On the Entanglement Properties of Quantum Ising Chains

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Abstract: We study the ground state properties of the one-dimensional quantum Ising model and its phase diagram through the lens of quantum information theory concepts. We begin by analysing the area law behaviour of entanglement entropy and its logarithmic violation at the critical point. Next, we introduce the classical-to-quantum correspondence to elucidate the structure of two-point correlation functions. Finally, we characterize the distinct phases of the model via its entanglement spectrum.
Keywords: Theoretical Physics, Many-body Quantum Systems, Quantum Phase Transitions, Quantum Information Theory, Condensed Matter, Area Laws, Entanglement Spectrum
SDGs: 4:Quality Education, 8:Decent Work and Economic Growth, 13:Climate Action

I. INTRODUCTION

At the heart of the quantum theory, lies one of the most dazzling and surprising features of our current description of reality: *entanglement.*

Entanglement can be defined as the system's property of exhibiting non-local correlations which have no classical counterpart [1]. The concept of entanglement, firstly coined by E. Schrödinger [2] in his famous response to the EPR paradox, has found numerous applications in the context quantum information theory (QIT). In the last decades, though, it has proven to be key in understanding the behaviour of correlations in many-body quantum systems undergoing a quantum phase transition (QPT) [3]. Contrary to classical phase transitions, QPT occur at $T = 0$ K and their origin is no longer explained by thermal fluctuations but rather Heisenberg's uncertainty principle [4].

The aim of this work is to present several novel techniques for discerning the different phases of a quantum system ground state and its properties at criticality from an entanglement point of view [5]. Hence, we will study the most paradigmatic and archetypal model: *The Ising model in a transverse field.*

This work is structured as follows: first, in Section II we introduce the studied model, some quantum information concepts for measuring our system's entanglement properties such as the entanglement entropy (EE) and the numerical methods used. Then, in Section III, we proceed by presenting the most important feature of EE: *the area law.* In Section IV, we compute the EE results at criticality and see their relationship with conformal field theory (CFT). In Section V, we introduce the so-called classical-to-quantum (CQ) correspondence which will lead us to understand the behaviour of the two-point correlation function. In Section VI, we consider a different way of describing the entanglement of our system: *the entanglement spectrum.* Finally, in Section VII, we discuss the conclusions of this work.

II. THEORETICAL BACKGROUND

1. The 1-D Ising model

We consider the 1-D Ising model in a transverse field, the physics of this model is solely determined by its Hamiltonian [4, 6]:

$$H_I = -J\left(\sum_i Z_i Z_{i+1} + g\sum_i X_i\right). \quad (1)$$

Here J represents the strength of the interaction between neighbouring spins and g is a dimensionless coupling of the transverse field, note that both $J > 0$ and $g > 0$. Also, Z_i and X_i are the Pauli matrices defined at the site i and we work with periodic boundary conditions (PBC). For this model, the first term represents a first-neighbour interaction while the second one represents the spin interaction with the external field.

Additionally, our model exhibits a phase diagram where the parameter g acts as a control parameter. The system displays two distinct phases: a ferromagnetic phase, where spin-spin interactions dominate, and a quantum paramagnetic phase, where the influence of the external field prevails. In between, at a critical value: g_c, the system will undergo a QPT (see Figure 1 for a schematic representation of both phases) [7].

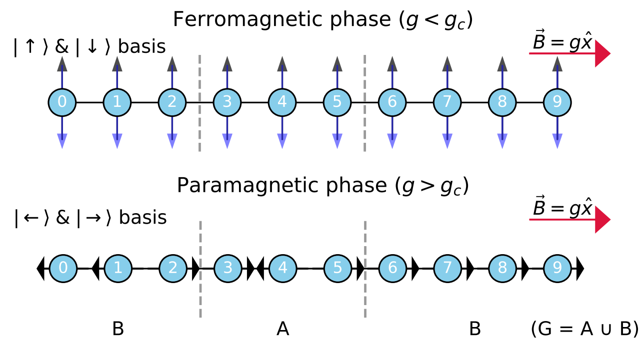

FIG. 1: Drawing of the two distinct phases of the ground state for the quantum Ising model generated by Eq. (1).

Furthermore, an interesting property of this model is that it fulfils the $\mathbb{Z}_2$ symmetry [8]. We can work on either the Z basis ($|\uparrow\rangle, |\downarrow\rangle$) or the X basis ($|\leftarrow\rangle, |\rightarrow\rangle$). They are related via: $|\rightarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$ and $|\leftarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)$.

First of all, we need to determine the ground state of our system. In the $g = 0$ and $g \to \infty$ limit, the ground state can be written as:

$$\begin{aligned} \left|\psi^{\text{Ferro}}_{(g\to 0)}\right\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\uparrow\uparrow \dots \uparrow\uparrow\uparrow\rangle \pm |\downarrow\downarrow\downarrow \dots \downarrow\downarrow\downarrow\rangle) \\ \left|\psi^{\text{Para}}_{(g\to \infty)}\right\rangle &= |\rightarrow\rightarrow\rightarrow \dots \rightarrow\rightarrow\rightarrow\rangle, \end{aligned} \tag{2}$$

where we note that the $g \to 0$ ground state has a two-fold degeneracy. For the remaining values of g of the phase diagram, we will compute them numerically.

2. *Von Neumann entropy*

In classical physics, the notion of entropy is associated to the amount of information that we lack in order to fully identify the microstate of the system compatible with its macrostate, in other words, it is related to the disorder in the system or randomness. Whereas, on the quantum realm, entropy may even arise with a complete knowledge of the state of the system, this happens due to a fundamental property of quantum systems: *entanglement* [9].

Such measure of entanglement is given via the von Neumann entropy or entanglement entropy (EE) [11]:

$$S(\rho) = -\text{Tr}[\rho \log(\rho)], \tag{3}$$

where $\rho = |\psi\rangle\langle\psi|$ stands for the density matrix.

Now, consider a bipartition of the system into subsystems A and B, each one defined by its orthonormal basis $\{|\varphi_i\rangle_A\}$ and $\{|\phi_i\rangle_B\}$. According to the Schmidt decomposition, we can express our state as [5]:

$$|\psi\rangle = \sum_i \sqrt{\lambda_i}\, |\varphi_i\rangle_A \otimes |\phi_i\rangle_B. \tag{4}$$

In our case, we are interested in the EE of a subregion A of our system (S_A), which can be defined as:

$$S_A(\rho_A) = -\text{Tr}[\rho_A \log(\rho_A)] = -\sum_i \lambda_i \log \lambda_i, \tag{5}$$

where $\text{Tr}_B[\hat{O}] = \sum_j \langle\phi_j|_B\, O\, |\phi_j\rangle_B$ and we have also defined the reduced density matrix (ρ_A) as:

$$\rho_A = \text{Tr}_B[\rho] = \sum_i \lambda_i |\phi_i\rangle_A \langle\phi_i|_A. \tag{6}$$

3. *Numerical methods*

Even though most of the known results for this model are for the thermodynamic limit, we have done numerical simulations to check it for finite-size systems (up to $N = 15$). Hence, our goal is to numerically compute the function $S_A = S_A(g)$ for each value of g in the phase diagram, the numerical procedure is the following:

1. Define the Hamiltonian via Eq. (1) for N sites.
2. Compute its ground state ($|\psi_{gs}\rangle$) and $\rho_{gs} = |\psi_{gs}\rangle\langle\psi_{gs}|$ through exact diagonalization of H_I.
3. Compute the reduced density matrix of a subregion Eq. (6), diagonalize it to obtain its eigenvalues λ_i.
4. Obtain $S_A(g)$ through Eq. (5).
5. Repeat the described process for each value of g.

III. AREA LAW

One of the most interesting properties of the subregion's entanglement entropy (S_A) is how it scales with its subregion size. A priori, one could argue that S_A would possess an extensive character, as its classical counterpart. Surprisingly, numerous ground state systems such as ours fulfil an area law, this means that they scale as $S_A \sim L^{d-1}$, here d represents the number of spatial dimensions [9, 10].

Claim: An area law holds if the system is gapped $\Delta E = E_{1e} - E_{gs} \neq 0$ and only has local interactions [12][†].

The above statement is rather a conjecture than a theorem as it has not been proven for every existing model. In our case, for the 1-D Ising model, a proof exists showcasing that in fact the ground state fulfils an area law.

Thus, practically, this means that the entanglement entropy of our subregion system should be bounded by a constant independently of the subregion size (L), hence: $S_A = \text{constant}\ \ \forall L$.

Intuitively, since interactions are short-ranged, quantum correlations can only build up across the points where the two regions connect—that is, through the boundary. In Figure 1, we clearly see that there are just two boundary points connecting regions A and B: the links 2–3 and 5–6. This remains true regardless of the subsystem size. It follows that: 1) S_A is constant, 2) it is independent of L, and 3) it satisfies the property $S_A = S_B$.

Despite the fact the area law result is stated in the thermodynamic limit, the EE difference between two subregions with different subregion sizes (ΔS_A) has been computed for a finite-size system of total length $N = 15$. As expected, their difference is zero—except at the peak around $g = 1$, (see Figure 2). Fitting the data with a parabola near the peak, we obtain: $g_{c,(\text{num.})} = (1.0002 \pm 1 \cdot 10^{-4})$. In fact, somewhat unexpectedly, we have identified the critical value $g_{c,(\text{theory})} = 1$ of the model with astonishing accuracy, where the QPT occurs [7]. In the next section, we will explore why the area law is violated at criticality.

[†] Actually, the condition $\Delta E \neq 0$ does not hold at $g = 0$ due to the presence of a double degeneracy (see Eq.(2)). In fact, degeneracy also affects the very definition of $\rho = |\psi\rangle\langle\psi|$. Therefore, we will focus on the limit $g \to 0$. A more detailed treatment of the case $g = 0$ lies beyond the scope of this project.

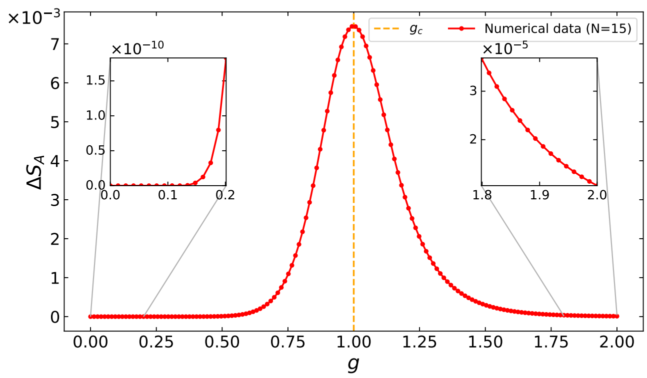

FIG. 2: Entropy difference: $S_A(L=7) - S_A(L=6)$. The peak of the function, marked with a dashed line, determines the critical value g_c of the system.

Even though an area law could be seen as a peculiar feature of our system, let me stress how important this result is. The greatest difficulty while simulating many-body systems is due to its complexity, as our Hilbert space $\mathcal{H}$ dimension grows exponentially with N as: 2^N. On the contrary, if an area law holds, the effective dimension of our system $\mathcal{H}$ is considerably lower [12]. This solely premise lies at the heart of numerical simulation methods that exploit this characteristic such as DMRG algorithms or Tensor Networks [13].

IV. CFT RESULTS

In this section we explain how criticality affects the area law behaviour for finite-size systems. Initially we had argued that for an area law to hold $\Delta E \neq 0$, but at criticality ($g_c = 1$), this model becomes gapless and a violation of the area law occurs [4, 6].

At criticality, the correlation length of the system diverges, and the system becomes scale-invariant. In this regime, the critical point can be described by a conformal field theory (CFT), which is characterized by its central charge, c. The central charge effectively counts the number of degrees of freedom at low energies and governs how entanglement scales at criticality [14]. In this context, a universal relation between $S_A(g_c = 1)$ and the central charge can be established [15, 16].

For a 1D finite-size system with PBC at $g_c = 1$, total system's size N, subregion size L, the expression reads:

$$S_A(L) = \frac{c}{3}\log\left(\frac{N}{\pi a}\sin\frac{\pi L}{N}\right) + D, \tag{7}$$

where a is the lattice spacing and D is a constant. The universality class of the 1D quantum Ising model is characterized by the central charge $c_{\text{theory}} = \frac{1}{2}$ [16].

Numerically, as shown in Figure 3, we obtain an excellent agreement with theory:

$$c_{\text{fit}} = (0.507 \pm 0.001) \;\;\&\;\; D_{\text{fit}} = (0.4752 \pm 0.0004). \tag{8}$$

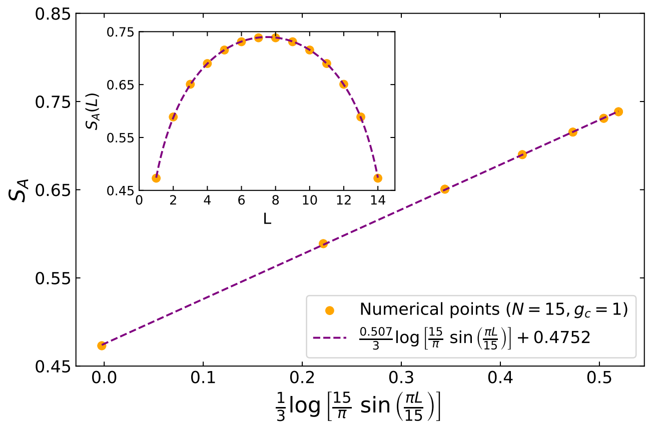

FIG. 3: Entanglement entropy at $g_c = 1$ as a function of the subsystem size L. Our numerical computations are reported with orange circles. The dashed line correspond to Eq. (7).

Let me also comment that apart from being able to determine the universality class of the model (by computing its central charge), violations of area laws are widely used for determining critical points for other not well studied systems, as they represent an alternative to renormalization group computations [17, 18].

V. TWO-POINT CORRELATION FUNCTION AND THE CQ CORRESPONDENCE

One of the most interesting features of our 1-D quantum model is how it can be mapped to a 2-D classical chain[§], thus to the famous Onsager's solution [19]:

$$H_{2d,c} = -\sum_{\langle i,j\rangle}\tilde{J}_{ij}S_iS_j \Longleftrightarrow H_{1d,q} = -J\sum_i\left(Z_iZ_{i+1} + gX_i\right). \tag{9}$$

This result is known as the classical-to-quantum correspondence and states that the partition functions of both models are the same $\mathcal{Z}_{2d,c} = \mathcal{Z}_{1d,q}$, as well as their critical exponents and the behaviour of the two-point correlation function [8, 20].

First, the 2-point X-Z-correlation function is defined as:

$$\begin{aligned} \mathcal{C}^{xx,(conn)}_{i,j} &= \langle 0|X_iX_j|0\rangle - \langle 0|X_i|0\rangle\langle 0|X_j|0\rangle \\ \mathcal{C}^{zz,(conn)}_{i,j} &= \langle 0|Z_iZ_j|0\rangle - \langle 0|Z_i|0\rangle\langle 0|Z_j|0\rangle. \end{aligned} \tag{10}$$

Now, thanks to the CQ correspondence, we consider the functional form of $C_{i,j}$ in the classical 2D model and use it to fit the data of our quantum 1D system [21, 22]:

$$\mathcal{C}^{(xx,zz)}_{i,j}(g \neq g_c) \sim e^{-\frac{|r_{ij}|}{\xi}} \;\;\&\;\; \mathcal{C}^{zz}_{i,j}(g_c) \sim \frac{1}{|r_{ij}|^{\eta}}. \tag{11}$$

[§] To be more precise, the ground state of the quantum system at $T_q = 0$ maps to the equilibrium state of the classical model at finite temperature $T_c \neq 0$.

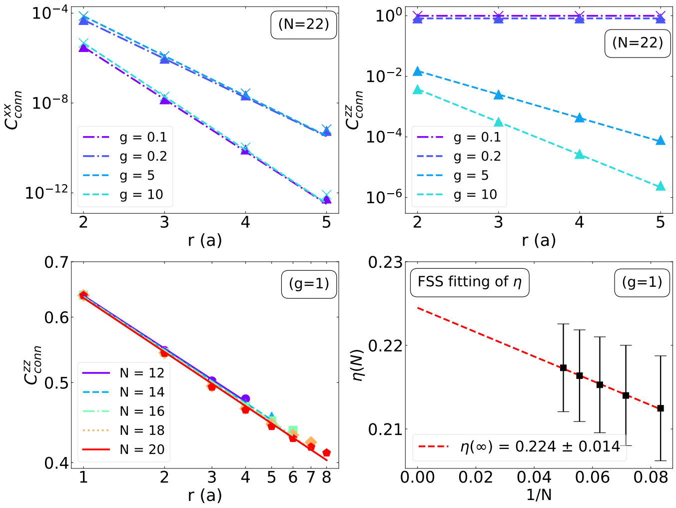

FIG. 4: Two-point correlation functions. Top-left: off-criticality X-direction lin-log scale. Top-right: off-criticality Z-direction lin-log scale. Bottom-left: criticality Z-direction log-log scale. Bottom-right: FSS of the η critical exponent

The numerically obtained results in/off criticality are in accordance with the CQ prediction (see Figure 4) with the exception of $C^{zz}(g < 1)$ which is constant due to present long-range order of the ferromagnetic phase. Additionally, the exponential decay of C_{ij} off-criticality is a necessary but not sufficient condition for an area law, reinforcing the initial idea of studying S_A directly [9].

Furthermore, we also determine the critical exponent of the correlation function η (see Eq. (11) for $g = g_c$) by using finite-size scaling (FSS) techniques [23].

An established Ansatz for this exponent is [24]:

$$\eta(N) = \eta(N \to \infty) + \frac{a}{N}. \tag{12}$$

As we said earlier, thanks to the CQ correspondence, the critical exponent $\eta^{(1d,q)}_{\text{FSS}}$ (see Figure 4, bottom-right) should coincide with the theoretical value predicted by Onsager's solution : $\eta^{(2d,c)}_{\text{theo}} = 0.25$. As expected, both results are compatible:

$$|\eta^{(2d,c)}_{\text{theo}} - \eta^{(1d,q)}_{\text{FSS}}| = 0.0255 < 2\ \eta^{(1d,q)}_{\text{FSS}} = 0.0284\ . \tag{13}$$

VI. ENTANGLEMENT SPECTRUM

Up to this point, we have uniquely been interested in the entanglement entropy of the subregion S_A. But, in principle, the reduced density matrix ρ_A contains more information that the single value S_A.

As proposed by Li and Haldane [25], the key insight lies in imagining that the reduced density matrix ρ_A can be spanned by an effective Hamiltonian H_{eff} that captures the behaviour of the subregion A. Mathematically:

$$\rho = \frac{1}{\mathcal{Z}} e^{-\beta H} \to \rho_A = \frac{1}{\mathcal{Z}_A} e^{-\beta H_{\text{eff}}}. \tag{14}$$

In reduced units, the above equation reads: $\rho_A = e^{-H_{\text{eff}}}$.

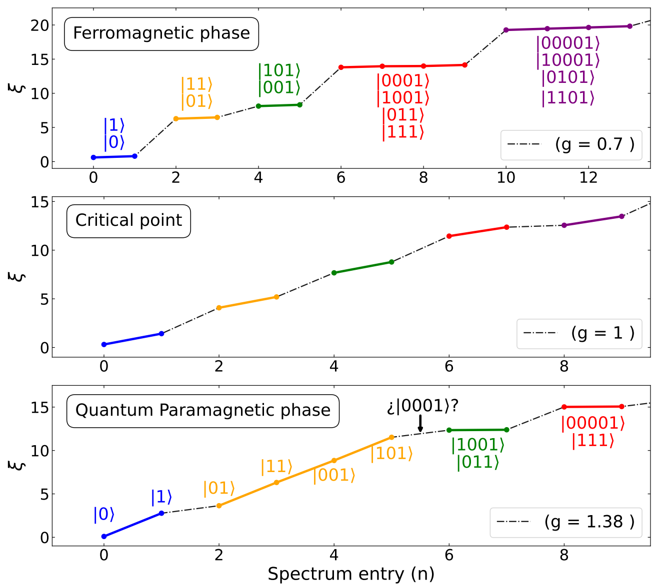

FIG. 5: Entanglement spectrum for a finite-size system ($N = 10$, $L = 5$) for both phases and at the critical point. The labelled states correspond with the ones shown in Table I.

From Eq. (6), we identify λ_i as the eigenvalues of ρ_A. If we then define $\lambda_i = e^{-\xi_i}$, comparing with Eq. (14), we can interpret ξ_i as the "energy levels" (also called entanglement spectrum) of our effective Hamiltonian (H_{eff}). Studying its spectra, one can deduce multiple properties of the real Hamiltonian given in Eq. (1) as well as characterize the distinct phases and determine some other properties at criticality [26].

Actually, for this model, the spectra of H_{eff} is known and can be found via the corner transfer matrix method. In the thermodynamic limit, it can be proven that H_{eff} can be written in terms of non-interacting fermions [27]:

$$H_{\text{eff}} = \sum_{j=0}^{\infty} \epsilon_j \hat{n}_j \quad \text{with} \quad \epsilon_j = \begin{cases} 2j\epsilon & \text{for } g < 1 \\ (2j+1)\epsilon & \text{for } g > 1\ . \end{cases} \tag{15}$$

Note that $\hat{n}$ represents the occupation number ($\hat{n} = \hat{c}^\dagger \hat{c}$) and ϵ is a constant that depends on the value of g.

State	$E_{(g<1)}$	$E_{(g>1)}$	n	**State**	$E_{(g<1)}$	$E_{(g>1)}$	n
$\|0\rangle$	0	0	0	$\|1001\rangle$	6ϵ	8ϵ	2
$\|1\rangle$	0	ϵ	1	$\|011\rangle$	6ϵ	8ϵ	2
$\|01\rangle$	2ϵ	3ϵ	1	$\|111\rangle$	6ϵ	9ϵ	3
$\|11\rangle$	2ϵ	4ϵ	2	$\|00001\rangle$	8ϵ	9ϵ	1
$\|001\rangle$	4ϵ	5ϵ	1	$\|10001\rangle$	8ϵ	10ϵ	3
$\|101\rangle$	4ϵ	6ϵ	2	$\|0101\rangle$	8ϵ	10ϵ	3
$\|0001\rangle$	6ϵ	7ϵ	1	$\|1101\rangle$	8ϵ	11ϵ	3

TABLE I: First entanglement spectrum levels of H_{eff} spanned by Eq. (15) for $g < 1$ and $g > 1$, grouped by the total number of fermions $n = \sum_j n_j$. Owing to the $\mathbb{Z}_2$ symmetry, the degeneracies always occur in even multiples. (Thermodynamic limit result, $N \to \infty$).

The first ξ_i values of ρ_A for a finite-size system (FS) of N=10 and L=5 have been numerically computed (see Figure 5). We then proceed to compare them with the thermodynamic limit results shown on Table I.

For the ferromagnetic phase, all the degeneracies of the first levels match with the exception that the spacing is not equidistant ($\Delta\xi \neq 2\epsilon$).

For the quantum paramagnetic phase, the 8ϵ and 9ϵ two-fold degeneracies are present as well as the missing 2ϵ level. On the contrary, the level $|00001\rangle$ is missing and the degenerate levels appear one spectrum entry earlier.

The above discrepancies can be explained through the fact that in a FS, there is no singularity at the critical point, and thus there cannot be a transition between both spectrums, as in the $N \to \infty$ case. Interestingly, for the FS system at $g = 1$, a sign of criticality still appears as all the two-fold and four-fold degeneracies disappear.

VII. CONCLUSIONS

In this work, we have analysed the phases and critical behaviour of the transverse field Ising model using a range of concepts from quantum information theory. The main conclusions are as follows:

The area law for the entanglement entropy of a subregion holds in finite-size systems. Its logarithmic violation at the critical point $g = 1$ is accurately captured by a conformal field theory with central charge $c = 1/2$.

The two-point correlation function $C_{i,j}$ exhibits an exponential decay in both phases ($g \neq 1$) and a power-law one at the critical point $g_c = 1$, in agreement with the classical-to-quantum correspondence prediction.

Finally, the entanglement spectrum provides a useful tool to characterize and distinguish the two phases of the system based on their entanglement structure.

As future work, we plan to apply the same theoretical framework to study thermal states and investigate how the phase diagram is modified by the introduction of disorder, as in the one-dimensional quantum random Ising model. Another promising direction is to explore the nonequilibrium dynamics of the model following a quantum quench.

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Estudi de les Propietats d'Entrellaçament de les Cadenes Quàntiques d'Ising

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Resum: Estudiem les propietats de l'estat fonamental del model d'Ising quàntic unidimensional i el seu diagrama de fases utilitzant conceptes de la teoria de la informació quàntica. Comencem analitzant el comportament de la llei d'àrea de l'entropia d'entrellaçament i la seva violació logarítmica al punt crític. A continuació, introduïm la correspondència entre sistemes clàssics i quàntics per deduïr el comportament de les funcions de correlació a dos punts. Finalment, caracteritzem les diferents fases del model a través del seu espectre d'entrellaçament.
Keywords: Física Teòrica, Sistemes Quàntics de Molts Cossos, Transicions de Fase Quàntiques, Teoria de la Informació Quàntica, Matèria Condensada, Lleis d'Àrea, Espectre d'Entrellaçament
SDGs: 4:Educació de Qualitat, 8:Treball Digne i Creixement Econòmic, 13:Acció Climàtica

Objectius de Desenvolupament Sostenible (ODSs o SDGs)

1. Fi de la es desigualtats		10. Reducció de les desigualtats	
2. Fam zero		11. Ciutats i comunitats sostenibles	
3. Salut i benestar		12. Consum i producció responsables	
4. Educació de qualitat	X	13. Acció climàtica	X
5. Igualtat de gènere		14. Vida submarina	
6. Aigua neta i sanejament		15. Vida terrestre	
7. Energia neta i sostenible		16. Pau, justícia i institucions sòlides	
8. Treball digne i creixement econòmic	X	17. Aliança pels objectius	
9. Indústria, innovació, infraestructures			

El contingut d'aquest TFG es relaciona directament amb l'ODS 4 (fita 4.4) per tractar-se d'un treball científic en l'àmbit universitari. També es relaciona amb l'ODS 8 (fita 8.5) a causa que el desenvolupament d'aquesta obra permet una inclusió digne al mercat laboral. Finalment, amb l'ODS 13 (fites 13.2, 13.3, 13.a, 13.b) ja que els resultats del projecte permeten la utilització d'algorismes molt més eficients i que requereixen menys recursos computacionals, mitigant així l'impacte mediambiental de les simulacions numèriques.

GRAPHICAL ABSTRACT