Quantitative verification of entanglement and fidelities from incomplete measurement data

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Many experiments in quantum information aim at creating multi-partite entangled states. Quantifying the amount of entanglement that was actually generated can, in principle, be accomplished using full-state tomography. This method requires the determination of a parameter set that is growing exponentially with the number of qubits and becomes infeasible even for moderate numbers of particles. Non-trivial bounds on experimentally prepared entanglement can however be obtained from partial information on the density matrix. The fundamental question that needs to be addressed in this context is then formulated as: What is the entanglement content of the least entangled quantum state that is compatible with the available measurement data?

We formulate the problem mathematically [1] employing methods from the theory of semi-definite programming and then address this problem for the case, where the goal of the experiment is the creation of graph states. The observables that we consider are the generators of the stabilizer group, thus the number of measurement settings grows only linearly in the number of qubits. We provide analytical solutions as well as numerical methods that may be applied directly to experiments, and compare the obtained bounds with results from full-state tomography for simulated data.

I. INTRODUCTION

Detecting and quantifying entanglement is one of the core problems in quantum information theory [2, 3]. The detection of entanglement can in principle be accomplished by measuring the complete quantum state and, thereafter, applying separability tests. However, the dimension of the density matrix grows exponentially with the number of constituents of the system. Therefore, full state tomography becomes very costly and experimentally infeasible already for a moderate number of particles. Thus, it is of interest to detect and quantify entanglement, even when only partial information on the density matrix is known. Entanglement Witnesses represent one way to verify the existence of entanglement with only a few measurements [4]. In [5] it was demonstrated that one may define an entanglement measure on the basis of witness operators and provide lower bounds on entanglement measures [6, 7].

However, the restriction to witness operators is unnecessary and may neglect information that is obtained when measuring the local operators into which the witness operator has been decomposed [1]. A direct calculation of the least amount of entanglement (in accordance with an entanglement measure of choice) that is compatible with the measured data of *arbitrary* observables is proposed in [1] and this approach is guaranteed to deliver the best lower bounds that can be obtained from the information that is available. The same philosophy may also be followed when bounding other quantities such as the fidelity with a desired target state. We apply the method described in [1] to the case where the goal of the experiment was the creation of cluster states. The observables we consider are the generators of the stabilizer group (for an introduction to the stabilizer formalism see e.g. [8]). Thus the number of measurement settings grows only linearly in the number of qubits.

This article is structured as follows: First, we describe how to provide lower bounds on the fidelity with a target state (here stabilizer states) in Sec. II and in Sec. III apply this to some simple examples. Sec. IV discusses the general approach to estimate robustness measures from incomplete information on the density matrix. Then, in Sec. V we utilize this approach to obtain lower bounds on the Global Robustness of Entanglement, and give closed formulae for systems consisting of two, three, and four qubits. A comparison of the obtained bounds with exact values for noisy cluster states is provided in Sec. VI.

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II. MINIMAL FIDELITY AND ENTANGLEMENT

In many experiments we aim at creating a particular pure quantum state $|\phi\rangle$. Needless to say, experimental imperfections and noise will usually lead to a noisy approximation to this state, i.e. a fidelity that is different from unity. This naturally raises the question as to how close we actually are to the target state. It is desirable to find simple sets of measurements that give us enough information to find useful lower bounds on the fidelity that has been achieved in the experiment. This problem may be solved with the methods that have been developed earlier in [1]. More formally, we will measure a set of observables $\{A_i\}$ and find measured mean values a_i. Then we will find the state ρ that predicts the mean values a_i and that has the least fidelity with the target state $|\phi\rangle$. Mathematically this is formulated as

$$F_{min} = min[tr[|\phi\rangle\langle\phi|\rho] : tr[A_i\rho] = a_i, \rho \geq 0]. \tag{1}$$

The solution to this problem is called the primal optimal. This problem is in fact numerically very efficiently solvable as it is linear program which is a special case of a semi-definite program. As such there are firstly very efficient numerical algorithms and, employing the concept of duality, one can also find lower bounds on the minimization problem [9]. Indeed, by duality we find that

$$F_{min} = max[min[tr[(|\phi\rangle\langle\phi| - \sum_i \lambda_i A_i)\rho] + \lambda_i a_i] \tag{2}$$

$$= max[\sum_i \lambda_i a_i : (|\phi\rangle\langle\phi| - \sum_i \lambda_i A_i) \geq 0]. \tag{3}$$

The solution to the latter, dual, problem is the dual optimal. That we really have equality, as we have implied here, is not trivial but is true for linear programs and for general semi-definite programs it is true under very mild conditions (see [9] for details) and is usually safe to assume at the beginning (though that this needs to be checked should be remembered when primal and dual optimum do not appear to coincide). The same methods can also be used to verify and quantify entanglement measures. In the bi-partite setting this can for example be done for the logarithmic negativity [2, 10, 11, 12] and simple analytical formulae can be given [1] for useful sets of observables. For multi-partite settings we have a variety of measures available [2, 3]. One may chose simple generalizations of the negativity measures but may also study robustness measures [13]. The method for the description of negativity measures can be deduced directly from [1]. In this note we will thus only present the basic approach for robustness measures.

III. EXAMPLES: ESTIMATE OF FIDELITY

A. GHZ States

The optimization problem formulated above may look somewhat daunting. Let us therefore consider some examples. First, we consider the quantitative verification of the fidelity with the EPR state $|\phi_2\rangle = \frac{1}{\sqrt{2}}(|00\rangle+|11\rangle)$. Let us measure the expectation values of the observables $A_1 = X_1 \otimes X_2$ and $A_2 = Z_1 \otimes Z_2$ where X (Z) is the Pauli x (z) operator. The unit trace condition on the density matrix is $tr[\rho]$ so that we have $A_3 = \mathbb{1}$. Then we find

$$F_{min} = \frac{a_1 + a_2}{2}. \tag{4}$$

This is seen from the choice

$$\rho = \begin{pmatrix} 1+a_2 & 0 & 0 & 2a_1+a_2-1 \\ 0 & 1-a_2 & 1-a_2 & 0 \\ 0 & 1-a_2 & 1-a_2 & 0 \\ 2a_1+a_2-1 & 0 & 0 & 1+a_2 \end{pmatrix} \tag{5}$$

and for the dual problem with the choice $\lambda_1 = \lambda_2 = \frac{1}{2}$ and $\lambda_3 = 0$. The verification of the GHZ-fidelity, that is the overlap with the state $|\phi\rangle = \frac{1}{2}(|000\rangle + |111\rangle)$ may also be considered. Here we measure the observables

$$A_1 = X_1 \otimes X_2 \otimes X_3 \tag{6}$$

$$A_2 = Z_1 \otimes Z_2 \otimes \mathbb{1} \tag{7}$$

$$A_3 = \mathbb{1} \otimes Z_2 \otimes Z_3. \tag{8}$$

Again $A_4 = \mathbb{1}$. Here it is a little harder to find the closed formula but it is actually

$$F_{min} = max[\frac{a_1 + a_2 + a_3 - 1}{2}, 0]. \tag{9}$$

The dual optimal is then of course $\lambda_1 = \lambda_2 = \lambda_3 = \frac{1}{2}$ and $\lambda_4 = -\frac{1}{2}$. The optimal ρ for the primal problem has $\rho_{1,1} = max[(a_2 + a_3)/4, 0]$, $\rho_{i,j} = \rho_{i,i} = \rho_{j,j} = \rho_{j,i}$ for $i, j \in [2, ..., 7]$ and $\rho_{1,8}$ such that the above optimal emerges.

For a general n-particle GHZ-state we measure for example

$$A_1 = X_1 \otimes \cdots \otimes X_n \tag{10}$$
$$A_2 = Z_1 \otimes Z_2 \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \tag{11}$$
$$A_3 = \mathbb{1} \otimes Z_2 \otimes Z_3 \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \tag{12}$$
$$\vdots$$
$$A_n = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes Z_{n-1} \otimes Z_n. \tag{13}$$

to find

$$F_{min} = max[\frac{a_1 + ... + a_n - n + 2}{2}, 0] \tag{14}$$

It is straightforward to read off the form of the dual optimal from this expression.

B. Cluster States

We find the same bounds on the fidelity for cluster states. As a matter of fact, these fidelity estimates are true for any observables which generate a stabilizer group. A proof is given in Appendix B.

IV. ENTANGLEMENT MEASURES

In this section we will discuss the estimation of entanglement measures from tomographically incomplete measurements . As mentioned, [1] discusses already the logarithmic negativity measures. For example, when one measures $X \otimes X$ and $Z \otimes Z$ and finds a_x and a_z then as demonstrated in [1]

$$E_{min} = max(0, log(|a_x| + |a_z|)) \tag{15}$$

and if one additionally measures $Y \otimes Y$ and finds a_y then

$$E_{min} = max(0, log(1 + |a_x| + |a_y| + |a_z|)). \tag{16}$$

Here we will present the approach for the Global Robustness of Entanglement. For bi-partite systems, this is defined as

$$E(\rho) = min[tr[\sigma] : \sigma \geq 0, \rho^{\Gamma} + \sigma^{\Gamma} \geq 0] \tag{17}$$

where σ must be Hermitian and positive-semidefinite, and Γ denotes partial transposition. For many particles, say n, a natural extension is

$$E(\rho) = min[tr[\sigma] : \sigma \geq 0, \rho^{\Gamma_\alpha} + \sigma^{\Gamma_\alpha} \geq 0, \forall \alpha \in \{1, \ldots, n\}]. \tag{18}$$

Again, given some expectation values $tr[\rho A_i] = a_i$, we would then determine

$$E_{min} = min[E(\rho) : tr(\rho A_i) = a_i, \rho \geq 0]. \tag{19}$$

This is again a semi-definite program and is thus rapidly solvable using numerical programs. For analytical work it will again be interesting to derive the dual which will allow us to find lower bounds on the above minimization. This derivation can be done in the following steps:

$$\begin{aligned}
E_{min} &= min[tr[\sigma] : tr(\rho A_i) = a_i, \rho^{\Gamma_\alpha} + \sigma^{\Gamma_\alpha} \geq 0, \rho \geq 0, \sigma \geq 0] \\
&= max[min\{tr[\sigma] - \sum_\alpha tr[\eta_\alpha(\rho^{\Gamma_\alpha} + \sigma^{\Gamma_\alpha})] \\
&\quad - \sum_i \mu_i(tr[\rho A_i] - a_i) : \rho, \sigma \geq 0\} : \eta_\alpha \geq 0, \mu] \\
&= max[min\{tr[\sigma(\mathbb{1} - \sum_\alpha \eta_\alpha^{\Gamma_\alpha})] - \sum_\alpha tr[\eta_\alpha^{\Gamma_\alpha}\rho]\} \\
&\quad - \sum_i \mu_i(tr[\rho A_i] - a_i) : \rho, \sigma \geq 0\} : \eta_\alpha \geq 0, \mu] \\
&= max[min\{-\sum_\alpha tr[\eta_\alpha^{\Gamma_\alpha}\rho] - \sum_i \mu_i(tr[\rho A_i] - a_i)\} : \eta_\alpha \geq 0, \mathbb{1} \geq \sum_\alpha \eta_\alpha^{\Gamma_\alpha}, \mu] \\
&= max[\sum_i \mu_i a_i : \mathbb{1} \geq \sum_\alpha \eta_\alpha^{\Gamma_\alpha}, \sum_\alpha \eta_\alpha^{\Gamma_\alpha} + \sum_i \mu_i A_i \leq 0, \eta_\alpha \geq 0, \mu] \qquad (20)
\end{aligned}$$

V. APPLICATION TO STABILIZER STATES

In this section we will utilize the approach described in the previous section to explicitly calculate lower bounds on the Global Robustness of Entanglement. We will see that the proper choice of observables transforms the optimization problem into a linear program, which may be solved analytically as well as numerically using well-known algorithms like the Simplex method.

We assume now that the goal of the experiment was to create either a cluster state with the associated adjacency matrix Γ_A or a GHZ state. Then a natural choice for the observables A_i would be the generators K_i of the abelian stabilizer group. For cluster states the stabilizers (or correlation operators) are given by $K_i = X_i Z_{N_i}$ where the subscript N_i is to be understood as applying Z-operators to all neighbors of the i-th qubit in the lattice defined by Γ_A. For N-qubit GHZ states the generators of the stabilizer group are: $K_1 = X_1 \otimes ... \otimes X_N$ and for $k = 2, ..., N$: $K_k = Z_{k-1}Z_k$. Due to the commutation relations fulfilled by these operators, it is easy to see that the symmetries that leave the observables $a_i = tr(\rho K_i)$ invariant are given by the transformation $\rho \longrightarrow \rho' = \sum_{i_1,...,i_N=0}^{1} K_1^{i_1}...K_N^{i_N} \rho K_1^{i_1}...K_N^{i_N}$. We may therefore restrict our attention to states of the form:

$$\rho = \sum_{i_1,...,i_N=0}^{1} c_{i_1...i_N} K_1^{i_1}...K_N^{i_N} \qquad (21)$$

with real coefficients $c_{i_1...i_N}$. We can further restrict the matrices η_α of the dual problem to have the same symmetries as the states ρ. The eigenvalues of ρ are:

$$\lambda_{j_1...j_N}(\rho) = \sum_{i_1,...,i_N=0}^{1} (-1)^{i_1 j_1}...(-1)^{i_N j_N} c_{i_1...i_N} \qquad (22)$$

where the $j_k \in [0, 1]$ form a binary index for λ.

The symmetries obeyed by ρ also implies that the (unnormalized) state σ has the same symmetries as (21). This can be seen as follows: One may define the completely positive map

$$\Lambda(\psi) = \sum_{i_1,...,i_N=0}^{1} K_1^{i_1}...K_N^{i_N} \psi K_1^{i_1}...K_N^{i_N} \qquad (23)$$

Then, assume we found E_{min} and the corresponding operator σ, such that $(\rho + \sigma)^{\Gamma_\alpha} \geq 0 \ \forall \alpha \in \{1, \ldots, N\}$. Since $\Lambda((\rho+\sigma)^{\Gamma_\alpha}) = \rho^{\Gamma_\alpha} + \Lambda(\sigma)^{\Gamma_\alpha}$, one concludes that σ must be invariant under rotations of the stabilizer group. Therefore:

$$\sigma = \sum_{i_1,...,i_N=0}^{1} d_{i_1...i_N} K_1^{i_1}...K_N^{i_N} \qquad (24)$$

and the eigenvectors of σ are given by

$$\lambda_{j_1 \dots j_N}(\sigma) = \sum_{i_1,\dots,i_N=0}^{1} (-1)^{i_1 j_1} \dots (-1)^{i_N j_N} d_{i_1 \dots i_N} \tag{25}$$

A. 2 Qubits

1. 2 Qubits: Upper Bound

In this section we will evaluate the entanglement for a composite system of two qubits, supposedly prepared as a cluster state. The measurements performed on this system result in $a_1 = tr(\rho K_1)$ and $a_2 = tr(\rho K_2)$, with $K_1 = X \otimes Z$ and $K_2 = Z \otimes X$. W.l.o.g. we restrict to the case of positive a_i but write the solutions of the more general case of arbitrary a_i. The primal problem reads

$$min[tr(\sigma) : (\rho + \sigma)^{\Gamma_1} \geq 0, \quad \rho \geq 0, \quad \sigma \geq 0, \quad tr(\rho K_i) = a_i] \tag{26}$$

We denote the eigenvalues of ρ resp. of its transpose by:

$$\lambda_{j_1 j_2}(\rho) = \sum_{i_1,i_2=0}^{1} (-1)^{i_1 j_1} (-1)^{i_2 j_2} c_{i_1 i_2} \tag{27}$$

$$\lambda_{j_1 j_2}(\rho^{\Gamma_1}) = \sum_{i_1,i_2=0}^{1} (-1)^{i_1 j_1} (-1)^{i_2 j_2} (-1)^{i_1 i_2} c_{i_1 i_2} \tag{28}$$

Eigenvalues of σ and σ^{Γ} are of the same form, and we denote the corresponding coefficients with $d_{i_1 i_2}$. The coefficients $c_{00} = 1/4$, $c_{10} = a_1/4$, $c_{01} = a_2/4$ are given by normalization and measurement constraints. In the case $a_1 + a_2 \leq 1$, one may set $c_{11} = 0$, which is the coefficient that changes sign under partial transposition. Thus, $\sigma = 0$ in this case. Otherwise, upper bounds on $tr(\sigma) = 4d_{00}$ are obtained by the choice $d_{00} = (a_1 + a_2 - 1)/4$, $d_{i_1 i_2} = -d_{00}/3$ else, and $c_{11} = -d_{00}$. The upper bound on the Global Robustness of Entanglement is thus given by:

$$E_{min} = max\{0, |a_1| + |a_2| - 1\}. \tag{29}$$

2. 2 Qubits: Lower Bound

Here we will derive a lower bound on the Global Robustness of Entanglement according to Eq. 20. We will see that this lower bound coincides with the upper bound derived in the previous section. First, one may restrict the matrices η_α to have the same symmetries as ρ:

$$\eta_\alpha = \sum_{i_1,i_2=0}^{1} c_{i_1 i_2}^{(\alpha)} K_1^{i_1} K_2^{i_2}. \tag{30}$$

Since the partial transposes Γ_1 and Γ_2 have the same impact on the η_α (both change the sign of the coefficient c_{11}), we may simplify the problem by setting $\eta_1 = \eta_2 = \eta/2$. Again we consider only the case of positive a_i's. The dual problem can now be formulated as the following eigenvalue problem in the form of a linear program:

$$max[\mu_0 + \mu_1 a_1 + \mu_2 a_2 : \mu_0 \mathbb{1} + \mu_1 K_1 + \mu_2 K_2 + \eta^{\Gamma_1} \leq 0, \ \eta \geq 0, \ \eta^{\Gamma_1} \leq \mathbb{1}]. \tag{31}$$

Besides the trivial solution (all variables equal zero), a little thought shows that the above system of inequalities is fulfilled by $-\mu_0 = \mu_1 = \mu_2 = 1$ and $c_{00} = -c_{10} = -c_{01} = c_{11} = 1/2$. Thus:

$$E_{min} = max\{0, |a_1| + |a_2| - 1\}. \tag{32}$$

which coincides with the upper bound presented in the previous subsection.

No. Qubits	exact value	estimated value	relative deviation
2	0.8142	0.8097	0.0055
3	0.8185	0.8097	0.0108
4	2.2995	2.2387	0.0264

TABLE I: Comparison of the Global Robustness of Entanglement (GRE) for 2, 3, and 4 qubit noisy cluster states with an estimate of the GRE from measurements of the generators of the stabilizer group only

B. 3 Qubits

If the goal of the experiment was the creation of a triangle cluster state, the observables are naturally $K_1 = X \otimes Z \otimes Z$, $K_2 = Z \otimes X \otimes Z$, and $K_3 = Z \otimes Z \otimes X$ with measurement outcomes $a_i = tr(K_i \rho)$, $i \in \{1, 2, 3\}$. Then, one finds a solution similar to the 2-qubit case, in the sense that it only depends on the two largest measurement outcomes:

$$E_{min} = max\{0, |a_1| + |a_2| + |a_3| - min(|a_1|, |a_2|, |a_3|) - 1\}. \tag{33}$$

C. 4 Qubits

Let us now consider the case, where the goal of the experiment was the creation of a 4-qubit cluster state associated with a square lattice graph (box cluster state). Then the four generators of the corresponding stabilizer group are given by $K_1 = X \otimes Z \otimes \mathbb{1} \otimes Z$, $K_2 = Z \otimes X \otimes Z \otimes \mathbb{1}$, $K_3 = \mathbb{1} \otimes Z \otimes X \otimes Z$, $K_4 = Z \otimes \mathbb{1} \otimes Z \otimes X$. The measurement outcomes are denoted by $a_i = tr(\rho K_i)$ for $i \in \{1, \ldots, 4\}$ and are assumed to be non-negative. Thus, the problem for the square lattice case reads:

$$max[\mu_0 + \sum_{i=1}^{4} \mu_i a_i : \sum \eta_\alpha^{\Gamma_\alpha} + \sum_{i=0}^{3} \mu_i K_i \leq 0,\ \eta_\alpha \geq 0,\ \ \sum \eta_\alpha^{\Gamma_\alpha} \leq 1] \tag{34}$$

where $K_0 = \mathbb{1}$. The matrices η_α are restricted to: $\eta_\alpha = \sum_{i_1,\ldots,i_4=0}^{1} c_{i_1\ldots i_4}^{(\alpha)} K_1^{i_1} \ldots K_4^{i_4}$. The partial transposes are therefore given by: $\eta_\alpha^{\Gamma_\alpha} = \sum_{i_1,\ldots,i_4=0}^{1} (-1)^{i_1 \sum_{N_\alpha} i_{N_\alpha}} c_{i_1\ldots i_4}^{(\alpha)} K_1^{i_1} \ldots K_4^{i_4}$.

Even though, this translates to a system of inequalities which looks rather complex, one may realize easily that the solution of the two-qubit case represents also a solution for this system. This means, $\mu_0 = -1$, $\mu_1 = \mu_2 = 1$ and $\mu_3 = \mu_4 = 0$, and regarding the η_α one obtains $c_{0000}^{(1)} = c_{1100}^{(1)} = \frac{1}{4}$, $c_{1000}^{(1)} = c_{0100}^{(1)} = -\frac{1}{4}$ and $\eta_2 = \eta_1$, $\eta_3 = \eta_4 = 0$. One may easily check, that another solution is given by the following set of parameters: $\mu_0 = -5,\ \mu_1 = 2,\ \mu_2 = 2,\ \mu_3 = 2,\ \mu_4 = 2$. and the coefficients of the operator sum representation of the η_α are listed in Tab. II. Summarizing these results gives:

$$E_{min} = max[0,\ (|a_1| + |a_2| - 1),\ 2(|a_1| + |a_2| + |a_3| + |a_4|) - 5] \tag{35}$$

VI. QUALITY OF THE ESTIMATE AND LOCAL STATISTICS

In order to check the usefulness of the obtained bounds, we compare these bounds with exact values for simulated noisy cluster states. We assume that after a perfect cluser state was created, the qubits are subject to local dephasing for a certain time (here we assume 10 ms). Then, the system is described by the following master equation:

$$\dot{\rho} = \frac{\gamma}{2} \sum_i (Z_i \rho Z_i - \rho) \tag{36}$$

where γ is the dephasing-rate, which we take to be $(10\,\mathrm{s})^{-1}$. A comparison between exact values of the Global Robustness with our estimate is given in Tab. I. It shows that the estimate deviates only a few per cent from the exact value. It is obvious that the bounds can be improved by considering any additional information on the density matrix. When one performs measurements on distant parties, the observables such as $\langle X \otimes X \rangle$ must be gained from local measurements. The entanglement depends mainly on the correlations, as we have seen in the above comparison. However, the obtained local statistics may be used to improve the bounds. Consider the measurements $\langle X \otimes X \rangle = 0.9$,

$\langle Z \otimes Z \rangle = 0.7$, $\langle Z \otimes \mathbb{1} \rangle = 0$, $\langle \mathbb{1} \otimes Z \rangle = 0.25$. In this example, the GRE yields 0.6 when one considers only the XX- and ZZ-observables. Taking into account the local statistics improves the GRE by more than ten per cent to 0.6671. This example shows that one should use all available information the measurements provide to obtain optimal bounds on entanglement.

VII. CONCLUSION AND OUTLOOK

In conclusion, we investigated how to obtain lower bounds on the fidelity and robustness measures from partial information on the density matrix of a multi-partite system. We utilized the symmetries of the stabilizer group to formulate the problem as a linear program, which can be treated analytically as well as numerically. Analytical solutions were obtained for two, three, and four qubit-systems. This method is of particular interest for experiments, since the number of measurement settings grows only linearly in the number of qubits, whereas full-state tomography requires an exponential number of settings. A comparison of the obtained bounds with exact values of the Global Robustness shows that the difference is in the order of only a few per cent.

For the future, it will be interesting to investigate if analytical solutions to our approach can be found for systems with an arbitrary number of constituents.

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APPENDIX A: SOLUTION TO THE DUAL PROBLEM FOR A 4 QUBIT MEASUREMENT

APPENDIX B: PROOF FOR THE FIDELITY OF NOISY CLUSTER STATES

Let $a_i = tr(K_i \rho)$, $i \in \{1, \ldots, N\}$ the mean values of the stabilizer operators. Twirling over the stabilizer group allows us to restrict to

$$\rho = \frac{1}{2^N} \sum_{i_1, \cdots, i_N = 0}^{1} c_{i_1 \ldots i_N} K_1^{i_1} \cdots K_N^{i_N} \tag{B1}$$

α	1	2	3	4
$c^{(\alpha)}_{0000}$	3/16	3/16	3/16	3/16
$c^{(\alpha)}_{1000}$	-1/16	-2/16	1/16	-2/16
$c^{(\alpha)}_{0100}$	-2/16	-1/16	-2/16	1/16
$c^{(\alpha)}_{0010}$	1/16	-2/16	-1/16	-2/16
$c^{(\alpha)}_{0001}$	-2/16	1/16	-2/16	-1/16
$c^{(\alpha)}_{1100}$	1/16	1/16	-1/16	-1/16
$c^{(\alpha)}_{1010}$	-3/16	1/16	-3/16	1/16
$c^{(\alpha)}_{1001}$	1/16	-1/16	-1/16	1/16
$c^{(\alpha)}_{0110}$	-1/16	1/16	1/16	-1/16
$c^{(\alpha)}_{0101}$	1/16	-3/16	1/16	-3/16
$c^{(\alpha)}_{0011}$	-1/16	-1/16	1/16	1/16
$c^{(\alpha)}_{1110}$	2/16	-1/16	2/16	1/16
$c^{(\alpha)}_{1101}$	-1/16	2/16	1/16	2/16
$c^{(\alpha)}_{1011}$	2/16	1/16	2/16	-1/16
$c^{(\alpha)}_{0111}$	1/16	2/16	-1/16	2/16
$c^{(\alpha)}_{1111}$	-1/16	-1/16	-1/16	-1/16

TABLE II: Coefficients for the operator sum representation of the operators η_α, where the goal of the experiment is a box cluster state

with eigenvalues

$$\lambda_{j_1,\ldots,j_N}(\rho) = \frac{1}{2^N} \sum_{i_1,\cdots,i_N=0}^{1} (-1)^{\sum_m i_m j_m} c_{i_1\ldots i_N} \tag{B2}$$

The target state may be written as

$$|\phi\rangle\langle\phi| = \frac{1}{2^N} \sum_{i_1,\cdots,i_N=0}^{1} K_1^{i_1} \cdots K_N^{i_N} \tag{B3}$$

Primal problem: Now we choose the coefficients

$$c_{i_1\ldots i_N} = \sum_{k=1}^{N} i_k a_k - \sum i_k + 1 \tag{B4}$$

Because $\forall\, m : K_m^2 = 1$, we find

$$tr(|\phi\rangle\langle\phi|\rho) = \frac{1}{2^N} \sum_{i_1,\ldots,i_N=0}^{1} c_{i_1\ldots i_N} \tag{B5}$$

$$= \frac{1}{2^N} \sum_{i_1,\ldots,i_N=0}^{1} (\sum_{k=1}^{N} i_k a_k - \sum i_k + 1) \tag{B6}$$

$$= \frac{1}{2}(\sum_k a_k - N + 2) \tag{B7}$$

Dual problem: The dual problem may be solved by the choice $\lambda_0 = N/2 - 1$ and $\lambda_i = 1/2$ for $i \geq 1$. In order to check the validity of this solution, one must prove that $\chi - \Xi \geq 0$ with $\chi = |\phi\rangle\langle\phi|$ and $\Xi = \frac{1}{2}\sum_{i=1}^{N} K_i - (1 - \frac{N}{2})\mathbb{1}$. The eigenvalues of Ξ are given by

$$\lambda_{j_1\ldots j_N}(\Xi) = \frac{N}{2} - 1 - \frac{1}{2}\sum_{i=1}^{N}(-1)^{j_i} \tag{B8}$$

This means $\lambda_{0\dots0}(\Xi) = -1$. Since $\lambda_{0\dots0}(\chi) = 1$, we have $\lambda_{0\dots0}(\chi+\Xi) = 0$. It is easy to see that $\lambda_{j_1\dots j_N}(\Xi) \geq 0$ for $(j_1,\dots,j_N) \neq (0,\dots,0)$, and $\lambda_{j_1\dots j_N}(\chi) = 0$ for these indices, thus $\chi+\Xi \geq 0$.

We assume N is even. One may set $c_{i_1\dots i_N} = \sum_{k=1}^N a_k - \sum i_k + 1$. We will now prove by induction that $\rho = \sum c_{i_1\dots i_N} K_1^{i_1}\dots K_N^{i_N} \geq 0$ with the above choice, provided that one can find pairs of measurement outcomes with $a_1 + a_2 \geq 1, ..., a_{N-1} + a_N \geq 0$, for $N \geq 4$.

It is convenient to begin the induction for $N = 2$. A simple calculation shows that the eigenvalues of ρ result in

$$\lambda_{00}(\rho) = \frac{1}{2}(a_1 + a_2) \tag{B9}$$
$$\lambda_{10}(\rho) = \frac{1}{2}(1 - a_1) \tag{B10}$$
$$\lambda_{01}(\rho) = \frac{1}{2}(1 - a_2) \tag{B11}$$
$$\lambda_{11}(\rho) = 0 \tag{B12}$$

Induction step: $N \longrightarrow N+2$:

$$\lambda_{j_1\dots j_N 00} = \sum_{i_1\dots i_{N+2}} (-1)^{i_1j_1+\dots+i_{N+2}j_{N+2}} c_{i_1\dots i_{N+2}} \tag{B13}$$
$$= \sum_{i_1\dots i_{N+2}} (-1)^{i_1j_1+\dots+i_{N+2}j_{N+2}} (c_{i_1\dots i_N} + a_{N+1} + a_{N+2} - i_{N+1} - i_{N+2}) \tag{B14}$$
$$= \sum_{i_1\dots i_{N+2}} (-1)^{i_1j_1+\dots+i_Nj_N} (c_{i_1\dots i_N} + a_{N+1} + a_{N+2} - i_{N+1} - i_{N+2}) \tag{B15}$$
$$= \sum_{i_1\dots i_{N+2}} (-1)^{i_1j_1+\dots+i_Nj_N} c_{i_1\dots i_N} + \tag{B16}$$
$$+ \sum_{i_1\dots i_{N+2}} (-1)^{i_1j_1+\dots+i_Nj_N} (a_{N+1} + a_{N+2} - i_{N+1} - i_{N+2}) \tag{B17}$$
$$= 4 \cdot \sum_{i_1\dots i_N} (-1)^{i_1j_1+\dots+i_Nj_N} c_{i_1\dots i_N} + \tag{B18}$$
$$+ \sum_{i_1\dots i_{N+2}} (-1)^{i_1j_1+\dots+i_Nj_N} (a_{N+1} + a_{N+2} - i_{N+1} - i_{N+2}) \tag{B19}$$

The first term is non-negative by assumption. Furthermore, we may write the last term as:

$$\sum_{i_{N+1},i_{N+2}} \sum_{i_1\dots i_N} (-1)^{i_1j_1+\dots+i_Nj_N} (a_{N+1} + a_{N+2} - i_{N+1} - i_{N+2}) \tag{B20}$$

Using the relation

$$\sum_{i_1\dots i_N=0}^{1} (-1)^{i_1j_1+\dots+i_Nj_N} \cdot A = \begin{cases} 2^N \cdot A & \text{, if } \vec{j} = 0; \\ 0 & \text{, otherwise;} \end{cases} \tag{B21}$$

the mentioned term becomes

$$\sum_{i_{N+1},i_{N+2}} 2^N (a_{N+1} + a_{N+2} - i_{N+1} - i_{N+2}) \tag{B22}$$

Performing the summation gives simply $2^N(4 \cdot (a_{N+1} + a_{N+2} - 1))$, which is also non-negative. Thus $\lambda_{j_1\dots j_N 00} \geq 0$.

$$\lambda_{j_1\dots j_N 10} = \sum_{i_1\dots i_{N+2}} (-1)^{i_1 j_1+\dots+i_{N+2} j_{N+2}} c_{i_1\dots i_{N+2}} \tag{B23}$$

$$= \sum_{i_1\dots i_{N+2}} (-1)^{i_1 j_1+\dots+i_{N+2} j_{N+2}} (c_{i_1\dots i_N} + a_{N+1} + a_{N+2} - i_{N+1} - i_{N+2}) \tag{B24}$$

$$= \sum_{i_1\dots i_{N+2}} (-1)^{i_1 j_1+\dots+i_N j_N + i_{N+1}} (c_{i_1\dots i_N} + a_{N+1} + a_{N+2} - i_{N+1} - i_{N+2}) \tag{B25}$$

$$= \sum_{i_1\dots i_{N+2}} (-1)^{i_1 j_1+\dots+i_N j_N + i_{N+1}} c_{i_1\dots i_N} + \tag{B26}$$

$$+ \sum_{i_1\dots i_{N+2}} (-1)^{i_1 j_1+\dots+i_N j_N + i_{N+1}} (a_{N+1} + a_{N+2} - i_{N+1} - i_{N+2}) \tag{B27}$$

$$= 2 \cdot \sum_{i_1\dots i_N} (-1)^{i_1 j_1+\dots+i_N j_N} c_{i_1\dots i_N} + \tag{B28}$$

$$+ \sum_{i_1,\dots,i_N,i_{N+2}} (-1)^{i_1 j_1+\dots+i_N j_N} (a_{N+1} + a_{N+2} + 1 - i_{N+2}) \tag{B29}$$

$$= 2 \cdot \sum_{i_1\dots i_N} (-1)^{i_1 j_1+\dots+i_N j_N} c_{i_1\dots i_N} + \tag{B30}$$

$$+ \sum_{i_1,\dots,i_N} (-1)^{i_1 j_1+\dots+i_N j_N} [(2(a_{N+1} + a_{N+2}) + 1] \tag{B31}$$

Again, the first term is non-negative by assumption, and the second term is non-zero only for $\vec{j}_N = 0$, in which case it is positive. Thus $\lambda_{j_1\dots j_N 10} \geq 0$. Analogously, one may show that $\lambda_{j_1\dots j_N 01} \geq 0$ and $\lambda_{j_1\dots j_N 11} \geq 0$.

For brevity, the proof is only given for systems with an even number of qubits. Similar thoughts may be applied for the case of uneven qubit numbers.