

Entanglement in pure and thermal cluster states

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Abstract. We present a closest separable state to cluster states, which in turn allows us to calculate the entanglement scaling using relative entropy of entanglement. We reproduce known results for pure cluster states and show how our method can be used in quantifying entanglement in noisy cluster states. Operational meaning is given to our method, which clearly demonstrates how these closest separable states can be constructed from two-qubit clusters in the case of pure states. We also discuss the issue of finding the critical temperature at which the cluster state becomes only classically correlated and the importance of this temperature to our method.

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1. Introduction

Entanglement plays an important role in modern physics and is the subject of intense research for both its implications in our fundamental understanding of nature [1] and its practical usefulness in quantum information processing [2, 3]. Different models of quantum computing have been devised to harness this usefulness. The most prominent ones include the circuit model [4], topological computing [5] and measurement-based computing [6].

Measurement-based quantum computation (or one-way quantum computation) differs from the circuit model by using an initially prepared highly entangled resource state. The algorithm proceeds as a set of local measurements on this state. The basis and order of these measurements characterize the algorithm, and outcomes of previous measurements are fed forward to make the computation deterministic.

The general resource for this computation model is graph states [7]. In this paper, we will concentrate on particular graph states, namely cluster states [8]. Unlike graph states, cluster states have regular square structure. One of the advantages of one-way quantum computation is that all the entanglement used in the algorithm is present right at the beginning. The subsequent measurements only consume it. This makes it easier to identify the role of entanglement in the information processing compared to the traditional circuit model. Recently it has also been shown both theoretically and experimentally in [9] that the quantum computational power of cluster states can be extended by replacing some projective measurements with generalized quantum measurements. This makes cluster state quantum computation a very attractive and promising prospect when it comes to constructing a quantum computer.

Due to its clear role as a resource in one-way quantum computation, it is highly desirable to know the entanglement properties of cluster states. Perhaps one of the most important problems in studying the properties of quantum states, and resource states for quantum computation in particular, is the quantification of entanglement itself. The entanglement scaling of pure d -dimensional graph states has been shown by Markham *et al* to be $N/2$ [10]. However, any realistic quantum computer will operate at finite temperatures, which makes it necessary to be able to characterize the entanglement of mixed states. Quantifying entanglement is a notoriously difficult task [11] and the exact scaling of entanglement in thermal cluster states is still unknown, although some advances have been made by investigating the localization of entanglement in noisy cluster states [12].

There are many entanglement measures that quantify the scaling of entanglement in quantum states. In this work, we use the relative entropy of entanglement (see [19, 20]) to quantify the scaling. In general, there are not many multipartite quantum states for which the relative entropy of entanglement can be calculated analytically. D -dimensional symmetric states are one of the few examples [13, 14]. How to find the closest separable state to a general entangled state is unknown, and the problem of closed form of the relative entropy still remains an open question. Although some progress has been made in this direction [15, 16], it is impossible to do this even for a general two-qubit state.

We present a method of constructing the closest separable state to a thermal cluster and show how it can reproduce the results of Markham *et al* [10] for pure cluster states in section 2. Thermal cluster states can be described by a Hamiltonian with many-body interactions, which is why they do not occur in nature. However, they can be approximated by naturally occurring two-body couplings using perturbative gadgets [17] and projected entangled pair states [18], which are outlined in section 3. Noisy cluster states also arise in experiments using neutral atoms in optical lattices due to magnetic sensitivity of the hyperfine levels of these atoms. In section 4,

we discuss how entanglement in these states can be quantified. We also show how bound entanglement complicates the procedure of finding the closest separable state for noisy cluster states.

2. Pure cluster states

The entanglement of cluster states is known to scale linearly with the size of the system as $N/2$. This result was first obtained by Markham *et al* [10]. The authors used a technique where they derived upper and lower bounds on the entanglement, and then they showed that these two bounds are equal.

In this section, we verify this result using geometrical ideas. To do this, we employ the relative entropy of entanglement [19, 20] $E(\sigma)$ defined as

$$E(\sigma) = \min_{\rho \in \mathcal{D}} S(\sigma \parallel \rho), \quad (1)$$

where σ is the entangled state. The minimization is taken over the set \mathcal{D} of all separable states ρ and $S(\sigma \parallel \rho) = \text{Tr}[\sigma \log \sigma - \sigma \log \rho]$ is the relative entropy. For pure states, this simplifies to $S(\sigma \parallel \rho) = -\text{Tr}[\sigma \log \rho]$. Since we are considering only qubits, we take the logarithm to base 2. The state that minimizes the relative entropy in (1) will be designated by ρ^* and will be called the closest separable state. In order to prove that this state ρ^* achieves the minimum of relative entropy, we employ the same approach as in [21]. Consider a small region around the closest separable state $(1-x)\rho^* + x\tau$ for a small parameter x . All we have to show now is that for a general separable state τ , the gradient of relative entropy is non-negative in this region. Due to convexity of the set of separable states, this will also mean that the minimum of relative entropy is global.

A cluster state can be thought of as a state whose qubits are first prepared in the $+1$ eigenstate of σ^x and then control-phase gates CZ are applied between nearest neighbours. For example, the two-qubit cluster state is $|\psi_2\rangle = CZ|+\rangle|+\rangle = \frac{1}{2}[|00\rangle + |01\rangle + |10\rangle - |11\rangle]$. It can be easily seen that the closest separable state ρ_2^* is

$$\rho_2^* = \frac{1}{4} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \end{pmatrix} \quad (2)$$

by calculating that $E(\sigma_2 \parallel \rho_2^*) = 1$, where $\sigma_2 = |\psi_2\rangle\langle\psi_2|$.

So far all the states have been expressed in the computational basis $\{|0\rangle, |1\rangle\}$. It is, however, more useful to write the states in what we call the ‘mixed’ basis $\{|0\rangle, |1\rangle, |+\rangle, |-\rangle\}$. So the state vector and the closest separable state for the case of two qubits now become

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}[|0+\rangle + |1-\rangle], \quad (3)$$

$$\rho_2^* = \frac{1}{2}[|0+\rangle\langle 0+| + |1-\rangle\langle 1-|]. \quad (4)$$

Similarly for four qubits the expressions take the following form:

$$|\psi_4\rangle = \frac{1}{2}[|0+0+\rangle + |0-1-\rangle + |1-0+\rangle + |1+1-\rangle], \quad (5)$$

$$\rho_4^* = \frac{1}{4}[|0+0+\rangle\langle 0+0+| + |0-1-\rangle\langle 0-1-| + |1-0+\rangle\langle 1-0+| + |1+1-\rangle\langle 1+1-|]. \quad (6)$$

| | Vector $ \psi_N\rangle$ | Cluster σ_N | Separable ρ_N^* |
|---------------------|-------------------------|--------------------|----------------------|
| Computational basis | $2^{-N/2}$ | 2^{-N} | 2^{-N} |
| 'Mixed' basis | $2^{-N/4}$ | $2^{-N/2}$ | $2^{-N/2}$ |

From the form of ρ_2^* , and ρ_4^* , we can see that the closest separable state is obtainable from the state vector by writing the density matrix in the 'mixed' basis and then keeping only the diagonal terms. This is why it is more instructive to work in the 'mixed' basis; one can immediately see the form of the closest separable state from the state vector. Of course, in the computational basis, not all off-diagonal terms are zero.

An important thing to notice is that the number of terms in the state vector of a cluster state is different in the computational basis and in the 'mixed' basis. In the computational basis all the coefficients are nonzero; they are either 1 or -1 . Hence for the N -qubit cluster state, there are 2^N basis coefficients. On the other hand, in the 'mixed' basis the number of coefficients drops to $2^{N/2}$. So when it comes to normalization coefficients for the density matrices, we have the coefficients summarized in the table on this page.

From the above, it is clear that the closest separable matrix ρ_N^* is of rank $2^{N/2}$. Another useful fact that will be used later is that when the matrices are expressed in the 'mixed' basis, it is easy to see that they commute with the cluster state $[\rho_N^*, \sigma_N] = 0$.

Before we start the proof for the closest separable state, a small note about our notation is in order. The proof contains places where instead of just writing σ_N or ρ_N^* , it is more instructive to write out the state explicitly, for instance for two qubits $\sigma = \frac{1}{2}(|0+\rangle + |1-\rangle) * (\langle 0+| + \langle 1-|)$. This is of course not possible in the case of general N . Therefore, we use the following notation:

$$\begin{aligned}
 \text{pure vector} & \quad |\psi_N\rangle = 2^{-N/4}(|\dots\rangle + \dots), \\
 \text{pure matrix} & \quad \sigma_N = 2^{-N/2}(|\dots\rangle + \dots) * (\langle \dots| + \dots), \\
 \text{closest sep. state} & \quad \rho_N^* = 2^{-N/2}(|\dots\rangle\langle \dots| + \dots).
 \end{aligned}$$

From the normalization factors it is clear that the states are in the 'mixed' basis. This also implies that each round bracket contains $2^{N/2}$ terms.

As mentioned above, to prove that states of the form ρ_2^* and ρ_4^* are really the closest separable states, we need to show that the gradient of relative entropy in a small region around ρ_N^* is non-negative:

$$\lim_{x \rightarrow 0} \frac{\partial}{\partial x} S(\sigma \parallel (1-x)\rho_N^* + x\tau) \geq 0. \quad (7)$$

Substituting $f(x, \tau) = S(\sigma \parallel (1-x)\rho_N^* + x\tau)$ and realizing that for a positive operator A we have the expression

$$\log A = \int_0^\infty \frac{At - 1}{A + t} \frac{dt}{1 + t^2},$$

condition (7) becomes

$$\frac{\partial f}{\partial x}(0, \tau) = \text{Tr} \left[\sigma \int_0^\infty (\rho_N^* + t)^{-1} (\rho_N^* - \tau) (\rho_N^* + t)^{-1} dt \right] \geq 0. \quad (8)$$

Starting with the first integral in equation (8)

$$\begin{aligned} &= \text{Tr} \left[\sigma \int_0^\infty (\rho_N^* + t)^{-1} \rho_N^* (\rho_N^* + t)^{-1} dt \right] \\ &= \text{Tr} \left[\sigma \int_0^\infty (\rho_N^* + t)^{-2} dt \rho_N^* \right]. \end{aligned} \quad (9)$$

Evaluating the integral in equation (9),

$$\begin{aligned} \int_0^\infty (\rho_N^* + t)^{-2} dt &= \int_0^\infty (2^{-N/2} + t)^{-2} dt (|\dots\rangle\langle\dots| + \dots) \\ &= \int_0^\infty (2^{-N/2} + t)^{-2} dt * 2^{N/2} \rho_N^* \\ &= 2^{N/2} * 2^{N/2} \rho_N^* \\ &= 2^N \rho_N^*. \end{aligned} \quad (10)$$

Substituting this back into equation (9),

$$\begin{aligned} \text{Tr}[\sigma * 2^N \rho_N^* \rho_N^*] &= 2^N [\sigma * 2^{-N} (|\dots\rangle\langle\dots| + \dots) * (|\dots\rangle\langle\dots| + \dots)] \\ &= \text{Tr}[\sigma (|\dots\rangle\langle\dots| + \dots)] \\ &= 2^{-N/2} * 2^{N/2} = 1. \end{aligned} \quad (11)$$

Now we turn our attention to the second integral in equation (8). Here we will use the fact that σ and ρ_N^* commute with each other,

$$\begin{aligned} &= \text{Tr} \left[\int_0^\infty (\rho_N^* + t)^{-1} \sigma (\rho_N^* + t)^{-1} dt \tau \right] \\ &= \text{Tr} \left[\int_0^\infty (\rho_N^* + t)^{-2} dt \sigma \tau \right] \\ &= 2^N \text{Tr}[\rho_N^* \sigma \tau] \\ &= 2^N \text{Tr}[2^{-N/2} 2^{-N/2} (|\dots\rangle\langle\dots| + \dots) * (|\dots\rangle + \dots) * (\langle\dots| + \dots) \tau] \\ &= \text{Tr}[(|\dots\rangle\langle\dots| + \dots) * (|\dots\rangle + \dots) * (\langle\dots| + \dots) \tau] \\ &= \text{Tr}[(|\dots\rangle + \dots) * (\langle\dots| + \dots) \tau] \\ &= 2^{N/2} [\sigma \tau]. \end{aligned} \quad (12)$$

So finally the gradient of the relative entropy in equation (8) can be written as

$$\frac{\partial f}{\partial x}(0, \tau) = 1 - 2^{N/2} \text{Tr}[\sigma \tau]. \quad (13)$$

In order for equation (13) to be non-negative, the trace needs to scale at most as $2^{-N/2}$. This is in fact the case as can be proven by induction. First, we will consider $\tau = |\alpha\beta\rangle\langle\alpha\beta|$. The inequality has been verified numerically for two, four and six qubits. In the case of two qubits, a graphical solution has been obtained as well in figure 1.

$$\begin{aligned} N = 2, \quad \text{Tr}[\sigma_2 \tau_2] &\leq \frac{1}{2} = 2^{-1}, \\ N = 4, \quad \text{Tr}[\sigma_4 \tau_4] &\leq \frac{1}{4} = 2^{-2}, \\ N = 6, \quad \text{Tr}[\sigma_6 \tau_6] &\leq \frac{1}{8} = 2^{-3}. \end{aligned} \quad (14)$$

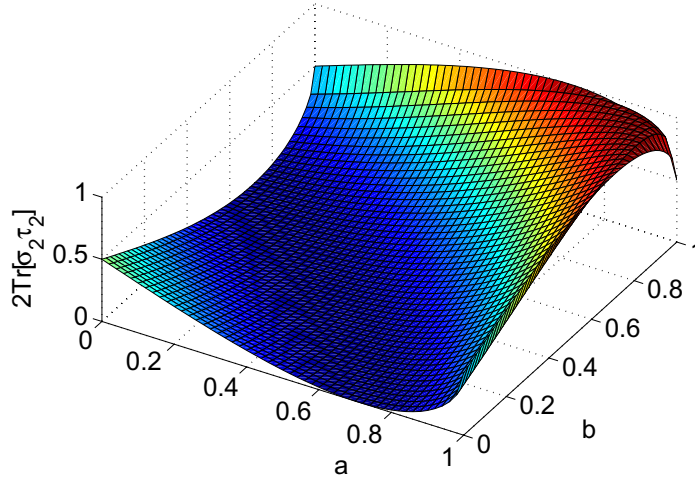


Figure 1. Plot of $2\text{Tr}[\sigma_2\tau_2]$ showing that the maximum of the trace is 1 and therefore the gradient of relative entropy is non-negative. Here a and b are parameters from τ representing the different amplitudes for the two subsystems. So $\tau = |\alpha\beta\rangle\langle\alpha\beta|$, where $|\alpha\rangle = a|0\rangle + \sqrt{1-|a|^2}|1\rangle$ and similarly $|\beta\rangle = b|0\rangle + \sqrt{1-|b|^2}|1\rangle$.

Assume that the above holds true for the case of $N = k$, namely $\text{Tr}[\sigma_k\tau_k] \leq 2^{-k/2}$. Now we need to prove, using the above assumption, that the case $N = k + 2$ holds true:

$$\text{Tr}[\sigma_{k+2}\tau_{k+2}] \leq 2^{-k/2-1}. \quad (15)$$

We start with the trace

$$\begin{aligned} \text{Tr}[\sigma_{k+2}\tau_{k+2}] &= \langle\psi_{k+2}|\tau_{k+2}|\psi_{k+2}\rangle \\ &= \langle\psi_k|\langle\psi_2|CZ^\dagger\tau_k \otimes \tau_2 CZ|\psi_k\rangle|\psi_2\rangle, \end{aligned} \quad (16)$$

where we have used the fact that $|\psi_{k+2}\rangle = CZ|\psi_k\rangle|\psi_2\rangle$ and $\tau_{k+2} = \tau_k \otimes \tau_2$. The control-phase gate acts on qubits k and $k+1$. Also the separable state τ does not commute with the controlled phase gate so their commutator is nonzero $[\tau_k \otimes \tau_2, CZ] = A$ and we can substitute $\tau_k \otimes \tau_2 CZ = A + CZ\tau_k \otimes \tau_2$ into equation (16).

$$\text{Tr}[\sigma_{k+2}\tau_{k+2}] = \langle\psi_k|\langle\psi_2|CZ^\dagger A|\psi_k\rangle|\psi_2\rangle + \langle\psi_k|\tau_k|\psi_k\rangle * \langle\psi_2|\tau_2|\psi_2\rangle. \quad (17)$$

Taking a closer look at the product $CZ^\dagger A$ and using the above commutation relation, we obtain $CZ^\dagger A = CZ^\dagger\tau_k \otimes \tau_2 CZ - \tau_k \otimes \tau_2$. Taking the trace of both sides,

$$\text{Tr}[CZ^\dagger A] = \text{Tr}[CZ^\dagger\tau_k \otimes \tau_2 CZ] - \text{Tr}[\tau_k \otimes \tau_2] = 0. \quad (18)$$

Using the assumption for $N = k$, this implies

$$\text{Tr}[\sigma_{k+2}\tau_{k+2}] = \langle\psi_k|\tau_k|\psi_k\rangle * \langle\psi_2|\tau_2|\psi_2\rangle \leq 2^{-k/2-1}. \quad (19)$$

Therefore $(\partial f/\partial x)(0, |\alpha\beta \dots\rangle\langle\alpha\beta \dots|) \geq 0$. Since any separable state can be written in the form $\rho = \sum_i p^i |\alpha^i \beta^i \dots\rangle\langle\alpha^i \beta^i \dots|$, we have

$$\frac{\partial f}{\partial x}(0, \rho) = \sum_i p^i \frac{\partial f}{\partial x}(0, |\alpha^i \beta^i \dots\rangle\langle\alpha^i \beta^i \dots|) \geq 0. \quad (20)$$

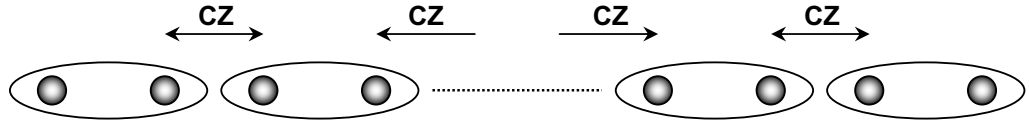


Figure 2. Closest separable state of N qubits. Each pair of qubits represents the closest separable state ρ_2^* .

Therefore ρ_N^* is the closest separable state to σ_N . Now we can compute the relative entropy between the cluster state σ_N and ρ_N^* :

$$\begin{aligned}
 E(\sigma_N) &= S(\sigma_N \parallel \rho_N^*) \\
 &= -\text{Tr}[\sigma_N \log \rho_N^*] \\
 &= -\langle \psi_N | \log \rho_N^* | \psi_N \rangle \\
 &= -\log \langle \psi_N | \rho_N^* | \psi_N \rangle \\
 &= -\log 2^{-N} 2^{N/2} \\
 &= -\log 2^{-N/2} = \frac{N}{2}.
 \end{aligned} \tag{21}$$

This concludes the proof that our closest separable state gives a linear scaling of entanglement and reproduces the results of Markham *et al* [10].

We can look at the form of the closest separable state from a more operational point of view. Imagine we are asked to prepare the closest separable state to an N -qubit one-dimensional cluster state. The only ingredients needed to construct this state are the two-qubit closest separable state ρ_2^* and the control-phase gates CZ . The state ρ_N^* can be written as

$$\rho_N^* = U * \underbrace{(\rho_2^* \otimes \rho_2^* \otimes \cdots \otimes \rho_2^*)}_{N/2} * U^\dagger, \tag{22}$$

where the unitarity applied has the form

$$U = I \otimes \underbrace{CZ \otimes CZ \otimes \cdots \otimes CZ}_{N/2-1} \otimes I. \tag{23}$$

All the unitary (23) implements are control-phase gates CZ between qubits 2–3 and 4–5 and so on. It connects the states ρ_2^* together in a chain as shown in figure 2. It is important to notice that although control-phase gates are entangling operations, they leave the state ρ_N^* in a separable form.

This can easily be seen if we consider two separable two-qubit states (2) joined by a control-phase operation. The total four-qubit state can be written as $\rho_4^* = CZ_{2,3} \rho_2^* \otimes \rho_2^* CZ_{2,3}^\dagger$. This state is locally equivalent to $\rho_4^* = \frac{1}{4} [|0000\rangle \langle 0000| + |0111\rangle \langle 0111| + |1011\rangle \langle 1011| + |1100\rangle \langle 1100|]$, where we have applied Hadamard operators on every second qubit $I \otimes H \otimes I \otimes H$. The transformed state ρ_4^* is clearly separable. Since identical analysis can be applied to ρ_N^* , we conclude that control-phase operations in the unitary (23) do not introduce any entanglement and ρ_N^* remains separable.

It is important to note that the form of the closest separable state is the same for cluster states in higher dimensions as well. The majority of the proof for closest separable states is independent of the dimension of our cluster state. The dimensionality becomes important only in equation (16), where we assume a one-dimensional cluster state by using $|\psi_{k+2}\rangle = CZ|\psi_k\rangle|\psi_2\rangle$,

where the control-phase gate is applied between qubits k and $k + 1$. For higher dimensions, the number of control-phase gates in equation (16) increases due to the larger number of neighbouring qubits. However, the logic of the proof remains unchanged. Therefore, it is possible to find the closest separable state to a pure cluster state of any dimensionality. This is crucial because unlike linear cluster chains, two- and higher-dimensional clusters are universal resources for quantum computation [6].

3. Thermal entanglement

Entanglement has been studied in the context of condensed matter in some simple spin chains, mainly the XY Heisenberg model and the transverse Ising model [22, 23]. Properties of entanglement were also computed in cluster states created in triangular optical lattices in [24]. These studies concentrate on the importance of quantum effects in both classical and quantum phase transitions where either the temperature or some external parameter is varied. This is achieved by looking at the diverging behaviour of entanglement length [25] between pairs of qubits. This approach is suited for the study of phase transitions where two-particle correlations play a fundamental role. However, by looking at only reduced density matrices of two-qubit systems, a large amount of information about the rest of the system and its correlations is discarded.

Our aim in this and the next section is to look at entanglement in cluster states at a finite temperature. By using the relative entropy of entanglement, no information is thrown away about quantum correlations in our system. The study of thermal entanglement is of great significance since any realistic scheme of implementing a quantum computer will operate at finite temperatures. We are interested in seeing at what temperature the thermal fluctuations destroy all the entanglement in our system. Doing this allows us to find new closest separable states to both pure and thermal cluster states.

Consider the cluster Hamiltonian

$$H = -J \sum_{j=1}^N \sigma_j^x \bigotimes_{i \in \mathcal{N}} \sigma_i^z, \quad (24)$$

where J is the coupling constant and \mathcal{N} is the neighbourhood of site j . The terms in the sum above are just a particular case of stabilizer operators [6]. Hence, Hamiltonian (24) is also referred to as the stabilizer Hamiltonian. The ground state of this Hamiltonian is the cluster state. Excited states are achieved by local σ_j^z flips. The ground state has energy $-NJ$ and is non-degenerate. The k th excited state has energy $J(-N + 2k)$ with degeneracy $N!/k!(N - k)!$ [26]. The energy gap is $2J$. All the states in the spectrum of the Hamiltonian are equally entangled since they are all some σ^z away from the ground state. Therefore our method of finding the closest separable state can also be used on these excited states.

Hamiltonians like the one in equation (24) contain many-body interaction terms and do not occur directly in nature. This has been formally proven by Nielsen [27], where he showed that the cluster state does not occur as the exact ground state of any physical system in nature. However, Hamiltonians of this type can be simulated using only two-body interaction Hamiltonians. To illustrate how this works, we will first explicitly calculate how a three-body one-dimensional stabilizer Hamiltonian can be simulated by two-body interactions using the approach of Dür *et al* [28]. This is a standard and most straightforward way of seeing how three-body interactions can be approximated using only two local Hamiltonians. Below we also present two general methods in approximating the stabilizer Hamiltonian. One approach relies

on the use of perturbative gadgets used by Kempe [17] and the other on projected entangled pair states (PEPS) introduced by Verstraete [18].

We start by demonstrating on a simple example how many-body interactions can be approximated by two local Hamiltonians. Consider applying different Hamiltonians in sequence for a short period of time δt . Then by a clever choice of these Hamiltonians, we can make all first-order terms in δt vanish in the Taylor expansion of the unitary that the Hamiltonians generate. Higher-order terms in δt will then contain many-body interactions [28].

Consider a unitary evolution given by applying four different Hamiltonians $U = e^{iH_4\delta t} e^{iH_3\delta t} e^{iH_2\delta t} e^{iH_1\delta t}$. Taylor expanding this unitary operator and setting $H_4 = -H_2$ and $H_3 = -H_1$, we obtain

$$U = e^{i2\delta t^2(-i/2)[H_1, H_2]} + O(\delta t^3). \quad (25)$$

Therefore, this sequence describes, up to higher order, the action of an effective Hamiltonian that is

$$H_{\text{eff}} = -(i/2)[H_1, H_2], \quad (26)$$

which can describe a three-body interaction. Choosing the two-body Hamiltonians to be $H_1 = \sigma_1^z \sigma_2^y$ and $H_2 = \sigma_2^z \sigma_3^z$ leads to the effective interaction $-(i/2)[H_1, H_2] = \sigma_1^z \sigma_2^x \sigma_3^z$. Hence, two-body interactions can simulate a one-dimensional cluster Hamiltonian. The same technique can be applied recursively to simulate general many-body interactions. However, note that there is a dilation factor of $2/\delta t$; hence the required physical time to implement a three-body interaction is longer.

The above example can be generalized by the use of perturbative gadgets [17], which were introduced to construct a two-local Hamiltonian whose low-energy effective Hamiltonian corresponds to a three-local interaction. They can also be used to obtain arbitrary k -local effective interaction by direct application of k th order perturbation theory as shown in [29]. The essence of this method is to make use of ancilla qubits to create an effective many-body interaction out of two-body couplings. Unfortunately, this method has one shortcoming in that the parameters in the perturbing Hamiltonian need to be controlled with precision that increases with the size of the system, which makes this approach unsuitable for simulating large systems.

A different approach to simulating the interactions in (24) by using only two local Hamiltonians is due to Verstraete and Cirac [18] and their use of PEPS. Cluster states can be obtained through a projection of a number of virtual qubits prepared in maximally entangled states to a smaller number of physical qubits. Imagine a lattice with c qubits placed at each site. This number depends on the total number of bonds that connect a qubit to other sites. In PEPS representation, we first prepare each pair of virtual qubits in the state $|C_2\rangle = \frac{1}{\sqrt{2}}(|0+\rangle + |1-\rangle)$. We proceed by projecting these qubits onto physical qubits using $P = |0\rangle\langle 00 \dots 0| + |1\rangle\langle 11 \dots 1|$ at each site to obtain the desired cluster state.

When reversed, this idea can be used to consider a larger number of physical qubits interacting through nearest-neighbour two-body couplings that are then projected down to a smaller number of logical qubits as proposed in [30] to simulate a cluster state. In this approach, a number of qubits, depending on the geometry of the lattice, are placed at each site. They interact through nearest-neighbour Ising interaction $H_0 = -\sum_{\mu} \sum_{\langle i, j \rangle} \sigma_{\mu, i}^z \otimes \sigma_{\mu, j}^z$. Here μ counts the number of lattice points and $\langle i, j \rangle$ represents the nearest-neighbouring qubits within a lattice site. The role of this Hamiltonian is to implement the projection P at each site onto logical states $|0\rangle$ and $|1\rangle$. This is achieved only when the qubits interact strongly within a site. Across the lattice sites a different interaction is introduced, $V = -\sum_{\mu} \sum_i \sigma_{(\mu, i)}^x \otimes \sigma_{(v(i), i)}^z$. The total

Hamiltonian can then be represented as $H = gH_0 + \lambda V$. Perturbation theory can then be applied when $g \gg \lambda > 0$. The effective stabilizer Hamiltonian is then obtained from higher-order terms in the perturbation. Due to the nature of this approach, the logical state will not be the exact cluster state, but the errors arising from perturbation can be made arbitrarily small by careful manipulation of the interaction strengths g and λ . This was performed on a square lattice in [30] and a more detailed calculation and a generalization for graph states were presented in [31].

The ground state of the stabilizer Hamiltonian is highly entangled and the entanglement scales linearly with the size of the cluster state as $N/2$ [10]. Using this Hamiltonian allows us to calculate the thermal state $\sigma(\beta) = e^{-\beta H} / \text{Tr}[e^{-\beta H}]$. Since the terms in the summation (24) commute with each other, the thermal state takes the form

$$\sigma(\beta) = \frac{1}{2^N} \prod_j^N [I + \tanh(\beta J) K_j], \quad (27)$$

where K_j is the stabilizer operator at site j [12]. Because the higher excitations can be achieved by local σ^z flips, we can introduce a completely positive map D acting on a state $D(\rho) = D_1 \otimes \cdots \otimes D_N(\rho)$ where the local dephasing channels take the form

$$D_i(\rho) = (1 - p)\rho + p\sigma_i^z \rho \sigma_i^z. \quad (28)$$

So with a probability p , a σ^z is applied to site j . The mixed state obtained after applying the dephasing channel D with equal probability for all sites $p = 1/(1 + e^{\beta J})$ is equivalent to the thermal state (27) as shown in [34].

Generating a cluster state requires implementing the stabilizer Hamiltonian and cooling the system to its ground state. Practically this is not possible because the state will always be at a finite temperature. Therefore, it will be mixed and have the form (27). Cluster states can also be generated by using neutral atoms trapped in a periodic potential of an optical lattice [35]. Allowing these atoms to interact with their nearest neighbours implements the control-phase gates needed for creation of a cluster state. These operations are massively parallel and the whole system can be entangled in one single step. The qubits are encoded into two magnetically sensitive hyperfine levels of the neutral atoms. This means that the state undergoes decoherence from stray magnetic fields. These errors take the form of local σ^z errors and therefore the state is described by the local dephasing channel (28). By applying our techniques of entanglement quantification from section 2, we directly study how the environment degrades quantum correlations in these experiments.

An interesting question to ask is whether this entanglement persists at finite temperatures and where is the critical point beyond which the thermal entangled state becomes separable. For simplicity, we will now consider a two-qubit thermal cluster state of the form

$$\sigma_2(\omega) = \frac{1}{4}(I + \omega\sigma^x \otimes \sigma^z)(I + \omega\sigma^z \otimes \sigma^x), \quad (29)$$

where $\omega = \tanh(\beta J)$. So in the low-temperature limit as $T \rightarrow 0$, we recover the pure state because $\omega \rightarrow 1$. As the temperature increases, $\omega \rightarrow 0$ and for $T \rightarrow \infty$ we obtain a maximally mixed state. To calculate the critical temperature at which the state becomes separable, we use the Peres–Horodecki criterion [32, 33]. To see when the state fails to be positive definite, we have to solve the following equation: $\omega_c^2 + 2\omega_c - 1 = 0$. This equation has two solutions, $\omega_c = -1 \pm \sqrt{2}$, but we will disregard the negative solution because it is not physical. Substituting this back into $\omega = \tanh(\beta J)$ finally gives us the critical temperature

$$T_c = -\frac{2J}{k_B \ln(\sqrt{2} - 1)}. \quad (30)$$

The entanglement for $T < T_c$ happens to be of useful distillable nature [34]. Therefore by using local operations and classical communication on multiple copies of the thermal cluster, pure entanglement can be distilled that can be subsequently used in quantum computation. The protocol to achieve this and a proof of the optimality of the rate of distillation is given in [34] as well. This critical temperature for distillable entanglement remains unchanged for higher dimensions and any system size N , as proven in [26]. For temperatures above the critical temperature, $T \geq T_c$, the N -qubit cluster state, where $N > 2$, is not fully separable but is bound entangled [36]. The critical temperature at which all entanglement vanishes is nontrivial to find because properties of bound entanglement are still not fully understood.

An interesting point to note about the value of the critical temperature is that it has the same form as the critical temperature for phase transition in the two-dimensional Ising model [37, 38]. A two-dimensional ferromagnet can be modelled by nearest-neighbour interactions between spin- $\frac{1}{2}$ particles on a square lattice by a Hamiltonian $H_I = -J \sum_{i=1}^{L_x} \sum_{j=1}^{L_y} (\sigma_{i,j} \sigma_{i+1,j} + \sigma_{i,j} \sigma_{i,j+1})$, where L_x and L_y count the size of the lattice in the horizontal and vertical directions, respectively. This system displays a phase transition at critical temperature (30). Above this temperature it is energetically more favourable for the spins to be completely disordered. Below this temperature the spins assume an ordered configuration, all pointing either up or down to minimize the free energy. An important fact to note is that the critical temperature of phase transition in the Ising model is not dimensionality independent like the one for survival of distillable entanglement in thermal cluster states. There is no finite critical temperature for the one-dimensional Ising chain and the critical temperature in a three-dimensional system has so far only been estimated numerically. Ising-type interaction is used when implementing the control-phase gate when generating the cluster state. Although other interesting parallels can be drawn between one-way quantum computation and theory of phase transitions as detailed in [39], why the two critical temperatures are identical in two completely different systems is still unknown.

We have already calculated the closest separable state for a two-qubit cluster. Now we will show that this state is not unique. In fact there are infinitely many states that satisfy condition (7). Since there is no bound entanglement for the case of two qubits, we know that the thermal cluster state at the critical temperature T_c is fully separable. It is natural to ask the question: what the distance is between this state and a pure cluster state in terms of the relative entropy. So we want to calculate $S(\sigma_2 \parallel \sigma_2(\omega_c))$, where $\sigma_2(\omega_c) = \frac{1}{4}(I + \omega_c \sigma^x \otimes \sigma^z)(I + \omega_c \sigma^z \otimes \sigma^x)$ and $\omega_c = \sqrt{2} - 1$. It can be quickly checked that $S(\sigma \parallel \sigma_2(\omega_c)) = 1$ and the gradient of relative entropy in a small region around $\sigma_2(\omega_c)$ is $(\partial f / \partial x)(0, \tau) = 1 - 2\text{Tr}[\sigma \tau] \geq 0$, as can be seen from equation (14). Therefore the two-qubit thermal cluster at critical temperature is another good closest separable state to the pure cluster state.

It is instructive to look at the thermal cluster state $\sigma_2(\omega)$ in the ‘mixed’ basis and compare it to the pure cluster closest separable state ρ_2^* . Transforming $\sigma_2(\omega)$ we have

$$(I \otimes H)\sigma_2(\omega)(I \otimes H)^\dagger = \frac{1}{4} \begin{pmatrix} A & 0 & 0 & \omega A \\ 0 & B & -\omega B & 0 \\ 0 & -\omega B & B & 0 \\ \omega A & 0 & 0 & A \end{pmatrix}, \quad (31)$$

where $A = 1 + \omega$ and $B = 1 - \omega$. From the form of the matrix, it can be seen that the only way that $\sigma_2(\omega) \rightarrow \rho_2^*$ is when all the terms apart from $1 + \omega$ vanish. So we arrive at the following four conditions that have to be satisfied simultaneously: $\omega(1 + \omega) = 1 - \omega = \omega(\omega - 1) = 0$ and

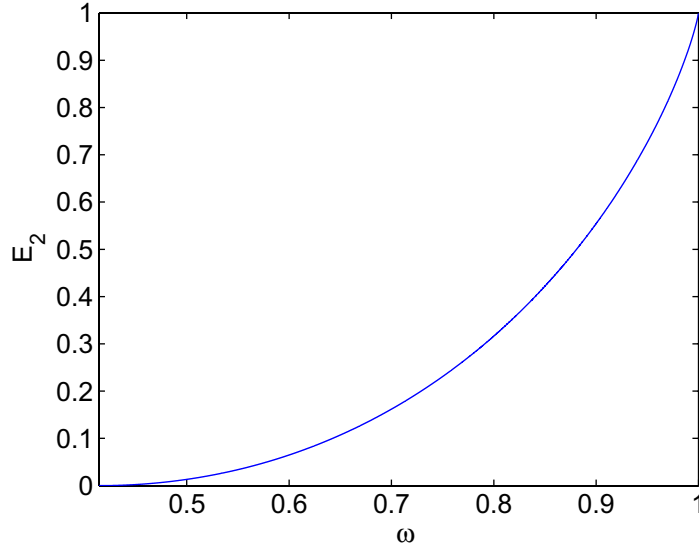


Figure 3. Scaling of entanglement of two and four qubits with increasing temperature. When the thermal coefficient $\omega = 1$, we recover the result for the pure cluster state. At the critical point $\omega_c = \sqrt{2} - 1$, the state is separable.

$1 + \omega = 2$. It is straightforward to see that these conditions are not simultaneously satisfied for any ω . Therefore as the temperature increases, the thermal cluster state does not approach the closest separable state ρ_2^* . This last result can also be seen from the fact that the relative entropy between these two states is nonzero, i.e. $S(\sigma_2(\omega_c) \parallel \rho_2^*) \neq 0$. The relative entropy between two states $S(A \parallel B)$ vanishes if and only if $A = B$ [40].

Taking a convex mixture of ρ_2^* and $\sigma_2(\omega_c)$ allows us to find a general form of the closest two-qubit separable state

$$\rho_2 = (1 - \lambda)\rho_2^* + \lambda\sigma_2(\omega_c), \quad (32)$$

where $\lambda \in [0, 1]$. This can be verified by computing the gradient of the relative entropy in the usual way, $(\partial f / \partial x)(0, \tau) = 1 - 2\text{Tr}[\sigma \tau] \geq 0$ for all $\lambda \in [0, 1]$.

4. Thermal cluster states

Now we are in a position to calculate the entanglement of thermal cluster states. We will use a similar approach as above to show that the form of the closest separable state is the same as in equation (32). However, this time the parameter λ that determines the mixture of our two closest separable states from equation (32) will not be completely free and its lower bound will depend on the temperature. We will show that as the temperature increases towards the critical temperature $T \rightarrow T_c$, the parameter λ increases towards unity.

We already have everything we need to compute the scaling of entanglement with temperature of a thermal two-qubit cluster state given by equation (29). The only thing that remains to be determined is a suitable candidate for the closest separable state. The most obvious choice would be $\sigma_2(\omega_c) = \frac{1}{4}(I + \omega_c \sigma^x \otimes \sigma^z)(I + \omega_c \sigma^z \otimes \sigma^x)$, where $\omega_c = \sqrt{2} - 1$. In fact this gives the correct behaviour of entanglement $E(\sigma_2(\omega)) = \text{Tr}[\sigma_2(\omega) \log \sigma_2(\omega) - \sigma_2(\omega) \log \sigma_2(\omega_c)]$, as can be seen in figure 3. The gradient of the relative entropy in the neighbourhood of the state $\sigma_2(\omega_c)$ is non-negative, $(\partial f / \partial x)(0, \tau) \geq 0$, as expected.

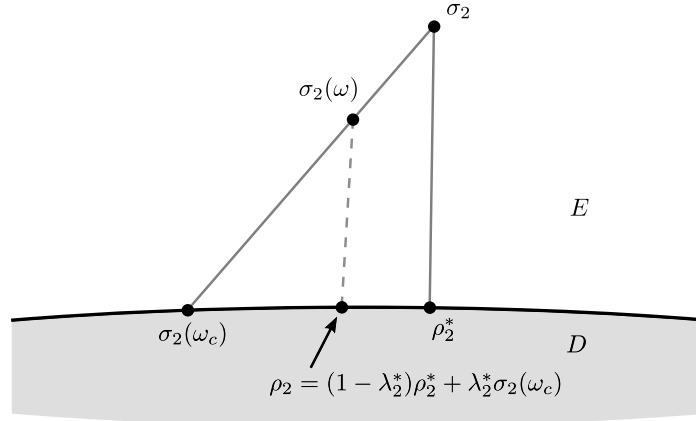


Figure 4. Section of Hilbert space of two qubits. The shaded area D represents the subspace of all separable states. E designates the set of all entangled states. As the temperature increases, the set of all separable states becomes smaller. This set is represented by all the points found on the E – D boundary between the states $\sigma_2(\omega_c)$ and ρ_2 .

Now that we know that for two qubits the cluster state at critical temperature is a closest separable state, we can ask whether there exists a more general form of the state just like in section 3. It turns out that this is in fact possible, albeit with some needed modifications. We have seen that as the temperature increases, the thermal cluster state does not approach the state ρ_N^* from section 2. This can also be seen from the non-vanishing distance between the separable states $\sigma_N(\omega_c)$ and ρ_N^* , i.e. $S(\sigma_N(\omega_c) \parallel \rho_N^*) \neq 0$. As the temperature increases, the distance between the cluster states $\sigma_N(\omega)$ and $\sigma_N(\omega_c)$ approaches zero, as expected. However, this is not true for the distance between $\sigma_N(\omega)$ and ρ_N^* due to the fact that $S(\sigma_N(\omega_c) \parallel \rho_N^*) \neq 0$.

This problem can be overcome by not allowing the parameter λ from equation (32) to take any value from the interval $[0, 1]$. Rather we require that the lower bound of the possible values of λ increases with temperature. We call this bound λ^* and require $\lambda^* = \lambda^*(\omega)$.

As before, we will first demonstrate the general principle at work on a two-qubit cluster state $\sigma_2(\omega)$. First, we need to find the new parameter λ^* by minimizing the distance between the thermal cluster state $\sigma_2(\omega)$ and the state (32) ρ_2 for a constant temperature. Solving $(\partial/\partial\lambda)S(\sigma_2(\omega) \parallel \rho_2) = 0$ for λ gives the new λ^* :

$$\lambda_2^* = \frac{2}{(\sqrt{2} - 2)(3 + \omega)}. \quad (33)$$

We can straightaway confirm that the separable state given by this new parameter $\rho_2 = (1 - \lambda_2^*)\rho_2^* + \lambda_2^*\sigma_2(\omega_c)$ is also a closest separable state by calculating the gradient of relative entropy at this state $(\partial f/\partial x)(0, \tau) \geq 0$. Therefore, we can construct a new general closest separable state

$$\rho_2(\omega) = (1 - \lambda)\rho_2^* + \lambda\sigma_2(\omega_c), \quad (34)$$

where this time $\lambda \in [\lambda_2^*, 1]$. The relative positions of all the above states in Hilbert space are illustrated in figure 4. However, the figure does not capture the fact that the distances $S(\sigma_2 \parallel \rho_2^*)$ and $S(\sigma_2 \parallel \sigma_2(\omega_c))$ are the same. This is because not all properties of Hilbert space can be pictured on a two-dimensional drawing.

This method of finding closest separable states can be extended to general N -qubit cluster states. The crucial part is to find the critical temperature at which the cluster becomes fully separable. Due to the presence of bound entanglement for $N \geq 3$, this is a nontrivial task and at present it is unclear how it can be achieved. Cavalcanti *et al* [36] calculated the upper and lower bounds on the value of the critical temperature for cluster states of different dimensions. However, all this changes is that the separable state $\sigma(\omega_c)$ would be shifted to the left of the state $\sigma_2(\omega_c)$ on the E – D boundary in figure 4 since the critical temperature for $N \geq 3$ is higher than for the one calculated here.

5. Conclusion

We have demonstrated a systematic way of constructing a closest separable state to N -qubit cluster states. Our method reproduces known results for pure states and also allows us to quantify entanglement for mixed cluster states.

For pure states, the method relies on writing the density matrix of the state in the ‘mixed’ basis and setting any off-diagonal elements to zero. Operationally we can construct this state from $N/2$ copies of the two-qubit closest separable state and join them together by applying control-phase gates as demonstrated in section 2. Our method applies to cluster states of all dimensions. This is particularly useful since cluster states of dimension $d \geq 2$ are a universal resource state for quantum computation.

It also turns out that state ρ_N^* is not the only closest separable state. The thermal cluster state at critical temperature $\sigma_N(\omega_c)$ is also another closest separable state to the pure cluster state. Therefore any convex mixture of these two states also minimizes the relative entropy. However, at the moment it is difficult to determine the precise temperature at which the cluster becomes fully separable for cases of more than two qubits due to the presence of bound entanglement.

Mixed states require an even more careful approach. When quantifying entanglement in thermal cluster states, a convex mixture of ρ_N^* and $\sigma_N(\omega_c)$ does not minimize the relative entropy anymore. Parameter λ that determines the mixture of these two states does not take any value from interval $[0, 1]$. Instead, as the temperature increases, the lower bound of this interval increases as well. Hence the range of values the parameter λ can take is constricted to $\lambda \in [\lambda^*, 1]$. The new lower bound λ^* is a function of temperature and as temperature approaches the critical value $\lambda^* \rightarrow 1$. In other words, both the thermal cluster σ_ω and the closest separable state ρ approach the same state.

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