Experimental Estimation of Average Fidelity of a Clifford Gate on a 7-qubit Quantum Processor

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Quantum gates in experiment are inherently prone to errors that need to be characterized before they can be corrected. Full characterization via quantum process tomography is impractical and often unnecessary. For most practical purposes, it is enough to estimate more general quantities such as the average fidelity. Here we use a unitary 2-design and twirling protocol for efficiently estimating the average fidelity of Clifford gates, to certify a 7-qubit entangling gate in a nuclear magnetic resonance quantum processor. Compared with more than 108 experiments required by full process tomography, we conducted 1656 experiments to satisfy a statistical confidence level of 99%. The average fidelity of this Clifford gate in experiment is 55.1%, and rises to 87.5% if the infidelity due to decoherence is removed. The entire protocol of certifying Clifford gates is efficient and scalable, and can easily be extended to any general quantum information processor with minor modifications.

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Introduction. Benchmarking protocols for characterizing the level of coherent control are fundamental in evaluating potential quantum information processing (QIP) devices. They provide an objective comparison of quantum control capabilities between diverse QIP devices, and also indicate the prospects of a given platform with respect to fault-tolerant quantum computation [1]. The traditional approach of using quantum process tomography (QPT) [2, 3] is useful for completely characterizing a quantum channel, and has been applied to at most 3-qubit systems in experiment [4–11]. However, QPT requires number of measurements that scale exponentially with number of qubits n \( \approx 2^{4n} \), making it impractical even in relatively small systems. Moreover, for many practical purposes, such as benchmarking, the full description of a particular quantum channel is not necessary and more accessible properties of the gates are sufficient. To benchmark a gate it is enough to estimate the distance between the implemented channel and the ideal gate. Several methods such as randomized benchmarking [12–14], twirling [15–17], and Monte Carlo estimations [18, 19] have been proposed to evaluate a particular quantum channel in an efficient manner, each with its own restrictions and drawbacks. Here, in order to benchmark our coherent controls on a 7-qubit nuclear magnetic resonance (NMR) system, we adopted the twirling protocol [17] to estimate the average fidelity of an important Clifford gate in QIP. The gate of interest generates maximal coherence from single coherence with the aid of local rotations, and is of critical importance to many QIP tasks such as the creation of a cat state in multi-qubit systems. The estimation method is scalable and independent of the number of qubits, and is straightforward to implement in other quantum information processing architectures.

For the twirling protocol we conducted only 1656 experiments compared with about \( 2.7 \times 10^8 \) experiments required for fully characterizing the 7-qubit gate via QPT. The average fidelity of the certified gate is 55.1% before accounting for decoherence and rises to 87.5% by separating the decoherence effect out. Moreover, the NMR spectra based on the application of this Clifford gate are in excellent agreement with the simulation results.

Theory. Let \( \mathcal{U} \) be a superoperator representation of the Clifford gate \( \mathcal{U} \) that we want to implement and \( \bar{\mathcal{U}} = \Lambda \circ \mathcal{U} \) be the superoperator representation of the real evolution in the laboratory experiment. We call \( \Lambda \) the noise superoperator and our task is to estimate its average fidelity with respect to the identity. The method described below is based on twirling [20] and the construction of a unitary 2-design [16].

Given a fiducial pure state \( |\psi\rangle \), the average fidelity (with respect to the identity) is the quantum fidelity \( \langle \psi | \Lambda (|\psi\rangle \langle \psi|) |\psi\rangle \) averaged over all pure states \( V |\psi\rangle \) where \( V \) is an arbitrary unitary transformation. Averaging over the entire Hilbert space can be done using the Haar mea-
sure $d\mu(V)$ [12], so

$$F(\Lambda) = \int d\mu(V)\langle\psi|V\Lambda^\dagger \circ \Lambda \circ V\langle\psi|\rangle|\psi\rangle. \quad (1)$$

Here $V$ is the superoperator representation of a unitary $V$ and $V\Lambda = U \circ V$. In this notation it is easy to see that the average fidelity depends only on $\Lambda$.

Using a unitary 2-design based on the Clifford group, it is possible to simplify Eq. (1) to

$$F(\Lambda) = \frac{1}{|C_n^1|} \sum_{C_i \in C_n} \langle\psi|C_i^\dagger \circ \Lambda \circ C_i\langle\psi|\rangle|\psi\rangle, \quad (2)$$

where $C_n$ is the n-qubit Clifford group $C_n$. The average fidelity is therefore equivalent to the fidelity of the average channel

$$\bar{\Lambda}_{C_n} = \frac{1}{|C_n|} \sum_{C_i \in C_n} C_i^\dagger \circ \Lambda \circ C_i. \quad (3)$$

This is a depolarizing channel $\bar{\Lambda}_{C_n}(\rho) = P_0\rho + [1 - P_0]I$ with $P_0$ the probability of no error. The average fidelity of Eq. (2) is therefore a function of the parameter $P_0$.

To estimate $P_0$ in a scalable way we can make use of an identification involving the $C_{1^n_2}^1\otimes n$-twirling channel. This is the channel $\Lambda$ twisted over the composition of the n-fold tensor product of the 1-qubit Clifford group $C^0_1$ and the permutation group $\Pi$

$$\bar{\Lambda}_{C^0_1\otimes n,\Pi} = \frac{1}{|C_{1^n_2}^1 \otimes \Pi|} \sum_{C_i \in C^0_1\otimes n,\Pi} C_i^\dagger \circ \Lambda \circ C_i. \quad (4)$$

It has a Pauli form

$$\bar{\Lambda}_{C^0_1\otimes n,\Pi}(\rho) = \sum_{w=0}^n \text{Pr}(w) \left( \frac{1}{3^w} \sum_{i=1}^{3^w} \rho_{i,w}\rho_{i,w}^{\dagger} \right), \quad (5)$$

where $\text{Pr}(w)$ is the probability that a Pauli error of weight $w$ occurs. The identification $P_0 = \text{Pr}(0)$ [21] gives

$$\bar{F}(\Lambda) = \frac{2^n\text{Pr}(0) + 1}{2^n + 1}. \quad (6)$$

The task of finding the average fidelity of the noisy channel $\Lambda$ is now reduced to finding $\text{Pr}(0)$, i.e. the probability that the twirled channel $\bar{\Lambda}_{C^0_1\otimes n,\Pi}$ does not cause an error.

To obtain $\text{Pr}(0)$, we can start from the input state $|0\rangle^{\otimes n}$, apply the $C^0_1\otimes n$ twirled channel, and measure the output state in the n-bit string basis [15]. Equivalently, for an ensemble system we can replace $|0\rangle^{\otimes n}$ by n distinct input states $\rho_{w} = Z^{\otimes w}f^{\otimes n-w}$ where $Z$ represents the Pauli matrix $\sigma_z$, followed by a permutation operation $\Pi_n$, and measure accordingly as shown in Fig. 1(a).

From an experimental perspective this is still a difficult task. Ideally we want to make as few assumptions as possible about the ability to perform arbitrary Clifford operations since in practice we can only implement $\Lambda = \Lambda \circ U_c$. Moussa et al. [17] modified the original twirling protocol in the following way. By inserting the identity $U_c \circ U_c^\dagger$ appropriately, the circuit depicted in the upper panel of Fig. 1(a) can be transformed to the lower one. The input state $\rho_i = C_i \circ \Pi_n(\rho_{w})$ is the input Pauli operator and the measurement $M_{\rho_i,\Lambda_c} = U_c(\rho_i)$ (that can be calculated efficiently [22]) is also a Pauli operator.

By implementing the circuit in the lower panel of Fig. 1(a), the probability of no error is [25]

$$\text{Pr}(0) = \frac{1}{4^n} \left( 1 + \frac{1}{2^n} \sum_{i=1}^{4^n-1} \text{Tr} \left( U_c(\rho_i) M_{\rho_i,\Lambda_c} \right) \right). \quad (7)$$

Then substituting Eq. (7) to Eq. (6) will yield the average fidelity of the faulty Clifford gate $\Lambda_c$.

Note that the above twirling protocol is limited to the certification of Clifford gates. For a general unitary gate, it is often impractical to realize the measurement operator $M_{\rho_i,\Lambda} = U \circ U_{\rho_i}^\dagger$, whereas for a Clifford gate it can be decomposed efficiently [22]. It is possible to develop fault-tolerant quantum computing where Clifford gates and magic state preparation are the basic building blocks [23, 24]. In these architectures they are the only gates that need to be benchmarked [? ]. For example, the encoding operation of the 3-qubit quantum error correction code is a Clifford gate comprising two controlled-NOT (CNOT) gates and a single qubit Hadamard gate, and has been certified in a 3-qubit solid-state NMR system [17].

In spite of the simplification of the aforementioned way to estimate the average fidelity of Clifford gates, the complexity remains exponential as $4^n - 1$ distinct Pauli states need to be prepared. Actually, measuring all of the expectation values is unnecessary if one only desires to approximate the average with a given confidence level and confidence interval [15]. Hoeffding’s inequality [26] states that if $x_1, ..., x_m$ are independent realizations of a random variable $x$, confined to the interval $[a, b]$ and with statistical mean $\mathbb{E}(x) = \mu$, then for any $\delta > 0$ we have

$$\text{Prob}(|\bar{x} - \mu| > \delta) \leq 2e^{-2\delta^2 m/(b-a)^2}, \quad (8)$$

where $\bar{x} = \frac{1}{m} \sum_{i=1}^{m} x_i$ is the estimator of the exact mean $\mu$, and $\text{Prob}(\epsilon)$ denotes the probability of event $\epsilon : |\bar{x} - \mu| > \delta$ which we want to minimize. Explicitly, Hoeffding’s inequality provides an upper bound on the probability that the estimated mean is off by a value greater than $\delta$. The confidence level and confidence interval are $1 - \text{Prob}(\epsilon)$ and $[\delta, \delta]$, respectively.

When $\mu$ is the average fidelity we have $a = 0$ and $b = 1$. Hence, for a given $\text{Prob}(\epsilon)$ and $\delta$, the number of experiments calculated by taking the log of Eq. (8) is

$$m \leq \frac{\ln(2/\text{Prob}(\epsilon))}{2\delta^2}. \quad (9)$$
Decoherence Error over the entire Pauli group, in distinct Pauli states, \( n \) (color online). (a) Twirling protocols for quantum memories (top) and Clifford gates (bottom). Top: \( \rho_w = C^\otimes n \Pi_s \Pi_U \rho \Pi_U \Pi_s C^\dagger \) spreads over the entire Pauli group \( \mathcal{P}_n \), \( \mathcal{U}_c = \mathcal{U}_c \circ \Lambda \) is the noisy Clifford gate, and \( M_{\rho,c} = \mathcal{U}_c \rho \mathcal{U}_c^\dagger \). (b) Molecular structure of Dichlorocyclobutanone derivative [28] shown in Fig. 1(b). (c) Pulse sequence for the creation of labeled PPS via the method in Ref. [27]. It consists of three parts: encoding, coherence selection (CS) and decoding. \( \mathcal{U}_c \), realized by a 80 ms GRAPE pulse, is the Clifford gate to be certified. The instantaneous states are (unnormalized) \( \rho_1 = |0\rangle \langle 0| \otimes Z, \rho_2 = |0\rangle \langle 0| \otimes Z^2, \rho_3 = |0\rangle \langle 0| \otimes Z^4 + |1\rangle \langle 1| \otimes Z^4 \), and \( \rho_4 = |0\rangle \langle 0| \otimes Z^3 \). (d) Experimental result for the certification of \( \rho_1 \). \( k \) is the number of Pauli operators for weight \( w \), and \( k_w \) is the number of experiments via the sampling; \( t \) is the typical time for the input Pauli state preparation, and \( F_i \) is the fidelity to observe the probability of no error, and \( F_{d,inc} \) is the same quantity but without decoherence effect \( E_d \). (e) Relationship among the experimental remaining signals (blue), decoherence effects (orange) and gate imperfections (gray) for different \( w \).

Note that the number of experiments is independent of number of qubits \( n \), once the desired \( \text{Prob}(\epsilon) \) and \( \delta \) have been given. This result reveals that the estimation of the average fidelity of Clifford gates via twirling protocol is efficient and scalable. For instance, given a 99% confidence level, \( \text{Prob}(\epsilon) = 1\% \) and \( \delta = 0.04 \), the total number of experiments is 1656, independent of \( n \).

Experiment. In the experiment we chose \( \mathcal{U}_c \) to be the Clifford gate used to generate maximal (7-qubit) coherence from single (1-qubit) coherence, up to single-qubit gates. It evolves \( Z_1 \otimes \cdots \otimes Z_n \) to \( Z_1^2 \otimes \cdots \otimes Z_n \) and is the basic encoding process for the pseudo-pure state (PPS) preparation method of Ref. [27] shown in Fig. 1(c). It also plays a role in the creation of cat states. The gate can be decomposed into a sequence of elementary Clifford gates of the type

\[
e^{-i\frac{\pi}{4}X_i} e^{-i\frac{\pi}{4}Z_i} Z_i e^{-i\frac{\pi}{4}Y_i},
\]

that increase the order of coherence by evolving \( Z_i \) to \( Z_i^2 \). Implementing \( \mathcal{U}_c \) in experiment is nontrivial as it requires \( 2(n-1) \) single qubit operations and \( (n-1) \) 2-qubit operations.

Our 7-qubit NMR processor is the per-\(^{13}\)C-labeled dichlorocyclobutanone derivative [28] shown in Fig. 1(b) dissolved in \( d_6 \)-acetone. The carbon nuclei labeled \( C_1 \) to \( C_7 \) denote the seven qubits. Details of the molecular process
structure can be found in the Supplementary Material [29]. \(^{1}H\) nuclei were decoupled by the Waltz-16 sequence throughout all experiments. The internal Hamiltonian of this system can be described as

\[
\mathcal{H}_{\text{int}} = \sum_{j=1}^{7} \pi \nu_j Z_j + \sum_{j<k=1}^{7} \frac{\pi}{2} J_{jk} Z_j Z_k,
\]

where \(\nu_j\) is the resonance frequency of the \(j\)th spin and \(J_{jk}\) is the scalar coupling strength between spins \(j\) and \(k\). All experiments were conducted on a Bruker DRX 700 MHz spectrometer at room temperature.

The entire procedure to estimate the average fidelity of \(\mathcal{U}_c\) can be divided into four parts, as follows:

(i) Sampling. To achieve a confidence level 99% and precision \(\delta = 0.04\), we computed that the required number of experiments is 1656 via Eq. (9). Then we randomly sampled 1656 distinct Pauli states out of the entire 7-qubit Pauli group, which has in total \(4^7 - 1 = 16383\) elements. We distributed all 1656 input Pauli states to seven subgroups according to their Pauli weights \(w = 1\) to \(w = 7\). The primary reason for this distribution is that a quantum gate such as \(\mathcal{U}_c\), here is usually more prone to error when applied to higher weight Pauli states. Additionally, the preparations of input Pauli states with different weights \(w\) are distinct.

The sampling result is shown in Fig. 1(d), where the number of sampled experiments \(k_w\) for weight \(w\) is around one tenth of the total number \(k = 3^{w}(\binom{w}{w})\).

(ii) Preparation and Calibration. For the creation of every input Pauli state, we employed an efficient sequence compiling program [30] to produce the corresponding pulse sequence. All pulses in the preparation sequences are selective and generated by Gaussian shapes. We then compared the state preparation results with the thermal equilibrium state as a calibration of the certification procedure, aiming to capture the errors in preparation and measurements. The typical duration \(t\) for preparing a weight \(w\) Pauli state and the related calibration results \(F_i\) are both listed in Fig. 1(d).

(iii) Evolution. The target operation \(\mathcal{U}_c\) was optimized by a GRadient Ascent Pulse Engineering (GRAPE) pulse [31]. Utilizing the GRAPE algorithm guarantees that \(\mathcal{U}_c\) is a Clifford gate to a very good approximation, as traditional state-dependent shape pulses for multiple qubits in NMR are unlikely to form a strict Clifford operation. The GRAPE pulse of \(\mathcal{U}_c\) was obtained with the pulse width chosen as 80 ms and a simulated fidelity of 0.99. A special calibration method was used in the experiment to ensure that the pulse acting on the spins was a very close approximation to the simulated (theoretical) pulse [5].

(iv) Measurement. After applying the GRAPE pulse of \(\mathcal{U}_c\) to each input Pauli state in the experiment, we measured the corresponding output Pauli state by local readout pulses, and recorded the ratio of the remaining signal to that of the reference input state. Next we averaged the results with respect to different weights \(w\), as shown by \(F_c\) in Fig. 1(d). It is expected that the ratio will decrease as \(w\) increases, since higher coherences are less robust to the decoherence occurring during \(\mathcal{U}_c\).

The probability of no error (\(F_c\) in Fig. 1(d)) is \(\text{Pr}(0) \approx 54.7\%\). The average fidelity of \(\mathcal{U}_c\) via Eq. (6) is then \(\bar{F}(\Lambda) \approx 55.1\%\). It is possible to decompose \(\mathcal{U}_c\) into twelve 1-qubit gates and six 2-qubit gates \([?]\), so the average error per sub-gate is \(\approx 2.5\%\). To quantify the decoherence contribution during \(\mathcal{U}_c\), we followed the approach of phase damping [32] to simulate the dynamical process step by step. The average signal attenuation due to decoherence is shown by \(E_d\) in Fig. 1(d). Under the assumption that the decoherence error can be factorized, the probability of no error \(\text{Pr}(0)\) after theoretically removing the decoherence is 87.4%, which means the average fidelity is 87.5%. The average error per sub-gate is then \(\approx 0.7\%\). The remaining errors are mainly attributed to imperfection in the design and implementation of the GRAPE pulse. Fig. 1(c) shows the relationship between the raw experimental results, decoherence effects and gate imperfections for each \(w\).

Fig. 2(a) shows the spectrum of \(Z^{\otimes 7}\) after \(\mathcal{U}_c(Z_7)\) under the observation of \(C_2\). Comparing the simulated and experimental spectra gives a qualitative indication of the level of coherent control achieved in this 7-qubit system. For another comparison we followed \(\mathcal{U}_c\) by a set of operations to extract the PPS as in Fig. 1(c). The PPS spectrum by observing the labeled spin \(C_7\) is shown in Fig. 2(b).

**Conclusion.** We estimated the average fidelity of a non-trivial 7-qubit Clifford gate using a twirling protocol.
together with a random sampling method. This is the largest gate-characterization reported in an experiment to date. The experimental spectra demonstrate reliable coherent control of this 7-qubit system while our benchmarking protocol gives an average gate fidelity of 55.1% before accounting for decoherence, and 87.5% after theoretically removing the contribution of decoherence. An important feature of the protocol is the relatively small number of experiments required: 1656 ($< 2^{11}$) compared to $2^7 \times 10^8$ ($\approx 2^{28}$) for process tomography. With further developments in experimental quantum information processing we expect that the methods used here will become standard tools for characterizing gate fidelities in larger processors.

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