Subsystem pseudopure states

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(Received 5 November 2006; published 18 April 2007)

A critical step in experimental quantum information processing (QIP) is to implement control of quantum systems protected against decoherence via informational encodings, such as quantum error-correcting codes, noiseless subsystems, and decoherence-free subspaces. These encodings lead to the promise of fault-tolerant QIP, but they come at the expense of resource overheads. Part of the challenge in studying control over multiple logical qubits is that QIP testbeds have not had sufficient resources to analyze encodings beyond the simplest ones. The most relevant resources are the number of available qubits and the cost to initialize and control them. Here we demonstrate an encoding of logical information that permits control over multiple logical qubits without full initialization, an issue that is particularly challenging in liquid-state NMR. The method of subsystem pseudopure states will allow the study of decoherence control schemes on up to six logical qubits using liquid-state NMR implementations.

DOI: 10.1103/PhysRevA.75.042321 PACS number(s): 03.67.Pp, 76.60.−k, 33.25.+k

I. INTRODUCTION

Liquid-state nuclear magnetic resonance (NMR) is a convenient testbed for new ideas in quantum information processing (QIP). NMR has been used to experimentally test quantum algorithms [1,2], control strategies [3–6], and steps toward fault-tolerant quantum computation [7–9]. Recently, the focus has turned to control of encoded information that will allow quantum processors to avoid decoherence. The advantages achieved by encoding information come at the expense of physical resources, as the encoding requires additional qubits as ancillas [10–12]. For liquid-state NMR to continue its role as a QIP testbed, the size of the systems used must increase. This is a critical issue because of the signal loss for pseudopure states accompanying each added qubit [13,14]. Here we propose a scheme to reduce this signal decrease, that will allow the study of 3–6 logical qubits with the current experimental instrumentation. We first review the sources of signal loss tied to the creation of pseudopure states in NMR and introduce a class of pure states that we call *subsystem* pseudopure states, for which this signal loss is significantly reduced. Before quantifying the gain in signal for a general encoding, we present an example drawn from a widely studied encoding. Finally, we discuss the experimental results with particular attention to the metrics of control that the subsystem pseudopure states allow us to measure and their ability to quantify the actual control reached in experimental tests.

II. SUBSYSTEM PSEUDOPURE STATES

At room temperature and in a high magnetic field, the NMR spin system is a highly mixed state described by the thermal density matrix ρ_{th}:

$$\rho_{th} \approxeq \frac{\mathbb{1}}{2^N} - \epsilon\rho_{eq} = \frac{\mathbb{1}}{2^N} - \frac{\epsilon}{2^N}\sum_{i=1}^{N}\sigma_z^i, \tag{1}$$

where the term $\epsilon\rho_{eq}$ is a small, traceless deviation from the identity, which gives rise to the observable signal. The ability to use this system as a quantum information testbed relies on effectively purifying the mixed equilibrium state. QIP can be performed on pseudopure states [14–16], states for which the dynamics of the observable operators are equivalent to the observables of a pure state. Unfortunately, the creation of pseudopure states comes at the expense of exponential consumption in experimental resources: time in the case of temporal averaging [15], signal in the case of spatial averaging [16], or usable Hilbert space in the case of logical labeling [14].

Since the eigenvalues of a pseudopure state are different from those of the mixed state [with the exception of SU(2)], a nonunitary completely positive operation T must be implemented:

$$\rho_P = T(\rho_{th}) = \frac{\mathbb{1}}{2^N} - \epsilon\alpha\left(\rho_{pp} - \frac{\mathbb{1}}{2^N}\right), \tag{2}$$

where ρ_{pp} is a density matrix describing a pure state. The scaling factor α determines the signal loss and is bounded by the spectral norm ratio (since $\|\rho_{eq}\| \geqslant \|T(\rho_{eq})\|$)

$$\alpha \leqslant \frac{\|\rho_{eq}\|}{\|\rho_{pp} - \mathbb{1}/2^N\|} \tag{3}$$

with $\|\rho_{eq}\| = N/2^N$. The signal-to-noise ratio (SNR) loss in the case of a full pseudopure state is thus $N/(2^N-1)$. This exponential loss of signal is one of the facts that disqualify liquid-state NMR as a scalable approach to QIP [17,18]. Even if algorithmic purification schemes [13,19,20] could be applied, if there were a sufficient number of spins over which we had high fidelity control, stronger spin-spin couplings and longer T_2 times would be required. Considering that we have the ability to coherently control 10–12 qubits [21] and possess spin systems responsive to such control, the loss of signal when preparing pseudopure states is also a serious limitation for benchmarking these systems.

To avoid this SNR loss when studying encoded operations, we can use the additional flexibility afforded since only the subsystems encoding the information need to be pseudopure, while all other subsystems can be left in a mixed state. This also reduces the complexity of the state prepara-

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tion. In a parallel way [22], it had been observed that imperfect state preparation is enough for the existence of decoherence-free subspaces (DFSs). To present the general structure that encoding imposes on the Hilbert space, we adopt the subsystem approach [23,24], which provides a unified description for quantum error correction (QEC) [25–27], decoherence-free subspaces [11,12,28], and noiseless subsystems (NSs) [29–32]. A Hilbert space $\mathcal{H}$ of dimension $d=2^N$ is used to encode $l\leqslant N$ qubits of information, protected against some noise $J=\{J_\alpha\}$. With a change of basis to a direct sum[1] $\mathcal{H}\cong\oplus_i\mathcal{L}_i\otimes\mathcal{S}_i$, the noise acts only on the subsystems $\mathcal{S}_i$ (the syndrome) while the subsystems $\mathcal{L}_i$ are noiseless (for simplicity, we will often refer to a decomposition $\mathcal{H}=\mathcal{L}\otimes\mathcal{S}\oplus\mathcal{R}$, with $\mathcal{R}$ an unprotected subspace).

To perform computations on logical qubits, they need to be prepared in a (pseudo)pure state. The remaining subsystems $\mathcal{S}_i$ can, however, remain in a mixed state. We require only that the logical state evolves as a pure state in the logical subsystem, under the action of logical operations.

If we are evolving the system with logical operators, the fact that they act only on the encoded subspace $\mathcal{L}$ ensures that information within this subspace will not leak out or mix with the orthogonal spaces during logical unitary transformations, thus preserving the purity of the encoded subspace under the noise model. An important requirement for the subsystem pseudopure states is the ability to decode: the use of a mixed state should not introduce a mixing of the information contained in the logical qubits and in the unprotected subsystems, even when the information is transferred back to physical qubits by decoding. For unital maps, setting the unprotected subsystem to the identity state will satisfy this requirement without any further action required on the decoded state (notice that other mixed states are possible for particular encodings). For a DFS or a NS, not being able to apply the simple decoding operation to transfer the full information back to the physical qubits is inconvenient, as logical observables are in general difficult to measure experimentally since they are usually given by many-body states in the basis of the physical system. In the case of QEC the decoding involves also a correction step. If the unprotected part of the Hilbert space has evolved, it is no longer possible to perform a unique correction operation, valid for any input state.

The state preparation procedure that bears the most resemblance to the method we propose is logical labeling [14], which uses a unitary transformation to change the equilibrium distribution of spin states into one where a subsystem of the Hilbert space is pseudopure conditional on a physical spin having some preferred orientation. The parts of Hilbert space that remain mixed are of no use to the computation. It can be shown that an m-qubit pseudopure state can be stored among the Hilbert space of N qubits provided the inequality $(2^m-1)\leqslant N!/[(N/2)!]^2$ is satisfied. A key insight is that in the study of encoded qubits, one need not take this m-qubit effective pure state and perform an encoding of l logical qubits under the hierarchy $l<m<N$: Instead, an l-qubit encoded state can be prepared directly from the equilibrium state of N qubits.

If information is encoded in a subsystem of dimension 2^l, with a corresponding syndrome subsystem $\mathcal{S}$ of dimension d_s that we can leave in a mixed state, the number of zero eigenvalues in this subsystem pseudopure state is $(2^l-1)d_s$. We can create a state that is pure on the logical degrees of freedom as long as there are at least as many zero eigenvalues in the thermal state as in the l-qubit pure state: $(2^l-1)\leqslant N!/[(N/2)!]^2 d_s$. However, the eigenvalue spectrum of the equilibrium state of an N-spin density matrix $[\lambda(\rho_{eq})=\{N,N-2,\ldots,-N\}]$ will most generally not generate the necessary eigenvalue spectrum required for decoding the l qubits of information into l physical qubits without error. So a combination of techniques must be used.

Before presenting a general model that allows us to quantify the SNR gain obtained by the subsystem pseudopure states, we will clarify the concept with an example.

III. EXAMPLE

In a DFS information is protected inside subspaces of the total Hilbert space that are invariant under the action of the noise generators. Here we consider collective σ_z noise, which describes a dephasing caused by completely correlated fluctuations of the local magnetic field $B_z\hat{z}$:

$$\mathcal{H}_{SE}=J_z\otimes B_z, \tag{4}$$

with $J_z=\Sigma_i\sigma_z^i$, the total spin angular momentum along the quantization axis z. In a Hilbert space of dimension 4, the eigenspace of the noise operator J_z with eigenvalue 0 is a two-dimensional DFS [8] and can be used to encode one qubit of information. The DFS is spanned by the basis vectors $|01\rangle$ and $|10\rangle$. A natural encoding of a logical qubit $|\psi\rangle_L$ is given by

$$\alpha|0\rangle_L+\beta|1\rangle_L\Leftrightarrow\alpha|01\rangle+\beta|10\rangle. \tag{5}$$

The encoded pure state for a DFS logical qubit is given by

$$|01\rangle\langle 01|=\frac{\mathbb{1}_L+\sigma_{z,L}}{2}=\frac{\mathbb{1}+\sigma_z^1-\sigma_z^2-\sigma_z^1\sigma_z^2}{4}. \tag{6}$$

In the case of this DFS, the Hilbert space can be written as a direct sum of the logical subspace $\mathcal{L}$ (spanned by the basis $|01\rangle$ and $|10\rangle$) and its complementary subspace $\mathcal{R}$ (spanned by the basis $|00\rangle$ and $|11\rangle$). If we add the identity on the $\mathcal{R}$ subspace to the logical pure state, we obtain a mixed state that is equivalent in terms of its behavior on the logical degrees of freedom:

$$\rho_{spps}=\frac{1}{2}|0\rangle\langle 0|_L+\frac{\mathbb{1}_R}{4}=\frac{1}{4}(\mathbb{1}+\sigma_{z,L})=\frac{1}{4}\left(\mathbb{1}+\frac{\sigma_z^1-\sigma_z^2}{2}\right). \tag{7}$$

The traceless part of this state is simply proportional to $\sigma_z^1-\sigma_z^2$: From thermal equilibrium, a unitary operation is sufficient to obtain this state, so no signal is lost. The subsystem pseudopure state that one obtains with this method requires less averaging to implement the nonunitary transformation.

[1]Further action of an appropriate operator A is required in the case of QEC codes [29].

We expect such transformation to result in general in a higher SNR, since less information about the system is neglected, and to have less complex state preparation, since the nonunitary transformation is less demanding.

As an example, consider the pure state of two logical qubits encoded into a four-physical-qubit DFS [33]:

$$|00\rangle\langle 00|_L = \frac{1}{4}(\mathbb{1}_L^1 + \sigma_{z,L}^1) \otimes (\mathbb{1}_L^2 + \sigma_{z,L}^2). \quad (8)$$

If we add $\mathbb{1}_R$ to the unprotected subspace of each logical qubit we obtain a state that is pseudopure within the subspace of the logical encoding:

$$\rho_{spps} = \frac{1}{16}(\mathbb{1}_L^1 + \mathbb{1}_R^1 + \sigma_{z,L}^1) \otimes (\mathbb{1}_L^2 + \mathbb{1}_R^2 + \sigma_{z,L}^2)$$
$$= \frac{1}{16}\left(\mathbb{1}^{1,2} + \frac{\sigma_z^1 - \sigma_z^2}{2}\right) \otimes \left(\mathbb{1}^{3,4} + \frac{\sigma_z^3 - \sigma_z^4}{2}\right). \quad (9)$$

We still need a nonunitary operation to obtain this state, but the resulting SNR is $2/3$ instead of $4/15$ as for creating the full pseudopure state. The preparation procedure is also less complex, since it only requires preparing up to two-body terms $(\sigma_z^i\sigma_z^j)$ instead of the four-body term $(\sigma_z^1\sigma_z^2\sigma_z^3\sigma_z^4)$ necessary for the full pseudopure state (in general an N-body term involves interactions among all N spins; usually only some of the couplings among spins are strong enough to permit fast two-qubit operations).

IV. GENERAL THEORY

To illustrate the advantages that subsystem pseudopure states bring, we now present a general scheme, looking for a quantitative bound on the increase in sensitivity with respect to full pseudopure states. When under a particular encoding the Hilbert space is transformed to $\mathcal{H} \cong \oplus_i \mathcal{L}_i \otimes \mathcal{S}_i$, in the encoded representation the state we want to prepare will have the form

$$\rho_{spps} = \bigoplus_i a_i \left(|\psi\rangle_L^i \langle\psi|_L^i \otimes \frac{\mathbb{1}_S^i}{d_{s_i}} \right). \quad (10)$$

The dimension of the ith syndrome is d_{s_i}; a_i are subspace weighting coefficients, such that $\Sigma_i a_i = 1$, ensuring a unit trace of ρ_{spps}. We analyze the conditions that give the optimal signal, given that some freedom in the construction of the subsystem pseudopure states is available.

If we wish to encode l logical qubits among N physical qubits, with a syndrome subsystem $\mathcal{S}$ of dimensions 2^s, the subsystem pseudopure state is

$$\rho_{spps} = a\left(|\psi\rangle\langle\psi|_L \otimes \frac{\mathbb{1}_S}{2^s} \right) + \frac{1-a}{2^N - 2^{s+l}} \mathbb{1}_R. \quad (11)$$

The signal as defined in the Appendix is given by $S(\rho) = a\epsilon\alpha S(|\psi\rangle\langle\psi|_l) \propto a\alpha l$, where $\alpha \leqslant \|\rho_{eq}\| / \|\rho_{spps} - \mathbb{1}/2^N\|$ and the signal-to-noise ratio is upper bounded by $\mathrm{SNR} \propto N 2^{s+1-N}$.

For more than one logical qubit, each being protected against some noise, or to concatenate different encodings, a tensor structure of encoded qubits arises naturally. We analyze also this second type of construction, which can bring a further enhancement of the signal. We assume here that we encode one logical qubit in n physical qubits—each being a subsystem pseudopure state—and we build a logical l-qubit state with the tensor product of these encoded qubits. The Hilbert space can be written as a tensor product of direct sums as $\mathcal{H} = \otimes_{i=1}^l (\mathcal{L}_i \otimes \mathcal{S}_i \oplus \mathcal{R}_i)$.

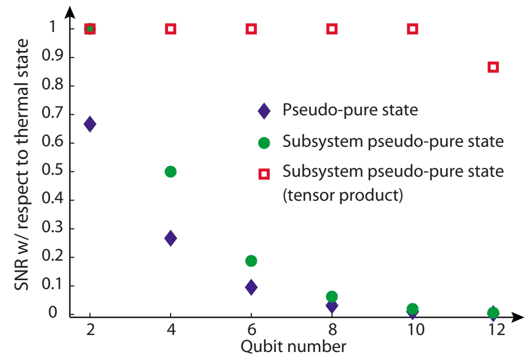

FIG. 1. (Color online) SNR (normalized to the SNR for the thermal state) for DFS encoding of one logical qubit on two physical qubits, as a function of the total physical qubit number.

The corresponding partially mixed states differ with respect to the previous ones, in that subspaces that are not actually used to store protected information are not maximally mixed:

$$\rho_{spps} = \left(a_1 |\psi\rangle\langle\psi|_{L1} \otimes \frac{\mathbb{1}_{s1}}{2^s} \oplus \frac{1-a_1}{2^n - 2^{s+1}} \mathbb{1}_{R1} \right)$$
$$\otimes \left(a_2 |\psi\rangle\langle\psi|_{L2} \otimes \frac{\mathbb{1}_{S2}}{2^s} \oplus \frac{1-a_1}{2^n - 2^{s+1}} \mathbb{1}_{R2} \right) \otimes \cdots . \quad (12)$$

The maximum SNR depends on the relative dimension of the logical subspace and the syndrome and on the number of encoded qubits. In particular, when $l < -1/\log_2(1-2^{s-n})$ the $\mathrm{SNR} \propto N 2^{s+1/l-n}$; and when $l > -1/\log_2(1-2^{s-n})$, instead, we obtain $\mathrm{SNR} \propto N 2^s (2^n - 2^s)^l / [2^N - (2^n - 2^s)^l]$.

In both cases, the SNR obtained with a tensor product structure is higher than for the first construction presented, as shown in Fig. 1 for the DFS encoding presented in the previous section example.

The improvement brought by the subsystem pseudopure states can be generalized to many types of encoding. We now present two examples, applying our scheme to the case of a three-qubit NS and a three-qubit QEC, to illustrate some possible applications of the scheme proposed.

A. Noiseless subsystems

The smallest code that protects a system against an arbitrary collective noise is realized with a three-physical-qubit NS [23,24,34–36]. The collective noise conserves the total angular momentum J of the system. In the case of a three-spin-$\frac{1}{2}$ system, the Hilbert space can immediately be written as $\mathcal{H} = \mathcal{H}_{3/2} \oplus \mathcal{H}_{1/2}$. The second subspace $(\mathcal{H}_{1/2})$ is doubly degenerate, so we identify in it a protected subsystem, reflecting a logical degree of freedom: $\mathcal{H}_{1/2}=\mathcal{L}\otimes\mathcal{S}$, where the second subsystem is associated with the j_z quantum number.

Since the information is all encoded in the subsystem $\mathcal{L}$, we can safely leave the subsystem $\mathcal{S}$ in a mixed state. The state we want to create has the form $|0\rangle\langle 0|_L\otimes\mathbb{1}_S/2$. In terms of physical operators, using the decoding operator in Ref. [34], this corresponds to

$$\rho_{spps}=(\mathbb{1}+\sigma_z^1+\sigma_z^2+\sigma_z^1\sigma_z^2)/8. \tag{13}$$

Only 1/3 of the equilibrium signal must be lost to create this state.

Notice that we can also set the subspace corresponding to $j=3/2$ to the identity state, with $a=\frac{1}{2}$ for the optimal SNR. With the encoding given in [34], the identity on the unprotected subspace $\mathcal{H}_{3/2}$ is $(\mathbb{1}-\sigma_z^1/2)/8$. The subsystem pseudopure state is then $\rho_{spps}=(2\times\mathbb{1}+\sigma_z^1/2+\sigma_z^2+\sigma_z^1\sigma_z^2)/16$ and 1/2 of the SNR is retained in obtaining this state instead of 3/7 for a full pseudopure state, a 16% increase.

B. QEC

When the noise does not present any useful symmetry, information can still be preserved by using QEC codes [10,26,27]. These codes are based on a two-step operation for protecting against the noise: first the information is encoded in an appropriate subspace and then, after a short time during which at most one error has occurred, the qubit is corrected based upon the state of the syndrome. To obtain a subsystem pseudopure state, the strategy is again to purify only the subspace encoding the information, while the ancillary subspaces are left in a mixed state. It could appear that this scheme cannot be applied, since when ancillas are not in the ground state but in a mixed state, they indicate that errors have already acted on the system: QEC codes can protect only for a finite number of errors. However, if we initially populate the orthogonal syndrome subspaces with the identity, recovery of the information is still possible and we obtain a subsystem pseudopure state with a higher SNR and the same observable dynamics as a full pseudopure state.

Consider, for example, the encoding for the three-qubit QEC [7,37], protecting against a single bit-flip error (σ_x^i). The code subspace is spanned by the basis set

$$|0\rangle_L=|000\rangle,\quad |1\rangle_L=|111\rangle. \tag{14}$$

The Hilbert space has an irreducible representation as the direct sum of four orthogonal subspaces: $\mathcal{H}=\mathcal{L}\oplus\mathcal{R}_1\oplus\mathcal{R}_2\oplus\mathcal{R}_3$, each $\mathcal{R}_i$ spanned by the basis $\sigma_x^i\{|0\rangle_L,|1\rangle_L\}$, $i=1,2,3$.

An error causes a swapping of the code subspace with one of the orthogonal subspaces, which is then corrected by the decoding operation. Starting from the pure state $|\psi\rangle|00\rangle$, which we encode following (14), the final state after an error and decoding is $|\psi\rangle|xy\rangle$ ($x,y\in\{0,1\}$) and the ancillas need to be reinitialized for the code to be effective against a second error. Since logical operations act only on the first subspace, we can set the other subspaces to the maximally mixed state. The state we want to prepare is thus given by

$$\begin{aligned}a|\psi\rangle\langle\psi|_L+(1-a)(\mathbb{1}_{R1}+\mathbb{1}_{R2}+\mathbb{1}_{R3})/6\\ =a|\psi\rangle\langle\psi|_L+(1-a)(\mathbb{1}-\mathbb{1}_L)/6.\end{aligned} \tag{15}$$

When we decode after an eventual error, we obtain the state $(a|\psi\rangle\langle\psi|_1-(1-a)\mathbb{1}_1/6)|xy\rangle\langle xy|+(1-a)\mathbb{1}/6$. Since the identity $\mathbb{1}_1$ is not observable in NMR, this state carries the same information content as the full pseudopure state. With $a=1/4$ we find that the SNR is reduced only to $\frac{3}{4}$SNR for this mixed state, while it would be 3/7 for the full pseudopure state.

Generalizing to other QEC codes, one can always find an encoding operation that transforms the Hilbert space to $\mathcal{H}\cong\mathcal{L}\oplus_i\mathcal{R}_i=\mathcal{L}\oplus\mathcal{R}$ and prepare a subsystem pseudopure state following the constructions for the DFS, setting the subspace $\mathcal{R}$ to identity. However, this encoding only allows one to correct for a finite number of errors; a recovery operation is needed to reinitialize the ancillas. The recovering operation could be in general accomplished by a strong measurement; however, this is not feasible in NMR; one must have fresh ancillas available (the problem posed by the need of resettable ancilla is not unique to NMR). To correct for two errors in the previous example, a partially mixed state with four ancillas should be prepared, so that two new fresh ancillas can be used for correcting the second error. In general, in addition to the three-qubit system that encodes the state, a separated reservoir (not affected by the noise) of $2n$ ancillas is needed for correcting n errors. Even if ancillas must all be prepared simultaneously, the creation of subsystem pseudopure states increases the SNR, so that the number of ancillas, and therefore of errors that can be corrected, can be increased in actual experiments.

V. METRICS OF CONTROL

The correlation of the experimental density matrix with the theory density matrix is a quantitative measure of control [38]. The attenuated correlation takes into account attenuation due to decoherent or incoherent processes:

$$C=\frac{\mathrm{Tr}(\rho_{th}\rho_{expt})}{\sqrt{\mathrm{Tr}\{\rho_{th}^2\}\mathrm{Tr}\{\rho_{in}^2\}}}. \tag{16}$$

Here $\rho_{th}=U\rho_{in}U^\dagger$, $\rho_{expt}=\mathcal{E}(\rho_{in})$, and ρ_{in} define the theoretical, experimental, and input states, respectively.

When we compare theoretical and experimental encoded states, their overlap has contributions that mirror the logical subsystem structure of the Hilbert space. Consider for simplicity a Hilbert space that can be written in terms of logical and nonlogical subspaces, $\mathcal{H}\cong\mathcal{L}\oplus\mathcal{R}$. Rewriting the experimental quantum process in terms of Kraus operators [39] A_μ $[\mathcal{E}(\rho)=\sum_\mu A_\mu\rho A_\mu^\dagger]$ we can separate them into three groups $\{A_{\mu,LL},A_{\mu,RR},A_{\mu,LR}\}$, which respectively describe the maps on the $\mathcal{L}$ subspace, $\mathcal{R}$ subspace, and the mixing of these two subspaces. The correlation will reflect these three contributions to the dynamics, $C=\alpha_{LL}C_{LL}+(\alpha_{LR}C_{LR}+\alpha_{RL}C_{RL})+\alpha_{RR}C_{RR}$, where

$$C_{KH}=\frac{\mathrm{Tr}(P_{K\rho_{th}}\sum_\mu A_{\mu,KH}(P_{H\rho_{in}}P_H)A_{\mu,KH}^\dagger)}{\sqrt{\mathrm{Tr}[(P_{H\rho_{in}})^2]\mathrm{Tr}[(P_{K\rho_{th}})^2]}}, \tag{17}$$

$$\alpha_{KH} = \sqrt{\frac{\mathrm{Tr}\{(P_{H\rho_{in}})^2\}\mathrm{Tr}\{(P_{K\rho_{th}})^2\}}{\mathrm{Tr}(\rho_{in}^2)\mathrm{Tr}(\rho_{th}^2)}}.$$

Here we define P_L (P_R) as the projector onto the encoded (nonlogical) subspace. Notice that if the ideal state is inside the logical subspace, its projection on the nonlogical subspace $P_R\rho_{th}$ is zero and the last term goes to zero, $C_{RR}=0$.

For encoded qubits, we limit state tomography to the logical subspace only, so that a reduced number of readouts is enough to characterize the information available from this subspace. The ability to preserve and manipulate the information inside the logical subspace can be better quantified by the correlation on this subspace C_{LL}, comparing the experimental logical state with the theoretical state inside the subspace only. If the input state of this process, ρ_{in}, is a full pseudopure state and inside the logical subspace, the correlation C_{LL} with the logical ideal state is the only contribution to the total correlation C.

If a pseudopure state over logical degrees of freedom is used instead, $C_{LR}\neq 0$, since the output state in the protected subspace may contain contributions arising from the action of the map $\mathcal{E}$ on the identity in the nonlogical subspace. Given an input state $\rho_{in}=a|\psi\rangle\langle\psi|_L+(1-a)\mathbb{1}_R/d_R$, from the experimental output state we can only measure the quantity (by observing only the l logical qubits or their phyisical equivalents)

$$\begin{aligned} C_{LL}^{*} &= aC_{LL} + (1-a)C_{LR} \\ &= aC_{LL} + (1-a)\frac{\mathrm{Tr}[U_{th}|\psi\rangle\langle\psi|_L U_{th}^{\dagger}\mathcal{E}(\mathbb{1}_R/d_R)]}{\sqrt{\mathrm{Tr}[(P_{L\rho_{in}}P_L)^2]}\sqrt{\mathrm{Tr}[(P_{L\rho_{th}}P_L)^2]}}. \end{aligned} \tag{18}$$

Note that in this case $C\neq C_{LL}^{*}$, since the contribution C_{RL} is not taken into account. The measured correlation is thus defined by two terms: the first takes into account the control over the encoded subspace only and the eventual leakage from it, while the second takes into account mixing from the $\mathcal{R}$ subspace to the $\mathcal{L}$ subspace. State tomography of the input state $\mathbb{1}_R$ after the algorithm allows one to calculate the correlation on the logical subspace C_{LL}.

To characterize the control of quantum gate operations most generally, many metrics have been suggested [38,40,41]. A good operational metric is, for example, the average gate fidelity (or fidelity of entanglement) that can be measured as the average of correlations of a complete orthonormal set of input states: $\bar{F}=\Sigma_j C^j=\Sigma_j \mathrm{Tr}[U_{th}\rho^j U_{th}\mathcal{E}(\rho^j)]$. Similarly, the encoded operational fidelity can be defined as the average correlation over an orthonormal set of operators spanning $\mathcal{L}$: $\bar{F}_L=\Sigma_j' C_{LL}^j=\Sigma_j' \mathrm{Tr}[U_{th}\rho_L^j U_{th}\mathcal{E}(\rho_L^j)]$.

The fidelity on the logical subspace focuses on the achieved control in the implementation of the desired transformation on the protected subspace; this new metric is immune to unitary or decoherent errors within $\mathcal{R}$ alone:

$$\begin{aligned} \bar{F}_L &= \sum_j{}' C_{LL}^j = \sum_j{}' \mathrm{Tr}\left[U_{th\rho_L^j}U_{th}\left(\sum_\mu A_\mu P_{L\rho_L^j}P_L A_\mu\right)\right] \\ &= \sum_\mu |U_{th}A_{\mu,L}|^2/N^2. \end{aligned} \tag{19}$$

The extent to which $U_{L,expt}$ is close to $U_{th,L}$ can be determined from $\bar{F}_L$, while the avoidance of subspace mixing will be specified by the gap between $\bar{F}$ to $\bar{F}_L$.

VI. CONCLUSIONS

Subsystem pseudopure states offer not only a greater SNR but also a less complex state preparation which is reflected in increased fidelity of the experimental results (as shown in a following paper). By no means does this logical encoding overcome the exponential loss of signal suffered by pseudopure states; however, for the corresponding state in the full Hilbert space, the gain is significant. As we explore control over multiple logical qubits, these advantages become tantamount.

In particular, this method coupled with the experimental control on a Hilbert space of about ten qubits would allow for the study of a repeated QEC code, the Shor code for protecting against single-qubit errors, or a multilayered encoding like QEC using three DFS-encoded qubits or vice versa. In addition encoded versions of gates essential to algorithms, like the quantum Fourier transform, can be carried out with liquid-phase NMR. The effective noise superoperator on the logical subspace can also be reconstructed [42], to gain insight into how various encoding schemes modify the noise structure. Some of the foreseeable experiments are synthesized in Table I.

By considering metrics of control for only the logical degrees of freedom of our system, we also reduce the number of input states needed to characterize a particular gate sequence, as long as only the behavior of the protected information is of interest.

The state initialization method proposed could also find application in a broader context, whenever exact purification of the system is possible, but costly. Quite generally, a qubit need not be identified with a physical two-level system, but rather with a subsystem whose operator algebra generators satisfy the usual commutation and anticommutation relationships. State initialization and purification could be performed on these subsystems only, thus allowing experimental advantages similar to the ones shown in the particular case of logical qubits.

ACKNOWLEDGMENTS

The authors thank N. Boulant and P. Zanardi for helpful discussions. This work was supported in part by the National Security Agency (NSA) under Army Research Office (ARO) Contracts No. W911NF-05-1-0469 and No. DAAD19-01-1-0519, by the Air Force Office of Scientific Research, and by the Quantum Technologies Group of the Cambridge-MIT Institute.

APPENDIX

Here we calculate the SNR upper bound for a general subsystem pseudopure state. As seen, there is some freedom in creating these states, given an encoding. This reflects a compromise between how much SNR is gained in leaving

TABLE I. Experiments of 4–9 qubits that will be achievable with the initialization method proposed. GHZ indicates the Greenberger-Horne-Zeilinger state: $(|000\rangle+|111\rangle)/\sqrt{2}$.

Four spins	DFS	One logical qubit. Isotropic noise.
		What differences from the three-qubit NS?
Five spins	NS	Two logical qubits. Create Bell state.
	QEC	Two errors. One logical qubit QEC for σ_x errors.
	QEC	Two logical qubits QEC for σ_x errors.
Six spins	DFS	Three logical qubits, σ_z noise. Create GHZ state.
	GHZ	Create two GHZ states and then encode them. σ_z noise.
	QEC	Concatenate two-qubit DFS with three-qubit QEC.
	DFS	
Nine spins	Shor's code	Nine-qubit QEC to correct all single-qubit errors.

the system mixed and how much of this SNR does come from the information-carrying part of the Hilbert space.

Since we are interested in the information that we can manipulate and observe, a good measure of the sensitivity gain is the SNR of the qubits storing the information after the decoding. Instead of the total magnetization, which is the observable in NMR, we are therefore interested in

$$\begin{aligned}\mathrm{SNR} &= \langle|\vec{M}|\rangle \propto S(\rho)\\ &= \sqrt{\mathrm{Tr}\Big(\sum \sigma_z^i\rho\Big)^2 + \mathrm{Tr}\Big(\sum \sigma_x^i\rho\Big)^2 + \mathrm{Tr}\Big(\sum \sigma_y^i\rho\Big)^2},\end{aligned} \tag{A1}$$

where the sum extends only over the l information-carrying qubits. Other metrics are of course conceivable, for example the total magnetization of the N spins or the spectral norm of the density matrix deviation, but they are not directly related to the signal arising from the information-carrying qubits.[2]

We begin with the first construction presented in the main text. For the sake of clarity, we consider to encode l logical qubits among N physical qubits, with a syndrome subsystem $\mathcal{S}$ of dimensions[3] 2^s (the Hilbert space can be written as $\mathcal{H}=\mathcal{L}\otimes\mathcal{S}\oplus\mathcal{R}$).

The encoding operation is, in general, defined by its action on the initial state $|\psi\rangle_l|00\ldots\rangle_{N-l}$, giving the encoded state $|\psi\rangle_L|0\rangle_S$. Hence, there is some flexibility in the choice of encoding operation (since it is defined only for ancillas initially in the ground state) but we can specify it with the assumption that the state in the encoded subsystem $\mathcal{S}$ is determined by the first s ancillas state:

$$U_{enc}|\psi\rangle_l|\phi\rangle_s|00\ldots\rangle_{N-l-s} = |\psi\rangle_L|\phi\rangle_S. \tag{A2}$$

The subsystem pseudopure state is

$$\rho_{spps} = a\left(|\psi\rangle\langle\psi|_L \otimes \frac{\mathbb{1}_S}{2^s}\right) + \frac{1-a}{2^N-2^{s+l}}\mathbb{1}_R, \tag{A3}$$

which after decoding following (A2) becomes

$$\begin{aligned}\rho_{spps} = \left(a|\psi\rangle\langle\psi| - \frac{1-a}{2^N-2^{s+l}}\mathbb{1}_l\right)\\ \times\frac{\mathbb{1}_s}{2^s}|00\ldots\rangle\Big\langle 00\ldots\Big|_{N-l-s} + \frac{1-a}{2^N-2^{s+l}}\mathbb{1}.\end{aligned} \tag{A4}$$

The signal is thus given by $S(\rho)=a\epsilon\alpha S(|\psi\rangle\langle\psi|_l)\propto a\alpha l$, where $\alpha\leqslant\|\rho_{eq}\|/\|\rho_{spps}-\mathbb{1}/2^N\|$. To obtain the spectral norm of the subsystem pseudopure state traceless part, we calculate its eigenvalues:

$$\left\{\frac{a}{2^s}-2^{-N},-2^{-N},\frac{1-a}{2^N-2^{s+l}}-2^{-N}\right\}. \tag{A5}$$

The upper bound for the signal is obtained for $a=2^{s+1-N}$ and we have $\mathrm{SNR}\propto N2^{s+1-N}$.

The second type of subsystem pseudopure state presented in Sec. IV can be most generally written as

$$\begin{aligned}\rho_{spps} = &\left(a_1|\psi\rangle\langle\psi|_{L1}\otimes\frac{\mathbb{1}_{S1}}{2^s}\right.\\ &\left.\oplus\frac{1-a_1}{2^n-2^{s+1}}\mathbb{1}_{R1}\right)\otimes\left(a_2|\psi\rangle\langle\psi|_{L2}\otimes\frac{\mathbb{1}_{S2}}{2^s}\oplus\frac{1-a_1}{2^n-2^{s+1}}\mathbb{1}_{R2}\right)\\ &\otimes\cdots.\end{aligned} \tag{A6}$$

Notice that we consider that all the qubits have the same encoding and to make the problem more tractable we choose $a_i=a\,\forall\, i$. Other choices of course exist, and may lead to a better SNR, but will not be explored here. Upon decoding, this state is transformed to

$$\begin{aligned}U_{enc}^{\dagger}\rho_{spps}U_{enc} = \otimes_{i=1}^{l}\Bigg[\left(a|\psi\rangle\langle\psi|_1-\frac{1-a}{2^n-2}\mathbb{1}_1\right)\otimes\frac{\mathbb{1}_s}{2^s}\\ \otimes|00\ldots\rangle\langle 00\ldots|+\frac{1-a}{2^n-2}\mathbb{1}_n\Bigg]_i.\end{aligned} \tag{A7}$$

[2]Notice that even the chosen metric can be misleading, since in the case $l>1$ some states give no signal (e.g., a nonobservable coherence). However, any of these states can be characterized by especially designed readout operations that transform it to an observable state, while preserving its information content. More specifically, we will consider only the ground-state $|00\ldots\rangle$ signal, since any other state is isomorphic to it, via a unitary operation.

[3]We consider only the case where we can map qubits on the subsystem S, even if in general the subsystem could not be mapped to qubits. The results would be the same, however, with slightly different notation.

The signal is again proportional to $a\alpha l$ and by varying a we can find the optimal state. The eigenvalues for the traceless part of the subsystem pseudopure state are

$$\prod_{i=1}^{l}\left(\left\{\frac{a}{2^s},0,\frac{1-a}{2^n-2^{s+1}}\right\}_i\right)-2^{-N}$$
$$=\left\{\left(\frac{a}{2^s}\right)^{l-p}\left(\frac{1-a}{2^n-2^{s+1}}\right)^p\Bigg\|_{p=0}^{l}-2^{-N},-2^{-N}\right\}. \quad \text{(A8)}$$

The maximum SNR depends on the relative dimension of the logical subspace and the syndrome and on the number of encoded qubits (notice that for $n \leqslant s$ there is no useful solution). Two cases are possible. (1) When $l < -1/\log_2(1-2^{s-n})$ the $\mathrm{SNR} \propto N2^{s+1/l-n}$ (the norm reaches the minimum value 2^{-N} for $a \leqslant 2^{s+1/l-n}$). (2) When $l > -1/\log_2(1-2^{s-n})$, instead we obtain $\mathrm{SNR} \propto N2^s(2^n-2^s)^l/[2^N-(2^n-2^s)^l]$: the minimum value for the norm $(2^n-2^s)^{-1}-2^N$ is obtained for $a/2^s=(1-a)/(2^n-2^{s+1})$, i.e., for $a=2^s/(2^n-2^s)$.

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