Classical simulation versus universality in measurement based quantum computation

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(Dated: February 1, 2008)

We investigate for which resource states an efficient classical simulation of measurement based quantum computation is possible. We show that the *Schmidt–rank width*, a measure recently introduced to assess universality of resource states, plays a crucial role in also this context. We relate Schmidt–rank width to the optimal description of states in terms of tree tensor networks and show that an efficient classical simulation of measurement based quantum computation is possible for all states with logarithmically bounded Schmidt–rank width (with respect to the system size). For graph states where the Schmidt–rank width scales in this way, we efficiently construct the optimal tree tensor network descriptions, and provide several examples. We highlight parallels in the efficient description of complex systems in quantum information theory and graph theory.

I. INTRODUCTION

The classical description of many–body quantum systems, and the classical simulation of their dynamics, is generically a hard problem, due to the exponential size of the associated Hilbert space [1, 2]. Nevertheless, under certain conditions an efficient description of states and/or their evolution is possible. This is, for instance, demonstrated by the density matrix renormalization group method [3], which allows one to successfully calculate ground states of strongly correlated spin systems in one spatial dimension using matrix product states [4]. In this context, the questions *'For which (families of) states does an efficient classical description exist?',* and *'When is an efficient classical simulation of the evolution of such states under a given dynamics possible?'* are naturally of central importance.

Apart from their practical importance, the above questions are directly related to more fundamental issues, in particular to the power of quantum computation and the identification of the essential properties that give quantum computers their additional power over classical devices; this relation to quantum computation will be central in this article. In particular, we will study these questions from the point of view of the *measurement based* approach to quantum computing, more specifically the model of the one–way quantum computer [5]. In this model, a highly entangled multi–qubit state, the 2D *cluster state* [6], is processed by performing sequences of adaptive single–qubit measurements, thereby realizing arbitrary quantum computations. The 2D cluster state serves as a *universal resource* for measurement based quantum computation (MQC), in the sense that any multi–qubit state can be prepared by performing sequences of local operations on a sufficiently large 2D cluster state.

When studying the fundamentals of the one–way model, two (related) questions naturally arise, which we will consider in the following; first, it is asked which resource states, other than the 2D cluster states, form universal resources for MQC; second, one may also consider the question whether MQC on a given state can be *efficiently simulated* on a classical computer. Naturally, these two issues are closely related, as one expects that an efficient classical simulation of MQC performed on (efficient) universal resource states is impossible. However, it is important to stress that classical simulation and non–universality are principally different issues.

The question of which other resource states are also universal has been investigated recently in Ref. [7], where the required entanglement resources enabling universality were investigated. In particular, it was proven that certain entanglement measures, in particular certain *entanglement width* measures, must diverge on any universal resource, thus providing necessary conditions for universality.

On the other hand, the issue of classical simulation of MQC evidently brings us back to the central introductory questions posed above. Results regarding the efficient simulation of MQC do exist, and it is e.g. known that any MQC implemented on a 1D cluster state can be simulated efficiently [8]. More generally, the efficient description of quantum states in terms of (tree) tensor networks turns out to play an important role in this context [9, 10].

In this article we strengthen the connection between classical simulation of MQC and non–universality. Our starting point will be the no–go results for universality obtained in Ref. [7], stating that the entanglement monotones *entropic entanglement width* and *Schmidt–rank width* must diverge on any universal resource; both measures are closely related, and we refer to section II A for definitions. We then focus on the Schmidt–rank width measure, and prove, as our first main result, that MQC can be efficiently simulated on every resource state which is ruled out by the above no–go result. More generally, we prove that MQC can be simulated efficiently on all states where the Schmidt–rank width grows at most logarithmically with the system size [11].

Second, along the way of proving the above results, we provide a natural interpretation of the Schmidt–rank width measure, as we show that this monotone quantifies what the optimal description of quantum states is in

terms of tree tensor networks; this shows that there is in fact a large overlap between the present research and the work performed in Ref. [10] regarding the simulation of quantum systems using tree tensor networks.

As our third main result, we show that the Schmidt–rank width (and entanglement width) – these are measures which are defined in terms of nontrivial optimization problems – can be computed efficiently for all graph states. Moreover, for all graph states where the Schmidt–rank width grows at most logarithmically with the number of qubits, we give efficient constructions of the optimal tree tensor networks describing these states.

We further remark that the origin of the Schmidt-rank width lies in fact in graph theory, and its definition is inspired by a graph invariant called *rank width*. It turns out that the study of rank width in graph theory shows strong similarities with the study of efficient descriptions and simulations of quantum systems, viz. the two introductory questions of this article. The similarity is due to the fact that, in certain aspects of both quantum information theory and graph theory, one is concerned with the efficient description of complex structures in terms of tree–like structures. We will comment on the existing parallels between these fields.

Finally, we emphasize that the present work is situated in two different dynamic areas of research within the field of quantum information theory; the first is the study of universality and classical simulation of measurement based quantum computation, and the second is the problem of efficiently describing quantum systems and their dynamics. An important aim of this article consists of bringing together existing results in both fields and showing that there is a strong connection between them; in particular, we find that the notion of Schmidt–rank width has been considered independently in Refs. [7] and [10] and plays an important role in both areas of research. In order to establish the connections between these two areas in a transparent manner, a substantial part of this article is devoted to giving a clear overview of which relevant results are known in both fields.

The paper is organized as follows. In section II we discuss entanglement width and Schmidt-rank width, and their role in universality and classical simulation of MQC. In Section III the description of states in terms of tree tensor networks is reviewed, and a connection to Schmidt-rank width is established. This Section also includes our main result, stating that any state with a logarithmically bounded Schmidt-rank width has, in principle, an efficient description in terms of a tree tensor network, and hence any MQC performed on such states can be efficiently simulated classically. In Section IV these results are applied to graph states, and we provide in addition an explicit way of obtaining the optimal tree tensor network. We discuss the relation between the treatment of complex systems in quantum information theory and graph theory in section V, and summarize and conclude in section VI.

II. ENTANGLEMENT WIDTH, UNIVERSALITY, AND CLASSICAL SIMULATION

In this section we introduce two related multipartite entanglement measures called *entropic entanglement width* and *Schmidt–rank width* and discuss their role in the studies of universality of resources for measurement based quantum computation (MQC) and in classical simulation of MQC.

These entanglement measures are defined in section II A. In section II B we review the definition of universal resources for MQC, and the use of the above measures in this study. In section II C we consider the basic notions regarding efficient classical simulation of MQC. Finally, in section II D we pose the two central questions of this article in a precise way; the first question asks about the interpretation of the measures entanglement width and Schmidt–rank width, and the second deals with the role of these measures in the context of classical simulation of MQC.

A. Entanglement width

The entropic entanglement width $E_{\mathrm{wd}}(|\psi\rangle)$ of an multi–party state $|\psi\rangle$ is an entanglement measure introduced in Ref. [7]. Qualitatively, this measure computes the minimal bipartite entanglement entropy in the state $|\psi\rangle$, where the minimum is taken over specific classes of bipartitions of the system. The precise definition is the following.

Let $|\psi\rangle$ be an n-party pure state. A *tree* is a graph with no cycles. Let T be a *subcubic* tree, which is a tree such that every vertex has exactly 1 or 3 incident edges. The vertices which are incident with exactly one edge are called the *leaves* of the tree. We consider trees T with exactly n leaves $V := \{1, \dots, n\}$, which are identified with the n local Hilbert spaces of the system. Letting $e = \{i, j\}$ be an arbitrary edge of T, we denote by $T \setminus e$ the graph obtained by deleting the edge e from T. The graph $T \setminus e$ then consists of exactly two connected components (see Fig. 1), which naturally induce a bipartition (A_T^e, B_T^e) of the set V. We denote the bipartite entanglement entropy of $|\psi\rangle$ with respect to the bipartition (A_T^e, B_T^e) by $E_{A_T^e, B_T^e}(|\psi\rangle)$. The entropic entanglement width of the state $|\psi\rangle$ is now defined by

$$E_{\mathrm{wd}}(|\psi\rangle) := \min_T \ \max_{e \in T} \ E_{A_T^e, B_T^e}(|\psi\rangle), \qquad (1)$$

where the minimization is taken over all subcubic trees T with n leaves, which are identified with the n parties in the system.

Thus, for a given tree T we consider the maximum, over all edges in T, of the quantity $E_{A_T^e, B_T^e}(|\psi\rangle)$; then the minimum, over all subcubic trees T, of such maxima is computed.

Similarly, one may use the Schmidt rank, i.e. the number of non–zero Schmidt coefficients, instead of the bipar-
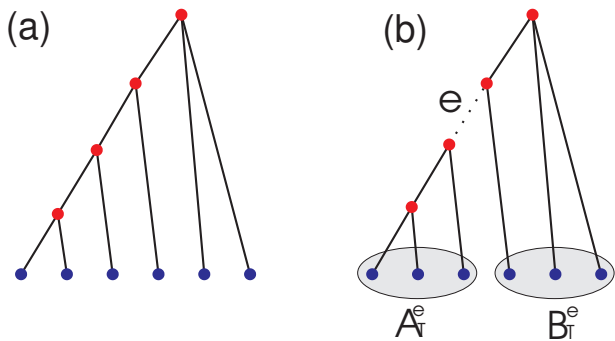
FIG. 1: (a) Example of a subcubic tree T with six leaves (indicated in blue). (b) Tree $T \setminus e$ obtained by removing edge e and induced bipartition (A_T^e, B_T^e).

tite entropy of entanglement as basic measure. One then obtains the *Schmidt–rank width*, or χ*–width*, denoted by $\chi_{\mathrm{wd}}(|\psi\rangle)$. The precise definition is the following. Letting $\chi_{A_T^e, B_T^e}(|\psi\rangle)$ denote the number of non–zero Schmidt coefficients of $|\psi\rangle$ with respect to a bipartition (A_T^e, B_T^e) of V as defined above, the χ–width of the state $|\psi\rangle$ is defined by

$$\chi_{\mathrm{wd}}(|\psi\rangle) := \min_T \max_{e \in T} \log_2 \chi_{A_T^e, B_T^e}(|\psi\rangle). \quad (2)$$

It is straightforward to show (cf. Ref. [7]) that E_{wd} is an entanglement monotone [12], i.e., this measure vanishes on product states, is a local invariant, and decreases on average under local operations and classical communication (LOCC). The proof can readily be extended to χ_{wd}, demonstrating that also χ–width is a valid entanglement measure. In fact, using that the Schmidt rank is non–increasing under *stochastic* LOCC, or SLOCC, it can be proven that the χ–width is also non–increasing under SLOCC.

Since the inequality

$$\log_2 \chi_{A,B}(|\psi\rangle) \geq E_{A,B}(|\psi\rangle) \quad (3)$$

holds for any bipartition (A, B) of the system and for any state $|\psi\rangle$, we have

$$\chi_{\mathrm{wd}}(|\psi\rangle) \geq E_{\mathrm{wd}}(|\psi\rangle). \quad (4)$$

Note, however, that these quantities can show a completely different (scaling) behavior.

It is clear that the definitions of entropic entanglement width and Schmidt–rank width are based upon similar constructions, where optimizations are performed over subcubic trees. Such constructions can of course be repeated for any bipartite entanglement measure; hence a whole class of multipartite entanglement measures is obtained, which we will call the class of *entanglement width measures*. The entropic entanglement width and

χ–width are two examples of entanglement width measures. It would be interesting to consider other examples of entanglement width measures, and investigate their possible role in quantum information theory.

The definitions of the above entanglement measures are inspired by a graph invariant called *rank width*, which was introduced in Ref. [13]. The connection with rank width is obtained by evaluating the entropic entanglement width or χ–width in *graph states*. This is explained next.

First we recall the definition of graph states. Let $\sigma_x, \sigma_y, \sigma_z$ denote the Pauli spin matrices. Let $G = (V, E)$ be a graph with vertex set $V := \{1, \ldots, n\}$ and edge set E. For every vertex $a \in V$, the set $N(a)$ denotes the set of neighbors of a, i.e., the collection of all vertices b which are connected to a by an edge $\{a, b\} \in E$. The graph state $|G\rangle$ is then defined to be the unique n-qubit state which is the joint eigenstate, with eigenvalues equal to 1, of the n commuting correlation operators

$$K_a := \sigma_x^{(a)} \bigotimes_{b \in N(a)} \sigma_z^{(b)}. \quad (5)$$

Standard examples of graph states include the GHZ states, and the 1D and 2D cluster states, which are obtained if the underlying graph is a 1D chain or a rectangular 2D grid, respectively. We refer to Ref. [14] for further details.

Let Γ be the $n \times n$ adjacency matrix of G, i.e, one has $\Gamma_{ab} = 1$ if $\{a, b\} \in E$ and $\Gamma_{ab} = 0$ otherwise. For every bipartition (A, B) of the vertex set V, define $\Gamma(A, B)$ to be the $|A| \times |B|$ submatrix of Γ defined by

$$\Gamma(A, B) := (\Gamma_{ab})_{a \in A, b \in B}. \quad (6)$$

Using standard graph state techniques it can then be shown (see e.g. [14]) that

$$\begin{aligned} \mathrm{rank}_{\mathbb{F}_2} \Gamma(A, B) &= \log_2 \chi_{A,B}(|G\rangle) \\ &= E_{A,B}(|G\rangle). \end{aligned} \quad (7)$$

where $\mathrm{rank}_{\mathbb{F}_2} X$ denotes the rank of a matrix X when arithmetic is performed over the finite field $\mathbb{F}_2 = \mathrm{GF}(2)$. Thus, the Schmidt rank and the bipartite entanglement entropy w.r.t. any bipartition (A, B) coincide for graph states, and are given by the rank of the matrix $\Gamma(A, B)$. Using the identity (7), one immediately finds that the χ–width (and entropic entanglement width) of the graph state $|G\rangle$ coincides with the *rank width* $\mathrm{rwd}(G)$ of the graph G. The explicit definition of $\mathrm{rwd}(G)$ reads [13]

$$\mathrm{rwd}(G) := \min_T \max_{e \in T} \mathrm{rank}_{\mathbb{F}_2} \Gamma(A_T^e, B_T^e) \quad (8)$$

(where the minimization is again over subcubic trees as in the definition of χ–width), which, using (7), indeed coincides with the χ–width of $|G\rangle$.

Note that the subcubic trees which are considered in the definition of rank width are not to be confused with the defining graph G of the graph state $|G\rangle$ (the latter can

be an arbitrary graph); the subcubic trees merely serve as a means of selecting certain bipartitions of the system, independent of the state which is considered. For instance, if we consider a linear cluster state $|L_6\rangle$ of six qubits, corresponding to a graph L_6 that is a linear chain, then the tree depicted in Fig. 1 corresponds to the optimal tree in the definition of the rank-width (and χ-width), leading to $\mathrm{rwd}(L_6) = \chi_{\mathrm{wd}}(|L_6\rangle) = 1$.

In section V we will further comment on the motivations for the definition of rank width, and we will draw parallels with the study of complex systems in quantum information theory.

B. Universal resources for MQC

In Ref. [7] a definition for universality of families of states for MQC was put forward, and the use of E_{wd} to assess non–universality of states was demonstrated. In this section we briefly review the definition and the corresponding results.

Consider an (infinitely large) family of qubit states

$$\Psi = \{|\psi_1\rangle, |\psi_2\rangle, \ldots\}, \qquad (9)$$

where $|\psi_i\rangle$ is a state on m_i qubits and $m_i < m_{i+1}$ for every $i = 1, 2, \ldots$. This family is called a *universal resource for MQC* if for each state $|\phi\rangle$ on n qubits there exists a state $|\psi_i\rangle \in \Psi$ on m_i qubits, with $m_i \geq n$, such that the transformation $|\psi_i\rangle \to |\phi\rangle |0\rangle^{m_i-n}$ is possible deterministically by means of LOCC. That is, any state $|\phi\rangle$ can be prepared using only states within the family Ψ as resource. Equivalently, the action of an arbitrary unitary operation U on a product input state $|0\rangle^n$ can be implemented, where now $|\phi\rangle := U|0\rangle^n$ in the above definition. This definition is in the spirit of the model of the one–way quantum computer, where sequences of adaptive single–qubit measurements performed on a sufficiently large 2D cluster state allow one to prepare any multi–qubit state. The definition of universal resource aims to identify the required resources, in terms of entanglement, that allow one to perform universal quantum computation in the sense specified above.

In the above definition of universality of a family Ψ, we have not yet considered the efficiency with which states can be prepared using members of Ψ. An *efficient* universal resource Ψ is a universal resource having the property that all states that can be efficiently generated with a quantum gate network should also be efficiently generated from universal resource Ψ. We refer to Ref. [15] for a detailed account on efficient universality.

In Ref. [7] it was found that any universal resource Ψ must satisfy the following property. Let $E(|\phi\rangle)$ be a functional which is defined on the set of *all* n-qubit states, for *all* $n \in \mathbb{N}$, and suppose that $E(|\phi\rangle)$ is non–increasing under LOCC. More precisely, if $|\phi\rangle$ and $|\phi'\rangle$ are states on n and n' qubits, respectively, then $E(|\phi\rangle) \geq E(|\phi'\rangle)$ whenever the transformation $|\phi\rangle \to |\phi'\rangle|0\rangle^{n-n'}$ is possible by means of LOCC. Moreover, let E^* denote the supremal value of $E(|\phi\rangle)$, when the supremum is taken over all n-qubit states, for all $n \in \mathbb{N}$ (the case $E^* = \infty$ is allowed). Then any universal resource Ψ must satisfy the property

$$\sup \{E(|\psi\rangle) \mid |\psi\rangle \in \Psi\} = E^*. \qquad (10)$$

That is, the supremal value of every entanglement measure E must be reached on every universal resource Ψ. Using the fact that there exist families of quantum states where the entropic entanglement width and χ–width grow unboundedly with the system size (the 2D cluster states are such examples), it is then straightforward to show that any universal family of states Ψ must have unbounded entropic entanglement width and χ–width as well. More precisely, one has [7]:

Theorem 1 *Let Ψ be a universal resource for MQC. Then the following statements hold:*

(i) $\sup \{E_{wd}(|\psi\rangle) \mid |\psi\rangle \in \Psi\} = \infty$;

(ii) $\sup \{\chi_{wd}(|\psi\rangle) \mid |\psi\rangle \in \Psi\} = \infty$.

In other words, families Ψ where the measures E_{wd} or χ_{wd} are *bounded*, cannot be universal. This insight, together with the relation between entropic entanglement width and χ–width and the graph theoretical measure rank width, allows one to identify classes of graph states as being non–universal since the rank width is bounded on such classes. Examples include linear cluster graphs, trees, cycle graphs, cographs, graphs locally equivalent to trees, graphs of bounded tree–width, graphs of bounded clique–width or distance–hereditary graphs. We refer to the literature for definitions.

In the remainder of this paper, we will focus on the χ–width measure.

C. Classical simulation of MQC

Rather than considering the question whether a family Ψ is a universal resource for MQC, one may also consider the question whether MQC on Ψ can be *efficiently simulated* on a classical computer. We will say that efficient classical simulation of MQC on a family of states Ψ is possible, if for every state $|\psi_i\rangle \in \Psi$ it is possible to simulate every LOCC protocol on a classical computer with overhead $\mathrm{poly}(m_i)$, where m_i denotes the number of qubits on which the state $|\psi_i\rangle$ is defined, as before. We remark that an efficient classical description of the initial states $|\psi_i\rangle$ is a necessary, but not necessarily a sufficient condition for efficient simulation on a classical computer.

The issue of classical simulation of MQC has recently been considered by several authors. At this point we remind the reader of what is already known in this context. Regarding simulation of MQC on *graph states*, we recall the following results:

- In Ref. [8] it was showed that MQC on 1D cluster states can be simulated efficiently classically;

- In Ref. [10] it was showed that MQC on tree graphs can be simulated efficiently classically;

- In Ref. [9] it was showed that MQC on graphs with logarithmically bounded tree width [16] can be simulated efficiently classically.

Note that the above result on tree width implies the two other results, as tree graphs (and thus also 1D cluster graphs) have tree width equal to 1 [17].

More general results, i.e., regarding *arbitrary states*, were obtained in Ref. [10], where it was shown that MQC can be simulated efficiently on all states allowing an efficient *tree tensor network* description. The description of quantum systems in terms of tree tensor networks will play an important role in the present analysis, and will be reviewed in detail in section III.

Although related, the issues of universality and classical simulation in MQC are fundamentally two different questions. Most of us expect that any family Ψ for which classical simulation of MQC is possible, will not be an efficient universal resource; this reflects the common belief that quantum computers are in some sense exponentially more powerful than classical machines – note, however, that so far there is no rigorous proof of this statement. While one expects the possibility of classical simulation of MQC to imply non–universality of a resource Ψ, the converse implication is certainly not believed to hold in general. Indeed, it is highly likely that many non–universal families could still be used to implement specific quantum algorithms.

D. Problem formulation

It is clear that regarding the notion of χ-width, and the above issues of universality and classical simulation of MQC, a number of open questions remain. In this section we formulate two central questions, (Q1) and (Q2), which will constitute the main research topics in this article. We will first state these questions and then discuss them.

(Q1) Does there exist a natural *interpretation* of the χ–width measure?

(Q2) Do there exist resources Ψ having bounded χ–width, which nevertheless *do not allow* an efficient classical simulation of MQC?

Question (Q1) is concerned with the fact that the definition of χ–width seems to be rather arbitrary and not intuitive, and solely motivated by the connection to the graph theoretical measure rank width. We will, however, provide a satisfactory interpretation of this measure in the context of quantum information in the next section.

Question (Q2) is concerned with the question whether non–universal resources can still be useful for quantum computation, in the sense that MQC performed on such states is more powerful than classical computation. As remarked above, it may well be that there exist

non–universal families of states where MQC is nevertheless hard to simulate classically. Previous results leave open this possibility, as the criteria for non–universality and classical simulatability do not coincide. For non–universal states detected by the χ–width criterion (i.e., theorem 1 (ii)), we will show that this is not the case. In section III C we will show that MQC can be simulated efficiently for any family Ψ which is ruled out by the χ–width criterion as being a non–universal resource.

III. ENTANGLEMENT–WIDTH AND TREE TENSOR NETWORKS

In this section we tackle questions (Q1) and (Q2) as stated in the previous section. First we will attach a natural interpretation to the χ–width measure, as we will show that $\chi_{\mathrm{wd}}(|\psi\rangle)$ quantifies the complexity of the optimal *tree tensor network* (TTN) describing the state $|\psi\rangle$, thus providing a satisfactory answer to question (Q1). Moreover, we shall see that this connection with tree tensor networks immediately allows us to give a negative answer to (Q2): we find that MQC can be simulated efficiently on all resources having a bounded χ–width.

These results will be obtained in three main steps. In section III A we review the notions of tensor networks and, more particularly, tree tensor networks. We also review results obtained in Ref. [10], where it was proved that LOCC on states specified in terms of efficient TTN descriptions can be simulated efficiently; the results in Ref. [10] will be central ingredients to our analysis. In section III B we show how to obtain TTN descriptions for arbitrary quantum states. Finally, in section III C we establish the connection between TTNs and χ–width.

A. Tree tensor networks and efficient simulation of quantum systems

In this section we review the basic notions regarding (tree) tensor networks (see also Ref. [9]), and the simulation of quantum systems described by TTNs as obtained in Ref. [10].

Consider a $d_1 \times \cdots \times d_n$ complex tensor [18]

$$A := A_{i_1 i_2 \ldots i_n}, \tag{11}$$

where each index i_α ranges from 1 to d_α, for every $\alpha = 1, \ldots, n$. The number of indices n is sometimes called the *rank* of the tensor A. We will call the number $D := \max_\alpha d_\alpha$ the *dimension* of A. For example, every pure n-qubit state expressed in a local basis,

$$|\phi\rangle = \sum_{i_1,\ldots,i_n=0}^{1} A_{i_1 \ldots i_n} |i_1 \ldots i_n\rangle \tag{12}$$

corresponds to an $2 \times \cdots \times 2$ tensor of rank n and dimension 2.

If $A^{(1)}$ and $A^{(2)}$ are two tensors of ranks n_1 and n_2, respectively, and s and t are integers with $1 \leq s \leq n_1$ and $1 \leq t \leq n_2$, and both the sth index of $A^{(1)}$ and the tth index of $A^{(2)}$ range from 1 to the same integer d, then a sum of the form

$$\sum_{j=1}^{d} A^{(1)}_{i_1 \ldots i_{s-1} \; j \; i_{s+1} \ldots i_n} A^{(2)}_{i_1 \ldots i_{t-1} \; j \; i_{t+1} \ldots i_n} \qquad (13)$$

yields a tensor of rank $n_1 + n_2 - 1$. This sum is called a *contraction* of the tensors $A^{(1)}$ and $A^{(2)}$. More specifically, one says that the sth index of $A^{(1)}$ is contracted with the tth index of $A^{(2)}$. A situation where several tensors $A^{(1)}, \ldots, A^{(N)}$ are contracted at various indices is called a *tensor network*. The maximal dimension of any tensor in the network, is called the *dimension* of the network, and will usually be denoted by D in the following. Note that every tensor network with n *open* indices (i.e., indices which are not contracted), can be associated in a natural way to an n-party pure quantum state.

We will only consider tensor networks where every index appears at most twice in the network. In this case, every tensor network can be represented by a *graph F* in the following way.

- For every tensor $A^{(\alpha)}$ a vertex α is drawn.

- Whenever two tensors $A^{(\alpha)}$ and $A^{(\beta)}$ are contracted, an edge is drawn between the corresponding vertices α and β in the graph.

- Finally, for every *open* index of a tensor $A^{(\alpha)}$, i.e., an index which is not contracted, one draws a new vertex and an edge connecting this vertex to the vertex α.

As an example, consider three tensors $A^{(1)}, A^{(2)}, A^{(3)}$ contracted as follows:

$$\sum_{jkl} A^{(1)}_{ajk} A^{(2)}_{bjl} A^{(3)}_{ckl}. \qquad (14)$$

This tensor network has 3 open indices a, b, c, and the indices j, k, l are contracted. The graph underlying this tensor network is depicted in Fig. 2a. The tensor network (14) is naturally associated with a 3–partite pure state

$$|\psi\rangle := \sum_{abc} \left\{ \sum_{jkl} A^{(1)}_{ajk} A^{(2)}_{bjl} A^{(3)}_{ckl} \right\} |a\rangle_1 |b\rangle_2 |c\rangle_3, \qquad (15)$$

where we introduced local bases $\{|a\rangle_1\}$, $\{|b\rangle_2\}$, and $\{|c\rangle_3\}$ (the subscripts denote the associated Hilbert spaces of the basis vectors). In fact, $|\psi\rangle$ is an example of a matrix product state. Writing

$$|\psi^{(1)}_{jk}\rangle := \sum_a A^{(1)}_{ajk} |a\rangle_1,$$

$$|\psi^{(2)}_{jl}\rangle := \sum_b A^{(2)}_{bjl} |b\rangle_2,$$

$$|\psi^{(3)}_{kl}\rangle := \sum_c A^{(3)}_{ckl} |c\rangle_3,$$

one obtains the shorthand notation

$$|\psi\rangle = \sum_{jkl} |\psi^{(1)}_{jk}\rangle |\psi^{(2)}_{jl}\rangle |\psi^{(3)}_{kl}\rangle. \qquad (16)$$

It is clear that similar shorthand expressions can be obtained for arbitrary tensor networks.

A *tree tensor network* (TTN) is a tensor network where the underlying graph is a tree, i.e., a graph with no cycles. An example of a TTN is

$$\sum_{ijklm} A^{(1)}_{abi} A^{(2)}_{ijk} A^{(3)}_{jlm} A^{(4)}_{cdl} A^{(5)}_{efm} A^{(6)}_{ghk}, \qquad (17)$$

and the corresponding tree graph is depicted in Fig. 2b. Note that (14) is an example of a tensor network which is *not* a TTN.
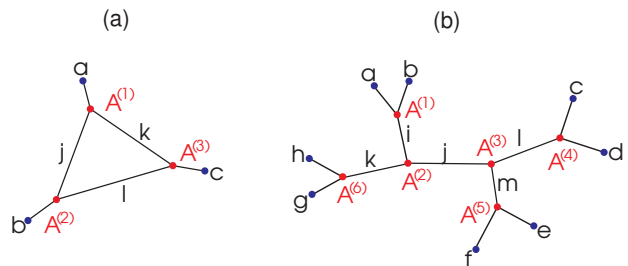

FIG. 2: Tensor network with three tensors $A^{(1)}_{ajk}, A^{(2)}_{bjl}, A^{(3)}_{ckl}$ and three open indices a, b, c corresponding to a cycle graph. (b) Tensor network with six tensors $A^{(1)}_{abi}, A^{(2)}_{ijk}, \ldots, A^{(6)}_{ghk}$ and eight open indices a, b, c, d, e, f, g, h corresponding to a tree graph.

The following definitions regarding TTNs will be important below (see theorem 3). Let T be a tree. An *open edge* is an edge which is incident with a leaf of T. An *inner edge* is an edge which is not an open edge. Consider a TTN with tree T having n open edges, corresponding to an n-party state $|\psi\rangle$. Let $e \in T$ be an inner edge, and let (A^e_T, B^e_T) be the corresponding bipartition of the system. By partitioning all tensors in the network in two classes as induced by the bipartition (A^e_T, B^e_T) and grouping all contractions which occur between tensor in the same class of the bipartition, one can write the network in the form

$$\sum_i |\phi^i_{A^e_T}\rangle |\xi^i_{B^e_T}\rangle. \qquad (18)$$

We say that the TTN is in *normal form w.r.t the bipartition* (A^e_T, B^e_T) if the vectors $\{|\phi^i_{A^e_T}\rangle\}$ and $\{|\xi^i_{B^e_T}\rangle\}$ are (up to a normalization) the Schmidt vectors of the state $|\psi\rangle$ w.r.t. the bipartition (A^e_T, B^e_T). We say that the TTN is in *normal form* if it is in normal form for all bipartitions (A^e_T, B^e_T), where e ranges over all inner edges in T [20].

The interest in TTNs in quantum information theory lies in the property that the representation of systems in terms of TTNs leads to efficient *descriptions* of states

as well as to the possibility of efficiently simulating the *dynamics* of the system. The main results in this context were obtained in Refs. [9] and [10]. The latter result will be particularly interesting for our purposes, and will be reviewed next.

We will be concerned with TTNs corresponding to subcubic trees. It can easily be verified that if a TTN corresponds to a subcubic tree, has n open indices, and has dimension D, then the TTN depends on at most $O(nD^3)$ complex parameters. Therefore, if an n-party state can be described by a TTN where D scales at most polynomially in n, then $|\psi\rangle$ can be described by poly(n) complex parameters by using this TTN. Hence a family of systems allowing an efficient description is obtained. What is more, it has been shown that also the *processing* of such systems can efficiently be simulated classically. The following result, obtained in Ref. [10], will play an important role in the subsequent analysis.

Theorem 2 *If an n-party pure quantum state $|\psi\rangle$ is specified in terms of a TTN of dimension D, where the underlying tree graph is subcubic, then any MQC performed on $|\psi\rangle$ can be classically simulated in $O(n\ poly(D))$ time.*

Therefore, if D grows at most polynomially with n, then the above simulation scheme is efficient. It is noted by the authors in Ref. [10] that there is no restriction in considering subcubic trees only, in the sense that any n-party state which can be represented by a TTN (with arbitrary underlying tree) with poly(n) parameters, can also be represented by a subcubic TTN with poly(n) parameters.

B. Description of quantum systems with TTNs

Theorem 2 shows that, if an efficient TTN description is *known* for a quantum state, then LOCC on this state can be simulated efficiently. However, this result does not give any information about *obtaining* an (efficient) TTN description of a given state. Note that, if a state is specified, there might exist several TTN descriptions, some of which might be efficient and some of which might not be. In fact, we will see below that, if a subcubic tree with n open edges is specified, then *any* n-party state $|\psi\rangle$ can be represented by a TTN with this specific tree structure – although generally tensors of exponential dimension in n are required. Therefore, the following two questions are naturally raised:

- If a state $|\psi\rangle$ and a subcubic tree T are given, what is the behavior of the dimension D of the associated TTN(s)?

- If only a state $|\psi\rangle$ is given, what is the optimal subcubic TTN describing this state, i.e., the one with the smallest dimension D?

Next it is shown that the entanglement in the state $|\psi\rangle$ as measured by the Schmidt–rank, plays a crucial role in answering the above questions. We prove the following result.

Theorem 3 *Let $|\psi\rangle$ be an n-party state and let T be a subcubic tree with n leaves which are identified with the n parties in the system. Then there exists a TTN description of $|\psi\rangle$ with underlying tree T, where the dimension D of this TTN is equal to*

$$\log_2 D = \max_{e \in T} \chi_{A_T^e, B_T^e}(|\psi\rangle). \tag{19}$$

Moreover, this TTN is in normal form.

Proof: the proof is constructive. The idea is to stepwise compute all tensors associated to the vertices of T, by traversing the tree from the leaves to the root, as depicted in Fig. 3. First we need some definitions. A vertex of T which is not a leaf is called an *inner* vertex; note that every inner vertex has degree 3. We fix one inner vertex r and call it the *root* of the tree T. The *depth* of a vertex is the length of the shortest path from this vertex to the root r. We denote by Δ the maximal depth of any inner vertex in T. We refer to Fig. 3 for a schematic representation.
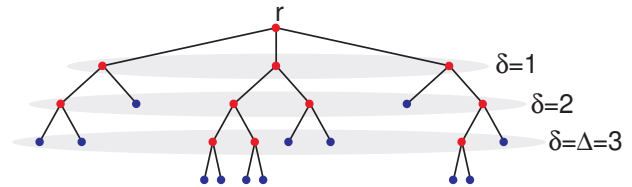

FIG. 3: Subcubic tree with root r, where leaves (corresponding to the $n = 13$ parties of the system) are indicated in blue, and inner vertices are indicated in red. The tree is arranged in such a way that all inner vertices of same depth δ are on the same horizontal line.

The construction is initialized by considering all inner vertices $\{v_1, \ldots, v_N\}$ of depth Δ. Every such vertex has two open edges, corresponding to two qubits in the system. We let $\{a_\alpha, b_\alpha\}$ be the vertices associated in this way to v_α, for every α. We then compute all Schmidt decompositions w.r.t. the bipartitions ($\{a_\alpha, b_\alpha\}$ – rest of the system), i.e.,

$$|\psi\rangle = \sum_i |\phi_i^{(\alpha)}\rangle |\xi_i^{(\alpha)}\rangle, \tag{20}$$

for every α. The vectors $|\phi_i^{(\alpha)}\rangle$ have support on the qubits $\{a_\alpha, b_\alpha\}$, the vectors $|\xi_i^{(\alpha)}\rangle$ have support on the rest of the system. The Schmidt coefficients are absorbed in the latter vectors.

One then proceeds by computing the tensors associated to the inner vertices of depth $\Delta - 1$, and then to the vertices of depth $\Delta - 2, \ldots$, up to depth equal to 1, by in

every step applying the procedure which will be outlined now.

Let $1 \leq \delta \leq \Delta - 1$. For every vertex v, let T_v be the unique subtree of T such that $v \in T_v$ and T_v is one of the two subtrees obtained by deleting the upper edge of v. Let T_v^* be the tree obtained by, first, adding one vertex v^* to T_v and connecting v^* to v with an edge $\{v, v^*\}$ and, second, drawing κ open edges at the vertex v^*, where κ is equal to the number of qubits which do not correspond to leaves of T_v.

Now, suppose that the following is true: *for all inner vertices w of depth $\delta + 1$, a TTN description for $|\psi\rangle$ is known with tree T_w^*, and all these TTNs are in normal form.* We then outline a procedure to obtain, for every inner vertex v of depth δ, a TTN description for $|\psi\rangle$ with tree T_v^*, and all these TTNs are in normal form.

Procedure.— Consider an inner vertex v of depth δ. Let e_1, e_2, e_3 denote the edges incident with v, such that e_1 and e_2 are the lower edges, and e_3 is the upper edge as in Fig. 4. Let (X_1, X_2, X_3) be the unique tripartition of the system defined by

$$
\begin{aligned}
(X_1, X_2 \cup X_3) &:= (A_T^{e_1}, B_T^{e_1}) \\
(X_2, X_1 \cup X_3) &:= (A_T^{e_2}, B_T^{e_2}) \\
(X_3, X_1 \cup X_2) &:= (A_T^{e_3}, B_T^{e_3}).
\end{aligned}
\tag{21}
$$

See also Fig. 4 for a simple pictorial definition.

We then make the distinction between the following cases:

(A) neither e_1 or e_2 are open edges, i.e., both edges connect v to other inner vertices;

(B) one of these two edges, say e_2, is an open edge.

First we consider case (A). Let v_1 (v_2) be the vertex connected to v by the edge e_1 (e_2). By assumption, we have TTN descriptions for $|\psi\rangle$ with trees $T_{v_1}^*$ and $T_{v_2}^*$ which are in normal form. Consider these TTN descriptions, and group all contractions in such a way that one obtains Schmidt decompositions of $|\psi\rangle$ with respect to the above bipartitions:

$$
|\psi\rangle = \sum_{i=1}^{d_\alpha} |\psi_{X_i}^i\rangle |\psi_{\bar{X}_i}^i\rangle,
\tag{22}
$$

for every $\alpha = 1, 2$, where $d_\alpha := \chi_{X_i, \bar{X}_i}(|\psi\rangle)$ denote the Schmidt ranks, and where $\bar{X}_i$ denotes the complement of X_i (e.g., $\bar{X}_1 = X_2 \cup X_3$). The Schmidt coefficients have been absorbed in the vectors $|\psi_{\bar{X}_i}^i\rangle$. Consider also the Schmidt decomposition of $|\psi\rangle$ w.r.t. the split $(X_3, X_1 \cup X_2)$, using an analogous notation

$$
|\psi\rangle = \sum_{i=1}^{d_3} |\psi_{X_3}^i\rangle |\psi_{\bar{X}_3}^i\rangle.
\tag{23}
$$

The latter decomposition is not given by TTN so far, and has to be calculated separately. Using the above 3
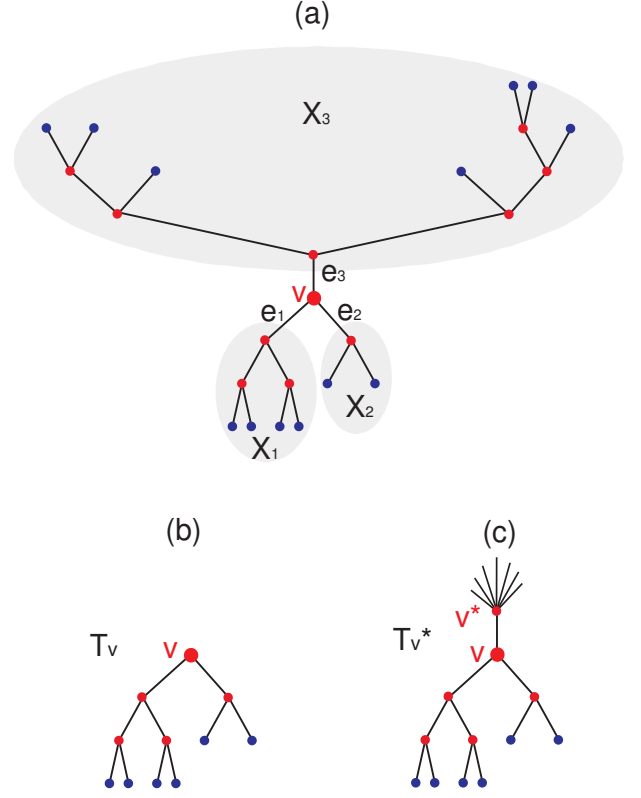

FIG. 4: (a) Same subcubic tree as depicted in Fig. 3, where vertices are re-arranged. We consider an inner vertex v of depth $\delta = 1$ with lower edges e_1, e_2 and upper edge e_3, and the corresponding tripartition of the system into groups X_1, X_2, X_3. (b) Subtree T_v and (c) tree T_v^* (for definition see text).

Schmidt decompositions, we can write

$$
|\psi\rangle = \sum_{i=1}^{d_1} |\psi_{X_1}^i\rangle |\psi_{X_2 \cup X_3}^i\rangle
\tag{24}
$$

$$
= \sum_{i=1}^{d_1} |\psi_{X_1}^i\rangle \langle \psi_{X_1}^i |\psi\rangle
\tag{25}
$$

$$
= \sum_{i=1}^{d_1} \sum_{j=1}^{d_2} |\psi_{X_1}^i\rangle |\psi_{X_2}^j\rangle \langle \psi_{X_1}^i \psi_{X_2}^j |\psi_{X_1 \cup X_3}^{}\rangle
\tag{26}
$$

$$
= \sum_{i=1}^{d_1} \sum_{j=1}^{d_2} \sum_{k=1}^{d_3} |\psi_{X_1}^i\rangle |\psi_{X_2}^j\rangle |\psi_{X_3}^k\rangle B^{ijk},
\tag{27}
$$

where we have used the following arguments and definitions. In order to go from (25) to (26), we have inserted equation (22) for $\alpha = 2$ in (25); to obtain the last equality (27), we have defined the tensor B^{ijk} by

$$
\langle \psi_{X_1}^i |\psi_{X_1 \cup X_3}^j\rangle = \sum_{k=1}^{d_3} B^{ijk} |\psi_{X_3}^k\rangle.
\tag{28}
$$

This yields a TTN description of $|\psi\rangle$ with underlying tree T_v^*. Note that (27) implies that the Schmidt vectors $|\psi_{X_1 \cup X_2}^k\rangle$ are recuperated as

$$|\psi_{X_1 \cup X_2}^k\rangle = \sum_{i,j} |\psi_{X_1}^i\rangle |\psi_{X_2}^j\rangle B^{ijk}, \tag{29}$$

which shows that the TTN is in normal form w.r.t.the bipartition $(X_3, X_1 \cup X_2)$. It then immediately follows that this TTN is in normal form. This concludes case (A).

Next we consider case (B). Let v_1 and v_2 be defined as above. Note that in this case $X_2 = \{v_2\}$. Consider again the TTN description and related Schmidt decomposition (22) for $\alpha = 1$, i.e., for the bipartition $(X_1, \{v_2\} \cup X_3)$. Note that the Schmidt decomposition for the split $(\{v_2\}, X_1 \cup X_3)$ is not available from the TTN since v_2 is not an inner vertex, but we will not need it. As in (A), consider also the Schmidt decomposition (23), i.e., for the bipartition $(X_3, X_1 \cup \{v_2\})$. We then write

$$|\psi\rangle = \sum_{i=1}^{d_1} |\psi_{X_1}^i\rangle \langle \psi_{X_1}^i |\psi\rangle \tag{30}$$

$$= \sum_{i=1}^{d_1} \sum_{k=1}^{d_3} |\psi_{X_1}^i\rangle |\psi_{X_3}^k\rangle \langle \psi_{X_1}^i |\psi_{X_1 \cup \{v_2\}}^k\rangle \tag{31}$$

$$= \sum_{i=1}^{d_1} \sum_{k=1}^{d_3} |\psi_{X_1}^i\rangle |\psi_{\{v_2\}}^{ik}\rangle |\psi_{X_3}^k\rangle \tag{32}$$

where we have used the definition

$$|\psi_{\{v_2\}}^{ik}\rangle := \langle \psi_{X_1}^i |\psi_{X_1 \cup \{v_2\}}^k\rangle. \tag{33}$$

This yields a TTN description of $|\psi\rangle$ with underlying tree T_v^* which is again in normal form. This concludes (B). This also ends the procedure.

Note that the assumption of the procedure is trivially fulfilled for $\delta = \Delta - 1$ after the Schmidt decompositions (20) have been computed. The procedure is then applied to $\delta = \Delta - 1, \Delta - 2, \dots, 1$. After this, all tensors in the desired TTN description are known, except the one associated to the root r of T. To obtain this final tensor, the following steps are taken. Let e_1, e_2, e_3 be the edges incident with r, let v_1, v_2, v_3 be the corresponding vertices of depth 1, and let the tripartition (X_1, X_2, X_3) be defined as before. From the previous steps in the algorithm, we have TTN descriptions for $|\psi\rangle$ with trees $T_{v_1}^*$, $T_{v_2}^*$ and $T_{v_3}^*$ which are in normal form. Consider these TTN descriptions, and group all contractions as above, in such a way that one obtains Schmidt decompositions of $|\psi\rangle$ with respect to the above bipartitions:

$$|\psi\rangle = \sum_{i=1}^{d_\alpha} |\psi_{X_i}^i\rangle |\psi_{\bar{X}_i}^i\rangle, \tag{34}$$

for every $\alpha = 1, 2, 3$. A similar derivation as (24)–(27) shows that $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_{i=1}^{d_1} \sum_{j=1}^{d_2} \sum_{k=1}^{d_3} |\psi_{X_1}^i\rangle |\psi_{X_2}^j\rangle |\psi_{X_3}^k\rangle B^{ijk}, \tag{35}$$

where B^{ijk} is defined similarly as above. This expression describes $|\psi\rangle$ as a TTN with tree T, as desired. Moreover, it follows from (35) that this TTN is in normal form w.r.t to the bipartitions $(X_\alpha, \bar{X}_\alpha)$ for $\alpha = 1, 2, 3$. Since the TTNs (34) were in normal form by construction, this implies that the TTN description (35) is in normal form altogether.

Finally, it immediately follows that the dimension of this TTN is equal to (19) [21]. This concludes the proof of theorem 3. $\qquad \square$

Note that theorem 3 proves that, if a subcubic tree with n open edges is specified, then any n-party state can be represented by a TTN with this specific tree structure. The construction presented in the proof of theorem 3 is similar to a procedure presented in Ref. [22] of how to obtain a matrix product description (which is a particular instance of a tensor network) for an arbitrary state $|\psi\rangle$; there, too, the dimension of the tensor network depends on the maximal Schmidt rank of $|\psi\rangle$ as measured w.r.t a specific class of bipartite splits, similar to (but different from) eq. (19).

C. Connection with χ−width

Theorem 3 now allows us to give a natural interpretation of the χ-width measure (2). Namely, for any state $|\psi\rangle$ one has:

- $\chi_{\mathrm{wd}}(|\psi\rangle)$ is the smallest possible dimension of a TTN associated to $|\psi\rangle$ through the Schmidt decomposition construction described in theorem 3;

- the tree T which yields the minimum in (2) corresponds to the optimal TTN, i.e., the one with smallest dimension [23].

These observations fully answer (Q1), the first of the two central questions put forward in section II D of this article. What is more, we now immediately arrive at a satisfactory answer to question (Q2), since theorems 2 and 3 (see also Ref. [10]) imply the following.

Theorem 4 *Let $|\psi\rangle$ be an n-party state. Denote $\chi := \chi_{wd}(|\psi\rangle)$, let T be a tree yielding the optimum in the definition of χ, and suppose that the TTN description of $|\psi\rangle$ with underlying tree T is known. Then any MQC on $|\psi\rangle$ can be simulated classically in $O(n \, poly(2^\chi))$ time.*

In particular, this result shows that, whenever χ_{wd} is *bounded* on a family of states $\Psi = \{|\psi_1\rangle, |\psi_2\rangle, \dots\}$, then any MQC on Ψ can be simulated efficiently classically – even in linear time in the system size n. This result fully

answers question (Q2) in the negative; i.e., the χ–width measure, which was originally introduced as a means to assess whether a resource Ψ is universal for MQC, can equally well be used to asses whether MQC on Ψ can be efficiently simulated classically. In particular, we have found that MQC can be simulated efficiently for *any family Ψ which is ruled out by the χ–width criterion (i.e., theorem 1 (ii)) as being a non–universal resource.*

Note that theorem 4 even allows one to conclude that efficient simulation is possible when χ_{wd} grows at most logarithmically with the system size – i.e., it may be unbounded. One observes that if χ_{wd} exhibits this scaling behavior on a family of states Ψ, then it is not detected by the χ–width universality criterion. This apparent paradox is resolved by considering the notion of *efficient universality*, which was briefly introduced in section II B. When this requirement is introduced in the definition of universality, the above paradox is resolved as follows. One can prove [15] that χ_{wd} (and E_{wd}) need to grow *faster than logarithmically with the system size* on any efficient universal resource. This clearly resolves the above apparent contradiction.

While the above results indeed settle questions (Q1) and (Q2), in practical situations one is of course faced with the problem whether, when a state $|\psi\rangle$ is specified, the optimal TTN can be computed efficiently. In particular, if theorem 4 is to be applied, the following quantities need to be computed:

(a) The quantity χ itself;

(b) an optimal subcubic tree T in the calculation of χ;

(c) the TTN description of $|\psi\rangle$ corresponding to the tree T.

It is clear that, for any of the above quantities to be efficiently computable, in the least one needs to have an efficient description of the state $|\psi\rangle$ in some form – say, a polynomial size quantum circuit leading to the preparation of the state, or, in the case where $|\psi\rangle$ is a graph state, the underlying graph or stabilizer description. If an efficient description is not available, quantities such as e.g. the Schmidt rank w.r.t. some bipartition can generally not be computed efficiently, and there is no hope of computing e.g. (a) in polynomial time. However, it is important to stress that the possibility of an efficient description is by no means sufficient to compute the quantities (a)–(b)–(c) efficiently.

Regarding (a) and (b), the optimization in the definition of the χ–width measure suggests that an explicit evaluation of χ_{wd} in a specified state, as well as the determination of the optimal subcubic tree, might be a highly nontrivial task. However, we note that general results in this context are known. In particular, we refer to Ref. [13], where optimization problems of the form

$$\min_{T} \max_{e \in T} f(A_T^e) \qquad (36)$$

are considered, where f is a function defined on subsets of $V := \{1, \dots, n\}$, $f : A \subseteq V \to f(A)$. It has been shown

that such optimizations can be performed in polynomial time in n, i.e., the optimum as well as the tree yielding the optimum can be determined efficiently, for a subclass of functions f which meet several technical requirements. In the next section we will see that the graph states form a class of states where these requirements are met, such that the calculation of the χ-width can be performed efficiently. However, the techniques presented in Ref. [13] might be used or generalized to calculate the χ–width efficiently for classes of states larger than the graph states.

Regarding (c), it is clear that the optimal TTN description of $|\psi\rangle$ can only be computed efficiently if this TTN description is itself efficient, i.e., if it depends on at most poly(n) parameters – this is exactly the case when χ scales as $\log(n)$. If χ scales in the latter way, then it follows from the procedure outlined in theorem 3, that the optimal TTN description of $|\psi\rangle$ can be obtained efficiently given one is able to determine the following quantities in poly(n) time:

(i) the Schmidt coefficients and Schmidt vectors for all bipartitions (A_T^e, B_T^e), where T is the optimal tree in the definition of the χ–width.

(ii) Certain overlaps between Schmidt vectors: in particular, the tensor coefficients

$$B^{ijk} = \langle \psi_{X_1}^i | \langle \psi_{X_3}^k | \psi_{X_1 \cup X_3}^j \rangle \qquad (37)$$

in eq. (28) and similar tensors in eq. (35), as well as the vectors

$$|\psi_{\{v_2\}}^{ik}\rangle := \langle \psi_{X_1}^i | \psi_{X_1 \cup \{v_2\}}^k \rangle \qquad (38)$$

in eq. (33).

Thus, a number of conditions need to be fulfilled to obtain an efficient TTN description, if it exists, for a given state. Remarkably, in the next section we show that the quantities (a), (b) and (c) can be computed efficiently for all *graph states*.

As a final remark in this section, note that an efficient TTN description (if it exists) of a state $|\psi\rangle$ w.r.t. a given tree T, can always we obtained efficiently if $|\psi\rangle$ is already specified in terms of an efficient TTN description w.r.t. a different tree T'.

IV. GRAPH STATES

In this section we specialize the results obtained in the previous section to graph states.

A. Simulation of MQC

Theorem 4 and the connection between χ–width of graph states and rank width of graphs, allows us to obtain the following result.

Theorem 5 *Let $|G\rangle$ be a graph state on n qubits. If the rank width of G grows at most logarithmically with n, then any MQC on $|G\rangle$ can efficiently be simulated classically.*

In particular, the above result shows that if $\mathrm{rwd}(G)$ is bounded on a family $\mathcal{G} = \{G_1, G_2, \dots\}$, then any MQC on the set $\Psi(\mathcal{G}) = \{|G_1\rangle, |G_2\rangle, \dots\}$ can efficiently be simulated classically. This provides a complementary result to the one obtained in Ref. [7], where it was proved that any family of graphs with bounded rank width cannot provide a universal resource for MQC. Therefore, all examples given in Ref. [7] of non–universal graph states (see also section II B) can also be given here as examples of resources on which MQC can be simulated efficiently classically.

Note that theorem 5 supersedes all known results (see section II C) on classical simulation of MQC on graph states. To see this, let us consider the result in Ref. [9] stating that MQC can be simulated efficiently on all graph states G with logarithmically bounded tree width $\mathrm{twd}(G)$. Using the inequality [24]

$$\mathrm{rwd}(G) \leq 4 \cdot \mathrm{twd}(G) + 2, \qquad (39)$$

one finds that, whenever $\mathrm{twd}(G)$ scales as $\log(n)$ (where n is the number of qubits in the system), then also $\mathrm{rwd}(G)$ scales at most as $\log(n)$. Thus, theorem 5 implies that MQC can be simulated efficiently on all graph states G with logarithmically bounded tree width, and the result in Ref. [9] is retrieved. This shows that theorem 5 fully recovers and generalizes the known results on simulation of MQC on graph states.

Finally, we emphasize that the rank width can be bounded on families of graphs which do *not at all* have any tree–like structure, i.e., graphs possibly having many cycles; therefore, the presence of cycles in a graph is no indication that efficient simulation of MQC on the associated state might be hard. One reason of this property is that a possible tree structure of a graph does not remain invariant under local operations; e.g., the fully connected graph and the star graph (one central vertex connected to all other vertices) are locally equivalent; the latter is a tree graph, the former is not – in fact, the tree width of the star graph is equal to 1, whereas the tree width of the fully connected graph on n vertices is $n - 1$ [17]. Contrary to e.g. the tree–width measure, the rank width is a local invariant, thus taking into account such cases. Due to these properties, our results prove a significant extension to the use of the tree width; indeed, the above example unambiguously illustrates the superiority of the rank width as a criterion to address the classical simulation of MQC on graph states.

B. TTNs for graph states

In this section we are concerned with the issue whether, if a graph state is given, the optimal TTN can be computed efficiently, i.e., we consider the quantities (a)–(b)–(c) as denoted in section III C.

Let G be a graph on n vertices. It was shown in Ref. [13] that, for a fixed integer k, the problem "*Is the rank width of G smaller than k?*" is in the complexity class P. Moreover, in Ref. [25] several polynomial–time so–called *approximation algorithms* for the rank width are constructed. When G is given as an input, the (most efficient) algorithm either confirms that $\mathrm{rwd}(G)$ is larger than k, or it outputs a subcubic tree T^* such that

$$\max_{e \in T^*} \mathrm{rank}_{\mathbb{F}_2} \Gamma(A_{T^*}^e, B_{T^*}^e) = 3k - 1, \qquad (40)$$

which implies that $\mathrm{rwd}(G) \leq 3k - 1$. The running time of the algorithm is $O(n^3)$.

These results immediately yield an efficient procedure to determine the qualitative behavior of the χ–width of graph states, and to determine the optimal subcubic tree in the calculation of the χ–width. More precisely, a possible (binary search) approach is the following: first run the above algorithm for $k = n/2$; if the algorithm confirms that $\mathrm{rwd}(G) \geq n/2$, then run the algorithm for $k = 3n/4$; if not, then run the algorithm for $k = n/4$, etc. This algorithm is guaranteed to terminate in $\mathrm{poly}(n)$ time. After the last run of the algorithm, the rank width, and the corresponding optimal subcubic tree, is obtained up to a factor 3.

Thus, both quantities (a) and (b) as defined in the discussion following theorem 4, can be computed efficiently for any graph state.

As for an efficient calculation of quantity (c), we note that, for any bipartition of the system, both the Schmidt coefficients and the Schmidt vectors can be computed efficiently for graph states using the stabilizer formalism; moreover, the Schmidt vectors can always be chosen to be stabilizer states themselves. This can be proved as follows (we only give a sketch of the argument, as it involves standard stabilizer techniques). Let $|G\rangle$ be a graph state on qubits $V := \{1, \dots, n\}$, and let (A, B) be a bipartition of V. Let $\mathcal{S}$ denote the stabilizer of $|G\rangle$, defined by

$$\mathcal{S} := \left\{ \prod_{a \in V} (K_a)^{x_a} \mid x_a \in \{0, 1\}, \forall\, a \in V \right\}, \qquad (41)$$

where the operators K_a have been defined in eq. (5). Thus, $\mathcal{S}$ is the commutative group generated by the operators K_a. One then has [14]

$$|G\rangle\langle G| \;=\; \frac{1}{2^n} \prod_{a \in V} (I + K_a) = l \frac{1}{2^n} \sum_{g \in \mathcal{S}} g. \qquad (42)$$

Let $\mathcal{S}_A$ be the subgroup of operators in $\mathcal{S}$ acting trivially on the qubits in $V \setminus A = B$. Then

$$\rho_A := \mathrm{Tr}_B |G\rangle\langle G| = \frac{1}{2^{|A|}} \sum_{g \in \mathcal{S}_A} g. \qquad (43)$$

This operator satisfies

$$
\begin{aligned}
(\rho_A)^2 &= \frac{1}{2^{2|A|}} \sum_{g \in \mathcal{S}_A} g \sum_{h \in \mathcal{S}_A} h \\
&= \frac{1}{2^{2|A|}} \sum_{g \in \mathcal{S}_A} \sum_{h \in \mathcal{S}_A} h = \frac{|\mathcal{S}_A|}{2^{|A|}} \rho_A.
\end{aligned}
\tag{44}
$$

The second equality holds since $\mathcal{S}_A$ is a group. Denoting $r := 2^{|A|}|\mathcal{S}_A|^{-1}$, it follows that $(r\rho_A)^2 = r\rho_A$, showing that $r\rho_A$ a projection operator. Thus, all nonzero eigenvalues of this operator are equal to 1. This shows that all nonzero eigenvalues of ρ_A (which are the squares of the Schmidt coefficients of $|G\rangle$ w.r.t. the bipartition (A, B)) are equal to $r^{-1} = 2^{-|A|}|\mathcal{S}_A|$. Moreover, as ρ_A has unit trace, it follows that

$$
r^{-1} \cdot \mathrm{rank}(\rho_A) = 1,
\tag{45}
$$

such that the number of nonzero eigenvalues of ρ_A is equal to $r = 2^{|A|}|\mathcal{S}_A|^{-1}$ [26].

The eigenvectors of ρ_A can be computed as follows. Let $\{K_1^A, \ldots, K_s^A\} \subseteq \mathcal{S}_A$ denote a minimal generating set of $\mathcal{S}_A$, where $s := \log_2 |\mathcal{S}_A|$. Let $\{K_{s+1}^A, \ldots, K_{|A|}^A\}$ be additional Pauli operators, chosen in such a way that

$$
\{K_1^A, \ldots, K_s^A, K_{s+1}^A, \ldots, K_{|A|}^A\}
\tag{46}
$$

is a set of commuting and independent operators; such a set always exists (though it is non–unique) and can be computed efficiently, by using the stabilizer formalism (see e.g. [14]). Note that (46) is the generating set of a stabilizer state $|\psi\rangle$ on the qubits in A, namely the state

$$
|\psi\rangle\langle\psi| := \frac{1}{2^{|A|}} \prod_{i=1}^{|A|} (I + K_i^A).
\tag{47}
$$

Moreover, this state is an eigenstate of ρ_A. To see this, note that $K_j^A |\psi\rangle\langle\psi| = |\psi\rangle\langle\psi|$, and thus $K_j^A |\psi\rangle = |\psi\rangle$, for every $j = 1, \ldots, s$. As $\{K_j^A\}_{j=1}^s$ is a generating set of the group $\mathcal{S}_A$, this last identity implies that $g|\psi\rangle = |\psi\rangle$ for every $g \in \mathcal{S}_A$, and therefore

$$
\rho_A |\psi\rangle = \frac{1}{2^{|A|}} \sum_{g \in \mathcal{S}_A} g|\psi\rangle = \frac{|\mathcal{S}_A|}{2^{|A|}} |\psi\rangle.
\tag{48}
$$

In order to obtain a basis of eigenvectors, one considers the $2^{|A|-s} = 2^{|A|}|\mathcal{S}_A|^{-1}$ stabilizer states $|\psi_{\alpha_{s+1}, \ldots, \alpha_{|A|}}\rangle$ with stabilizers generated by

$$
\{K_1^A, \ldots, K_s^A, \alpha_{s+1} K_{s+1}^A, \ldots, \alpha_{|A|} K_{|A|}^A\},
\tag{49}
$$

where $\alpha_k = \pm 1$, for every $k = s+1, \ldots, |A|$. One can, with arguments analogous to above, show that all these states are eigenvectors of ρ_A. Moreover, all these states are mutually orthogonal; one has

$$
\begin{aligned}
&\langle \psi_{\alpha_{s+1}, \ldots, \alpha_{|A|}} | \psi_{\beta_{s+1}, \ldots, \beta_{|A|}} \rangle \\
&= (-1)^{\alpha_k} \langle \psi_{\alpha_{s+1}, \ldots, \alpha_{|A|}} | K_k^A | \psi_{\beta_{s+1}, \ldots, \beta_{|A|}} \rangle \\
&= (-1)^{\alpha_k + \beta_k} \langle \psi_{\alpha_{s+1}, \ldots, \alpha_{|A|}} | \psi_{\beta_{s+1}, \ldots, \beta_{|A|}} \rangle,,
\end{aligned}
\tag{50}
$$

for every $k = s+1, \ldots, |A|$, where we have respectively used that

$$
\langle \psi_{\alpha_{s+1}, \ldots, \alpha_{|A|}} | = (-1)^{\alpha_k} \langle \psi_{\alpha_{s+1}, \ldots, \alpha_{|A|}} | K_k^A
\tag{51}
$$

and

$$
K_k^A |\psi_{\beta_{s+1}, \ldots, \beta_{|A|}}\rangle = (-1)^{\beta_k} |\psi_{\beta_{s+1}, \ldots, \beta_{|A|}}\rangle.
\tag{52}
$$

It immediately follows from the identity (50) that the states $|\psi_{\alpha_{s+1}, \ldots, \alpha_{|A|}}\rangle$ are mutually orthogonal. Since there are exactly $2^{|A|}|\mathcal{S}_A|^{-1}$ such vectors, as many as there are nonzero Schmidt coefficients, we have computed all Schmidt vectors of $|G\rangle$ w.r.t. the bipartition (A, B). Remark that at this point we only have a stabilizer description of the Schmidt vectors; if necessary, the expansion of these vectors in the computational basis can be computed using the results in Ref. [27].

This shows that both Schmidt coefficients and Schmidt vectors of $|G\rangle$ w.r.t. any bipartition (A, B) can be computed efficiently, and that the Schmidt vectors can always be chosen to be stabilizer states. Moreover, note that overlaps between stabilizer states can be computed efficiently using stabilizer techniques, and we refer to [28], where this problem was considered.

Thus, all necessary ingredients (cf. (i)–(ii) in section III C) needed for the efficient construction of the optimal TTN of a graph state $|G\rangle$, can be computed efficiently when $\mathrm{rwd}(G)$ scales as $\log(n)$.

We then arrive at the following result.

Theorem 6 *Let $|G\rangle$ be a graph state on n qubits and denote $\chi := \chi_{wd}(|G\rangle)$. Then an optimal subcubic tree T in the definition of χ can be computed in $\mathrm{poly}(n)$ time. Moreover, if χ scales as $\log(n)$ then the TTN description of $|G\rangle$ corresponding to T can be computed in $\mathrm{poly}(n)$ time.*

Note that, in particular, the conditions of the above theorem are fulfilled for all classes of graphs having bounded rank width, and thus efficient TTNs can be computed in $\mathrm{poly}(n)$ time for all such classes.

C. Example for the cycle graph on $n = 6$ qubits

In this section we give an explicit example of the computation of the rank width, the optimal subcubic tree, and the corresponding TTN description of a particular graph state, namely the 6-qubit state $|C_6\rangle$ associated to the *cycle graph* (or *ring graph*) C_6 on 6 vertices. The adjacency matrix Γ of C_6 is the 6×6 matrix

$$
\begin{bmatrix}
\cdot & 1 & \cdot & \cdot & \cdot & 1 \\
1 & \cdot & 1 & \cdot & \cdot & \cdot \\
\cdot & 1 & \cdot & 1 & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & 1 & \cdot \\
\cdot & \cdot & \cdot & 1 & \cdot & 1 \\
1 & \cdot & \cdot & \cdot & 1 & \cdot
\end{bmatrix},
\tag{53}
$$

where ' $\cdot$ ' denotes an entry equal to zero.

1. Rank width and optimal tree

First we compute the rank width of the graph C_6. In fact, we will prove that $\mathrm{rwd}(C_6) = 2$. To show this, consider the subcubic tree T depicted in Fig. 1. The leaves of T are associated to the vertices of C_6 in the following natural way: first, fix an arbitrary vertex of C_6 and denote this to be vertex 1; then, starting from vertex 1, traverse the vertices of C_6 in a counterclockwise way, and denote the vertices by 2, 3, 4, 5 and 6, respectively; these vertices are now associated to the leaves of T by identifying vertex 1 with the leftmost leaf of T, vertex 2 with the second leaf from the left, etc.

It is now straightforward to show that

$$\max_{e \in T} \ \mathrm{rank}_{\mathbb{F}_2} \ \Gamma(A_T^e, B_T^e) = 2. \tag{54}$$

This can be showed by simply computing the ranks of all matrices $\Gamma(A_T^e, B_T^e)$ and picking the largest of these ranks. Furthermore, one has

$$\alpha_{T'}(C_6) := \max_{e \in T'} \ \mathrm{rank}_{\mathbb{F}_2} \ \Gamma(A_{T'}^e, B_{T'}^e) \geq 2 \tag{55}$$

for every subcubic tree T'. This can be seen as follows: first, note that $\alpha_{T'}(C_6) \geq 1$ for every T', since

$$\mathrm{rank}_{\mathbb{F}_2} \Gamma(A, B) \geq 1 \tag{56}$$

for every bipartition (A, B). Second, suppose that T' is a subcubic tree such that $\alpha_{T'}(C_6) = 1$; we will show that this leads to a contradiction. Note that $\mathrm{rank}_{\mathbb{F}_2} \Gamma(A, B)$ is equal to 1 if and only if (A, B) is a bipartition of the form (one vertex – rest). Moreover, if $\alpha_{T'}(C_6) = 1$, then one must have

$$\mathrm{rank}_{\mathbb{F}_2} \ \Gamma(A_{T'}^e, B_{T'}^e) = 1 \tag{57}$$

for every $e \in T'$. Thus, every bipartition $(A_{T'}^e, B_{T'}^e)$ must be of the form (one vertex – rest); this leads to a contradiction. This shows that the inequality (55) is correct. We can therefore conclude that

$$\mathrm{rwd}(C_6) := \min_{T'} \alpha_{T'}(C_6) = 2 \tag{58}$$

and that the tree T as depicted in Fig. 1 yields the optimum.

At this point we note that here ad hoc methods have been used to obtain the above result; however, we remind the reader that general algorithms exist to calculate the rank width and the optimal tree, as cited in section IV A.

2. TTN description

The computation of the TTN description of $|C_6\rangle$ with underlying tree T is performed in Appendix A. The result is the following:

$$\langle x_1 \dots x_6 | C_6 \rangle = \frac{1}{2^3} \sum_{abcdef} \psi_{abx_1x_2}^{(1)} \psi_{abcdx_3}^{(2)} \psi_{cdefx_4}^{(3)} \psi_{efx_5x_6}^{(4)}, \tag{59}$$

where $x_1, \dots, x_6 \in \{0, 1\}$ and where all indices in the sum run from 0 to 1. The pair ab should be regarded as one index taking 4 different values, as well as the pairs cd and ef. Moreover, one has the following definitions:

$$\begin{aligned}
\psi_{abx_1x_2}^{(1)} &:= \delta_{a,x_1} \delta_{b,x_2} \\
\psi_{abcdx_3}^{(2)} &:= (-1)^{ac+ab+bx_3+dx_3} \\
\psi_{cdefx_4}^{(3)} &:= \delta_{f,c} \delta_{d,x_4} (-1)^{de+ec} \\
\psi_{efx_5x_6}^{(4)} &:= \delta_{e,x_5} \delta_{f,x_6}.
\end{aligned} \tag{60}$$

V. COMPLEX SYSTEMS VERSUS TREE STRUCTURES IN QIT AND GRAPH THEORY

We have seen that the χ–width of a graph state is equal to the rank width of the underlying graph. There is in fact a striking parallel between the *motivations* for the definitions of rank width of graphs and of χ–width of general quantum states, on which we comment here.

As explained above, the χ–width gives information about the optimal TTN which describes a given quantum state. The interest in such TTNs naturally arises due to the fact that the dynamics of quantum systems which allow TTN descriptions with sufficiently small dimension D, can be simulated efficiently on a classical computer. These and similar techniques (cf. e.g. the matrix product states formalism) are invoked because the efficient classical simulation of *general* quantum systems can be a very difficult problem. Thus, in spite of the general hardness of this simulation problem, it becomes tractable when restricted to the class of those systems with efficient TTN descriptions.

In graph theory an analogous situation occurs. While many interesting problems are hard to compute on general graphs, they become tractable for those classes of graphs which can be associated, through certain constructions, with tree structures. The simplest examples are of course the tree graphs themselves, which are in some sense the simplest instances of graphs; and indeed, many difficult problems become efficiently solvable, or even trivial, on trees. However, this is far from the whole story. In graph theory one has considered a variety of so–called *width parameters*, which all measure, in different ways, how similar a graph is to a tree graph. Examples are rank width, tree width, clique–width, path–width, and branch–width. It has been shown that for families of graphs where a given width parameter is *bounded*, large classes of (NP–)hard problems have efficient solutions. For example, the problem of deciding whether a graph is 3–colorable, which is a NP–hard, is efficiently solvable when restricted to classes of graphs of bounded rank width. The graph theoretical results in this context are often very general and far–reaching; e.g., it has been show that all graph problems which can be formulated in terms of a certain mathematical logic calculus, have efficient solutions when restricted to graphs of bounded rank

width. We refer to Ref. [29] for an accessible treatment of these and related issues.

Thus, in certain aspects of both quantum information theory and graph theory there is a natural interest in using tree structures for the approximation of complex systems. Moreover, there seems to be a strong parallel in the explicit constructions which are used in both fields. A striking example is obtained here, as the rank width of graphs exactly coincides with the χ–width measure on graph states. As a second example, it was found in Ref. [9] that the efficient contraction of large tensor network is directly related to the tree width of the underlying graphs. The present authors believe that the aforementioned parallel can significantly be exploited further.

VI. CONCLUSION

In this paper we have considered the possibility to classically simulate measurement based quantum computation. We have shown that all states with a bounded or logarithmically growing Schmidt–rank width can in fact be described efficiently, and moreover any one–way quantum computation performed on such states can also be simulated efficiently. We have given an interpretation of the Schmidt–rank width, a measure that has its origin in graph theory, in terms of the optimal tree tensor network describing a state. We have also provided a constructive procedure how to obtain the optimal TTN, and discussed the requirements that this can be done efficiently. For graph states, we have explicitly constructed the corresponding TTN, and provided an efficient algorithm to do this for any graph state where the underlying graph has bounded or logarithmically growing rank width. These results on efficient simulation complement recent findings on universality of states, in the sense that all states that are found to be non–universal resources for MQC using the Schmidt–rank width criteria (i.e. which have bounded Schmidt–rank width) can also be simulated efficiently on a classical computer. The connection to complexity issues in graph theory, also highlighted in this paper, seems to provide future possibilities for a fruitful interchange of concepts and methods between the fields of quantum information and graph theory.

Acknowledgments

APPENDIX A: OPTIMAL TTN DESCRIPTION OF $|C_6\rangle$

We now compute the TTN description of $|C_6\rangle$ w.r.t. the tree T depicted in Fig. 1, using the procedure out-

lined in theorem 3. Consider the following Schmidt decompositions of $|C_6\rangle$:

$$|C_6\rangle = \frac{1}{\chi^{(1)}} \sum_i |\phi_i^{(1)}\rangle_{12} |\xi_i^{(1)}\rangle_{3456} \qquad (A1)$$

$$= \frac{1}{\chi^{(2)}} \sum_j |\phi_j^{(2)}\rangle_{123} |\xi_j^{(2)}\rangle_{456} \qquad (A2)$$

$$= \frac{1}{\chi^{(3)}} \sum_k |\phi_k^{(3)}\rangle_{1234} |\xi_k^{(3)}\rangle_{56}. \qquad (A3)$$

These decompositions are taken w.r.t. the bipartitions $(\{1,2\},\{3,4,5,6\})$, $(\{1,2,3\},\{4,5,6\})$ and $(\{1,2,3,4\},\{5,6\})$, respectively; these correspond to the bipartitions (A_T^e, B_T^e), where e runs over all inner edges of T. All Schmidt vectors in (A1) are normalized, and the $\chi^{(\alpha)}$ are the square roots of the Schmidt ranks of the corresponding bipartitions [30].

We now show how the TTN description of $|C_6\rangle$ w.r.t the tree T is obtained, by applying the procedure presented in theorem 3. First, note that the depth Δ of T is equal to 3. We start by considering the single inner vertex of depth 3; this is the vertex which has leaves 1 and 2 as lower vertices. We then compute the Schmidt decomposition (A1), corresponding to the bipartition which is obtained by deleting the upper edge of this vertex. In a second step, we consider the single vertex in T having depth 2, and compute the corresponding Schmidt decomposition (A2). Moreover, we write

$$|C_6\rangle = \frac{1}{\chi^{(1)}} \sum_i |\phi_i^{(1)}\rangle \langle\phi_i^{(1)}|C_6\rangle$$
$$= \frac{1}{\chi^{(1)}\chi^{(2)}} \sum_{i,j} |\phi_i^{(1)}\rangle \langle\phi_i^{(1)}|\phi_j^{(2)}\rangle |\xi_j^{(2)}\rangle, \quad (A4)$$

(where we have omitted the subscripts of the Schmidt vectors). Finally, we consider the Schmidt decomposition (A3) (corresponding to the uper edge of the unique depth 1 vertex), and write it as

$$|C_6\rangle = \frac{1}{\chi^{(3)}} \sum_k |\xi_k^{(3)}\rangle \langle\xi_k^{(3)}|C_6\rangle \qquad (A5)$$

Combining eqs. (A5) and (A4) then shows that $|C_6\rangle$ can be written as follows [31]:

$$|C_6\rangle = \frac{1}{\chi^{(1)}\chi^{(2)}\chi^{(3)}} \sum_{ijk} |\phi_i^{(1)}\rangle \langle\phi_i^{(1)}|\phi_j^{(2)}\rangle |\xi_k^{(3)}\rangle \langle\xi_k^{(3)}|\xi_j^{(2)}\rangle. \qquad (A6)$$

Note that the states $\langle\phi_i^{(1)}|\phi_j^{(2)}\rangle$ are defined on qubit 3, for every i and j, and that the states $\langle\xi_k^{(3)}|\xi_j^{(2)}\rangle$ are defined on qubit 4, for every j and k.

Next we explicitly compute the Schmidt coefficients and Schmidt vectors in the above expansions, using the stabilizer formalism.

As for the Schmidt coefficients, note that

$$
\begin{aligned}
2 &= \text{rank}_{\mathbb{F}_2} \, \Gamma(\{1,2\}, \{3,4,5,6\}) \\
&= \text{rank}_{\mathbb{F}_2} \, \Gamma(\{1,2,3\}, \{4,5,6\}) \\
&= \text{rank}_{\mathbb{F}_2} \, \Gamma(\{1,2,3,4\}, \{5,6\}),
\end{aligned}
\tag{A7}
$$

and therefore (using (7)) all the Schmidt ranks of the above bipartitions are equal to $2^2 = 4$. Thus, the indices i, j, k in eq. (A6) all run from 1 to 4, and we also have

$$
\chi^{(1)} = \chi^{(2)} = \chi^{(3)} = \sqrt{4} = 2.
\tag{A8}
$$

It will be convenient to write the indices i, j, k as pairs of bits, and we will use the notations $i \equiv ab$, $j \equiv cd$, $k \equiv ef$, where $a, b, c, d \in \{0, 1\}$.

We now consider the Schmidt vectors w.r.t. the above bipartitions. We start with the bipartition $(\{1,2\}, \{3,4,5,6\})$. Here one finds that

$$
\text{Tr}_{\{3,4,5,6\}}(|C_6\rangle\langle C_6|) = \frac{1}{4}I.
\tag{A9}
$$

Thus, a Schmidt basis for the subset $\{1, 2\}$ could simply be chosen to be the computational basis; in other words, we take

$$
|\phi_{ab}^{(1)}\rangle = |a\rangle \otimes |b\rangle \equiv |ab\rangle,
\tag{A10}
$$

defined on the qubits $\{1, 2\}$, for every $a, b \in \{0, 1\}$.

The same argument can be repeated for the vectors $\{|\xi_{ef}^{(3)}\rangle\}$, where we can take $|\xi_{ef}^{(3)}\rangle = |ef\rangle$, defined on the qubits $\{5, 6\}$, for every $e, f \in \{0, 1\}$.

As for the bipartition $(\{1,2,3\}, \{4,5,6\})$, one can easily show that

$$
\text{Tr}_{\{4,5,6\}}(|C_6\rangle\langle C_6|) = \frac{1}{8}(I + \sigma_z \otimes \sigma_x \otimes \sigma_z)
\tag{A11}
$$

and that, hence, the states

$$
|\phi_{cd}^{(2)}\rangle = \sigma_z^c \otimes I \otimes \sigma_z^d |L_3\rangle
\tag{A12}
$$

form a valid Schmidt basis, where $c, d \in \{0, 1\}$ and where $|L_3\rangle$ is the linear cluster state on 3 qubits, defined on the qubits $\{1, 2, 3\}$.

To compute the vectors $\{|\xi_{cd}^{(2)}\rangle\}$, note that one has

$$
|\xi_{cd}^{(2)}\rangle = 2\langle\phi_{cd}^{(2)}|C_6\rangle.
\tag{A13}
$$

Therefore, we have to compute expressions of the form

$$
[(\langle L_3|\sigma_z^c \otimes I \otimes \sigma_z^d) \otimes I]|C_6\rangle,
\tag{A14}
$$

for every $c, d = 0, 1$. To do so, we use that every n-qubit graph state $|G\rangle$ with adjacency Γ can be written as [14]

$$
|G\rangle = \frac{1}{2^{n/2}} \sum_{u \in \{0,1\}^n} (-1)^{q_G(u)}|u\rangle,
\tag{A15}
$$

where $\{|u\rangle \mid u \in \{0,1\}^n\}$ is the n-qubit computational basis and where

$$
q_G(u) := \frac{1}{2}u^T\Gamma u.
\tag{A16}
$$

One then finds that (A14) is equal to (omitting multiplicative constants)

$$
\sum_{u,v,w} \left(\sum_{x,y,z} (-1)^{q_{C_6}(x,y,z,u,v,w)+q_{L_3}(x,y,z)+xc+zd} \right) |uvw\rangle.
\tag{A17}
$$

Straightforward algebra then shows that the power of -1 in the above expression is equal to

$$
x(w+c) + z(d+u) + q_{L_3}(u,v,w).
\tag{A18}
$$

Moreover, one has

$$
\sum_{x,y,z} (-1)^{x(w+c)+z(d+u)} = \begin{cases} 2^3 & w = c \text{ and } d = u \\ 0 & \text{else} \end{cases}
\tag{A19}
$$

We then find that (A17) is equal to

$$
|d\rangle \left(\sum_{v=0}^{1} (-1)^{q_{L_3}(d,v,c)}|v\rangle \right) |c\rangle,
\tag{A20}
$$

for every $c, d = 0, 1$. Thus, these 4 states form the set $\{|\xi_{cd}^{(2)}\rangle\}_{j=1}^4$, defined on qubits $\{4, 5, 6\}$.

The only remaining task is the computation of the states $\langle\phi_{ab}^{(1)}|\phi_{cd}^{(2)}\rangle$ and $\langle\xi_{ef}^{(3)}|\xi_{cd}^{(2)}\rangle$. To compute the former of these states, it follows from the above that one has to compute, for every $a, b, c, d \in \{0, 1\}$, overlaps of the form

$$
\begin{aligned}
\langle\phi_{ab}^{(1)}|\phi_{cd}^{(2)}\rangle &= (\langle a| \otimes \langle b| \otimes I) \left(\sigma_z^c \otimes I \otimes \sigma_z^d|L_3\rangle\right) \\
&= (-1)^{ac}\langle a| \otimes \langle b| \otimes \sigma_z^d|L_3\rangle.
\end{aligned}
\tag{A21}
$$

Using the expansion (A15), it is then easy to show that (A21) is equal to

$$
(-1)^{ac} \sum_{v=0}^{1} (-1)^{q_{L_3}(a,b,v)+dv}|v\rangle,
\tag{A22}
$$

for every $a, b, c, d \in \{0, 1\}$, and these states are defined on qubit 3. A similar calculation can be performed to obtain

$$
\langle\xi_{ef}^{(3)}|\xi_{cd}^{(2)}\rangle = \delta_{f,c}(-1)^{q_{L_3}(d,e,c)}|d\rangle,
\tag{A23}
$$

for every $c, d, e, f \in \{0, 1\}$, and these states are defined on qubit 4.

We can now write down the TTN description of the state $|C_6\rangle$ w.r.t. the tree T depicted in Fig. 1:

$$
|C_6\rangle = \frac{1}{2^3} \sum_{abcdef} \left\{ |ab\rangle_{12} \left(\sum_v (-1)^{ac+q_{L_3}(a,b,v)+dv}|v\rangle_3 \right) \times \right.
$$
$$
\left. \left(\delta_{f,c}(-1)^{q_{L_3}(d,e,c)}|d\rangle_4 \right) |ef\rangle_{56} \right\},
\tag{A24}
$$

where we have again indicated subscripts to specify on which qubits the states are defined.

Recalling the definition of q_{L_3}, namely

$$q_{L_3}(t_1, t_2, t_3) := t_1 t_2 + t_2 t_3, \qquad (A25)$$

for every $t_1, t_2, t_3 \in \{0, 1\}$, we recover expression (59). Note that one can easily check that (59) is correct, by summing out all indices $a, \ldots, f$:

$$
\begin{aligned}
\langle x_1 \ldots x_6 | C_6 \rangle &= \frac{1}{2^3} \sum_{abcdef} \left\{ \delta_{a,x_1} \delta_{b,x_2} (-1)^{ac+ab+bx_3+dx_3} \right. \\
&\qquad \left. \delta_{f,c} \delta_{d,x_4} (-1)^{de+ec} \delta_{e,x_5} \delta_{f,x_6} \right\} \\
&= \frac{1}{2^3} (-1)^{x_6 x_1 + x_1 x_2 + \cdots + x_5 x_6} \\
&= \frac{1}{2^3} (-1)^{q_{C_6}(x_1, \ldots, x_6)}, \qquad (A26)
\end{aligned}
$$

where in the last equality we indeed obtain the correct computational basis expansion of $|C_6\rangle$.

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