Single-Shot Quantum Process Tomography
Abhishek Shukla and T. S. Mahesh∗
Department of Physics and NMR Research Center,
Indian Institute of Science Education and Research, Pune 411008, India

The standard procedure for quantum process tomography (QPT) involves applying the quantum process on a system initialized in each of a complete set of orthonormal states. The corresponding outputs are then characterized by quantum state tomography (QST), which itself requires the measurement of non-commuting observables realized by independent experiments on identically prepared system states. Thus QPT procedure demands a number of independent measurements, and moreover, this number increases rapidly with the size of the system. However, the total number of independent measurements can be greatly reduced with the availability of ancilla qubits. Ancilla assisted process tomography (AAPT) has earlier been shown to require a single QST of system-ancilla space. Ancilla assisted quantum state tomography (AAQST) has also been shown to perform QST in a single measurement. Here we combine AAPT with AAQST to realize a ‘single-shot QPT’ (SSPT), a procedure to characterize a general quantum process in a single collective measurement of a set of commuting observables. We demonstrate experimental SSPT by characterizing several single-qubit processes using a three-qubit NMR quantum register. Furthermore, using the SSPT procedure we experimentally characterize the twirling process and compare the results with theory.

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I. INTRODUCTION

An open quantum system may undergo an evolution due to intentional control fields as well as due to unintentional interactions with stray fields caused by environmental fluctuations. Even the carefully designed control fields may be imperfect to the extent that one might need to characterize the overall process acting on the quantum system. Such a characterization, achieved by a procedure called quantum process tomography (QPT), is crucial in the physical realization of a fault-tolerant quantum processor [1, 2]. QPT is realized by considering the quantum process as a map from a complete set of initial states to final states, and experimentally characterizing each of the final states using quantum state tomography (QST) [3]. Since the spectral decomposition of a density matrix may involve noncommuting observables, Heisenberg’s uncertainty principle demands multiple experiments to characterize the quantum state. Thus QST by itself involves the measurement of a series of observables after identical preparations of the system in the quantum state. Hence, QPT in general requires a number of independent experiments, each involving initialization of the quantum system, applying the process to be characterized, and finally QST. Furthermore, the total number of independent measurements required for QPT increases exponentially with the size of the system undergoing the process.

The physical realization of QPT has been demonstrated on various experimental setups such as NMR [4, 5], linear optics [6–9], ion traps [10, 11], superconducting qubits [12–17], and NV center qubit [18]. Several developments in the methodology of QPT have also been reported [19, 20]. In particular, it has been shown that ancilla assisted process tomography (AAPT) can characterize a process with a single QST [6, 7, 21, 22]. However, it still requires multiple measurements each taken over a set of commuting observables. On the other hand, if sufficient ancilla qubits are available, QST can be carried out with a single joint measurement over the entire system-ancilla space. This procedure, known as ancilla assisted quantum state tomography (AAQST), has been studied both theoretically and experimentally [23–26]. Here we combine AAPT with AAQST and realize a ‘single-shot quantum process tomography’ (SSPT), which can characterize a general process in a single collective measurement of the system-ancilla state.

In the next section, after briefly revising QPT and AAPT, we describe SSPT procedure. In section III, we illustrate SSPT using a three-qubit nuclear magnetic resonance (NMR) quantum register. We characterize certain unitary processes corresponding to standard quantum gates. We also characterize a nonunitary process, namely twirling operation. Finally we conclude in section IV.

II. THEORY

A. Quantum Process Tomography (QPT)

A process $\varepsilon$ maps a quantum state $\rho$ to another state $\varepsilon(\rho)$. Here we consider an $n$-qubit system with $N^2 (= 2^{2n})$-dimensional Liouville space $S$. In order to characterize $\varepsilon$, we let the process act on each linearly independent element of a complete basis set $\{\rho_1, \rho_2, \cdots, \rho_{N^2}\}$.

∗ mahesh.ts@iiserpune.ac.in
Expressing each output state in the complete basis we obtain
\[ \varepsilon(\rho_j) = \sum_k \lambda_{jk} \rho_k, \]
where the complex coefficients \( \lambda_{jk} \) can be extracted after QST.

The outcome of a trace-preserving quantum process \( \varepsilon \) also has an operator-sum representation
\[ \varepsilon(\rho) = \sum_i E_i \rho E_i^\dagger, \]
where the Kraus operators \( E_i \) satisfy the completeness relation \( \sum_i E_i^\dagger E_i = I \). To assist experimental characterization of the process, we utilize a fixed set of basis operators \( \{ \hat{E}_m \} \), and express \( E_i = \sum_m e_{im} \hat{E}_m \). The process is now described by
\[ \varepsilon(\rho) = \sum_{mn} \hat{E}_m \rho \hat{E}_n^\dagger \chi_{mn}, \]
where \( \chi_{mn} = \sum_i e_{im} e_{in}^* \) form a complex matrix which completely characterizes the process \( \varepsilon \). Since the set \( \{ \rho_k \} \) forms a complete basis, it is also possible to express
\[ \hat{E}_m \rho_j \hat{E}_n^\dagger = \sum_k \beta_{jk}^{mn} \rho_k, \]
where \( \beta_{jk}^{mn} \) can be calculated theoretically. Eqns. 1, 3 and 4 lead to
\[ \varepsilon(\rho_j) = \sum_k \lambda_{jk} \rho_k = \sum_k \sum_{mn} \beta_{jk}^{mn} \chi_{mn} \rho_k. \]

Exploiting the linear independence of \( \{ \rho_k \} \), one obtains the matrix equation
\[ \beta \chi = \lambda, \]
from which \( \chi \)-matrix can be extracted by standard methods in linear algebra.

For example, in the case of a single qubit, one can choose the linearly independent basis \( \{ |0\rangle, |1\rangle \} \) (see Fig. 1a). While the middle-two elements are non-Hermitian, they can be realized as a linear combination of Hermitian density operators [27]. A fixed set of operators \( \{ I, X, -iY, Z \} \) can be used to express the \( \chi \) matrix. Thus the standard single-qubit QPT procedure requires four QST experiments.

QPT on an \( N \)-dimensional system requires \( N^2 \)-QST experiments, and a single QST involves several quantum measurements each taken jointly over a set of commuting observables. The exact number of measurements may depend on the properties of available detectors. In the case of an \( n \)-qubit NMR system with a well resolved spectrum [28], QST requires \( \lceil \frac{N}{2} \rceil \) measurements, where \( \lceil \cdot \rceil \) rounds the argument to next integer [26]. Therefore an \( n \)-qubit QPT needs a total of \( M_{QPT} \approx N^2 \lceil \frac{N}{2} \rceil \) measurements. Estimates of \( M \) for a small number of qubits shown in the first column of Table 1 illustrate the exponential increase of \( M_{QPT} \) with \( n \).

### B. Ancilla-Assisted Process Tomography (AAPT)

If sufficient number of ancillary qubits are available, ancilla assisted process tomography (AAPT) can be carried out by simultaneously encoding all the basis elements onto a higher dimensional system-ancilla Liouville space \( S \otimes A_1 \) [6, 7, 21, 22]. AAPT requires a single final QST, thus greatly reducing the number of independent measurements. For example, a single-qubit process tomography can be carried out with the help of an ancillary qubit by preparing the \( n \)-qubit cat state \( |\psi_n\rangle = (|00\cdots0\rangle + |11\cdots1\rangle)/\sqrt{2} \), applying the process

\[ \begin{array}{c|c|c}
 n & M_{QPT} & M_{AAPT} (n_{A1}) \\
 \hline
 1 & 8 & 2 \ (1) \\
 2 & 32 & 4 \ (2) \\
 3 & 192 & 11 \ (3) \\
 4 & 1024 & 32 \ (4) \\
 5 & 7168 & 103 \ (5) \\
\end{array} \]

TABLE I. Comparison of number of independent measurements and number of ancilla qubits (in parenthesis) required for \( n \)-qubit QPT, AAPT, and SSPT.

where \( \beta_{jk}^{mn} \)
on the system-qubit, and finally carrying out QST of the two-qubit state (see Fig. 1b). Although only two independent measurements are needed for a two-qubit QST, this number grows exponentially with the total number of qubits.

All the $N^2$ basis elements of the $n$-qubit system can be encoded simultaneously in independent subspaces of a single $N^2 \times N^2$ Liouville operator belonging to $2n$-qubit space $S \otimes A_1$. Thus exactly $n$-ancilla qubits are needed to carry out AAPT on an $n$-qubit system. Therefore AAPT requires $M_{\text{AAPT}} \approx \frac{N^2}{2n}$ independent measurements. The minimum number of experiments for a few system-qubits are shown in the second column of Table I. While AAPT requires significantly lesser number of measurements compared to QPT, it still scales exponentially with the number of system-qubits.

C. Single-Shot Process Tomography (SSPT)

It had been shown earlier that, if sufficient number of ancillary qubits are available, QST of a general density matrix of arbitrary dimension can be performed with a single joint measurement of a set of commuting observables [23–26]. This method, known as ancilla assisted quantum state tomography (AAQST) is based on the redistribution of all elements of the system density matrix on to a joint density matrix in the combined system-ancilla Liouville space. Initially ancilla register for AAQST is prepared in a maximally mixed state thus erasing all information in it and redistribution of matrix elements is achieved by an optimized joint unitary operator [26].

By combining AAPT with AAQST, process tomography can be achieved with a single joint measurement of all the qubits (see Fig. 1c and 3rd column of Table I). If AAQST is carried out with an ancilla space (A2) of $n_{A2}$-qubits, the combined space $S \otimes A_1 \otimes A_2$ corresponds to $\tilde{n} = 2n + n_{A2}$ qubits. A single joint measurement suffices if the total number of observables is equal to or exceeds the number of real unknowns (i.e., $N^4 - 1$) in the $2n$-qubit density matrix, i.e., if $\tilde{n}N \geq (N^4 - 1)$, where $\tilde{N} = 2^n$ [26]. The number of ancillary qubits $n_{A1}$ and $n_{A2}$ required for SSPT are shown in the third column of Table I.

The complete circuit for SSPT is shown in Fig. 2. It involves two ancilla registers, one for AAPT and the other for AAQST. Initially AAQST register is prepared in a maximally mixed state and the other two registers are set to $|0\rangle^{\otimes \tilde{n}}$ states. Hadamard gates on the AAPT ancilla followed by C-NOT gates (on system qubits controlled by ancilla) prepare state $|\psi_{\tilde{n}}\rangle$, which simultaneously encodes all the basis elements required for QPT. A single application of the process $\varepsilon$, on the system qubits, acts simultaneously and independently on all the basis elements $\{\rho_j\}$. The final AAQST operation allows estimation of all the elements of the $2n$-qubit density matrix $\sum_j \varepsilon(\rho_j) \otimes A_1^{(j)}$, where $A_1^{(j)}$ identifies the $j$th subspace. The output of each subspace $\varepsilon(\rho_j)$ can now be extracted, and the coefficients $\lambda_{jk} = Tr[\varepsilon(\rho_j)\rho_k^{\dagger}]$ can be calculated.

III. EXPERIMENTS

We used iodotrifuoroethylene (C$_2$F$_3$I) dissolved in acetone-D$_6$ as a 3-qubit system. The molecular structure and labelling scheme are shown in Fig. 3 (a). All the experiments described below are carried out on a Bruker 500 MHz NMR spectrometer at an ambient temperature of 300 K using high-resolution NMR techniques. The NMR Hamiltonian in this case can be expressed as

$$\mathcal{H} = -\pi \sum_{i=1}^{3} \nu_i \sigma^z_i + \pi \sum_{i=1,j>i}^{3,3} J_{ij} \sigma^+_i \sigma^-_j / 2$$

FIG. 2. (Color online) Quantum circuit for SSPT.

FIG. 3. (Color online) Molecular structure of iodotrifuoroethylene (a), and the table of Hamiltonian and relaxation parameters (b), NMR pulse-sequence to demonstrate SSPT (c). Pulse sequence for preparing $|00\rangle$ pseudopure state is shown in the inset of (c).
where $\sigma^z_i$ and $\sigma^z_j$ are Pauli z-operators of $i$th and $j$th qubits [28]. The chemical shifts $\nu_i$, coupling constants $J_{ij}$, and relaxation parameters ($T_1$ and $T_2$) are shown in Fig. 3 (b). All the pulses are realized using gradient ascent pulse engineering (GRAPE) technique [29] and had average fidelities above 0.99 over 20% inhomogeneous RF fields.

We utilize spins $F_1$, $F_2$, and $F_3$ respectively as the system qubit ($S$), AAPT ancilla ($A_1$), and AAQST ancilla ($A_2$). The NMR pulse-sequence for SSPT experiments are shown in Fig. 3(c). It begins with preparing $A_2$ qubit in the maximally mixed state by bringing its magnetization into transverse direction using a Hadamard gate, and subsequently dephasing it using a PFG. The remaining qubits are initialized into a pseudopure $|00\rangle$ state by applying the standard pulse-sequence shown in the inset of Fig. 3c [30]. The Bell state $|\psi_2\rangle$ prepared using a Hadamard-CNOT combination had a fidelity of over 0.99. After preparing this state, we applied the process $\varepsilon$ on the system qubit. The final AAQST consists of $(\pi/2)_y$ and $(\pi/2)_y$ pulses on all the qubits separated by delays $\tau_1 = 6.7783$ ms and $\tau_2 = 8.0182$ ms [26]. A single joint measurement of all the qubits now leads to a complex signal of 12 transitions, from which all the 15 real unknowns of the 2-qubit density matrix $\rho_{S,A_1} = \sum_j \varepsilon(\rho_j) \otimes A_1^{(j)}$ of $F_1$ and $F_2$ can be estimated [26]. In our choice of fixed set of operators and basis elements

$$
\rho_{S,A_1} = \begin{bmatrix}
\lambda_{11} & \lambda_{12} & \lambda_{21} & \lambda_{22} \\
\lambda_{13} & \lambda_{14} & \lambda_{23} & \lambda_{24} \\
\lambda_{31} & \lambda_{32} & \lambda_{11} & \lambda_{12} \\
\lambda_{33} & \lambda_{34} & \lambda_{13} & \lambda_{14}
\end{bmatrix}
$$

[31]. The $\chi$ matrix characterizing the complete process can now be obtained by solving the eqn. 6.

A. SSPT of quantum gates

We now describe experimental characterization of several single-qubit unitary processes. The quantum gates to be characterized are introduced as process $\varepsilon$ on $F_1$ qubit in Fig. 3c. The experimental $\chi$-matrices for NOP (identity process), NOT-X ($e^{-i\pi X /2}$), NOT-Y ($e^{-i\pi Y /2}$), Hadamard, Phase-$\pi$ ($e^{i\pi Z}$), and Phase-$\pi/4$ ($e^{i\pi Z/8}$) are shown in Fig. 4. Starting from thermal equilibrium, each SSPT experiment characterizing an entire one-qubit process took less than four seconds. A measure of overlap of the experimental process $\chi_{\text{exp}}$ with the theoretically expected process $\chi_{\text{th}}$ is given by the gate fidelity [18]

$$
F(\chi_{\text{exp}}, \chi_{\text{th}}) = \frac{|Tr[\chi_{\text{exp}}^{\dagger}\chi_{\text{th}}]|}{\sqrt{Tr[\chi_{\text{exp}}^{\dagger}\chi_{\text{exp}}] Tr[\chi_{\text{th}}^{\dagger}\chi_{\text{th}}]}}
$$

The gate fidelities for all the six processes are indicated in Fig. 4. Except in the cases of Hadamard and Phase-$\pi/4$, the gate fidelities were about 0.99. The lower fidelities in Hadamard (0.95) and Phase-$\pi/4$ (0.97) are mainly due to imperfections in the RF pulses implementing these processes.

In order to study the robustness of SSPT procedure we first considered an ideal process, simulated the corresponding spectral intensities, and reconstructed the final density matrix $\rho_{S,A_1}$. Using eqn. 8 we obtained $\lambda_{jk}$ values and calculated the matrix $\chi_0$ simulating the noise-free SSPT procedure. We then introduced noise by adding random numbers in the range $[-\eta, \eta]$ to the spectral intensities and used the resulting data calculating $\chi_\eta$ simulating the noisy SSPT procedure. The variations of average gate fidelities $F(\chi_0, \chi_\eta)$ for various processes versus noise amplitude $\eta$ are shown in Fig. 5. Interestingly, the noise has similar effects on fidelities of all the simulated processes. We also observe that fidelities remained above 0.9 for $\eta < 0.1$, indicating that SSPT is fairly robust against the noise in this range.

![FIG. 5. (Color online) Simulated fidelity of various processes as a function of noise $\eta$.
]
B. SSPT of twirling process

Twirling is essentially a nonunitary process usually realized by an ensemble average of a set of unitary operations. It was first introduced by Bennett et al. [32] for extracting singlet states from a mixture of Bell states. Twirling has been studied in detail [33–37] and various modified twirling protocols have also been suggested [38, 39].

In NMR, twirling can be achieved with the help of a pulsed field gradient (PFG), which produces a continuous space-dependent spin-rotation, such that the ensemble average effectively emulates a nonunitary process [40]. A $\hat{z}$ PFG produces a space-dependent unitary $U_\phi = \exp \left(-i \frac{\phi}{2} \sum_{j=1}^{n} s_{jz} \right)$ with $\phi \in [-\Phi, \Phi]$, where $j$ is the summation index over all the qubits, and the maximum phase $\Phi$ depends on the strength and duration of the PFG and the sample volume. When the $\hat{z}$ PFG acts on an initial $n$-qubit density matrix $\rho_{in} = \sum_{lm} \rho_{lm} |l\rangle \langle m|$, the resultant output density matrix is,

$$
\rho_{out} = \frac{1}{2\Phi} \int_{-\Phi}^{\Phi} d\phi \, U_\phi \rho_{in} U_\phi^\dagger = \sum_{lm} \rho_{lm} |l\rangle \langle m| \, \text{sinc}(q_{lm} \Phi). \quad (10)
$$

Here $\text{sinc}(x) = \frac{\sin(x)}{x}$ and $q_{lm} = \frac{1}{2} \sum_{j} [(-1)^{m_j} - (-1)^{n_j}]$ is the quantum number of the element $|l_1 l_2 \cdots l_n\rangle |m_1 m_2 \cdots m_n\rangle$, i.e., the difference in the spin-quantum numbers of the corresponding basis states. While the diagonal elements $|l\rangle \langle l|$ and other zero-quantum elements are unaffected by twirling, the off-diagonal elements with $q_{lm} \neq 0$ undergo decaying oscillations with increasing $\Phi$ values.

SSPT of twirling process is carried out using the procedure described in Fig. 3c after introducing $\delta$-PFG-$\delta$ in place of the process $\varepsilon$, where $\delta$ is a short delay for switching the gradient. Applying PFG selectively on the system qubit is not simple, and is also unnecessary. Since the $F_3$ qubit (AAQT ancilla) is already in a maximally mixed state, twirling has no effect on it. For the Bell state $|\psi_2\rangle$, applying a strong twirling on either or both spins ($F_1$, $F_2$) has the same effect, i.e., a strong measurement reducing the joint-state to a maximally mixed state. However, since $|\psi_2\rangle$ corresponds to a two-quantum coherence (i.e., $q_{00,11} = 2$), its dephasing is double that of a single-quantum coherence. Assuming the initial state $\rho_{in} = |\psi_2\rangle \langle \psi_2|$, and using expressions 1 and 10, we find that the non-zero elements of $\lambda$ are

$$
\lambda_{11} = \lambda_{44} = 1, \quad \text{and} \quad \lambda_{22} = \lambda_{33} = \text{sinc}(2\Phi). \quad (11)
$$

Solving expression 6, we obtain a real $\chi$ matrix with only non-zero elements

$$
\chi_{EE} = \frac{1 + \text{sinc}(2\Phi)}{2} \quad \text{and} \quad \chi_{ZZ} = \frac{1 - \text{sinc}(2\Phi)}{2}. \quad (12)
$$

In our experiments, the duration of PFG and $\delta$ are set to 300 $\mu$s and 52.05 $\mu$s respectively, such that the chemical shift evolutions and $J$-evolutions are negligible. The strength of twirling is slowly varied by increasing the PFG strength from 0 to 2.4 G/cm in steps of 0.05 G/cm. The results of the experiments are shown in Fig. 6. The filled squares (circles) in Fig. 6(a) correspond to experimentally obtained values for $|\chi_{EE}|$ (|$\chi_{ZZ}$|). Small imaginary parts observed in experimental $\chi$ matrices are due to minor experimental imperfections. The smooth (dashed) lines indicate corresponding theoretical values obtained from eqns. 12. The crosses indicate the gate fidelities $F(\chi_{exp}, \chi_{th})$ calculated using eqn 9. The barplots show experimental $|\chi|$ matrices for (b) $\Phi = 0$, (c) $\Phi = 0.64\pi$, (d) $\Phi = \pi$, and (e) $\Phi = 3.43\pi$, and $\chi_{EE}$ and $\chi_{ZZ}$ values in Fig 6(a) corresponding to these $\Phi$ values are circled out.

At zero twirling, the process is essentially a NOP process as is clear from the bar plot in Fig. 6(b), wherein $|\chi_{EE}| \approx 1$ and $|\chi_{ZZ}| \approx 0$. When $\Phi = k\pi/2$ with an integer $k$, the ensemble initially prepared in state $|\psi_2\rangle$ undergoes an overall phase distribution over $[-k\pi, k\pi]$, and at this stage $\chi_{EE} = \chi_{ZZ} = 0.5$ (e.g. Fig. 6 d). Further increase in $\Phi$ leads to oscillations of $\chi_{EE}$ and $\chi_{ZZ}$ about 0.5, and for large $\Phi$ values, both of these elements damp towards 0.5 and all other elements vanish (e.g. Fig. 6 c). The errors in experimental $\chi_{EE}$ and $\chi_{ZZ}$ values were less than 8%. The good agreement of the experimental values with theory indicates the overall success of SSPT procedure. The average of the gate fidelities was over 0.96. Small deviations of the experimental values from theory are due to nonlinearities in PFG profile as well as due to imperfections in RF pulses implementing the SSPT procedure.
IV. CONCLUSIONS

Information processing requires two important physical resources, namely, the size of the register and the number of operations. Often there exists an equivalence between these two resources which allows trading one resource with another. Likewise, in the present work we show that, if some extra qubits are available, it is possible to carry out quantum process tomography of the system qubits with a single joint measurement over a set of commuting observables. We have illustrated this method on a single system qubit and two ancillary qubits using NMR quantum computing methods. In particular, we extracted the $\chi$ matrices characterizing certain quantum gates and obtained their gate fidelities with the help of a single measurement of a three qubit system in each case. We studied the robustness of SSPT procedure using numerical simulations. We also characterized twirling operation which is essentially a nonunitary process. The overall procedure of SSPT is general and can be applied to other fields such as optical qubits, trapped ions, or superconducting qubits.

A potential application of single-shot process tomography could be in high throughput characterization of dynamic processes. The standard methods require repeated applications of the same process either to collect independent outputs from all the basis states or to allow quantum state tomography. However, the present method requires only one application of the process for the entire characterization.

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