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QUANTUM INFORMATICS

Comparison of Tomography Methods for Pure and Almost Pure Quantum States

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Quantum tomography is the most informative tool for estimating the quality of preparation and transformation of quantum states. Its development is crucially necessary for debugging of developed quantum processors. Many existing methods of quantum tomography differ in types of performed measurements and in procedures of their processing. The practical implementation of quantum tomography requires the comparison of different methods, which is complicated because of the absence of a general methodology of estimation. A universal methodology based on numerical experiments has been proposed in this work to estimate the quality of quantum state tomography methods. The developed methodology has been applied to three quantum tomography methods (root approach, compressed sensing, and adaptive tomography) efficiently operating with almost pure states, which is relevant for the current technological foundation of the experiments.

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1. INTRODUCTION

The technologies of quantum computing implementation developed in last several years allow operating quantum registers containing more than 50 qubits [1, 2], but the accuracy of state preparation in such quantum systems is still insufficient for the successful solution of applied problems. Quantum key distribution methods should soon allow exchange of large messages in an almost absolute secret mode [3, 4]. For the debugging and control of quality of the state preparation in these systems, it is necessary to use *quantum tomography* methods [5–8]. The choice of a certain method depends on a number of factors, such as the difficulty of experimental implementation, types of considered states, and computational difficulty of processing of the measurement results. Although most of the methods are considered as universal, their accuracy can strongly depend on these factors.

It is important to note that almost pure quantum states can be prepared in modern quantum registers. All but one eigenvalues of the density matrix of an almost pure state are close to zero. Furthermore, at low sample size, such a weak mixing of the state is negligibly low compared to statistical fluctuations, and states themselves are manifested as pure [9]. Under such conditions, methods for reconstructing the general density matrix are inefficient because they introduce an excessive number of parameters in the quantum state model. Among such methods are linear inversion with projection [10], standard convex optimization [11], method based on the Cholesky decomposition [12], and projected gradient descent [13, 14].

It is known that the tomography of reduced-rank quantum states by means of such inefficient methods results in the convergence of infidelity by the law $\propto 1/N^{1/2}$, where N is the total sample size from all measurements (the number of representatives of a quantum statistical ensemble) [9, 15–18]. At the same time, the most efficient tomography methods can provide convergence rate $\propto 1/N$.

For the problem under consideration, a number of existing methods tend to approach convergence rate $\propto 1/N$. The practical application of quantum tomography methods requires the comparison of their efficiency. This comparison is also important for the development of new quantum tomography methods. However, the problem of comparison is difficult because of the absence of a common methodology of estimates: different problems and testing conditions are considered in different works, and also different efficiency indicators are used. In particular, representing compressed sensing tomography results, the authors of [19] mainly focused on the comparison of measurement protocols with different sizes, whereas less attention was paid to the dependence on the sample size. In [20], the root tomography approach was demonstrated in application to a single mixed state. Comparison of adaptive tomography methods was performed in [9] only for random (in the Haar measure) pure states and random (in the Bures measure) mixed states, which cannot reveal the efficiency of the method in application to almost pure states.

The described problem is also complicated because the implementation of most of the quantum tomography methods is difficult. This does not allow the fast comparison of methods in some particular cases in order to determine the most efficient of them.

In this work, we propose a universal methodology for the practical estimate of the quality of quantum state tomography methods and apply it to the methods based on convex optimization, root approach, compressed sensing, and adaptive tomography. The methods are briefly described in Section 2. For each method, we perform numerical experiments under the same conditions and, then, analyze the results in terms of the prespecified benchmarks formulated in Section 3. Using the analysis results, we perform the comparison of methods in Section 4, which reveals their relative efficiencies with respect to each other and some very significant fine differences.

2. DESCRIPTION OF THE METHODS

Below, we briefly describe all methods under consideration. Each method is specified by both the type of performed measurements and the procedure of measurements results processing. Note that all methods under consideration are based on factorized measurements (each qubit is measured independently), because such measurements are the simplest and most relevant for practical realization.

2.1. Factorized Measurements in Mutually Unbiased Bases, Least Squares Method for the Density Matrix (FMUB–LSDM)

The method is based on the determination of the parameters of the general density matrix by minimizing the squares of differences between theoretical (from the estimate of the density matrix) and experimental frequencies of various events. To ensure a physically correct result, this minimization is performed under a positive semidefinite constraint on the density matrix. This problem is efficiently solved by convex optimization methods [11]. As a measurement protocol, we use the protocol of factorized mutually unbiased bases (FMUB protocol): each qubit is measured independently in three mutually unbiased bases corresponding to the Pauli operators σ_x, σ_y, and σ_z [21]. In this case, the measurement of each basis involves the same number of representatives of the statistical ensemble. The optimization problem is solved with the open-source software for the convex optimization CVX [22].

2.2. Maximum Likelihood Method with Root Approach

The maximum likelihood method is one of the most widespread methods of statistical reconstruction of quantum states. This method has the optimal asymptotic properties under certain quite general conditions [23].

2.2.1. Factorized measurements in mutually unbiased bases, root approach with a known rank (FMUB–RootTR). In the root estimation approach, the square root of the density matrix, i.e., a $d \times r$ matrix ψ such that $\rho = \psi\psi^\dagger$ is the density matrix, is considered instead of the density matrix itself. Here, the rank of the state r can be from 1 to d (d is the dimension of the Hilbert space). Search for the maximum likelihood for ψ is reduced to the solution of a quasilinear equation by the fixed-point iteration method [20, 24].

The rank $r = 1$ corresponds to the pure quantum state, whereas the rank $r = d$ describes the completely mixed state. Within the FMUB–RootTR method, we use the true rank (TR) r_t of the quantum state density matrix, which is considered as a priori known. It is noteworthy that the estimate with $r = d$ numerically coincides with estimates by the methods based on the Cholesky decomposition [12] and projected gradient descent [13, 14].

As in the FMUB–LSDM method, we consider the FMUB protocol. The reconstruction of a quantum state with the root approach is performed using its open program implementation [25].

2.2.2. Factorized measurements in mutually unbiased bases, root approach with the adequate rank (FMUB–RootAR). The true rank of an experimentally studied quantum state is often unknown a priori. In this case, the adequate rank (AR) is chosen using the χ^2 test [20]. To this end, we reconstruct a state by varying r from 1 to d and estimating p-value P_r of each model using the χ^2 test. If $P_r \geq \alpha$, where $\alpha = 5\%$ is the significance level, is satisfied for a certain rank r, the procedure is stopped and this rank is taken as the true rank: $r_t = r$. The procedure is also stopped if $P_{r+1} < P_r$ and $r_t = r$ is accepted. This algorithm means that a state with the minimum rank (in particular, a pure state) is taken as the null statistical hypothesis; in this case, $\alpha = 5\%$ specifies the so-called probability of a type I error (probability of rejecting the null hypothesis under the condition that it is true). In addition, this procedure can ensure a certain reduction of the computational cost because of a rare resort to higher rank models.

2.3. Measurement of Pauli Operators, Compressed Sensing Approach (Pauli–CS).

The compressed sensing (CS) approach is the expansion of the least squares method, where the trace of the density matrix is minimized together with the sum of squares [19, 26]:

$$\rho = \arg\min_{X\geq 0}\left[\frac{1}{2}\|O_{\mathrm{T}}(X) - O_{\mathrm{M}}\|_2^2 + \frac{4M}{\sqrt{N}}\mathrm{Tr}X\right]. \qquad (1)$$

Here, $O_{\mathrm{T}}(X)$ and O_{M} are the vectors of the theoretical (based on the density matrix X) and experimental average values of observables corresponding to different measurements, respectively. The measurement protocol is specified by the tensor product of a set of Pauli operators together with the identity operator σ_0: $P_n = \{\sigma_0, \sigma_x, \sigma_y, \sigma_z\}^{\otimes n}$. A measurement of each observable involves the same number of representatives of a statistical ensemble. The authors of [19, 26] also considered protocols formed by subsets of operators from P_n that are not informationally complete for general density matrices. Here, we consider only the complete set of 4^n measurements.

To solve the optimization problem given by Eq. (1), we used the open-source software for the convex optimization CVX [22].

2.4. Adaptive Tomography

In the Introduction, we mentioned that methods reconstructing a general density matrix are inefficient for the tomography of pure and almost pure states. This disadvantage can be eliminated by choosing an appropriate measurement protocol that increases information on components of the density matrix with small weights. This choice is ensured by the suitable rotation of the multiqubit measurement protocol for one of the projectors to be orthogonal to the maximum number of principal components of the density matrix of the studied state. Since the true state is unknown, this could be reached adaptively: the density matrix is estimated when new results of measurements appear and appropriate measurements for the next iteration are selected [9, 18, 27–29].

2.4.1. Factorized orthogonal measurements, maximum likelihood estimation of the density matrix (FO–MLDM). The adaptive protocol of factorized orthogonal (FO) measurements proposed in [9] involves an iterative procedure each step of which includes the estimation of the density matrix $\hat{\rho}$ using all previously performed measurements. After that, a factorized n-qubit vector $|\varphi\rangle_1 \otimes \ldots \otimes |\varphi\rangle_n$ orthogonal to no more than $K_{\max} = n$ principal components of $\hat{\rho}$ is constructed. Then, the vectors $|\varphi\rangle_1, \ldots, |\varphi\rangle_n$ are complemented to the orthonormal single-qubit bases, which are used in next measurements. The estimation of the density matrix $\hat{\rho}$ at each iteration step is performed by the maximum likelihood estimation of the density matrix (MLDM). The authors of [9] performed this procedure using accelerated projected gradient descent. In simulation, we used the full-rank root approach (see Section 2.2.1). As in [9], the measurement in a new basis involves $N_k = \max(100, \lfloor N_0/30 \rfloor)$ representatives of the statistical ensemble. Here, N_0 is the total number of representatives measured in preceding iterations.

2.4.2. Factorized orthogonal measurements in mutually unbiased bases, maximum likelihood estimation of the density matrix (FOMUB–MLDM). The FO–MLDM method cannot be applied to tomography of a single qubit, because orthogonal measurements in this case are always unambiguous and iterations do not provide information completeness.[1] Furthermore, the computational difficulty of the method caused by the necessity of search for the optimal basis at each adaptive step complicates its repeated simulation for acquiring a sufficient statistical ensemble, particularly when the analysis is required for large N values. These features stimulate us to develop a new adaptive protocol based on the FO–MLDM method supplemented by a unitary "rotation" of the single-qubit sets of MUB at each iteration step such that one of its vectors coincides with $|\varphi\rangle_j$ ($j = 1, \ldots, n$). Thus, informationally complete measurements of each qubit are formed at each adaptive step and one of them coincides with that performed at each iteration within the FO–MLDM method.[2] This approach can be applied to analyze single-qubit states and requires searching the orthogonal factorized measurements fewer times.

We also take N_k as the number of representatives of the ensemble per each measurement basis.

3. METHODOLOGY OF THE ANALYSIS

One of the main characteristics of quantum tomography is the accuracy of reconstruction of the unknown quantum state that can be obtained having a certain number of representatives of the statistical ensemble N (sample size). As a measure of accuracy, we use the widely used *fidelity* measure specifying the probability of coincidence of the true σ and reconstructed ρ density matrices: $F = \left(\mathrm{Tr}\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right)^2$ [30]. However, the inverse question is often formulated in real experiments: How many resources are necessary to ensure the required fidelity level (*fidelity benchmark*) F_{B}? We consider the following basic resources:

—The sample size N_{B} determines the required number of identically prepared representatives of an unknown quantum state.

[1] Information completeness with respect to the current estimate of the state can be reached by adding new measurements close to the constructed one [32].

[2] This is valid only for the two-level subsystems considered here. For subsystems with a dimension of 3 or higher, the completion of $|\varphi\rangle_j$ to the basis is ambiguous and, consequently, does not usually coincide with any of the bases of the transformed MUB.

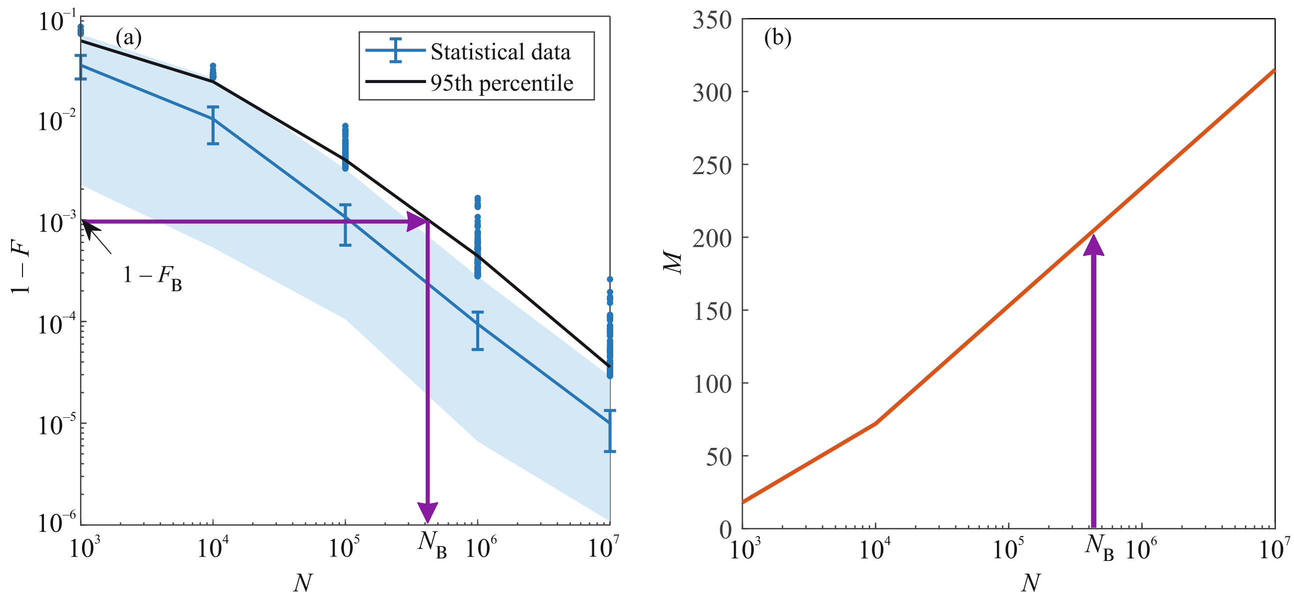

Fig. 1. (Color online) Method of determination of resources from the statistical data. (a) Calculation of the 95th percentile of infidelity for each total sample size N. The required N_B value is calculated with linear interpolation (on a logarithmic scale) for a chosen benchmark fidelity F_B. (b) Calculation of the number of measurements by the value at the point N_B.

—The number of *different* measurement bases M_B describes the number of necessary rearrangements of the configuration of the measuring instrument during a single tomography experiment.

The listed characteristics are calculated for two different classes of states: random pure states and depolarized random pure states. We consider systems of n qubits. The corresponding quantum states are defined in a Hilbert space with the dimension $d = 2^n$. Since the accuracy itself is a random variable, numerous numerical tomographic experiments should be performed to determine the studied characteristics. We note that the quality of some tomography protocols can often be estimated a priori using a universal accuracy distribution [20]. Furthermore, the accuracy depends on the studied states chosen randomly in each experiment. A random pure state $|\psi\rangle$ is generated in the Haar measure [31]. The density matrix for a depolarized random pure state is chosen on the basis of a random pure state by the formula $\rho = (1-p)|\psi\rangle\langle\psi| + pI_d/d$, where I_d is the $d\times d$ identity matrix and p is the random variable uniformly distributed from 0 to 0.1.

To calculate resources required for the quantum tomography method, we use the following algorithm (Fig. 1).

(i) A series of 1000 independent numerical quantum tomography experiments are performed for different sample sizes N. In each experiment, a random state is generated and the Monte Carlo simulation of its measurements is performed. The measurement protocol is determined by a certain quantum tomography method. The state is reconstructed from the results of the measurements and the fidelity F is determined.

(ii) The 95th percentile of infidelity $[1-F]_{95}$ is calculated for each N value.

(iii) The fidelity benchmark F_B is chosen.

(iv) The dependence of $\log[1-F]_{95}$ on $\log N$ is linearly interpolated and the sample size N_B for which $[1-F]_{95} = 1-F_B$ is determined.

(v) The dependence of M on $\log N$ is linearly interpolated and the M_B value at the point $\log N_B$ is determined.

The use of the 95th percentile of infidelity implies that, having N_B representatives of quantum state, the method makes it possible to obtain a fidelity of no worse than F_B with a probability of 95%. The linear interpolation of the dependence of $\log[1-F]_{95}$ on $\log N$ is chosen because, as mentioned above, quantum tomography is characterized by the dependence $1-F \propto 1/N^q$, where $0 < q \leq 1$.

4. COMPARISON OF THE METHODS

Below, we present the results of comparison of different tomography methods in application to the same random states in systems of one, two, and three qubits. The fidelity benchmark $F_B = 99.9\%$ was taken and the same statistical data were used for methods based on identical measurement protocols (e.g., FMUB protocol).

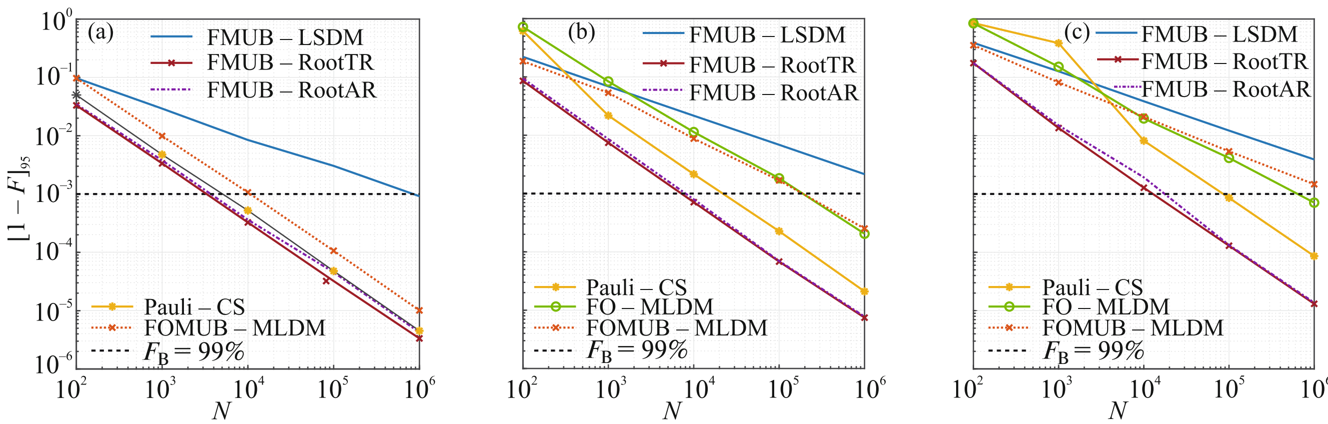

Fig. 2. (Color online) Infidelity 95th percentiles for various tomography methods versus the sample size for the tomography of random pure states for (a) one, (b) two, and (c) three qubits. The horizontal dashed straight line marks the infidelity benchmark $1 - F_B$.

4.1. Random Pure States

Figure 2 shows the results of simulation for the test of random (in the Haar measure) pure states. The corresponding quantitative estimates are summarized in Table 1.

4.2. Depolarized Random Pure States

Figure 3 and Table 2 present the results of simulation for depolarized random pure states. The FO–MLDM method was not analyzed under these conditions because of a large computational difficulty. We note that the estimate of a quantum state using the root approach with a known rank (FMUB–RootTR) in this case where the rank of the true quantum state is full ($r_t = d$) is numerically equivalent to any maximum likelihood estimate of the density matrix (MLDM).

5. DISCUSSION

Numerous quantum tomography methods have already been reported. It is difficult to analyze the efficiencies of various methods using only the corresponding publications because conditions under which these methods are tested can be significantly different. In this work, we have proposed a general methodology of quantitative comparison of different quantum tomography methods. This methodology is based on the simulation of real experimental conditions identical for all considered tomography methods. We calculate resources needed for each method to reach a certain fidelity benchmark in a quantum tomography experiment.

The results obtained show fine and very significant differences between several tomography methods for pure and almost pure quantum states in systems of one to three qubits. The root approach (FMUB–RootTR, FMUB–RootAR), compressed sensing (Pauli–CS), and factorized orthogonal measurements (FO–MLDM) for pure states allow approaching the infidelity convergence rate $\propto 1/N$ with different coefficients. The root approach demonstrates the best characteristics in the required resources. The difference in the coefficient of proportionality for the Pauli–CS method can possibly be compensated in part by the transition from the analysis of the average values of observables to the frequencies of various outcomes. The authors of [9] mentioned that the characteristics

Table 1. Quantitative estimates of resources spent by different quantum tomography methods to reach the fidelity $F_B = 99.9\%$ in the case of the random pure state test

	1 qubit		2 qubits		3 qubits	
	N_B	M_B	N_B	M_B	N_B	M_B
FMUB–LSDM	847475	3	$>10^6$	9	$>10^6$	64
FMUB–RootTR	3302	3	7163	9	12796	27
FMUB–RootAR	3690	3	8022	9	17596	27
Pauli–CS	5080	4	21859	16	85581	64
FO–MLDM	–	–	188490	157	638732	194
FOMUB–MLDM	10667	71	187391	175	$>10^6$	>297

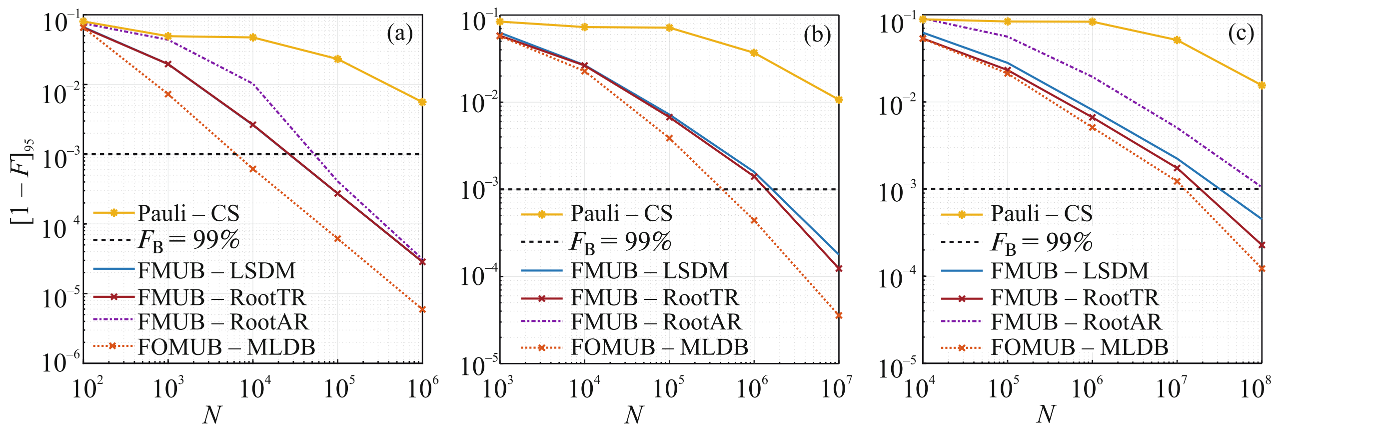

Fig. 3. (Color online) Infidelity 95th percentiles for various tomography methods versus the sample size for the tomography of depolarized random pure states for (a) one, (b) two, and (c) three qubits. The horizontal dashed straight line marks the infidelity benchmark $1 - F_B$.

of the FO–MLDM method can be improved by considering the density matrix with a limited rank at each adaptive step instead of the reconstruction of the general density matrix. As expected, when reconstructing the general density matrix by the least squares method FMUB–LSDM, infidelity decreases approximately as $1/N^{1/2}$. When simulating and comparing different methods, we developed a new adaptive FOMUB–MLDM method based on the measurement protocol in factorized mutually unbiased bases, which is a kind of combination of the FMUB–LSDM and FO–MLDM methods. In its application to pure states, the convergence of infidelity decreases gradually with an increase in the system dimension from the law $1/N$ to the law $1/N^{1/2}$.

The estimate of the general density matrix by the maximum likelihood or least squares method gives an optimal convergence rate $1/N$ for mixed states, but only if all eigenvalues of the density matrix are large enough. Otherwise, such convergence is observed only in the case of a very large sample size. Our quantitative analysis for the case of almost pure states shows that the transition to the law of $1/N$ can be ensured at smaller N values using the FOMUB–MLDM method, where single-qubit sets of MUB are "rotated" at each adaptive step orthogonally to the current estimate of the state.

The FMUB–RootAR and Pauli–CS methods provide a much lower accuracy for the problem of tomography of almost pure states, but the universality of the FMUB–RootAR method, which is due to the possibility of adaptation of the quantum state model rank to the existing statistical data, provides a transition to a law of $1/N$ much earlier than the Pauli–CS method. It is noteworthy that the adaptive compressed sensing method described in [29] can ensure a high accuracy for states with an arbitrary purity level. However, as any other existing adaptive method, this method requires significant resources for the calculation of the protocol and for the repeated tuning of the instruments to change the measurement basis.

The development of the proposed methodology together with other tomography methods will allow systematizing data in this field and obtaining the general picture of the efficiency of methods in application to different practically important problems.

Table 2. Quantitative estimates of resources spent by different quantum tomography methods to reach the fidelity $F_B = 99.9\%$ in the case of the depolarized random pure states test

	1 qubit		2 qubits		3 qubits	
	N_B	M_B	N_B	M_B	N_B	M_B
FMUB–LSDM	26732	3	1624133	9	31844790	27
FMUB–RootTR	26862	3	1379537	9	18751495	27
FMUB–RootAR	52829	3	4388900	9	$>10^8$	27
Pauli–CS	$>10^6$	4	$>10^7$	16	$>10^8$	64
FOMUB–MLDM	6361	58	420015	203	12261609	388

6. CONCLUSIONS

To summarize, an approach based on numerical experiments has been proposed to estimate the quality of quantum tomography methods in application to the reconstruction of pure and almost pure states. The main comparison measure is the number of measurements necessary to reach a given accuracy, which is relevant for modern experimental problems. Six modern quantum tomography methods have been analyzed and compared. The results obtained and the methodology itself can be used to choose the method and number of measurements in a given experiment, as well as to develop and optimize new quantum tomography methods. For almost pure quantum states, a further development of adaptive strategies of quantum measurements is actual. Such strategies should provide the maximum amount of information on components of the density matrix with small weights with given restrictions on the existing experimental resources.

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