \{ |\tilde{j}\rangle \} \) belong to the invariant subspace of some one-dimensional irrep of our subgroup.

Assume that the \( A_d \) have been redefined to incorporate the (constant) unitary transformation \( \tilde{U} \) such that Eq. (4.1) becomes \( A_d|\tilde{j}\rangle = c_d|\tilde{j}\rangle \). Expand the state \( |\tilde{j}\rangle \) as in Eq. (4.9):\(^6\)

\[
|\tilde{j}\rangle = \sum_{k} \sum_{\mu=1}^{d_k} \bar{\vartheta}^k_{\mu} |\psi^k_{\mu}\rangle \tag{4.17}
\]

where \( P^k_{\mu\mu} |\phi\rangle = \bar{\vartheta}^k_{\mu} |\psi^k_{\mu}\rangle \). Now, using Eq. (4.10),

\[
A_d|\tilde{j}\rangle = c_d|\tilde{j}\rangle
\]

\[
= \sum_{k} \sum_{\mu=1}^{d_k} \bar{\vartheta}^k_{\mu} A_d|\psi^k_{\mu}\rangle
\]

\[
= \sum_{k} \sum_{\mu=1}^{d_k} \bar{\vartheta}^k_{\mu} \sum_{n} a_{d,n} G_n |\psi^k_{\mu}\rangle \tag{4.18}
\]

\[
= \sum_{k} \sum_{\mu=1}^{d_k} \bar{\vartheta}^k_{\mu} \sum_{n} a_{d,n} \sum_{\lambda=1}^{d_k} \Gamma^k(G_n)_{\lambda\mu} |\psi^k_{\lambda}\rangle \tag{4.19}
\]

and taking inner products [using Eq. (4.6)]

\[
\langle \psi^k_{\lambda}|A_d|\tilde{j}\rangle = c_d \sum_{\mu=1}^{d_k} \bar{\vartheta}^k_{\mu} \langle \psi^k_{\lambda}|\psi^k_{\mu}\rangle
\]

\[
= c_d \bar{\vartheta}^k_{\mu}
\]

\[
= \sum_{k} \sum_{\mu=1}^{d_k} \bar{\vartheta}^k_{\mu} \sum_{n} a_{d,n} \sum_{\lambda=1}^{d_k} \Gamma^k(G_n)_{\lambda\mu} \langle \psi^k_{\lambda}|\psi^k_{\mu}\rangle
\]

\[
= \sum_{k} \sum_{\mu=1}^{d_k} \bar{\vartheta}^k_{\mu} \sum_{n} a_{d,n} \Gamma^k(G_n)_{\mu\mu}. \tag{4.20}
\]

Using this result we would like to show that the \( \Gamma^k(G_n)_{\mu\mu} \) that appear here must be one-dimensional irreps. Let us establish “generic” conditions for this purpose.

Equation (4.20) can be rewritten as an eigenvalue equation

\[
A_d^l \bar{\vartheta}^l_l = c_d \bar{\vartheta}^l_l, \tag{4.21}
\]

where

\[
A_d^l = \sum_{n} a_{d,n} \Gamma^l(G_n). \tag{4.22}
\]

\(^6\)For notational simplicity we avoid introducing another index for the multiplicity of the irrep here. That such superpositions are allowed for DF states is clear from Eq. (4.15).
The vector \( \tilde{\theta}_j \) may be zero for a given irrep \( \Gamma' \), in which case Eq. (4.21) is trivially satisfied. Let us assume this is not the case for some \( j \) (it cannot be the case for all \( l \), by Eq. (4.17)). Then the most general way in which Eq. (4.21) can be satisfied is for \( \tilde{\theta}_j \) to be an eigenvector of \( A'_{ij} \) for all codewords \( |j\rangle \), with eigenvalue \( c_d \). However, while this is the most general condition, it is nongeneric. By generic we mean that we take the errors to be arbitrary, i.e., we do not want to make any assumptions on the \( a_{d,n} \). Now, if the eigenvalue equation were to be satisfied, the vector of coefficients \( \tilde{\theta}_j \) would have to be “special.” In other words, it would have to be adjusted to be an eigenvector of \( A'_d \). To make this adjustment would require two conditions: (i) having a priori knowledge of the \( a_{d,n} \) and (ii) being able to control \( \tilde{\theta}_j \). We would like to avoid assuming (i) because fine-tuning the bath is physically unacceptable. In contrast, control of \( \tilde{\theta}_j \) is certainly desirable. However, we would like to avoid the situation where only certain special choices of \( \tilde{\theta}_j \), compatible with specific bath parameters, yield decoherence-free states \( |\tilde{j}\rangle \).\(^7\) We thus conclude that to avoid fine-tuning of the bath parameters and/or special initial conditions, \( A'_{ij} \) must be proportional to the identity. But since \( \Gamma' \) is an irrep this is only possible if it is one dimensional, i.e., \( \Gamma'(G_n)_{\mu\nu} = \gamma'_{\mu\nu}, \mu, \nu = 1, \) and \( c_d = \Sigma_n a_{d,n} \gamma'_{n,i} \). In addition we see that \( c_d \) can only be \( i \) independent if the DFS states \( |\tilde{j}\rangle \) are spanned only by basis states of copies of the same irrep \( \Gamma' \). Q.E.D.

We summarize with the following theorem.

**Theorem 1.** Suppose that the Kraus operators belong to the group algebra of some group \( G = \{G_n\} \), i.e., \( A_d = \Sigma_{n=1}^N a_{d,n} G_n \). If a set of states \( \{|j\rangle\} \) belong to a given one-dimensional irrep \( \Gamma^k \) of \( G \), then the DFS condition \( A_d |j\rangle = c_d |j\rangle \) holds. If no assumptions are made on the bath coefficients \( \{a_{d,n}\} \), then the DFS condition \( A_d |j\rangle = c_d |j\rangle \) implies that \( |j\rangle \) belongs to a one-dimensional irrep \( \Gamma^k \) of \( G \).

For completeness we give in Appendix B an example of the “nongeneric DFSs,” which result from “accidentally” satisfying Eq. (4.21) with irreps of dimension greater than 1.

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### V. EXAMPLES OF SUBGROUPS WITH DECOHERENCE-FREE STATES

The general considerations from the previous section will now be illustrated with some examples. To simplify the notation, let \( X, Y, Z \) represent the \( \sigma^x, \sigma^y, \sigma^z \) Pauli matrices, and let us drop the tensor product symbol (i.e., let \( ZI=Z \otimes I, X^2=X \otimes X, \) etc.). Also, we will ignore normalization factors in this section.

---

\(^7\)This statement of what are generic conditions that lead to a DFS is very similar to that in Ref. [8].
The multiplicity of each of the four one-dimensional irreps in the reducible representation generated here by the $K=4$ qubits is 4. To see this, recall the multiplicity formula Eq. (4.4). In the present case, the given representation yields $\chi = \{16,0,0,0\}$ (for $I^2, X^2, Y^2, X^2Y^2, X^2$ respectively) and so, with $\chi^k(I^4)=1, m_k = \frac{1}{4}\chi^k(I^4)16=4$ for all $k$.

Now, let us explicitly find the decoherence-free states. To do so we can pick an arbitrary, convenient four-qubit state and project it onto a given irrep. For example, starting with $|0000\rangle$:

$$P^1|0000\rangle = |0000\rangle + |1100\rangle + |0011\rangle + |1111\rangle = |\psi_1^1\rangle,$$

$$P^2|0000\rangle = |0000\rangle + |1100\rangle - |0011\rangle - |1111\rangle = |\psi_1^2\rangle,$$

$$P^3|0000\rangle = |0000\rangle - |1100\rangle + |0011\rangle - |1111\rangle = |\psi_1^3\rangle,$$

$$P^4|0000\rangle = |0000\rangle - |1100\rangle - |0011\rangle + |1111\rangle = |\psi_1^4\rangle.$$ (5.5)

Each of these four states belongs to a different irrep, and thus to a different DFS, which can be verified by applying an arbitrary Kraus operator, as in Eq. (5.3). For example,

$$A_d|\psi_1^1\rangle = a_{d,0}|0000\rangle + a_{d,1}|1100\rangle + a_{d,2}|0011\rangle + a_{d,3}|1111\rangle$$

$$+ a_{d,1}(|1100\rangle + |0000\rangle + |1111\rangle + |0011\rangle)$$

$$+ a_{d,2}(|0011\rangle + |1111\rangle + |0000\rangle + |1100\rangle)$$

$$+ a_{d,3}(|1111\rangle + |0011\rangle + |1100\rangle + |0000\rangle)$$

$$= (a_{d,0} + a_{d,1} + a_{d,2} + a_{d,3})|\psi_1^1\rangle.$$ (5.6)

Similarly,

$$A_d|\psi_1^2\rangle = (a_{d,0} + a_{d,1} - a_{d,2} - a_{d,3})|\psi_1^2\rangle,$$

$$A_d|\psi_1^3\rangle = (a_{d,0} - a_{d,1} + a_{d,2} - a_{d,3})|\psi_1^3\rangle,$$

$$A_d|\psi_1^4\rangle = (a_{d,0} - a_{d,1} - a_{d,2} + a_{d,3})|\psi_1^4\rangle.$$ (5.7)

This is in agreement with Eq. (4.16).

Now, recall that each irrep appears four times. This means we should be able to find three more independent states belonging to each of the irreps. Indeed, by performing projections on the states $|0001\rangle$, $|0100\rangle$, and $|1001\rangle$ (using $|0010\rangle$ and $|1000\rangle$ does not produce new states) we obtain the complete basis for the DFSs. For example,

$$P^1|0001\rangle = |0001\rangle + |1101\rangle + |0010\rangle + |1110\rangle = |\psi_2^1\rangle,$$

$$P^1|0100\rangle = |0100\rangle + |1000\rangle + |0111\rangle + |1111\rangle = |\psi_3^1\rangle,$$

$$P^1|1001\rangle = |1001\rangle + |0101\rangle + |1010\rangle + |0110\rangle = |\psi_4^1\rangle.$$ (5.8)

And again

$$A_d|\psi_2^1\rangle = (a_{d,0} + a_{d,1} + a_{d,2} + a_{d,3})|\psi_2^1\rangle,$$

$$P^2|0001\rangle = (a_{d,0} + a_{d,1} + a_{d,2} + a_{d,3})|\psi_2^1\rangle.$$ (5.9)

with similar results for the other states. All of this is in agreement with the general results of Sec. IV B. Finally, we may consider an arbitrary superposition of decoherence-free states taken from the multiple appearances of a given irrep, $|\psi^k\rangle = \sum \phi_k^k|\psi_k^k\rangle$, and this will again be decoherence-free.

2. The subgroup $Q_4$

In this case the Kraus operators can be written as

$$A_d = a_{d,0}I^4 + a_{d,1}X^4 + a_{d,2}Y^4 + a_{d,3}Z^4.$$ (5.10)

Again, using the general arguments of Sec. IV B, in the case of $Q_4$ we can just read off the matrix elements of the four (one-dimensional) irreps from the table in Eq. (5.2). Thus the four projection operators are

$$P^1 = I^4 + X^4 + Y^4 + Z^4,$$

$$P^2 = I^4 + X^4 - Y^4 - Z^4,$$

$$P^3 = I^4 - X^4 + Y^4 - Z^4,$$

$$P^4 = I^4 - X^4 - Y^4 + Z^4.$$ (5.11)

Using the multiplicity formula, Eq. (4.4), the given representation again yields $\chi = \{16,0,0,0\}$ (for $I^4, X^4, Y^4, Z^4$ respectively) and so once more $m_k = \frac{1}{4}\chi^k(I^4)16=4$ for all $k$.

To find the decoherence-free states let us start again with $|0000\rangle$. We find

$$P^1|0000\rangle = 2(|0000\rangle + |1111\rangle) = |\psi_1^1\rangle,$$

$$P^2|0000\rangle = |0000\rangle + |1111\rangle - |0000\rangle - |1111\rangle = 0,$$

$$P^3|0000\rangle = |0000\rangle - |1111\rangle + |0000\rangle - |1111\rangle = 0,$$

$$P^4|0000\rangle = 2(|0000\rangle - |1111\rangle) = |\psi_1^1\rangle.$$ (5.12)

The vanishing of the projections of $P^2$ and $P^3$ implies that $|0000\rangle$ has no components in the irreps $I^2$ and $I^3$. Thus a different starting state is needed, e.g., $|0001\rangle$. Then

$$P^2|0001\rangle = 2(|0001\rangle + |1111\rangle) = |\psi_1^2\rangle,$$

$$P^3|0001\rangle = 2(|0001\rangle - |1111\rangle) = |\psi_1^3\rangle.$$ (5.13)

That these states are decoherence-free is again easily verified by application of an arbitrary Kraus operator, e.g.,

$$A_d|\psi_2^2\rangle = (a_{d,0}I^4 + a_{d,1}X^4 + a_{d,2}Y^4 + a_{d,3}Z^4)$$

$$\times 2(|0001\rangle + |1111\rangle)$$

$$= (a_{d,0} + a_{d,1} - a_{d,2} - a_{d,3})|\psi_2^2\rangle.$$ (5.14)

etc. The full DFS corresponding to the projection $P^1$ is found by applying $P^1$ to the initial states $|0011\rangle, |0101\rangle, |1001\rangle,$
\[ P^1|0011\rangle = 2(|0011\rangle + |1100\rangle) = |\psi_1^4\rangle, \]
\[ P^1|0101\rangle = 2(|0101\rangle + |1010\rangle) = |\psi_1^4\rangle, \]
\[ P^1|1001\rangle = 2(|1001\rangle + |0110\rangle) = |\psi_1^4\rangle. \quad (5.15) \]

in addition to \(|\psi_1^4\rangle\) above.

Since the decoherence process described by \(Q_4\) is different from that of \(Q_X\), the decoherence-free states are, not surprisingly, different in the two cases.

### 3. The subgroup \(Q_Z\)

As another example of an Abelian subgroup, assume now that the Kraus operators, for \(K=2\) qubits, can be written as
\[ A_d = a_{d,0}I^2 + a_{d,1}IZ + a_{d,2}IZ + a_{d,3}Z^2. \quad (5.16) \]

The four projection operators are thus
\[ P^1 = I^2 + ZI + IZ + Z^2, \quad P^2 = I^2 + ZI - IZ - Z^2, \]
\[ P^3 = I^2 - ZI + IZ - Z^2, \quad P^4 = I^2 - ZI - IZ + Z^2. \quad (5.17) \]

In this case, the given representation on two qubits yields \(\chi = \{4,0,0,0\}\) (for \(I^2, ZI, IZ, Z^2\), respectively) and so \(m_\chi = \frac{1}{2}\chi(\tilde{I}^2)4 = 1\) for all \(k\). Thus, as expected (since the representation is four-dimensional), the multiplicity of each of the four one-dimensional irreps is 1.

Let us again explicitly find the decoherence-free states:
\[ P^1|00\rangle = 4|00\rangle = |\psi_1\rangle, \]
\[ P^2|01\rangle = 4|01\rangle = |\psi_2\rangle, \]
\[ P^3|10\rangle = 4|10\rangle = |\psi_3\rangle, \]
\[ P^4|11\rangle = 4|11\rangle = |\psi_4\rangle. \quad (5.18) \]

And indeed
\[ A_d|\psi^k\rangle = (a_{d,0} + a_{d,1} + a_{d,2} + a_{d,3})|\psi^k\rangle, \quad k = 1, \ldots, 4. \]

This means that each of the four "computational basis states" \(|\psi^k\rangle\) is by itself a DFS. However, since these DFSs belong to different irreps, a superposition is not decoherence-free. This agrees with the well known fact that phase damping leads to decay of the off diagonal elements of the density matrix in the computational basis, but does not cause any population decay.

### 4. The subgroup \(Q_{2Z}\)

As a final example of an Abelian subgroup, let us return to the anisotropic dipolar-coupling Hamiltonian [Eq. (3.14)] discussed in Sec. III. Note first that it is necessary to transform from the \(\sigma^z\) basis used there to \(\sigma^{1,2}\) in order for our Pauli-group-based discussion to apply. Having done that, it is clear that unless anisotropy is imposed this Hamiltonian generates the entire Pauli group, since all bilinear combinations \(\sigma^a \otimes \sigma^b\) appear in it. Assume therefore that we have a four-spin molecule constrained to rotate only about the \(z\) axis. This amounts to setting \(s_{jk}^{ab} = \delta_{a0}\delta_{b0}s_{jk}\) in Eq. (3.14), so that only \(\sigma_j^z \otimes \sigma_k^z\) terms remain. The corresponding subgroup is
\[ Q_{2Z} = \{\tilde{IIII}, \tilde{ZZII}, \tilde{ZIIZ}, \tilde{IIZZ}, \tilde{ZIIZ}, \tilde{IZII}, \tilde{IZIZ}, \tilde{ZZZZ}\}. \quad (5.19) \]

To find the DFS under \(Q_{2Z}\), construct the projector \(P^1 = \frac{1}{2}E_g = \sum_{g \in Q_{2Z}} q\) corresponding to the identity irrep of \(Q_{2Z}\). Applying this projector to the initial states \(|0000\rangle\) and \(|1111\rangle\) we find a two-dimensional DFS, spanned by these two states. This DFS thus encodes a single qubit.

### B. Non-Abelian subgroups?

It would have been interesting to find examples of non-Abelian subgroups that have one-dimensional irreps and thus support a DFS. However, no such subgroups exist in the case of the Pauli group, as we now prove.

Each two elements of the Pauli group \(P_E\) either commute or anticommute (Appendix A). Let \(Q\) be a non-Abelian subgroup of \(P_E\). Then there must be at least two elements of \(Q\), say \(q_1\) and \(q_2\), that anticommute. Assume that the state \(|i\rangle\) belongs to a one-dimensional irrep \(\tilde{\Gamma}\) of \(Q\). Then \(\tilde{\Gamma}(q_1)|i\rangle = c_1|i\rangle\) and \(\tilde{\Gamma}(q_2)|i\rangle = c_2|i\rangle\), where \(c_1, c_2\) are numbers. Now, by assumption \(\tilde{\Gamma}(q_2q_1) = \tilde{\Gamma}(-q_1q_2)\). Therefore \(\tilde{\Gamma}(q_1q_2)|i\rangle = \tilde{\Gamma}(q_1)|\tilde{\Gamma}(q_2)|i\rangle = c_1c_2|i\rangle\), and also \(\tilde{\Gamma}(q_1q_2)|i\rangle = \tilde{\Gamma}(-q_2q_1)|i\rangle = c_1\tilde{\Gamma}(-q_2)|i\rangle\). If \(\tilde{\Gamma}(-q_2) = -\tilde{\Gamma}(q_2)\) then we have \(\tilde{\Gamma}(q_2q_1)|i\rangle = -c_1c_2|i\rangle\) so that \(c_1c_2 = -c_1c_2\). This implies that at least one of \(c_1\) and \(c_2\) is zero. However, this cannot be true since the representation is unitary. Is there another possibility? Note that \(\tilde{\Gamma}(-q_2) = \tilde{\Gamma}(q_2)\), so the question boils down to the value of \(a\) in \(\tilde{\Gamma}(a) = a\tilde{\Gamma}(I)\). But since \(-I\tilde{I}\tilde{I} = I\tilde{I}\\tilde{I}\) it follows that \(\tilde{\Gamma}(I)\tilde{\Gamma}(I) = \tilde{\Gamma}(I) = 1\), so that \(\tilde{\Gamma}(I) = \pm 1\). Assume then that the other case, \(\tilde{\Gamma}(I) = 1\), holds. Let us use Eq. (4.4) while recalling that only the four multiples of the identity have nonvanishing trace:
\[ m_\chi = \frac{1}{N} \sum_{n=1}^N \chi[\Gamma^n(I)] \cdot \chi[\Gamma^n(I)] \]
\[ = \frac{1}{N} \left[ \chi[\Gamma(I)](2^K) + \chi[\Gamma(-I)](-2^K) + \chi[\Gamma^I(iI)](i2^K) + \chi[\Gamma^I(-I)](-i2^K) \right]. \quad (5.20) \]

Since the irrep \(\Gamma^I\) is one dimensional, \(\chi[\Gamma^I] = \Gamma^I\), i.e., the character is the element itself. Now let \(I^2 = \tilde{I}I\). Then since \(\tilde{\Gamma}(-I) = 1\), and using \(\Gamma^I(-I) = \tilde{\Gamma}(-I)\\tilde{I}\\tilde{I}\), we find \(\tilde{m} = 0\). Therefore such irreps do not appear at all.
Thus an anticommuting pair of elements in $Q$ is incompatible with a one-dimensional irrep, so that if $Q$ has a one-dimensional irrep, it must be Abelian.\footnote{We thank Dr. P. Zanardi for discussions regarding this point.}

Recall that the DFS condition of theorem 1 applies to arbitrary groups. Groups other than the Pauli group may support non-Abelian subgroups with one-dimensional irreps (the above proof relied strongly on a property specific to the Pauli group, that its elements either commute or anticommute). However, at least within the Hamiltonian framework expounded in Secs. II and III, it is the Pauli group that appears naturally for the group algebra to which the Kraus operators belong.

VI. DIMENSION OF THE DECOHERENCE-FREE SUBSPACES

We showed in the previous section that for the Pauli group DFSs can exist only for Abelian subgroups. This observation allows us to calculate the dimension of these DFSs. Recall from the general discussion in Sec. IV B that in the generic case a superposition of states belonging to different irreps will decohere, whereas a superposition of states within copies of a given irrep will be decoherence-free (see also the examples in the previous section). Also, by the Abelian property, each such copy supports only a single decoherence-free state. Hence the dimension of the DFS associated with a given irrep $\Gamma^k$ is simply its multiplicity $m_k$.

Let $Q$ be an order-$N$ Abelian subgroup of the Pauli group on $K$ qubits. Using Eq. (5.20) and $\Gamma^k(-I) = \pm 1$ again, we have two (and only two) cases: (i) If $\Gamma^k(-I) = 1$ then $m_k = 0$, so such irreps do not support a DFS; (ii) If $\Gamma^k(-I) = -1$ then

$$m_k = 2^{k+2}/N.$$  

This shows that all irreps that support a DFS have the same multiplicity, and thus all these DFSs have the same dimension.

If the subgroup does not include elements with the $\pm 1, \pm i$ factors, as in the examples in Sec. V, then only the term $\Gamma^k(I)$ appears in Eq. (5.20), and consequently

$$m_k = 2^k/N, \quad \text{no } \{\pm 1, \pm i\} \text{ factors}.$$  

In any case, the dimension of the DFS is inversely proportional to the order of the subgroup. This implies a trade-off between the number of errors that can be dealt with by the code ($N$) and the number of decoherence-free qubits ($\log_2 m_k$).

As an interesting corollary we see that the largest Abelian subgroup of the Pauli group has order $2^{K+2}$ (since $m_k \geq 1$ implies $N \approx 2^{K+2}$). Examples of such subgroups are (1) the group generated by all the single-qubit $X'$s (or $Y'$s or $Z'$s) with $\pm 1, \pm i$; (2) the group generated by $XXI\cdots II, YYI\cdots II, ZZI\cdots II, IXXI\cdots II, IYYI\cdots II, HZZI\cdots II, \ldots, II\cdots IZZ$ with $\pm 1, \pm i$.

These groups support only one-dimensional DFSs. The last group is relevant for errors due to exchange on pairs of identical qubits [46], and we see that the corresponding decoherence-free state is automatically immune to exchange errors. (See Ref. [21] for a discussion of protection of DFSs against exchange errors arising in the spatially correlated collective decoherence case.)

VII. SUMMARY AND CONCLUSIONS

Decoherence-free subspaces are associated most commonly with the existence of a spatial symmetry in the system-bath coupling, as in the collective decoherence model. Here we have considered the case when no such symmetry is assumed, and have shown that one can nevertheless find DFSs under certain conditions. The essential assumptions are that either to lowest order only multiple-qubit errors are possible, meaning that the bath can couple only to multiple system excitations; or that only one type of error process (such as phase damping) occurs, which can be relevant for NMR quantum computer schemes and optical lattices (or any other realization where scattering-induced phase shifts are the dominant decoherence mechanism). In either case, instead of the full Pauli group of errors, only a subgroup needs to be considered. Barring certain nongeneric cases, the DFSs then correspond to states that transform according to the one-dimensional irreducible representations of such a subgroup. This characterization of DFSs, while formally similar to previous results, is different in that it trades the assumption of spatial symmetry for one of multiple-qubit coupling to the bath.

We show in a sequel paper [25] how to perform universal fault tolerant quantum computation on the DFSs found in this paper using only one- and two-body Hamiltonians. It would further be desirable to identify in detail the physical conditions under which the Pauli subgroup model is relevant for current proposals for quantum computers. An important example we have discussed is the dipolar-coupling-induced decoherence in NMR.

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APPENDIX A: THE PAULI GROUP

The Pauli matrices are

$$\sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$  \hspace{1cm} (A1)

They have the following properties:

$$\sigma^2 = I, \quad \alpha = 0,x,y,z,$$
\[ \begin{align*}
\{ \sigma_\alpha, \sigma_\beta \} &= 2i \epsilon_{\alpha\beta\gamma} \sigma_\gamma, \\
\{ \sigma_\alpha, \sigma_\beta \} &= 2 \delta_{\alpha\beta} I, \\
\sigma_\alpha \sigma_\beta &= i \epsilon_{\alpha\beta\gamma} \sigma_\gamma + \delta_{\alpha\beta} I, \\
\text{Tr}(\sigma_\alpha) &= 0, \quad \alpha = x, y, z.
\end{align*} \] (A2)

The Pauli group of order K is the set of all \( 4^{K+1} \) possible tensor products of K of the Pauli matrices and \( \pm, \pm i: \)

\[ P_K = \pm, \pm i \{ \otimes_{k=1}^K \sigma_{\alpha_k} \}. \] (A3)

Some of its useful properties are the following.

(i) Let \( p_1, p_2 \in P_K \). Since either \( \{ \sigma_{\alpha, k}, \sigma_{\beta, k} \} = 0 \) or \( \{ \sigma_{\alpha, k}, \sigma_{\beta, k} \} \neq 0 \) it follows that

\[ \text{either } [p_1, p_2] = 0 \quad \text{or} \quad \{p_1, p_2\} = 0. \] (A4)

(ii) Since \( \sigma_\alpha \) are all unitary, so are all \( p \in P_K \).

(iii) Since \( \sigma_\alpha \) are all Hermitian but we allow for \( \pm i \) factors, \( p \in P_K \) is either Hermitian or anti-Hermitian. Thus if \( p \in P_K \) then \( p^\dagger \in P_K \).

(iv) Since \( \text{Tr}(A \otimes B) = \text{Tr} A \times \text{Tr} B \), the only elements in \( P_K \) that are not traceless are the four \( \pm, \pm i \) multiples of the identity, and each has trace \( 2^K \).

**APPENDIX B: EXAMPLES OF NONGENERIC DECOHERENCE-FREE SUBSPACES**

We will show here an example of a DFS that arises out of a two-dimensional irrep of a non-Abelian subgroup, in the "nongeneric" case. Let us consider the non-Abelian eight-element subgroup \( Q_8 = \{ \pm 111, \pm XXI, \pm IZZ, \pm iXYZ \} \). In this standard representation it is reducible and splits into four copies of a two-dimensional irreducible representation of \( Q_8 \). Since there is just one irrep, we drop the irrep index \( k \) on \( \Gamma^k \), etc. The two-dimensional representation of \( Q_8 \) is the following:

\[ \begin{align*}
\Gamma(\pm111) &= \pm \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \Gamma(\pm XXI) = \pm \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}, \\
\Gamma(\pm IZZ) &= \pm \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \Gamma(\pm iXYZ) = \pm \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.
\end{align*} \] (B1)

The eight-dimensional Hilbert space is split into four irreducible subspaces \( V^\gamma \) (corresponding to the four copies of \( \Gamma \)) spanned by

\[ \begin{align*}
V^1 &= (|\psi_{01}^1\rangle, |\psi_{11}^1\rangle) = (|00\rangle, |11\rangle), \\
V^2 &= (|\psi_{02}^2\rangle, |\psi_{12}^2\rangle) = (|11\rangle, |00\rangle), \\
V^3 &= (|\psi_{03}^3\rangle, |\psi_{13}^3\rangle) = (|10\rangle, |01\rangle), \\
V^4 &= (|\psi_{04}^4\rangle, |\psi_{14}^4\rangle) = (|01\rangle, |10\rangle).
\end{align*} \] (B2)

On each of these two-dimensional subspaces the group acts like \( \Gamma \). A codeword in the DFS can be expanded as \( |\vec{j}\rangle = \Sigma_{z=0}^{1} \Sigma_{\mu=0}^{1} \theta_{\mu,z}^\gamma |\psi_{\mu}\rangle \). Let us take as our code just the first basis vector of each irreducible subspace, i.e.,

\[ C = \{|0\overline{1}\rangle, |2\overline{2}\rangle, |3\overline{1}\rangle, |4\overline{0}\rangle\} = \{ |00\rangle, |11\rangle, |10\rangle, |01\rangle \}. \] (B3)

Denoting the vector of coefficients as \( \vec{\theta}^\gamma = (\theta_{00}^\gamma, \theta_{10}^\gamma) \), this means that \( \vec{\theta}^0 = (1,0) \) and \( \vec{\theta}^{\pi z} = (0,0) \). In this case we can show that there are Kraus operators \( A_d \) that satisfy the DFS condition on the code, by searching for matrices \( A_d \) that have \( \vec{\theta}^\gamma \) as eigenvectors. An example is

\[ A_1 = \begin{pmatrix} c_1 & d_1 \\ 0 & e_1 \end{pmatrix}, \quad A_2 = \begin{pmatrix} c_2 & d_2 \\ 0 & e_2 \end{pmatrix}, \] (B4)

with the conditions \( c_1^2 + d_1^2 = 0 \), \( c_2^2 + c_4^2 = 1 \), and \( |d_1|^2 + |d_2|^2 + |e_1|^2 + |e_2|^2 = 1 \) for normalization [Eq. (3.9)]. The corresponding Kraus operators are

\[ \begin{align*}
A_1^\dagger &= \frac{c_1 + e_1}{2} \Gamma_{III} + \frac{d_1}{2} \Gamma_{XXI} + \frac{e_1}{2} \Gamma_{IZZ} + \frac{d_1}{2} \Gamma_{iXYZ}, \\
A_2^\dagger &= \frac{c_2 + e_4}{2} \Gamma_{III} + \frac{d_2}{2} \Gamma_{XXI} + \frac{e_2}{2} \Gamma_{IZZ} + \frac{d_2}{2} \Gamma_{iXYZ}.
\end{align*} \] (B5)

The code \( C \) is a DFS. It is the particular equality (i.e., the "conspiring," nongeneric or accidental relationship) between the coefficients of the \( XXI \) and \( XYZ \) terms that is responsible for the existence of this DFS.

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