The Kirchhoff’s Matrix-Tree Theorem revisited:
counting spanning trees with the quantum relative entropy

Vittorio Giovannetti∗ Simone Severini†

January 12, 2013

Abstract

By revisiting the Kirchhoff’s Matrix-Tree Theorem, we give an exact formula for the number
of spanning trees of a graph in terms of the quantum relative entropy between the maximally
mixed state and another state specifically obtained from the graph. We use properties of the
quantum relative entropy to prove tight bounds for the number of spanning trees in terms of
basic parameters like degrees and number of vertices.

1 Introduction

The Kirchhoff’s Matrix-Tree Theorem is a classic result stating that the total number of spanning
trees of a graph is exactly the determinant of any principal minor of the Laplacian matrix of the
graph. The theorem can be traced back to 1847 [8]. The number of spanning trees of a graph,
which is also called the complexity of the graph, is a valuable invariant (i.e., a quantity that does
not depend on the ordering of the vertices). There are various and diverse applications of the
number of spanning trees: an important role in the theory of electrical networks, for example, in
computing driving point resistances [4]; a wide use in the study of graph-theoretic problems, like
routing, counting Eulerian tours, etc. [15]; the computation of network reliability [5]; and chemical
modeling [6]. In quantum field theory, it is well-known that the value of a Feynman integral can
be written in terms of spanning trees [11]. The Tutte polynomial, object with a variety of uses in
statistical mechanics, can be characterized via spanning trees [19].

By reinterpreting the Kirchhoff’s Matrix-Tree Theorem in the context of quantum informa-
tion theory, we give an exact formula to count spanning trees based on the notion of quantum
relative entropy. This function is the quantum mechanical analog of the relative entropy. It is
central in the quantification and manipulation of quantum entanglement, quantum data compres-
sion, communication costs, etc. [14] [17]. It is traditionally interpreted as a parameter to quantify
the distinguishability between two quantum states. We show that the number of spanning trees
is proportional to the distinguishability/distance between a certain density matrix associated to
the graph in context and the maximally mixed state, i.e., the state with maximum von Neumann
entropy, or, equivalently, maximum amount of classical uncertainty.

∗NEST, Scuola Normale Superiore and Istituto Nanoscienze-CNR, Piazza dei Cavalieri 7, I-56126 Pisa, Italy;
v.giovannetti@sns.it.
†Department of Physics and Astronomy, University College London, Gower St., WC1E 6BT London, United
Kingdom; simoseve@gmail.com.
By using standard machinery from quantum information theory, we study bounds on the number of spanning trees obtained from basic quantities like the number of vertices, edges, and degrees. We exhibit a tight bound; equality is obtained for stars and certain multigraphs obtained by adding multiple edges to stars. Even if the bound is tight, it performs poorly in general. A potential improvement could be obtained by allowing different coefficients in the quantum state associated to the graph.

The remainder of the paper is structured as follows: Section 2 contains the mathematical setup and the main result; Section 3 gives lower and upper bounds; Section 4 proposes a brief discussion and draws some conclusions. We give particular attention to a plausible operational meaning for the number of spanning trees, when considering our class of quantum states.

2 Main result

A graph is an ordered pair $G = (V, E)$, where $V$ is a set of elements called vertices and $E \subseteq V \times V - \{\{i, i\}\}$, for every $i \in V$, is set of unordered pairs of vertices called edges. Despite we mainly consider simple graphs, our treatment can be easily generalized to multigraphs, i.e., graph with multiple edges. A graph $H = (W, F)$ is a subgraph of $G$ if $W \subseteq V$ and $F \subseteq E$. The subgraph $H$ is spanning if $W = V$. A cycle is a graph with set of vertices $\{0, 1, ..., k - 1\}$ and set of edges $\{\{i, (i + 1) \mod k\} : i = 0, 1, ..., k - 1\}$. A tree is a graph without cycles as subgraphs. Denoting by $|S|$ the number of elements in a set $S$, the degree of a vertex $i$ is the nonnegative integer $d(i) = |\{j : \{i, j\} \in E\}|$. The (combinatorial) Laplacian of $G$ is the $n \times n$ matrix $L = \Delta - A$, where $\Delta_{ij} = d(i) \delta_{ij}$ (the Kronecker delta); $A_{ij} = 1$ if $\{i, j\} \in E$ and $A_{ij} = 0$, otherwise. The determinant of the $n - 1 \times n - 1$ matrix $L'_{ij}$ obtained by deleting the $\ell$-th row and column of $L$ is independent of $\ell$. The Kirchhoff’s Matrix-Tree Theorem (see, e.g., [16], Theorem VI.29) states that for the number of spanning trees of a graph $G$, $\tau(G)$, we have

$$\tau(G) = \det \left(L'_{ij}\right). \tag{1}$$

Let $\mathcal{H}$ be an Hilbert space of dimension $n$ with standard basis $\{|1\}, ..., |n\}$, where the vector $|i\rangle$ is associated to the vertex $i \in V$. The volume of $G$ is denoted and defined as $\text{vol}(G) = \sum_{i \in V} d(i)$. By the Handshake Lemma, $\text{vol}(G) = 2|E|$. Denoting by $\langle i|\psi\rangle$ the functional that sends $|j\rangle$ to the inner product $\langle i|j\rangle$, for each $i, j = 1, ..., n$, we define the matrix

$$\rho = \frac{1}{\text{vol}(G)} \sum_{\{i, j\} \in E} |i\rangle\langle j|, \tag{2}$$

where $|i\rangle\langle j| := |i\rangle - |j\rangle$. It is promptly verified that $\rho = L/\text{Tr}(\Delta) = L/\text{vol}(G)$ [3]. In what follows, we write $d = \text{vol}(G)$, in order to simplify the notation. We can treat $\rho$ as the state of a quantum system with assigned Hilbert space $\mathcal{H}$, given that $\rho$ is a density matrix, being positive-semidefinite, and trace-one. In particular, we shall use two notions from the tool-box of quantum information theory: CPTP maps and the quantum relative entropy.

Axiomatically, the evolution of a state $\sigma$ may be governed by a completely positive trace-preserving (for short, CPTP) map $\Phi \rightarrow \Phi(\sigma) = \sum_j K_j\sigma K_j^\dagger$, for some set $\{K_j\}$ of operators on $\mathcal{H}$ such that $\sum_j K_j^\dagger K_j = I$, where $I$ is the identity matrix (see, e.g., [12]). The von Neumann entropy of a density matrix $\sigma$ is defined by $S(\sigma) = -\text{Tr}(\sigma \ln \sigma)$. Given density matrices $\sigma_1$ and $\sigma_2$, the
quantum relative entropy of $\sigma_1$ with respect to $\sigma_2$ measures the difficulty of distinguishing between these states and it is defined by

$$S(\sigma_1 \| \sigma_2) = \text{Tr}(\sigma_1 \ln \sigma_1) - \text{Tr}(\sigma_1 \ln \sigma_2).$$

The Kirchhoff’s Matrix-Tree Theorem tells us that the number of spanning trees of a graph $G$ on $n$ vertices, $\tau(G)$, can be expressed in terms of the density matrix $\rho$. From Eqs. (1) and (2), we are prompted to the next statement:

**Theorem 1** Let $G$ be a graph on $n$ vertices and $d/2$ edges. The number of spanning trees of $G$ is

$$\tau(G) = \left(\frac{d}{n-1}\right)^{n-1} e^{-(n-1)S(\frac{\Pi_{\ell}}{\rho}^{\|\Phi_{\ell}(\rho)})},$$

and also

$$\tau(G) = \left(\frac{d}{n-1}\right)^{n-1} e^{-\sum_{\ell=1}^{n} S(\frac{\Pi_{\ell}}{\rho}^{\|\Phi_{\ell}(\rho)})}.$$  
(3)

Here, $\Pi_{\ell}$ is a projection operator onto the $n-1$ dimensional space spanned by all the elements of the standard basis associated to $G$, but the $\ell$-th; $\Phi_{\ell}$ is the CPTP map defined by

$$\Phi_{\ell}(\rho) = \Pi_{\ell}\rho \Pi_{\ell} + Q_{\ell}\rho Q_{\ell},$$

where

$$Q_{\ell} = I - \Pi_{\ell} = |\ell\rangle\langle\ell|,$$

is the complementary projector of $\Pi_{\ell}$.

(In matrix theory, the above transformation is called pinching and consists of removing all the off-diagonal terms related to the $\ell$-th vertex of the graph.) The derivation of Eq. (3) is simple and ultimately follows from the identity

$$\exp(-S(I/n\parallel M)) = N(\det M)^{1/n},$$

which holds for all positive semidefinite $n \times n$ matrices $M$. For a more explicit derivation, we firstly construct the $n \times n$ matrix which has zeros in the $\ell$-th row and in the $\ell$-th column, but it is identical to the Laplacian $L$ in the remaining entries. We can express it as

$$\Pi_{\ell}L\Pi_{\ell} = d\Pi_{\ell}\rho\Pi_{\ell}.$$  
(6)

By construction, the matrix $\Pi_{\ell}L\Pi_{\ell}$ will have the same spectrum of $L'_{\ell}$ plus an extra zero eigenvalue. Recall in fact that $L'_{\ell}$ is an $(n-1) \times (n-1)$ matrix, while $\Pi_{\ell}L\Pi_{\ell}$ is $n \times n$. Such an extra zero eigenvalue is associated with the eigenvector $|\ell\rangle$. Therefore, denoting by $\lambda'_{i}$ the eigenvalues of $L'_{\ell}$, we can write

$$\tau(G) = \det(L'_{\ell}) = \prod_{i \in S'} \lambda'_{i},$$

where the set $S'$ contains all eigenvalues of $\Pi_{\ell}L\Pi_{\ell}$ but the extra zero. This formula implies

$$\ln \tau(G) = \sum_{i \in S'} \ln \lambda'_{i} = \text{Tr}(\Pi_{\ell} \ln(\Pi_{\ell}L\Pi_{\ell})).$$
(We adopt the standard convention 0 ln 0 = 0.) Thus, by Eqs. (5, 6),

\[ \ln \tau(G) = (n - 1) \text{Tr}(\frac{\Pi_\ell}{n-1} \ln(d\Pi_\ell\rho)) \]
\[ = (n - 1) \text{Tr}(\frac{\Pi_\ell}{n-1} \ln(\Pi_\ell\rho)) + (n - 1) \ln d \]
\[ = (n - 1) \text{Tr}(\frac{\Pi_\ell}{n-1} \ln \Phi_\ell(\rho)) + (n - 1) \ln d, \]

where in the last identity we used the fact that since \( Q_\ell \) and \( \Pi_\ell \) are orthogonal projectors we have

\[ \ln(\Pi_\ell \rho \Pi_\ell + Q_\ell \rho Q_\ell) = \ln(\Pi_\ell \rho \Pi_\ell) + \ln(Q_\ell \rho Q_\ell). \]

Noticing that \( \Pi_\ell / (n - 1) \) is positive semi-definite and has trace one, we can identify this operator with a density matrix. Indeed, it is the density matrix describing a maximally mixed state of the subspace orthogonal to \( |\ell\rangle \). It follows that

\[ \text{Tr}(\frac{\Pi_\ell}{n-1} \ln \Phi_\ell(\rho)) = - S(\frac{\Pi_\ell}{n-1} \parallel \Phi_\ell(\rho)) \]
\[ = - \ln(n - 1) - S(\frac{\Pi_\ell}{n-1} \parallel \Phi_\ell(\rho)). \]

Hence,

\[ \ln \tau(G) = -(n - 1) S(\frac{\Pi_\ell}{n-1} \parallel \Phi_\ell(\rho)) + (n - 1) \ln \frac{\text{vol}(G)}{n-1}, \]

which reduces to Eq. (3) by exponentiating it – Eq. (4) is then a trivial consequence of Eq. (3).

If the graph does not have isolated vertices \( i.e. \) if \( \Delta \) is invertible, or \( d(i) > 0 \) for every \( i \in V \) an alternative (but equivalent) expression can be obtained as follows:

\[ \tau(G) = \left( \frac{d}{n} \right)^n e^{-\frac{n S(\frac{1}{n} \parallel \Phi_\ell(\rho))}{\Delta_\ell}} \]
\[ = \left( \frac{d}{n} \right)^n e^{-\frac{\sum_{\ell=1}^n S(\frac{1}{n} \parallel \Phi_\ell(\rho))}{\det(\Delta)^{1/n}}}, \]

where, for \( \ell \in \{1, \ldots, n\}, \ \Delta_\ell \) is the \( \ell \)-th diagonal element of the degree matrix \( \Delta \). If \( \Delta \) is not invertible, \( i.e. \), if it has at least a zero diagonal entry, the graph \( G \) has no spanning tree. In this case, one can verify that Eq. (5) still applies under the assumption that \( \ell \) is not an isolated vertex of the graph. On the other hand, Eq. (9) cannot be used, as the denominator diverges. To include this case, we should simply say that if \( \det(\Delta) = 0 \) then \( \tau(G) = 0 \), while if \( \det(\Delta) \neq 0 \) then Eq. (9) applies. To prove the above identity, it is sufficient to verify Eq. (5), since Eq. (9) is obtained by multiplying such term over all possible values of \( \ell \) and by taking \( n \)-th root of the result. For Eq. (8), we go back to Eq. (7) and notice that

\[ \ln \tau(G) = \text{Tr}(\Pi_\ell \ln(d\Pi_\ell \rho)) \]
\[ = \text{Tr}(\Pi_\ell \ln(\Pi_\ell \rho \Pi_\ell)) + (n - 1) \ln d \]
\[ = \text{Tr}(\ln \Phi_\ell(\rho)) - \ln(\Delta_\ell/d) + (n - 1) \ln d \]
\[ = \text{Tr}(\ln \Phi_\ell(\rho)) - \ln(\Delta_\ell) + n \ln d, \]

where we used the fact that

\[ \ln \Phi_\ell(\rho) = \Pi_\ell \ln(\Pi_\ell \rho \Pi_\ell) + Q_\ell \ln(Q_\ell \rho Q_\ell) \]
\[ = \Pi_\ell \ln(\Pi_\ell \rho \Pi_\ell) + Q_\ell \ln(\Delta_\ell/d). \]
Eq. (8) finally follows from
\[ \text{Tr}(\ln \Phi_\ell(\rho)) = n \text{Tr}(\frac{1}{n} \ln \Phi_\ell(\rho)) = -n S(\frac{1}{n}||\Phi_\ell(\rho)) - n \ln n. \]

Eqs. (3,4,8,9) allow us to express \( \tau(G) \) in terms of the density matrix \( \rho \) and the relative entropy. It is worth noticing that it is possible to recast these equations in the following form:
\[ \tau(G) = \left(\frac{d-\Delta_\ell}{n-1}\right)^{n-1} e^{-(n-1) S(\frac{1}{n}||\rho_\ell')}, \]

now \( \rho_\ell' \) is the density matrix obtained by normalizing \( L_\ell \), i.e.,
\[ \rho_\ell' = \frac{L_\ell}{d-\Delta_\ell} \sim \frac{\Pi_\ell L \Pi_\ell}{d-\Delta_\ell}, \]

where \( \sim \) denotes equivalence. (Notice that the last term is an \( n \times n \) matrix with a zero column and a zero row.) The derivation of this expression is exactly on the same line as the previous ones.

3 Bounds

We can derive lower and upper bounds on \( \tau(G) \) by exploiting known facts about the quantum relative entropy. On the other hand, deriving meaningful, simple lower bounds on \( \tau(G) \) with our technique does not seem to be natural. A first attempt based on the monotonicity of the relative entropy fails to produce even a trivial result, which is \( \tau(G) \geq 0 \). We discuss this case here only as an exercise. Firstly, observe that \( i \) \( \Phi_\ell \) is a unital quantum channel (i.e., it maps the identity operator into itself \( \Phi_\ell(I) = I \)) and that \( ii \) the relative entropy is not increasing under CPTP maps, an important and nontrivial property:
\[ S(\rho_1||\rho_2) \geq S(\Phi(\rho_1)||\Phi(\rho_2)). \]

Using these two facts we can exhibit a lower bound for \( \tau(G) \):
\[ S(\frac{1}{n}||\Phi_\ell(\rho)) = S(\Phi_\ell(\frac{1}{n})||\Phi_\ell(\rho)) \leq S(\frac{1}{n}||\rho) = -\ln n - \frac{1}{n} \sum_{j=1}^{n} \ln \lambda_j, \]

where \( \lambda_j \) is the \( j \)-th eigenvalues of \( \rho \). Replacing this into Eq. (8), we thus get
\[ \tau(G) = \frac{d^n}{\Delta_\ell n^2} e^{-n S(\frac{1}{n}||\Phi_\ell(\rho))} \geq \frac{d^n}{\Delta_\ell} e^{\sum_{j=1}^{n} \ln \lambda_j} \]
\[ = \frac{d^n \det(\rho)}{\Delta_\ell} = \frac{\det(L)}{\Delta_\ell}, \]

which is true for all \( \ell \). Therefore taking the minimum over \( \ell \), we can write
\[ \tau(G) \geq \frac{\det(L)}{\delta_{\text{min}}}, \]

where \( \delta_{\text{min}} \) denotes the minimum degree of the graph. Similarly, replacing Eq. (11) into Eq. (9), we get the inequality \( \tau(G) \geq \det(L)/(\det \Delta)^{1/n} \). Notice that these lower bounds are both trivial.
Indeed, since $L$ has at least a null eigenvalue we have that $\det(L) = 0$ and thus the above inequalities simply states that $\tau(G) \geq 0$. It is worth observing that one could in principle get something less trivial by replacing the density $\rho$ which appears in the r.h.s. of Eq. (11) with a generic $\tilde{\rho}$ state which satisfies the condition $\Phi_\ell(\tilde{\rho}) = \Phi_\ell(\rho)$ (notice that such $\tilde{\rho}$ can be easily constructed and that they have the property of having the same diagonal elements of $\rho$). This would allow us to rewrite Eq. (13) as $\tau(G) \geq \det(\bar{L})/\delta_{\min}$, where $\bar{L} = \bar{\rho}d$ (in this case $\det(\bar{L})$ needs not to be zero).

Using the results in [1], we can determine upper bound on $S(\cdot\|\cdot)$ which, through our expressions, will result on bounds on $\tau(G)$. None of the bounds seem to be particularly relevant (they are too weak and require to compute quantities which are not easily computable). As an example we just report here one of them which is obtained through the inequality

$$S(\rho_1\|\rho_2) \leq \frac{\text{Tr}((\rho_1 - \rho_2)^2)}{\lambda_{\min}(\rho_2)},$$

where $\lambda_{\min}(\rho_2)$ is the smallest nonzero eigenvalues of $\rho_2$. We apply this inequality to the identity of Eq. (8). In this case, $\rho_1 = I/n$ and $\rho_2 = \Phi_\ell(\rho)$. Hence, exploiting the properties of $\rho$,

$$\text{Tr}((I/n - \Phi_\ell(\rho))^2) = -1/n + \frac{\text{Tr}(\Delta^2) + \text{Tr}(\Delta) - 2\Delta_\ell}{d^2}.$$
All the bounds in the theorem should be compared with the trivial value \( \tau_{\text{trivial}} = \left( \frac{\text{Tr}(\Delta/2)}{n-1} \right) \), which simply follows by observing that any spanning tree has exactly \( n-1 \) edges and that \( \text{Tr}(\Delta/2) \) is the total number of edges of the graph. It turns out that there is not a definitive ordering among \( \tau_{\text{trivial}} \) and the bounds that we derived above. Indeed, our bounds perform better on some graphs only.

As an example, let us consider the following cases:

- **The complete graph, \( K_n \).** According to the Cayley formula, \( \tau(K_n) = n^{n-2} \). For \( K_n \), we have \( \Delta = (n-1)I, \Delta_{\text{max}} = n-1, \text{Tr}(\Delta) = n(n-1), \) and \( \det \Delta = (n-1)^n \). Hence, all our bounds coincide, i.e., \( \tau_0 = \tau_A = \tau_B = \tau_C = \tau_D = \tau_E = (n-1)^{n-1} \), while \( \tau_{\text{trivial}} = \left( \frac{n(n-1)/2}{n-1} \right) \), which for \( n \geq 7 \) is already larger than \( (n-1)^{n-1} \).

- **The star, \( K_{1,n-1} \).** In this case, \( \Delta \) has one eigenvalue equal to \( n-1 \) (in fact, \( \Delta_{\text{max}} = n-1 \)) and \( n-1 \) eigenvalues equal to 1. Clearly, \( \tau(K_{1,n-1}) = 1 \). We have that \( \tau_0 = \tau_E = 1 \), a tight bound, while \( \tau_A = (n-1)^{n-1}, \tau_B = \left( \frac{2(n-1)}{n} \right)^{n-1}, \tau_C = \left( \frac{2(n-1)}{n} \right)^{n-1} \frac{1}{(n-1)^{n-1}}, \tau_D = \left( \frac{2(n-1)}{n} \right)^{n-1} \frac{1}{n-1} \). Notice that in this case \( \tau_A < \tau_D \) for \( n \geq 6 \) and \( \tau_A > \tau_D \) for \( n < 6 \).

- **Consider the graph with \( n = 4 \) vertices and edges \{1,2\}, \{2,3\}, \{3,4\}, \{2,4\}.** One can easily verify that \( \tau(G) = 3 \). For this graph, we have \( \tau_0 = \tau_{\text{trivial}} = 4, \) while \( \tau_A \approx 6.45, \tau_B = 8, \tau_C = 8.6, \tau_D \approx 5.33, \) and \( \tau_E \approx 4.62 \). Notice that in this case \( \tau_A > \tau_D \).

To prove the optimality of \( \tau_0 \), we firstly observe that each graph \( G \) with \( n = 2 \) and multiple edges saturate the bound. Those graphs are only characterized by the number \( k \) of edges which connects the two element of \( V \): therefore \( \Delta = \text{diag}(k,k) \) and \( \tau_0(G) = k \). For multigraphs on an arbitrary number of vertices \( n > 2 \), we consider stars with multiple edges only between an arbitrary but fixed pair of adjacent vertices. W.l.o.g. we may assume \( k \) edges between vertices 1 and 2 only. These multigraphs are denoted by \( K_{1,n,k} \). It is clear that \( \tau(K_{1,n,k}) = k \). Furthermore, since \( \Delta = \text{diag}(k+(n-1),k,1,\cdots,1) \), then also \( \tau_0(K_{0,1,k}) = k \).

Both these bounds follow from the Klein inequality: the relative entropy of two states is always positive semi-definite. On the basis of Eq. (8), we can conclude that

\[
\tau(G) \leq \frac{d^n}{n^n \Delta_{\ell}} = \frac{\text{Tr}(\Delta^n/n)}{\Delta_{\ell}}, \tag{14}
\]

for all \( \ell \). Minimizing the r.h.s. with respect to such index, we can then write

\[
\tau(G) \leq \frac{d^n}{n^n \Delta_{\text{max}}} = \frac{\text{Tr}(\Delta^n/n)}{\Delta_{\text{max}}} = \tau_D, \tag{15}
\]

Similarly, from Eq. (9),

\[
\tau(G) \leq \frac{d^n}{n^n \det(\Delta)^{1/n}} = \frac{\text{Tr}(\Delta^n/n)}{\det(\Delta)^{1/n}} = \tau_C. \tag{16}
\]

Since \( \Delta_{\text{max}} \geq \det(\Delta)^{1/n} \geq \delta_{\min} \), if follows that \( \tau_D \leq \tau_C \).

7
A more refined bound can be obtained by exploiting the following inequality (see [10]):

\[
\sum_i p_i S(r_i\|s_i) \geq S(\sum_i p_i r_i\|\sum_j q_j s_j) - \sum_i p_i \ln(p_i/q_i);
\]

this is valid if \( r_i, s_i \) are density matrices and \( p_i \) and \( q_i \) are generic probability distributions. Let us apply this to \( \sum_{\ell=1}^n S(I/n\|\Phi_\ell(\rho)) \), with \( p_i = q_i = 1/n \):

\[
\frac{1}{n} \sum_{\ell} S(\frac{\rho}{n}\|\Phi_\ell(\rho)) \geq S(\frac{\rho}{n}\|\sum_\ell \Phi_\ell(\rho)/n) - \frac{(1/n) \ln(n/n) = S(\frac{\rho}{n}\|\sigma)}{n^2}.
\]

where

\[
\sigma = \sum_\ell \Phi_\ell(\rho)/n = \sum_\ell (\Pi_\ell \rho \Pi_\ell + Q_\ell \rho Q_\ell)/n = \frac{\Delta}{d} - \frac{n-2A}{n} \frac{A}{d}
\]

(17)

With the use of Eq. (9), we finally can write

\[
\tau(G) \leq \frac{d^n}{n^d |\text{det}(\Delta)|^{1/n}} e^{nS(\frac{\rho}{n}\|\sigma)} = \frac{d \text{det}(\sigma)}{\text{det}(\Delta)^{1/n}}
\]

\[
= \frac{\text{det}(\Delta - \frac{n-2A}{n} A)}{\text{det}(\Delta)^{1/n}} = \frac{\text{det}(\Delta + 2A/n)}{\text{det}(\Delta)^{1/n}}.
\]

(18)

The bound is interesting but it still involves the computation of a determinant. We can however do better by using again the fact that the relative entropy is decreasing under the action of CPTP maps. Consider the CPTP map

\[
\Psi = \frac{1}{n} \sum_{\ell=1}^n \Phi_\ell;
\]

(19)

\[
\Psi(\Delta) = \Delta, \quad \Psi(A) = \frac{n-2A}{n}.
\]

Now,

\[
\Psi^k(\sigma) = \Psi^{k+1}(\rho) = \frac{\Delta}{d} - \left(\frac{n-2A}{n}\right)^{k+1} \frac{A}{d},
\]

where \( \Psi^k \) represent the CPTP map obtained by concatenating \( k \) times the map \( \Psi \) (i.e. \( \Psi \) is applied to \( \sigma \) exactly \( k \) times). For \( k \gg 1 \) this yields (in any norm),

\[
\lim_{k \to \infty} \Psi^k(\sigma) = \frac{\Delta}{d}.
\]

Therefore,

\[
S(\frac{\rho}{n}\|\sigma) \geq S(\Psi(\frac{\rho}{n})\|\Psi^k(\sigma)) = S(\frac{\rho}{n}\|\Psi^k(\sigma)) = S(\frac{\rho}{n}\|\Psi(\frac{\rho}{n})) - \left(\frac{n-2A}{n}\right)^{k+1} \frac{A}{d},
\]

which in the limit of large \( k \) gives

\[
S(\frac{\rho}{n}\|\sigma) \geq S(\frac{\rho}{n}\|\frac{\Delta}{d}).
\]
Replacing this into the first line of Eq. (18), we finally obtain
\[
\tau(G) \leq \frac{d^n}{n^n \det(\Delta)^{1/n}} e^{-nS(\frac{L}{n}\|\sigma)} \\
\leq \frac{d^n}{n^n \det(\Delta)^{1/n}} e^{-nS(\frac{L}{n}\|\Delta)} = \det(\Delta)^{1-1/n} = \tau_A. \tag{20}
\]
This upper bound, as the one of Eq. (16), is just a function of the matrix $\Delta$. It is natural to ask which of the two bounds is better: the bound (20) is always better than (16). To prove this, take
\[
\frac{\tau_A}{\tau_C} = \frac{\det(\Delta)}{\text{Tr}(\hat{\Delta})^{n}} \leq 1,
\tag{21}
\]
which can be easily verified by exploiting the fact that $\ln(x)$ is a concave function of its argument. This clarify the relation between $\tau_A$ and $\tau_C$.

For the bound $\tau_B$, we start form observing that Eq. (8) and (9) imply that the following inequality should apply for any $\ell$:
\[
\Delta_\ell = \det(\Delta)^{1/n} \frac{e^{-nS(\frac{L}{n}\|\Phi_\ell(\rho))}}{e^{-\sum_{\ell=1}^{n} S(\frac{L}{n}\|\Phi_\ell(\rho))}} \leq \frac{\det(\Delta)^{1/n}}{e^{-\sum_{\ell=1}^{n} S(\frac{L}{n}\|\Phi_\ell(\rho))}}.
\]
where the last step is (again) a consequence of the Klein inequality. Now,
\[
\text{Tr}(\Delta) \leq \frac{n \det(\Delta)^{1/n}}{e^{-\sum_{\ell=1}^{n} S(\frac{L}{n}\|\Phi_\ell(\rho))}} \implies \frac{e^{-\sum_{\ell=1}^{n} S(\frac{L}{n}\|\Phi_\ell(\rho))}}{\det(\Delta)^{1/n}} \leq \frac{n}{\text{Tr}(\Delta)}.
\]
Recalling that $\text{Tr}(\Delta) = \text{vol}(G)$ and replacing this into Eq. (9), we have
\[
\tau(G) \leq \text{Tr}(\hat{\Delta})^{n-1} = \tau_B.
\]
We can now compare $\tau_B$ to $\tau_A$ and $\tau_C$. Begin by writing
\[
\frac{\tau_B}{\tau_C} = \left( \frac{\det(\Delta)}{\text{Tr}(\hat{\Delta})^{n}} \right)^{1/n} = \left( \frac{\tau_A}{\tau_C} \right)^{1/n}.
\]
Thanks to Eq. (21), we can thus conclude that
\[
1 \geq \frac{\tau_B}{\tau_C} \geq \frac{\tau_A}{\tau_C},
\]
which implies $\tau_C \geq \tau_B \geq \tau_A$.

For $\tau_0$, we start from Eq. (8) which we specify for $\Delta_\ell = \Delta_{\max}$, i.e.,
\[
\tau(G) = \left( \frac{d}{n} \right)^n e^{-nS(\frac{L}{n}\|\Phi_\ell(\rho))} \frac{\Delta_{\max}}{\Delta_{\max}}, \tag{22}
\]
where $\hat{\ell}$ is the value of $\ell$ achieving $\Delta_{\max}$. We then use the monotonicity of the relative entropy to write
\[
S(\frac{L}{n}\|\Phi_\ell(\rho)) \geq S(\Psi^k(\frac{L}{n})\|\Psi^k(\Phi_\ell(\rho))) = S(\frac{L}{n}\|\Phi_\ell(\Psi^k(\rho))) \\
\simeq S(\frac{L}{n}\|\Phi_\ell(\hat{\Delta})) = S(\frac{L}{n}\|\hat{\Delta}),
\]
where $\Psi$ is the unital CPTP map introduced in Eq. (19). In writing the last passage of the first line we used the fact that since for each $\ell$ and $\ell'$ the channels $\Phi_\ell$ and $\Phi_{\ell'}$ commute, also $\Psi$ (and thus $\Psi^k$) commute with $\Phi_\ell$. The first identity in the second line is obtained for large $k$ using the fact that $\Psi^k(\rho) \simeq \Delta/\text{vol}(G)$, and finally the last passage follows from the fact that for $\ell$, $\Phi_\ell(\Delta) = \Delta$. Replacing this into Eq. (22), we finally get

$$\tau(G) \leq \left(\frac{d}{n}\right)^n e^{-nS(\frac{I}{n} \parallel \frac{\Delta}{d})} = \left(\frac{d}{n}\right)^n \frac{n^n \det(\frac{\Delta}{d})}{\Delta_{\text{max}}^n} = \frac{\det(\Delta)}{\Delta_{\text{max}}} = \tau_0.$$ 

To clarify the relations with the other bounds, we need only to observe that

$$\frac{\tau_0}{\tau_A} = \frac{\det(\Delta)^{1/n}}{\Delta_{\text{max}}} \leq 1.$$ 

To derive $\tau_E$ we use Eq. (21) and the Klein inequality, as we have already done above. This yields

$$\tau(G) = \left(\frac{d-\Delta}{n-1}\right)^{n-1} e^{-(n-1)S(\frac{I}{n} \parallel \Phi_\ell(\rho))} \leq \left(\frac{d-\Delta}{n-1}\right)^{n-1} = \nu(n \parallel \Phi_\ell(\rho)),$$

for all $\ell$. The case $\Delta_\ell = \Delta_{\text{max}}$ gives $\tau_E$; $\tau_E > \tau_0$ follows from the concavity of $\log(x)$; $\tau_E < \tau_B$ follows from $\Delta_{\text{max}} \geq \text{Tr}(\Delta)/n$.

By repeating the derivation of $\tau_A$, starting from Eq. (3) instead of Eq. (8), we can derive a new upper bound, $\tau_F$. However, this turns out to be weaker than $\tau_A$. Specifically, we get the following inequality:

$$\tau(G) \leq \left(\frac{n}{n-1}\right)^{n-1} \det(\Delta)^{1-1/n} = \tau_F.$$ 

(23)

To verify this, we use the joint convexity of the relative entropy and then its monotonicity under CPTP maps:

$$\frac{1}{n} \sum_{\ell=1}^n S(\frac{\Pi_\ell}{n-1} \parallel \Phi_\ell(\rho)) \geq S(\sum_{\ell=1}^n \frac{\Pi_\ell}{n-1} \parallel \sum_{\ell=1}^n \Phi_\ell(\rho))$$

$$= S(I/n \parallel \Psi(\rho)) \geq S(\Psi^k(I/n \parallel \Psi^{k+1}(\rho))$$

$$= S(I/n \parallel \Psi^{k+1}(\rho)) \simeq S(I/n \parallel \Delta/d),$$

where $\Psi$ is the unital CPTP map introduced in Eq. (19) and where the last identity holds for $k \to \infty$. Replacing this inequality into Eq. (21) and where the last identity holds for $k \to \infty$. Replacing this inequality into Eq. (23), we finally obtain

$$\tau(G) \leq \left(\frac{d}{n-1} e^{-S(I/n \parallel \Delta/d)}\right)^{n-1} = \left(\frac{d}{n-1} n \det(\Delta/d)^{1/n}\right)^{n-1},$$

which coincides with (23).

4 Conclusions

We comment on the expressions that we have derived to see if these could help us in providing an operational meaning to $\tau(G)$ or more generally to $\rho$. We notice that all the expressions derived so far allow us to write $\tau(G)$ as a product of two quantities: a first term which is typically greater
than one and which depends only on the degree matrix of the graph; an exponential which is always smaller than one and which depends on the relative entropy between a density matrix obtained via some processing of \( \rho \) and a totally mixed density operator. In particular, we may point out that, apart from the cases of \( \text{(8)} \) and \( \text{(9)} \) where there is an extra factor inversely proportional to \( \Delta \ell \), the first contribution goes like \( \sim (d/n)^n \), where \( d \) is the sum of the degrees. Since the quantity \( d/n \) measures the average degree, \( (d/n)^n \) counts the average number of independent walks one would obtain while hopping randomly \( n - 1 \) times along the edges of the graph while starting from a generic vertex. This number is clearly much larger than the number of spanning tree of \( G \) (the latter being just a proper subset of the trajectories generated by the hopping). The exponential term of our expressions can then be interpreted as the fraction of the trajectories which indeed correspond to a spanning tree of \( G \). Their values are obtained by computing the relative entropy between a density matrix associated with \( G \) and a totally mixed state (either \( n \) dimensional or \( n - 1 \) dimensional).

Invoking the quantum Stein’s Lemma we can provide these quantities with an operational meaning in the context of the (asymmetric) quantum hypothesis testing problem (see \([2]\)). It is known that \( S(\rho_1 | \rho_2) \) represents the optimal upper bound on type-II error rate for any sequence of measurements used to decide whether a given state is \( \rho_1 \) or \( \rho_2 \), under the conditions of bounded type-I error. Let us recall that in the hypothesis testing problem, type-II (or false negative) errors are those in which we have mistaken \( \rho_2 \) with \( \rho_1 \); for type-I (or false positive) errors are those in which we have mistaken \( \rho_1 \) with \( \rho_2 \). This implies that the exponential quantities in our expressions quantify how different is the quantum state associated to our graph from the totally mixed state.

The study of the relation between relative entropy and the complexity of a graph which we have carried on in this paper is probably not exhaustive. It is plausible to believe that allowing freedom to add arbitrary coefficients to the projectors in the definition of \( \rho \) we can push the relative entropy closer to the effective number of spanning trees or even to a different graph-theoretic quantity. The associated problem would then closely resemble scenarios where we aim to optimize some quantity over a matrix fitting a graph under specific constraints (see, e.g., the Lovász theta function, the Colin de Verdière parameter, etc.). This appears to be an open research direction involving the relative entropy and possibly other standard notions from quantum information theory.

Acknowledgments. We would like to thank Koenraad Audenaert for important discussion. VG acknowledges support from the Institut Mittag-Leffler (Stockholm), where he was visiting while part of this work was done. SS is supported by a Newton International Fellowship.

References

[1] K. M. R. Audenaert and J. Eisert, Continuity bounds on the quantum relative entropy, *J. Math. Phys.* **46**, 102104 (2005).

[2] K. M. R. Audenaert, M. Nussbaum, A. Szkola, F. Verstraete, Asymptotic Error Rates in Quantum Hypothesis Testing, *Comm. Math. Phys.* **279**, 251-283 (2008).

[3] S. Braunstein, S. Ghosh, and S. Severini, The laplacian of a graph as a density matrix: a basic combinatorial approach to separability of mixed states, *Ann. Comb.*, Vol. 10, no 3 (2006), 291-317.

[4] B. Bollobás, *Modern Graph Theory*, Springer Verlag, New York, 1998.
[5] I. B. Gertsbakh, Y. Shpungin, *Models of Network Reliability: Analysis, Combinatorics, and Monte Carlo*, CRC Press, 2009.

[6] A. Hinchcliffe (Editor), *Chemical Modelling: Applications and Theory, Volume 2*, The Royal Society of Chemistry (2002).

[7] A. S. Holevo, Bounds for the quantity of information transmitted by a quantum communication channel, *Prob. Inf. Transm. (USSR)* 9, 177–83 (1973).

[8] G. Kirchhoff, Über die Auflösung der Gleichungen, auf welche man bei der untersuchung der linearen verteilung galvanischer Ströme geführt wird, *Ann. Phys. Chem.* 72, 497-508, 1847.

[9] W. Ochs, A new axiomatic characterization of the von Neumann entropy, *Rep. Math. Phys.* 8 (1975), 109–120.

[10] A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*, Cambridge Series on Information and the Natural Sciences, 2000.

[11] N. Nakanishi, *Graph Theory and Feynman Integrals*, Gordon and Breach, New York, 1971.

[12] V. Paulsen, *Completely Bounded Maps and Operator Algebras*, Cambridge University Press, Cambridge, 2002.

[13] A. Rényi, *Probability Theory*, Amsterdam: North-Holland, 1970.

[14] B. Schumacher and M. Westmoreland, Relative entropy in quantum information theory. *American Mathematical Society Contemporary Mathematics Series: Quantum Information and Quantum Computation*, 305, American Mathematical Society, Providence, 2002.

[15] R. P. Stanley, *Enumerative combinatorics, vol. I.*, Wadsworth and Brooks/Cole, Monterey, 1986.

[16] W. T. Tutte, *Graph Theory*, Encyclopedia of Mathematics and its Applications, 21, Addison-Wesley, 1984.

[17] V. Vedral, The Role of Relative Entropy in Quantum Information Theory, *Rev. Mod. Phys.* 74, 197–234 (2002).

[18] W. Watkins, The Laplacian matrix of a graph: Unimodular congruence, *Linear and Multilinear Algebra* 28:35-43 (1990).

[19] D. Welsh, *The Tutte polynomial. Random Structures Algorithms*, 15(3-4):210–228, 1999. Statistical physics methods in discrete probability, combinatorics, and theoretical computer science (Princeton, NJ, 1997).