A-Exam Question #1

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Abrupt, or first-order, phase transitions are characterized by kinks in the free energy at the transition, which lead to discontinuities in certain thermodynamic quantities [11]. With the appropriate tuning, systems with abrupt phase transitions can be brought into a regime where the phase on neither side of the transition is stable, and the two phases coexist in finite domains. This coexistence is usually imagined as involving finite domains which are compact in space; after all, most of our statistical models involve local interactions, which means it is compact spatial regions whose potential for correlation is strongest. However, this is not a rule. We will see through some examples (and previous results) how phase coexistence can arise and make sense in systems whose interactions are *nonlocal* and disordered.

Consider the Hamiltonian defined for $Q \in \mathrm{SO}(n)$ by

$$H(Q) = -\sqrt{n}\sum_{i=1}^n\sum_{j=1}^n |Q_{ij}| \tag{1}$$

This model may seem trivial and uncoupled, but it is not; the requirement that Q be orthogonal restricts the $n\times n$ matrix elements to a $\frac12 n\times(n-1)$ dimensional manifold. To see this, take an analogous model, where $Q \in S^n$. In spherical coordinates, the Hamiltonian is

$$\begin{aligned}H(Q) = -\sqrt{n}\big\{&|\sin\phi_1\cdots\sin\phi_n| + |\cos\phi_1| \\ &+ |\sin\phi_1\cos\phi_2| + \cdots + |\sin\phi_1\cdots\sin\phi_{n-1}\cos\phi_n|\big\}\end{aligned}$$

which is coupled in a complex way. Unfortunately, there is no closed-form parameterization of $\mathrm{SO}(n)$, so an explicit expression for the Hamiltonian like that for the n-sphere is not possible [12].

One can run metropolis simulations on a Lie group G by forming an orthogonal basis $\{e_i\}$ of its Lie algebra $\mathfrak{g}$ and then mapping that basis to near-identity elements of the Lie group using the exponential map. For an element $X \in \mathfrak{g}$, $\exp(\epsilon X)$ for some small value ϵ is a linear transformation which shifts an element $g \in G$ by a small step. For the orthogonal group, $\mathfrak{g}$ is the set of skew-symmetric matrices. Choosing as a basis of $\mathfrak{g}$ matrices with $A_{ij} = 1$, $A_{ji} = -1$ for some $i \neq j$ and $A_{kl} = 0$ otherwise, the resulting transformation $\exp(\epsilon A)$ is simply a Givens rotation in the plane i–j. In the course of this question, we will also be

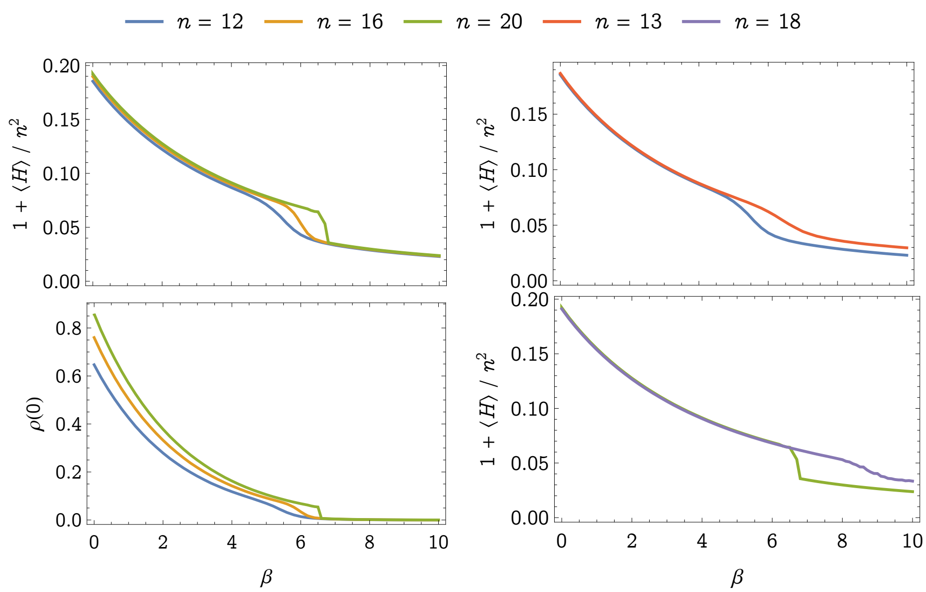

Figure 1: Top Left: The normalized expectation value of the Hamiltonian (1) for $Q \in \mathrm{SO}(n)$ and $n = 12$, 16, and 20 as a function of inverse temperature β. Bottom Left: The distribution of matrix elements evaluated at $Q_{ij} = 0$. Top Right: The expectation value of the Hamiltonian for $n = 12, 13$. Bottom Right: The expectation value of the Hamiltonian for $n = 18, 20$.

investigating transitions in other Lie groups—namely, the special unitary group SO(n) and the compact symplectic group[1] Sp(n). For the unitary group, the algebra is composed of skew-Hermitian matrices, and for the compact symplectic group it is composed of quaternionic skew-Hermitian matrices.

The model (1) is interesting because, when simulated as described above, it undergoes an abrupt phase transition. This is evidenced in Fig. 1, which shows a discontinuity in the expectation value of the Hamiltonian as a function of inverse temperature. It has been suggested that an order parameter for this transition is the probability density ρ of value of the elements Q_{ij} evaluated at $Q_{ij} = 0$ [3]. This is shown in Fig. 1 as well. Notice that, as n is increased, the transition becomes both more abrupt and decreases in temperature. This can be accounted for if the entropy and energy change of the ordered phase are non-extensive. For some values of n, this model's ground state consists of real Hadamard matrices, or $Q \in \mathrm{SO}(n)$ for which $|Q_{ij}| = 1/\sqrt{n}$ for all i, j. Hadamard matrices can only exist for $n = 1, 2$ and n that are multiples of 4, and in those dimensions there are usually many such matrices [6]. For instance, in $n = 16$ there are four Hadamard matrices inequivalent under transposition, negating rows or columns, or exchanging rows or columns, and with those operations many can be generated. However, there need not exist Hadamard matrices for a given n for this transition to exist. The upper right of Fig. 1 shows the transition in a system with $n = 13$, for which Hadamard matrices certainly do not exist, and indeed we found in numerics that this transition occurs for every n. For non-Hadamard n, the discontinuity is not as large, since the ground state cannot be as low-energy, and the transition temperature is often shifted dramatically from that for Hadamard-n nearby. See, for instance, the comparison of $n = 18$ and $n = 20$ in the bottom right of Fig. 1.

Does this transition occur in analogous systems? The Hamiltonian (1) for $Q \in \mathrm{SU}(n)$ or $Q \in \mathrm{Sp}(n)$ does not exhibit this transition, as seen at the top of Fig. 2. However, the Hamiltonian

$$H(Q) = -\sqrt{n} \sum_{i=1}^{n} \sum_{j=1}^{n} \left\{ |\Re(Q_{ij})| + |\Im(Q_{ij})| \right\} \tag{2}$$

(and its natural extension for quanterions) for these same groups does exhibit the transition, shown at the bottom of Fig. 2. In the former case, Hadamard matrices still comprise the group state, but those matrices are now complex (or qaternion) and equivalent Hadamard matrices form continuous surfaces connected by shifting phase. The fact this transition does not exist for those systems but does for (2) suggests that the discrete, disconnected nature of the ground states is important. This transition also does not happen for $Q \in S^n$ (Fig. 3), which may be surprising, as for all n this model has many disconnected ground states: $\{\pm\frac{1}{\sqrt{n}}, \ldots, \pm\frac{1}{\sqrt{n}}\}$ for all combinations of $\pm$.

[1]The compact symplectic group, which is isomorphic to $\mathrm{U}(2n) \cap \mathrm{Sp}(2n, \mathbb{C})$ (unitary symplectic matrices of dimension $2n$), is also $\mathrm{U}(n, \mathbb{H})$, or the quaternionic unitary group of dimension n.

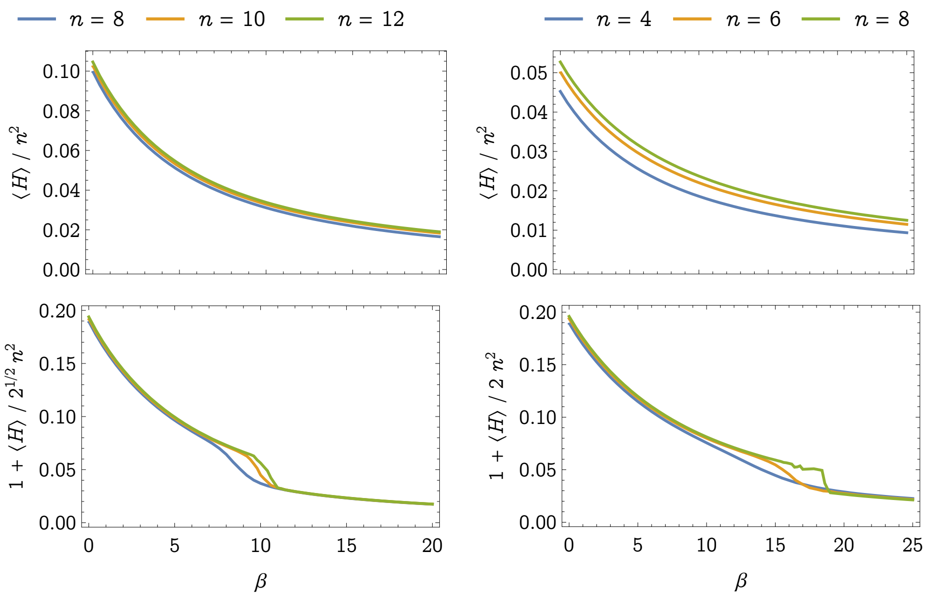

Figure 2: Top Left: The expectation value of (1) on the space SO(n). Top Right: The expectation value of (1) on the space Sp(n). Bottom Left: The expectation value of (2) on the space SO(n). Bottom Right: The expectation value of (2) on the space Sp(n).

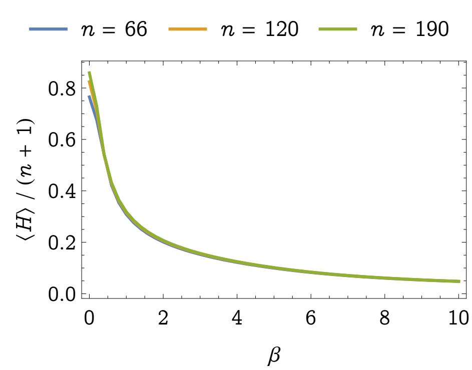

Figure 3: Expectation value of (1) on the space S^n.

What is going on here? We put forth the following conjecture: the model (1) for $Q \in \mathrm{SO}(n)$ can be thought of as a model of $\frac{n}{2}$ (where integer division is used) two-component spins with annealed disordered couplings. The spins undergo an abrupt paramagnetic–spin-glass transition. The non-extensive nature of the energy and entropy in the transition is explained by the fact that there are only $\frac{n}{2}$ spins which transition compared to $\frac{1}{2}n(n-1)$ coupling degrees of freedom.

How does this conjecture take shape? In the theory of Lie groups, a torus in a compact Lie group G is a compact, connected, abelian Lie subgroup of G [13]. Since the only compact, connected, abelian Lie group of dimension n is $\mathrm{T}^n = S^1 \times \cdots \times S^1$, such a subgroup is isomorphic to the torus. A *maximal torus* of a Lie group is the torus in that Lie group of highest dimension. For $\mathrm{SO}(n)$, the only maximal torus is dimension $\frac{n}{2}$ and corresponds to the subgroup of the form

$$\begin{bmatrix} R_1 & & 0 \\ & \ddots & \\ 0 & & R_{n/2} \end{bmatrix}$$

where the R_i are two-dimensional rotation matrices. In the case of odd n, the subspace is orthogonal to

$$\begin{bmatrix} R_1 & & 0 & \\ & \ddots & & \\ 0 & & R_{n/2} & \\ & & & 1 \end{bmatrix}$$

Any member of a Lie group G can be decomposed into the form PJP^{-1}, where J acts on orthogonal directions along the maximal torus and $P \in G$. In particular, this is true for orthogonal matrices: for any $Q \in \mathrm{SO}(n)$, we can write $Q = PJP^{\mathrm{T}}$ with $P \in \mathrm{SO}(n)$ and

$$J = \begin{bmatrix} s_1 & & 0 \\ & \ddots & \\ 0 & & s_{n/2} \end{bmatrix}$$

for

$$S_i = \begin{bmatrix} s_i^x & s_i^y \\ -s_i^y & s_i^x \end{bmatrix}$$

We have chose notation for the 2×2 matrices along the diagonal of J which is purposely provocative: such rotation matrices encode the value of a two-component spin s_i. In this notation, the elements of the original matrix Q are given by

$$Q_{ij} = \sum_{k=1}^{n/2} \Big[\big(P_{i(2k)} P_{j(2k)} + P_{i(2k+1)} P_{j(2k+1)} \big) s_k^x + \big(P_{i(2k+1)} P_{j(2k)} - P_{i(2k)} P_{j(2k+1)} \big) s_k^y \Big]$$

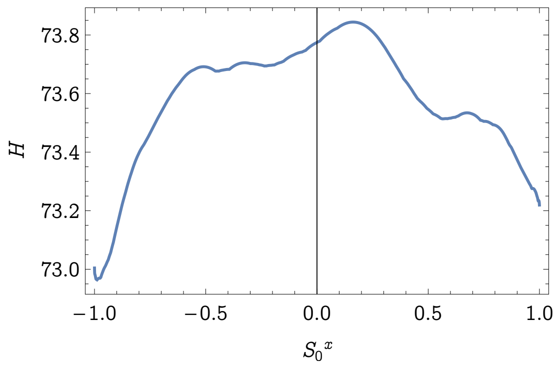

Figure 4: The energy landscape for the spin component S_0^x with $n = 20$ when all other spins are fixed at random orientations.

and the effect of the Hamiltonian (1) is to couple the spins in nontrivial ways. The energy landscape of one spin with others fixed and $P \in \mathrm{SO}(20)$ chosen randomly is shown in Fig 4.

When $P = I$, this is simply a model of uncoupled spins. For fixed P[2] disorder is quenched. In this case, a paramagnetic–spin glass transition happens (Fig. 5). For most random P, this transition does not exhibit a significant discontinuity in the expectation value of the Hamiltonian, but does have a discontinuity in the expectation value $\langle s_i^x \rangle$ and $\langle s_i^y \rangle$ from zero in the high-temperature phase to nonzero values which depend on the particular ground state in the low temperature phase. When P is taken from $PJP^T = H$ where H is Hadamard, the discontinuity becomes visible in the energy again (also Fig. 5). This is presumably because, for fixed random P, the ground state well is not very deep, while for Hadamard-derived P it is much more significant.

We can confirm more formally that this is indeed a spin-glass transition by simulating replicas of our model at various fixed random P and measuring the spin-glass order parameter

$$q = \tfrac{2}{n} \sum_{i=1}^{n/2} s_i^\alpha \cdot s_i^\beta$$

where the replica index $\alpha = 1, \ldots m$ [1, 9]. Simulations suggest that the model does indeed undergo a paramagnetic–spin-glass transition that breaks replica symmetry, as seen in Fig. 6, though the simulations were only started on Saturday and haven't yet made it all the way through the transition as of this writing.

When we allow P to vary (as is done in the original model), disorder is annealed. Simulating this case also results in a transition, as evidenced in Fig. 7. The discontinuity in energy persists, and is in fact broken into small jumps

[2] Which we can randomly generate by taking a sufficiently long random walk to approach the Harr measure of $\mathrm{SO}(n)$ [10].

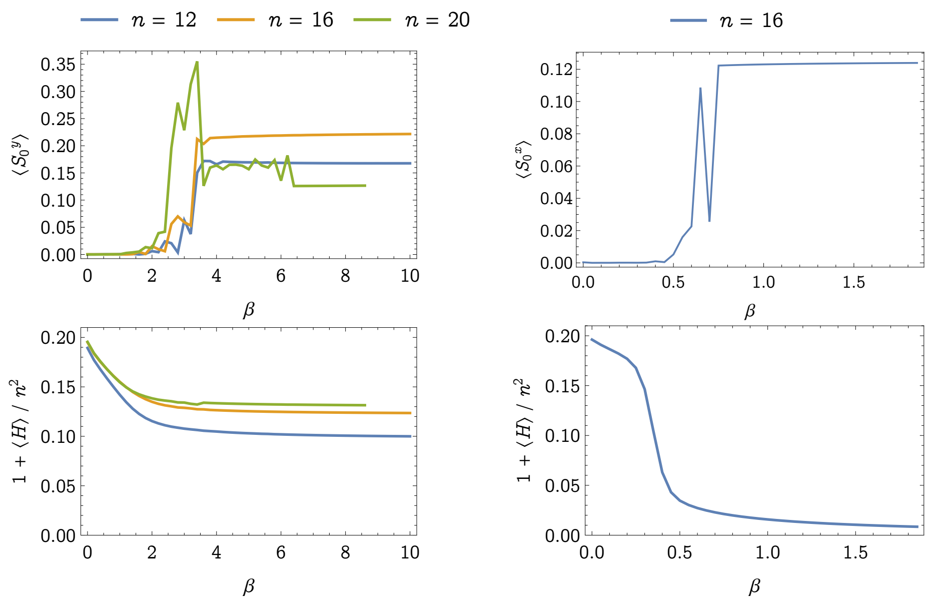

Figure 5: Top left: The expected value of the spin component s^y as a function of β for quenched disorder with random P. Bottom left: The expected value of the Hamiltonian for quenched disorder with random P. Top right: The expected value of the spin component s^x for quenched disorder with P from a Hadamard decomposition. Bottom right: The expected value of the Hamiltonian for quenched disorder with P from a Hadamard decomposition.

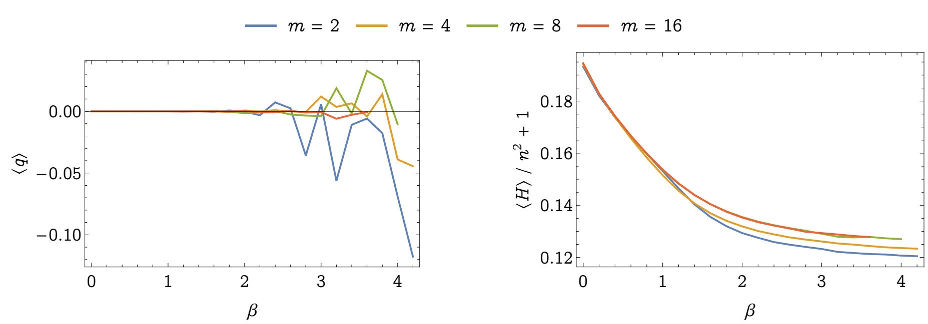

Figure 6: (Note: this simulation hasn't made it all the way through the transition yet. I only had this idea a week ago!) Left: The expectation value of the replica symmetry breaking order parameter for $n = 16$ and various numbers of replicas m. Right: The expectation of the Hamiltonian averaged over replicas.

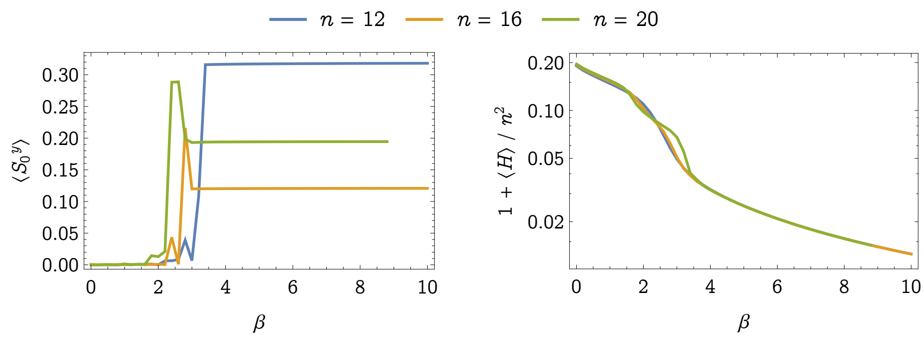

Figure 7: Left: The expectation value of a spin component with annealed disorder. Right: The expectation value of the Hamiltonian with annealed disorder.

which correspond with jumps in the expectation value of the spin—presumably the energies of metastable states the simulation is found in before reaching the ground state. Notice also that the transition temperature is shifted from the original case. This can be explained by the form of the metropolis algorithm used here: taking a step in spin space is just as likely as taking a step in disorder space, while taking a step in spin space in the original model is disfavored. This change in step preference affects the entropy of spins relative to disorder. The shift in the transition temperature with n also vanishes for the same reason: the number of free variables is simply $\frac{n}{2}$, not n^2 as before.

The final test of this principle is to return to our original model and investigate whether the expectation value of the spins as defined by the positions along the maximal torus undergo the transition we've discussed. In our metropolis simulation we implemented an efficient solver for the decomposition detailed above by modifying the result of the GSL Schur decomposition of $Q \in \mathrm{SO}(n)$ [5]. The results of those simulations are shown in Fig. 8. As can be seen, the transition corresponds to a discontinuity in the expectation value of spin components. Also shown in that figure are the distribution of spin components for $n = 16$ at various temperatures. The distribution stays nearly identical to its $\beta = 0$ infinite temperature form until $\beta \sim 5$, at which point it changes rapidly to the red curve before β reaches 7, where it remains stable in a ground state which is notably not Hadamard (for which all spins have $s^x = \pm 1$).

What of the fact of phase coexistence in this system? Phase coexistence in infinite-range spin-glasses has been recognized since the 1980s [4] and was discovered in another spin-glass model more recently [2]. Many experimentalists have also found evidence of spin-glass and ferro- or paramagnetic ordering coexisting [8, 7, 14]. In no case do the authors share any thought on the nature of the coexistence they discover in their infinite-range theory, just that it is present. One can speculate, however, that it occurs in the same way it does in the case of local interactions, but the phase domains no longer have a relation to spatial position of spins, and instead correspond to collections of components

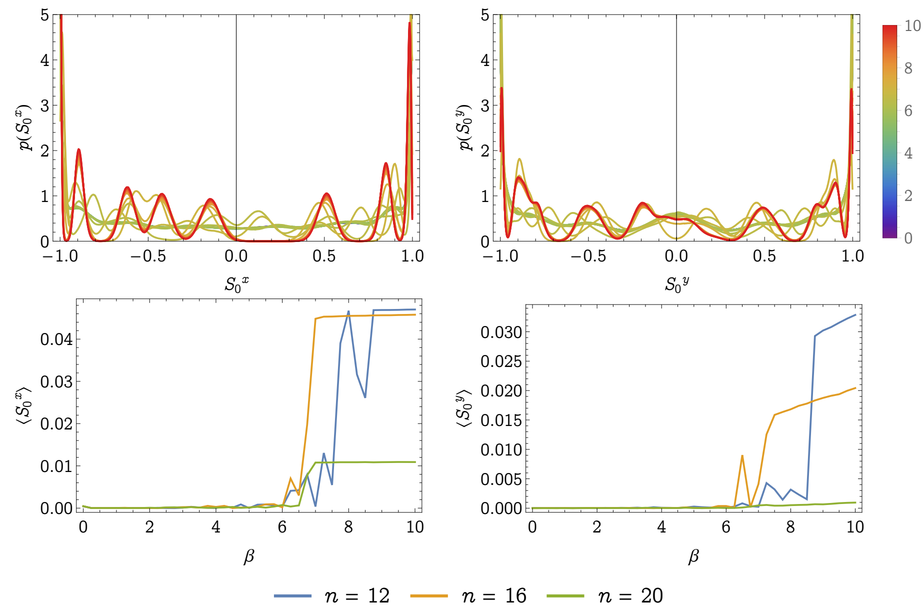

Figure 8: Results of simulating the original model and decomposing each step into spins and couplings. Top Left: The distribution of s^x for $n = 16$ at various β (shown by coloration). Top Right: The distribution of s^y for $n = 16$ at various β. Bottom Left: The expectation value of s^x. Bottom Right: The expectation value of s^y.

which happen to be coupled strongly. One could imagine embedding a nonlocal system in sufficiently many spatial dimensions so that the strength of its couplings is related in a monotonic way to the distance between the elements coupled; in this high-dimension embedding, the low-dimensional nonlocal system would have spatially segregated phases and behave as a high-dimensional local system.

In any case, we have at least reduced the problem of a first-order transition in this model of orthogonal matrices to that of first-order transitions in spin-glasses. In the process, we have reduced the matrix model to that of two-component spins coupled with annealed disorder, and have demonstrated how such a reduction can be done for any compact Lie group. The resulting spin model undergoes a paramagnetic–spin-glass transition for various forms of disorder and for any n.

References

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