

Quantum state tomography with a single measurement setup: supplementary material

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Coupler Description

The linear, passive coupler U of M modes is represented by a unitary matrix of dimension M , $U \in U(M)$, where $U(M)$ is the unitary group of order M . The coupler U is sampled from the Haar measure on $U(M)$, which is the uniform measure on the unitary group.

The photons entering the coupler evolve according to

$$a_i^\dagger \mapsto \sum_j U_{ij} a_j^\dagger. \quad (S\ 1)$$

Here, a_i^\dagger is the photon creation operator at port i . The photon evolution induces a unitary evolution in the entire space $\mathcal{U} \in U(D)$, where D is the dimension of the truncated Fock space $D = \binom{M-1+N}{N}$ for N photons. Thus, the density matrix at the input ρ evolves at the output to

$$\rho \mapsto \rho_{\text{out}} = \mathcal{U} \rho \mathcal{U}^\dagger. \quad (S\ 2)$$

Observable Details

For M ports, N photons, $M > N$, define the following observable

$$A = \sum_{\{n\}^i} i |\{n\}^i\rangle \langle \{n\}^i|. \quad (S\ 3)$$

Here, $\{n\}^i = (n_1^i \dots n_M^i)$, $\sum_q n_q^i = N$ is the i th configuration of N photons in M ports. The different projections are obtained from all Fock states of M ports, N photons. It is indeed an observable, since $A^\dagger = A$. Experimentally, each projection corresponds to a different N -fold correlation measurement. For example, $|1_{q_1} \dots 1_{q_N}\rangle \langle 1_{q_1} \dots 1_{q_N}|$ corresponds to measuring a single photon in port q_1 , a single photon in port q_2 and so on.

The addition of the linear coupler $U \in U(M)$ is represented by a unitary matrix of dimensions $M \times M$ (see Coupler section in this supplementary), dictating an evolution of the photons as in eq. (S 1).

To find the probability of each measurement outcome, we can use the evolution of the density matrix, as in eq. (S 2). Alternatively, we may fix the input state and evolve the observable as

$$A' = \mathcal{U}^\dagger A \mathcal{U}. \quad (S\ 4)$$

The probability for each N -fold correlation is

$$p(|\{n\}^i\rangle|\rho) = \text{Tr}(\rho \mathcal{U}^\dagger |\{n\}^i\rangle \langle \{n\}^i| \mathcal{U}) \quad (S\ 5)$$

$$= \langle \{n\}^i | \mathcal{U} \rho \mathcal{U}^\dagger | \{n\}^i \rangle, \quad i \in \{1, \dots, D\}.$$

Since these are all correlations after propagation in a single coupler U , they require a single experimental setup.

Recovery Methods

The problem of recovering the density matrix from measurements can be described as finding the density matrix ρ such that the measurement outcomes derived from ρ fit the experimental results. If we denote the linear transformation of the density matrix due to the observables being measured by $\mathcal{A}_i: \mathbb{C}^{d \times d} \rightarrow \mathbb{R}_+^d$, $\mathcal{A}_i(\rho) = y_i$, $i \in \{1, \dots, d\}$, where d is dimension of the system, then our problem can be described mathematically as: Find $\rho \in \mathbb{C}^{d \times d}$ such that $\rho^\dagger = \rho$, $\rho \geq 0$, $\text{Tr} \rho = 1$ and $\mathcal{A}_i(\rho) = y_i$ for $i = 1, \dots, d$. The first constraints result from ρ being a density matrix, while the rest arise from the requirement to conform to the measurements. This problem can be formulated as the optimization problem

$$\min_{\rho} \sum_{i=1}^d \|\mathcal{A}_i(\rho) - y_i\|_2^2 \quad (\text{S } 6)$$

subject to $\rho^\dagger = \rho, \rho \geq 0, \text{Tr} \rho = 1$.

In our problem, we wish to find the density matrix at the input ρ_0 , such that the derived measurements after the coupler, with the addition of the ancilla, conform to the measured data. Since we use a single observable in the larger system of dimension D , the measurements are described by the linear transformation $\mathcal{A}: \mathbb{C}^{D \times D} \rightarrow \mathbb{R}_+^D$, $\mathcal{A}(\rho_0 \otimes \rho_{\text{ancilla}}) = y$ with the y_j given by eq. (S 5).

In our scheme, we use prior knowledge, namely that the state is close to a pure state or can be approximated by one. In terms of the density matrix, the prior knowledge takes the form of the density matrix having a small number of nonzero eigenvalues. In other words, the density matrix has low rank, or can be approximated by a low rank matrix. To harness this knowledge for the purpose of state recovery, we consider the following optimization problem

$$\min_{\rho_0} \text{rank}(\rho_0) \quad (\text{S } 7)$$

subject to $\rho_0^\dagger = \rho_0, \rho_0 \geq 0, \text{Tr} \rho_0 = 1$,

$$\mathcal{A}(\rho_0 \otimes \rho_{\text{ancilla}}) = y.$$

Here, ρ_0 is the state at the input that we wish to recover, ρ_{ancilla} is the state of the ancilla at the input (known to us) and y is the experimentally measured data. With the realistic addition of experimental noise on the measurements, we can modify (S 7) to

$$\min_{\rho_0} \text{rank}(\rho_0) \quad (\text{S } 8)$$

subject to $\rho_0^\dagger = \rho_0, \rho_0 \geq 0, \text{Tr} \rho_0 = 1$,

$$\|\mathcal{A}(\rho_0 \otimes \rho_{\text{ancilla}}) - y\|_2^2 \leq \epsilon,$$

where ϵ relates to the amount of measurement noise.

The problem formulated in eq. (S 8) is not convex due to the rank objective. To approximate the solution, we use the LogDet heuristic [1], in which the non-convex rank function is replaced by a surrogate function, the log of the determinant, which promotes low rank solutions. The LogDet function is then linearized at the vicinity of a proposed solution to yield an iterative algorithm. In the k th iteration, the optimization problem to be solved is

$$\min_{X_k} \text{Tr}(X_{k-1} + \delta I)^{-1} X_k \quad (\text{S } 9)$$

subject to $X_k \geq 0, \text{Tr}(X_k) = 1$,

$$\|\mathcal{A}(\rho_0 \otimes \rho_{\text{ancilla}}) - y\|_2^2 \leq \epsilon.$$

Here, X_k is the matrix we are looking for in iteration k , X_{k-1} is the matrix found in the previous iteration, and δ is a small regularization parameter. Once X_k, X_{k-1} are close to each other in the Frobenius norm sense, no further iterations are preformed, and the low rank density matrix is X_k .

A second approach to solving (S 8) is to drop the low-rank requirement and solve the problem

$$\min_{\rho_0} \|\mathcal{A}(\rho_0 \otimes \rho_{\text{ancilla}}) - y\|_2^2 \quad (\text{S } 10)$$

subject to $\rho_0^\dagger = \rho_0, \rho_0 \geq 0, \text{Tr} \rho_0 = 1$.

In this case, the prior knowledge is not used explicitly. However, for certain measurement matrices, the mere structure of the density matrix, namely the positive-definiteness, results in a unique low rank solution [2,3]. Thus, in these cases, the low rank solution is found regardless of the algorithm used. A comparison between LogDet (eq. (S 9)) and the constrained least squares problem (eq. (S 10)) is presented in Fig. S1. The results are very similar, with the LogDet somewhat superior.

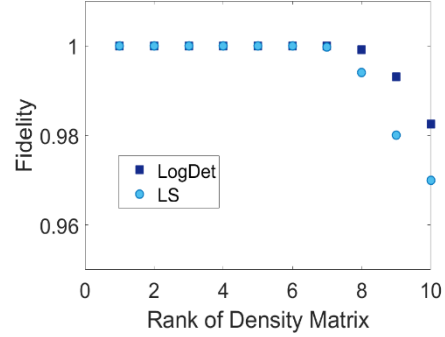


Fig. S1: A comparison between the recovery fidelity for $N = 3$ photons in $m = 4$ input ports, $M = 11$ output ports, using LogDet (eq. (S 9)) and constrained LeastSquares (eq. (S 10)).

Sampling Mixed States

The problem of sampling quantum states from the entire Hilbert space has theoretical importance, as well as direct consequences on benchmarking of quantum circuits and quantum state recovery methods. For pure states, described by density matrices with rank 1, there exists a unique uniform measure, the Haar measure, on the unitary group of dimensions corresponding to the dimension of the system. This measure is invariant to unitary transformations, thus all pure states are equivalent.

While the question of sampling pure states has a clear answer, the answer to the corresponding problem with mixed states remains elusive [4]. The density matrix, as a positive semidefinite matrix with trace 1, can be described by its spectral decomposition $\rho = \sum_i \lambda_i |i\rangle\langle i|$, where λ_i are the eigenvalues and $|i\rangle$ are the eigenvectors. Thus, a measure μ on the set of density matrices depends on the eigenvalues and eigenvectors $\mu = \mu(\lambda_1, \dots, \lambda_D; |1\rangle, \dots, |D\rangle)$. In the spirit of the unitary invariance satisfied by the uniform measure on pure states, we can define measures on the set of density matrices which are product measures on the eigenvalues and eigenvectors [5]

$$\mu = \mu_\lambda(\lambda_1, \dots, \lambda_D) \times \mu_i(|1\rangle, \dots, |D\rangle), \quad (\text{S } 11)$$

where the measure on the eigenvectors μ_i is the Haar measure. Other measures include, for example, the measure induced by pure states in a larger system [4]. They are sampled uniformly, and then a part of the system is traced over to produce a mixed state of the original dimension.

As explained in the main text, to demonstrate our quantum state recovery method, we preform several simulations. In these simulations, a large number (typically several hundreds) of density matrices are generated, they evolve in the system of a single observable, and the measurement outcomes are calculated according to eq. (S 5). We then add noise to the measurements, and apply our method to recover the state at the input of the system. The recovered density matrix is compared to the original one. Thus, we need to sample a large number of density matrices describing mixed states.

Due to the appeal and physical motivation of unitary invariance, we choose to sample from a product measure on the eigenvalues and eigenvectors (eq. (S 11)), where we take the eigenvectors measure to be Haar, leading to invariance of the measure under unitary evolution. The measure on the eigenvalues is chosen to be the uniform measure on the $r - 1$ dimensional unit simplex, where r is the desired rank of the density matrix.

Dependence on the Realization of the Coupler

The mixing component in our scheme is realized in the optical setting by a linear random coupler. The coupler is sampled from the Haar measure on the corresponding unitary group. It is natural to ask how strongly, if at all, the specific realization of the coupler affects the ability to recover the quantum state. To answer this question, we sample 30 different couplers from the same distribution and use them to recover a single density matrix of rank 2, describing 3 photons in 4 input modes, with 10 output modes (thus ~ 0.55 of the measurements required for tomography are used). The results are shown in Fig. S2(a). The mean fidelity in this scenario is 0.996. As evident from the figure, the fidelity does not depend on the specific realization of the coupler. In Fig. S2(b), the fidelity for each coupler is averaged over 30 density matrices, again showing no dependence on the specific realization of the coupler, as long as it is sampled uniformly.

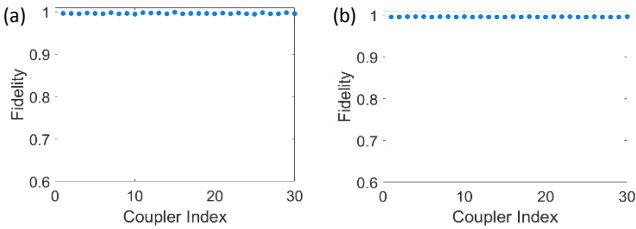


Fig. S2: (a) Fidelity obtained with different couplers, a single density matrix. (b) Fidelity obtained with different couplers, averaged over 30 density matrices.

A POVM Set of the Measurements

The ancilla added to the original system increases the dimension of the system, resulting in addition of measurements. However, the evolution in the system has to couple between the ancilla and the original system to indeed yield more informative measurements. This can be shown using a Positive Operator Valued Measurements (POVM) formulation of the measurements performed in our scheme. POVM measurements are generalized quantum measurements, described by a set of operators $\{E_i\}_{i=1}^n$ satisfying $E_i \geq 0, \sum_i E_i = I$. The probability of each outcome is $p(i|\rho) = \text{Tr}(E_i \rho)$. They are called generalized measurements since the operators E_i do not have to be orthogonal to each other, unlike the case of ordinary measurements in quantum mechanics, called projective measurements.

The physical realization of a POVM set $\{E_i\}_{i=1}^n$ is obtained by extending the original Hilbert space using an ancilla, and performing projective measurements in the larger space, as described in Neumark's Theorem [6,7]. In the process of realizing the POVM set, we start with a set of operators on the original Hilbert space as described earlier. We then obtain an ancilla and a set of projective measurements in the combined Hilbert space of the original system and the ancilla. The POVM elements are derived from the projective measurements by tracing over the ancilla degrees of freedom. In our scheme, we describe a set of projective measurements, namely the spectral decomposition of (S

4), and an ancilla $\rho_{\text{ancilla}} = |0\rangle\langle 0|$. By deriving the corresponding POVM set on the Hilbert space of our original density matrix ρ_0 , we can investigate the interplay between the coupler and the ancilla.

As in the main text, we denote the dimension of the original system as d , and that of the extended system (with the ancilla) as D , such that $\rho_0 \in \mathbb{C}^{d \times d}, \rho_{\text{in}} = \rho_0 \otimes \rho_{\text{ancilla}} \in \mathbb{C}^{D \times D}$. The original system consists of ports $i \in I_{\text{original}}, |I_{\text{original}}| = m$, while the ancilla consists of ports $i \in I_{\text{ancilla}}, |I_{\text{original}} \cup I_{\text{ancilla}}| = M$. The projective measurements are $P_i = w_i w_i^\dagger, i \in \{1, \dots, D\}$, where $w_i = \mathcal{U}|\{n\}^i\rangle$. There are indeed D such orthogonal vectors, since the Fock states $\{|\{n\}^i\rangle\}_{i=1}^D$ form an orthonormal basis, and the evolution operator \mathcal{U} is unitary.

The POVM elements E_i are related to the w_i by a projection onto the original subspace [7]

$$E_i = \text{Tr}_{\text{ancilla}}(v_i v_i^\dagger), \quad i \in \{1, \dots, D\} \quad (\text{S } 12)$$

$$v_i = P_{\text{original}}(w_i),$$

where the projection onto the original space is defined as

$$P_{\text{original}}\left(\sum_{i=1}^D \beta_i |\{n\}^i\rangle\right) = \sum_{i \in I} \beta_i |\{n\}^i\rangle \quad (\text{S } 13)$$

$$I = \{i \in \{1, \dots, D\} \mid n_q^i = 0 \forall q \in I_{\text{ancilla}}\}.$$

That is, the projection eliminates all the coefficients of the vectors in the large space having a nonzero number of photons in the ancilla ports. For the vectors defining the projections, we have

$$v_i = P_{\text{original}}(w_i) = \sum_{j \in I} u_{ij} |\{n\}^j\rangle \quad (\text{S } 14)$$

and therefore, the POVM operators are

$$E_i = \text{Tr}_{\text{ancilla}}\left(\sum_{j, j' \in I} u_{ij} u_{j'i}^\dagger |\{n\}^j\rangle\langle\{n\}^{j'}|\right), \quad (\text{S } 15)$$

These are indeed operators on the desired space, since $\forall j \in I$, we have zero photons in the ancilla ports. Therefore, we can write

$$E_i = \text{Tr}_{\text{ancilla}}\left(\sum_{j, j' \in I} u_{ij} u_{j'i}^\dagger |n_1^j \dots n_m^j\rangle\langle n_1^{j'} \dots n_m^{j'}| \otimes |0\rangle\langle 0|\right) \quad (\text{S } 16)$$

$$= \sum_{j, j' \in I} u_{ij} u_{j'i}^\dagger |n_1^j \dots n_m^j\rangle\langle n_1^{j'} \dots n_m^{j'}|.$$

Here, $i \in \{1, \dots, D\}$ and $j, j' \in I$. The operators E_i form a resolution of the identity

$$\sum_{i \in \{1, \dots, D\}} E_i = \sum_{i \in \{1, \dots, D\}} \sum_{j, j' \in I} u_{ij} u_{j'i}^\dagger |n_1^j \dots n_m^j\rangle\langle n_1^{j'} \dots n_m^{j'}| \quad (\text{S } 17)$$

$$= \sum_{j, j' \in I} \sum_{i \in \{1, \dots, D\}} u_{ij} u_{j'i}^\dagger |n_1^j \dots n_m^j\rangle\langle n_1^{j'} \dots n_m^{j'}|$$

$$= \sum_{j, j' \in I} \delta_{jj'} |n_1^j \dots n_m^j\rangle\langle n_1^{j'} \dots n_m^{j'}|$$

$$= \sum_{j \in I} |n_1^j \dots n_m^j\rangle\langle n_1^j \dots n_m^j| = I.$$

They are also rank-1 operators, since

$$E_i = |q_i\rangle\langle q_i| \quad (S 18)$$

$$|q_i\rangle = \sum_{j \in I} u_{ij} |n_1^j \dots n_m^j\rangle.$$

Therefore they are positive semidefinite $\langle \psi | E_i | \psi \rangle = |\langle \psi | q_i \rangle|^2 \geq 0 \forall |\psi\rangle$. Thus, the set $\{E_i\}_{i=1}^D$ forms a POVM.

The measurement-state relation can be formulated in the following manner

$$y = \mathcal{A} \rho_{CS}. \quad (S 19)$$

Here, $y \in \mathbb{R}_+^D$, $\mathcal{A} \in \mathbb{C}^{D \times d^2}$ and $\rho_{CS} \in \mathbb{C}^{d^2}$ is the original density matrix in vector form, obtained by column stacking. The matrix \mathcal{A} describes the measurement operator. Define a set of D matrices $B^k \in \mathbb{C}^{d \times d}$, $k \in \{1, \dots, D\}$ with elements

$$B_{ij}^k = u_{ki} u_{kj}^*. \quad (S 20)$$

Here, \mathcal{U} is the evolution operator. Then the k th row of \mathcal{A} is the row stacking of B^k . To estimate the usability of the measurements, we sampled 100 random linear couplers from the Haar measure of varying dimensions, and plotted in Fig. S3 the average rank of the measurement matrix \mathcal{A} versus the number of measurements D . The original system dimension is $d = 20$. As evident in the figure, the measurement matrix has full row rank, up to the point where $D > d^2$.

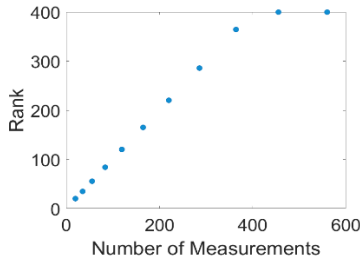


Fig. S3: Average rank of \mathcal{A} (eq. (S 19)) versus the number of measurements D .

Notice that for an interaction-less coupler $\mathcal{U} = \mathcal{U}_{\text{original}} \otimes \mathcal{U}_{\text{ancilla}}$, we have in eq. (S 14)

$$v_i = \sum_{j \in I} u_{ij} |n_1^j \dots n_m^j\rangle \otimes |0\rangle. \quad (S 21)$$

Due to the tensor product, the v_i are linearly dependent. In that case, there are only at most d linearly independent v_i , and the rank is lower than d .

Performance Analysis without Knowing the Original State

In the main text, we evaluate our method by randomly generating density matrices, calculating their propagation in the coupler, deriving the measurement outcomes, adding noise, and trying to recover the state. The fidelity between the recovered state and the original one is calculated and used as a measure of the recovery quality (Fig. 2b-d, Fig. 4b). This figure can be used to estimate the number of measurements needed for each rank of the density matrix. However, in an experiment, the original state is not known. Thus, to take full advantage of the small number of degrees of freedom in low rank states, the experimentalist would need some

estimate of the rank, which is generally unknown in advance. Moreover, with only the measurements at hand taken with a given coupler, some method is required to assess if the recovery can be trusted – without fabricating multiple couplers unnecessarily. Therefore, a way to find the information in Fig. 2b (the ranks for which the recovery works well) without knowing the original state, and to check the validity of the reconstruction and the number of measurements taken, is needed.

We propose the following approach. First, an upper bound on the rank is estimated, dictating the number of measurements and coupler size used. Then, the measurements are taken in the lab with a given coupler, and a reconstruction is found using the method described in the main text. Next, to gain confidence in the obtained solution and number of measurements taken, the following (computational) procedure is employed, requiring only the measurements at hand (which were already obtained) and the measurement matrix (the structure of the coupler, known to the experimentalist):

1. The number of measurements is reduced artificially by 5%, by randomly deleting rows from the measurement matrix and the corresponding measurements.
2. A second reconstruction is obtained with the smaller sample.
3. The two reconstructions are compared (for example, using a normalized Frobenius norm). If the difference between the two reconstructions is small, then the original solution (and number of measurements taken) is trusted.

Thus, if we took enough measurements to begin with, then the reconstruction should not be sensitive to a small reduction in the number of measurements. This procedure does not require more measurements or any further experimental effort. It only uses the measurements taken originally for the purpose of reconstruction.

To test this method, we attempt to recover the ranks for which the reconstruction was perfect in Fig. 2b in the main text, without using the original states. The results are shown in Fig. S4. The solid curves are the ones appearing in Fig. 2b in the main text. They were obtained with the knowledge of the original state, as well as averaging over density matrices and coupler realizations. The yellow areas are those obtained by the method described in this section, with a single random density matrix for each rank, and a single coupler for each of the figures. For each rank, a density matrix is generated, propagated in the coupler, and the measurements are calculated. Then, the measurements, along with the sampling matrix, were used to obtain a "trust/do not trust" flag. As evident in the figure, this approach captures the transition from having enough measurements to allow perfect recovery, to not having sufficient measurements, without using any knowledge of the input state.

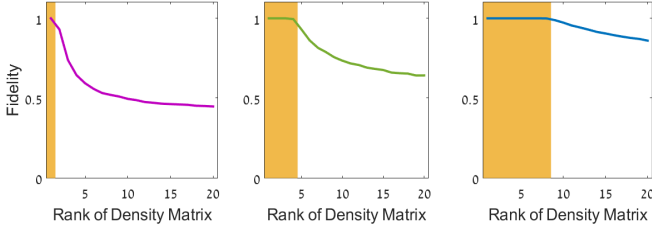


Fig. S4: Average recovery fidelity using the original state (solid lines) and the ranks for which the "trust the solution" flag has been raised, according to the procedure described in this section (without the original state).

Of course, the suggested criterion is a simplification of a more flexible test that can be performed. In a similar manner (and without using the original unknown state or taking any more measurements), once the measurements are taken and the state is recovered, successive attempts to recover are performed, each using a smaller, random sample of the measurements. The normalized difference between consecutive reconstructions is calculated and plotted against the iteration. If enough measurements are taken, a plateau is expected. An example is seen in Fig. S5. On the left, the result of such a process, with a 5% reduction in the number of measurements at each iteration, is presented for a coupler of 9 ports and rank 2 state at the input. The reconstruction should work in this case, as predicted by Fig. 2b in the main text. Indeed, we see a plateau, meaning that the reconstruction is insensitive to a reduction in the number of measurements. On the right, a similar scenario is presented, only with a rank 10 state at the input. This time, not enough measurements are used, and no plateau is observed.

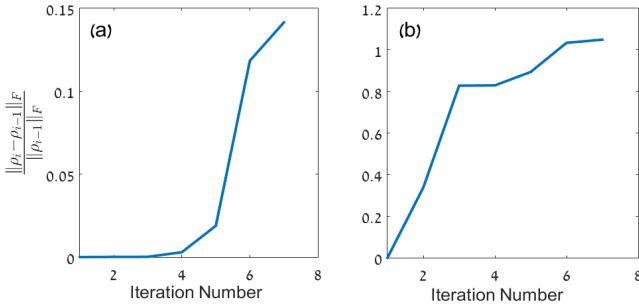


Fig. S5: Norm difference between successive solutions, with a measurement reduction between them. In (a), enough measurements have been taken, while in (b) the number of measurements is insufficient.

Finally, the results described so far use smaller couplers according to the number of actual degrees of freedom in the sought state. However, an alternative is to use a large coupler according to a conservative overestimate of the rank, and take a subset of the measurements in the larger coupler. In Fig. S6, the recovery fidelity is plotted versus the rank for the same conditions as in Fig. 2b in the main text, with an 11 port coupler, but with the number of measurements found in a 9 port coupler.

In combination with the method described here to gain confidence in the solution, an optimal number of measurements (a low number allowing for a reliable recovery) can be achieved in the following manner. First, loosely bound the rank from above to choose the coupler. Then, loosely bound the rank from below and perform a small number of measurements, according to the

underestimated rank and the known statistics (in Fig. 2b, for example). Check the confidence level of the solution. If it is not trustworthy, perform some more measurements and try to recover again. Repeat this process until a good solution emerges.

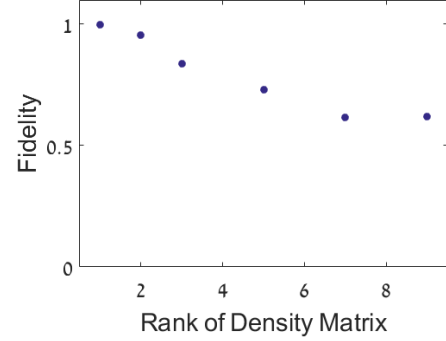


Fig. S6: Mean recovery fidelity using the number of measurements available in a 9 port coupler, using an 11 port coupler (the measurements are chosen randomly).

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