Matrix product states: Symmetries and two-body Hamiltonians

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We characterize the conditions under which a translationally invariant matrix product state (MPS) is invariant under local transformations. This allows us to relate the symmetry group of a given state to the symmetry group of a simple tensor. We exploit this result in order to prove and extend a version of the Lieb-Schultz-Mattis theorem, one of the basic results in many-body physics, in the context of MPS. We illustrate the results with an exhaustive search of SU(2)-invariant two-body Hamiltonians which have such MPS as exact ground states or excitations.

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I. INTRODUCTION

Matrix product states (MPSs) [1,2] encapsulate many of the physical properties of quantum spin chains. Of particular interest in various physical contexts is the subset of translationally invariant (TI) MPS, originally introduced as finitely correlated states [1]. Their importance stems from the fact that with a simple tensor, A, one can fully describe relevant states of N spins, which, at least in principle, should require one to deal with an exponential number of parameters when written in a basis in the corresponding Hilbert space $\mathcal{H}^{\otimes N}$. Thus, all the physical properties of such states are contained in A. It is therefore important to obtain methods to extract the physical properties directly from such a tensor without having to resort to $\mathcal{H}^{\otimes N}$.

An important physical property of a TI state, Ψ, is the symmetry group under which it is invariant. That is, the group G such that

$$u_g^{\otimes N}|\Psi\rangle = e^{i\theta_g}|\Psi\rangle, \tag{1}$$

where $g \in G$ and u_g is a unitary representation on $\mathcal{H}$. In a recent paper [3] we showed that for a certain kind of MPS (those fulfilling the so-called injectivity condition [1,2]), this symmetry group is uniquely determined by the symmetry group of A (with a tensor product representation). Roughly speaking this means that by studying the symmetries of A we can obtain those for the whole state Ψ. This result allows us, for example, to shed a different perspective into string order [3], a key concept in strongly correlated states in many-body quantum systems.

Another relevant property of MPS is that they are all exact ground states (GSs) of short-range interacting (frustration-free) Hamiltonians [1,2]. In particular, for every TIMPS we can always build a (so-called) "parent" Hamiltonian for which it is the ground state. Of particular interests are TIMPS with two-body parent Hamiltonians, that is, whose parent Hamiltonian consists of two-body interactions only, and among those, the ones which have a large symmetry group, such as SU(2). The reason is that those are the ones that naturally appear in condensed-matter problems. Two prominent examples are the AKLT [4] and the Majumdar-Ghosh [5] states, which have two-body parent Hamiltonians with SU(2) symmetry. They have served as toy models to understand certain physical behavior in real physical systems, such as the existence of a Haldane gap [6] in spin chains with integer spin or the phenomenon of dimerization [5], respectively. Despite their key role in the understanding of spin chains, there are very few other examples known of TIMPS with SU(2) symmetry and with a two-body parent Hamiltonian [1,7,8].

In this work we first generalize the results of Ref. [3] to arbitrary TIMPS. This enables us to derive some generic properties about those states, as well as to obtain a simple proof for a version of the Lieb-Schultz-Mattis theorem [9,10]. This celebrated theorem states that all Hamiltonians with SU(2) symmetry are gapless for semi-integer spin $[\dim(\mathcal{H})=n+1/2,\ n=0,1,\ldots]$. In our case, we can prove that all TIMPS corresponding to systems with semi-integer spins cannot be the unique ground state of a local frustration-free Hamiltonian. Furthermore, we can extend the proof to other groups, such as U(1) for spin 1/2 systems, and find counterexamples for this last case when the spin is 5/2 or larger.

In the second part of our work we concentrate on MPS that are eigenstates (not necessarily grounds states) of a (so-called "parent") Hamiltonian which has SU(2) symmetry and contains two-body interactions only. We find other families of Hamiltonians beyond the well-known Affleck-Kennedy-Lieb-Tasaki (AKLT) and Majumdar-Ghosh with those features. Furthermore, we find the first examples of MPS that correspond to excited states of SU(2)-invariant Hamiltonians. There is another example of state with spin 1, which is never the ground state of any frustration-free SU(2)-invariant two-body Hamiltonian. In order to make a systematic search of all those MPS we develop a simple technique that allows for a numerical systematic search.

This paper is organized as follows. In Sec. II we review some of the basic properties of TIMPS and establish the notation that will be needed in the following. In Sec. III we establish the relation between the symmetry group of a TIMPS and that of the tensor A defining the MPS. For continuous symmetries, such as SU(2), we will see that the set of symmetric TIMPS is intimately related to the set of Clebsch-Gordan coefficients. Section IV then provides an MPS version of the Lieb-Schultz-Mattis theorem, and in Sec. V we

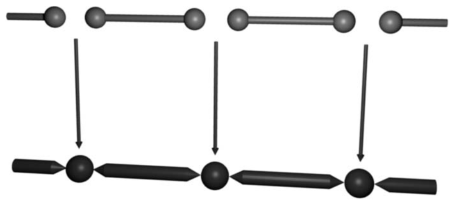

FIG. 1. This figure represents the MPS construction. A pair of virtual spins which are connected to their neighbors via a maximally entangled state $|\Omega\rangle = \Sigma_{\alpha=1}^{d}|\alpha\alpha\rangle$ are mapped into the physical spins (below). All properties of the state originate from the mapping between physical and virtual system.

give a detailed investigation of the SU(2) symmetric TIMPS which are eigenstates of two-body Hamiltonians.

II. MATRIX PRODUCT STATES

Let us consider a system with periodic boundary conditions of N (large but finite) sites, each of them with an associated d-dimensional Hilbert space. A translationally invariant MPS on this system can be defined with a valence bond construction in the following way. Let us consider another couple of D-dimensional ancillary/virtual Hilbert spaces associated to each site and connected to the real/physical d-dimensional space by a map $\mathcal{A} = \Sigma_{i\alpha\beta} A_{i,\alpha\beta}|i\rangle\langle\alpha\beta|$ (Fig. 1). Then, by introducing maximally entangled states connecting every pair of neighboring virtual Hilbert spaces (usually called entangled *bonds*), it is not difficult to prove that the state can be written as

$$|\Phi\rangle = \sum_{i_1,\ldots,i_N} \mathrm{tr}[A_{i_1}\cdots A_{i_N}]|i_1\cdots i_N\rangle,$$

where we call the matrices $\mathcal{K} = \{A_i \in \mathcal{M}_D, i = 1, \ldots, d\}$ as *Kraus operators*. A way to work simultaneously with all of them is to define the map

$$V = \sum_i A_i \otimes |i\rangle. \tag{2}$$

For each MPS there exists a canonical form ([2], theorem III7 and lemma IV4) which assures that one may choose all matrices A_i with a block-diagonal structure [12], in such a way that after gathering enough spins together, the Kraus operators fulfil the following.

Property 1: span property—the set of products $\mathcal{P} = \{A_{i_1}\cdots A_{i_n}\}$, with n as the collected spins, spans the vector space of all matrices with the same block-diagonal structure. It is an open conjecture stated in [2] and verified in many particular cases that an upper bound for the number of sites which have to be gathered to achieve property 1 depends only on the dimension D of the Kraus operators. When there is only one block in the above *canonical decomposition* the MPS is usually called *injective*, since the linear operator mapping boundary conditions to the resulting states is indeed injective [1,2] when taking sufficiently many particles. The definition reads as follows.

Property 2: injectivity—there exists n such that the map $\Gamma_n(X) = \Sigma_{i_1,\ldots,i_n} \mathrm{tr}(XA_{i_1}\cdots A_{i_n})|i_1\cdots i_n\rangle$ is injective. For each MPS $|\psi\rangle$ one can construct a Hamiltonian, called *parent Hamiltonian*, for which $|\psi\rangle$ is an eigenstate with eigenvalue 0.

Definition 3: parent Hamiltonian—let $\rho^{(k)}$ be the reduced density matrix of $|\psi\rangle$ for k particles (k will be called the *interaction length* of the parent Hamiltonian). Let us suppose that $\{|v_i\rangle\}_{i=1}^{r}$, with $r \geq 1$, is an orthonormal basis for $\ker[\rho^{(k)}]$. Taking any linear combination of projectors $h(\vec{a}) = \Sigma_{i=1}^{r} a_i|v_i\rangle\langle v_i|$, we define $H = \Sigma_i \tau_i(h) \otimes \mathbb{1}_{\mathrm{rest}}$, where τ_i is the translation operator.

If $a_i \geq 0$, then the Hamiltonian is positive semidefinite and $|\psi\rangle$ is indeed a ground state. Moreover H is *frustration free* since $|\psi\rangle$ minimizes the energy locally. Injectivity has now a deep physical significance. If it is reached for n particles and every $a_i > 0$, it ensures that the MPS is the *only* ground state of its $(n+1)$-local parent Hamiltonian, that it is an exponentially clustering state, and that there is a gap above the ground-state energy [1,2].

In this work we will focus on symmetries of *states* instead of *Hamiltonians*. There is however a close connection between the two approaches. On one hand, it is clear that the unique ground state of a symmetric Hamiltonian has to keep the symmetry. On the other hand, we have the following proposition.

Proposition 4—if an MPS $|\psi\rangle$ is invariant under a representation of a group, one can choose its parent Hamiltonian H invariant under the same representation. To see that it is enough to notice that the symmetry in state (1) implies the invariance of $\ker[\rho^{(k)}]$ under the same symmetry. Symmetrizing $\ker[\rho^{(k)}]$ (i.e., averaging it) with respect to the considered group will then yield a symmetric h which still constitutes a parent Hamiltonian.

III. LOCALLY SYMMETRIC MPS

In this section we analyze the implications of a given symmetry for a MPS. First, we show that the symmetry transfers to the Kraus operators—generalizing the findings of [1,3]. In a second step we show that the symmetry in the Kraus operators imposes that they are essentially uniquely defined in terms of the Clebsch-Gordan coefficients. Finally, for the special case of SU(2) one can simplify even further and analyze the qualitative differences between integer and semi-integer spin.

A. Characterization of symmetries

It was demonstrated in [3] that the Kraus operators which describe any injective state symmetric under a group G fulfil the condition $\Sigma_i u_{ij}^{g} A_i = U_g A_j U_g^{\dagger}$, where u and U are representations of G (Fig. 2). We provide in this section a generalization in which injectivity is not required. The N appearing in the proof must be sufficiently large to obtain property 1 after collecting $N/5$ spins.

We start by proving the case of discrete symmetries, extending the demonstration to continuous groups below. Theorem 5: discrete symmetries—let $\{A_i\}_{i=1}^{d}$ be the Kraus operators which describe a locally invariant MPS $|\psi\rangle$ with respect to a single unitary u, i.e., $u^{\otimes N}|\psi\rangle = e^{i\theta}|\psi\rangle$. Then, the symmetry in the physical level can be replaced by a local transformation in the virtual level. This means that there exists a unitary U—which can be taken as block diagonal with the same block structure as the A's in the MPS and composed with a permutation matrix among blocks, i.e., $U=P(\oplus_b V_b)$—such that

$$\sum_j u_{ij}A_j = WUA_iU^\dagger, \tag{3}$$

with $W=\oplus_b e^{i\theta_b}\mathbb{1}_b$.

Proof: we follow here a reasoning as in the proof of [2] (lemma IV4). We collect the spins in five different blocks, each one of them with property 1. Applying $u^{\otimes N}$ gives us the same MPS (we incorporate the global phase in the new matrices) with different matrices B's but with the same block-diagonal form and also (after gathering) with property 1. We now require the following lemma, which is demonstrated below.

Lemma 6: for each block in the A's, for instance, the one given by matrices A_i^1, there is a block in the B's, given by matrices B_i^1, which expands the same MPS. Since both are now canonical forms of the same injective MPS, by ([2], theorem 311) [13], they must be related by a unitary and a phase, $V_1A_i^1V_1^\dagger=e^{i\theta_1}B_i^1$, which finishes the proof of the theorem.

Let us prove now the lemma. By using property 1 and summing with appropriate coefficients, it is possible to show that there exists a block-diagonal $D\times D$ matrix $X\neq 0$ such that

$$\mathrm{tr}[A_{i_2}^1\cdots A_{i_5}^1] = \mathrm{tr}[XB_{i_2}\cdots B_{i_5}], \quad \forall\, i_2,\ldots,i_5.$$

Since $X\neq 0$, there exists one block, let us say X_1, different from 0. Then, summing with appropriate coefficients again we get that there exists a matrix $Y\neq 0$ such that

$$\mathrm{tr}[YA_{i_3}^1A_{i_4}^1A_{i_5}^1] = \mathrm{tr}[X_1B_{i_3}^1B_{i_4}^1B_{i_5}^1], \quad \forall\, i_3,i_4,i_5.$$

We can now argue as in [2] (lemma IV4) to conclude the proof. □

If we have now a symmetry given by a compact connected Lie group G, that is, Eq. (1) holds for any $g\in G$ and a representation $g\mapsto u_g$, we obtain the following. Theorem 7: (continuous symmetries)—the map $g\mapsto P_g$ is a representation of G and therefore the trivial one. The maps $g\mapsto e^{i\theta_g^b}$ and $g\mapsto V_g^b$ are also representations of G.

Proof: let us start with the map $g\mapsto P_g$. From Eq. (3) we get

$$W_{g_2g_1}U_{g_2g_1}A_hU_{g_2g_1}^\dagger = \sum_j u_{jh}^{g_2g_1}A_j = \sum_{jk} u_{jk}^{g_2}u_{kh}^{g_1}A_j$$
$$= W_{g_2}W_{g_1,P_{g_2}}U_{g_2}U_{g_1}A_hU_{g_1}^\dagger U_{g_2}^\dagger, \tag{4}$$

where $W_{g_1,P_{g_2}}$ is the same unitary as W_{g_1} but with the blocks permuted according to the permutation P_{g_2}. Since $P_{g'}W_g=W_{g,P_{g'}}P_{g'}$ and W_g commutes with all other terms appearing in Eq. (4), we can multiply successively and use property 1 (with L as the required block size) to get, for all $n\geq L$ and all X block diagonal,

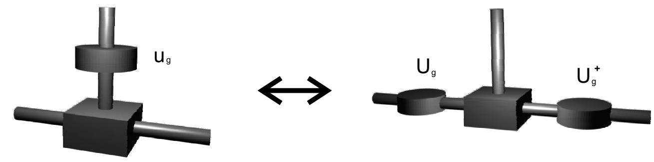

FIG. 2. The unitary u_g applied on the physical level is reflected in the virtual level as a pair of unitaries U_g.

$$W_{g_2g_1}^nU_{g_2g_1}XU_{g_2g_1}^\dagger = (W_{g_2}W_{g_1,P_{g_2}})^nU_{g_2}U_{g_1}XU_{g_1}^\dagger U_{g_2}^\dagger. \tag{5}$$

By taking $X=\mathbb{1}_b$ for each block b, we get that $P_{g_2}P_{g_1}$ must be $P_{g_2g_1}$. But since we are assuming the group G connected, this in turn implies that $P_g=\mathbb{1}$ for all g. With this we can split Eq. (5) into blocks to get, for each b, each $n\geq L$ and each matrix X,

$$e^{in\theta_{g_2g_1}^b}V_{g_2g_1}^bXV_{g_2g_1}^{b\dagger} = e^{in(\theta_{g_1}^b+\theta_{g_2}^b)}V_{g_2}^bV_{g_1}^bXV_{g_1}^{b\dagger}V_{g_2}^{b\dagger}. \tag{6}$$

Taking $X=\mathbb{1}$ we obtain

$$e^{in(\theta_{g_2g_1}^b)} = e^{in(\theta_{g_1}^b+\theta_{g_2}^b)}.$$

In particular, when $n=L$, we get that $L(\theta_{g_2g_1}^b)=L(\theta_{g_1}^b+\theta_{g_2}^b)+2k_0\pi$ and when $n=L+1$ we get that $(L+1)(\theta_{g_2g_1}^b)=(L+1)(\theta_{g_1}^b+\theta_{g_2}^b)+2k_1\pi$. Gathering both results, the L can be removed and we obtain $\theta_{g_2g_1}^b=\theta_{g_1}^b+\theta_{g_2}^b+2(k_1-k_0)\pi$. Finally, to show that $g\mapsto V_g^b$ is a representation, it is enough to notice that Eq. (6) implies that $V_{g_1}^{b\dagger}V_{g_2}^{b\dagger}V_{g_2g_1}^b$ commutes with every matrix. □

A trivial consequence of these theorems is the fact that having an *irreducible* representation U_g in the virtual level implies that the MPS has to be injective. We give an alternative proof of this fact in Appendixes A and B without having to rely on the MPS canonical form. There we analyze also when the reverse implication holds.

B. Uniqueness of the construction method

Once the theorem which provides the condition that the Kraus operators fulfill in order to generate invariant MPS has been established; the next step is to prove that they can always be constructed by means of Clebsch-Gordan coefficients. To do that, it is more convenient to work with the map V defined in Eq. (2). From the definition it is clear that the condition $\sum_i u_{ij}^gA_i=U_gA_jU_g^\dagger$ reads then $U_g\otimes u_gV=VU_g$. Notice that we have removed the dependence on the phase. By theorem 7 this can be done for groups with a complex enough structure, as SU(2), for which there is no nontrivial one-dimensional (1D) representation.

Given a compact group G, the tensor product of two irreps—we are choosing a single representative for each class of equivalent irreps—can always be decomposed as a direct sum of irreps,

$$u_g\otimes v_gC = C\bigoplus_i c_g^i,$$

where C is a unitary whose elements are called Clebsch-Gordan coefficients. In what follows we will denote by

$\phi_i: \mathbb{C}^{d_i} \rightarrow \mathbb{C}^d \otimes \mathbb{C}^{d'}$ the matrix associated to the restriction of C to the d_i-dimensional invariant subspace $\mathcal{H}_i$ associated to the irrep c_g^i, with d and d' being the dimensions of the representations u_g and v_g, respectively.

We are interested in possible solutions of

$$u_g \otimes v_g \Omega = \Omega w_g \quad \forall\, g, \tag{7}$$

where u_g, v_g, and w_g are irreps of a given compact group G. It is clear that taking

$$\Omega = \sum_i \beta_i \phi_i \tag{8}$$

does the job if we sum over i's corresponding to equivalent representations $c_g^i = w_g$. The next lemma guarantees that this is all.

Lemma 8: all possible solutions of Eq. (7) are given by Eq. (8). Proof: any Ω verifying Eq. (7) gives

$$\Omega^\dagger \Omega = w_g \Omega^\dagger \Omega w_g^\dagger,$$

which means by Schur's lemma that $\Omega^\dagger \Omega = \alpha \mathbb{1}$ and we may assume that if there is a nonzero solution, it can be taken as an isometry. Moreover, introducing $V = C^\dagger \Omega$, which verifies $V^\dagger V = \mathbb{1}$, one has

$$V w_g = (\oplus_i c_g^i) V. \tag{9}$$

From there one gets that $P = VV^\dagger$ is a rank d projector (d is the dimension of the representation w_g) that commutes with $(\oplus_i c_g^i)$ for all g. By Schur's lemma, it is supported on $\oplus_i \mathcal{H}_i$ with i's such that $c_g^i = w_g$, and in this subspace it is of the form

$$\begin{pmatrix} |\beta_1|^2 \mathbb{1}_d & \bar{\beta}_1 \beta_2 \mathbb{1}_d & \cdots \\ \beta_1 \bar{\beta}_2 \mathbb{1}_d & |\beta_2|^2 \mathbb{1}_d & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix} = |\beta\rangle\langle\beta| \otimes \mathbb{1}_d.$$

This implies that $V = |\beta\rangle \otimes W$ for a given $d \times d$ unitary W. But if we substitute this in Eq. (9), since we are assuming a unique fixed representative for each class of equivalent representations, we get $W = \mathbb{1}_d$ and $\Omega = \Sigma_i \beta_i \phi_i$. $\square$

From this we can now conclude. Theorem 9: let us consider a group G and two representations u_g (irrep) and $U_g = \oplus_i U_g^{D_i}$. Then, the structure of all possible maps V fulfilling $U_g \otimes u_g V = V U_g$ is

$$V = \begin{pmatrix} \alpha_{11} V_{D_1}^{D_1} & \alpha_{12} V_{D_1}^{D_2} & \cdots & \alpha_{1n} V_{D_1}^{D_n} \\ \alpha_{21} V_{D_2}^{D_1} & \alpha_{22} V_{D_2}^{D_2} & \cdots & \alpha_{2n} V_{D_2}^{D_n} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{n1} V_{D_n}^{D_1} & \alpha_{n2} V_{D_n}^{D_2} & \cdots & \alpha_{nn} V_{D_n}^{D_n} \end{pmatrix}, \tag{10}$$

where $V_{D_i}^{D_j}$ is a solution, according to lemma 8, to $U_g^{D_i} \otimes u_g V_{D_i}^{D_j} = V_{D_i}^{D_j} U_g^{D_i}$.

C. The case of SU(2)

Let us apply the results of Sec. III B to the case in which $G = \mathrm{SU}(2)$. Our construction is a natural generalization of the one used in [1,14].

We consider from now on irreducible representations u_g of the symmetry on the physical spin. Nevertheless, a substantial part of the results can be straightforwardly extended to the reducible case. Hence, we are interested in analyzing the restrictions that SU(2) impose in the general solution given by theorem 9 to the equation

$$(U \otimes J) V = V U, \tag{11}$$

where, with some abuse of notation, J is the SU(2) irrep corresponding to spin J and $U = (i_1 \oplus \cdots \oplus i_n \oplus s_1 \oplus \cdots \oplus s_m)$ is the virtual representation composed of n integer irreps and m semi-integer irreps. Note that in the Clebsch-Gordan decomposition of SU(2) all representations appear with multiplicity one. Therefore there is only one term in the sum in Eq. (8). At this point one should distinguish the cases of J integer or semi-integer. If J is integer, zero is the only solution to $(i_j \otimes J)\Omega = \Omega s_k$ and $(s_k \otimes J)\Omega = \Omega i_j$ for all j and k, and we get in Eq. (10) a block-diagonal structure,

$$V = \begin{pmatrix} \alpha_1^1 V_{i_1}^{i_1} & \cdots & \alpha_1^n V_{i_1}^{i_n} & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \alpha_n^1 V_{i_n}^{i_1} & \cdots & \alpha_n^n V_{i_n}^{i_n} & 0 & \cdots & 0 \\ 0 & \cdots & 0 & \alpha_{n+1}^{n+1} V_{s_1}^{s_1} & \cdots & \alpha_{n+1}^{n+m} V_{s_1}^{s_m} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \alpha_{n+m}^{n+1} V_{s_m}^{s_1} & \cdots & \alpha_{n+m}^{n+m} V_{s_m}^{s_m} \end{pmatrix}.$$

The paradigmatic example in this case is the AKLT state [4], which corresponds to the case of $J=1$ and $U=1/2$ in Eq. (11). In [1], the authors generalized the AKLT model to arbitrary integers J and irreducible U. We will call the resulting MPS as *FNW states*. It is shown in [1] how for $U = \frac{J}{2}$ FNW states are unique ground states of frustration-free nearest-neighbor interactions. An alternative construction focused on the restrictions imposed by the SU(2) symmetry on the density matrix instead of the Kraus operators can be found in [15].

If J is semi-integer, 0 is the only solution to $(s_j \otimes J)\Omega = \Omega s_k$ and $(i_k \otimes J)\Omega = \Omega i_j$ for all j and k, and we get in Eq. (10) an off-diagonal structure

$$V = \begin{pmatrix} 0 & \cdots & 0 & \alpha_1^{n+1} V_{i_1}^{s_1} & \cdots & \alpha_1^{n+m} V_{i_1}^{s_m} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & \alpha_n^{n+1} V_{i_n}^{s_1} & \cdots & \alpha_n^{n+m} V_{i_n}^{s_m} \\ \alpha_{n+1}^1 V_{s_1}^{i_1} & \cdots & \alpha_{n+1}^n V_{s_1}^{i_n} & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \alpha_{n+m}^1 V_{s_m}^{i_1} & \cdots & \alpha_{n+m}^n V_{s_m}^{i_n} & 0 & \cdots & 0 \end{pmatrix}.$$

It is clear that the virtual representations must be reducible now, which is very much related to the Lieb-Schultz-Mattis theorem, as we will show in Sec. V. The paradigmatic example in this case is the *Majumdar-Ghosh model* [5], which corresponds to $J = \frac{1}{2}$ and $U = \frac{1}{2} \oplus 0$. A generalization of this model for the case of arbitrary J and $U = F \oplus 0$ was recently proposed in [8]. In general, it is possible to find a set of representations which fits into any model with SU(2) symmetry, for instance [7,16–19,22].

IV. LIEB-SCHULTZ-MATTIS THEOREM

The Lieb-Schultz-Mattis theorem states that for semi-integer spin, a SU(2)-invariant 1D Hamiltonian cannot have a uniform (independent of the size of the system) energy gap above a unique ground state. That is, symmetry imposes strong restrictions on the possible behaviors of a system. In this section we want to go a step further and analyze which implications one can obtain from having a *single* symmetric state in a semi-integer spin chain. By restricting our attention to the class of MPS we will show the following.

Theorem 10—any MPS with an SU(2) symmetry in the sense of Eq. (1) with u_g irrep and even physical dimension d cannot be injective. By theorem 11 of [2] this implies that it cannot be the unique ground state of any frustration-free Hamiltonian.

Proof: let us assume that the MPS is injective and prove the theorem by contradiction. Theorems 5 and 7 guarantee that

$$\sum_j u_{jk}^g A_j = U_g A_k U_g^\dagger. \tag{12}$$

We consider $u=e^{iJ_z}$ with $(J_z)_{j,k}=\delta_{j,k}[k-(d+1)/2]$, $k=1,\ldots,d$. Then, Eq. (12) gives

$$e^{i\varphi_k}A_k = UA_kU^\dagger \tag{13}$$

for a unitary U and φ_k half integer. We finish by proving that if N is odd, $\mathrm{tr}(A_{k_1}\cdots A_{k_N})=0$ and hence the MPS cannot be injective. From Eq. (13) we get $\mathrm{tr}(A_{k_1}\cdots A_{k_N})=0$ unless $\Sigma_{i=1}^N \varphi_{k_i}=N(d+1)/2$. The latter is, however, impossible for odd N as the left-hand side (lhs) is an integer whereas the right-hand side (rhs) is a half integer. □

From the proof one may get the impression that only the U(1) symmetry is required, and this is indeed the case if the generator of such symmetry has eigenvalues $-m/2,\ldots,m/2$ as above. The next example shows that this is, however, not true for *any* U(1) symmetry, which in turn shows that a larger symmetry such as SU(2) is required for the Lieb-Schultz-Mattis theorem.

Example 11: let us consider a local symmetry generated by $G=e^{i\beta H}$ for a Hermitian matrix H. Let us choose the physical dimension $d=D^2-D$, which is always even, and the set of Kraus operators $\mathcal{K}=\{A_{(i,j)}=|i\rangle\langle j|, i\neq j\}$. We select $\alpha_1,\ldots,\alpha_D\in\mathbb{R}$ such that $\alpha_i-\alpha_j\neq 0$ if $i\neq j$ and H is the diagonal matrix $H=\Sigma_{i\neq j}(\alpha_i-\alpha_j)|(i,j)\rangle\langle(i,j)|$ (which has in addition only nonzero eigenvalues). With $U_\beta=e^{i\beta\Omega}$ where $\Omega=\mathrm{diag}[\alpha_1\ldots\alpha_D]$ it is clear that

$$e^{i\beta(\alpha_i-\alpha_j)}A_{(i,j)} = U_\beta A_{(i,j)}U_\beta^\dagger,$$

so the MPS generated by means of the Kraus operators $\mathcal{K}$ has the local symmetry G. Moreover, the MPS is trivially injective when $D\geq 3$. We can prove this by choosing arbitrary k and k'. Since $D\geq 3$, we can always find an l such that $k'\neq l\neq k$ and then $|k\rangle\langle k'|=|k\rangle\langle l|l\rangle\langle k'|=A_{(k,l)}A_{(l,k')}$.

Let us remark that this counterexample is applicable to spin $\geq\frac{5}{2}$. Indeed, one can prove theorem 2 for U(1) and spin $\frac{1}{2}$, which is the content of the following proposition. The case of spin 3/2 remains an open question.

Proposition 12: if $|\Phi\rangle$ is an MPS with physical dimension $d=2$ and invariant under U(1), then $|\Phi\rangle$ cannot be injective. Proof: we will show it by contradiction. By choosing a basis where the physical unitary u is diagonal, the condition on the Kraus operators becomes

$$e^{i\lambda_n\phi}A_n = e^{iH\phi}A_ne^{-iH\phi},$$

where H is the Hermitian generator of the symmetry. Let us expand the expression for infinitesimal angles

$$[H,A_n] = \lambda_n A_n,$$

which is the equation of eigenvalues for the operator $L(\bullet)=[H,\bullet]$. This can be transformed into an ordinary eigenvalue equation for the matrix operator $L=H\otimes\mathbb{1}-\mathbb{1}\otimes\bar{H}$. The diagonalization can be easily performed by taking the spectral decomposition of $H=\Sigma_i\mu_iP_i$, where P_i are orthogonal projectors. It straightforwardly follows that the eigenvalues of L are $\lambda_{ij}=\mu_i-\mu_j$ and the corresponding eigenoperators fulfil $A_{ij}=P_iA_{ij}P_j$.

Let us focus now on the case where $d=2$. Then, we have $A_1=P_1A_1P_\alpha$ and $A_2=P_\beta A_2P_\gamma$ for some α,β,γ. If $\beta=1$ $P_1X=X$ for all $X\in\mathrm{span}\{A_{i_1}\cdots A_{i_n}\}$ and the MPS cannot be injective. The same happens if $\alpha=\gamma$. So let us assume that $\beta\neq 1$ and $\gamma\neq\alpha$. Now if $\alpha=1$, we have $A_1=P_1A_1P_1$, $A_2=(\mathbb{1}-P_1)A_2(\mathbb{1}-P_1)$, and the MPS is block diagonal and hence noninjective. The same happens if $\beta=\gamma$. So $\alpha\neq 1$ and $\beta\neq\gamma$ and this gives $A_1^2=0=A_2^2$ which implies that $\mathrm{span}\{A_{i_1}\cdots A_{i_n}\}=\mathrm{span}\{A_1A_2A_1A_2\cdots A_2A_1A_2A_1\cdots\}$ has dimension ≤ 2. □

V. GENERAL CONSTRUCTION OF SU(2) TWO-BODY HAMILTONIANS WITH MPS EIGENSTATES

We have seen in definition (3) a way, called the parent Hamiltonian method, to construct local SU(2)-symmetric Hamiltonians with MPS as eigenstates. In this section we first prove that this method is the most general one to find Hamiltonians having a given MPS as *local eigenstate*, that is, being an eigenstate of each local term in the Hamiltonian. Then, we show examples (including the AKLT and Majumdar-Ghosh states) of MPS that are *excited* eigenstates of local two-body translationally invariant SU(2)-symmetric Hamiltonians. More examples are then provided in Appendix B.

A. Completeness of the parent Hamiltonian method

Theorem 13: given an MPS $|\psi\rangle$, any translational invariant Hamiltonian having it as a local eigenstate is of the form $a\mathbb{1}+H$ where H is a parent Hamiltonian for $|\psi\rangle$ in the sense of definition 3. Proof: let us call h the local Hamiltonian. By hypothesis of local eigenstate,

$$h\rho = \lambda\rho \tag{14}$$

for certain $\lambda\in\mathbb{R}$. This implies $[\rho,h]=0$, and hence one can find a set of projectors $\mathcal{P}=\{P_i, i=1,\ldots,r|\Sigma_iP_i=\mathbb{1}\}$ such that we can decompose both ρ and h by means of them, i.e., $h=\Sigma_i a_i P_i$ and $\rho=\Sigma_{j\in C} b_j P_j$, where C represents the set of projectors which describe the support of ρ. Using Eq. (14) with this decomposition gives that $a_i=\lambda$ for all $i\in C$, and hence

$$h=\sum_{i\in C^{\perp}} a_i P_i+\lambda\sum_{i\in C} P_i=\sum_{i\in C^{\perp}}(a_i-\lambda)P_i+\lambda\mathbb{1}.$$

Then, the translational invariance Hamiltonian is $H=\Sigma_j \tau^j(h)\otimes\mathbb{1}_{\mathrm{rest}}$, where τ is the translation operator. The theorem follows from replacing the result for the local Hamiltonian and comparing this with definition 3 of the parent Hamiltonian. □

This theorem shows that given an MPS $|\psi\rangle$, looking for all possible parent Hamiltonians of interaction length k is equivalent to looking for all possible solutions to the equation

$$h\rho^{(k)}=\lambda\rho^{(k)}, \tag{15}$$

with $\lambda=\mathrm{tr}[h\rho^{(k)}]$. The next lemma gives yet another equivalent formulation, which is the one that we will use in the sequel.

Lemma 14: given a Hermitian matrix h and a density matrix ρ, $h\rho=\lambda\rho$ if and only if

$$\mathrm{tr}[h^2\rho]-\mathrm{tr}[h\rho]^2=0. \tag{16}$$

Proof: one implication is clear. For the other, let us write $\langle h\rangle$ for $\mathrm{tr}[h\rho]\mathbb{1}$. By assumption

$$\mathrm{tr}[(h-\langle h\rangle)^2\rho]=\mathrm{tr}[h^2\rho]-\mathrm{tr}[h\rho]^2=0.$$

So $\rho^{1/2}(h-\langle h\rangle)^2\rho^{1/2}=0$, since it is a positive operator with trace 0. This implies that $(h-\langle h\rangle)\rho=0$ and hence $h\rho=\lambda\rho$. □

With this at hand we can systematically search for MPS that are excited *local eigenstates* of SU(2)-invariant Hamiltonians with two-body interactions. We will proceed as follows. We start with a given SU(2)-symmetric MPS $|\psi\rangle$ and fix the interaction length n. Then we look for possible solutions to Eq. (16) of the form

$$h=\sum_{i<j\leq n}\sum_{\alpha=1}^{2J} a_{ij}^{(\alpha)}(\vec{S}_i\circ\vec{S}_j)^{\alpha}+a_0\mathbb{1} \tag{17}$$

to ensure SU(2) symmetry and two-body interactions in the Hamiltonian. Finally, to guarantee that the MPS $|\psi\rangle$ is an excited state, we will find another SU(2)-symmetric MPS with less energy that will act as a witness. In Sec. V B we will illustrate this procedure starting with $|\psi\rangle$ the AKLT, the Majumdar-Ghosh state, and generalizations. Throughout we work in the thermodynamical limit $N\to\infty$.

B. Examples of SU(2) two-body Hamiltonians

1. Spin 1

Let us consider the AKLT state as a first example. Its Kraus operators are $A_{-1}=-\sqrt{2}\sigma^-$, $A_0=\sigma^z$, and $A_1=\sqrt{2}\sigma^+$.

In the case where $n=2$ the only solution to Eq. (16) is the AKLT Hamiltonian. In the case where $n=3$, the solutions are given by

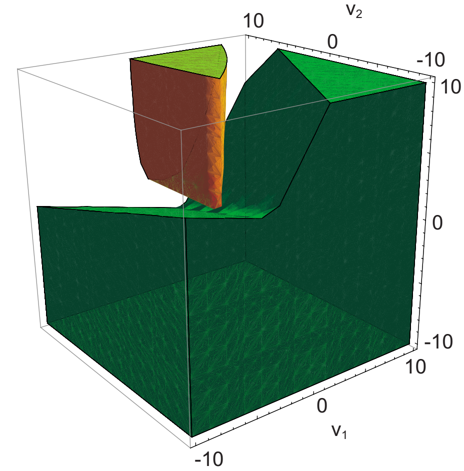

FIG. 3. (Color online) Space of parameters of the local Hamiltonian h for the AKLT state and $n=3$. The orange (small) volume represents the points where the state is the local (and hence the global) ground state. The green (large) volume represents points corresponding to excited states detected with the witness $\frac{3}{2}\oplus\frac{1}{2}$.

$$\begin{aligned}h=&(-3v_1+v_2+3v_3)(\vec{S}_1\circ\vec{S}_2)+v_3(\vec{S}_1\circ\vec{S}_2)^2\\&+\frac{1}{2}(-3v_1+v_2)(\vec{S}_1\circ\vec{S}_3)-\frac{1}{2}(-3v_1+v_2)(\vec{S}_1\circ\vec{S}_3)^2\\&+v_2(\vec{S}_2\circ\vec{S}_3)+v_1(\vec{S}_2\circ\vec{S}_3)^2,\end{aligned}$$

where the eigenvalue corresponding to the AKLT state is $7v_1-3v_2-2v_3$. The total translational invariant Hamiltonian is then

$$\begin{aligned}H=\sum_i&(-3v_1+2v_2+3v_3)(\vec{S}_i\circ\vec{S}_{i+1})+(v_1+v_3)(\vec{S}_i\circ\vec{S}_{i+1})^2\\&+\frac{1}{2}(-3v_1+v_2)(\vec{S}_i\circ\vec{S}_{i+2})-\frac{1}{2}(-3v_1+v_2)(\vec{S}_i\circ\vec{S}_{i+2})^2,\end{aligned}$$

which contains the usual AKLT model. It is not difficult to check that there is a region in the parameter space where the AKLT state is still the ground state of this Hamiltonian. To find regions where it is an excited eigenstate we will use as a witness the SU(2)-symmetric MPS associated to the virtual representation $\frac{3}{2}\oplus\frac{1}{2}$ (see Sec. III). The result is plotted in Fig. 3, where one sees the existence of points in this family of spin 1 Hamiltonians for which the AKLT state is an excited state.

Note that it is possible to perform a change of variables in the total Hamiltonian, for instance $a\to\frac{1}{2}(-3v_1+v_2)$ and $b\to v_1+v_3$, such that it depends only on two parameters. However, the number of parameters that the local Hamiltonian h depends on cannot be reduced, which means that there are nonphysical parameters in it. In Fig. 4 we have represented the problem above ($n=3$ and AKLT state) in terms of the physical parameters. The positive axis b corresponds there to the usual AKLT Hamiltonian.

Concerning FNW states, that is, integer spin J and virtual irrep j, we have performed an exhaustive search and Table I gathers the main results. The study has been carried out by

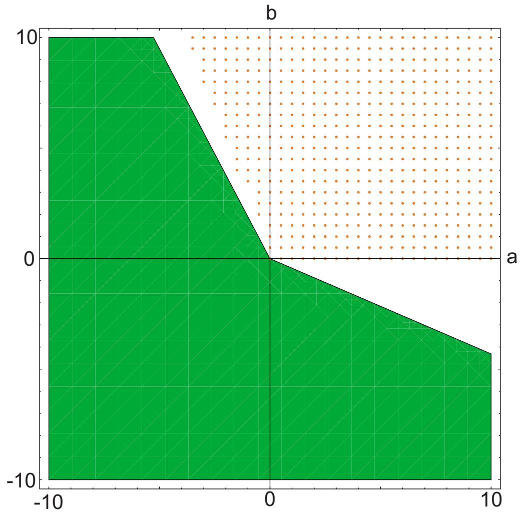

FIG. 4. (Color online) Space of physical parameters of the global Hamiltonian H corresponding to $n=3$ and the AKLT state. The points (orange) represent where the state is the local (and hence the global) GS. The surface (green) represents points corresponding to excited states detected by means of the witness $\frac{3}{2}\oplus\frac{1}{2}$.

increasing n and studying the number of parameters which the family of Hamiltonians depends on (notice that the case of interaction length n contains the case of interaction length $n-1$). We have increased n until the number of parameters stops growing. In all the cases considered in the table, a saturation occurs when $n>3$, i.e., considering that more than three particles apparently does not add new Hamiltonians.

Let us also introduce a new state of spin 1 with virtual spin 1, given by the Kraus operators

$$A_1=\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\0&0&1\\0&0&0\end{pmatrix},\quad A_0=\frac{1}{\sqrt{2}}\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix},$$

$$A_{-1}=\frac{1}{\sqrt{2}}\begin{pmatrix}0&0&0\\-1&0&0\\0&-1&0\end{pmatrix}.$$

The total translational invariant Hamiltonian which has this state as eigenstate is

TABLE I. Table of results for FNW states with physical spin J and virtual spin j. The numbers in the table are the number of parameters which the obtained families of Hamiltonians depend on. The ■ represent the cases for which no solution was found.

	(j)						
J	$\frac{1}{2}$	1	$\frac{3}{2}$	2	$\frac{5}{2}$	3	$\frac{7}{2}$
1	2	1	■	■	■	■	■
2		5	3	■	■	■	■
3			4	2	2	1	■

$$H=\sum_i(\vec{S}_i\circ\vec{S}_{i+1})^2-(\vec{S}_i\circ\vec{S}_{i+2})-(\vec{S}_i\circ\vec{S}_{i+2})^2.$$

This state is injective and a local excited state. The fact that this state is an excited state of the global Hamiltonian can be checked as above by means of the witness $1\oplus 0$.

2. Spin $\frac{1}{2}$

Let us consider now the Majumdar-Ghosh state as an example with semi-integer spin. The Kraus operators are now

$$A_{-1/2}=\begin{pmatrix}0&\frac{1}{\sqrt{2}}&0\\0&0&-1\\0&0&0\end{pmatrix},\quad A_{1/2}=\begin{pmatrix}0&0&0\\1&0&0\\0&\frac{1}{\sqrt{2}}&0\end{pmatrix}.$$

As in the previous case, we do not find any solution for $n=2$ and only the Majumdar-Ghosh Hamiltonian for the cases $n=3$ and $n=4$. For $n=5$ the solutions to Eq. (16) are given by

$$\begin{aligned}h={}&(v_1-v_2+v_4)(\vec{S}_1\circ\vec{S}_2)+(v_1-v_2+v_4)(\vec{S}_1\circ\vec{S}_3)\\&+v_3(\vec{S}_1\circ\vec{S}_4)+v_3(\vec{S}_1\circ\vec{S}_5)+v_4(\vec{S}_2\circ\vec{S}_3)\\&+(-v_1+v_2+v_3)(\vec{S}_2\circ\vec{S}_4)+v_3(\vec{S}_2\circ\vec{S}_5)+v_2(\vec{S}_3\circ\vec{S}_4)\\&+v_1(\vec{S}_3\circ\vec{S}_5)+v_1(\vec{S}_4\circ\vec{S}_5)\end{aligned}\tag{18}$$

and the energy associated to the state is $-\frac{3}{4}(v_1+v_4)$. The total Hamiltonian $H=\Sigma_i\tau_i(h)$ is given by

$$\begin{aligned}H=\sum_i{}&2(v_1+v_4)(\vec{S}_i\circ\vec{S}_{i+1})+(v_1+v_3+v_4)(\vec{S}_i\circ\vec{S}_{i+2})\\&+2v_3(\vec{S}_i\circ\vec{S}_{i+3})+v_3(\vec{S}_i\circ\vec{S}_{i+4}).\end{aligned}\tag{19}$$

As in the AKLT case, by means of a change of variables $a\rightarrow v_3$ and $b\rightarrow v_1+v_4$, the number of physical parameters in the total Hamiltonian is 2, compared with the four parameters the local Hamiltonian depends on. The Majumdar-Ghosh state is an excited local eigenstate for a region in the space of parameters, which in this case is detected by the witness $\frac{1}{2}\oplus 1\oplus 0$, as shown in Fig. 5. The usual Majumdar-Ghosh Hamiltonian [20] corresponds to the positive axis b.

3. Spin $\frac{3}{2}$

Let us consider as final example the SU(2)-symmetric MPS corresponding to spin $\frac{3}{2}$ and virtual representation $\frac{3}{2}\oplus 0$. For $n=3$, the solutions to Eq. (16) are given by

$$\begin{aligned}h={}&v_3(\vec{S}_1\circ\vec{S}_2)+v_2(\vec{S}_1\circ\vec{S}_2)^2+v_1(\vec{S}_1\circ\vec{S}_2)^3\\&+(2v_1-v_2+v_3)(\vec{S}_1\circ\vec{S}_3)+(4v_1-v_2)(\vec{S}_1\circ\vec{S}_3)^2\\&+v_1(\vec{S}_1\circ\vec{S}_3)^3+v_3(\vec{S}_2\circ\vec{S}_3)+v_2(\vec{S}_2\circ\vec{S}_3)^2+v_1(\vec{S}_2\circ\vec{S}_3)^3\end{aligned}\tag{20}$$

and the energy associated to the MPS is in this case $-\frac{15}{64}(165v_1-60v_2+16v_3)$. The global Hamiltonian now reads

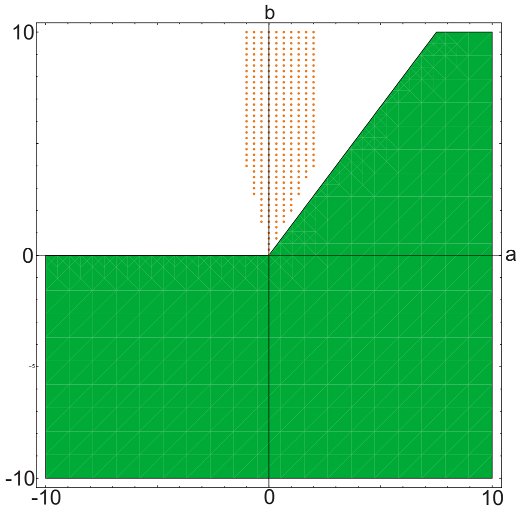

FIG. 5. (Color online) Space of physical parameters of the total Hamiltonian for $n=5$ associated to the Majumdar-Ghosh state. The points (orange) represent where the state is the local (and hence the global) ground state. The surface (green) represents points corresponding to excited states detected by means of the witness $\frac{1}{2}\oplus 1\oplus 0$.

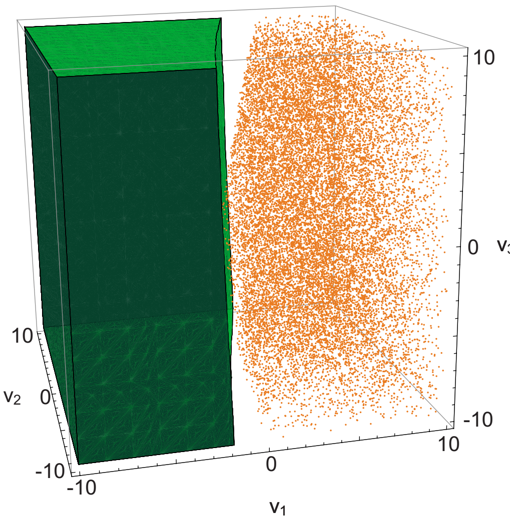

FIG. 6. (Color online) Space of parameters of the spin $\frac{3}{2}$ model. The points (orange) are obtained numerically and they represent values of the parameters where the MPS state is the GS. The volume (green) represents points corresponding to excited states detected with the witness $\frac{3}{2}\oplus 1\oplus 0$.

$$H=\sum_i 2v_3(\vec{S}_i\circ\vec{S}_{i+1})+2v_2(\vec{S}_i\circ\vec{S}_{i+1})^2+2v_1(\vec{S}_i\circ\vec{S}_{i+1})^3 + (2v_1-v_2+v_3)(\vec{S}_i\circ\vec{S}_{i+2})+(4v_1-v_2)(\vec{S}_i\circ\vec{S}_{i+2})^2 + v_1(\vec{S}_i\circ\vec{S}_{i+2})^3. \tag{21}$$

It is remarkable that in this case there are no spurious parameters in the local Hamiltonian h. Considering the family of states whose virtual representation is $\frac{3}{2}\oplus 1\oplus 0$ as a witness, it is possible to demonstrate that there is a region in the space of parameters of the Hamiltonian for which the MPS is an excited eigenstate, as shown in Fig. 6.

VI. CONCLUSIONS

Despite the fact that all our results are restricted to the family of TIMPS, their relevance is manifested by the fact that those states approximate all ground states of one-dimensional Hamiltonians with short-range interactions [11]. Thus, one would expect that the properties derived for MPS would be relevant in a more general context. Moreover, due to their simplicity, MPS can be then thought as a "laboratory" for which some generic mathematical and physical properties of states that are relevant in one-dimensional spin chains can be searched. Later on, one may use more powerful mathematical methods to try to extrapolate those properties to general spin chains. Furthermore, many of the techniques used in the present work are amenable of an extension to higher spatial dimensions, where projected entangled pair state (PEPS) play the role of MPS. In Ref. [3] some first results in this direction were derived, which will be generalized in a further publication.

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APPENDIX A: RELATIONS BETWEEN IRREDUCIBILITY AND INJECTIVITY

In this appendix we give a direct proof of the fact that an irreducible representation in the virtual level of a symmetric MPS implies that the MPS is injective. We also see that the reverse inclusion is not true in general but it holds under some conditions on the Kraus operators.

We have to recall that given a set of Kraus operators defining an MPS $\mathcal{K}=\{A_1,\dots,A_d\}$, we can define an associated *completely positive map* $\mathbb{E}(X)=\Sigma_{i=1}^d A_i X A_i^\dagger$. The symmetry in the MPS transfers then to the *covariance* of the channel, that is, $\mathbb{E}(U_g X U_g^\dagger)=U_g\mathbb{E}(X)U_g^\dagger$ for all X. It is shown in [1,2] that if $\mathbb{E}$ is trace preserving and has $\mathbb{1}$ as its unique fixed point, then the MPS is injective. Moreover, it is trivial to see that if $\mathbb{E}$ is the ideal channel [$\mathbb{E}(X)=X$ for all X], then the MPS is a product state. Therefore, the desired result that *irrep implies injectivity* is a consequence of the following theorem.

Theorem 15: let us take a completely positive map $\mathbb{E}:\mathcal{M}_D\to\mathcal{M}_D$ that is covariant for an irrep of a compact connected Lie group G. Then, either $\mathbb{E}$ is the ideal channel or it is trace preserving and the identity is its only fixed point.

Proof: let us consider a fixed point Δ of $\mathbb{E}$. Then $U_g\Delta U_g^\dagger$ is also a fixed point because of the covariance. Therefore, integrating under the Haar measure and using Schur's lemma, $\mathbb{1}$ is also a fixed point. A similar argument shows that $\mathbb{E}$ is also trace preserving.

Now we can apply Lüders' theorem [21], which ensures that the set of fixed points $\mathcal{P}$ of $\mathbb{E}$ coincides with the commutant $\mathcal{K}'$ of the set of Kraus operators of $\mathbb{E}$. This is trivially a C^* subalgebra of $\mathcal{M}_D$. Moreover, we know by the classification of the C^* subalgebras in $\mathcal{M}_D$ that there exists a unitary $V \in \mathcal{M}_D$ such that $V\mathcal{P}V^\dagger = \oplus_i (M_{n_i} \otimes \mathbb{1}_{n_i'}) = \mathcal{A}$.

The equivalent representation $V_g = VU_gV^\dagger$ is also an irrep and fulfils $V_g \mathcal{A} V_g^\dagger = \mathcal{A}$. This means that the block structure of $\mathcal{A}$ remains invariant under the action of V_g by conjugation. Now we use

$$V_g \mathcal{A} V_g^\dagger \subset \mathcal{A} \Leftrightarrow [J, \mathcal{A}] \subset \mathcal{A} \text{ for all generators } J. \tag{A1}$$

This implies that J has the same block structure as $\mathcal{A}$. If there is more than one block, the representation is reducible. If $\mathcal{A} = M_n \otimes \mathbb{1}_{n'}$, then we use again Eq. (A1).

The Schmidt decomposition allows us to take $J = \Sigma_i A_i \otimes B_i$ where the B_i's form a basis of $M_{n'}$, with $B_1 = \mathbb{1}$. Then, Eq. (A1) gives $\Sigma_i [A_i, M_n] \otimes B_i = C \otimes \mathbb{1}$, which implies that A_i is proportional to $\mathbb{1}$ for all $i \geq 2$. This gives $J = \mathbb{1} \otimes X + Y \otimes \mathbb{1}$ and hence $V_g = V_1^g \otimes V_2^g$, which is reducible unless $\mathcal{A} = \mathbb{1}$ or $\mathcal{A} = M_N$ (which implies that $\mathbb{E}$ is the ideal channel). □

Although the implication in the opposite direction could also seem true, it is not, as shown by the following example. Example 16: let us consider the family of SU(2)-symmetric MPS of spin 1 with a reducible virtual representation $\frac{1}{2} \oplus \frac{3}{2}$ given by the following maps (see Sec. III):

$$\tilde{V} = \begin{pmatrix} e^{i\alpha_{11}} \cos \theta_1 V_{1/2}^{1/2} & e^{i\alpha_{12}} \sin \theta_2 V_{1/2}^{3/2} \\ e^{i\alpha_{21}} \sin \theta_1 V_{3/2}^{1/2} & e^{i\alpha_{22}} \cos \theta_2 V_{3/2}^{3/2} \end{pmatrix}.$$

It is not difficult to check that the MPS is injective except in particular directions in space, such as those for which the isometry breaks into blocks, i.e., $\theta_i = n\frac{\pi}{2}$.

Although the equivalence is not true in general, we can still give a sufficient condition which applies, for instance, to the AKLT and other FNW states. Let us recall from [3] or theorems 5 and 7 that an injective symmetric MPS verifies

$$\sum_i u_{ij}^g A_i = e^{i\theta_g} U_g A_j U_g^\dagger, \tag{A2}$$

where in addition one may ask for $\Sigma_i A_i^\dagger A_i = \mathbb{1}$ [2].

Proposition 17: if u_g is irreducible and $\{A_i^\dagger A_j\}_{i,j}$ spans the whole space of matrices, then the virtual representation U_g of Eq. (A2) is also irreducible.

Proof: from Eq. (A2) one gets

$$\sum_{i_1,i_2} \bar{u}_{i_1 j_1}^g u_{i_2 j_2}^g A_{i_1}^\dagger A_{i_2} = U_g A_{j_1}^\dagger A_{j_2} U_g^\dagger.$$

Integrating now with respect to the Haar measure, the lhs is simplified by the irreducibility of u_g and the orthogonality relations. The result is $\delta_{j_1 j_2} \Sigma_i A_i^\dagger A_i = \delta_{j_1 j_2} \mathbb{1}$. This means that $\int_G U_g X U_g^\dagger \propto \mathbb{1}$, $\forall X \in \mathcal{M}_D$, since we can span the complete space of matrices. But this implies that U_g is an irrep by means of the inverse of Schur's lemma. □

APPENDIX B: LIST OF PARENT HAMILTONIANS

The following lists SU(2)-invariant two-body Hamiltonians for which the MPS with physical spin J (irrep) and virtual spin j is an exact eigenstate with energy ϵ.

1. Spin $J=\frac{1}{2}$

For $j = \frac{1}{2} \oplus 0$ and $\epsilon = -\frac{3}{4}(v_1 + v_4)$,

$$H = \sum_i 2(v_1 + v_4)(\vec{S}_i \circ \vec{S}_{i+1}) + (v_1 + v_3 + v_4)(\vec{S}_i \circ \vec{S}_{i+2}) + 2v_3(\vec{S}_i \circ \vec{S}_{i+3}) + v_3(\vec{S}_i \circ \vec{S}_{i+4}).$$

There are no solutions found (with $n \leq 6$) for $j = \frac{1}{2} \oplus 1$, $\frac{3}{2} \oplus 1$, $\frac{3}{2} \oplus 2$, and $\frac{5}{2} \oplus 2$.

2. Spin $J=1$

For $j = \frac{1}{2}$ and $\epsilon = 7v_1 - 3v_2 - 2v_3$,

$$H = \sum_i (-3v_1 + 2v_2 + 3v_3)(\vec{S}_i \circ \vec{S}_{i+1}) + (v_1 + v_3)(\vec{S}_i \circ \vec{S}_{i+1})^2 + \frac{1}{2}(-3v_1 + v_2)(\vec{S}_i \circ \vec{S}_{i+2}) - \frac{1}{2}(-3v_1 + v_2)(\vec{S}_i \circ \vec{S}_{i+2})^2.$$

For $j = 1$ and $\epsilon = 1$,

$$H = \sum_i (\vec{S}_i \circ \vec{S}_{i+1})^2 - (\vec{S}_i \circ \vec{S}_{i+2}) - (\vec{S}_i \circ \vec{S}_{i+2})^2.$$

There are no solutions found (with $n \leq 4$) for $j = \frac{3}{2}$, 2, $\frac{5}{2}$, and 3.

3. Spin $J=\frac{3}{2}$

For $j = \frac{3}{2} \oplus 0$ and $\epsilon = -\frac{15}{64}(165v_1 - 60v_2 + 16v_3)$,

$$H = \sum_i 2v_3(\vec{S}_i \circ \vec{S}_{i+1}) + 2v_2(\vec{S}_i \circ \vec{S}_{i+1})^2 + 2v_1(\vec{S}_i \circ \vec{S}_{i+1})^3 + (2v_1 - v_2 + v_3)(\vec{S}_i \circ \vec{S}_{i+2}) + (4v_1 - v_2)(\vec{S}_i \circ \vec{S}_{i+2})^2 + v_1(\vec{S}_i \circ \vec{S}_{i+2})^3.$$

For $j = \frac{1}{2} \oplus 1$ and $\epsilon = -\frac{495}{64}$,

$$H = \sum_i \frac{243}{16}(\vec{S}_i \circ \vec{S}_{i+1}) + \frac{29}{4}(\vec{S}_i \circ \vec{S}_{i+1})^2 + (\vec{S}_i \circ \vec{S}_{i+1})^3.$$

There are no solutions found (with $n \leq 4$) for $j = \frac{3}{2} \oplus 1$, $\frac{5}{2} \oplus 1$, $\frac{1}{2} \oplus 2$, and $\frac{3}{2} \oplus 2$.

4. Spin $J=2$

For $j=1$ and $\epsilon=(-6986v_1+778v_2-62v_3+1260v_4-90v_5)$,

$$
\begin{aligned}
H = \sum_i & (2400v_1 - 63v_2 + 24v_3 - 792v_4 + 63v_5)(\vec{S}_i \circ \vec{S}_{i+1}) \\
& + (133v_1 - 14v_2 + 2v_3 - 133v_4 + 14v_5)(\vec{S}_i \circ \vec{S}_{i+1})^2 \\
& + (v_2 + v_5)(\vec{S}_i \circ \vec{S}_{i+1})^3 + (v_1 + v_4)(\vec{S}_i \circ \vec{S}_{i+1})^4 \\
& + \left(\frac{1729}{2}v_1 - 91v_2 + \frac{13}{2}v_3\right)(\vec{S}_i \circ \vec{S}_{i+2}) \\
& + \left(\frac{5719}{36}v_1 - \frac{301}{18}v_2 + \frac{43}{36}v_3\right)(\vec{S}_i \circ \vec{S}_{i+2})^2 \\
& + \left(-\frac{665}{18}v_1 + \frac{35}{9}v_2 - \frac{5}{16}v_3\right)(\vec{S}_i \circ \vec{S}_{i+2})^3 \\
& + \left(-\frac{133}{12}v_1 + \frac{7}{6}v_2 - \frac{1}{12}v_3\right)(\vec{S}_i \circ \vec{S}_{i+2})^4.
\end{aligned}
$$

For $j=\frac{3}{2}$ and $\epsilon=0$,

$$
\begin{aligned}
H = \sum_i & (580v_1) - 80v_2 + 10v_3 - 330v_4 + 30v_5(\vec{S}_i \circ \vec{S}_{i+1}) \\
& + (91v_1 - 11v_2 2v_3 - 91v_4 11v_5)(\vec{S}_i \circ \vec{S}_{i+1})^2 \\
& + (v_2 + v_5)(\vec{S}_i \circ \vec{S}_{i+1})^3 + (v_1 + v_4)(\vec{S}_i \circ \vec{S}_{i+1})^4 \\
& + \frac{1}{6}(2275v_1 - 275v_2 + 25v_3)(\vec{S}_i \circ \vec{S}_{i+2}) \\
& + \frac{1}{36}(455v_1 - 55v_2 + 5v_3)(\vec{S}_i \circ \vec{S}_{i+2})^2 \\
& + \frac{1}{18}(-455v_1 + 55v_2 - 5v_3)(\vec{S}_i \circ \vec{S}_{i+2})^3 \\
& + \frac{1}{36}(-91v_1 + 11v_2 - v_3)(\vec{S}_i \circ \vec{S}_{i+2})^4.
\end{aligned}
$$

There are no solutions found (with $n \leq 4$) for $j=2$ and $\frac{5}{2}$.

5. Spin $J=3$

Solutions (mostly cumbersome ones) were found for $j=1(n=3)$, $j=2(n=2)$, and $j=5/2(n=2)$.

[1] M. Fannes, B. Nachtergaele, and R. W. Werner, Commun. Math. Phys. **144**, 443 (1992).

[2] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, Quantum. Inf. Comput. **7**, 401 (2007).

[3] D. Perez-Garcia, M. M. Wolf, M. Sanz, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **100**, 167202 (2008).

[4] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Commun. Math. Phys. **115**, 477 (1988).

[5] C. K. Majumdar and D. K. Ghosh, J. Math. Phys. **10**, 1399 (1969).

[6] F. D. M. Haldane, Phys. Lett. A **93**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983).

[7] A. Klümper, A. Schadschneider, and J. Zittartz, Europhys. Lett. **24**, 293 (1993).

[8] V. Karimipour and L. Memarzadeh, Phys. Rev. B **77**, 094416 (2008).

[9] E. Lieb, T. Schultz, and D. Mattis, Ann. Phys. **16**, 407 (1961).

[10] M. B. Hastings, Phys. Rev. B **69**, 104431 (2004).

[11] F. Verstraete and J. I. Cirac, Phys. Rev. B **73**, 094423 (2006).

[12] Eventually after gathering some spins together to neglect the periodic components—something that we will always assume.

[13] The condition of Ref. [2] (theorem 311) that the canonical form in the OBC must be unique can be dropped by Eq. (3) of L. Lamata *et al.*, Phys. Rev. Lett. **101**, 180506 (2008).

[14] S. Singh, H.-Q. Zhou, and G. Vidal, e-print arXiv:cond-mat/0701427.

[15] J. Dukelsky, M. A. Martin-Delgado, T. Nishino, and G. Sierra, Europhys. Lett. **43**, 457 (1998).

[16] B. Kumar, Phys. Rev. B **66**, 024406 (2002).

[17] J. M. Roman, G. Sierra, J. Dukelsky, and M. A. Martin-Delgado, J. Phys. A **31**, 9729 (1998).

[18] S. Rachel and M. Greiter, Phys. Rev. B **78**, 134415 (2008).

[19] D. Sen and N. Surendran, Phys. Rev. B **75**, 104411 (2007).

[20] The family of Hamiltonians constructed in [16] is quite remarkable. In this paper the ground state of the Hamiltonian which corresponds to $b=2a$ is calculated and fits perfectly to our results.

[21] O. Bratteli, P. E. T. Jorgensen, A. Kishimoto, and R. F. Werner, J. Oper. Theory **43**, 97 (2000).

[22] Hong-Hao Tu, Guang-Ming Zhang, and Tao Xiang, Phys. Rev. B **78**, 094404 (2008).