Practical experimental certification of computational quantum gates via twirling

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Due to the technical difficulty of building large quantum computers, it is important to be able to estimate how faithful a given implementation is to an ideal quantum computer. The common approach of completely characterizing the computation process via quantum process tomography requires an exponential amount of resources, and thus is not practical even for relatively small devices. We solve this problem by demonstrating that twirling experiments previously used to characterize the average fidelity of quantum memories efficiently can be easily adapted to estimate the average fidelity of the experimental implementation of important quantum computation processes, such as unitaries in the Clifford group, in a practical and efficient manner with applicability in current quantum devices. Using this procedure, we demonstrate state-of-the-art coherent control of an ensemble of magnetic moments of nuclear spins in a single crystal solid by implementing the encoding operation for a 3 qubit code with only a 1% degradation in average fidelity discounting preparation and measurement errors. We also highlight one of the advances that was instrumental in achieving such high fidelity control.

**Introduction** – Due to the technical challenges of building quantum computers, only small building blocks of such devices have been demonstrated so far in a number of different physical systems. In order to quantify how closely these demonstrations come to the desired ideal operations, the experiments are fully characterized via quantum process tomography (QPT) [1,2]. When, often, the average fidelity [3,4] between the experiment and the ideal operator is calculated from the description of the estimated process. The main drawback of this approach is that the current experimental state of the art. Here we solve this problem by showing that, for an important class of quantum operations, the average fidelity can be estimated efficiently, requiring a number of experiments which is independent of the system size. This new proposal is also practical, and enables the demonstration of processes which could not have been possible due to the complexity of QPT. We use this protocol to demonstrate state-of-the-art coherent control of the magnetic moments of an ensemble of nuclear spins in a single crystal solid, and highlight one of the advances that was instrumental in achieving such high fidelity control.

**Twirling** – It has been recently shown that if one wishes to compare an experimental implementation of a quantum process to the identity process (i.e. a process where the system state remains unchanged, such as in the case of ideal quantum memories), then it is possible to estimate the average fidelity via a technique known as twirling [6,10], with a number of experiments which depends only on the desired accuracy of the estimate, not on the system size — moreover, these experiments are simple to implement, requiring only local operations and measurements [6]. The twirling procedure consists of applying a random unitary before the process to be characterized, followed by the inverse of this randomly chosen unitary. When these unitaries obey certain symmetry properties, the resulting invariant information about the noise under this symmetry can be extracted by repeating the experiment with different random choices. For example, if the twirling gates are random permutations followed by tensor products of single-qubit Cliffs then information about the weights of the noise terms can be determined [8]. The schematic for such an experiment is depicted in Fig. 1(a), where the process we would like to compare to the identity process, $\mathcal{E}$, is conjugated with $C_i$, an appropriately chosen randomizing local operation, and $M_j$ is the measurement of the parity of a subset of qubits in the computational basis.

For more general processes, in order to compare a given process to a desired unitary evolution one could in principle apply the physical process under consideration, and then apply the inverse of the unitary evolution we would like to compare it against, finally measuring the overlap between the
initial state and the resulting state for a set of initial states — this is, in essence, the definition of the average fidelity. The obstacle to implementing such a protocol is that often one is attempting to demonstrate or certify the implementation of a unitary, and a noiseless implementation of its inverse cannot be assumed to be available. One way \[6, 11\] to address this problem is to estimate the average fidelity over a set of quantum processes that form a group by considering random sequences of such processes chosen to result in the identity process — examples of such sets include the group of all unitary processes, as well as the Clifford group \[13\]. Such motion-reversal benchmarking schemes suffer from two shortcomings: they apply only to noise satisfying certain strength conditions \[12\], and they only provide information about the average over a set of processes instead of specific information about a particular process. While this information is useful, what is experimentally most useful is to diagnose coherent control implementation errors, which, in our experience, are highly process-dependent. Therefore, it is critical for the experimentalist to be able to characterize a particular process.

Certification procedure — The result we report here, which side-steps many of the shortcomings listed above, is that the average fidelity between any physical process on multiple qubits and any particular element of the Clifford group can be estimated efficiently by a simple modification to the twirling protocol, leading to the same favourable scaling as experiments which compare a physical process to the identity. If we define \(\mathcal{U}\) to be the desired element of the Clifford group, then the noisy implementation \(\hat{\mathcal{U}}\) can be thought of as some noisy process \(\mathcal{E}\) followed by the application of \(\mathcal{U}\), i.e. \(\hat{\mathcal{U}} = \mathcal{U} \otimes \mathcal{E}\). Unitaries in the Clifford group include operations needed to encode and decode quantum information to protect it from noise \[14\] — in current approaches to fault-tolerance these operations comprise the vast majority of (if not all) operations. Clifford group operations can also be used to achieve universal fault-tolerant quantum computation with the aid of especially prepared resource states \[13, 15\], so these operations are of great importance and utility for quantum computation.

In order to see why the average fidelity can be estimated efficiently for these operations, consider Fig. 1(b), which modifies the original twirling protocol \[8\] by inserting the identity process — in this case written as \(\mathcal{U} \otimes \mathcal{U}\). One can in principle combine all processes after the first application of \(\mathcal{U}\) in (b) into a new measurement. For a general unitary process this new measurement will be as hard to implement as performing the process \(\mathcal{U}\) itself. However, if \(\mathcal{U}\) is an element of the Clifford group \[16\], this results in the measurement of the parity of a different set of qubits in a different local basis (or equivalently, the measurement of a different Pauli operator \[13\]) which can be precomputed efficiently given \(\mathcal{U}\), the local randomizing Clifford operation \(\mathcal{C}_i\), and the original measurement \(\hat{M}_j\), as depicted in Fig. 1(c), where \(f(\hat{M}_j, \mathcal{C}_i, \mathcal{U}) = \mathcal{U}(C_i \hat{M}_j C_i^\dagger)\). In essence, the protocol in Fig. 1(c) is the experiment, but the data is analyzed according to Fig. 1(a) as described in \[8, 9\], which separates the noise \(\mathcal{E}\) from the unitary \(\mathcal{U}\).

As the parity measurement is equivalent to local measurement followed by simple data post-processing, and the initial states required are product states locally equivalent to the all-zeros state, it is important that precise local operation be available. In other words, the problem of implementing the inverse of a multibody Clifford unitary \(\mathcal{U}\) can be translated into the problem of implementing classical data processing and local (single-body) quantum operations reliably. These operations are often readily available at high fidelities, as randomizing benchmarking results have demonstrated \[11, 17, 18\]. Thus the average fidelity of any implementation of a Clifford group operation can be estimated using a number of experiments that depends only on the desired accuracy, as is the case for twirling experiments with quantum memories \[8\].

Due to this connection to twirling protocols, our proposal also enables the estimation of other parameters beyond the gate fidelity, such as the probability of errors of a given weight. Recent proposals for Monte Carlo estimation of state and gate fidelity have the same scaling as the protocol we describe here (in the case of Clifford gates) \[19, 20\]. However, the probability of errors of a given weight are not natural parameters to be considered in the Monte Carlo sampling protocols, demonstrating the advantage of considering twirling protocols in this context. The simplicity of the experiments also shows that our proposal is of practical significance in the benchmarking of these important operations. Moreover, because the estimation of the average fidelity in the twirling protocol corresponds to the estimation of the probability of no errors having occurred (a single parameter that is accessible with an accuracy that does not depend on the number of qubits \[8\]), Bayesian estimation of such a probability is straightforward, as is the calculation of uncertainties associated with these estimates.

Experiment — A common task for an experimentalist is to optimize and tweak the performance of a particular gate on the system. The experimenter has many potential knobs to adjust and he/she needs a reliable robust method for certifying whether any changes actually improved the performance. A trivial example is calibrating the power of a pulse but here we demonstrate how we can easily quantify the improvement from more subtle and sophisticated control improvements.

Building on the success of liquid-state NMR as a test bed of QIP ideas, Solid-state NMR systems offer \[21, 12\] intrinsically larger couplings, longer coherence times, the ability to pump entropy out of the system of interest into a spin bath \[23, 24\] and the potential for much higher initial polarizations. This comes at the cost of a more complicated internal Hamiltonian, which makes the system harder to control in practice.

Methods inspired by optimal control theory have been successful in aiding pulse design for small systems. However, for these pulses to achieve the designed fidelity, it is important that the implemented control fields at the sample match the designed ones. That is to say, any systematic deviations from the designed pulses, due to the finite bandwidth of the resonant probe circuit or the non-linearities in the pulse gen-
To this end, a feedback system can be employed to correct for these systematic imperfections [23]. We use an antenna to measure the fields in the vicinity of the sample, then this data is fed back for comparison with the target pulse, and a new pulse form that attempts to compensate for the imperfections is computed and sent back to the signal generation unit. This loop is repeated a number of times to reach a satisfactory pulse form [26, 27]. Fig. 2 shows a typical example of the measured pulse forms of the initial and corrected attempts to match a target pulse shape. The development of this feedback pulse rectification protocol has led to a great improvement in the fidelity of coherent control of nuclear spins in the solid state – the certification scheme is used herein to demonstrate and quantify the typical improvement in fidelity resulting from using the feedback system.

The specific computational register under investigation is an ensemble of molecular nuclear spins in a macroscopic single crystal of Malonic Acid (C₃H₄O₄). A small fraction (≈ 3%) of the molecules are triply labeled with (spin-½)¹³C to form an ensemble of 3-qubit processor molecules, spatially buffered from one another by molecules of the same compound but with natural abundance (≈ 1%) carbon nuclei. During computation, the processors are decoupled from the 100% abundant spin-½ protons in the crystal by applying a decoupling pulse sequence to the protons.

The experiments were performed at room temperature in a static field of 7.1T using a purpose-built NMR probe. Shown in Fig. 3 is a proton-decoupled ¹³C spectrum, following polarization-transfer from the abundant protons, for the particular orientation of the crystal used in this experiment. A precise spectral fit gives the Hamiltonian parameters (listed in the inset table in Fig. 3), as well as the free-induction dephasing times, T₂, for the various transitions; these average at ≈ 2ms. The dominant contribution to T₂ is Zeeman-shift dispersion, which is largely refocused by the control pulses, leading to effective dephasing times much larger than T₂ [22]. The carbon control pulses are numerically optimized to implement the required unitary gates using the Gradient Ascent Pulse Engineering (GRAPE) [28] algorithm, and are typically designed [29] to have an average Hilbert-Schmidt fidelity of 99.8% over appropriate distributions of Zeeman-shift dispersion and control-fields inhomogeneity.

**Preparation and measurement** – The first step in the initial preparation procedure for all experiments described below is a selective polarization transfer from one of the methylene protons (Hₘ₁) to the methylene carbon (Cₘ). This is realized using a short [30] Hartman-Hahn cross-polarization sequence [31] after tipping the proton polarization to the transverse plane, and is sufficient because the coupling strength between these two nuclei is more than an order of magnitude larger than any other coupling. The state of the three carbon nuclei after this polarization can be described as ρₚ = .iOS3 + αIX, where α quantifies the amount of polarization transferred from the proton, and is on the order of 10⁻³ for protons in 7.1T at room temperature. A free induction decay is collected for this initial state to establish a reference for α, against which all subsequent experiments are compared. Simple coherence-transfer pulses can then be used to prepare all states of the form ρₚ = .iOS3 + αX⊗w.iOS⁻³⁻w, and their permutations over 3 qubits, for w = 1, 2, 3. From these states, pulses realizing single qubit π/2 rotations are all that is required.
for preparing a state with non-zero projection on any arbitrary 3-qubit Pauli operator. The same set of pulses are sufficient to transform any output state into an observable in an NMR experiment.

These single-qubit $\frac{\pi}{2}$ rotations can be realized with very high fidelity, which we now demonstrate using single qubit randomized benchmarking. The average fidelity of randomized sequences of $\frac{\pi}{2}$ pulses on each of the three qubits. Each data point is the average fidelity of 24 sequences. Fitting the data to $\log(F - \frac{1}{2}) = \log A_0 + m \log p$, we extract an average error per gate of $1.6 \pm 0.4 \times 10^{-3}$ for $C_1$ (blue diamonds), $3.8 \pm 0.7 \times 10^{-3}$ for $C_2$ (red squares), and $4.4 \pm 0.6 \times 10^{-3}$ for $C_3$ (green circles).

Appendix A: Experimental procedure with example

In this section, we describe in some detail the proposed protocol for estimating the average fidelity of a noisy implementation $\hat{U}$ to an ideal $n$-qubit Clifford gate $U$. For illustrative purposes, we use the encoding circuit $[34]$ of the five-qubit code $[35]$ (shown in Fig. 6) as a running example of the unitary process to be certified. As mentioned in the main text, this protocol can be viewed as a variation on a local-Cliffords-and-permutations twirling scheme described in ref. $[8]$, and detailed in ref. $[9]$ as the parity monitoring protocol.

In order to estimate the average fidelity between a physical implementation $\hat{U}$ and the ideal encoding circuit $U$, one can use the following procedure.

1. Offline, for each $w \in 1, \ldots, n$:
   
   (a) Choose an operator $\hat{M}_w$ with weight $w$ from the Pauli group on $n$-qubits. The overall sign of the Pauli operator should also be chosen uniformly at random. This is a tensor product of $n$ single-qubit Pauli operators, where $n - w$ of them are the identity. This step amounts to picking a random string of $2w + 1$ bits, and choosing $w$ qubits at random on which to act with the non-identity Paulis.

   (b) For the running example, one such choice for, say, $w = 3$ would be $\hat{M}_1 = I \otimes Y \otimes I \otimes X \otimes Z$.

   (c) Repeat this procedure $k_w = O(1/\epsilon^2)$ times in order to achieve a final accuracy of $\epsilon$ $[8]$.

2. In the laboratory:
   
   (a) For each choice of $\hat{M}_w$, prepare a state $\hat{\rho}_w$ such that
      
      $$ r_k := \langle \hat{M}_k \rangle_{\hat{\rho}_k} = \text{tr} \hat{\rho}_k \hat{M}_k \neq 0. $$

   (1)
Experiment ± 1.000

| Target | Experiment | $w$ | $k_{1w}$ | $\lambda_{1w}$ | Probability of no error $\bar{F}$ |
|--------|------------|-----|---------|-------------|-------------------------------|
| a      |            | 1   | 6       | 0.967 ± 0.010 | 0.983 ± 0.007 |
|        |            | 2   | 21      | 1.000 ± 0.009 | 0.863 ± 0.013 |
|        |            | 3   | 7       | 0.978 ± 0.017 | 0.973 ± 0.009 |
| b      |            | 1   | 8       | 0.848 ± 0.022 | 0.959 ± 0.014 |
|        |            | 2   | 21      | 0.883 ± 0.017 | 0.989 ± 0.013 |
|        |            | 3   | 8       | 0.799 ± 0.023 | 0.964 ± 0.016 |
| c      |            | 1   | 6       | 0.959 ± 0.014 |                  |
|        |            | 2   | 21      | 0.989 ± 0.013 |                  |
|        |            | 3   | 8       | 0.964 ± 0.016 |                  |

FIG. 5. Summary of the experimental parameters and results for the three sets of certification experiments – the Target column shows the quantum circuit representation of the ideal process; the Experiment column represents the experimental setup to certify the corresponding implementation, including state preparation and measurement using local readout pulses as described in the text; $k_{1w}$ and $\lambda_{1w}$ are, respectively, the number of performed experiments, and the average surviving polarization, partitioned by the Pauli-weight, $w$, of the input preparation (for more details, see Appendix A.) Shown also are the Bayesian estimated probability density functions for the probability of no error in the experimental implementation of the target gate, as well as the estimated average fidelity. The three sets of experiments are (a) State preparation and measurement compared to the Identity operation - this can be thought of as a calibration for the certification procedure; (b) the target is the encoding operation for the 3-qubit phase quantum error correcting code, and the experimental implementation is a numerically designed pulse using GRAPE; and (c) is the same as (b) but the pulse is corrected for implementation errors using the feedback procedure described in the text.

FIG. 6. Encoding network for the $[[5,1,3]]$ stabilizer code [34].

This, for example, can always be achieved by applying local Cliffords to the state $|0\rangle^\otimes n$. For $M_1 = \hat{I} \otimes \hat{Y} \otimes \hat{I} \otimes \hat{X} \otimes \hat{Z}$, one choice of local operations which achieves this is $\hat{C}_1 = \hat{I} \otimes \hat{P} \hat{H} \otimes \hat{I} \otimes \hat{H} \otimes \hat{I}$, where $\hat{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ and $\hat{P} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, resulting in $r_1 = 1$.

(b) Apply the noisy implementation $\hat{U}$ to the prepared state $\hat{\rho}_k$

(c) Measure the expectation value

$$t_k := \langle f(\hat{M}_k, C_1, U) | \hat{U}(\hat{\rho}_k) \rangle = \langle U(C_1 \hat{M}_k C_1^\dagger) | \hat{U}(\hat{\rho}_k) \rangle = \text{tr} \left[ C_1^\dagger \chi(C_1^\dagger |0\rangle^\otimes n C_1^\dagger C_1 \hat{M}_k \right].$$

If, for example, one had access only to projective measurements in the Pauli $Z$ eigenbasis on the individual qubits, a measurement of $f(\hat{M}_k, C_1, U)$ can be accomplished by a basis change which is a tensor product of single-qubit Clifford transformations. For the running example, $f(\hat{M}_1, C_1, U) = \hat{Z} \otimes \hat{Z} \otimes \hat{I} \otimes \hat{Y} \otimes \hat{X}$, so that the transformation needed to change Pauli $Z$ measurements into this observable would be $\hat{C}_1 = \hat{I} \otimes \hat{I} \otimes \hat{I} \otimes \hat{P} \hat{H} \otimes \hat{H}$.

3. The average fidelity should be estimated as follows:

(a) For each weight $w$, $\lambda_w$ is the average of the ratio $t_k / r_k$ for all $\hat{M}_k$ of weight $w$ ($\lambda_0$ is taken to be 1).

(b) $\text{Pr}(\text{no error})$ is the inner product of $\lambda_w$ and the first row of $\Omega^{-1}$, which is a matrix described in refs. [8][9]. This results in

$$\text{Pr}(\text{no error}) = \sum_{w=0}^{n} 3^w w^n / 4^n \lambda_w.$$  (3)

(c) The average fidelity $\bar{F}$ between $\hat{U}$ and $\hat{U}$ is finally...
given by

\[ F = \frac{2^n \Pr(\text{no error}) + 1}{2^n + 1} \quad (4) \]

Appendix B: Software

A simple script which automates the computation of the transformed Pauli operators given some Clifford operation can be found at [http://github.com/marcusps/TransPauli](http://github.com/marcusps/TransPauli)

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