Hyperdeterminant of 4-qubit spin chains

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Abstract: The properties of the hyperdeterminant, a genuine multipartite entanglement figure of merit for 4 qubits, are studied. We analyze when the hyperdeterminant detects quantum phase transitions and how it is related to the wave function of the system. By studying the ground state of two well-known quantum hamiltonians, Ising and XXZ, we analyze how entanglement behaves in terms of the hyperdeterminant. To conclude, we introduce finite temperature effects which leads us to explore the full spectrum of energies of both models.

I. INTRODUCTION

Recent developments in technology have allowed the study of quantum systems with low number of qubits to become a reality. These systems allows us to test various properties of Quantum Mechanics directly from the experiments. The feature from this theory that is most intriguing, and has no classic analogous, is entanglement. This non-local property of Quantum Mechanics is the one responsible for most of its striking features such as teleportation, secret sharing and Quantum Computation, as can be seen in Ref.[1], or Quantum Phase Transitions (QPT) Ref.[2]. Classical phase transitions are driven by thermal fluctuations, as explained in Ref.[3], and it is a well known fact that the correlation length of the system diverges on the vicinity of the critical point. On the other hand, QPT happen at absolute zero temperature. By modifying an external field parameter or a coupling constant of the hamiltonian, QPT are driven by quantum fluctuations. Similarly as its classical counterpart, close to a critical point, the system becomes correlated at all scales. This is why we expect the entanglement of the system to peak around these transitions. Quantum Sensing takes advantage of this feature of quantum many-body systems and uses it to improve accuracy on detection devices as explained in Ref.[4].

Since entanglement is the core of both quantum many-body systems and Quantum Information Theory, it is crucial to know how to describe, and more importantly, quantify it. Describing multipartite entanglement is a non-trivial task that occupies physicists all around the world. It is widely known that the Von Neuman entropy perfectly describes bipartite entanglement due to its natural connection to the Schmidt decomposition. Multipartite entanglement is not fully understood, and multiple figures of merit have been proposed as candidates to detect when a certain state is entangled in a multipartite way. As Miyake and Wadati showed in Ref.[5], hyperdeterminants are thought to be the natural generalization of more simple entanglement measures, such as the concurrence or 3-tangle for 2 or 3 qubits respectively. In the following sections we will study a multipartite entanglement figure of merit, the hyperdeterminant, of a 4-qubit chain.

The paper is organized as follows. In Section II we describe the invariants we will use to describe multipartite entanglement and some of its properties. In Section III we study the Transverse Ising model, starting from its ground state to later study the whole spectrum, in order to introduce finite temperature effects. In Section IV we perform a similar study for the XXZ hamiltonian. In Section V we present our conclusions and summarize our results while also exploring possible applications in Quantum Sensing and Metrology.

II. HYPERDETERMINANT, POLYNOMIAL INVARIANTS AND FINITE TEMPERATURE EFFECTS

The wave function for a general 4-qubit chain state reads:

$$|\psi\rangle \equiv \sum_{i,j,k,l=0,1} a_{ijkl}|ijkl\rangle, \tag{1}$$

where $a_{ijkl} \in \mathbb{C}$ and must satisfy normalization of the wave function. Since entanglement must not grow, on average, by Local Operations and Classical Computation (LOCC), multipartite entanglement can be classified in terms of this group and its stochastic version, SLOCC. As it can be seen in Ref.[5], the different classes and states can be classified in terms of the hyperdeterminant.

The hyperdeterminant is a mathematical construction discovered by Cayley in Ref.[6], who first gave the expression for a 2x2x2 tensor. In the general case, it is defined as a discriminant for a multilinear map $f : V_1 \otimes V_2 \otimes \cdots \otimes V_r \to K$ from finite-dimensional vector spaces V_i to their underlying field K which may be $\mathbb{R}$ or $\mathbb{C}$. The hyperdeterminant, $\mathrm{Hdet}(f)$, is a polynomial in components of the tensor f which is zero if and only if the map f has a non-trivial point where all partial derivatives with respect to the components of its vector arguments vanish.

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In this paper, we define the hyperdeterminant of a wave function as

$$\mathrm{Hdet}(|\psi\rangle) \equiv \mathrm{Hdet}(a_{ijkl}). \tag{2}$$

The definition given above does not allow for a clear construction of the hyperdeterminant. Following the Schläfli's construction as in Ref.[5], the hyperdeterminant for 4 qubits can be built as :

$$\begin{aligned} &\mathrm{Hdet}_2(C) = c_{00}c_{11} - c_{10}c_{01}, \\ &P_3(x) = \mathrm{Hdet}_2/.c_{ij} \to (b_{ij0} + b_{ij1}x), \\ &\mathrm{Hdet}_3(B) = \Delta(P_3(x)), \\ &P_4(x) = \mathrm{Hdet}_3/.b_{ijk} \to (a_{ijk0} + a_{ijk1}x), \\ &\mathrm{Hdet}_4(B) = \frac{1}{256}\Delta(P_4(x)), \end{aligned} \tag{3}$$

where C, B, A are arbitrary matrices, /. means "replace", $P_{3,4}(x)$ are polynomials and Δ is the discriminant of the polynomial. We could also construct the hyperdeterminant for the 4-qubit chain in terms of lower degree invariants of the SLOCC group, $SL(2,\mathbb{C})^4$. In terms of the fundamental polynomial invariants the hyperdeterminant reads:

$$\mathrm{Hdet}(|\psi\rangle) = S^3 - 27T^2 \tag{4}$$

where S and T can be constructed via tensor contractions or from low degree polynomial invariants as can be seen in Ref.[7].

If the wave function of the system can be expressed as a product state of any partition of the system, then it is easy to prove that

$$\begin{aligned} &i) \quad |\psi\rangle = |\xi\rangle_1 \otimes |\varphi\rangle_{234} \Rightarrow \mathrm{Hdet}(|\psi\rangle) = 0, \\ &ii) \quad |\psi\rangle = |\xi\rangle_{12} \otimes |\varphi\rangle_{34} \Rightarrow \mathrm{Hdet}(|\psi\rangle) = 0, \end{aligned} \tag{5}$$

where $|\xi\rangle$ and $|\varphi\rangle$ are different general wave functions for the qubits that the exterior index of the ket indicates, thus allowing for a prediction of the value of the invariants. In the case of any partition like *i)* we can show that all invariants are strictly zero, meaning that the hyperdeterminant is zero. This is not a surprising result, since genuine quadripartite entanglement can not be present if only 3 qubits are entangled. On the other hand, partitions such as *ii)* behave differently. For the partition shown in Eq.(5), S, T and the hyperdeterminant are strictly zero. The invariants reflecting the properties of the wave function in this case are the fundamental invariants of $SL(2,\mathbb{C})^4$, whose explicit form can be found in Ref.[7]. Depending on the partition, these invariants either become proportional to the concurrence of 2 qubits or zero. This lower degree invariants reflect more clearly the structure of the wave function as they have much less terms than S,T and the hyperdeterminant, which is a polynomial of around 4 million terms. The invariants, and hence the hyperdeterminant, are not only zero due to factorizations, since symmetries can make exact cancellations between the coefficients occur.

Let us also introduce temperature as quantum statistical mechanics dictates, Ref.[8], the density matrix of the system in thermal equilibrium with an external reservoir is given by:

$$\rho_\beta \equiv \frac{e^{-\beta \mathrm{H}}}{\mathcal{Z}}, \tag{6}$$

where $\mathcal{Z} = \mathrm{Tr}\left(e^{-\beta \mathrm{H}}\right)$ is the quantum canonical function, $\beta = \frac{1}{k_b T}$ and k_b the Maxwell-Boltzman constant. For all numerical calculations we will set this constant to 1 in order to avoid numerical fluctuations. To compute the hyperdeterminant in terms of temperature we use the following definition:

$$\mathrm{Hdet}(\rho_\beta) \equiv \frac{1}{\mathcal{Z}} \sum_{i=0,15} e^{-\beta E_i} \mathrm{Hdet}\left(|\psi_i\rangle\right), \tag{7}$$

where $\mathrm{H}|\psi_i\rangle = E_i|\psi_i\rangle$ and the sum runs over all the spectrum of eigenenergies and eigenstates. Using this model we can see how the ground state will dominate at low temperatures whether at high temperatures all eigenstates will contribute with the same weight to the sum.

In the upcoming sections we will consider a state to be quadripartitely entangled under the hyperdeterminant if it is different from zero. If the S and T invariants are different from zero but an exact cancellation occurs, which makes the hyperdeterminant null, we will also consider the state to be quadripartitely entangled under it. There are certain states, such as $|W\rangle = \frac{1}{2}(|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle)$, that have null hyperdeterminant and S, T are also zero, although the state is clearly entangled. This means that the hyperdeterminant is unable to capture all types of quadripartite entanglement.

The study of the upcoming hamiltonians has been wrought with a code developed in Python using mostly functions from the library *mpmath* Ref.[9] for arbitrary precision numerics. All calculations have been carried to an arbitrary precision of 100 decimals. All simulations have been done on a 4-qubit chain with periodic boundary conditions.

III. TRANVERSE ISING MODEL

The ferromagnetic Ising Model is defined by the following quantum hamiltonian:

$$\mathrm{H} = -\sum_i \sigma_i^x \sigma_{i+1}^x + \lambda \sigma_i^z, \tag{8}$$

Where σ are the well known Pauli matrices for $s = \frac{1}{2}$ spins. This model is known for having a critical point at $\lambda = 1$ where the infinite system switches from an ordered ferromagnetic phase to a disordered paramagnetic phase. Since we are working with a finite chain it is to expect that finite-size effects will affect our simulation. As

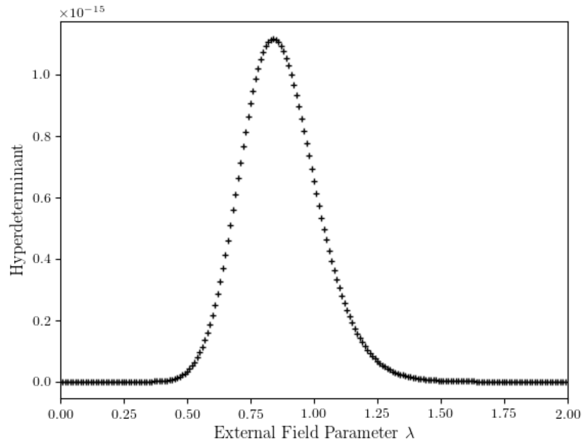

FIG. 1: The dependence of the hyperdeterminant of the transverse Ising model around the QPT is shown.

per our chain, the hyperdeterminant behaves as shown in Fig.1.

We see how the hyperdeterminant peaks closely to the infinite chain transition point. In fact, it peaks at $\lambda \sim 0.84$ and attains a value of $\text{Hdet}(|\psi_0^{\text{Ising}}\rangle) \sim 1.116 \cdot 10^{-15}$. Comparing this value with the absolute maximum hyperdeterminant obtained in Ref.[10], $\text{Hdet}(|\text{HD}\rangle) \sim 1.98 \cdot 10^{-5}$, we see how our model gets multipartite entanglement, but it is still very weak.

As we have seen in Section II, we need to compute the full spectrum of eigenstates in order to introduce temperature. The excited states of the Ising model can be classified in 3 types:

1. $S = T = 0$ which imply $\text{Hdet}(|\psi\rangle)$=0, due to factorizations of the wave function.
2. $S = T = ct. \neq 0$ which cancel out to give $\text{Hdet}(|\psi\rangle)$=0
3. $S = f(\lambda); T = f'(\lambda)$ and $\text{Hdet}(|\psi\rangle) = f(\lambda)$ or 0 due to factorizations when both functions are zero.

This classification also applies for the XXZ model shown in Section IV. The analysis of all the spectrum is given in Table I.

From it we see that only the ground state and the second excited state (and their symmetrics, the 13^{th} and 15^{th}) have non zero hyperdeterminant. Not only so, but the peak of the second excited state is also five orders of magnitude greater than the one associated to the ground state. This is due to the fact that the greatest possible number of configurations of the system happens when two spins are excited.

To compute the hyperdeterminant with finite temperature effects we use Eq.(7) in order to generate Fig.2 where we can see how the hyperdeterminant saturates approximately when $T \sim 10$. Its fast saturation is due to the fact, that the only other state contributing to it is the

	Hdet	S	T
$E_{0,15}$	$f(\lambda)$	$s_1(\lambda)$	$t_1(\lambda)$
$E_{1,5}$	0	$s_2(\lambda)$	$t_2(\lambda)$
$E_{2,13}$	$f'(\lambda)$	$s_3(\lambda)$	$t_3(\lambda)$
$E_{3,4,8,9,11,12}$	0	0	0
$E_{6,7}$	0	ct_s	ct_t
$E_{10,14}$	0	$s_4(\lambda)$	$t_4(\lambda)$

TABLE I: Summary of the different invariant values for all excited states for the Ising Model. E_i indicates how many times the state is exited above the ground state. All terms just indicate how the invariant depends on external parameters and have been calculated up to $\lambda = \frac{3}{2}$ since for larger λ the different energies start crossing and switching their roles between excited or ground states.

second excited state. It is from this state where the unexpected change in magnitude order comes, as explained in the previous paragraph. We also see how the maximum of the hyperdeterminant jumps abruptly due to the low energy difference between the ground state and the 2^{nd} excited state.

This peculiar behavior of the second excited state may play an important role in Quantum Sensing and Metrology, where temperature can not be neglected and thermal fluctuations of the states appear. As we can see in Fig.2, the peak smoothens and moves to $\lambda \sim 1.25$.

We have seen for the Ising model how the hyperdeterminant detects the QPT and all states generated follow the properties presented in Section II. In order to ensure the hyperdeterminant is a good figure of merit to detect QPT we will study the XXZ Model.

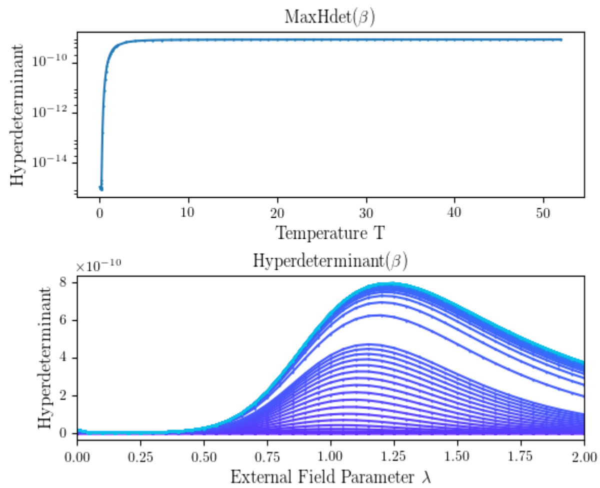

FIG. 2: The evolution of the hyperdeterminant over some chosen values of temperature is shown. A lighter color in the upper curves means a higher temperature.

IV. XXZ MODEL

The XXZ model is defined by the following quantum hamiltonian

$$\mathrm{H} = \sum_i \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z + \lambda \sigma_i^z. \quad (9)$$

If we set $\lambda = 0$, as we can see in Ref.[11], this model is in the ferromagnetic phase for $\Delta < -1$, in the critical XY spin-glass phase for $-1^+ \leq \Delta \leq 1$ and in the Néel antiferromagnetic phase for $\Delta > 1$.

Surprisingly, the hyperdeterminant $\forall \Delta$ and $\forall \lambda$ is exactly zero. Due to this fact, the hyperdeterminant is not able to detect any QPT for this model, but on the other hand, S and T are able to do so, as shown in Fig.3.

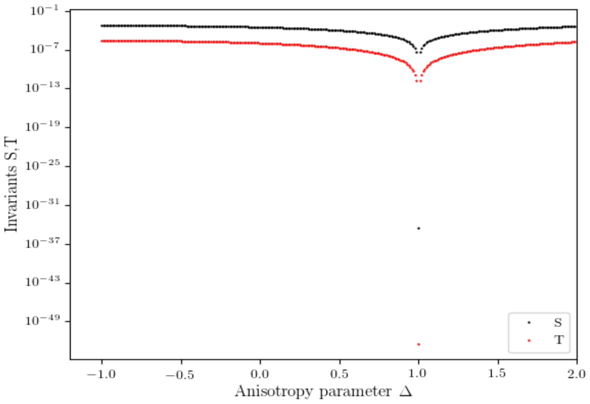

FIG. 3: It shows the dependence of the S,T invariants of the XXZ model over the anisotropy parameter. The region $-2 < \Delta < -1$ is empty because there both invariants are strictly 0 and the logarithmic scale is unable to show it.

We see how both invariants are able to detect both QPT, but they cancel out exactly to make the hyperdeterminant 0. This can be explained in terms of the explicit form of the ground state. For the ferromagnetic phase we clearly have a product state $|\psi_0\rangle = |1111\rangle$ or $|0000\rangle$ which has no entanglement at all. For the Néel phase, the non normalized state is given by

$$|\psi_0(\Delta)\rangle = |0011\rangle + |0110\rangle + |1100\rangle + |1001\rangle - \frac{1}{2}\left(\Delta + \sqrt{8+\Delta^2}\right)(|0101\rangle + |1010\rangle), \quad (10)$$

which is an entangled state. If we set $\Delta = 1$ then the state reads

$$|\psi_0(1)\rangle = |\psi^-\rangle_{23}|\psi^+\rangle_{14} + |\psi^-\rangle_{34}|\psi^+\rangle_{12} \quad (11)$$

where $|\psi^\pm\rangle = |01\rangle \pm |10\rangle$. If we are able to factorize the system into subsystems which are entangled between them, then we could justify S and T being zero. Since in this case the factorization is in terms of two pairs, the fact that the invariants are zero is due to symmetry. The XXZ chain is U(1) symmetric $\forall \Delta$ but when $\Delta = 1$, SU(2) symmetry is also fulfilled, hence making the invariants 0 (Ref.[12],[13]).

In a similar fashion as we did in the last section, the XXZ model exhibits analogous features regarding the invariants. As before, by performing the same analysis as in Section III, we can construct Table II in which now we show the different dependencies of the energy E(Δ) instead of the excited states for the sake of simplicity.

E=	Hdet	S	T
-4	0	0	0
4	0	0	0
0	0	0	0
0_1	0	ct_s	ct_t
-4Δ	0	ct_s	ct_t
4Δ	0	0	0
$E'(\Delta)$	0	$s(\lambda)$	$t(\lambda)$

TABLE II: Summary of the different invariant values for all excited states for the XXZ Model. All terms just indicate how the invariant depends on external parameters and $E'(\Delta) = -2(\Delta \pm \sqrt{8+\Delta^2})$. The energy 0_1 corresponds to the only state which has a different structure than the rest of the states with null energy, hence leading to a different behavior of the invariants. The terms $ct_{s/t}$ simply mean that the invariants are constant and with different values.

All states generated can be studied under the classification of Verstraete *et al.*in Ref.[14] and is left for upcoming studies.

As we have seen, the hyperdeterminant is completely null for all eigenstates of the XXZ Hamiltonian, hence it is mandatory to compute the thermal average, in an analogous way as Eq.(7), for the invariants S and T. In order to keep the figure simple, we only show the S invariant in the region of low temperatures in Fig. 4.

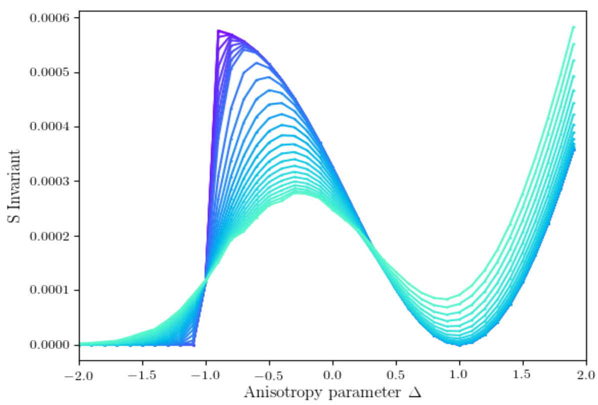

FIG. 4: The evolution of the S invariant over some chosen values of temperature is shown. A lighter color in the lower curves means a higher temperature.

We see how when higher energy states are contributing to the average, S slowly loses its ability to detect both QPT. It is worth noting that introducing temperature as in Eq.(7) we preserve the properties of the invariants regarding the detection of entangled states, while changing its properties regarding the detection of QPT.

Unlike the Ising model, XXZ behaves as we would expect when temperature is introduced, making the detection of QPT vanish when thermal fluctuations are contributing to the system. This holds great importance in any experimental quantum setup, where decoherence plays a decisive role in how the system evolves and hence may prove useful for Quantum Sensing and Metrology.

V. CONCLUSIONS

We have studied a multipartite generalization of the 2-qubit concurrence, the hyperdeterminant. We have studied its behavior for both the Ising and the XXZ model, successfully detecting the QPT in the first case. Since the hyperdeterminant can not detect QPT in the XXZ model we decided to explore the behavior of more fundamental invariants, S and T, since they reflect clearly the properties of the wave function. Finally, we introduced finite temperature effects by means of the quantum canonical partition function from statistical mechanics.

Multipartite entanglement is not yet fully understood. It is clear how to generalize concurrence and other lower dimension invariants but the hyperdeterminant is still not able to capture the essence of entanglement in a similar fashion as the Von Neuman entropy does. Further studies will consist on a deeper analysis of the polynomial invariants in hope of finding a general way to quantify and detect QPT, and more importantly, entanglement.

Quantum Sensing and Metrology takes advantage of entangled systems in order to measure experimentally little variations of macroscopic quantities, such as the magnetic field. As it is seen in Ref.[4] or Ref.[15], entangled states play a key role in achieving the Heisenberg limit of measurements where the uncertainty of a measure scales as $\frac{1}{N}$, whereas the standard quantum limit for a single qubit system scales as $\frac{1}{\sqrt{N}}$.

The main problem of those systems is that any improvement on the sensitivity scaling gets usually worsened due to decoherence of the system. For instance, GHZ states pose an improvement of sensitivity of $\sqrt{N}$. But, on the other hand, GHZ has a decoherence rate N times faster than a product state, hence leaving no real improvement overall on the sensitivity attained.

Since ground states are the most stable of all, the use of highly entangled spin chain may play an important role in extending the coherence time of systems that achieve the Heisenberg limit. As we have seen, if we are able to set up a spin chain in a QPT we expect the system to have maximum entanglement. In this case we would be able to approach the Heisenberg limit with a state that is the most stable over all the spectrum. Regarding our 4-qubit chain, it is left for further studies to find out which hamiltonian produces the maximally entangled state under the hyperdeterminant, the $|\text{HD}\rangle$ state.

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