Universal Quantum Computation and Leakage Reduction in the 3-Qubit Decoherence Free Subsystem

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Abstract
We describe exchange-only universal quantum computation and leakage reduction in the 3-qubit decoherence free subsystem (DFS). We discuss the angular momentum structure of the DFS, the proper forms for the DFS CNOT and leakage reduction operators in the total angular momentum basis, and new exchange-only pulse sequences for the CNOT and leakage reduction operators. Our new DFS CNOT sequence requires 22 pulses in 13 time steps. The DFS leakage reduction sequence, the first explicit leakage reduction sequence of its kind, requires 30 pulses in 20 time steps. Although the search for sequences was performed numerically using a genetic algorithm, the solutions presented here are exact, with closed-form expressions.

1 Introduction
Interest and research in semiconductor quantum dots for quantum information processing has continued to grow since the original proposal by Loss and Di-Vincenzo [1, 2]. In semiconductor quantum dot systems, with a single electron spin as a qubit, two qubit gates using electron exchange interactions can be performed on sub-nanosecond time scales [3]. In contrast, single qubit operations based on electron spin resonance may be two orders of magnitude slower or more [4, 5]. The slow and technically challenging single electron operations can be avoided by using an encoding in which exchange interactions give encoded universality. The possibility of universal computation using only the exchange
interaction, and its connection to decoherence free (DF) subsystems, has been demonstrated in [6, 7, 8]. Bacon et al. [6] describe the 4-qubit DF subspace, giving exchange-based Hamiltonians that generate encoded universal computation. Kempe et al. [7, 8] give a general theory for decoherence free subspaces and subsystems, and prove the universality properties of these encodings employing only exchange or other two-body interactions. Experiments on a single three-spin exchange-only encoded qubit have also recently been reported [9].

Any implementation of exchange-only quantum computing, however, requires explicit gate sequences for a universal set of encoded gates. For the 3-qubit decoherence free subspace, DiVincenzo et al. [10] found explicit exchange gate pulse sequences for single encoded qubit gates, as well as for an encoded two-qubit gate locally equivalent to a CNOT. (A two-qubit gate is locally equivalent to a second two-qubit gate if they differ only by single qubit gates [11].) Kawano et al. [12] showed that DiVincenzo’s numerically obtained locally equivalent CNOT sequence using 19 gate pulses in 13 time steps in fact approximates a true, analytical, solution.

The DiVincenzo 19 gate locally equivalent CNOT pulse sequence is valid only for the 3-qubit DF subspace, and not for the entire 3-qubit DF subsystem. Computation in the DF subsystem offers two major advantages compared to the subspace: initialization of encoded subsystem states requires no magnetic field, and the subsystem states are immune to all global decoherence mechanisms, not just global decoherence in a single direction. To exploit these features of the 3-qubit subsystem, an analytic CNOT gate sequence for the entire subsystem was found by Bonesteel et al. [13], which requires approximately 50 exchange gates. Using a genetic algorithm, we have significantly improved on the Bonesteel et al. solution, finding a new analytic pulse sequence for the encoded subsystem CNOT that requires just 22 exchange gates in 13 time steps. Additionally, our solution is for the full encoded CNOT, and not just the locally equivalent CNOT. The 4-qubit DF subspace possesses the same magnetic field-free initialization and global decoherence immunity as the 3-qubit subsystem. An encoded CNOT gate sequence has also been found for the 4-qubit encoding [14], requiring 50 exchange gates in 27 time steps. With a CNOT gate sequence that is more than twice as expensive as our 3-qubit CNOT solution, and the additional overhead of an extra physical qubit per encoded qubit, the 4-qubit encoding is apparently inferior to the 3-qubit encoding.

Computation with the 3-qubit DF subsystem requires not only a universal set of encoded gates, but also an effective means of recovering from errors. Though the subsystem protects against global decoherence, local decoherence mechanisms such as nuclear hyperfine and electron-electron dipole-dipole coupling still exist, and give rise to both encoded errors and leakage from the encoded subsystem. Encoded errors can be corrected using standard quantum error correction procedures [15], but leakage errors must be converted, or reduced, to encoded errors in the course of applying quantum error correction. The incorporation of leakage reduction units into fault tolerant quantum error correction circuits is described in [16]. Kempe et al. [8] describe a “SWAP If Leaked” (SIL) operator that performs leakage reduction for the 3-qubit DF sub-
Table 1: Quantum numbers of commuting operators that uniquely specify all basis vectors in a three qubit, eight-dimensional Hilbert space. $S$ is the total spin of all three qubits and specifies whether the DFS qubit has leaked; $S = \frac{1}{2}$ is unleaked, $S = \frac{3}{2}$ is leaked. $S_{1,2}$ is the total spin of the first two qubits and gives the logical or encoded state for unleaked states. $S_z$ is the total spin-z of all three qubits and is the gauge quantum number. The top line gives the index labels of the basis vectors, which correspond to Eqs. (1)–(8).

|   | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  |
|---|----|----|----|----|----|----|----|----|
| $S$| $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{3}{2}$ | $\frac{3}{2}$ |
| $S_{1,2}$ | 0 | 0 | 1 | 1 | 1 | 1 | 1 | 1 |
| $S_z$ | $\frac{1}{2}$ | $-\frac{1}{2}$ | $\frac{1}{2}$ | $-\frac{1}{2}$ | $\frac{1}{2}$ | $-\frac{1}{2}$ | $\frac{1}{2}$ | $-\frac{1}{2}$ |

2 Angular Momentum Structure of DFS

The basis states of the Hilbert space containing three qubits can be described by three angular momentum quantum numbers $S$, $S_{1,2}$, and $S_z$. $S$ is the total spin of the three qubits, corresponding to the eigenvalues of the operator $S^2 \equiv S_x^2 + S_y^2 + S_z^2$, where $S_j \equiv 1/2(\sigma_j^{(1)} + \sigma_j^{(2)} + \sigma_j^{(3)})$ is the total angular momentum in the $j$ direction, $\sigma_j^{(n)}$ is the $j$th Pauli matrix on the $n$th qubit, and $\hbar \equiv 1$. The eigenvalues of $S^2$ are $S(S + 1)$. $S_{1,2}$ is similarly the total spin of the first two qubits, and $S_z$ the total $z$ spin of all three qubits. The eigenstates described by these quantum numbers are shown in Table 1. Their corresponding eigenvectors
can be written in the computational basis via Clebsch-Gordan coefficients:

\[ |1\rangle = \frac{1}{\sqrt{2}} (|010\rangle - |100\rangle) = |S_0\rangle |0\rangle \]  
\[ |2\rangle = \frac{1}{\sqrt{2}} (|011\rangle - |101\rangle) = |S_0\rangle |1\rangle \]  
\[ |3\rangle = \frac{\sqrt{2}}{3} |001\rangle - \frac{1}{\sqrt{6}} |010\rangle - \frac{1}{\sqrt{6}} |100\rangle = \frac{1}{\sqrt{3}} (\sqrt{2} |T_+\rangle |1\rangle - |T_0\rangle |0\rangle) \]  
\[ |4\rangle = \frac{1}{\sqrt{6}} (|011\rangle + |101\rangle - \sqrt{\frac{2}{3}} |110\rangle) = \frac{1}{\sqrt{3}} (|T_0\rangle |1\rangle - \sqrt{2} |T_-\rangle |0\rangle) \]  
\[ |5\rangle = |000\rangle = |T_+\rangle |0\rangle \]  
\[ |6\rangle = \frac{1}{\sqrt{3}} (|001\rangle + |010\rangle + |100\rangle) = \frac{1}{\sqrt{3}} (|T_+\rangle |1\rangle + \sqrt{2} |T_0\rangle |0\rangle) \]  
\[ |7\rangle = \frac{1}{\sqrt{3}} (|011\rangle + |101\rangle + |110\rangle) = \frac{1}{\sqrt{3}} (\sqrt{2} |T_0\rangle |1\rangle + |T_-\rangle |0\rangle) \]  
\[ |8\rangle = |111\rangle = |T_-\rangle |1\rangle \]  

where the singlet \( |S_0\rangle \) and triplet \( |T_\mu\rangle \) states are defined as:

\[ |S_0\rangle = \frac{1}{\sqrt{2}} (|01\rangle - |10\rangle) \]  
\[ |T_+\rangle = |00\rangle \]  
\[ |T_0\rangle = \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \]  
\[ |T_-\rangle = |11\rangle \]  

The singlet and triplets are eigenstates of the \( S_{1,2}^z \) operator.

The 3-qubit DFS is spanned by the first four eigenstates in Table [1]. The total spin quantum number \( S \) distinguishes between states in the valid unlocked subspace (\( S = \frac{1}{2} \)) and leaked states (\( S = \frac{5}{2} \)). Within the unlocked subspace a valid state of the 3-qubit DF subsystem has encoded (or logical) quantum number \( S_{1,2} \) and gauge quantum number \( S_z \) that are unentangled: valid states are factorizable states of the abstract (rather than physical) subsystems corresponding to \( S_{1,2} \) and \( S_z \) quantum numbers. Valid DFS subsystem states are given by \( \alpha(|\gamma| |1\rangle + \delta |2\rangle) + \beta(|\gamma| |3\rangle + \delta |4\rangle) \). In terms of the \( S_{1,2} \) and \( S_z \) quantum numbers we see the factorizability explicitly:

\[ \alpha(|\gamma| |1\rangle + \delta |2\rangle) + \beta(|\gamma| |3\rangle + \delta |4\rangle) \]  
\[ = \alpha(|\gamma| S = 1/2, S_{1,2} = 0, S_z = 1/2) + \delta |1/2, 0, -1/2\rangle + \beta(|\gamma| S = 1/2, 1, 1/2) + \delta |1/2, 1, -1/2\rangle \]  

Global decoherence mechanisms couple only to the \( S_z \) quantum number, and thus modify the gauge state only and not the encoded information. A 3-qubit DFS state can be initialized as a singlet in the first two qubits and an arbitrary spin in the third qubit, giving the state \( \gamma |1\rangle + \delta |2\rangle \). The initialized state has encoded quantum number \( S_{1,2} = 0 \) and an undefined gauge state unentangled
with the encoded quantum number. Assuming that the 3-qubit DFS is not leaked, measurement of the total spin $S_{1,2}$ on the first two qubits distinguishes between singlet and triplet states and gives the logical content of the DFS.

Encoded operations on the 3-qubit DFS are performed using the exchange interaction between its constituent qubits. The exchange interaction between qubits $m$ and $n$ is defined as

$$H_{m,n}^{ex} = \frac{1}{4} (\sigma_z^{(m)} \cdot \sigma_z^{(n)} + \sigma_y^{(m)} \cdot \sigma_y^{(n)} + \sigma_z^{(m)} \cdot \sigma_z^{(n)}).$$

The exchange interaction generates the SWAP operation between qubits $m$ and $n$, with a partial swap operation given by

$$U_{m,n}^{ex}(p) = \exp(-i\pi p H_{m,n}^{ex});$$

$U_{m,n}^{ex}(p = \pm 1)$ gives the usual SWAP operation up to a global phase. Because the exchange interaction generates swaps between qubits making up the 3-qubit DFS, it cannot change any total angular momentum quantum numbers: it commutes with both $S$ and $S_z$ (as well as $S_x$ and $S_y$). The exchange interaction does change the $S_{1,2}$ quantum number and hence the encoded state: exchange between qubits 1 and 2 generates an encoded $z$ rotation, and exchange between qubits 2 and 3 generates an encoded rotation about the $\hat{n} = \{\sqrt{3}/2, 0, -1/2\}$ axis.

The fact that the exchange interaction cannot change total angular momentum quantum numbers motivates the choice for the set of quantum numbers describing two 3-qubit DFS’s or six physical qubits. For DFS qubits $A$ and $B$, a valid basis set is simply the “product basis” of the $A$ and $B$ eigenvectors given in Table 1. None of the quantum numbers of the product basis commutes with all of the possible exchange operations between the six physical qubits. However, if we use the total angular momentum basis consisting of quantum numbers $S_{tot}$, $S_z$ tot, $S_A$, $S_B$, $S_{A,1,2}$, and $S_{B,1,2}$, the conservation of $S$ tot and $S_z$ tot leads to a partial diagonalization of the exchange-constructed operator and the block structure described below. $S_{tot}$ is the total spin of all six physical qubits and $S_z$ tot is the total $z$ spin of all six physical qubits. $S_A$ ($S_B$) is the total spin of DFS qubit $A$ ($B$), with $S_A = \frac{3}{2}$ and $S_B = \frac{5}{2}$ corresponding to unleaked states. $S_{A,1,2}$ ($S_{B,1,2}$) is the spin of the first two qubits of DFS qubit $A$ ($B$) and gives the logical information encoded in DFS qubit $A$ ($B$).

The structure of a six-qubit system is given in [4]. It consists of five spin-0 subspaces, nine spin-1 subspaces, five spin-2 subspaces, and one spin-3 subspace [17]. Each total spin subspace is further divided into $S_{z, tot}$ subspaces. Tables 2–4 show the quantum numbers for the basis states of $S_{tot} = 0, 1, 2$, respectively ($S_{tot} = 3$ is not needed in the following). Table 2 gives the five-dimensional spin-0 subspace of the six physical qubit system. Table 3 gives the nine-dimensional $S_{tot} = 1$, $S_{z, tot} = -1$ subspace; $S_{tot} = 1$, $S_{z, tot} = 0$ or 1 have analogous nine-dimensional subspaces. Table 4 gives the five-dimensional $S_{tot} = 2$, $S_{z, tot} = -2$ subspace; similarly, $S_{tot} = 2$ and $S_{z, tot} = -1, 0, 1, 2$ have analogous five-dimensional subspaces. The 64-dimensional basis vectors can again be written in terms of the computational basis of six spin-1/2 particles using Clebsch-Gordan coefficients.

Because the exchange interaction commutes with $S_{tot}$ and $S_{z, tot}$, any operator constructed from exchange gates cannot mix subspaces with different
Table 2: Quantum numbers for two DFS qubits in the total spin-0 subspace. 

|       | 1   | 2   | 3   | 4   | 5   |
|-------|-----|-----|-----|-----|-----|
| \(S_{\text{tot}}\) | 0   | 0   | 0   | 0   | 0   |
| \(S_{z,\text{tot}}\) | 0   | 0   | 0   | 0   | 0   |
| \(S_A\) | 1   | 1   | 1   | 1   | 3   |
| \(S_B\) | \(\frac{3}{2}\) | \(\frac{3}{2}\) | \(\frac{3}{2}\) | \(\frac{3}{2}\) | \(\frac{3}{2}\) |
| \(S_{A,1,2}\) | 0   | 0   | 1   | 1   | 1   |
| \(S_{B,1,2}\) | 0   | 1   | 0   | 1   | 1   |

\(S_{\text{tot}}\) and \(S_{z,\text{tot}}\). Additionally, because the exchange interaction also commutes with \(S_{z,\text{tot}}\) and \(S_{y,\text{tot}}\), exchange-constructed operators must have exactly the same matrix entries on subspaces with the same \(S_{\text{tot}}\) but different \(S_{z,\text{tot}}\). That is, the matrix entries of an exchange-constructed operator on the \(S_{\text{tot}} = 1\), \(S_{z,\text{tot}} = -1\) subspace are exactly the same on the \(S_{\text{tot}} = 1\), \(S_{z,\text{tot}} = 0\) and \(S_{\text{tot}} = 1\), \(S_{z,\text{tot}} = 1\) subspaces, and similarly for \(S_{\text{tot}} = 2\), \(S_{z,\text{tot}} = -2\), -1, 0, 1, 2. When written in the total angular momentum basis, an exchange-constructed operator is a block diagonal matrix, whose diagonal blocks are one 5×5 spin-0 block, three identical 9×9 spin-1 blocks, five identical 5×5 spin-2 blocks, and a spin-3 block consisting of a 7×7 identity matrix times a phase factor; none of these blocks couples to another. If we define the generator of swap to be 

\[ H_{\text{sw}}^{m,n} = H_{m,n}^{x} - 1/4, \]

so that \(\exp(-i\pi H_{\text{sw}}^{m,n})\) gives a full SWAP, including the global phase, the swap-generated group is \(SU(5) \times SU(9) \times SU(5) \times U(1)\). The \(S_{\text{tot}} = 3\) subspace transforms as the identity under swaps, so the \(U(1)\) phase factor must be \(\exp(-i\theta[S_{\text{tot}}(S_{\text{tot}} + 1) - 12])\). The algebraic origin of the block structure is described in \[7, 8\]. Constructing DFS operators on the two DFS qubits amounts to finding exchange gate sequences that satisfy the desired forms of the block matrix in the total angular momentum basis.

### 3 DFS CNOT Pulse Sequence

The CNOT operation on two unleaked 3-qubit DFS’s must perform a CNOT gate on the logical DFS information contained in the quantum numbers \(S_{A,1,2}\) and \(S_{B,1,2}\), independent of the gauge state. We seek an exchange pulse sequence, i.e., a sequence of unitary operators generated by the exchange interaction, whose product in the total angular momentum basis gives the required CNOT operation on the encoded quantum numbers. Because of the structure of exchange-constructed matrices described in Section 2, we need only constrain
Table 3: Quantum numbers for two DFS qubits in the total spin-1, $S_{z,\text{tot}} = -1$ subspace. Basis vectors 6–9 are valid encoded states; basis vectors are leaked states, with one or both of the constituent DFS qubits leaked. Basis vectors 10 and 11 are unleaked in DFS qubit $A$. See Table 2 for operator definitions.

|       | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 |
|-------|---|---|---|---|----|----|----|----|----|
| $S_{\text{tot}}$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $S_{z,\text{tot}}$ | $-1$ | $-1$ | $-1$ | $-1$ | $-1$ | $-1$ | $-1$ | $-1$ | $-1$ |
| $S_A$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ |
| $S_B$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ |
| $S_{A,1,2}$ | 0 | 0 | 1 | 1 | 0 | 1 | 1 | 1 | 1 |
| $S_{B,1,2}$ | 0 | 1 | 0 | 1 | 1 | 1 | 0 | 1 | 1 |

Table 4: Quantum numbers for two DFS qubits in the total spin-2, $S_{z,\text{tot}} = -2$ subspace. Basis vectors 15 and 16 are unleaked in DFS qubit $A$. See Table 2 for operator definitions.

|       | 15 | 16 | 17 | 18 | 19 |
|-------|----|----|----|----|----|
| $S_{\text{tot}}$ | 2 | 2 | 2 | 2 | 2 |
| $S_{z,\text{tot}}$ | $-2$ | $-2$ | $-2$ | $-2$ | $-2$ |
| $S_A$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ |
| $S_B$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ | $\frac{\sqrt{2}}{2}$ |
| $S_{A,1,2}$ | 0 | 1 | 1 | 1 | 1 |
| $S_{B,1,2}$ | 1 | 1 | 0 | 1 | 1 |
appropriately for the DFS CNOT. In the \( S_{\text{tot}} = 0, S_{z,\text{tot}} = 0 \) block the CNOT matrix must take the following form:

\[
e^{i\theta_0}
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & e^{i\phi_0}
\end{pmatrix},
\]

(15)

where \( \theta_0 \) and \( \phi_0 \) are arbitrary phases, and the rows and columns correspond to the basis vectors 1–5 in Table 2. The upper left 4 \( \times \) 4 block is the usual CNOT operation on the unleaked, logical states; unitarity requires that the leaked state with \( S_{\text{tot}} = 0 \), basis vector 5, be uncoupled from the unleaked states. In the three 9 \( \times \) 9 spin-1 blocks the CNOT matrix must be

\[
e^{i\theta_1}
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & c_{1,1} & c_{1,2} & c_{1,3} & c_{1,4} & c_{1,5} \\
0 & 0 & 0 & 0 & c_{2,1} & c_{2,2} & c_{2,3} & c_{2,4} & c_{2,5} \\
0 & 0 & 0 & 0 & c_{3,1} & c_{3,2} & c_{3,3} & c_{3,4} & c_{3,5} \\
0 & 0 & 0 & 0 & c_{4,1} & c_{4,2} & c_{4,3} & c_{4,4} & c_{4,5} \\
0 & 0 & 0 & 0 & c_{5,1} & c_{5,2} & c_{5,3} & c_{5,4} & c_{5,5}
\end{pmatrix}
\]

(16)

where again \( \theta_1 \) is an arbitrary phase and the rows and columns correspond to basis vectors 6–14 in Table 3. The upper left 4 \( \times \) 4 block must be the CNOT on the encoded basis vectors, and the lower right 5 \( \times \) 5 block \( \{c_{i,j}\} \) is an arbitrary unitary matrix on the leaked states 10–14. Again, the leaked and unleaked states must not couple. The three 9 \( \times \) 9 spin-1 blocks are automatically identical when constructed out of exchange gates, so they need not be constrained separately. The CNOT matrix on the spin-2 and spin-3 subspaces is completely unconstrained, aside from unitarity, which is automatically satisfied with the exchange gates.

An objective function for the CNOT search is constructed from the constraints shown in Eqs. (15) and (16). Let \( U \) be the product of exchange gate unitaries in the total angular momentum basis, ordered so that basis vectors 1–5 correspond to Table 2 and basis vectors 6–14 correspond to Table 3. The objective function for the CNOT search is

\[
f_{\text{CNOT}}(U) = \sqrt{2 - \frac{1}{4}|U_{1,1} + U_{2,2} + U_{3,4} + U_{4,3}| - \frac{1}{4}|U_{6,6} + U_{7,7} + U_{8,9} + U_{9,8}|}.
\]

(17)

Since \( U \) is unitary by construction, its entries have modulus at most 1. The objective function is zero only when \( U_{1,1}, U_{2,2}, U_{3,4}, \) and \( U_{4,3} \) have modulus 1 and a common phase, and \( U_{6,6}, U_{7,7}, U_{8,9}, \) and \( U_{9,8} \) also have modulus 1 and
A_3

A_2

A_1

B_1

p_1

-1/2

1

-1/2

B_2

p_2

-1/2

1

-1/2

B_3

1 - p_2

Figure 1: Twenty-two pulse, 13 time step, exchange gate sequence for DFS CNOT. DFS qubits $A$ (control) and $B$ (target) are arranged as shown. Subscripts on $A$ and $B$ label the constituent physical qubits. Each gate corresponds to an exchange unitary $U^\text{ex}_{m,n}(p)$ [Eq. (14)], with the swap powers $p$ displayed explicitly in the gates. $p = 1$ corresponds to a full SWAP operation, up to a global phase. $p_1 = \arccos(-1/\sqrt{3})/\pi$ and $p_2 = \arcsin(1/3)/\pi$.

A (generally different) common phase. This objective function is used in the genetic algorithm described in Section 5. The two DFS qubits $A$ (control) and $B$ (target) are laid out in a linear array, in the order $A_3, A_2, A_1, B_1, B_2, B_3$. Only nearest neighbor exchange gates are permitted.

Figure 1 shows the best solution found by the genetic algorithm requiring 22 pulses in 13 time steps. Though the genetic algorithm uses approximate (finite precision) numbers, the final solution found is analytic, with the exchange gate powers shown in the figure. Writing the exchange unitaries given in Figure 1 in the total angular momentum basis and taking their product yields the following matrix for the spin-0 subspace:

$$
e^{i \theta_C} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 \end{pmatrix},$$

and for the spin-1 subspaces:

$$
e^{i \theta_C} \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{11}{16} & -\frac{5\sqrt{3}}{16} & 0 & 0 & -\frac{\sqrt{15}}{2} \\ 0 & 0 & 0 & -\frac{5\sqrt{3}}{16} & -\frac{1}{16} & 0 & 0 & 3\frac{\sqrt{5}}{8} \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{15}}{8} & 3\frac{\sqrt{5}}{8} & 0 & 0 & -\frac{1}{4} \end{pmatrix}.$$ (19)

The spin-0 and spin-1 subspaces have the same global phase. The matrices in Eqs. (18) and (19) clearly satisfy the constraints given in Eqs. (15) and (16).
The pulse sequence shown in Figure 1 thus gives the full (not merely locally equivalent) CNOT solution for the 3-qubit DF subsystem. Removing the \( p_1, p_2, -p_1, \) and \( 1 - p_2 \) gates results in a locally equivalent CNOT solution of 18 pulses in 11 time steps for the DF subsystem, which is shorter than the locally equivalent CNOT pulse sequence for the DF subspace only [10].

4 DFS Leakage Reduction Pulse Sequence

Given a possibly leaked DFS qubit A and a fiducial, unleaked DFS qubit B, the DFS leakage reduction operator has the following specification. If A is unleaked (a superposition of basis states 1–4 in Table 1), leakage reduction leaves the encoded quantum number \( S_{A,1} \) unchanged, but may possibly alter the gauge quantum number \( S_{A,z} \). If A is leaked, leakage reduction returns A to any state in the unleaked subspace. The state of DFS qubit B after leakage reduction is unconstrained, and will generally be leaked. Since we desire an exchange-only leakage reduction operator, the second, fiducial DFS qubit B is required. A single, leaked DFS qubit has total spin \( S = \frac{3}{2} \), which cannot be converted to an unleaked \( S = \frac{1}{2} \) state by exchange operations on the single DFS qubit alone.

Though the leakage reduction operator returns leaked states to the valid unleaked subspace, the final unleaked state is not necessarily a valid subsystem state—the reset state will not generally be a factorizable state of the encoded qubit and gauge qubit. After leakage reduction of a leaked state in DFS qubit A, the A wavefunction will be

\[
|\psi_A\rangle = \alpha_I |\psi_\lambda\rangle |\phi_{g,I}\rangle + \alpha_X Y_\lambda |\psi_\lambda\rangle |\phi_{g,X}\rangle + \alpha Y Z_\lambda |\psi_\lambda\rangle |\phi_{g,Y}\rangle + \alpha Z X_\lambda |\psi_\lambda\rangle |\phi_{g,Z}\rangle,
\]

(20)

where \( \alpha_\mu \) are complex amplitudes, \( |\psi_\lambda\rangle \) is the wavefunction of the encoded qubit, \( |\phi_{g,\mu}\rangle \) are wavefunctions of the gauge qubit, and \( X_\lambda, Y_\lambda, \) and \( Z_\lambda \) are single encoded qubit Pauli operators acting on the encoded wavefunction alone. The leakage reduced state thus generally appears as a superposition of the correct encoded state with Pauli-errors on the encoded state coupled to different gauge states. Standard quantum error correction will return such a superposition state in the unleaked subspace to a valid factorizable subsystem state. Quantum error correction procedures are constructed from DFS encoded gates such as the DFS CNOT, Hadamard, and Pauli gates. All the DFS gates have been constructed to act independently of the gauge state, so that quantum error correction on the encoded parts of Eq. (20) proceeds as usual. A projective measurement in the course of the error correction procedure selects one of the terms in Eq. (20), resulting in a valid factorizable DFS state. A similar argument holds in the case of fully coherent error correction.

The leakage reduction operator in the total angular momentum basis must have the following form. In the spin-0 subspace the leakage reduction matrix
must be
\[
\begin{pmatrix}
  d_{1,1} & d_{1,2} & 0 & 0 & 0 \\
  d_{2,1} & d_{2,2} & 0 & 0 & 0 \\
  0 & 0 & d_{1,1} & d_{1,2} & 0 \\
  0 & 0 & d_{2,1} & d_{2,2} & 0 \\
  0 & 0 & 0 & 0 & e^{i\phi}
\end{pmatrix}, \tag{21}
\]
where \(\{d_{i,j}\}\) is an arbitrary 2 \(\times\) 2 unitary matrix. The upper left 4 \(\times\) 4 block is the outer product of the identity on the encoded quantum number of DFS qubit \(A\) and an arbitrary unitary matrix on the encoded quantum number of DFS qubit \(B\). It ensures that the encoded quantum number of DFS qubit \(A\) is unchanged, with no constraint on the unitary evolution of DFS qubit \(B\)'s encoded quantum number, in the \(S_{\text{tot}} = 0, S_{z,\text{tot}} = 0\) gauge state. The decoupling of the fifth basis vector from the others ensures that no leakage from DFS qubit \(A\) occurs.

In the spin-1 subspaces the leakage reduction matrix must be
\[
\begin{pmatrix}
  e_{1,1} & e_{1,2} & 0 & 0 & 0 & 0 & f_{1,1}e_{1,3} & f_{1,2}e_{1,3} & 0 \\
  e_{2,1} & e_{2,2} & 0 & 0 & 0 & 0 & f_{1,1}e_{2,3} & f_{1,2}e_{2,3} & 0 \\
  0 & 0 & e_{1,1} & e_{1,2} & 0 & 0 & f_{2,1}e_{1,3} & f_{2,2}e_{1,3} & 0 \\
  0 & 0 & e_{2,1} & e_{2,2} & 0 & 0 & f_{2,1}e_{2,3} & f_{2,2}e_{2,3} & 0 \\
  e_{3,1} & e_{3,2} & 0 & 0 & 0 & 0 & f_{1,1}e_{3,3} & f_{1,2}e_{3,3} & 0 \\
  0 & 0 & e_{3,1} & e_{3,2} & 0 & 0 & f_{2,1}e_{3,3} & f_{2,2}e_{3,3} & 0 \\
  0 & 0 & 0 & 0 & g_{1,1} & g_{1,2} & 0 & 0 & g_{1,3} \\
  0 & 0 & 0 & 0 & g_{2,1} & g_{2,2} & 0 & 0 & g_{2,3} \\
  0 & 0 & 0 & 0 & g_{3,1} & g_{3,2} & 0 & 0 & g_{3,3}
\end{pmatrix}, \tag{22}
\]
where \(\{e_{i,j}\}, \{f_{i,j}\},\) and \(\{g_{i,j}\}\) are all arbitrary unitary matrices. The ordering of matrix entries again corresponds to the basis vector ordering in Table 3. Column 1 of Eq. \(22\) gives the action of the leakage reduction operator on basis vector 6 in Table 3. Basis vector 6 can be brought to basis vectors 6,7, and 10, in any complex linear combination: this action preserves the encoded 0 quantum number of DFS qubit \(A\) and keeps \(A\) unleaked, while allowing DFS qubit \(B\) to change its encoded state, or even leak. Basis vector 7 (column 2) has a similar evolution as basis vector 6. Columns 3 and 4 must be the same as columns 1 and 2, albeit with shifted entries; this ensures the identity is applied on the encoded quantum number of DFS qubit \(A\). The constraints on columns 1–4 and the constraints on the spin-0 matrix together ensure that the identity is applied on the encoded quantum number of DFS qubit \(A\) regardless of gauge state, assuming an unleaked DFS qubit \(B\).

The remaining columns of Eq. \(22\) repair leaked states of DFS qubit \(A\) in the spin-1 subspaces. Columns 7 and 8 (basis vectors 12 and 13) bring a leaked DFS qubit \(A\) into basis vectors 6–11, which are all unleaked in DFS qubit \(A\), leaving no components in the leaked basis vectors 12–14. Unitarity of Eq. \(22\) forces the entwining of the \(\{e_{i,j}\}\) and \(\{f_{i,j}\}\) matrices. Unitarity again forces columns 5, 6, and 9 to have 0 entries in their first six components, leaving \(\{g_{i,j}\}\) to be an arbitrary 3 \(\times\) 3 unitary matrix.

Leaked states of DFS qubit \(A\) also exist in the spin-2 subspaces and must be reduced to unleaked states. In the spin-2 subspace the leakage reduction matrix
must be
\[
\begin{pmatrix}
0 & 0 & h_{1,1} & h_{1,2} & 0 \\
0 & 0 & h_{2,1} & h_{2,2} & 0 \\
k_{1,1} & k_{1,2} & 0 & 0 & k_{1,3} \\
k_{2,1} & k_{2,2} & 0 & 0 & k_{2,3} \\
k_{3,1} & k_{3,2} & 0 & 0 & k_{3,3}
\end{pmatrix},
\]  
(23)

where \(\{h_{i,j}\}\) and \(\{k_{i,j}\}\) are arbitrary unitary matrices. The ordering of matrix entries in Eq. (23) corresponds to the basis vector ordering in Table 4. Columns 3 and 4 ensure that basis vectors 17 and 18, which are leaked in DFS qubit A and unleaked in DFS qubit B, are brought to basis vectors 15 and 16, which are unleaked in DFS qubit A. We stress that here and in the other spin subspaces, DFS qubit B must be unleaked, or leakage reduction of DFS qubit A will fail. The spin-3 subspace of the leakage reduction operator acts only on basis vectors that have both DFS qubits leaked and is unconstrained aside from unitarity.

An objective function for the leakage reduction operator is constructed from the constraints given in Eqs. (21)–(23). We additionally constrain \(\{f_{i,j}\} = \{h_{i,j}\}\), which forces a leaked state in DFS qubit A to be reset to a factorizable state of encoded and gauge quantum numbers. (This constraint is not necessary, but enabled us to find an analytic solution.) Again, let \(U\) be the product of exchange gate unitaries in the total angular momentum basis, and order the basis vectors according to Tables 2–4. We define the following matrices, constructed from components of \(U\):

\[
D^{(1)} = \begin{pmatrix} U_{1,1} & U_{1,2} \\ U_{2,1} & U_{2,2} \end{pmatrix},
\]
(24)
\[
D^{(2)} = \begin{pmatrix} U_{3,3} & U_{3,4} \\ U_{4,3} & U_{4,4} \end{pmatrix},
\]
(25)
\[
L^{(1)} = \begin{pmatrix} U_{6,12} & U_{6,13} \\ U_{8,12} & U_{8,13} \end{pmatrix},
\]
(26)
\[
L^{(2)} = \begin{pmatrix} U_{7,12} & U_{7,13} \\ U_{9,12} & U_{9,13} \end{pmatrix},
\]
(27)
\[
L^{(3)} = \begin{pmatrix} U_{10,12} & U_{10,13} \\ U_{11,12} & U_{11,13} \end{pmatrix},
\]
(28)
\[
H = \begin{pmatrix} U_{15,17} & U_{15,18} \\ U_{16,17} & U_{16,18} \end{pmatrix},
\]
(29)

with \(M^{(j)} = H^\dagger L^{(j)}\), and

\[
E^{(1)} = \begin{pmatrix} U_{6,6} & U_{6,7} & M^{(1)}_{1,1} \\ U_{7,6} & U_{7,7} & M^{(2)}_{1,1} \\ U_{10,6} & U_{10,7} & M^{(3)}_{1,1} \end{pmatrix},
\]
(30)
\[
E^{(2)} = \begin{pmatrix} U_{8,8} & U_{8,9} & M^{(1)}_{2,2} \\ U_{9,8} & U_{9,9} & M^{(2)}_{2,2} \\ U_{11,8} & U_{11,9} & M^{(3)}_{2,2} \end{pmatrix}.
\]
(31)
Figure 2: Thirty pulse, 20 time step, exchange gate sequence for DFS leakage reduction operator. DFS qubits \( A \) (potentially leaked) and \( B \) (fiducial, unleaked) are arranged as shown. Swap powers are displayed explicitly in the gates. \( q_1 = \arccos(1/3)/\pi \) and \( q_2 = \arcsin(1/\sqrt{3})/\pi \).
With these definitions the leakage reduction operator objective function is

\[
 f_{\text{LRO}}(U) = \left\| \frac{1}{4} (D^{(1)} + D^{(2)})^\dagger (D^{(1)} + D^{(2)}) - I_2 \right\|
 + \left\| \frac{1}{4} (E^{(1)} + E^{(2)})^\dagger (E^{(1)} + E^{(2)}) - I_3 \right\|
 + \| H^\dagger H - I_2 \|,
\]

where \( I_n \) is the \( n \times n \) identity matrix. The objective function is zero when: \( D^{(1)} = D^{(2)} \) and each is unitary, satisfying Eq. (21); \( H \) is unitary, satisfying Eq. (23); and \( E^{(1)} = E^{(2)} \) and each is unitary, satisfying Eq. (22) and the additional constraint that \( \{ f_{i,j} \} = \{ h_{i,j} \} \).

Figure 2 shows the best solution found by the genetic algorithm, requiring 30 pulses in 20 time steps. Again, the solution found is analytic, with the exchange gate powers shown in the figure. In the total angular momentum basis the product of the exchange gate unitaries satisfies the forms given in Eqs. (21)–(23). In Eq. (21) the free phase satisfies \( e^{i\phi} = 1 \), while the constituent unitary matrices, up to a common global phase, are explicitly:

\[
\{ d_{i,j} \} = \begin{pmatrix}
0 & \frac{1}{6} (i + \sqrt{3}) (3i + \sqrt{3}) \\
(-1)^{5/6} & 0
\end{pmatrix},
\]

\[
\{ e_{i,j} \} = \begin{pmatrix}
0 & \frac{1}{6} (i + \sqrt{3}) (3i + \sqrt{3}) & 0 & -\frac{2\sqrt{3}}{3} \\
\frac{1}{2\sqrt{2}} (-i + \sqrt{3}) & 0 & \frac{1}{3}
\end{pmatrix},
\]

\[
\{ f_{i,j} \} = \begin{pmatrix}
\frac{1}{12} (-i + 2\sqrt{2}) (3i + \sqrt{3}) & \frac{1}{12} (1 - i\sqrt{2}) (3i + \sqrt{3}) \\
\frac{1}{4} (-i + \sqrt{3}) & -\frac{1}{4} (-i + \sqrt{3}) (-i + \sqrt{3})
\end{pmatrix},
\]

\[
\{ g_{i,j} \} = \begin{pmatrix}
-\frac{1}{2} & \sqrt{-\frac{7}{12} + \frac{i\sqrt{3}}{3}} & 0 \\
-\frac{7}{24} \sqrt{2} \frac{1}{24} & \frac{1}{18} & -\frac{1}{9}
\end{pmatrix},
\]

\[
\{ h_{i,j} \} = \{ f_{i,j} \},
\]

\[
\{ k_{i,j} \} = \begin{pmatrix}
\frac{1}{2} & \sqrt{-\frac{7}{12} + \frac{i\sqrt{3}}{3}} & 0 \\
0 & -\frac{1}{2} & 0 \\
0 & 0 & -1
\end{pmatrix}.
\]

5 Genetic Algorithm

The DFS CNOT and leakage reduction operator gate sequences were constructed using the genetic method to minimize objective functions associated with the desired CNOT and leakage reduction operator block matrix forms. Although simple genetic algorithms can be quite slow, finding sequences of the lengths needed for the CNOT and leakage reduction operators (fewer than 40
gates) can be accomplished using a rather naive programming approach in a few weeks of evolution on an Apple XServe computer. (We also attempted optimization by simulated annealing, but the gate sequences we present here for the CNOT and leakage reduction operator were both found by genetic methods.) It helps that the time consuming part of the computation is embarrassingly parallel.

Our genetic approach iterates random changes on some population of gate configurations, each given by a list of powers of swap between adjacent physical qubits. At each iteration (“generation”) we augment the population with “mutations” and “mating”, and then apply “natural selection” that favors those configurations with low value of the objective function. We augment the objective functions given in Eqs. (17) and (32) by adding a “gate penalty” term which is simply the length of the sequence times some positive constant, the gate penalty parameter. The gate penalty parameter is adjusted as the evolution progresses to give a reasonable tradeoff between lowering the objective function and lowering the gate count.

The code was written in Mathematica Version 7.0 [18], using the built-in parallel processing capability. The two key Mathematica functions used were FindMinimum and RandomSample. FindMinimum searches for a local minimum of a function using a variety of local descent methods; RandomSample gives a pseudorandom sampling of a list with optionally weighted probability. Further description of these functions may be found in the Mathematica documentation [18].

5.1 Mutations

We have programmed five different types of mutations, chosen at random. We have varied the probabilities of each mutation, but for our CNOT and leakage reduction operator solutions, the probabilities are as shown:

**RefineOne (8%)**: randomly chooses one gate of a configuration and uses FindMinimum to optimize its power of swap, starting with the current value.

**RefineTwo (8%)**: randomly chooses an adjacent pair of gates and simultaneously minimizes the objective with respect to both powers of swap.

**RefineAll (4%)**: runs FindMinimum on all powers in the configuration. The time required to do this grows rapidly with the number of variables and is much larger than that of the previous two mutations. The Mathematica AccuracyGoal and PrecisionGoal Options of FindMinimum are set to modest values (< 5) so that this operation runs in a tolerable length of time.

**InsertGate (40%)**: inserts a gate at a random location with a random power, followed by RefineOne.
DeleteGate (40%): deletes a gate at a random location, followed by RefineTwo on the gates that were adjacent to the one removed. If the removed gate was the first or last, the RefineOne is used.

5.2 Mating

The initial population (unmutated) is divided into pairs. We take the beginning of one gate configuration and append the end of the other, and then run RefineAll. The length of the resultant “offspring” is chosen to be the minimum of that of the parent configurations and the number of gates from each parent is chosen at random. Because of RefineAll, this is a time consuming operation—but without the RefineAll very few of the offspring would survive natural selection. The genetic algorithm can be used without mating, but the diversity of the population suffers.

5.3 Natural Selection

Surviving gate configurations are selected using the Mathematica function RandomSample. The sampling weight, which is proportional to the probability of a member of the population appearing in the sample, is given by the inverse of the objective function augmented by the gate penalty term. Configurations with a small value of the objective function and low gate count are most likely to survive. The population size is specified by a parameter under user control. After the survivors are determined, gates between the same pair of qubits that are not separated by any noncommuting gates are combined into one gate, by simply adding their powers.

6 Conclusion

Using a genetic algorithm, we have found new, exact exchange gate pulse sequences for the encoded CNOT operation on two 3-qubit DFS qubits, as well as for the DFS leakage reduction operator. Our CNOT solution gives the most efficient sequence yet found for either the 3-qubit subspace or subsystem, while our leakage reduction solution is the first explicit sequence for any exchange-only subspace or subsystem encoding. We have found a wide range of other solutions for the DFS CNOT and leakage reduction operator, but the sequences presented here are the most efficient thus far. Other solutions that place additional constraints on the evolution of the leaked states may have superior error propagation properties when combined with fault tolerant error correction procedures; further investigation of such sequences is underway.

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