Thermodynamic cost of creating correlations

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We investigate the fundamental limitations imposed by thermodynamics for creating correlations. Considering a collection of initially uncorrelated thermal quantum systems, we ask how much classical and quantum correlations can be obtained via a cyclic Hamiltonian process. We derive bounds on both the mutual information and entanglement of formation, as a function of the temperature of the systems and the available energy. We also characterize the maximal temperature that allows for creating quantum entanglement. In the multipartite case, we consider several types of entanglement, in particular genuine multipartite and bipartite entanglement. This approach may find applications, e.g. in quantum information processing, for physical platforms in which thermodynamical considerations cannot be ignored.

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Introduction.—Thermodynamics is intimately connected to information theory. In recent years, this connection has been explored and extended in the quantum world [1]. Making use of the concepts and tools of quantum information theory, this research line brought tremendous progress in our understanding of the thermodynamics of quantum systems, see e.g. [2][5]. Given the power of quantum information processing, it is natural to investigate the possibilities offered by quantum effects (such as coherence and entanglement) in the context of thermodynamics [6][11].

The main question explored in this work is the following: what is the thermodynamic cost of establishing classical and quantum correlations? Our goal here is to find what are the fundamental limitations imposed by thermodynamics for creating correlations.

Here we investigate these issues using a particularly simple model. We consider an isolated quantum system, composed of two (or more) uncorrelated subsystems, all initially in a thermal state. In order to establish correlations between the subsystems, we allow ourselves to perform any possible unitary operation on the entire system. Performing such a unitary will in general cost us some energy.

The first question we seek to answer is how much correlation can be created in our system, and how much energy this will cost. We find the minimal amount of energy required to create a certain amount of correlations, quantified here by the quantum mutual information. We also discuss the state featuring the maximal amount of correlations [12], depending on the energy spectrum and the temperature.

Second, we investigate how much quantum entanglement can be established, and how much energy this will cost. We start here by considering a bipartite system, and ask what is the maximal amount of entanglement that can be achieved. We discuss in detail the case of a two-qubit system, presenting a protocol for creating the maximal amount of entanglement, and showing that there is a threshold temperature above which no entanglement can be created. Moving to the case of $n$ subsystems, we investigate similar questions, considering here different forms of entanglement, in particular genuine multipartite entanglement among the $n$ subsystems. Again, we consider the question of what is the threshold temperature at which entanglement can be created. We present protocols for which this temperature scales linearly in the number of subsystems, for all types of entanglement. Finally, we derive upper bounds considering the geometry of quantum states.

These results demonstrate the limitations on creating correlations that arise from thermodynamics. We envisage therefore that they will be relevant for discussing quantum information tasks in physical systems where thermodynamical considerations cannot be ignored. One example where similar issues were raised is NMR [13][14]. From a more theoretical point of view, our approach lies in between the resource theories of entanglement [15][16] and thermodynamics [3][4], i.e. we quantify the impact of resources from one on the other.

Framework.—We consider a system of $n$ initially uncorrelated $d$-dimensional quantum subsystems. Each subsystem is taken to have the same (arbitrary) local Hamiltonian $H$, and the same temperature $k_B T = 1/\beta$. Hence the initial state of the system is $\tau_\beta^n$, where $\tau_\beta = \frac{\exp(-\beta H)}{Z}$ and $Z = \text{Tr} (e^{-\beta H})$ is the partition function. When discussing qubits we will denote by $E$ the energy of the excited state and $p = \frac{1}{1+e^{-\beta}}$ the ground state probability. Allowing ourselves the use of arbitrary (global) unitaries $U$ acting on the system, we want to characterise (i) what is the energy cost $W$ of creating correlations (either classical or quantum), where $W$ is
given by $W = \text{Tr} \left( H_{\text{tot}}(\rho_f - \tau_\beta^2) \right)$, $\rho_f = U \tau_\beta^2 U^\dagger$ is the final state and $H_{\text{tot}} = \sum_i H^{(i)}$ is the total Hamiltonian; (ii) what are the limitations imposed by the initial temperature on the available correlations.

**General correlations.**—We consider the case of a two-qudit system, i.e. $n = 2$ and arbitrary $d$. Correlations between the subsystems (referred to as $A_1$ and $A_2$) are measured here using the quantum mutual information $I(A_1 : A_2) = S(A_1) + S(A_2) - S(A_1 A_2)$ where $S(X) = -\text{Tr}(\rho_X \log \rho_X)$ is the von Neumann entropy of system $X$. The goal is then to maximize $I(A_1 : A_2)$ over all global unitaries constrained by $W \leq \Delta E$. In other words, given some energy $\Delta E$ at our disposal, what is the maximal amount of correlations $\Delta I_{\text{E}}$ that we can create?

Note first that initially $I(A_1 : A_2) = 0$, as the initial state factorizes. Now, to create correlations we must apply a global unitary that will increase the local entropies $S(A_i)$ of $\rho_f$, since the total entropy $S(A_1 A_2) = 2S(\tau_\beta)$ will clearly not change. Recalling that the thermal state maximizes the entropy of a system with fixed average energy (see, for example, [17]), we find that

$$I_{\Delta E} \leq 2[S(\tau_{\beta'}) - S(\tau_\beta)], \quad (1)$$

where $\beta'$ is chosen such that $\Delta E = \text{Tr}[H_{\text{tot}}(\tau_{\beta'}^2 - \tau_\beta^2)]$. Hence in order to obtain correlations at minimal energy cost, one should look for a protocol such that the local states of $\rho_f$ are thermal states at equal temperature, i.e., $\text{Tr}_{A_i}(\rho_f) = \text{Tr}_{A_i}(\tau_\beta)$. In appendix A we construct such a protocol, thus reaching the bound [1], for Hamiltonians with equally spaced energy levels and for arbitrary Hamiltonians if the temperature difference is big enough. The case $\beta' \to \infty$ deserves particular attention, since here the maximal amount of correlations

$$I_{\max} = 2[\log d - S(\tau_\beta)] \quad (2)$$

is obtained, with corresponding energy cost

$$W = 2 \left( \frac{1}{2} \text{Tr} \, H - \frac{1}{2} \text{Tr} \, H e^{-\beta H} \right). \quad (3)$$

The bound [2] can always be reached by rotating the energy eigenbasis to the generalized Bell basis [12, 13]. For all $d$ we define the unitary operators $X = \sum_{i,j} |i+1 \mod d \rangle \langle i|$ and $Z = \sum_i \omega^i |i \rangle \langle i|$ with $\omega = e^{2\pi i/d}$ as generalisations of the (qubit) Pauli operators $\sigma_x$ and $\sigma_z$. The Bell basis is then given by $|\phi_{ij}\rangle = Z^i \otimes X^j |\psi\rangle$, where $|\psi\rangle = \frac{1}{\sqrt{d}} \sum_i |i\rangle$. Since all states which are diagonal in this basis have maximally mixed marginals, i.e. $\text{Tr}_{A_i}(|\phi_{ij}\rangle \langle \phi_{ij}|) = 1/d$, the bound [2] is achieved.

**Entanglement.**—We now consider the creation of quantum correlations, i.e. entanglement, in the system. Focusing first on the simplest case of a two-qubit system, we ask how much entanglement of formation, or equivalently concurrence $C$, [19], can be created. This question was addressed in Refs. [20, 21], where the authors characterized the state (the so called maximally entangled mixed states) featuring the largest amount of entanglement in the unitary orbit of any two-qubit state. Denoting by $\{\lambda_i\}$ the eigenvalues arranged in non-increasing order of the initial state, the maximal amount of concurrence is given by $C = \lambda_1 - \lambda_2 - 2\sqrt{\lambda_2 \lambda_3}$ (for $C \geq 0$). Applied to the present case, we find

$$C_{\max} = 2p^2 - p - 2(1 - p)\sqrt{p(1-p)}. \quad (4)$$

Hence it follows that there is a threshold temperature, $k_B T / E \gtrsim 1.19$ (or equivalently a threshold population $p \lesssim 0.698$), above which no entanglement can be created between the two qubits.

Next we derive the cost of creating entanglement. Consider first the case $T = 0$, i.e. $\tau = |0\rangle \langle 0|$. Here, it can be shown that for a given amount of available energy $\Delta E$, the unitary generating the most entanglement is simply a rotation in the $|00\rangle$, $|11\rangle$ subspace. From this we find the relation

$$C = \sqrt{\frac{\Delta E}{E}} (2 - \frac{\Delta E}{E}). \quad (5)$$

Moving to non-zero temperature, finding the optimal unitary is no longer straightforward. Nevertheless the problem can be attacked from two directions. First, we maximize $C$ numerically, with respect to all possible unitaries, for a given cost $W$. Second, we use an ansatz protocol, inspired by the optimal unitaries to achieve $C_{\max}$. These unitaries have the form of first rotating in the subspace of $|10\rangle$ and $|11\rangle$, followed by rotating in the subspace of $|00\rangle$ and $|11\rangle$. Our ansatz is to optimise over such unitaries, now a much simpler optimisation over the two unknown angles (one for each rotation). The results are presented in Fig. [2] where the solid line shows the result of the full optimisation and the dashed line shows the results of the ansatz. We see that when there is no restriction on the amount of available energy $W$, then our ansatz protocol performs optimally. However, this is not the case
FIG. 2. Main: Concurrence vs. available energy, for various values of $k_B T / E$. Solid lines show the optimal protocol, found numerically by optimising over the unitary group. The dashed lines show performance of simpler protocol, described in main text, which is seen to perform well, especially for smaller temperatures. Moreover, if the available energy is not limited, our ansatz is optimal. Inset (a) shows the behaviour of the maximal concurrence $C_{max}$ as a function of $k_B T / E$, while inset (b) shows the energy needed to leave the separable set, as a function of $k_B T / E$.

when $W$ is limited. Note that the amount of energy required to reach $C_{max}$ is decreasing as $T$ increases, shown in inset (a), where we also see that for low temperatures ($k_B T / E \lesssim 0.1$), we can generate essentially one e-bit, i.e. $C_{max} \simeq 1$. Moreover, for any $T > 0$, there is minimal amount of energy required for generating entanglement, shown in inset (b). This is because some energy is always needed to leave the set of separable states.

**Multipartite case.**— Let us now move to the multipartite case. Here, finding optimal unitaries is in general a difficult problem (almost intractable). Nevertheless, we can say relevant things by (i) considering specific protocols, (ii) using known results on the geometry of quantum states (i.e. bounds on the radius of separable states etc.). This will allow us to do the following: (i) study creation of entanglement and genuine multipartite entanglement (considering both GHZ and W states as exemplary instances), (ii) put bounds on the threshold temperature and on the cost for creating these forms of entanglement.

To start our discussion, we consider the case of $n$ qubits and a straightforward generalization of the above two-qubit protocol. That is, we consider a rotation in the $|0\rangle^\otimes n$, $|1\rangle^\otimes n$ subspace, of the form

$$U = |\phi\rangle \langle 0|^{\otimes n} + |\phi'\rangle \langle 1|^{\otimes n} + 1 - (|0\rangle \langle 0|)^{\otimes n} - (|1\rangle \langle 1|)^{\otimes n}$$

where $|\phi\rangle$ is the GHZ state and $|\phi'\rangle = Z_1 |\phi\rangle$. For a given bipartition $A|\bar{A}$, the concurrence in the final state $\rho_f$ can be conveniently lower bounded using the relation \cite{22,23}

$$C \geq 2\left(|\langle 0|^{\otimes n} \rho_f |1|^{\otimes n} | - \sqrt{\langle 0|^{\otimes n} \Pi_{A|\bar{A}} \rho_f \Pi_{A|\bar{A}} |0|^{\otimes n} |1|^{\otimes n} } \right) \tag{6}$$

where $\Pi_{A|\bar{A}}$ is the permutation operator acting on the two-copy Hilbert space exchanging partition $A$ between the two copies. Note that this protocol generates the same amount of entanglement along every possible bipartition and these bounds are proven to be tight for this protocol \cite{24}. This allows us to characterise the maximal temperature at which entanglement across all bipartitions can be created as a function of $n$. We find a surprisingly good scaling, which is linear in $n$, i.e. the critical temperature $T_E$ for below which entanglement creation is proven to be possible scales as $k_B T_E \gtrsim T / n$. Although this represents only a lower bound on the threshold temperature, numerical evidence suggests optimality of the linear scaling. Hence it follows that entanglement across all bipartitions can always be generated starting from an arbitrary temperature $T$, by considering a sufficiently large number of qubits $n$. The cost of such a linear scaling on the other hand is surprisingly small: at maximum performance the cost of creating entanglement across all bipartitions is $W = n E (1 - e^{-\beta E}) / (2(1 + e^{-\beta E}))$, i.e. exponentially small in $n$ for any $T > 0$.

The above protocol also allows us to discuss the creation of the strongest form of multipartite entanglement, namely genuine multipartite entanglement (GME). Since for the above protocol the final state $\rho_f$ is diagonal in the GHZ basis, the techniques of Ref. \cite{22} give us necessary and sufficient conditions for the creation of GME \cite{25}. The lower bound on the threshold temperature for creating genuine multipartite entanglement $T_{GME}$ with this protocol turns out to be asymptotically independent of $n$, and given by $k_B T_{GME} / E \gtrsim \frac{1}{2n(\ln(2))}$.

However this protocol performs far from optimal for creating GME. In fact it is much more favorable to create W type entanglement compared to GHZ type entanglement (as the above protocol). This can be intuitively understood from the fact that the entanglement of W states is much more robust to noise compared to GHZ states \cite{26,27}. The main idea of the following protocol, which is discussed in detail in Appendix B, is to aim at the creation of W type entanglement by first permuting the largest eigenvalue, $p^n$, and then the remaining smallest eigenvalues, $p(1 - p)^{n-1}$, in the degenerate subspace of energy $E$, and then rotate to a complete orthonormal basis consisting of W-like states. Note also that it is beneficial in terms of entanglement creation to shift the smallest eigenvalue, $(1 - p)^n$, to the ground state $|0\rangle^\otimes n$ as the entanglement of W states is fragile with respect to noise of the form $|0\rangle^\otimes n$. For this protocol, the
threshold temperature for creating GME scales almost linearly, as

\[ k_B T_{GME} = \frac{n}{2 \ln n} + O \left( \frac{n}{(\ln n)^2} \right). \]  

(7)

Hence, it is possible to generate GME among all \( n \) systems for an arbitrarily high temperature \( T < \infty \), by considering a sufficient number of qubits \( n \). The cost of this protocol is much higher than the one above used for GHZ type GME, however still exponentially small in \( n \) (See Appendix B). It is important to note here that the criterion used, while constituting a lower bound for an entropic measure of GME [22], is not optimal in its noise robustness [28], leaving open the possibility already for this particular protocol to scale linear in \( n \) at exponentially small energy cost.

Finally, it is also worth considering the task of creating entanglement on a single bipartition for the state \( \rho_f \). While the above protocols can indeed be used here, they are not optimal. A more efficient protocol can be deduced by realizing that, upon choosing a given bipartition, it is enough to focus on a subspace of dimension \( 4 \times 4 \) of \( \tau^\otimes n \) and then apply the two-qubit protocol [22]. To create the largest possible amount of entanglement in this subspace, one then looks for the purest \( 4 \times 4 \) subspace by choosing two orthogonal vectors for each subsystem of the bipartition. For \( \tau^\otimes n \), we thus consider the subspace spanned by the eigenvectors with the largest eigenvalue, \( p^0 \), and three smallest ones, \( (1-p)^0 \) and twice \( p(1-p)^{n-1} \). Applying finally the two-qubit protocol, we find that for large \( T \)

\[ k_B T_E = \frac{n}{2 \ln n} + O \left( \frac{n}{(\ln n)^2} \right). \]  

(8)

Hence the threshold temperature for the creation of bipartite entanglement using this protocol is also linear in \( n \) (for high temperatures), improving on the GHZ protocol discussed above by a factor of two.

So far, we have investigated explicit protocols, which allowed us to place lower bounds on the threshold temperature that still allows for the creation of entanglement. To study the limitations imposed by a thermal background it is also relevant to find upper bounds, which can be derived using results on the geometry of quantum states. In particular, it is known that the maximally mixed state is always surrounded by a volume of finite size that contains only separable states [14], and it is possible to place lower bounds on the radius of the ball of separable states. A state \( \rho \) of \( n \) qubits is fully separable if \( \| \rho - \frac{1}{2^n} \|_2 \leq \frac{1}{2} \sqrt{\frac{1}{n}} \) and is biseparable (hence does not feature GME) if \( \| \rho - \frac{1}{2^n} \|_2 \leq \frac{1}{2^n} \) [29] [30]. Since the distance to the maximally mixed state is invariant under a global unitary, it is enough here to check whether the initial state \( \tau^\otimes n \) is sufficiently close to the identity. From the bounds of Ref. [29] [30], we obtain the upper bounds on the threshold temperature

\[ \frac{k_B T_E}{E} \leq 2 \tan^{-1} \sqrt{\left( 1 + \frac{9}{4} 3^{n/2} \right)^{1/n} - 1} \]  

(9)

for the creation of entanglement, and

\[ \frac{k_B T_{GME}}{E} \leq 2 \tan^{-1} \sqrt{\left( 1 + \frac{1}{2} \right)^{1/n} - 1} \]  

(10)

for the creation of GME.

These bounds feature a scaling that is completely different compared to the lower bounds we derived previously. Hence, we get an exponential gap between our upper and lower bounds, both for the creation of entanglement and GME. We believe however that these upper bounds are far from optimal, and that much better bounds can be derived by using the form of the initial state \( \tau^\otimes n \), in particular using the fact that it is always full-rank with a specific spectrum. Moreover, we conducted a numerical search for the cases \( n = 2, 3, 4 \), suggesting an optimal scaling that is linear in \( n \).

Conclusion. — We have investigated the limitations on establishing correlations in the context of quantum thermodynamics. Starting from a system of product thermal states, we discussed the creation of the two most prominent and useful types of correlations, namely mutual information and entanglement. We introduced explicit protocols, and discussed their optimality. Moreover, we studied the thermodynamic limitations on the process of creating correlations, in terms of temperature and energy cost. From a more general perspective, the present work fits in a line of research investigating the interplay between quantum effects (such as entanglement) and ther-
modynamics. Beyond the fundamental interest, these questions are also relevant for information processing in systems where thermodynamical considerations cannot be ignored.

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APPENDIX A

In this appendix we prove that for equal energy spacings \( (E_k = k E_0) \) any local temperature \( T' > T \) lies in the unitary orbit of thermal product states at temperature \( T \). Furthermore this proof provides a constructive protocol that in this context reaches any amount of mutual information at minimally possible energy costs. Furthermore for general Hamiltonians this protocols provides a means to reach any sufficiently larger \( T' \) (for an exact condition see below) at minimal energy costs. First let us adopt the following convenient notation for the eigenvalue distribution of the marginal \( \tilde{p}^i_A := \text{diag}(\rho_A) \), which is sufficient for our purposes as the thermal states will always just be diagonal in energy eigenbasis. The general idea of the protocol that follows is that the global unitary should induce a doubly stochastic transformation \( M \) on the marginal probability vector, while ensuring that no coherences are created in any subsystem. First we decompose the marginal vectors as

\[
\text{diag}(\rho_A) = \sum_{i=0}^{d-1} \tilde{p}^i \quad \text{(11)}
\]

\[
\text{diag}(\rho_B) = \sum_{i=0}^{d-1} \Pi^i \tilde{p}^i \quad \text{(12)}
\]

with \( p^i_j = |j+\rangle \otimes |j+i\rangle \otimes |j+i\rangle = e^{-\beta(E_j+E_{j+1})/2Z^2} \) and \( \Pi = \sum_k |k\rangle \langle k+1| \). It will be useful to consider again the following generalized Bell states

\[
|B_{i,j}\rangle = \sum_{k=0}^{d-1} \omega^{k i} |k\rangle \otimes |k+j\rangle , \quad \text{(13)}
\]

with \( \omega = e^{2\pi i/d} \). Now it is straightforward to see that rotating in the subspaces spanned by \( S_i = \text{span}\{|B_{i,j}, B_{i,j}, \ldots, B_{d-1,j}\} \) ensures that every diagonal element that can be created by these rotations is being traced over. The unitarity ensures that rotations on the subspaces \( S_i \) induce a doubly stochastic transformation of the diagonal part of the density matrix in this subspace. Now all that is left is to observe that the probabilities in the decomposition of the subsystems correspond exactly to the rotations in the subspaces spanned...
by the maximally entangled states defined before, i.e.
\[
\text{diag}(\text{Tr}_B(U\rho U^\dagger)) = \sum_i M_i \tilde{p}_i
\]
(14)
\[
\text{diag}(\text{Tr}_A(U\rho U^\dagger)) = \sum_i \Pi'(M_i \tilde{p}_i)
\]
(15)
where each \(M_i\) is a doubly stochastic matrix. Now we can use the symmetry of the initial state, i.e. \(p_{ij} = p_{ji}\), and define a target doubly stochastic matrix \(M\) that should describe the transformation of both marginals. Since the vector \(\tilde{p}_0\) is equal for both marginals it is evident that \(M_0 = M\) already takes the first part out of the picture without restricting the generality of stochastic transformations.

In general if every doubly stochastic is equal, i.e. \(M_i = M\) and commutes with all \(\Pi'\), i.e. is a circulant matrix, it is evident (due to \(\sum_{i=0}^{d-1} \tilde{p}_i = \sum_{i=0}^{d-1} \Pi' \tilde{p}_i\)) that both subsystems’ probability vector will just be transformed by \(M\). In other words it is easily achievable to transform the subsystems probability distribution by any doubly stochastic matrix that commutes with all cyclic permutations, i.e. a circulant matrix.

The final question is thus whether circulant doubly stochastic transformations of the form \(T = \sum_i \alpha_i \Pi'\) are sufficient to reach any temperature, i.e. \(T \tilde{p}(\beta) = \tilde{p}(\beta')\forall \beta \geq \beta'\). Obviously starting from \(\beta = \infty\) one can reach all temperatures via choosing \(\alpha_i = p_i(\beta')\) and from any \(\beta\) one can reach the infinite temperature distribution via all \(\alpha_i = \frac{1}{\beta}\).

To address this question to its fullest extent we will first construct a general convex sum of cyclic permutations that achieves this general task and then check whether all coefficients are positive. We require that
\[
\sum_i \alpha_i \Pi' p_i(\beta) = p_\alpha(\beta')
\]
(16)
For sake of simplicity we will first define \(\alpha_i' = \alpha_i \frac{Z}{Z'}\) such that the condition is simplified to
\[
\sum_i \alpha_i' e^{-\beta E_{i+k}} = e^{-\beta' E_k}
\]
(17)
A set of \(\alpha_i'\) solving this equation system is given by
\[
\alpha_i' = \frac{\epsilon_{12}(...)(n-1-k) e^{-\beta E_{1} - \beta E_{2} - ... - \beta E_{n-1-k}}}{\epsilon_{12}(...)(n-1-k) e^{-\beta E_{1} - \beta E_{2} - ... - \beta E_{n-1-k}}}
\]
(18)
From this explicit form we can easily find negative coefficients and thus prove that circulant matrices are insufficient to reach any arbitrarily higher temperature. On the other hand we immediately see from very simple geometric considerations that for a sufficiently high difference in temperatures \(\Delta T = T' - T\) circulant matrices are always sufficient. Since the original probability vector is linearly independent from all its cyclic permutations and all of them are equally far in Euclidean distance from the infinite temperature distribution we can study the convex cone with \(\Pi' \tilde{p}_A\) as extremal rays. Since all of the extremal rays share the same distance to the center ray (infinite temperature), we know that a sufficient condition for circulant matrices to achieve the higher temperature Boltzmann distribution is simply given by the minimal distance from the central ray to all faces of the cone. This is always easily calculable for any energy distribution and gives a sufficient condition on \(\Delta T\) for this protocol to work.

Furthermore we can use the explicit solution to find Hamiltonians for which this protocol always works. One important example is equal energy spacing between the different levels, i.e. \(E_k = k E_0\). In this case the explicit solution for the \(\alpha_k\) is given as
\[
\alpha_k = 1 - \frac{Z' p'_i}{1 - Z p_1} \left( \delta_{0,k} + \frac{Z' p'_i - Z p_1}{1 - Z' p'_1} \delta_{k+d_0,k-1} \right)
\]
(19)
which is positive for all \(k\) due to the fact that \(p_0 > p'_0\), i.e. we have derived a protocol that delivers the maximally possible amount of mutual information at minimum energy costs for all Hamiltonians with equal energy spacing (and thus qubits as a special case).

**APPENDIX B**

Given an \(n\)-qubit thermal state \(\Omega = \sum e^{-\beta E} |\Omega\rangle\rangle\) we here find the \(n \gg 1\) asymptotics of the maximal temperature \(T_{GME}\) that allows to unitarily create genuinely multipartite entanglement (GME) in the ensemble with the W-state protocol and also calculate the energy cost of the protocol. Here \(T_{\beta} = \text{diag}(p, v)\), where \(p = 1/(1 + v)\) and \(v = e^{-\beta E}\) is the Boltzmann weight. If the eigenvectors corresponding to the first excited level of the total Hamiltonian are \(|w_1(1)\rangle_{i=1}^n\) and the ones corresponding to the second excited level are \(|w_2(1)\rangle_{i=1}^n\), then the measure we use has the form \(E[\Omega] = \sum_{i,j} \Omega_{ij} |2\sqrt{\Omega_{00}} \sum_a \sqrt{\Omega_{aa}} - (n-2)\sum_i \Omega_{ii}|20\)

where \(\Omega_{ij} = \langle w_1(1)|\Omega|w_j(1)\rangle\) and \(\Omega_{ab} = \langle w_1(2)|\Omega|w_2(2)\rangle\).

In short, the W-state protocol is the maximization of \(E\) over all such unitary operations that generate nondiagonal elements only in the eigensubspace of the first excited level (which we denote by \(W_1\)). These unitaries can be represented as \(UIU\), where \(UI\) is a permutation operation on the initial state and \(U\) is a general \(n \times n\) unitary living in \(W_1\). As this representation suggests, we divide the optimization procedure in two steps: (i) maximization over Us for a given \(I\), and (ii) maximization over\(I\). After \(I\) acts, the state becomes \(\Pi^U = I \rho U\Pi\) and its projection on \(W_1\) we denote by \(\omega^U\). Now, the operation \(U\) will act only on \(\omega^U\) and take it to \(\omega' = U\omega^U U^\dagger\) and since \(U\) is unitary, the traces of \(\omega'\) and \(\omega^U\) will be the same. Therefore, we
can rewrite (20) as
\[ E[U|\Omega|U] = -2\sqrt{\Omega_{|\alpha}} \sum_{\alpha} \sqrt{\Omega_{|\alpha}} - (n-2) \sum \omega_{ii}^\Pi. \] (21)

This shows that the maximization of \( E \) over \( U \) is reduced to the maximization of \( \sum_{i \neq j} |\omega_{ij}'|^2 \) over \( U \). To find this maximum, we first observe that due to the unitarity of \( U \), \( \text{Tr} ((\omega')^2) = \text{Tr} ((\omega^\Pi)^2) \); whence,
\[ \sum_{i \neq j} |\omega_{ij}'|^2 = \frac{\text{Tr} ((\omega^\Pi)^2) - \sum_i (\omega_i)^2}{2}. \] (22)

We now relax for the moment the constraint that \( \omega' \) and \( \omega^\Pi \) are unitarily connected and only require that \( \text{Tr} (\omega') = \text{Tr} (\omega^\Pi) \equiv \alpha \) and \( \text{Tr} ((\omega')^2) = \text{Tr} ((\omega^\Pi)^2) \equiv \alpha^2 \lambda \). Here we again divide the optimization in two steps:
1) maximize \( \sum_{i \neq j} |\omega_{ij}'|^2 \) with \( \sum_{i \neq j} |\omega_{ij}'|^2 \) fixed and 2) maximize the latter. Now we notice that
1) The maximum is reached for \( |\omega_{ij}'| = |\omega_{ij}'| \) and therefore
\[ \max \sum_{i \neq j} |\omega_{ij}'|^2 = \sqrt{n(n-1)/2} \sum_{i \neq j} |\omega_{ij}'|^2. \]
2) From (22), the maximum for \( \sum_{i \neq j} |\omega_{ij}'|^2 \) is reached when \( \sum_i (\omega_i)^2 \) is minimal. Since \( \sum_i \omega_i = \alpha \) is fixed, the minimum for \( \sum_i (\omega_i)^2 \) is reached when all \( \omega_i = \alpha/n \), i.e.,
\[ \max \sum_{i \neq j} |\omega_{ij}'|^2 = \alpha^2 (\lambda - 1/n)/2. \]
Finally,
\[ \max \sum_{i \neq j} |\omega_{ij}'|^2 = \alpha \sqrt{n(n-1)(\lambda - 1/n)}, \] (23)
and on this maximum, \( \omega' \) has the following form:
\[ \alpha \left( \frac{\frac{1}{n}}{e^{\phi_{12}} \sqrt{n/(n-1)}} \ldots e^{\phi_{1n}} \sqrt{n/(n-1)} \right) \ldots \left( \frac{e^{\phi_{n1}} \sqrt{n/(n-1)}}{e^{\phi_{n2}} \sqrt{n/(n-1)}} \ldots \frac{1}{n} \right). \] (24)

Obviously, being obtained in less restrictive conditions, (23) upper-bounds the sought \( \max U \sum_{i \neq j} |\omega_{ij}'|^2 \). Nevertheless, one can prove, that for suitably chosen \( \{\phi_{ij}\} \) the matrix in (24) can always be unitarily reached from \( \omega^\Pi \). The proof is slightly more involved and is conducted by first proving the statement for \( n = 3 \) by explicitly calculating the corresponding phases (only one phase is necessary to adjust there) and then proving the statement by induction for any \( n \).

Now, having done the maximization over \( U \), we turn to finding the \( \Pi \) with largest
\[ E^\Pi = \alpha \left( \sqrt{n(n-1)(\lambda - 1/n)} - n + 2 \right) - 2\sqrt{\Omega_{|\alpha}} \sum_{\alpha} \sqrt{\Omega_{|\alpha}}. \] (25)
where we have plugged (23) in (21). The quantity \( \lambda \) is defined above as the sum of the squares of the normalized elements of \( \omega^\Pi \). Therefore, it is never bigger than 1 which implies that in the \( n \rightarrow \infty \) limit, \( E^\Pi \) in (25) will be nonnegative only if \( \lambda \rightarrow 1 \). On the other hand, choosing a bigger \( \alpha \) and smaller elements in the eigensubspace of the second excited level (which we denote by \( W_2 \)) and on the ground state will also make \( E^\Pi \) bigger. To fulfill all this we choose \( \Pi \) so that it takes the smallest element of \( \Omega \), \( p^n v^n \), to the ground state, the biggest one, \( p^n \), to \( W_1 \). The rest of \( (n-1) \) elements in \( W_1 \) are chosen so that they are significantly smaller than \( p^n \). We will take them to be all equal (so that they keep \( \alpha \) as big as possible) and to be \( p^n v^{n-k} \) with some \( k \) that will be discussed later on.

Also, we will choose the elements in \( W_2 \) to be \( p^n v^{n-m} \) with some \( m \) that is small and independent of \( n \). At this point we do not know which exact choice of \( k \) and \( m \) will maximize \( E^\Pi \), but fortunately the existing information about them is enough to deduce the asymptotics we need.

With above described \( \Pi \) we have
\[ \lambda = \frac{1 + (n-1)v^{2(n-k)}}{1 + (n-1)v^{n-k)}}. \] (27)

So, to have \( \lambda \rightarrow \infty \), \( m^{n-k} \) must \( \rightarrow 0 \). With this condition and some algebraic manipulations employing Taylor expansions, we arrive at the following asymptotical expansion:
\[ \frac{E^\Pi}{p^n} = 1 - n^2 v^{n-k-m/2} C_n + O \left[ n^3 v^{2(n-k)} \right], \] (28)
where \( C_n = (1 - 1/n)^2 (v^{m/2} + v^k n/(n-1)) \) and is always \( O[1] \) since \( v < 1 \) and \( k \) and \( m \) are positive. With this, we rewrite (28) as
\[ \frac{E^\Pi}{p^n} = 1 - n^2 v^{n-k-m/2} C_n \left( 1 + O \left[ nv^{n-k} \right] \right). \] (29)

Having in mind that \( n^{n-k} \rightarrow 0 \) and explicitly indicating the dependence of \( k \) and \( T \) (and hence \( v \)) on \( n \) we obtain from (29) the asymptotic condition of the positivity of \( E^\Pi \) in the following form:
\[ 1 \geq n^2 v^{n-k-m/2} C_n = e^{\ln C_n + 2 \ln n - \frac{n-k-m/2}{\Omega_{GME}^0}}. \] (30)

From formula (30) it is now obvious that to maximize \( T_{GME} \), \( k_n \) has to be as small as possible. So, whatever the \( k_n \) and \( m \) delivering the maximum are, they are finite numbers independent of \( n \). Therefore,
\[ T_{GME}^{\max} = \frac{n}{2 \ln n} + O \left[ \frac{n}{(\ln n)^2} \right]. \] (31)
degenerate subspace. Adding the cost of all the permutations above gives the rather cumbersome formula for the energy cost of the W-state protocol as

\[
W = E(1 - e^{-\beta E})^{-n} (n-1)(e^{-\beta E} - e^{-\beta E(n-1)}) + \\
(1 - e^{-\beta E}) + n(e^{-\beta E(n-3)} - e^{-\beta En}) + \\
(n^2 - n)(e^{-2\beta E} - e^{-(n-2)\beta E}) + \\
3(e^{-\beta En} - e^{-\beta E(n-3)})
\]

which while seemingly complicated due to the numerous required permutations still remains exponentially small in \(n\) for any \(T > 0\).