Characterizing Bell non-locality using tensor network formalism

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Abstract: In quantum mechanics, the classical tenet that the degrees of freedom are independent of the act of their measurement, is no longer valid. The experimental footprint of quantum mechanics is the Bell inequalities violation, highlighting Bell non-locality. Alas, the computational cost of proving Bell non-locality scales exponentially with the system size, making it a formidable challenge to prove. Here we present a different approach to prove and validate Bell non-locality, by solving inverse Ising problems using tensor network formalism. We will show as examples of this validation a Bell-pair system and a Quantum Heisenberg Antiferromagnet (QHAF) in 1D.

I. INTRODUCTION

In quantum mechanics, particles can share correlations as entanglement [1] or Bell correlations [2, 3] that are stronger than any classical theory allows. That is the reason why we need to validate if a system can be treated as classical, or we need quantum mechanics in order to describe its nature.

Bell non-locality was found by Bell in 1964 [4], and proved that quantum theory cannot be reproduced by any classical *Local Variable* (LV) model. As it will be shown in section IV.A the original formulation of Bell inequalities requires two particles with spin 1/2. There are two observers, each having access only to one of the particles. The experiment requires that each party randomly chooses to perform one measurement from a set of two incompatible measurements. If the state of the particles is a Bell-pair, the statistics of the measurements violates the historic Bell inequality [4] known as the *Clauser-Horne-Shimony-Holt* (CHSH) inequality [5]:

$$\langle \sigma_0^{(1)}\sigma_0^{(2)} + \sigma_1^{(1)}\sigma_1^{(2)} + \sigma_0^{(1)}\sigma_1^{(2)} - \sigma_1^{(1)}\sigma_0^{(2)} \rangle_{LV} \geq -B_c = -2 \tag{1}$$

In the last decades, there has been a huge effort in order to prove and validate Bell inequalities in many-body systems, which cost scales exponentially with the system size, as it will be explained in the next section.

In this paper we will try to reproduce the procedure used in [6], but instead of using classical Monte Carlo algorithms and its formalism, we will use this other formalism called *Tensor network* [7–9], a relatively new way to proceed with many-body quantum mechanics. Which allows to proceed in a more rapid and customized way than other formalism's. This formalism allows us to represent sets of correlated data, to found the system wavefunction in many body systems or partition functions or even represent multi-dimensional data [7].

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II. BELL NON-LOCALITY

As explained in [6], we will use the device independent (DI) certification, which only assumes that the device can be controlled experimentally. We shall define a (N, k, p) scenario to verify Bell tests. We define N spatially separated degrees of freedom – that we imagine arranged over a lattice – on which we can measure k observable (inputs) with p possible results (outputs). We indicate as $\sigma_a^{(i)}$ the p possible results of the a-th observable on the i-th degree of freedom, with $a = \{0, ..., k-1\}$ and $i = \{1, ..., N\}$. In the DI approach, the actual quantum operators $\hat{M}_a^{(i)}$ and the Hilbert space associated to the N degrees of freedom, are not required. Moreover, we will denote the quantum data as the average over repeated measurements on the quantum system, $\langle f(\boldsymbol{\sigma}) \rangle_Q$ (where $\boldsymbol{\sigma} = \{\sigma_a^{(i)}\}$).

The strongest form of quantum correlations – Bell non-locality – is certified by the DI approach when the quantum data violates a Bell inequality [2, 3]. Which means that you can not construct a LV model whose correlation attains the value measured in the quantum system. Such models rely on a joint probability distribution for all the measurement outcomes, $P_{LV}(\boldsymbol{\sigma})$ [10]. Similarly to the classical statistics physics, LV models treat the measurement outputs $\sigma_a^{(i)}$ as random variables that fulfill a certain probability distribution. If two operators do not commute $[\hat{M}_a^{(i)}, \hat{M}_b^{(i)}] \neq 0$, then, there are some states for which we can find the joint of probability and others that we can not.

The most general form of Bell inequalities involving two body correlations have as an expression:

$$\sum_{i=1}^{N}\sum_{a=1}^{k} \alpha_a^{(i)} \langle \sigma_a^{(i)} \rangle_{LV} + \sum_{i,j=1}^{N}\sum_{a,b=1}^{k} \beta_{a,b}^{(i,j)} \langle \sigma_a^{(i)} \sigma_b^{(j)} \rangle_{LV} + ... \geq -B_C \tag{2}$$

where $\langle ... \rangle_{LV}$ is how we shall indicate the average over P_{LV} distribution and $-B_C$ is so called the classical

bound. Geometrically, each term of the Eq.(2) define an hyperplane in the correlation space defining two regions. The intersection between the half-spaces define a geometrical structure in the correlation space, called local polytope. If our data set is somewhere inside the local polytope our data fulfills the Bell inequality, otherwise our data violates the inequality highlighting the shortcomings of the LV model. This procedure defines also the closest facet of the local polytope to the quantum data.

If we consider an N particles many-body system, given a quantum data set $\{\langle f_r\rangle_Q; r = 1, ..., R\}$, where f_r are arbitrary functions of the measurement outputs, the local polytope has $p^{kN} + p^{2KN^2} + ...$ vertices, and its full reconstruction has therefore an exponential cost. Which means that it requires an incredible computational power and time to validate.

There have recently been developed some strategies in order to reduce this computational cost, either restricting the search of Bell inequalities to the invariants under change of lattice-site indices (namely $\alpha_a^{(i)} = \alpha_a, \beta_{a,b}^{(i,j)} = \beta_{a,b}$,etc. in Eq.(2)) [11] reducing the computational cost, but losing generality; or approximating the local polytope from the outside [12], which requires an exponential cost to converge to the actual polytope.

To reproduce the quantum data, we use the following approach, taking into account that our local variable model must satisfy the condition:

$$\langle f_r(\boldsymbol{\sigma})\rangle_Q = \langle f_r(\boldsymbol{\sigma})\rangle_{LV} \quad (r = 1, ..., k) \tag{3}$$

This Local Variable model will have an Ising Hamiltonian as $\mathcal{H}(\boldsymbol{\sigma}, \boldsymbol{K}) = -\sum_r K_r f_r(\boldsymbol{\sigma})$ where K_r are the Lagrange multipliers that minimize the "free-energy" functional:

$$F[P_{LV}] = \sum_{\boldsymbol{\sigma}} P_{LV} \log P_{LV} - \sum_r K_r(\langle f_r\rangle_{LV} - \langle f_r\rangle_Q) \tag{4}$$

Which is known to take the form of a Boltzmann distribution:

$$P_{LV} = \exp[\sum_r K_r f_f(\boldsymbol{\sigma})]/\mathcal{Z} \tag{5}$$

where $\mathcal{Z}$ is the partition function. This is called an *inverse Ising problem* [13] and has a convex convergence with a cost function as:

$$\mathcal{L}(\boldsymbol{K}) = \log \mathcal{Z}(\boldsymbol{K}) - \sum_r K_r \langle f_r\rangle_Q \tag{6}$$

This convexity of the cost implies a gradient-descendent algorithm:

$$G_r = \frac{\partial \mathcal{L}}{\partial K_r} = \langle f_r\rangle_{LV} - \langle f_r\rangle_Q \tag{7}$$

that converges to the global minimum. This algorithm presents two possibilities: 1) If the system can be represented as a classical system i.e. the quantum data lie inside the local polytope and the gradient will eventually be zero. 2) otherwise, our quantum data lies outside the local polytope, and the gradient will converge in practice when the distance:

$$|G_\infty|^2 = \min_{LV} \sum_r (\langle f_r\rangle_{LV} - \langle f_r\rangle_Q) \tag{8}$$

Geometrically, this means that our LV model has hit from inside a facet of the local polytope, nearest to the quantum data, or that it arrives to one of the vertices of the local polytope.

Note that in this case, the LV model will have a Hamiltonian which is not the actual quantum Hamiltonian, it is an effective Hamiltonian $\mathcal{K}(\boldsymbol{\sigma}) = \sum_r G_{r,\infty} f_r(\boldsymbol{\sigma})$, which will be necessarily frustrated as it is not obtained minimizing each term independently.

III. TENSOR NETWORKS

As previously mentioned, tensor networks is a formalism used in a variety of different situations, but usually in a many-body system. In this paper, we will use different algorithms of this formalism as *Projected entangled states* [14], describing a two-dimensional lattice (2D). We will introduce this formalism by explaining some examples to contextualize the actual paradigm, and we will proceed explaining some methods according to the system about to solve.

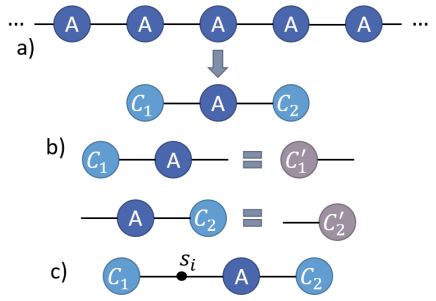

FIG. 1: Diagrammatic representation 1D classical infinite Ising model. a) Contraction of the system environment. b) Redefinition of the new corner matrices. c) Expected value of s_i.

A. 1D infinite Antiferromagnetic Ising Model

First, we will show the easiest system we can describe, which is a 1D Infinite Antiferromagnetic Ising Model. This well-known system follows the Hamiltonian $\mathcal{H} = J\sum_{\langle i,j\rangle} s_i s_j + h\sum_i s_i$. As it is the antiferromagnetic case $J = -1$, and h is the external magnetic field applied. The procedure will be: 1) We define the tensor A as:

$$A_{s_i s_j} = \exp(-\beta H_{s_i s_j}) \tag{9}$$

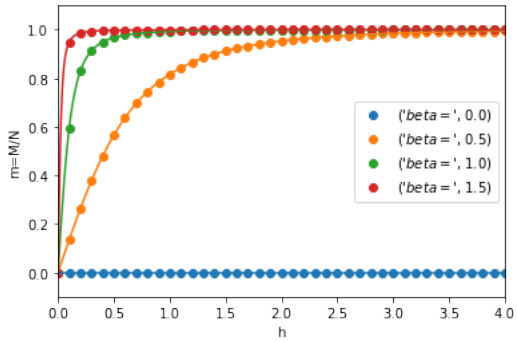

FIG. 2: Diagrammatic representation of 1D antiferromagnetic infinite chain under the effect of an external field h. The solid line is the exact solution and the points are the computed values.

This tensor will be a 2 by 2, as $s = \pm 1/2$. In each position of which, we will find the Boltzmann weight associated to each possible configurations of the spins s_i and s_j. 2) Then we need to contract the environment. We will proceed as following. We define two tensors C1 and C2 that can be random, one-dimensional, named corner matrices. These will be the environment of the system, and in order to reproduce an infinite system, we will contract each tensor C with a tensor A, obtaining a new tensor C'. Then we repeat this procedure, redefining the C' as C. We will proceed iterating until the difference between all the components of the two tensors, C and C' are smaller than a certain precision that we will name ξ. This procedure is very useful as we do not need to use *Markov chains* with contour conditions to reproduce a system [6], as you obtain an exact value with in an error ξ.

To calculate the expected value of an observable, we will proceed as follows. To compute the magnetization per particle, for example, we will sum the expected values of s_i from each site. The expected values will be calculated as shown in FIG.[1 c)], contracting the operator associated with the tensor A and then contracted with the environment. Which is equivalent to:

$$\langle s_i \rangle = \frac{\sum_i s_i \exp(-\beta \mathcal{H})}{\mathcal{Z}} \tag{10}$$

The results obtained for the magnetization of the system are shown in the FIG.[2].

B. 2D infinite Antiferromagnetic Ising Model

As an example of a more complex system, we will study the 2D lattice Ising model. Which has a Hamiltonian as:

$$H_{s_1 s_2 s_3 s_4} = J(s_1 s_2 + s_2 s_3 + s_3 s_4 + s_4 s_1) - h(s_1 + s_2 + s_3 + s_4) \tag{11}$$

With s being the spin on each intersection of the lattice. For simplicity, we will consider an antiferromagnetic

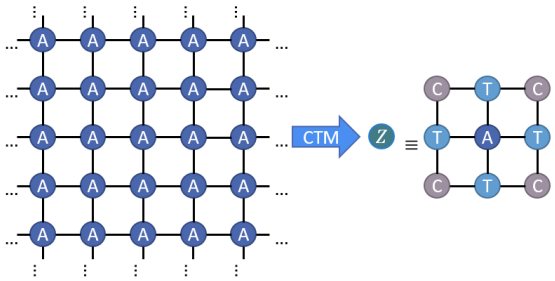

FIG. 3: Diagrammatic representation of the classical corner transfer matrix contraction.

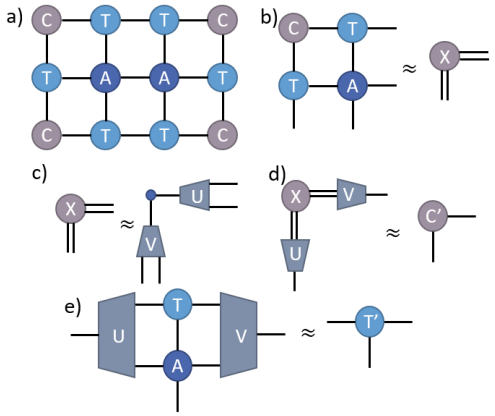

FIG. 4: CTM procedure. a) Insertion of a new column. b) Contraction of the tensors T-C-T-A as X. d) and e) Definition of C and T respectively.

case with $J = -1$ and the magnetic field applied h constant, with $s = \pm\frac{1}{2}$. Doing this approach we can define the tensor A, as

$$A_{s_1 s_2 s_3 s_4} = \exp\left(-\beta H_{s_i s_j s_k s_l}\right) \tag{12}$$

As in the previous case, this tensor contains all the possible states of four spins and the respective Boltzmann weight associated. The procedure to compute the environment of this tensor will be similar to the one used before. We will introduce the *Corner Transfer Matrix* (CTM) [15] which contracts the environment as follows. We define 8 tensors, 4 as corner matrices that we name C's and 4 site tensors that we name T's, as it is showed in the FIG.[3]. In order to reproduce the environment of the tensor, which is an infinite lattice, we will need to contract tensors until the resultant tensors converges. In this case, as our system is homogeneous and invariant under 90 degrees rotations, our system will have the same C's and T's in each direction. If it was not the case, we will have to treat each direction separately as in [15]. The contraction procedure of CTM shall be as follows:

1. Insertion: we add a new column T-A-T, between the columns C-T-C and the column T-A-T.

2. Absorption: we contract [16] the tensors T-C-T-A, as shown in FIG.[4 b)] and we obtain a new tensor that we will call X. Doing the eigenvalue decomposition of this tensor renormalized as a two leg tensor, with each leg with a dimension as the dimension product of T and A. By doing this, we obtain two tensors U and V, where $U = V^*$. These tensors have three legs. The two connected to X, have the same dimension as X and the other is of dimension χ, being χ the number of eigenvalues bigger than a certain precision, and has been defined from bigger to smaller. We shall now contract U-X-V to obtain C' and contract U-T-A-V to obtain T', as showed in FIG.[4 c) to e)].

3. Renormalization: Now we renormalize the tensors in order to be able to find convergence. We can obtain that goal by dividing C' and T' by the biggest eigenvalue of X. Then redefine these as C and T.

Now, we can compute the expected value of the magnetization of the system as a function of β, i.e. as a function of the system temperature. Where $\beta = \frac{1}{k_B T}$. We must compute the expected value of s in each direction and make the average (in our case, because its invariance under rotations, the four spins will be the same). The expected value is similarly computed to the case 1D. We contract the environment with the tensor A', where A' is the tensor A contracted with the tensor $s = \sigma_z$, being σ_z the Pauli matrix z. We then define the magnetization per particle as $m = \frac{1}{4}\sum_{i=1}^{4}\langle s_i\rangle$, FIG.[5].

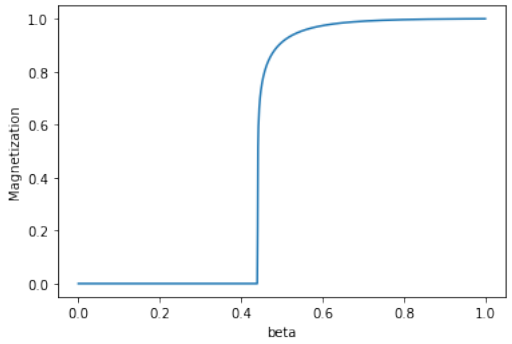

FIG. 5: Antiferromagnetic phase transition of classical Ising antiferromagnet.

IV. PROVING BELL NON-LOCALITY

Finally, we will try to prove Bell Non-locality using tensor networks, for a Bell-pair and a 1D *Quantum Heisenberg Antiferromagnet model* (QHAF). This two systems are well-known quantum cases and have been presented in many papers as quantum systems [6].

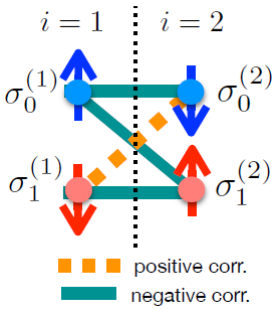

FIG. 6: Frustrated correlation pattern, that an LV model have to reproduce to realize the correlations on a Bell-pair $(|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle)/\sqrt{2}$ (from [6]).

A. Bell-pair

We will show as a first example of this procedure, a Bell-pair $(|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle)/\sqrt{2}$ of spin $S = 1/2$, and compare it with the results obtained in [6]. In this case we have a $(2, 2, 2)$ scenario. Choosing our quantum measurement basis as $\sigma_0^{(1)} = \sigma_x$, $\sigma_1^{(1)} = \sigma_y$, $\sigma_0^{(2)} = \cos(\theta)\sigma_x + \sin(\theta)\sigma_y$, $\sigma_1^{(2)} = \cos(\theta)\sigma_x - \sin(\theta)\sigma_y$, we obtain the quantum correlation functions are: $\langle\sigma_0^{(1)}\sigma_0^{(2)}\rangle_Q = \langle\sigma_1^{(1)}\sigma_1^{(2)}\rangle_Q = -\cos\theta$ and $\langle\sigma_1^{(1)}\sigma_0^{(2)}\rangle_Q = \langle\sigma_0^{(1)}\sigma_1^{(2)}\rangle_Q = -\sin\theta$. Choosing the optimal angle $\theta = \pi/4$, we obtain all quantum correlators with the common value $1/\sqrt{2}$, but we shall notice a fully frustrated correlation loop, as showed in FIG.[6].

We can use an Ising Model as $\mathcal{H} = -\sum_{a,b} K_{ab} s_a s_b$ to try to reproduce these values. Using tensor networks, this system is really simple to compute and to optimize its K_{ab}, to obtain the best approximation of $\langle s_i s_j\rangle_{LV}$ to the $\langle\sigma_{a_i}^{(i)}\sigma_{a_j}^{(j)}\rangle_Q$ i.e. to arrive to the local polytope facet from inside. This optimization can be computed with a large amount of different searching algorithms such as least-squares algorithm [17], minimizing the difference Eq.[8].

Because of the system's symmetry, we shall obtain the classical expected values as an average over the observables. Because of the antiferromagnetic frustration, we obtain: $\langle\sigma_0^{(1)}\sigma_0^{(2)}\rangle_{LV} = \langle\sigma_1^{(1)}\sigma_1^{(2)}\rangle_{LV} = \langle\sigma_0^{(1)}\sigma_1^{(2)}\rangle_{LV} = -\langle\sigma_1^{(1)}\sigma_0^{(2)}\rangle_{LV} = -1/4$. We shall define an effective Hamiltonian $\hat{\mathcal{H}}$ which has the same form as $\mathcal{H}$ and reproduces the (CHSH) inequality Eq.[1] (whereas the quantum data achieves $-2\sqrt{2}$, violating this inequality).

B. Quantum Heisenberg Antiferromagnet (QHAF)

We will end this paper by searching for Bell inequalities in a 1D Quantum Heisenberg Antiferromagnet (QHAF) with a Hamiltonian $\hat{\mathcal{H}} = J\sum_{\langle i,j\rangle}\hat{S}^{(i)}\cdot\hat{S}^{(j)}$ where $\hat{S}^{(i)}$ are the quantum $S = 1/2$ operators and $\langle i, j\rangle$ implies the

sum to nearest neighbours.

The ground state of this system is a many-body generalization of the Bell-pair considered above. We will focus on a $(20, 4, 2)$ scenario because for $k = 4$ we obtain the largest value of Bell inequalities, as showed in [6].

We consider a uniform measurement strategy in which the axes are coplanar and form an $a\pi/4$ angle for $a = \{0, 1, 2, 3\}$. So our correlations end up being: $\langle \sigma_a^{(i)} \sigma_b^{(j)} \rangle_Q = \cos(\theta_a)\cos(\theta_b)\sigma_x\sigma_x + \sin(\theta_a)\sin(\theta_b)\sigma_y\sigma_y + \cos(\theta_a)\sin(\theta_b)\sigma_x\sigma_y + \sin(\theta_a)\cos(\theta_b)\sigma_y\sigma_x$

From the quantum expected values obtained from Tenpy open source library [18], we define our classical model to approach the quantum model, like mentioned above. As $k = 4$, our tensor A must be a (2,2,2,2) tensor, with a Hamiltonian as $\mathcal{H} = -\sum_r K_r (s_i s_j)^{(r)}$, where the sum on r goes from 0 to 15, which indicates the possible $4 \times 4 = 16$ combinations of spins, and K_r are the respective Boltzmann weigh.

Using the least squares optimization algorithm, we have found a possible candidate for a Bell inequality, as our optimization process may have found a local minimum, but not necessarily the global one. The inequality fulfilled is

$$\langle \mathcal{B} \rangle_{LV} = \frac{1}{N} \sum_i \sum_{a,b} |\langle \sigma_a^{(i)} \sigma_b^{(i+1)} \rangle| \leq 1,446944364 \quad (13)$$

being the quantum value $\frac{3+3\sqrt{2}}{5} \approx 1,448528137$. This variation is less than 0,01 %, which will be very hard to prove experimentally.

V. CONCLUSIONS

We have reformulated the approach discussed in [6] in the context of tensor network. This gives us the possibility to directly construct the local variable distribution, getting rid of the Markov chain. The approach can be used to discover if a set of quantum data presents no local correlation and to identify possible candidates of Bell inequality. In Eq.[13] we found this candidate for the QHAF in 1D. Before claiming it is a new Bell inequality we must search in the literature. Something we are currently doing.

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