Tensor networks for frustrated systems: emergence of order from simplex entanglement

Daniel Alsina\(^1\) and José I. Latorre\(^1,2\)

\(^1\) Departament d’Estructura i Constituents de la Matèria, Universitat de Barcelona, Barcelona, Spain
\(^2\) Center for Quantum Technologies, National University of Singapore, Singapore

We consider a frustrated anti-ferromagnetic triangular lattice Hamiltonian and show that the properties of the manifold of its degenerated ground state are represented by a novel type of tensor networks. These tensor networks are not based on ancillary maximally entangled pairs, but rather on triangular W-like simplices. Anti-ferromagnetic triangular frustration is then related to ancillary W-states in contrast to ferromagnetic order which emerges from the contraction of GHZ-like triangular simplices. We further discuss the outwards entangling power of various simplices. This analysis suggests the emergence of distinct macroscopic types of order from the classification of entanglement residing on the simplices that define a tensor network.

Tensor networks stand as a powerful variational approach to quantum mechanical systems that escapes the sign problem that hampers Monte Carlo simulation \([1]\). Popular tensor networks are those that adapt their connectivity to the natural setting of a particular system. Relevant instances of tensor networks include Matrix Product States (MPS) \([2]\) and Projected Entangled Pairs States (PEPS) \([3]\) for translational invariant systems in one and two dimensions respectively, and MERA structures \([4]\) for scale invariant dynamics. All these approximation techniques are based on the use of ancillary maximally entangled states that are projected in different manners along the network. Yet, this strategy seems to capture the physics of frustration in a poor way. We here shall propose the construction of a novel type of tensor networks based on triangular ancillary states which are related to W-type entanglement and, as a consequence, are suited to describe geometric frustration.

We first should note that the word frustration is used with different meanings in classical \([5]\) and quantum physics \([6]\). For quantum systems, frustration often describes the situation where a Hamiltonian is made of terms that do not commute and, hence, there is no global eigenstate that minimizes each of the terms in the Hamiltonian. The system then develops entanglement. There is a different type of frustration which is found both in quantum and classical systems where the Hamiltonian is made out of commuting pieces, yet the state of minimum energy does not minimize each term due to constraints emerging from geometry. The prototype example of this kind of geometrical frustration is modeled by the anti-ferromagnetic triangular lattice model that we present in its quantum version

\[
H = J \sum_{\{i,j\} \in T} \sigma_i^z \sigma_j^z + \lambda \sum_i \sigma_i^z ,
\]

where \(\sigma^z\) and \(\sigma^x\) are the Pauli matrices, \(\{i,j\} \in T\) represents nearest neighbor interaction on the triangular geometry shown in Fig. 1. \(J > 0\) corresponds to the anti-ferromagnetic interaction and \(\lambda\) is the external transverse field. It is easy to see that even in the case of \(\lambda = 0\) and \(J > 0\) there is no arrangement of spins that minimize every term in the Hamiltonian.

Let us recall that the classical counterpart of the anti-ferromagnetic model displays a large degeneracy of ground states. In a triangular lattice made of \(n\) spins and \(\lambda = 0\), Wannier found that the number of states \(M\) with the same minimum energy \(E_0 = -n/3\) scales as the volume of the system, that is \(M \sim 2^{n}\), where \(a \sim .488\) \([7]\). This large degeneracy translates to the quantum case in the form of a large subspace of possible ground states \(|\psi_i\rangle, i = 1, \ldots, M\), where each \(|\psi_i\rangle\) corresponds to the quantum transcription of a classical solution into the computational basis. We may then consider the equal superpositions of all valid states on the computational basis that carry the same minimum energy \(E_0 = -n/3\),

\[
|\psi_0\rangle = \frac{1}{\sqrt{M}} \sum_i |\psi_i\rangle \quad H|\psi_i\rangle = E_0|\psi_i\rangle, \quad i = 1, \ldots, M
\]

where \(M\) corresponds to the degeneracy of the ground state manifold. The degeneracy is lifted when an external transverse field is applied. The special case where \(\lambda \rightarrow 0\) produces a particular combination of all \(|\psi_i\rangle\). In both cases, namely in the equal superposition or in the limit to zero of the external field, the resulting states carry a large entropy, as we shall discuss later.

The question we shall address here is whether a frus-
treated state such as $|\psi_0\rangle$ accepts a natural representation in terms of tensor networks. Let us start by observing that in the case of 3 spins forming a triangle, the equal superposition of valid ground states is

$$|\psi_0\rangle = \frac{1}{\sqrt{6}} (|001\rangle + |010\rangle + |100\rangle + |011\rangle + |101\rangle + |110\rangle),$$

where $|W\rangle = \frac{1}{\sqrt{3}} (|001\rangle + |010\rangle + |100\rangle)$ and $|\bar{W}\rangle = \frac{1}{\sqrt{3}} (|011\rangle + |101\rangle + |110\rangle)$. This introduces in a natural way $W$-states which are attached to a class of tripartite entanglement in quantum information theory. Frustration in this state amounts to equally superpose all the possibilities of assigning frustrated triangles, hence the emergence of $W$-type entanglement. Note that if we relax the requirement of equal superposition of possible ground states but retain isotropy, a freedom on the relative weight of $|W\rangle$ vs. $|\bar{W}\rangle$ states appears.

We next consider a larger structure, as the one shown in Fig. 1 and compute the ground state in the limit of zero external transverse field. The result reads

$$|\psi_0\rangle = \alpha (|001100\rangle + |010001\rangle + |011101\rangle) + \beta (|001101\rangle + |010010\rangle + |011110\rangle + |010101\rangle + |011001\rangle + |001101\rangle) + \gamma (|001010\rangle + |010010\rangle + |010100\rangle) + \delta |011010\rangle,$$  

with $\alpha \sim -.24$, $\beta \sim .19$, $\gamma \sim -.16$ and $\delta \sim .15$. It is convenient to analyze this state by looking at the distribution of spins on all triangles pointing up, since the triangles pointing down only provide a redundant description of the system. There are three up-triangles to be considered, respectively formed by the qubits $\{1,2,3\}$, $\{3,4,5\}$ and $\{3,5,6\}$. The relevant observation is that each state forming the superposition of the ground state in Eq. 4 is formed by a member of either a $W$ state or a $\bar{W}$ state. It is furthermore possible to verify that all the states in the equal superposition of valid ground states are made of elements of $W$- and $\bar{W}$-like states in the up-triangles. Though we may find a down-triangle with the configuration 111, this does not invalidate the fact that all up-triangles remain a member of genuine $W$ tripartite entanglement.

Let us now prove that this is the general case, namely that the equal superposition of valid ground states $|\psi_0\rangle$ is made of all possible combinations of $W$ and $\bar{W}$ configurations on all ancillary simplices. To prove this result we first consider the Hamiltonian

$$H_W = \sum_{i,j,k \in T^*} (z_i + z_j + z_k - 1)^2, \quad (5)$$

where $z_i = \frac{1+2\sigma_i^z}{2}$ and $T^*$ spans the set of up-triangles. Expanding this Hamiltonian we find

$$H_W = \frac{1}{2} \sum_{i,j \in T} \sigma_i^z \sigma_j^z + \sum_i \sigma_i^z + 1, \quad (6)$$

This construction shows that the ground state of the Hamiltonian $H_W$ belongs to the manifold spanned by $W$ states and that it carries $E_0 = 0$ energy.

This intuitive technique to construct frustrated Hamiltonians indicates that the way to represent the frustrated triangular dynamics needs to cancel the linear terms in $\sigma^z$. This can be done as follows

$$H = \sum_{i,j \in T} \left( (z_i + z_j + z_k - 1)^2 \right.$$

$$\left. + (z_i + z_j + z_k - 2)^2 - 2 \right), \quad (7)$$

where now $i,j,k$ are indexes of the sites that form up-triangles $T^*$. The original anti-ferromagnetic triangular Hamiltonian is recovered as a sum of two conditions, one trying to produce a superposition of $W$ states and another of $\bar{W}$ states. Both conditions can not be fulfilled simultaneously, so that the energy picks a penalization of one unit for each up-triangle coming from one of the two terms, hence $E_0 = -n/3$, which is the number of up-triangles.

The above arguments allow for the construction of a tensor network that represents the state $|\psi_0\rangle$ in an exact way. We first consider the filing of up-triangles all across the triangular lattice with $W$ and $\bar{W}$ ancillary states, that is ancillary quantum degrees of freedom of dimension $\chi = 2$, as shown in Fig. 2.

![FIG. 2: Tensor network based on a triangular simplex described by the tensor $A_{\alpha\beta\gamma}$, which projects the underlying ancillary indexes onto a physical one.](image)
that the contraction of ancillary indexes for this tensor network reproduces the state $|\psi_0\rangle$. Notably, a similar construction based on the use of GHZ states at each simplex does describe global ferromagnetic order. The interplay between GHZ and $W$ entanglement at the level of ancillary simplices is the key to distinct types of order at large scales.

A first consequence from the above construction is to observe that the entanglement of the state $|\psi_0\rangle$ is bounded to obey area law scaling at most. As mentioned previously, $|\psi_0\rangle$ is made of an exponential superposition of states. Thus, in principle, this state could display a volume law scaling of entanglement. Yet, $|\psi_0\rangle$ is described by a local tensor network that only links each spin to its nearest neighbor. That immediately sets a bound on the entropy of the state. Indeed, the entanglement entropy of the state $|\psi_0\rangle$ will scale as the area law at most. Moreover the ancillary states carry dimension $\chi = 2$, so the bound for the entanglement entropy of a region $A$ with boundary $\partial A$ is just $S(A) \leq \log 3 \partial A$, being the options that emerge outwards from each qubit. This is fully consistent with the idea that local interactions of translational invariant systems produce ground states that obey area law scaling for the entanglement entropy [11].

Let us now show that the triangular frustrated system is a particular case of the Exact Cover NP-complete problem, closely related to 3-SAT problem. Exact Cover is a decision problem based on the fulfillment of 3-bit clauses. To be precise, we are asked to decide whether a set of $n$ bits accept an assignment such that a set of clauses involving three bits are all satisfied. Each clause is obeyed if the three bits involved in it take values 001, 010 or 100. It was proven in Ref. [12] that there is an exact tensor network that describes the possible solutions of this problem and that the hard part of deciding the instance is found in the contraction of the tensor network.

In our case, the construction we have proposed previously can be seen as the particularization of the Exact Cover to the problem of a regular triangular lattice. This implies that triangular frustration is a sort of simple and regular version of Exact Cover. Indeed, Exact Cover clauses involve bits that have no geometrical proximity relation.

This observation can be translated to a statement about frustration cycles. The triangular model produces frustration at the level of single triangles. Instead, Exact Cover produces frustration over a non-local and non-homogeneous triangular lattice. Typical cycles of frustration in Exact Cover are of log $n$ size: therefore, the NP Exact Cover problem is much harder than regular triangular lattices models because of the long scale cycles for frustration.

We now turn to the issue of how ancillary entanglement develops into large scale correlations. We shall refer to this property as outwards entangling power of an ancillary simplex. We may visualize this process by first focusing on a single ancillary triangle. The different superpositions which are accepted on this ancillary state propagate outwards distinct configurations. For instance, the trivial case where the internal state corresponds to a 000 configuration can only propagate a global product state made of zeros. In the case where a $W$ ancillary state is used, the global state retains only a small amount of entanglement due to the dominant role of 0 versus 1 ancillary states. A remarkable jump in entanglement entropy is obtained when $W$ and $\bar{W}$ are accepted at the ancillary level. Then the global state gains a complex structure, and entanglement appears to scale. The outwards growth of entanglement from an ancillary triangle can be systematically analyzed. In Fig. 4 and Table I we present how much entanglement is observed as the size of the system increases.

![FIG. 3: Detail of the way three concurrent qubits with indexes $\alpha$, $\beta$ and $\gamma$, coming from entangled triangles are projected into a physical index $i$ defining the tensor $A_{\alpha\beta\gamma}^i$. The triangular anti-ferromagnetic equal superposition of ground states is obtained if $|\psi\rangle = \frac{1}{\sqrt{2}} (|W\rangle + |\bar{W}\rangle)$ and $A_{\alpha\beta\gamma}^i = \delta^i_\alpha \delta^i_\beta \delta^i_\gamma$.](image)

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![FIG. 4: Outwards entangling power of simplices can be assessed by computing the entropy of the reduced density matrix corresponding to the red (or dark) area made of $n_A$ spins, with $n_A = 3, 6, 10$ in this figure.](image)

The relation between GHZ and $W$ entanglement on triangular ancillary states and the emergence of distinct types of long distance order suggest interesting generalizations for larger simplices.

Let us here analyze the case of a tensor network created from a four-qubit simplex. We shall constrain our anal-
The above results suggest a connection between microscopic entanglement at the level of a simplex and the emerging of long-range correlations in the system. It is tempting to argue that distinct classes of entanglement might be responsible for different types of long-range order, as we found in the case of the triangular lattice. For four qubits, it is known that there are nine classes of 4-qubit states under the action of LOCC operations [13]. There are the corresponding analogues of GHZ and W states with four qubits, but there are further novel ways to entangle them. States with maximal hyperdeterminant may play a special role in 3D networks based on tetrahedrons.

Similarly, the spatial symmetries which are found on a simplex are related to symmetries at large scales. It is easy to see that if the triangular couplings are chosen as positive in the diagonal directions and negative in the horizontal direction, then frustration disappears and the exact simplex describing the model is a superposition of $|001\rangle$ and $|110\rangle$ states.

Therefore, we conclude that tensor networks constructed from non-trivial simplices are an interesting tool and could be the natural way to encode different levels of entanglement and symmetries at large order.

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| Simplex | $n_A = 3$ | $n_A = 6$ | $n_A = 10$ |
|---------|----------|----------|----------|
| $|GHZ\rangle$ | 1        | 1        | 1        |
| $|W\rangle$ | $\log_3$ | $\log_3$ | $\log_2$ |
| $|W\rangle,|\bar{1}\rangle$ | 2        | 3        | 4        |
| $|W\rangle,|\bar{0}\rangle$ | 2.183    | 3.126    | 5.053    |
| $|W\rangle,|\bar{1}\rangle,|\bar{0}\rangle$ | 1.815    | 2.756    | 4.314    |

TABLE I: Outward entanglement power of different triangular simplices. At each simplex, an equal supersposition of its allowed states (on the left) propagates the entanglement entropy (on the right, in ebits) to the rest of the system.

We then consider a tensor network as shown in Fig. 5, where every checked square contains an ancillary state and all links are counted just once. The tensor defined at every site is the product of delta functions of the physical index with each of the two ancillary qubits meeting there. For the case of 24 qubits shown in Fig. 5, we have scanned the entropy of the inner square as a function of the coefficients of this ancillary state. Maximum entanglement is obtained for the state corresponding to $\alpha_0 = \alpha_2 = \alpha_3 = \alpha_4 = -\alpha_1$.

![FIG. 5: Square network of 24 spins, with the red (or dark) area showing the 4 spins from which we are computing the entanglement entropy.](image-url)