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Unfrustrated qudit chains and their ground states

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We investigate chains of d-dimensional quantum spins (qudits) on a line with generic nearest-neighbor interactions without translational invariance. We find the conditions under which these systems are not frustrated, that is, when the ground states are also the common ground states of all the local terms in the Hamiltonians. The states of a quantum spin chain are naturally represented in the matrix product states (MPS) framework. Using imaginary time evolution in the MPS ansatz, we numerically investigate the range of parameters in which we expect the ground states to be highly entangled and find them hard to approximate using our MPS method.

I. INTRODUCTION

A system with local interactions is *not frustrated* if the global ground state of the Hamiltonian $H = \sum_k H_k$ is also a ground state of all the local terms H_k, each of which involves only a few particles. Frustration in a classical or quantum system (e.g., a spin glass [1]) is often the reason why finding its ground-state properties is hard. A locally constrained unfrustrated system could still have ground states that are hard to find (e.g., 3-SAT where one needs to test whether a Boolean formula, made up of 3-literal clauses, is satisfiable by an assignment of the Boolean variables [2]).

We choose to investigate chains of d-dimensional quantum spins (qudits) with two-local nearest-neighbor interactions. Our first result is an analytic derivation of the necessary and sufficient conditions for such quantum systems to be unfrustrated. Second, we look at their ground-state properties and find a range of parameters where we conjecture that these states are highly entangled and thus may be difficult to find computationally. We then corroborate this by a numerical investigation using a matrix product state (MPS) method.

The MPS description of a quantum state has proved to be a very useful tool for the investigation of one-dimensional (1D) quantum spin chains [3–5]. A pure state of a system of N interacting d-dimensional quantum spins can be written in the computational basis as $|\Psi\rangle = \sum_{i_k=1}^{d} \psi^{i_1 i_2 ... i_N} |i_1\rangle |i_2\rangle \cdots |i_N\rangle$, with d^N parameters $\psi^{\{i\}}$. For a 1D chain the coefficients $\psi^{\{i\}}$ can be conveniently expressed in an MPS form [6,7],

$$\psi^{i_1 i_2 ... i_N} = \sum_{\alpha_1, ..., \alpha_{N-1}=1}^{\chi} \Gamma_{\alpha_1}^{i_1,[1]} \Gamma_{\alpha_1,\alpha_2}^{i_2,[2]} \cdots \Gamma_{\alpha_{N-1}}^{i_N,[N]}, \qquad (1)$$

providing a local description of the system in terms of matrices $\Gamma^{i_k,[k]}$. One arrives at this form using a sequence of Schmidt decompositions [8]. The required size of the matrices is related to the number χ of nonzero Schmidt coefficients required for a decomposition of the state into two subsystems. In general, χ needs to grow like $d^{N/2}$ for the MPS to be exact.

Is it possible to capture the essential physics of the system accurately enough with an efficient simulation with a much smaller $\chi \sim \text{poly}(N)$, spanning only a small part of the full Hilbert space of the system? In our case, the qudits are arranged on a 1D lattice and only have nearest-neighbor interactions. We could thus expect that a reduced space might suffice for our needs. This concept is common for the various approaches proposed for efficient (tractable on a classical computer) numerical investigation of quantum many-body systems such as the density matrix renormalization group [9], MPSs [6], tensor product states [10], and projected entangled pair states (PEPSs) [11].

While the MPS formulation has been shown to work very well numerically for most 1D particle systems, complexity theory issues seem to show that there must be exceptions to this rule. Finding the ground-state energy of a 1D qudit chain with $d = 11$ has been shown to be as hard as any problem in quantum Merlin Arthur (QMA) [12,13]. It is believed that classical computers cannot efficiently solve problems in QMA. However, to our knowledge, until now there have not been any concrete examples (except at phase transitions) for which MPS methods do not appear to work reasonably well. This research was undertaken to try to discover natural examples of Hamiltonians for which MPS cannot efficiently find or approximate the ground states.

The paper is organized as follows. First, in Sec. II we show that the question of nonfrustration for qudit-chain Hamiltonians with general nearest-neighbor interactions can be addressed using only Hamiltonians that are sums of projector terms [14]. We then analytically show under what conditions zero-energy ground states for this system exist. Second, in Sec. III we show how to search for and approximate the ground states numerically and analyze the efficiency of finding the required MPS. We identify an interesting class of unfrustrated qudit-chain Hamiltonians, for which our MPS methods do not work well. Led by our numerical work, we conjecture that these ground states are highly entangled. Finally, we summarize our results and conclude with an outlook to further work in Sec. IV.

II. WHEN IS A QUDIT CHAIN UNFRUSTRATED?

We investigate chains of d-dimensional quantum particles (qudits) with nearest-neighbor interactions. The Hamiltonian
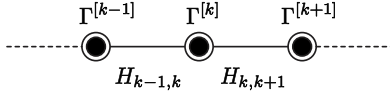
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FIG. 1. A qudit chain with nearest-neighbor interactions $H_{k,k+1}$ given by (2). The matrices $\Gamma^{[k]}$ are a local MPS description, (1), of the state.

of the system,

$$H = \sum_{k=1}^{N-1} H_{k,k+1},\tag{2}$$

is two-local (each $H_{k,k+1}$ acts nontrivially only on two neighboring qudits) (Fig. 1). Our goal is to find the necessary and sufficient conditions for the quantum system to be *unfrustrated*—its ground state is also a common ground state of all of the local terms $H_{k,k+1}$. The local terms can be written as

$$H_{k,k+1} = E_0^{(k)} P_{k,k+1}^{(0)} + \sum_p E_p^{(k)} P_{k,k+1}^{(p)},\tag{3}$$

where $E_0^{(k)}$ is the ground-state energy of $H_{k,k+1}$ and each $P_{k,k+1}^{(p)}$ is a projector onto the subspace spanned by the eigenstates of $H_{k,k+1}$ with energy $E_p^{(k)}$. The question of existence of a common ground state of all the local terms is equivalent to asking the same question for a Hamiltonian whose interaction terms are

$$H'_{k,k+1} = \mathbb{I}_{1,\dots,k-1} \otimes P_{k,k+1} \otimes \mathbb{I}_{k+1,\dots,N},\tag{4}$$

with $P_{k,k+1} = \sum_{p=1}^r P_{k,k+1}^{(p)}$ projecting onto the excited states of each original interaction term $H_{k,k+1}$. When this modified system is unfrustrated, its ground-state energy is 0 (all the terms are positive semidefinite). The unfrustrated ground state belongs to the intersection of the ground-state subspaces of each original $H_{k,k+1}$ and is annihilated by all the projector terms.

We now choose to focus on a class of Hamiltonians for which each

$$P_{k,k+1} = \sum_{p=1}^r |v_{k,k+1}^p\rangle\langle v_{k,k+1}^p|\tag{5}$$

is a *random* rank r projector acting on a d^2-dimensional Hilbert space of two qudits, chosen by picking an orthonormal set of r random vectors (a different set for every qudit pair; we are not assuming translational invariance).

We now find conditions governing the existence of zero-energy ground states (from now on, called solutions in short). We do so by counting the number of solutions possible for a subset of the chain and then adding another site and imposing the constraints given by the Hamiltonian.

Suppose we have a set of s_n linearly independent solutions for the first n sites of the chain in the form

$$\psi_{\alpha_n}^{i_1,\dots,i_n} = \Gamma_{\alpha_1}^{i_1,[1]} \Gamma_{\alpha_1\alpha_2}^{i_2,[2]} \dots \Gamma_{\alpha_{n-2},\alpha_{n-1}}^{i_{n-1},[n-1]} \Gamma_{\alpha_{n-1},\alpha_n}^{i_n,[n]},\tag{6}$$

similar to MPS, with $i_k = 1,\dots,d$ and $\alpha_k = 1,\dots,s_k$; here and henceforth all the repeated indices are summed over. The

Γs satisfy the linear independence conditions:[1]

$$\Gamma_{\alpha_{k-1},\alpha_k}^{i_k,[k]} x_{\alpha_k} = 0, \forall i_k, \quad \alpha_{k-1} \Longleftrightarrow x_{\alpha_k} = 0, \quad \forall \alpha_k.$$

We now add one more site to the chain, impose the constraint $P_{n,n+1}$, and look for the zero-energy ground states for $n+1$ sites in the form

$$\psi_{\alpha_{n+1}}^{i_1,\dots,i_{n+1}} = \psi_{\alpha_{n-1}}^{i_1,\dots,i_{n-1}} \Gamma_{\alpha_{n-1},\alpha_n}^{i_n,[n]} \Gamma_{\alpha_n,\alpha_{n+1}}^{i_{n+1},[n+1]}.\tag{7}$$

The unknown matrix $\Gamma_{\alpha_n,\alpha_{n+1}}^{i_{n+1},[n+1]}$ must satisfy

$$\langle v_{n,n+1}^p | i_n i_{n+1}\rangle \Gamma_{\alpha_{n-1},\alpha_n}^{i_n,[n]} \Gamma_{\alpha_n,\alpha_{n+1}}^{i_{n+1},[n+1]} = 0\tag{8}$$

for all values of $\alpha_{n-1}, \alpha_{n+1}$ and p, with $|v_{n,n+1}^p\rangle$ vectors defined in (5). This results in a system of linear equations,

$$C_{p\alpha_{n-1},i_{n+1}\alpha_n} \Gamma_{\alpha_n,\alpha_{n+1}}^{i_{n+1},[n+1]} = 0,\tag{9}$$

with $C_{p\alpha_{n-1},i_{n+1}\alpha_n} = \langle v_{n,n+1}^p | i_n i_{n+1}\rangle \Gamma_{\alpha_{n-1},\alpha_n}^{i_n,[n]}$ a matrix with dimensions $rs_{n-1} \times ds_n$. If $ds_n \geqslant rs_{n-1}$ and the matrix C has rank rs_{n-1}, the conditions (9) are independent and we can construct $ds_n - rs_{n-1}$ linearly independent, $\Gamma_{\alpha_n,\alpha_{n+1}}^{i_{n+1},[n+1]}$, corresponding to solutions for the $n+1$ qudit chain (see the Appendix for further discussion of the rank of C). The freedom we have now is to use only a subset of them for constructing solutions. Thus, we obtain the formula

$$s_{n+1} \leqslant ds_n - rs_{n-1},\tag{10}$$

valid for all n. The question now is how to choose s_n as we go along the chain.

The only constraint on $\Gamma_{\alpha_1}^{[1],i_1}$ is linear independence, which requires $s_1 \leqslant d$ ($s_0 = 1$, as the first pair has r constraints). If we choose the equality sign in the recursion relationship, Eq. (10), at each step, we obtain D_n linearly independent zero-energy states, where

$$D_n = dD_{n-1} - rD_{n-2},\tag{11}$$

for all n with $D_0 = 1$ and $D_1 = d$. The solution of this recursion relation is

$$D_n = \frac{f^{n+1} - g^{n+1}}{f - g},$$

with $f + g = d$ and $fg = r$. Hence,

$$f = \frac{d}{2} + \sqrt{\frac{d^2}{4} - r}, \quad g = \frac{d}{2} - \sqrt{\frac{d^2}{4} - r}.$$

There are three interesting regimes for r and d, which yield different behaviors of D_n (Fig. 2):

1. $r > \frac{d^2}{4}$ gives $D_n = r^{\frac{n}{2}} \frac{\sin(n+1)\theta}{\sin\theta}$ with $\cos\theta = \frac{d}{2\sqrt{r}}$. D_n becomes negative when $n + 1 > \frac{\pi}{\theta}$, and thus no zero-energy states can be constructed for a long chain if $r > \frac{d^2}{4}$.

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[1]Note that this is not the standard MPS form, which also requires linear independence in the other direction, that is,

$$y_{\alpha_{k-1}} \Gamma_{\alpha_{k-1},\alpha_k}^{i_k,[k]} = 0, \forall i_k, \quad \alpha_k \Longleftrightarrow y_{\alpha_{k-1}} = 0, \quad \forall \alpha_{k-1}.$$

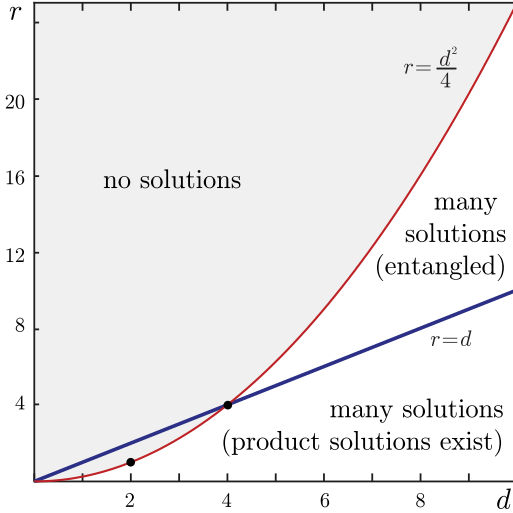In this case s_k would be the Schmidt rank for the partition of the qudits into $(1,\dots,k)$ and $(k+1,\dots,n)$.

FIG. 2. (Color online) The existence of zero-energy ground states for a qudit chain with d-dimensional qudits and r projectors per pair. We highlight two notable cases: $d = 2, r = 1$ and $d = 4, r = 4$.

2. $r = \frac{d^2}{4}$ results in $D_n = (\frac{d}{2})^n(n+1)$, an exponential growth in n (except when $d = 2$, which gives linear growth).

3. $r < \frac{d^2}{4}$ implies $f > \frac{d}{2}$ and $f > g$, so for large n, $D_n \sim f^n(1 - \frac{g}{f})^{-1}$ and the number of zero-energy states grows exponentially.

Any set of s_n that satisfies the inequality (10) must have $s_n \leqslant D_n$. To show this, we rewrite (10) as

$$s_0 = 1,$$
$$s_1 - ds_0 = -u_1,$$
$$s_n - ds_{n-1} + rs_{n-2} = -u_n, \quad n \geqslant 2,$$
$$\text{with} \quad u_n \geqslant 0, \quad n \geqslant 1.$$

These relations can be inverted to give

$$s_n = D_n - \sum_{l=1}^{n} u_l D_{n-l}, \quad n \geqslant 1,$$

from which $s_n \leqslant D_n$ follows at once.

This means that in regime 1, it is still not possible to construct solutions for a long chain. In regimes 2 and 3, we can construct sets of states with s_n growing more slowly than D_n.

1. For example when $d \leqslant r \leqslant \frac{d^2}{4}$, the recursion relation (10) can be satisfied also by $s_n = h^n$, provided that $h^2 - dh + r \leqslant 0$. This requires $g \leqslant h \leqslant f$, so the lower bound on h is the least integer $\geqslant g$.

2. In contrast, for $r < d$ the simple choice $s_n = 1$ also satisfies the recursion (10). This means that one can just solve the system from left to right as a linear system of equations. This results in a product state solution in the form

$$\psi^{i_1 i_2 \ldots i_n} = \psi^{[1], i_1} \psi^{[2], i_2} \cdots \psi^{[n], i_n}, \quad (12)$$

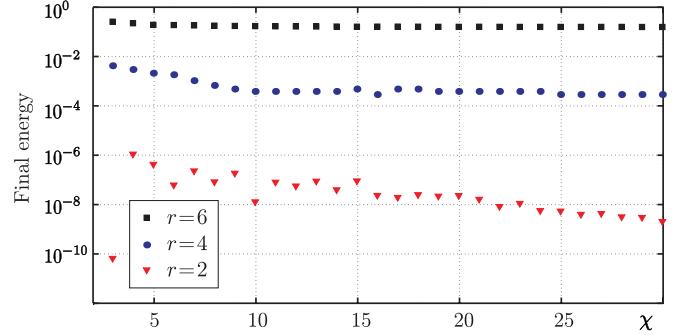which we can construct by starting with any $\psi^{[1]}$ and finding every $\psi^{[n+1]}$ from the previous ones.

FIG. 3. (Color online) Ground-state energy from imaginary time evolution vs. χ for different ranks of the Hamiltonian. This is a plot for a chain of $N = 20$ particles, with $d = 4$ states per site, and projector ranks of 2, 4, and 6. Exact description would require $\chi = d^{N/2} \approx 10^3$.

III. NUMERICAL INVESTIGATION USING MATRIX PRODUCT STATES

In this section we numerically search for the ground states of our class of random projector Hamiltonians (4). We probe the relations obtained in the previous section and see how well the energy coming from our small-χ MPS imaginary time evolution converges to 0. The numerical technique we use is similar to Vidal's [7,15]. We use imaginary time evolution to bring the system from a known state to its ground state: $|\Psi_{\text{grd}}\rangle = \lim_{\tau \to \infty} \frac{e^{-H\tau}|\Psi_0\rangle}{||e^{-H\tau}|\Psi_0\rangle||}$. In our numerical work we normalize the state after every time step [5]. We start from a uniform superposition of all the states and Trotterize by evolving first the odd pairs of sites and then the even pairs. Our experimentation with the parameters for a linear chain of length $N = 20$ is shown in Figs. 3–5; all the plots are on semi-log scale and the quantities being plotted are dimensionless.

We see that for $r < d$ the final energy converges to the zero-energy ground state relatively rapidly with $\chi \ll d^{N/2}$. This can be seen in Figs. 3–5 by the lowest curves (downward triangles). As shown, the final energy obtained from imaginary time evolution tends toward 0 with a steep slope, indicating that the ground state can be approximated efficiently with a small χ in the MPS ansatz.

The $r > d^2/4$ case, represented by squares, is shown as the top curve in Figs. 3–5. One sees that the final energy plateaus relatively quickly in all three cases. This shows that
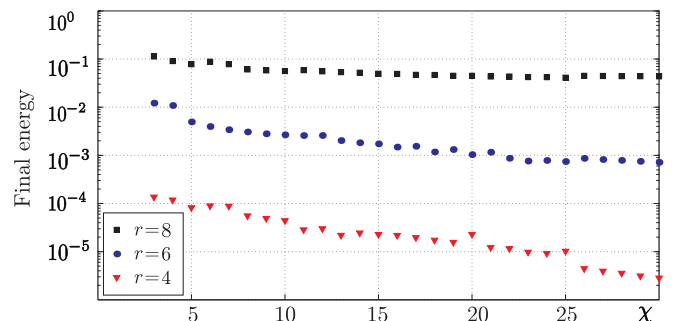

FIG. 4. (Color online) Final energy vs. χ for $N = 20$, $d = 5$, and projector ranks of 4, 6, and 8. Exact description would require $\chi \approx 10^5$.
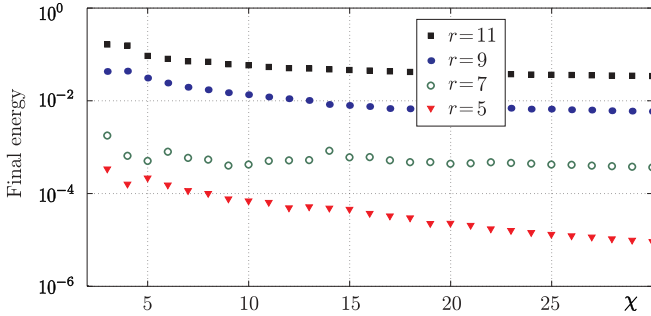
FIG. 5. (Color online) Final energy vs. χ for $N = 20$, $d = 6$, and projector ranks 5, 7, 9, and 11. Exact description in general would require $\chi \approx 10^8$.

the numerics have converged to a nonzero value and that increasing χ will not yield a lower value of energy. Therefore, the numerical results suggest that there are no ground states with zero energy.

In the previous section we analytically showed that when $d \leqslant r \leqslant d^2/4$, there are many zero-energy ground states. However, when we try to find these states numerically we see that the final energy converges to 0 slowly. This is shown in Figs. 3–5 by the middle curves (circles). Of these, there are the critical cases, where $r = \frac{d^2}{4}$. These correspond to the curves with circles in Figs. 3 and 5. The numerical investigation of the case $d \leqslant r \leqslant d^2/4$ is interesting because it suggests that for a large number of spins, finding the ground state with small χ, tractable on a normal computer, is very hard. We interpret this as a high amount of entanglement among the zero-energy ground states and leave the analytical proof of this statement for a follow-up paper.

IV. CONCLUSIONS

We have investigated the no-frustration conditions for a system of qudits on a line with d states per site and random rank r local projector Hamiltonians acting between the nearest-neighbor sites. We proved that there are no ground states with zero energy for $r > \frac{d^2}{4}$ and sufficiently large N. The system is not frustrated for $r \leqslant \frac{d^2}{4}$. This second parameter region further splits into two. For $d \leqslant r \leqslant \frac{d^2}{4}$, many entangled zero-energy ground states exist. In contrast, for $r < d$ we can also construct separable zero-energy ground states (see also Fig. 2).

We have verified the preceding statements numerically; in particular, we have shown that when $d \leqslant r \leqslant d^2/4$, approximating the ground-state energy (finding the ground states) is hard, as the states seem to be highly entangled. Future work entails the investigation of the energy gap [16] and the amount of entanglement in the system as a function of the parameters of the chain. Furthermore, we would like to address how far from an eigenstate of the Hamiltonian the wave function is after the truncations are made (i.e., as a function of χ). Finally, we would like to quantify the nature of the convergence to the ground state starting from an arbitrary state in this framework.

APPENDIX

We now address the question of the rank of the matrix C in Eq. (9). This C, which gives the constraints on $\Gamma^{[n+1]}$, depends on $|v_{n,n+1}^p\rangle$ and, through $\Gamma^{[n]}$, on all the $|v_{k,k+1}^p\rangle$ with $k < n$. We would like to say that for random $|v\rangle$ and when $s_k < D_k$ for random choices of the s_k-dimensional subspace, the rank of C is generically the maximum rank allowed, $\min(rs_{n-1}, ds_n)$. This is not obviously true. In particular, for the case $s_k = D_k$ in the regime $r \leqslant \frac{d^2}{4}$, to which we restrict ourselves henceforth, D_n grows exponentially in n, while the number of parameters in the $|v_{k,k+1}^p\rangle$ on which C depends only grows linearly. Thus C is far from a generic matrix of its size, but we now prove that its rank is indeed rD_{n-1}.

The argument used by Laumann *et al.* [17] to prove their "geometrization theorem" also applies to our problem. It shows that for a chain of N qudits with random $|v_{k,k+1}^p\rangle$, that is, for a Hamiltonian H as in Eqs. (2), (4), and (5), the number of zero-energy states, namely, dim[ker(H)], is, with probability 1 (which is what we mean by generic), equal to its minimum value. The calculation in Sec. II leading to the recursion relation (11) and its solution shows that in the regime $r \leqslant d^2/4$, this minimum is $\geqslant D_N$, since if the rank of the $rD_{k-1} \times dD_k$ matrix C is ever less than rD_{k-1}, we can choose $s_{k+1} = D_{k+1}$. Hence it is sufficient to find a single set of $|v_{k,k+1}^p\rangle$ for which dim[ker(H)] $= D_N$ to prove that D_N is the generic value, that is, that greater values occur with probability 0. This implies that the rank of each C is generically rD_{k-1}, since otherwise, at the first k where C had a smaller rank, we could construct more than D_{k+1} solutions for a chain of length $k + 1$.

We construct $|v_{k,k+1}^p\rangle$ with the property $\langle v_{k,k+1}^p | i_k i_{k+1}\rangle = 0$ unless $i_k \leqslant \frac{d}{2}$ and $i_{k+1} > \frac{d}{2}$. This can be done for r linearly independent $|v^p\rangle$ if $r \leqslant \frac{d^2}{4}$. We now assume that d is even; the modifications for d odd are obvious. We proceed by induction on n. Assume that in each $\Gamma_{\alpha_{k-1},\alpha_k}^{i_k,[k]}$ with $k \leqslant n$, α_k runs from 1 to D_k. From the definition of C [following Eq. (9)] and the special choice of $|v\rangle$, $C_{p\alpha_{n-1},i_{n+1}\alpha_n} = 0$ for $i_{n+1} \leqslant \frac{d}{2}$ and so from Eq. (9) $\Gamma_{\alpha_n,\alpha_{n+1}}^{i_{n+1},[n+1]}$ is unconstrained for $i_{n+1} \leqslant \frac{d}{2}$. This allows us to choose, for

$1 \leqslant \alpha_{n+1} \leqslant \frac{d}{2} D_n$,

$$\Gamma^{i_{n+1},[n+1]}_{\alpha_n,\alpha_{n+1}} = 1 \quad \text{when} \quad \alpha_{n+1} = \frac{d}{2}(\alpha_n - 1) + i_{n+1},$$

with $1 \leqslant \alpha_n \leqslant D_n$, $1 \leqslant i_{n+1} \leqslant \frac{d}{2}$, and

$$\Gamma^{i_{n+1},[n+1]}_{\alpha_n,\alpha_{n+1}} = 0 \quad \text{otherwise}.$$

As part of our induction, we assume that for $1 \leqslant \alpha_n \leqslant \frac{d}{2} D_{n-1}$,

$$\Gamma^{i_n,[n]}_{\alpha_{n-1},\alpha_n} = 1 \quad \text{when} \quad \alpha_n = \frac{d}{2}(\alpha_{n-1} - 1) + i_n,$$

with $1 \leqslant \alpha_{n-1} \leqslant D_{n-1}$, $1 \leqslant i_n \leqslant \frac{d}{2}$, and

$$\Gamma^{i_n,[n]}_{\alpha_{n-1},\alpha_n} = 0 \quad \text{otherwise}.$$

Now we can show that the rows of $C_{p\alpha_{n-1},i_{n+1}\alpha_n}$ are linearly independent: for if $\sum_{p,\alpha_{n-1}} y_{p,\alpha_{n-1}} C_{p\alpha_{n-1},i_{n+1}\alpha_n} = 0$ for all i_{n+1}, α_n this is true, in particular, for all $i_{n+1} > d/2$, $\alpha_n \leqslant \frac{d}{2} D_{n-1}$, when it becomes $\sum_p y_{p\alpha_{n-1}} \langle v^p_{n,n+1} | i_n i_{n+1} \rangle = 0$ for all $i_n \leqslant \frac{d}{2}$, $i_{n+1} > \frac{d}{2}$, and $\alpha_{n-1} \leqslant D_{n-1}$. Since the $|v^p\rangle$ are linearly independent, this is only true if $y_{p\alpha_{n-1}} = 0$ for all p, α_{n-1}. Hence the rank of C is $r D_{n-1}$, and α_{n+1} can take altogether $d D_n - r D_{n-1} = D_{n+1}$ values, which is what we wanted to prove.

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