Scaling of entanglement entropy for chains of arbitrary spin

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Abstract: We investigate the entanglement entropy of a 1D Hamiltonian written in terms of the generalized Gell-Mann matrices that shares some properties with the spin-1/2 XXZ model. In particular, we study the point that marks the boundary between a critical phase and a ferromagnetic phase. This point cannot be described by a conformal field theory and its ground state is infinitely degenerate in the thermodynamic limit. We find an analytical expression for the ground state and its Schmidt decomposition, and show that the entanglement entropy scales as $s \log_2 L$ in the leading order, where L is the size of the subsystem and s is the spin. The scaling is related to the symmetric-like structure of the ground state.

I. INTRODUCTION

Entanglement lies at the interplay between quantum information and many-body physics, and both fields have benefited from the advances in its study. From a quantum information perspective, entanglement is a resource used in protocols such as quantum teleportation [1] or superdense coding, and it is thought to be at the heart of the speed up of quantum computers [2]. Therefore, the study of entanglement in many-body systems provides a connection between quantum protocols and their implementation. From a many-body point of view, entanglement appears naturally in a variety of phenomena, like topological insulators [3] or quantum phase transitions [4], and provides a way to efficiently simulate certain quantum systems through Tensor Networks [5].

In this work we will study the bipartite entanglement of a many-body system close to a quantum phase transition. In quantum phase transitions, the appearance of long-range correlations can be explained by means of the entanglement of the ground state. Consider a quantum system in the pure state $|\Psi\rangle$, and a bipartition of it in parts A and B. As a measure of entanglement, we will use the von Neumann entropy of the reduced density matrix of either part A or B [2],

$$S(\rho_A) = -\mathrm{Tr}\rho_A \log_2 \rho_A = S(\rho_B). \tag{1}$$

The reduced density matrix of subsystem A is obtained by tracing out B from the density matrix of the system, $\rho_A = \mathrm{Tr}_B(|\Psi\rangle\langle\Psi|)$. It is convenient to write the reduced density matrix in terms of the Schmidt coefficients. The Schmidt decomposition of $|\Psi\rangle$ is

$$|\Psi\rangle = \sum_i \alpha_i |\varphi_i\rangle_A \otimes |\varphi_i\rangle_B, \tag{2}$$

where $|\varphi_i\rangle_A$ and $|\varphi_i\rangle_B$ are orthonormal basis of subsystems A and B, and the Schmidt coefficients α_i fulfill $\sum_i |\alpha_i|^2 = 1$. Tracing out either subsystem shows that, in these basis, ρ_A and ρ_B are the same diagonal matrix, one whose non-zero diagonal entries are $|\alpha_i|^2$. The entanglement entropy is, then,

$$S(\rho_A) = -\sum_i |\alpha_i|^2 \log_2 |\alpha_i|^2 \tag{3}$$

In 1D quantum systems out of criticality, the entanglement entropy is known to fulfill an area law [7]: the entanglement entropy of subsystem A grows as the area of A. This means that in 1D systems, the entanglement entropy is bounded. At critical points, however, the entanglement entropy violates the area law. In most cases the violation is by a factor of $\log L$, where L is the volume of A [8], although there are cases of Hamiltonians whose entanglement entropy can violate the area law by a power law [9, 10]. When the system is conformally invariant, it can be described by a conformal field theory, and the entropy of entanglement is known to scale as

$$S \sim \frac{c+\bar{c}}{6} \log_2 L, \tag{4}$$

when the chain has periodic boundary conditions [6]. Here, c and $\bar{c}$ are the central charges for the holomorphic and antiholomorphic sectors of the conformal field theory. Recent studies show that, even in non-conformally invariant points, a very high degeneracy of the ground state can also lead to violations of the area law [11].

The paper is organized as follows. In section II we introduce a Hamiltonian based on the generalized Gell-Mann matrices (henceforth, GGM), review the spin-1/2 XXZ model phase diagram, and show evidence of criticality and high entanglement entropy on a specific point of the Hamiltonian. We then study the properties of the ground state at that point. To do so, in section III we find the ground state of the GGM Hamiltonian. The ground state is found by writing the Hamiltonian as a sum of local projectors, a computation that is shown in appendix VI. In section IV we compute the Schmidt decomposition of the ground state and we find the scaling of the entanglement entropy, showing that it violates the area law by a factor of $\log_2 L$. Finally, we summarize the results in section V.

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II. THE GGM HAMILTONIAN

We will study the following 1D Hamiltonian with local interactions and periodic boundary conditions (PBC):

$$\mathcal{H}_d = \sum_{i=1}^{N} \left(\sum_{\lambda \notin \mathcal{D}} \lambda_i \lambda_{i+1} + \Delta \sum_{\lambda \in \mathcal{D}} \lambda_i \lambda_{i+1} \right), \qquad (5)$$

where the λ operators are the generalized Gell-Mann matrices of dimension d, the generators of the SU (d) group. $\mathcal{D}$ is the subset of diagonal GGM. When considering particles of spin s, the dimension is $d = 2s+1$.

For dimension 2 (spin-1/2), the GGM are the Pauli matrices, and the Hamiltonian in Eq. (5) reads

$$\mathcal{H}_2 = \sum_{i=1}^{N} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z \right). \qquad (6)$$

This is the Hamiltonian of the XXZ model, where Δ is an anisotropy parameter in the z axis. Thus, the Hamiltonian given in Eq. (5) can be seen as a generalization of the spin-1/2 XXZ model to any spin s. Usually, generalizations of this model to higher spins are done by substituting the Pauli matrices with the spin operators. In that case, the Hamiltonian can be written in terms of the S^z operator and the ladder operators, S^+ and S^-.

The XXZ model is known to exhibit critical behaviour in the $\Delta \in [-1, 1]$ region, known as the XY phase [12]. For $\Delta < -1$ the system is in the ferromagnetic Ising phase, while for $\Delta > 1$ it is in the Néel phase. The critical region is conformally invariant in the range $\Delta \in (-1, 1]$, and therefore it can be described by a conformal field theory. For the XXZ model, $c = \bar{c} = 1$ and the entanglement entropy scales with the size of the chain as $S \sim \frac{1}{3} \log_2 L$, according to Eq. (4).

However, the $\Delta = -1$ point is not conformally invariant, and Eq. (4) is no longer valid. This point is the boundary between the XY phase and the ferromagnetic phase, and is characterized by crossing of energy levels and a very high degeneracy. In the spin-1/2 case, the $\Delta = -1$ point can be mapped to the SU(2)-invariant Heisenberg antiferromagnetic model by the unitary transformation $\prod_{i=1}^{N/2} \sigma_{2i}^z$, that inverts every other spin. The SU(2) invariance can be used to determine the ground state multiplet and, since the transformation does not change the entanglement, the entanglement entropy of the XXZ $\Delta = -1$ point can be computed [13]. One could try to generalize this transformation with the set of diagonal GGM, but for higher spins each diagonal GGM would introduce different prefactors on each operator $\lambda_i \lambda_{i+1}$.

The ferromagnetic $\Delta = -1$ point retains some properties of the XXZ model when considering the GGM Hamiltonian. It is still a critical point where many energy levels cross, characterized by a high degeneracy that is partially broken in the ferromagnetic phase. As $\Delta \to -1^+$, the entanglement entropy of the system grows, while at $\Delta < -1$ the ground state is a product state and the entropy of entanglement vanishes. Figs. (1 and 2) show the energy crossing at $\Delta = -1$ and the behaviour of the entanglement entropy for different chains. The data has been obtained by numerical diagonalization of the Hamiltonian.

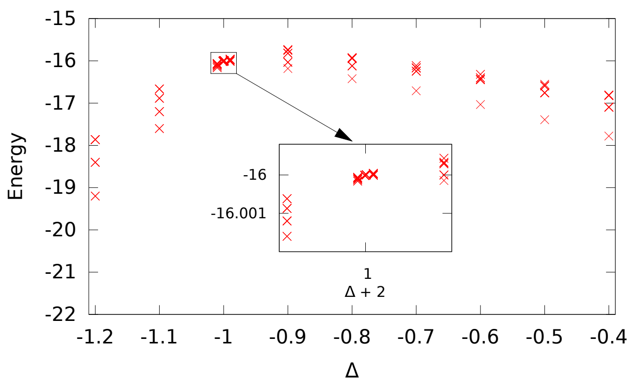

FIG. 1: Energy of the ground state and the first excited states of the GGM Hamiltonian for spin-1 and a chain of $N = 12$ particles. At $\Delta = -1$, the energies converge to $-2N\left(1 - \frac{1}{d}\right) = -16$. The inner plot's x axis is logarithmic. The behaviour around the ferromagnetic point is similar for other spin dimensions.

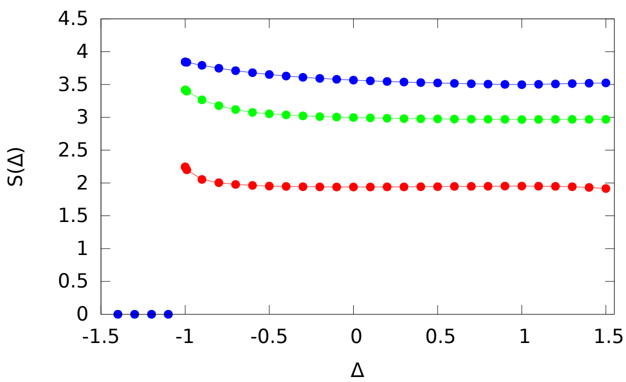

FIG. 2: Entanglement entropy of half a chain as a function of Δ for different chains. The upper, blue curve is a spin-3/2 chain with 8 lattice sites; the central, green curve is a spin-1 chain with 12 lattice sites; and the lower, red curve is a spin-1/2 chain of 20 lattice sites. As $\Delta \to -1^+$ the entanglement entropy increases, and for $\Delta < -1$ it vanishes because the ground state is a product state with all spins aligned in the same direction. The upper curve seems to grow slowly due to the small size of the chain.

III. GROUND STATE AT THE $\Delta = -1^+$ POINT

In the appendix (VI) we compute how the GGM Hamiltonian acts on a state. Using Eq. (23), in the $\Delta = -1$ point the Hamiltonian can be written as a sum of projectors and a constant term,

$$\mathcal{H}_d = 2\sum_{i=1}^{N}\left(\sum_{j\neq k} |kj\rangle_{i,i+1}\langle jk| + |jk\rangle_{i,i+1}\langle jk|\right) + E_0. \tag{7}$$

The indices j and k run from 0 to $d-1$. E_0 is the energy of the ground state, whose value is $E_0 = -2N\left(1-\frac{1}{d}\right)$. The structure of the ground state does not depend on E_0 or the factor 2, and is determined by the sum of positive local projectors, making the Hamiltonian frustration free. By inspection, one can see that there are two possibilities for the projectors acting on positions $i, i+1$ to annihilate a state. The sum of projectors only contains terms where $j \neq k$, and therefore states where both spins are equal are annihilated. A state where both spins are different will be annihilated if it is antisymmetric with respect to the swapping of the spins,

$$\left(\sum_{j\neq k} |kj\rangle\langle jk| + |jk\rangle\langle jk|\right)(|lm\rangle - |ml\rangle) = \\ |ml\rangle + |lm\rangle - |lm\rangle - |ml\rangle = 0 \tag{8}$$

Generalizing this result to the Hamiltonian acting on each pair of particles we can see that the ground states at the ferromagnetic point are equal weight superpositions of states that are antisymmetric with respect to the swapping of any two consecutive, different-valued spins.

Since the Hamiltonian in Eq. 7 can only swap the spins, the set of numbers $\{N_i\}$, $i = 0,\ldots,d-1$, where N_i is the number of i-valued spins, is a good quantum number. This is the main difference with the XXZ Hamiltonian, that can change the value of the spins by a unity. For the spin-1/2 case, both operations are the same, but for higher spins they are not. For each valid set $\{N_i\}$ there will be a ground state

$$|\{N_i\}\rangle = \frac{1}{\sqrt{C_{\{N_i\}}}}\sum_P (-1)^m |0\ldots d-1\rangle, \tag{9}$$

where each spin i is repeated N_i times. The sum is over all multiset permutations of the spins, and m is the number of swaps of consecutive, different-valued spins, in order to fulfill the condition we have found. The normalization factor is the multinomial coefficient

$$C_{\{N_i\}} = \binom{N}{N_0,\ldots,N_{d-1}} = \frac{N!}{N_0!\ldots N_{d-1}!}. \tag{10}$$

The structure of the ground state is similar to that of a permutation invariant state, but each state of the superposition has a sign that is obtained by swapping consecutive pairs of different spins, making it different to both the completely symmetric and antisymmetric states.

As an example, all five ground states for spin 1/2 and four lattice sites are:

$$\begin{aligned}
&|N_0=4,N_1=0\rangle = |0000\rangle\,,\\
&|N_0=3,N_1=1\rangle = \frac{1}{2}\left(|0001\rangle - |0010\rangle + |0100\rangle - |1000\rangle\right),\\
&|N_0=2,N_1=2\rangle = \frac{1}{\sqrt{6}}\left(|0011\rangle - |0101\rangle + |0110\rangle\right.\\
&\qquad\qquad\left.+\,|1001\rangle - |1010\rangle + |1100\rangle\right),\\
&|N_0=1,N_1=3\rangle = \frac{1}{2}\left(|0111\rangle - |1011\rangle + |1101\rangle - |1110\rangle\right),\\
&|N_0=0,N_1=4\rangle = |1111\rangle\,.
\end{aligned} \tag{11}$$

It is worth noting that the periodic boundary conditions impose a restriction on which sets $\{N_i\}$ can produce a ground state. If we start with a state $|0\ldots0\ldots d-1\ldots d-1\rangle$ and move the last i-valued spin to the front of its group using the PBC, we would need $N-N_i$ swaps and the resulting state would be a cyclic permutation of all the spins, now with a 0 in the last position. If we now swap the last 0 back to the last place of its group, we would need $N-N_0$ changes to get back the original state. Therefore the total number of changes is $2N-N_i-N_0$, and the sign of the resulting state would be $(-1)^{2N-N_i-N_0} = (-1)^{N_i+N_0}$. Only when the parity of N_i and N_0 is the same, the sign will be positive. If $N_0 = 0$, the reasoning in the same but replacing the 0 with the first value present in the state. We conclude then that only those sets $\{N_i\}$ in which all the $N_i \neq 0$ have the same parity can produce a ground state. As an example, the state $|001\rangle$ is not valid, since moving the 1 to the right twice and then the last 0 to the left once produces

$$|001\rangle \to -|100\rangle \to |010\rangle \to -|001\rangle\,. \tag{12}$$

However, in the thermodynamic limit there are still an infinite number of valid sets, and the ground state is infinitely degenerate. For open boundary conditions there is no restriction and all the sets are valid.

IV. BIPARTITE ENTANGLEMENT ENTROPY OF THE GROUND STATE AT THE $\Delta = -1^+$ POINT

The entanglement entropy can be computed using the fact that the ground state has the structure of the symmetric state with some signs changed. The relative phases between the superposition states do not change the Schmidt coefficients, so their entanglement must be the same. The entropy of the symmetric states of arbitrary local dimension has been studied [14, 15], and it is known to scale as

$$S \sim s\log_2 L. \tag{13}$$

In order to verify this result, we will compute the Schmidt decomposition of the ground state and the entanglement of a particular sector. Consider a bipartition of the chain with L and $N-L$ consecutive spins. Restricting to the block of L spins and a set $\{N_i^L\}$ compatible with $\{N_i\}$ (i.e. $N_i^L \leq N_i$ for all i), the possible states of the L spins will be all the multiset permutations of any state with N_i^L i-valued spins. This is the $\left|\{N_i^L\}\right\rangle$ given by Eq. (9), but now there is no restriction on the possible sets because the boundary conditions are open (the L-th spin is not interacting with the first). For the same reason, the possible states of the rest of the chain, containing $N-L$ particles, will be of the form of $\left|\{N_i^{N-L}\}\right\rangle_O$, where the subscript indicates that the boundary conditions are again open. For a given ground state of the whole chain of N particles, $\{N_i\}$ is fixed, so it must be $N_i^{N-L} = N_i - N_i^L$ for all i. Up to a sign that can be absorbed by either state, the Schmidt decomposition in subsystems of length L and $N-L$ can be written in terms of the OBC ground states of both bipartitions,

$$|\{N_i\}\rangle = \sum_{\{N_i^L\}} \sqrt{\frac{C_{\{N_i^L\}} C_{\{N_i - N_i^L\}}}{C_{\{N_i\}}}} \left|\{N_i^L\}\right\rangle_O \otimes \left|\{N_i - N_i^L\}\right\rangle_O , \quad (14)$$

Once we know the Schmidt coefficients, the bipartite entanglement entropy can be computed numerically for large blocks and spin dimensions using Eq. (3). In particular, we considered the ground states with the largest entanglement entropy, given by the sets $\{N_i\}$ in which all N_i are equal. This is also the state approached by the unique ground state in the $\Delta \to -1^+$ limit. The numerics show that for spins 1/2, 1, 3/2 and 2, and chains up to 500 lattice sites, the entanglement entropy of half a chain scales as Eq. (13) (see Fig. (3)).

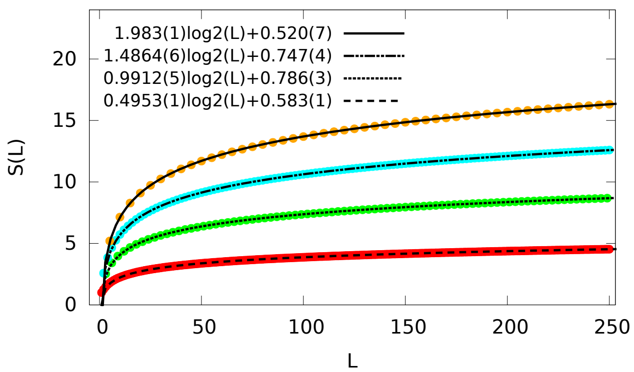

FIG. 3: Entanglement entropy of half a chain as a function of the chain length L. From up to down, the different curves are for spin 2, 3/2, 1 and 1/2. The lines are logarithmic fits starting from the first $L \geq 10$ to minimize finite size effects.

V. CONCLUSIONS

The GGM Hamiltonian at the ferromagnetic point $\Delta = -1$ generalizes some properties of the entanglement entropy of the spin-1/2 XXZ model. We have shown that the ground state at this point is infinitely degenerate in the thermodynamic limit, giving rise to a high entanglement. In particular, we have seen that the entanglement entropy scales as $S \sim s \log_2 L$ with the size of the subsystem. Therefore, it violates the area law by a logarithmic factor, although the system is not conformally invariant.

In this work we have computed the ground state analytically, instead of performing a local unitary transformation that leaves the entanglement unchanged, as can be done in the spin-1/2 XXZ model. However, we have proved that the ground state has the same structure, up to some signs, as the totally symmetric states. This fact suggests that such a transformation could exist, since that is the ground state of the Hamiltonian $\mathcal{H} = -\sum_i \left(\sum_\lambda \lambda_i \lambda_{i+1}\right)$.

VI. APPENDIX. ACTION OF THE GGM HAMILTONIAN ON A STATE

The generalized Gell-Mann matrices of dimension n are the generators of the SU(n) Lie group. They can be divided in three sets. The non-diagonal ones are either real symmetric or imaginary antisymmetric, which we will write as λ_s^{jk} and λ_a^{jk}, respectively. The third set are the diagonal matrices, which we will write as λ^l. In the standard qudit basis, the GGM of dimension d can be constructed as follows [16].

1. The real symmetric matrices are:

$$\lambda_s^{jk} = |j\rangle\langle k| + |k\rangle\langle j|, \qquad 0 \leq j < k \leq d-1. \quad (15)$$

2. The imaginary antisymmetric are:

$$\lambda_a^{jk} = -i\left(|j\rangle\langle k| - |k\rangle\langle j|\right), \qquad 0 \leq j < k \leq d-1. \quad (16)$$

3. And the diagonal matrices are:

$$\lambda^l = \sqrt{\frac{2}{l(l+1)}} \left(\sum_{m=0}^{l-1} |m\rangle\langle m| - l\,|l\rangle\langle l|\right), \qquad 1 \leq l \leq d-1. \quad (17)$$

There are $\frac{d(d-1)}{2}$ symmetric, $\frac{d(d-1)}{2}$ antisymmetric and $d-1$ diagonal GGM, and d^2-1 in total.

We will now compute the action of the Hamiltonian of Eq. (5) on a given state $|\Psi\rangle$. Since the Hamiltonian is local, we can restrict to states of two particles, $|\Psi\rangle = |jk\rangle$, and later generalize the results. We will work in the standard qudit basis, where j and k run from 0 to $d-1$.

Consider first the non-diagonal part of the Hamiltonian. For each real symmetric GGM (Eq. (15)) there is an imaginary, hermitian GGM (Eq. (16)) with entries in the same positions. Matrices other than λ_s^{jk} and λ_a^{jk} will annihilate $|jk\rangle$. The real matrix λ_s^{jk} (or λ_s^{kj} if $j > k$) acting on $|jk\rangle$ changes spin j to k and vice versa. The imaginary matrix λ_a^{jk} does so but introducing a phase i if acting on a j-valued spin, and $-$i if acting on a k-valued spin. Therefore, for pairs of equal-valued spins the action of the real and imaginary GGM cancel out, and for different-valued spins it is doubled. The action of all the non-diagonal part of the Hamiltonian is then:

$$\sum_{\lambda\notin\mathcal{D}} \lambda_i\lambda_{i+1} |jk\rangle_{i,i+1} = 2\,|kj\rangle_{i,i+1} \quad \text{if } j \neq k, \tag{18}$$

The action of the diagonal part of the Hamiltonian is

$$\Delta\sum_{\lambda\in\mathcal{D}} \lambda_i\lambda_{i+1} |jk\rangle_{i,i+1} = \Delta\sum_{l=1}^{d-1} \lambda_i^l\lambda_{i+1}^l |jk\rangle_{i,i+1}. \tag{19}$$

Since this part of the Hamiltonian is diagonal, the state will not change. We can compute the prefactor using Eq. (17). For a single particle in state $|j\rangle$,

$$\begin{aligned}\langle j|\,\lambda^l\,|j\rangle &= \sqrt{\frac{2}{l(l+1)}}\left(\sum_{m=0}^{l-1}\langle j|m\rangle\langle m|j\rangle - l\,\langle j|l\rangle\langle l|j\rangle\right)\\ &= \sqrt{\frac{2}{l(l+1)}} \times \begin{cases} 0, & \text{if } l<j\\ -l, & \text{if } l=j\\ 1, & \text{if } l>j\end{cases}\end{aligned} \tag{20}$$

For a pair of consecutive particles we can suppose $j \geq k$, without loss of generality. Then, the action of the Hamiltonian is

$$\begin{aligned}&\sum_{l=1}^{d-1}\langle j|\,\lambda^l\,|j\rangle\langle k|\,\lambda^l\,|k\rangle =\\ &=\sum_{l=1}^{d-1}\frac{2}{l(l+1)} \times \begin{cases} 0, & \text{if } l<j\\ -l, & \text{if } l=j\\ 1, & \text{if } l>j\end{cases} \times \begin{cases} 0, & \text{if } l<k\\ -l, & \text{if } l=k\\ 1, & \text{if } l>k\end{cases}\\ &=\sum_{l=1}^{d-1}\frac{2}{l(l+1)} \times \begin{cases} 0, & \text{if } l<j\\ l^2, & \text{if } l=j=k\\ -l, & \text{if } l=j>k\\ 1, & \text{if } l>j\end{cases}\\ &=\frac{2j}{j+1}\delta_{jk} - \frac{2}{j+1}(1-\delta_{jk}) + \sum_{l=j+1}^{d-1}\frac{2}{l(l+1)}\\ &= 2\delta_{jk} - \frac{2}{j+1} + \sum_{l=j+1}^{d-1}\frac{2}{l(l+1)}\\ &= 2\delta_{jk} - \frac{2}{j+1} + \frac{2}{d}\frac{d-j-1}{j+1} = 2\delta_{jk} - \frac{2}{d}\end{aligned} \tag{21}$$

As can be seen in the last expression, the action of the diagonal part of the Hamiltonian does not depend on the values of the spins, only on whether they are equal or different. This action can be written in the following form,

$$\Delta\sum_{\lambda\in\mathcal{D}} \lambda_i\lambda_{i+1} |jk\rangle_{i,i+1} = \begin{cases} \frac{2\Delta(d-1)}{d}\,|jk\rangle_{i,i+1}, & \text{if } j=k\\ -\frac{2\Delta}{d}\,|jk\rangle_{i,i+1}, & \text{if } j\neq k\end{cases}. \tag{22}$$

Finally, from Eqs. (18 and 22) the action of the Hamiltonian restricted to sites $i, i+1$ can be written as

$$\mathcal{H}_{i,i+1}|jk\rangle_{i,i+1} = \begin{cases} \frac{2\Delta(d-1)}{d}\,|jk\rangle_{i,i+1}, & \text{if } j=k\\ 2\,|kj\rangle_{i,i+1} - \frac{2\Delta}{d}\,|jk\rangle_{i,i+1}, & \text{if } j\neq k\end{cases}. \tag{23}$$

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