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FAST TRACK COMMUNICATION

Tensor 2-sums and entanglement

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Abstract
To define a minimal mathematical framework for isolating some of the characteristic properties of quantum entanglement, we introduce a generalization of the tensor product of graphs. Inspired by the notion of a density matrix, the generalization is a simple one: every graph can be obtained by addition modulo two, possibly with many summands, of tensor products of adjacency matrices. In light of this, we are still able to prove a combinatorial analogue of the Peres–Horodecki criterion for testing separability.

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1. Introduction

In this communication we attempt to define a minimal mathematical framework for isolating some of the characteristic properties of quantum entanglement. The proposed model is such that we hope the communication is amenable to be read by two audiences with different interests: those interested in algebraic and structural graph theory and those interested in entanglement theory.

The tensor product has a fundamental role in the standard formulation of quantum mechanics as the axiomatically designed operation for combining Hilbert spaces associated with the parties of a distributed quantum mechanical system (see, e.g. [5]). The definition of entanglement is in such a way so essentially dependent on the tensor product that we can only speak about entanglement in the presence of this operation. In the light of such a fact, mathematical criteria for detecting and classifying entanglement are mainly based on tools that give information, in most of the cases only partial, about the tensor product structure of quantum states or their dynamical operators.

It is plausible that some characteristic properties of significance in the quantum context remain associated with the tensor product even when we impoverish the mathematical structure used in quantum mechanics itself. In different terms, it is conceivable that certain properties of entanglement can be studied outside quantum mechanics, in a more controlled mathematical laboratory, where we keep features designated as essential and throw away redundant or 'less important' material. It is clear that such an experiment would imply a loss of some kind.

The goal of this communication is to define a toy setting with 'fake quantum states', which are still combined by using the notion of a tensor product. We do not ask whether we can actually define a physical theory with a state-space equivalent to the one proper of quantum mechanics, but obtain it with a restricted mathematical tool box. As we have stated above, what we do aim for is to picture a scenery with mathematical objects poorer than general quantum mechanical states, but still exhibiting some of their characteristic features.

The idea is then to distil a likely analogue of entanglement but in a slimmer mathematical setting. Specifically, we should be able to (i) define an operation for mixing states, that is, to obtain statistical mixtures of pure states, and to (ii) define an operation for combining states. Labelled graphs provide a versatile language for this intent: we mix by sum modulo two of adjacency matrices; we combine by a tensor product of graphs. The latter operation is well studied in graph theory. Indeed, it appeared in many different contexts with a number of equivalent names: tensor product in [1, 21], but also a direct product [3, 8] and a categorical product [19, 20], just to mention the most important ones. See also the recent papers [9, 13, 16], while for a general treatment of this graph product we refer to the book [12].

Graph tensor products have found a variety of applications. For example, let us just mention here that recently Leskovec *et al* [15] proposed tensor powers of graphs for modelling complex networks. The Kronecker product not only allows an investigation using analytical tools (which is not surprising since this is a well-understood operation), but the construction itself results very close to real-world networks.

The remainder of this communication is organized as follows. In the next section we provide the required preliminary definitions. Then, in section 3, theorem 6 gives a combinatorial characterization of tensor 2-sums. In section 4, theorem 8 gives a combinatorial analogue of the Peres–Horodecki criterion (see, e.g., [18]) for testing separability. The concluding section contains several topics for further research and related problems. In particular, it is an open question to establish computational complexity results concerning the recognition problem of tensor 2-sums.

2. Definitions

We consider graphs with a finite number of vertices, without multiple edges and without self-loops. The tensor product of graphs (see figure 1 for two examples) is defined as follows.

Definition 1. *The tensor product, $K = G \otimes H$, of graphs $G = (V(G), E(G))$ and $H = (V(H), E(H))$ is the graph with vertex set $V(K) = V(G) \times V(H)$ and $\{(g, h), (g', h')\} \in E(K)$ if and only if $\{g, g'\} \in E(G)$ and $\{h, h'\} \in E(H)$.*

Note that the product graph K is undirected, since $\{(g, h), (g', h')\} \in E(K)$ if and only if we have $\{(g', h'), (g, h)\} \in E(K)$. Let G be a graph with $V(G) = \{g_1, g_2, \ldots, g_n\}$. Recall that the *adjacency matrix* $A(G)$ of G is an $n \times n$ matrix with $A(G)_{i,j} = 1$ if $\{g_i, g_j\} \in E(G)$ and $A(G)_{i,j} = 0$, otherwise. Note that $A(G)$ is symmetric and that its labelling depends on the ordering of the vertices of G. Let H be another graph with $V(H) = \{h_1, h_2, \ldots, h_m\}$. Then, unless stated otherwise, the adjacency matrix of the tensor product $G \otimes H$ will be understood with respect to the lexicographic ordering

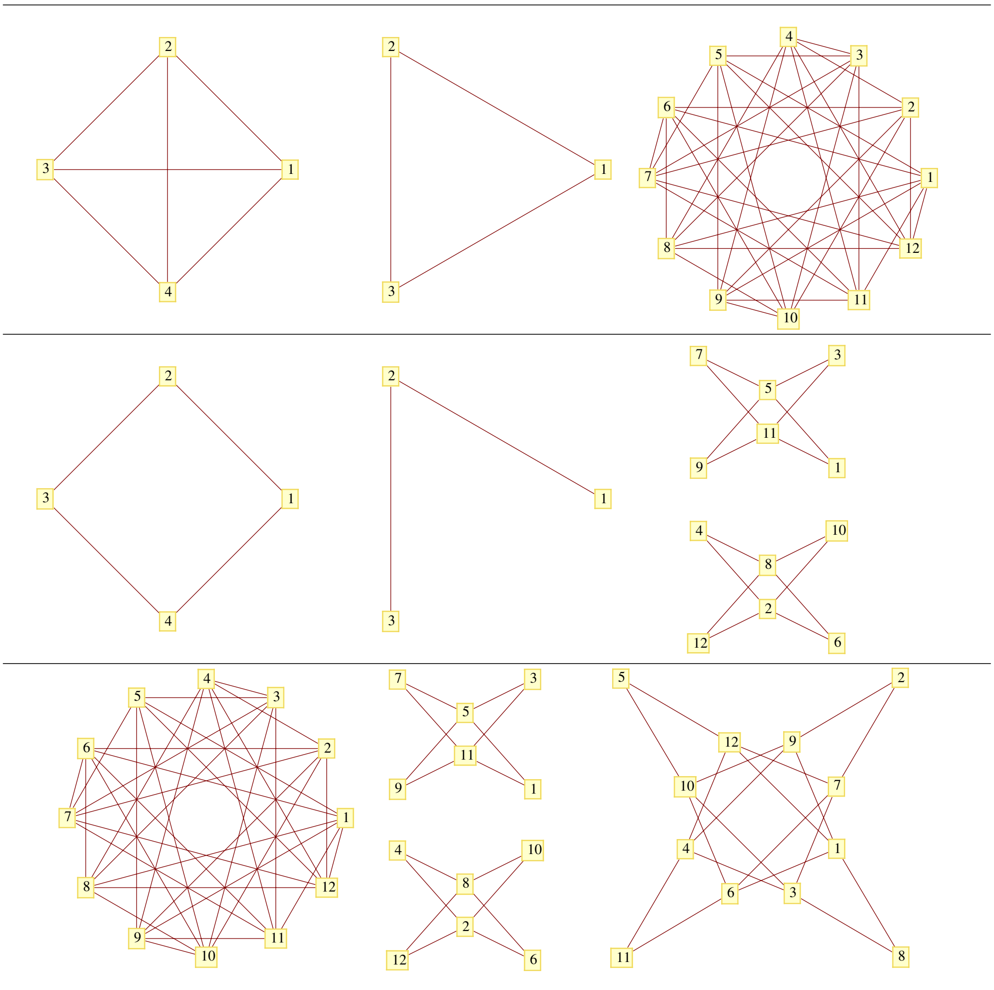

Figure 1. The figure consists of three rows. In the top row (from left to right) are drawn the complete graphs K_4 and K_3, and their tensor product $K_4 \otimes K_3$. In the middle row are drawn the cycle C_4, the path P_3 and their tensor product $C_4 \otimes P_3$. In the bottom row are drawn the graph $G = K_4 \otimes K_3$, $H = C_4 \otimes P_3$, and their 2-sum $G \oplus H$.

(This figure is in colour only in the electronic version)

of $V(G \otimes H)$: $(g_1, h_1), \ldots, (g_1, h_m), (g_2, h_1), \ldots, (g_2, h_m), \ldots, (g_n, h_m)$. Under this agreement, the following statement is a well-known useful fact: if $K = G \otimes H$ then $A(K) = A(G) \otimes A(H)$.

Our generalization of the tensor product of graphs requires an additional operation that is reminiscent of the symmetric difference, but producing a graph on the same vertex set of the operands.

Definition 2. *Let G and H be graphs with $V(G) = V(H)$. The sum modulo 2 or 2-sum for short, $K = G \oplus H$, of G and H is the graph with the same vertex set as G (and as H) such that $\{u, v\} \in E(K)$ if and only if either (i) $\{u, v\} \in E(G)$ and $\{u, v\} \notin E(H)$ or (ii) $\{u, v\} \notin E(G)$ and $\{u, v\} \in E(H)$.*

The right-hand side of the figure gives an example of the 2-sum of two graphs (in fact, of two tensor product graphs). The graph $K = G \oplus H$ has adjacency matrix with ijth entry $(A(K))_{i,j} = ((A(G))_{i,j} + (A(H))_{i,j}) \bmod 2$.

We are now ready to give the following definition, where by a nontrivial graph we mean a graph with at least one edge.

Definition 3. *A graph K is a tensor 2-sum if there exist a positive integer l, nontrivial graphs $G_1, \ldots, G_l$, and nontrivial graphs $H_1, \ldots, H_l$, such that*

$$K = \bigoplus_{k=1}^{l} (G_k \otimes H_k).$$

Here, $V(G_i) = V(G_j)$ and $V(H_i) = V(H_j)$, for every i and j.

Note that the case $l = 1$ reduces to the standard tensor product.

3. Characterization

Let $\mathcal{K}(p, q)$ be the set of graphs that are a tensor 2-sum in which the factors of the corresponding tensor products are of sizes p and q, respectively. Hence $|V(K)| = n = pq$ for $K \in \mathcal{K}(p, q)$. Note that if $K \in \mathcal{K}(p, q)$, then

$$|E(K)| \leqslant \binom{pq}{2} - q\binom{p}{2} - p\binom{q}{2} = 2\binom{p}{2}\binom{q}{2},$$

with the equality if and only if $K = K_p \otimes K_q$. Let $p \geqslant 2$ and $q \geqslant 2$ be arbitrary but fixed integers. Let G and H be arbitrary graphs on the p and q vertices, respectively. For our purposes, we may assume that $V(G) = \{g_1, \ldots, g_p\}$ for an arbitrary graph G on p vertices and $V(H) = \{h_1, \ldots, h_q\}$ for an arbitrary graph H on q vertices, that is, all graphs on a fixed number of vertices will have the same vertex set. Assume $K \in \mathcal{K}(p, q)$ and let $G_1, \ldots, G_l$ and $H_1, \ldots, H_l$ be graphs such that $K = \bigoplus_{k=1}^{l} (G_k \otimes H_k)$. Thus, by the above assumption, $V(K) = \{(g_i, h_j) \mid 1 \leqslant i \leqslant p, 1 \leqslant j \leqslant q\}$. The next notions will be useful for theorem 6:

Definition 4. *Let K be a (spanning) subgraph of the tensor product $G \otimes H$. Then K is a cross-like subgraph if $\{(g_i, h_j), (g_{i'}, h_{j'})\} \in E(K)$ implies that $\{(g_i, h_{j'}), (g_{i'}, h_j)\} \in E(K)$ as well.*

Definition 5. *Let G and H be graphs on vertex sets $\{g_1, \ldots, g_p\}$ and $\{h_1, \ldots, h_q\}$, respectively, with $E(G) = \{\{g_i, g_{i'}\}\}$ and $E(H) = \{\{h_j, h_{j'}\}\}$. Let us denote the tensor product $G \otimes H$ with $E(i, i'; j, j')$ and call it a tensor-elementary graph.*

Using these concepts, the graphs in the set $\mathcal{K}(p, q)$ can be characterized follows.

Theorem 6. *For a graph K, the following statements are equivalent.*

(i) $K \in \mathcal{K}(p, q)$;
(ii) K is a spanning, cross-like subgraph of $K_p \otimes K_q$;
(iii) K is a 2-sum of tensor-elementary graphs.

Proof. $(i) \Rightarrow (ii)$. Let $K = \bigoplus_{k=1}^{l} (G_k \otimes H_k)$. Then $V(K) = \{(g_i, h_j) \mid 1 \leqslant i \leqslant p, 1 \leqslant j \leqslant q\}$. Consider vertices (g_i, h_j) and $(g_i, h_{j'})$ of K, where $j \neq j'$. Since $\{(g_i, h_j), (g_i, h_{j'})\} \notin E(G_k \otimes H_k)$, $1 \leqslant k \leqslant l$, we infer that $\{(g_i, h_j), (g_i, h_{j'})\} \notin E(K)$. Analogously, $\{(g_i, h_j), (g_{i'}, h_j)\} \notin E(K)$ for any i and any $j \neq j'$. It follows that K is a spanning subgraph of $K_p \otimes K_q$.

Assume next that $\{(g_i, h_j), (g_{i'}, h_{j'})\} \in E(K)$. Then $\{(g_i, h_j), (g_{i'}, h_{j'})\} \in E(G_i \otimes H_i)$ for an odd number of indices k, say $k = k_1, \ldots, k_{2r+1}, r \geqslant 0$. Consequently, the edges $\{g_i, g_{i'}\}$ and $\{h_j, h_{j'}\}$ are simultaneously present precisely in the products $E(G_k \otimes H_k), k = k_1, \ldots, k_{2r+1}$. Therefore $\{(g_i, h_{j'}), (g_{i'}, h_j)\} \in E(K)$ as well. We conclude that K is also cross like.

$(ii) \Rightarrow (iii)$. Let K be a spanning, cross-like subgraph of $K_p \otimes K_q$. To each pair $\{(g_i, h_j), (g_{i'}, h_{j'})\}, \{(g_i, h_{j'}), (g_{i'}, h_j)\}$ of K assign the tensor-elementary graph $E(i, i'; j, j')$. Then it is straightforward to see that

$$K = \bigoplus_{\substack{\{(g_i,h_j),(g_{i'},h_{j'})\}\in E(K)\\ \{(g_i,h_{j'}),(g_{i'},h_j)\}\in E(K)}} E(i, i'; j, j').$$

$(iii) \Rightarrow (i)$. This implication is obvious. □

A sum modulo 2 of tensor products is not unique. More formally, given a tensor 2-sum graph K, there may be different representations of the form $K = \bigoplus_{k=1}^{l} (G_k \otimes H_k)$. This is trivially analogous to the situation for density matrices, where a mixed state does not capture all the information about the ensemble of pure states from which it arises.

To see that a representation need not be unique it is enough to recall that the prime factor decomposition of graph with respect to the tensor product is not unique in the class of bipartite graphs, see [12] for the general case and [2] for factorization of hypercubes. On the other hand, the prime factor decomposition is unique for connected nonbipartite graphs [17]. To see that this does not hold for tensor 2-sum representations, observe first that the 2-sum is commutative and associative. Moreover, it is not difficult to verify the distributivity law:

$$G \otimes (H_1 \oplus H_2) = (G \otimes H_1) \oplus (G \otimes H_2). \tag{1}$$

Consider now a tensor 2-sum graph K in which the first factor is fixed, that is

$$K = \bigoplus_{k=1}^{l} (G \otimes H_k).$$

Then by (1) we can also write K as

$$K = G \otimes \left(\oplus_{k=1}^{l} H_k\right).$$

Moreover, by the commutativity and associativity of the 2-sum, the graphs H_i can be arbitrarily combined to get numerous different representations of K.

4. Partial transpose

The Peres–Horodecki criterion for testing separability of quantum states is based on the partial transpose of a density matrix (see, e.g., [18]). The criterion states that if the density matrix (or, equivalently, the state) of a quantum mechanical system with composite dimension pq is entangled, with respect to the subsystems of dimension p and q, then its partial transpose is positive. For generic matrices, this operation is defined as follows.

Definition 7. *Let M be an $n \times n$ matrix, where $n = pq$, $p, q > 1$. Consider M as partitioned into p^2 blocks each of size $q \times q$. The partial transpose of M, denoted by M^{Γ_p}, is the matrix* *obtained from M, by transposing independently each of its p^2 blocks. Formally,*

$$M = \begin{pmatrix} \mathcal{B}_{1,1} & \cdots & \mathcal{B}_{1,p} \\ \vdots & \ddots & \vdots \\ \mathcal{B}_{p,1} & \cdots & \mathcal{B}_{p,p} \end{pmatrix} \Longrightarrow M^{\Gamma_p} = \begin{pmatrix} \mathcal{B}_{1,1}^T & \cdots & \mathcal{B}_{1,p}^T \\ \vdots & \ddots & \vdots \\ \mathcal{B}_{p,1}^T & \cdots & \mathcal{B}_{p,p}^T \end{pmatrix},$$

where $\mathcal{B}_{i,j}^T$ denotes the transpose of the block $\mathcal{B}_{i,j}$, for $1 \leqslant i, j \leqslant p$.

It is clear that we can have a partial transpose of a graph via its adjacency matrix. The next result translates the Peres–Horodecki criterion in our restricted setting. In a stronger way, the positivity is substituted by the equality. This observation closely resembles the result obtained in [4], when considering normalized Laplacians. However, here we drop the constraints of positivity and unit trace. The only property of relevance for this criterion to hold is then symmetry, apart from the fact that here we have only matrices of zeros and ones.

Theorem 8. *Let $K \in \mathcal{K}(p, q)$. Then $A(K) = A(K)^{\Gamma_p}$.*

Proof. Let $K = \bigoplus_{k=1}^{l}(G_k \otimes H_k)$. As earlier we can assume that $V(K) = \{(g_i, h_j) \mid 1 \leqslant i \leqslant p, 1 \leqslant j \leqslant q\}$. Also, $A(K)$ is assumed to be constructed with respect to the lexicographic order of the vertices of K: $(g_1, h_1), \ldots, (g_1, h_q), (g_2, h_1), \ldots, (g_2, h_q), \ldots, (g_p, h_q)$. To simplify the notation, identify the vertices of K in this order with the sequence $1, \ldots, q, q + 1, \ldots, 2q, \ldots, pq$. Then any i, $1 \leqslant i \leqslant pq$, can be (uniquely) written as $i = sq + r$ for some $0 \leqslant s \leqslant p - 1$ and $1 \leqslant r \leqslant q$. Consider an arbitrary block $\mathcal{B}_{s_1,s_2}$, $0 \leqslant s_1, s_2 \leqslant p - 1$, of $A(K)$. Note first that by the lexicographic order, $\mathcal{B}_{s_1,s_2} = 0$ if $s_1 = s_2$. Hence assume without loss of generality $s_1 < s_2$. Let the (r_1, r_2)th entry of $\mathcal{B}_{s_1,s_2}$ be equal to 1: $\left(\mathcal{B}_{s_1,s_2}\right)_{r_1,r_2} = 1$. Then $r_1 \neq r_2$. So $s_1q + r_1$ is adjacent to $s_2q + r_2$. Hence by theorem 6 (ii), $s_2q + r_1$ is adjacent to $s_1q + r_2$. But then $\left(\mathcal{B}_{s_1,s_2}\right)_{r_2,r_1} = 1$ which implies that $\mathcal{B}_{s_1,s_2} = \left(\mathcal{B}_{s_1,s_2}\right)^T$ as claimed. □

The converse of theorem 8 does not hold. Consider, for instance, the path on 4 vertices P_4 and label its consecutive vertices with 4, 1, 3, 2. Then the corresponding adjacency matrix is

$$\begin{pmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

which can be partitioned into 2×2 symmetric blocks. However, $P_4 \notin \mathcal{K}(p, q)$ since it has an odd number of edges.

While all separable quantum states belong to a set of PPT states (or, *positive partial transpose*states), it is not immediate to construct a general PPT state (see [18]). For graphs we have a simple method described in the next result, where $\cup$ denotes the disjoint union of graphs.

Theorem 9. *Let G be a graph on n vertices and with m edges. Then the graph*

$$G \cup mK_2 \cup (n^2 - n - 2m)K_1$$

belongs to $\mathcal{K}(n, n)$.

Proof. Let $V(G) = \{g_1, g_2, \ldots, g_n\}$ and let G' be an isomorphic copy of G with $V(G') = \{g_1', g_2', \ldots, g_n'\}$. Let H be the graph with the vertex set $V(H) = \{(g_i, g_j') \mid 1 \leqslant i \leqslant p, 1 \leqslant j \leqslant q\}$ and the edge set $E(H) = \{\{(g_i, g_i'), (g_j, g_j')\}, \{(g_i, g_j'), (g_j, g_i')\} \mid \{g_i, g_j\} \in E(G)\}$. Then it is straightforward to see that the connected components of H are G, n copies of K_2, and the remaining $n^2 - n - 2m$ components are K_1. In other words, $H = G \cup mK_2 \cup (n^2 - n - 2m)K_1$. Moreover, H is a spanning, cross-like subgraph of $K_n \otimes K_n$ so we conclude that $H \in \mathcal{K}(n, n)$. □

5. Conclusions and open problems

In an attempt to define a minimal mathematical framework for isolating some of the characteristic properties of quantum entanglement, we have introduced a generalization of the tensor product of graphs. The generalization consists of obtaining every graph by the addition modulo two, possibly with many summands, of tensor products of adjacency matrices. Then, we have proved a combinatorial analogue of the Peres–Horodecki criterion, by substituting positivity with equality.

The tensor 2-sum operation gives numerous interesting issues worth of investigation. Here is a selection of such open topics and problems.

- We have seen that a given graph K can have (and in most of the cases it does) different representation as a tensor 2-sum graph. Hence it is natural to define $T_2(K)$ as the smallest integer l (if it exists) such that K has a representation of the form $K = \bigoplus_{k=1}^{l}(G_k \otimes H_k)$. Clearly, $T_2(K) < \infty$ if and only if $K \in \mathcal{K}(p, q)$, for some p and q. The representation of $K \in \mathcal{K}(p, q)$ from theorem 6 (iii) can have an arbitrarily larger number of modulo 2 summands than $\mathrm{Kron}(K)$. Consider, for instance, $K = K_p \otimes K_q$. Clearly, $\mathrm{Kron}(K) = 1$, on the other hand the representation of theorem 6 (iii) requires pq summands. However, let $K = \bigoplus_{i=1}^{p-1} E(i, i+1; i, i+1)$. Then $T_2(K) = p$. Note also that $T_2(K) = 1$ if and only if K is not prime with respect to the tensor product. Is there a neat characterization of graphs K with $T_2(K)$? More generally, it would be good to have a classification of graphs in terms of the minimum number of summands required for their constructions as a sum of tensor products (that is, in terms of T_2).
- Theorem 6 gives two necessary and sufficient conditions for a graph to belong to $\mathcal{K}(p, q)$. However, these conditions are not efficient, so it remains to determine the computational complexity of the following decision problem.
  - Given: a graph G on $n = pq$ vertices.
  - Task: is $G \in \mathcal{K}(p, q)$?

  We feel that recent investigations of the so-called approximate graph products [10] might be useful in solving this problem. In this respect we add that the unique prime factorization of nonbipartite connected graphs can be found in polynomial time [11]. The problem of determining separability of generic quantum states is NP-hard [6, 7, 14]. The proof of this result requires some machinery. No separation between the two problems would give a simpler proof method.
- Assume K is a tensor 2-sum graph with a representation $K = \bigoplus_{k=1}^{l}(G_k \otimes H_k)$. Then the only condition we imposed on the graphs G_i and H_i is that each has at least one edge. One might want to be more restrictive by imposing that all G_i's and H_i's must be connected. What can be said of such restricted representations?
- It would be interesting to introduce a dynamics in addition to the static picture. Initially, this could be done by defining families of graphs obtained by *local permutation congruence*. The idea would be to describe a form of local unitary operations. For graphs, these are essentially permutations. Intuitively, testing equivalence under local unitaries can be seen as a special case of the subgraph isomorphism problem.

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