Estimating mixed quantum states

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We discuss single adaptive measurements for the estimation of mixed quantum states of qubits. The results are compared to the optimal estimation schemes using collective measurements. We also demonstrate that the advantage of collective measurements increases when the degree of mixing of the quantum states increases.

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I. INTRODUCTION

One of the best distinctions between classical and quantum systems can be formulated using the language of state measurements. The state of a single classical system is an observable: it is in principle always possible to measure generalized coordinates and generalized momenta at a certain time \( t \). This information is complete in the sense that it allows us to calculate the classical state at any time if the forces are known.

Quantum mechanics shows a different picture. In general, the state of a single quantum system cannot be determined since any measurement will lead to a reduction of the quantum state. As a consequence the complete reconstruction of a quantum state is only possible if we measure specific observables on an infinite ensemble of identically prepared systems. Such measurements have been intensively discussed experimentally as well as theoretically in recent years [1].

The interest in such questions has been renewed in the field of quantum information. In particular, it has been investigated how well one can estimate a quantum state from a finite ensemble of identical systems. For pure spin systems this problem has been solved [2–5]. The intriguing result is that one can learn more about the finite ensemble by performing a measurement on all quantum systems simultaneously [4]. In fact one can optimize the readout of quantum information via simultaneous strategies. Such a joint measurement may, however, pose practical problems since we may not have all systems available at a time or cannot realize the required complicated measurement operators experimentally. Hence we have recently analyzed how close one can come to such optimal joint estimation schemes by using single adaptive quantum measurements [6].

Also for mixed spin states the optimal generalized measurement has been constructed for a finite ensemble [7]. In addition it has been shown [8] how the gain of information of generalized measurements increases when the estimated state approaches a pure quantum state.

In the present paper we shall analyze the estimation of mixed states of qubits using single adaptive measurements. As a criteria for adaption the Kullback information gain turns out to be suited. We will compare our results to the optimal measurements discussed in [4].

The paper is organized as follows. In Sec. II we present the quantum system we are dealing with and introduce the corresponding notation. Sec. III contains the description of our adaptive measurement scheme. The optimization strategies used in these adaptive schemes are then described in detail in Sec. IV. In Sec. V and VI we show the estimation results for the cases of estimation without and with a priori information regarding the radial distribution of quantum states inside the Bloch sphere. We conclude with Sec. VII.

II. QUANTUM SYSTEM AND MEASUREMENT OPERATOR

Suppose we are given \( N \) two-level systems (qubits) identically prepared in the mixed state \( \hat{\rho} \). The task is to adaptively estimate \( \hat{\rho} \) by using experimentally realizable single measurements on the two-level systems.

Let us first define the notation and the key elements of our analysis. Any mixed quantum state \( \hat{\rho} \) of a two-level system (qubit) can be written down in the Bloch-sphere representation

\[
\hat{\rho}(r, \theta, \phi) = \frac{1}{2} \left( 1 + \vec{r}(r, \theta, \phi) \vec{\sigma} \right)
\]

with the Pauli-spin-vector \( \vec{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)^T \) and the Bloch vector

\[
\vec{r}(r, \theta, \phi) = r \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix}
\]

expressed in spherical coordinates. The parameters \( r \in [0, 1] \), \( \theta \in [0, \pi] \), \( \phi \in [0, 2\pi] \) uniquely determine the quantum state inside the Bloch sphere. Using the matrix representation of \( \vec{\sigma} \) the density matrix reads

\[
\hat{\rho}(r, \theta, \phi) = \frac{1}{2} \left( 1 + r \cos \theta \begin{pmatrix} \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} \\ r \cos \theta \end{pmatrix} \begin{pmatrix} \sin \theta e^{i\phi} \\ \sin \theta e^{-i\phi} \\ r \cos \theta \end{pmatrix} \right).
\]

This parametrization also allows us to represent the estimated state \( \hat{\rho}^{\text{est}} \) obtained after a certain measurement sequence. By introducing the probability density \( w(r, \theta, \phi) \) we can write
The integration based on an algorithm, cf. Fig. 1, which consists of five stages if an adaptive measurement strategy. This strategy is therefore defined as follows: 

1. We take the first, \( n = 1 \), of the \( N \) quantum systems and perform a measurement with randomly chosen direction \((\theta_1, \phi_1)\).

2. The \( n \)th measurement along the direction \((\theta_n, \phi_n)\) yields one of the two possible outcomes that we denote by \( i = 0 \) and \( i = 1 \). By using this information we modify the distribution \( w_{n-1}(r, \theta, \phi) \) of the estimated density operator

\[
\hat{\rho}_{n-1}^{(\text{est})} = \int dV w_{n-1}(r, \theta, \phi) \hat{\rho}(r, \theta, \phi)
\]

after \( n - 1 \) steps according to Bayes’ rule \([11]\)

\[
w_n(r, \theta, \phi) = Z^{-1} P_i(r, \theta, \phi | \theta_n, \phi_n) w_{n-1}(r, \theta, \phi).
\]

Hence with the help of the probabilities \( P_i \), Eq. (8), we update our current knowledge about the finite ensemble as formulated by the distribution \( w_n \). The normalization constant reads

\[
Z = \int dV P_i(r, \theta, \phi | \theta_n, \phi_n) w_{n-1}(r, \theta, \phi).
\]

Before we have acquired any information about the system, we assume our knowledge to be homogeneously distributed over the Bloch sphere; that is, we start from the initial distribution

\[
w_0(r, \theta, \phi) = \frac{3}{4\pi}
\]

thereby assuming that each volume element \( dV = r^2 \sin \theta dr d\theta d\phi \) is equally probable.

3. The updated probability distribution \( w_n(r, \theta, \phi) \) describes our present knowledge about the quantum state. With its help we determine the next measuring operator, i.e., the direction \((\theta_{n+1}, \phi_{n+1})\) of the measurement step \( n + 1 \). The new measuring operator should be designed in such a way that it allows us to gain the maximum amount of additional information about the unknown quantum state \( \hat{\rho} \).

For this purpose we have to apply a criterion by which we quantify the notion of maximum information gain. The different criterions that we use in this context will be described in detail in the next section. This step reflects the adaptive aspect of our algorithm, because the choice of a measuring operator is based on \( \hat{\rho}_n \) and thereby on the history of all previous measurement outcomes.

4. Once having found the next measuring operator \((\theta_{n+1}, \phi_{n+1})\) we now take one of the remaining quantum systems and measure it. If we still have quantum systems left, we continue with step 2.

III. ADAPTIVE MEASUREMENTS

We now propose an adaptive measurement strategy to improve the estimation of a quantum state \( \hat{\rho}(R, \Theta, \Phi) \) from a finite ensemble of \( N \) identically prepared quantum systems. Note that the Bloch vector coordinates \( R, \Theta \) and \( \Phi \) are the same for all \( N \) systems. Despite the fact that we restrict ourselves to simple projection measurements on single quantum systems we will show that it is possible to improve the estimation quality by using an adaptive measurement strategy. This strategy is based on an algorithm, cf. Fig. 1, which consists of five steps:

\[
\hat{\rho}^{(\text{est})} = \int dV w(r, \theta, \phi) \hat{\rho}(r, \theta, \phi)
\]

with normalization

\[
\int dV w(r, \theta, \phi) = 1.
\]
5. After we have used up all $N$ mixed qubits we arrive at the final probability distribution $w_N(r, \theta, \phi)$ which allows us to construct the corresponding estimated state $\hat{\rho}_N^{\text{est}}$.

As the measure of our state estimation quality we will use the fidelity $F_N$ defined as

$$F_N \left( \hat{\rho}, \hat{\rho}_N^{\text{est}} \right) = \text{Tr}^2 \sqrt{\hat{\rho}_N^{\text{est}} \hat{\rho}(R, \Theta, \Phi) \hat{\rho}_N^{\text{est}}} \, ,$$

for mixed quantum states which reduces to

$$F_N = \frac{1}{2} \left[ 1 + r_N^{\text{est}}(R, \Theta, \Phi) \right] + \sqrt{1 - (r_N^{\text{est}})^2} \sqrt{1 - (\bar{r}(R, \Theta, \Phi))^2}$$

for two-level systems with Bloch vectors $r_N^{\text{est}}$ and $\bar{r}(R, \Theta, \Phi)$. Note that this fidelity of course depends on the number $N$ of quantum systems at our disposal.

IV. MEASUREMENT STRATEGIES

In this section we will describe the strategies that we have applied to find the direction $(\theta_n, \phi_n)$ for the $n$th measurement by learning from the results of earlier measurements.

A. Random selection from all axes

A straightforward way to select a new measurement direction $(\theta_n, \phi_n)$ is to choose the parameters $\theta_n$ and $\phi_n$ randomly on the Bloch sphere, independent of any knowledge already acquired about the state. That is, each infinitesimal surface element $\sin \theta_n d\theta_n d\phi_n$ occurs with the same probability $1/4\pi$. Clearly this strategy is not adaptive because $(\theta_n, \phi_n)$ does not depend on any previous measurement outcome. Nevertheless, the estimated density operator $\hat{\rho}_n^{\text{est}}$ can still be updated after each measurement as described in step 2 of our algorithm.

The random selection implements a measurement protocol lacking any constructive strategy. Thus the results of this method will serve as a reference to which we can compare the outcomes of the optimization strategies described below.

B. Minimal measurements along three axes

In principle it is possible to determine any mixed state by measurements along three axes if an infinite number of quantum systems prepared in this state is available. Without loss of generality one can choose the Pauli operators $\sigma_x$, $\sigma_y$ and $\sigma_z$ to represent measurements along three orthogonal directions on the Bloch sphere. This set of measurement operators represents a minimal measurement or – in other words – corresponds to a minimal quorum.

Thus it is interesting to compare the efficiency of such a minimal measurement to our adaptive methods in the case of a finite number $N$ of available quantum systems. Then the measurement scheme consists of projecting an average number of $N/3$ systems using each of the directions $(\pi/2, 0)$, $(\pi/2, \pi/2)$ and $(0, 0)$.

C. Maximization of Kullback information gain

If we look at the measurement procedure from an information theoretic point of view then our aim will be to maximize the information that we can get in the measurement step from $n-1$ to $n$. A measure for the average information gain in the $n$th measurement is the so called Kullback information $\tilde{K}(\theta_n, \phi_n)$ that can be defined as

$$\tilde{K}(\theta_n, \phi_n) = \sum_{i=0}^{1} p_i^{\text{est}}(\theta_n, \phi_n) \times \int dV w_n^{(i)}(r, \theta, \phi) \log_2 \frac{w_n^{(i)}(r, \theta, \phi)}{w_{n-1}(r, \theta, \phi)}$$

with

$$p_i^{\text{est}}(\theta_n, \phi_n) = \langle \theta_n, \phi_n \mid \rho_n^{\text{est}} \mid \theta_n, \phi_n \rangle$$

and

$$p_0^{\text{est}} = 1 - p_1^{\text{est}}$$

being the estimated probabilities for the outcomes $i = 0, 1$ based on our current knowledge, i.e., based on the density operator $\rho_n^{\text{est}}$. Consequently, also the probability density

$$w_n^{(i)} = Z^{-1} p_i^{\text{est}}(\theta_n, \phi_n) w_{n-1}$$

explicitly depends on the outcome $i$ and on the direction $(\theta_n, \phi_n)$. Hence our expression, Eq. (15), for the Kullback information is a function of $(\theta_n, \phi_n)$ which can be maximized. In order to see that $\tilde{K}$ describes an estimated average information gain we rewrite it in the form

$$\tilde{K}(\theta_n, \phi_n) = \sum_{i=0}^{1} p_i^{\text{est}}(\theta_n, \phi_n) \times \int dV w_n^{(i)}(r, \theta, \phi) \log_2 w_n^{(i)}(r, \theta, \phi) - \int dV w_{n-1}(r, \theta, \phi) \log_2 w_{n-1}(r, \theta, \phi)$$

$$= S_{n-1} - \sum_{i=0}^{1} p_i^{\text{est}}(\theta_n, \phi_n) S_n^{(i)}(\theta_n, \phi_n).$$

The entropy $S_{n-1}$ describes our knowledge before the measurement, whereas the entropy $S_n^{(i)}$ stands for the estimated entropy provided we find the result $i$. 

Hence we can maximize the difference of entropies before and after the measurement by adjusting the parameters \((\theta_n, \phi_n)\). We therefore select the measuring direction \((\theta_n, \phi_n)\) that yields the maximum average information gain.

The estimated state \(\hat{\rho}_N^{(\text{est})}\) is finally again determined from \(w_N\). This strategy can be applied in the case that all measurement directions are possible as well as in the case that only the three measurement directions along \(\sigma_x, \sigma_y\) and \(\sigma_z\) are allowed. In the latter case the maximization described before is done only for the directions \((\pi/2, 0), (\pi/2, \pi/2)\) and \((0, 0)\). We will discuss the resulting estimation precisions in the next section.

### V. ESTIMATION WITHOUT A PRIORI INFORMATION

In this section we numerically evaluate the average fidelities for the state estimation schemes described above. Only such an average fidelity is a reasonable measure of quality of a specific estimation procedure, since we assume to have no prior information about \(\hat{\rho}\).

These average fidelities will depend on the number \(N\) of identically prepared quantum systems that we have at our disposal. Thus one state estimation experiment consists of a sequence of \(N\) measurements performed on \(N\) identical systems in state \(\hat{\rho}(R, \Theta, \Phi)\) and a subsequent estimation of a mixed state \(\hat{\rho}_N^{(\text{est})}\). The fidelity \(F_N\), Eq. (14), of the state estimation is then calculated by comparing both states.

However, in order to get the average fidelity

\[
\langle F_N \rangle = \left\langle F \left( \hat{\rho}(R, \Theta, \Phi), \hat{\rho}_N^{(\text{est})} \right) \right\rangle_{\hat{\rho}}
\]

we have to perform such a single run of the (numerical) experiment over and over again for different initial states \(\hat{\rho}(R, \Theta, \Phi)\), i.e., for different coordinates \((R, \Theta, \Phi)\). Hence the initial states \(\hat{\rho}(R, \Theta, \Phi)\), Eq. (3), are chosen randomly from an isotropic and homogenous probability distribution \(3/(4\pi)\) for each volume element \(R^2 \sin \Theta dR d\Theta d\Phi\) of the Bloch sphere. Using this homogenous probability distribution ensures that the performance of an estimation strategy is not biased by any specific choice of initial states. For more details on the averaging procedure see Appendix A.

The average fidelity for each \(N\) was obtained by averaging over \(10^4\) experiments, i.e., \(10^4\) initial states equally distributed inside the Bloch sphere. For the sake of a clear graphical presentation not the average fidelities themselves but the average errors

\[
f_N = 1 - \langle F_N \rangle
\]

are calculated for different \(N\).

In Fig. 2 the average errors \(f_N\) are compared to the average error \(f_N^{\text{rand}}\) of the random selection scheme by plotting the ratio

\[
\gamma_N = \frac{f_N}{f_N^{\text{rand}}}
\]
VI. ESTIMATION WITH RADIAL A PRIORI INFORMATION

Inspired by these findings we finally discuss how the precision of our estimation schemes depends on the degree of mixing of the initial states. In our case the adequate measure of precision is the estimation error \( f_N \), Eq. (21). For a quantitative check of the relation between estimation quality and degree of mixing of the initial states we have chosen the initial states no longer according to a homogenous probability distribution inside the Bloch sphere but from a probability distribution

\[
w_0(r, \theta, \phi; \alpha) dV = \frac{\alpha + 1}{4\pi} r^\alpha \sin \theta dr d\theta d\phi
\]

which clearly depends on the radius \( r \). Please note that we get the homogenous distribution for \( \alpha = 2 \) again. A larger parameter \( \alpha \geq 0 \) means a growing average radius

\[
\bar{r} = \frac{\alpha + 1}{\alpha + 2}
\]

which indicates a decreasing degree of mixing of the initial states. Thus a variation of the parameter \( \alpha \) allows us to study the influence of the degree of mixing onto the estimation precision of our schemes in which we have of course also adapted the initial probability \( w_0 \).

However, our previously described estimation scheme does not converge towards the estimation scheme for pure states \( 0 \) for \( \alpha \to \infty \). The cause of this behaviour is the final readout of the estimated radius \( r^{(est)} \). Please remember that this radius is found via the integration

\[
\int dV w_N(r, \theta, \phi) \tilde{\rho}(r, \theta, \phi)
\]

which yields the estimated state \( \tilde{\rho}^{(est)}(r^{(est)}, \theta^{(est)}, \phi^{(est)}) \). Thus even for solely pure initial states the estimated state will never be pure itself. That is, the readout of the estimated state does not properly account for our a priori information. For larger \( \alpha \) the estimated radius will always be too small compared to the average radius \( \bar{r} \), Eq. (24), of our initial distribution \( w_0 \), Eq. (23).

To overcome this non-convergence we now introduce an alternative readout scheme for the radius \( r^{(est)} \). The estimated parameters \( \theta^{(est)} \) and \( \phi^{(est)} \) are still obtained in the same way as before, that is, via Bloch representation of \( \tilde{\rho}^{(est)} \). The estimated radius \( r^{(est)} \), however, is now chosen as the average radius

\[
r^{(est)} = \int dV r w_N(r, \theta, \phi)
\]

of the final distribution \( w_N(r, \theta, \phi) \). It is easy to show that — even before the first measurement — this estimated radius tends to 1 for large \( \alpha \) and merges into the pure state estimation scheme for \( \alpha \to \infty \) \[13\].

Using this readout scheme we compare the resulting errors \( f_N \) to the errors \( f_N^{(opt)} \) that could be achieved by an optimal collective estimation scheme \[9\]. The errors \( f_N \) are based on a simple 3-axes estimation as described in Sec. IV.

In Fig. 4 we plotted the ratio \( f_N^{(opt)}/f_N \) versus \( N \). As one would expect our estimations are always worse than the optimal ones. We also find a very clear dependence of the ratio on the radial distribution described by the parameter \( \alpha \). The smaller \( \alpha \) the smaller is the ratio and vice versa. This means that for highly mixed states the optimal collective measurements offer a bigger advantage compared to separate measurements than for states with a small degree of mixing. Or, in other words, the bigger \( r \), Eq. (24), the closer can we come to the optimal limits using separate measurements. It is interesting to note that this statement is true for all \( N \) and not only in the limit \( N \to \infty \) as shown in \[17\].

VII. CONCLUSION

We have presented estimation methods based on separate adaptive measurements on single qubits. We have demonstrated the measurement schemes for estimating mixed quantum states of qubits. An algorithm is used to update the knowledge about the true quantum state after each measurement and to choose the best measuring operator for the next measurement. With this scheme we have been able to reduce the estimation errors compared to non-adaptive strategies. The best results can be obtained by using schemes related to Kullback information measures. Maximizing this information gain leads to considerable improvements in the estimation quality.

We have also shown that the advantage of collective measurements decreases with decreasing degree of mixing of the initial qubits for all \( N \), thereby confirming asymptotic results for \( N \to \infty \) found by Gill and Massar \[17\].

We have restricted ourselves to simple separate measurements which can be easily realized with nowadays technology. An additional advantage of our scheme is that there is no need to have all \( N \) quantum systems available at the same time. In contrast to optimal measurement schemes, for which one needs to perform complicated collective measurements on all the systems, our schemes can also be used if the \( N \) quantum systems can only be prepared one after the other. These features ensure the applicability of our scheme to experiments and practical state estimation problems in quantum information theory.

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APPENDIX A: AVERAGING OVER THE BLOCH SPHERE

In order to quantify the performance of our adaptive methods we have introduced the average fidelity $\bar{F}_N$, Eq. (20). In this Appendix we shortly describe the averaging procedure. In principle the calculation of $\langle F_N \rangle$ consists of two steps. First we have to determine the average fidelity $\bar{F}_N(\hat{\rho})$ for $N$ identical quantum systems prepared in state $\hat{\rho} = \hat{\rho}(R, \Theta, \Phi)$ by summing over all possible measurement paths $J$. Given a specific adaptive method each path is uniquely determined by the initial measurement direction $(\theta_1, \phi_1)$ and by the sequence of measurement results forming a string of 0’s and 1’s. That is, we have $J = J(\theta_1, \phi_1; \{0,1\}^N)$. With the fidelity $F_N(\hat{\rho}, J)$ for each path we arrive at

$$\bar{F}_N(\hat{\rho}) = \bar{F}_N(R, \Theta, \Phi) = \langle F_N(\hat{\rho}(R, \Theta, \Phi), J) \rangle_j.$$  

(A1)

In principle a simulation of this expression would be straightforward. We choose an initial measuring direction $(\theta_1, \phi_1)$ and therefore measures the performance of any estimation method.

However, this averaging procedure can be simplified, if we take the following into account. The fidelity $F_N(\hat{\rho}, J)$ is rotationally invariant. For a density operator rotated sufficiently many measurement sequences of length $N$. This should be repeated for a dense set of initial measurement directions on the Bloch sphere.

The second step of our averaging procedure consists of averaging $F_N(R, \Theta, \Phi)$ over all density operators $\hat{\rho} = \hat{\rho}(R, \Theta, \Phi)$ isotropically distributed over the Bloch sphere. In this way we find the fidelity

$$\langle F_N \rangle = \langle \bar{F}_N(R, \Theta, \Phi) \rangle_{(R, \Theta, \Phi)}$$  

(A2)

which is not biased by any specific choice of density operator and therefore measures the performance of any estimation method.

Therefore, we numerically simulate $\langle F_N \rangle$ by choosing sufficiently many points $(R, \Theta, \Phi)$ isotropically distributed over the Bloch sphere together with a randomly chosen path $J$.

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Design of optimized \((n+1)\)th measurement

\(n\)th measurement: result 0 or 1

\(\hat{\rho}_{n-1}\)

\(\downarrow\)

\(\hat{\rho}_n\)

\(n \rightarrow n + 1\)

FIG. 1. Schematic picture showing the sequence of steps in the adaptive algorithm. The algorithm starts with performing the \(n\)th experiment. The measurement result is then used to update the estimated density operator \(\hat{\rho}_{n-1}\). With the help of the updated density operator \(\hat{\rho}_n\), the measuring operator for the \((n+1)\)th measurement is selected and the algorithm restarts.

\(<F_N>/ <F_N^{(opt)}>\)

FIG. 3. Ratio of average fidelity \(\langle F \rangle\) and optimal average fidelity \(\langle F_{opt} \rangle\) plotted versus \(N\). Triangles (stars) again describe the adaptive strategies without (with) restriction to three axes. In addition the ratio for the random selection scheme is also plotted (diamonds).

\(\gamma_N\)

FIG. 2. Relative error \(\gamma_N\), Eq. (22), plotted versus number of quantum systems \(N\). The boxes show the results for the 3-axes measurement scheme, whereas the triangles (stars) visualize the relative errors of the Kullback information gain strategies without (with) restriction to only three possible measurement axes.

\(f_N^{(opt)}/ f_N\)

FIG. 4. Ratio of optimal estimation error \(f_N^{(opt)}\) and error of 3-axes estimation scheme \(f_N\) plotted versus \(N\) for different radial distributions of initial states parametrized by \(\alpha\), Eq. (23). From bottom to top the lines correspond to \(\alpha = 0, 2, 5, 10, 100\). We clearly see an increasing ratio for growing \(\alpha\).