



Valence bond solid states with symplectic symmetry

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We introduce a one-dimensional valence bond solid (VBS) state with symplectic symmetry $SP(n)$ and construct the corresponding parent Hamiltonian. We argue that there is a gap in the spectrum. We calculate exactly the static correlation functions, which fall off exponentially. Hence the model introduced here shares all properties of the Haldane scenario for integer-spin quantum antiferromagnets. We further show that the VBS state possesses string order and discuss its generalization to higher dimensions.

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I. INTRODUCTION

In 1987 Affleck, Kennedy, Lieb, and Tasaki (AKLT)¹ introduced the $SU(2)$ valence bond solid (VBS) state and showed that it is the unique ground state of a special antiferromagnetic spin-1 chain. This model possesses all properties of the Haldane scenario for integer-spin quantum antiferromagnets,² namely a unique ground state, an energy gap between the ground state and the excitations, and exponentially decaying correlations in the ground state. Soon after its discovery the VBS state was reformulated in terms of Schwinger bosons.^{3,4} This formulation revealed a striking analogy between the VBS state and the Laughlin state in the fractional quantum Hall effect,⁵ and enabled the analysis of the excitations above the AKLT state using a single-mode approximation.³ Following these developments the AKLT model was widely used to study general properties of spin-1 chains, for example the appearance of hidden string order⁶ and a $\mathbb{Z}_2 \times \mathbb{Z}_2$ -symmetry breaking in the Haldane phase.⁷ This success has also motivated the study of q -deformed AKLT chains,⁸ as well as $SU(n)$ generalizations of the VBS construction.^{9,10} Very recently, Tu *et al.*¹¹ extended the investigation of hidden string order to $SO(n)$ symmetric Hamiltonians.

Another important invention was the formulation of generalized VBS states in terms of finitely correlated or matrix product states,^{12,13} which in particular allows the relatively easy calculation of correlation functions. Östlund and Rommer¹⁴ showed that the wave functions appearing in the density matrix renormalization group (DMRG) method¹⁵ are represented by matrix product states. Since then DMRG algorithms, which make direct use of the matrix product state formulation, have been developed.¹⁶

On the other hand, large- n techniques based on symplectic symmetry were introduced by Read and Sachdev¹⁷ to study frustrated antiferromagnets on a square lattice. If one places symplectic spins transforming under a given representation of $SP(n)$ on an arbitrary lattice, it is always possible to form singlet bonds between any two sites. This is not true for unitary spins transforming under $SU(n)$, where the formation of singlets is in general only possible on bonds between a representation and their complex conjugate representation. This restricts the applicability of $SU(n)$ techniques to bipartite lattices. The $SP(n)$ technique was afterwards widely used

to study frustrated antiferromagnets on various lattices,¹⁸ doped antiferromagnets,¹⁹ paired Fermi gases,²⁰ stripes in high-temperature superconductors,²¹ and heavy-fermion systems.²² Recently, Flint *et al.*²³ introduced the “symplectic- n ” approach, which links time reversal and symplectic symmetry of spins by eliminating unwanted dipole moment operators in the decoupling procedure. This enabled the treatment of superconductivity on an equal footing with the Kondo effect. Moreover, Wu *et al.*²⁴ pointed out that the model of ultracold spin-3/2 fermions with contact interaction enjoys a generic $SP(4)$ symmetry, which led to further applications of the symplectic symmetry in the context of ultracold fermionic gases.²⁵

In this paper we will combine these aspects and generalize the VBS state to symplectic symmetry. We derive an exact parent Hamiltonian and argue that there exists a finite gap in the excitation spectrum. We then use the representation of the VBS state in terms of a matrix product state to calculate the static correlation functions and the expectation values of various string operators. Finally we discuss the VBS state and possible parent Hamiltonians on higher-dimensional lattices.

II. SYMPLECTIC SYMMETRY

One of the key features of the group $SU(2)$ is that two spins of arbitrary length S can always combine into a singlet, which is an essential condition for a proper description of frustrated antiferromagnetism. The analog statement is not true for spins transforming under $SU(n)$ with $n \geq 3$, where one has to deal with the tensor product of a representation and its complex conjugate one in order to form a singlet. In the language of antiferromagnetism this requires a bipartite lattice structure where one can place spins transforming under one representation of $SU(n)$ on one sublattice and the complex conjugated spins on the other sublattice. One way to overcome this problem¹⁷ is the generalization of $SU(2)$ spins to spins transforming under the symplectic group $SP(n)$, for which the formation of a singlet from two spins is always possible.

The symplectic group $SP(n)$ is the set of all unitary $n \times n$ -matrices U such that^{26,27}

$$U^t U = I, \quad (1)$$

where t denotes the transposed matrix and

TABLE I. Simplest irreducible representations of $SP(n)$, their dimensions, and the eigenvalues of the quadratic Casimir operator J^2 . We note that the representations $(110\dots 0)$, $(220\dots 0)$, and $(310\dots 0)$ do not exist for $SP(2) \cong SU(2)$. In this case the remaining representations are the singlet 0, the spinor representation $\frac{1}{2}$, the triplet 1, and the spin-2 representation 2.

Irreducible representation	dimension	Eigenvalue of J^2
$(00\dots 0)$	1	0
$(10\dots 0)$	n	$\frac{n+1}{4}$
$(110\dots 0)$	$\frac{1}{2}(n-2)(n+1)$	$\frac{n}{2}$
$(20\dots 0)$	$\frac{n}{2}(n+1)$	$\frac{n+2}{2}$
$(220\dots 0)$	$\frac{n}{12}(n-2)(n-1)(n+3)$	$n+1$
$(310\dots 0)$	$\frac{n}{8}(n-2)(n+1)(n+3)$	$n+2$
$(40\dots 0)$	$\frac{n}{24}(n+1)(n+2)(n+3)$	$n+4$

$$I = \begin{pmatrix} 0 & 1 & \cdots & 0 & 0 \\ -1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & -1 & 0 \end{pmatrix}. \quad (2)$$

As the matrix I is built up from blocks of 2×2 matrices, n has to be even. The generators of $SP(n)$, which we denote by A^a , $a=1, \dots, n(n+1)/2$, have to satisfy

$$(A^a)^t I + I A^a = 0. \quad (3)$$

The elements in the group are obtained by $U = \exp(i \sum_a \theta_a A^a)$ with real parameters θ_a . The matrices A^a play the same role as the Pauli matrices for $SU(2)$ and equal them in the case $n=2$. Hence there exists an isomorphism between $SP(2)$ and $SU(2)$; in particular the representations of $SP(2)$ equal those of $SU(2)$. An explicit representation of the matrices A^a for $SP(4)$ is given in Appendix A. The irreducible representations of $SP(n)$ can be labeled²⁶ by $(\lambda_1 \dots \lambda_{n/2})$, where the non-negative integers λ_i have to satisfy $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{n/2}$. Explicit formulas for the dimensions of the irreducible representations, the eigenvalues of the quadratic Casimir operator, and results on the decomposition of tensor products of irreducible representations are stated in Appendix B. In Table I we have tabulated these properties for those irreducible representations which we will use to construct the VBS chain below.

As a side note we mention that the symplectic group $SP(n)$ naturally arises in Hamiltonian mechanics.²⁸ The n -dimensional phase space M contains the generalized coordinates $q_1, \dots, q_{n/2}$ and their conjugated momenta $p_1, \dots, p_{n/2}$, which implies that n has to be even. The Hamiltonian $H: M \rightarrow \mathbb{R}$ induces the time evolution via its vector field. The phase space is equipped with a skew scalar product on its cotangent bundle T^*M , i.e., a bilinear map $\langle \cdot, \cdot \rangle: T^*M \times T^*M \rightarrow \mathbb{R}$, which satisfies $\langle x, y \rangle = -\langle y, x \rangle$. This skew scalar product defines a volume element on the phase space. The symplectic group is now the set of all linear transformation under which this skew scalar product is invariant.

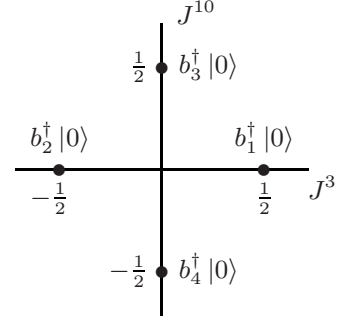


FIG. 1. Weight diagram of the fundamental representation of $SP(4)$. The states are labeled using the bosonic creation operators introduced in Eq. (4). J^3 and J^{10} denote the diagonal spin operators, their eigenvalues are easily obtained using Eq. (6).

In particular, the time evolution generated by the Hamiltonian is a symplectic transformation, which implies for example Liouville's theorem.

III. DIMER CHAIN

As a warmup exercise we first construct the $SP(n)$ generalization of the Majumdar-Ghosh model.²⁹ Let us consider a chain with N lattice sites and periodic boundary conditions, where we assume N to be even. On each lattice site we place an $SP(n)$ spin transforming under the fundamental n -dimensional representation $(10\dots 0)$. A basis at each lattice site i may be written in terms of bosonic creation and annihilation operators $b_{\sigma,i}^\dagger$ and $b_{\sigma,i}$ as³⁰

$$|\sigma\rangle_i = b_{\sigma,i}^\dagger |0\rangle_i, \quad \sigma = 1, \dots, n, \quad (4)$$

where $|0\rangle_i$ denotes the vacuum at site i . The weight diagram of the fundamental representation of $SP(4)$ is shown in Fig. 1. The action of the $SP(n)$ spin operators J^a on these basis states is given by

$$J_i = \frac{1}{2} \sum_{\sigma, \sigma'=1}^n b_{\sigma,i}^\dagger \mathbf{A}_{\sigma\sigma'} b_{\sigma',i}, \quad (5)$$

where we have introduced the vector notation $\mathbf{J} = (J^1, \dots, J^{n(n+1)/2})^t$. The eigenvalue of the quadratic Casimir operator on each lattice site equals $J_i^2 = (n+1)/4$. Using the explicit expressions for the generators of $SP(4)$ given in Appendix A, one finds for example

$$J_i^1 = \frac{1}{2}(b_{1,i}^\dagger b_{2,i} + b_{2,i}^\dagger b_{1,i}), \quad J_i^2 = \frac{i}{2}(b_{2,i}^\dagger b_{1,i} - b_{1,i}^\dagger b_{2,i}),$$

$$J_i^3 = \frac{1}{2}(b_{1,i}^\dagger b_{1,i} - b_{2,i}^\dagger b_{2,i}),$$

$$J_i^4 = \frac{1}{\sqrt{8}}(b_{1,i}^\dagger b_{4,i} + b_{2,i}^\dagger b_{3,i} + b_{3,i}^\dagger b_{2,i} + b_{4,i}^\dagger b_{1,i}),$$

$$J_i^5 = \frac{i}{\sqrt{8}}(b_{4,i}^\dagger b_{1,i} - b_{3,i}^\dagger b_{2,i} + b_{2,i}^\dagger b_{3,i} - b_{1,i}^\dagger b_{4,i}),$$

$$\begin{aligned}
 J_i^6 &= \frac{1}{\sqrt{8}}(b_{1,i}^\dagger b_{3,i} - b_{2,i}^\dagger b_{4,i} + b_{3,i}^\dagger b_{1,i} - b_{4,i}^\dagger b_{2,i}), \\
 J_i^7 &= \frac{i}{\sqrt{8}}(b_{1,i}^\dagger b_{3,i} + b_{2,i}^\dagger b_{4,i} - b_{3,i}^\dagger b_{1,i} - b_{4,i}^\dagger b_{2,i}), \\
 J_i^8 &= \frac{1}{2}(b_{3,i}^\dagger b_{4,i} + b_{4,i}^\dagger b_{3,i}), \quad J_i^9 = \frac{i}{2}(b_{4,i}^\dagger b_{3,i} - b_{3,i}^\dagger b_{4,i}), \\
 J_i^{10} &= \frac{1}{2}(b_{3,i}^\dagger b_{3,i} - b_{4,i}^\dagger b_{4,i}). \quad (6)
 \end{aligned}$$

We stress that the operators J^1 , J^2 , and J^3 as well as J^8 , J^9 , and J^{10} span two copies of the usual spin algebra $SU(2)$.

On this $SP(n)$ chain we consider the two linearly independent states represented by

$$\begin{aligned}
 | \circ - \circ \quad \circ - \circ \quad \circ - \circ \quad \circ - \circ \rangle & \quad \text{“odd”}, \\
 | \circ - \circ \quad \circ - \circ \quad \circ - \circ \quad \circ - \circ \rangle & \quad \text{“even”}, \quad (7)
 \end{aligned}$$

where the symbol $\circ - \circ$ stands for an $SP(n)$ singlet or dimer formed by the spins on two neighboring lattice sites. In the state labeled as “odd” the $SP(n)$ singlets are located on the bonds $(2i-1, 2i)$, whereas in the state labeled as “even” the $SP(n)$ singlets are located on the bonds $(2i, 2i+1)$. In the “even” state the right- and left-most spins also form an $SP(n)$ singlet due to the assumed periodic boundary conditions. In order to construct a parent Hamiltonian, i.e., a Hamiltonian which has the two states [Eq. (7)] as its unique ground states, we note that the total $SP(n)$ spin on each three neighboring sites has to contain a singlet and thus transforms under the fundamental representation $(10\dots 0)$. Hence, for all lattice sites i the operator $(\mathbf{J}_i + \mathbf{J}_{i+1} + \mathbf{J}_{i+2})^2 - (n+1)/4$ annihilates the dimer states [Eq. (7)], and by taking the sum over all lattice sites we arrive at

$$H_{\text{dimer}} = \sum_{i=1}^N \left(\mathbf{J}_i \mathbf{J}_{i+1} + \frac{1}{2} \mathbf{J}_i \mathbf{J}_{i+2} + \frac{n+1}{8} \right). \quad (8)$$

We have checked numerically for $n=4$ and $N=8$ that model (8) possesses exactly two zero-energy ground states. For $n=2$ one obtains the original Majumdar-Ghosh model.²⁹

IV. VBS CHAIN

In this section we construct the $SP(n)$ VBS state on a chain and derive the corresponding parent Hamiltonian. In Secs. V–VII we will then discuss the excitations above the VBS state, its static correlation functions, and the appearance of string order.

Let us consider again a chain with N lattice sites and periodic boundary conditions, but now N may be even or odd. At each lattice site we place two copies of the fundamental representation $(10\dots 0)$, i.e., we obtain the tensor product (the decomposition of tensor products in irreducible representations was derived in Refs. 31 and 32 and is presented in Appendix B)

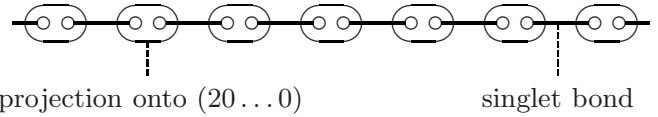


FIG. 2. Graphical representation of the VBS state $|\Psi_{\text{VBS}}\rangle$, the unique ground state of Eq. (12). Each circle stands for a fundamental representation $(10\dots 0)$, each line joining two circles for a singlet bond, and each oval for a lattice site on which we project onto the adjoint representation $(20\dots 0)$.

$$(10\dots 0) \otimes (10\dots 0) = (20\dots 0) \oplus (110\dots 0) \oplus (0\dots 0). \quad (9)$$

We note that for $n=2$ the representation $(110\dots 0)$ does not exist and we recover $\frac{1}{2} \otimes \frac{1}{2} = \mathbf{1} \oplus \mathbf{0}$. In the tensor product [Eq. (9)] we now project onto the adjoint, $n(n+1)/2$ -dimensional representation $(20\dots 0)$. An explicit basis for this representation can be constructed³⁰ from the bosonic basis of the fundamental representation (4). For $n=4$ this basis will be stated explicitly in Sec. VI. With this procedure we construct a chain of adjoint representations, which is the direct generalization of a spin-1 chain for $SU(2)$. If we consider the total $SP(n)$ spin of two neighboring sites we find the decomposition

$$\begin{aligned}
 (20\dots 0) \otimes (20\dots 0) &= (40\dots 0) \oplus (310\dots 0) \\
 &\oplus (220\dots 0) \oplus (20\dots 0) \\
 &\oplus (110\dots 0) \oplus (0\dots 0). \quad (10)
 \end{aligned}$$

For $n=2$ the second, third, and fifth representation on the right-hand side do not exist and Eq. (10) simplifies to $\mathbf{1} \otimes \mathbf{1} = \mathbf{2} \oplus \mathbf{1} \oplus \mathbf{0}$.

Starting with such a chain of adjoint representations, we can construct the VBS state as follows: We form a singlet between one of the fundamental representations $(10\dots 0)$ on lattice site i with one of the $(10\dots 0)$'s on the neighboring site $i-1$, while we form another singlet with the second representation $(10\dots 0)$ on lattice site i with one of the $(10\dots 0)$'s on the neighboring site $i+1$. We stress that the formation of these singlets is imposed in addition to the already implemented projection onto the adjoint representation at each lattice site. If we further impose periodic boundary conditions this yields a unique VBS state $|\Psi_{\text{VBS}}\rangle$, which is translationally invariant and can be represented graphically as shown in Fig. 2.

The parent Hamiltonian for the VBS state is constructed by noting that on each two neighboring sites in the VBS state, we find one singlet and two uncoupled fundamental representations. Hence, the total $SP(n)$ spin on two neighboring sites is given by the tensor product $(10\dots 0) \otimes (10\dots 0)$ given in Eq. (9). If we construct an operator which is identical to zero on Eq. (9) but takes strictly positive values on the complement of Eq. (9) in $(20\dots 0) \otimes (20\dots 0)$, we will obtain the VBS state as zero-energy ground state. This operation is most easily implemented using the quadratic Casimir operator $(\mathbf{J}_i + \mathbf{J}_{i+1})^2$ on the bond $(i, i+1)$, which takes the values $(n+2)/2$, $n/2$, and 0 on the representations in

Eq. (9) and $n+4$, $n+2$, and $n+1$ on the remaining representations in Eq. (10), respectively. Explicitly we will use on each bond $(i, i+1)$

$$P_{i,i+1} = \frac{1}{n} \frac{2}{5n^2 + 26n + 32} [(J_i + J_{i+1})^2] \times \left[(J_i + J_{i+1})^2 - \frac{n+2}{2} \right] \left[(J_i + J_{i+1})^2 - \frac{n}{2} \right]. \quad (11)$$

We stress that the operators $P_{i,i+1}$ are not simple projectors as $P_{i,i+1}$ takes different values on the subspaces $(220\dots 0)$, $(310\dots 0)$, and $(40\dots 0)$. We note that for $n=2$ the last factor in Eq. (11) is not necessary as the corresponding representation $(110\dots 0)$ does not exist. The normalization of $P_{i,i+1}$ is chosen in order to obtain a finite expectation value for the energy of each individual bond in the limit $n \rightarrow \infty$. In this limit the operator [Eq. (11)] becomes an orthogonal projector (up to the multiplicative constant $1/10$) onto the complement of Eq. (9) in Eq. (10). The parent Hamiltonian for the VBS state $|\Psi_{\text{VBS}}\rangle$ is now obtained by $H = \sum_i P_{i,i+1}$, together with $J_i^2 = (n+2)/2$,

$$H = \frac{1}{n} \sum_{i=1}^N \left[J_i J_{i+1} + \frac{16n+40}{5n^2+26n+32} (J_i J_{i+1})^2 + \frac{16}{5n^2+26n+32} (J_i J_{i+1})^3 + \frac{n^2+6n+8}{10n+32} \right]. \quad (12)$$

Here the operators J_i^a live in the adjoined representation and can be represented by $n(n+1)/2 \times n(n+1)/2$ matrices. As the operator [Eq. (11)] takes strictly positive values on $(220\dots 0)$, $(310\dots 0)$, and $(40\dots 0)$, all states except the VBS state are lifted to higher energies. We have checked numerically for $n=4$ and $N=3$ that the VBS state is the unique ground state of Eq. (12). A proof of the uniqueness can be obtained by generalizing the proof of the uniqueness of the ground state of the q -deformed VBS model.⁸ The Hamiltonian contains cubic terms as we had to use three factors in the operators [Eq. (11)]. As explained above the third factor is superfluous for $n=2$, omitting it yields the original AKLT model.¹ By keeping the third factor, however, we obtain an alternative parent Hamiltonian for the spin-1 VBS state.

The VBS construction described above can also be done for a chain with open boundary conditions. In this case we are left with one uncoupled fundamental representation at each end of the chain and we hence find n^2 linearly independent VBS states. The parent Hamiltonian for these states is given by Eq. (12) with the summation restricted to $1 \leq i \leq N-1$.

V. EXCITATIONS AND ENERGY GAP

The Hamiltonian [Eq. (12)] was constructed to be the exact parent Hamiltonian for the VBS state $|\Psi_{\text{VBS}}\rangle$. Although its ground state is known in all detail it is much harder to get results on the excitations above it. The simplest operation on the state $|\Psi_{\text{VBS}}\rangle$ one can imagine is to break one of the singlets, say the singlet on the bond $(i, i+1)$. Doing so we find two uncoupled $\text{SP}(n)$ spins, each transforming under the fun-

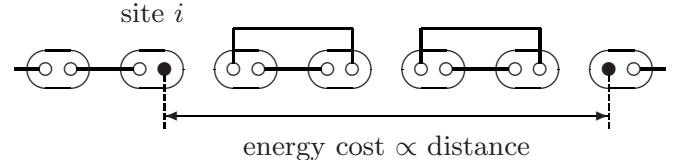


FIG. 3. If two spins (represented by the full circles) move apart from each other, the region between them will not have the same structure as in the ground state [we have sketched one way of how the $\text{SP}(n)$ spins may rearrange into singlets]. This causes an energy cost proportional to their distance and results in spinon confinement.

damental representation, which we will call spinons in the following. The resulting state is clearly not an eigenstate of Eq. (12). Nevertheless, the spinons are useful to perform the following Gedankenexperiment: Let us pin the first spinon at site i and move the other spinon to the right (see Fig. 3). The region between them has now a different structure than the ground state and is not annihilated by Eq. (12). As the energy cost grows linearly with the distance, the spinons are subject to a linear confinement potential and hence can only appear in bound states. The relative motion of the spinons will be described by a nonharmonic oscillator whose zero-point energy yields a finite gap for the creation of spinon-spinon bound states. This is consistent with the picture that the origin of the Haldane gap is a confinement force between spinons.^{10,33} A similar argumentation was applied by Greiter³⁴ to the excitations of the two-leg t - J ladder. Although this Gedankenexperiment suggests the appearance of an energy gap, we stress that the spinon bound states may not constitute good trial wave functions for the actual low-lying excitations in the model.

A possible way to prove the existence of a gap above the ground state is provided by the extension of results by Knabe³⁵ on a class of $\text{SU}(2)$ VBS Hamiltonians including the original AKLT model (details of the derivation are given in Appendix C). Let us consider a Hamiltonian of the form

$$H = \sum_{i=1}^N P_{i,i+1} \quad (13)$$

with periodic boundary conditions. We assume that $0 \leq P_{i,i+1} \leq 1$, as well as the existence of at least one zero-energy ground state of Eq. (13). The idea is to establish the inequality

$$H^2 \geq \epsilon H, \quad \epsilon > 0, \quad (14)$$

which implies that the lowest nonvanishing eigenvalue of H is larger than ϵ . As we show in Appendix C, Eq. (14) can be derived if the same model on a chain with $m+1$ sites and open boundary conditions satisfies

$$h_{i,m}^2 \geq \epsilon_m h_{i,m}, \quad \epsilon_m > \frac{1}{m}, \quad (15)$$

where $m \geq 2$ and

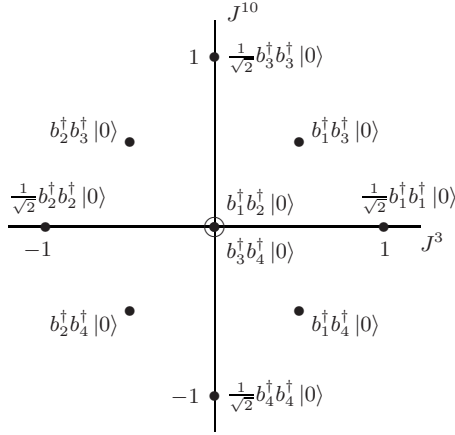


FIG. 4. Weight diagram of the adjoint representation of $SP(4)$. The state with $J^3=J^{10}=0$ is doubly degenerate. The states are labeled using the bosonic creation operators as in Eq. (17).

$$h_{i,m} = \sum_{k=i}^{i+m-1} P_{k,k+1}. \quad (16)$$

Hence the proof is finished if we can show that Eq. (15) is satisfied for a suitable integer m . This was achieved in Ref. 35 for $SU(2)$ VBS chains with spins $S=1, 3/2, 2$, and $5/2$ on each lattice site. Unfortunately, exact diagonalization of the $SP(4)$ model [Eq. (12)] with open boundary conditions for $m=2$ suggests that in order to establish the inequality $\epsilon_m > 1/m$, one has to study chains with at least ten lattice sites.

VI. STATIC CORRELATION FUNCTIONS

The VBS state $|\Psi_{\text{VBS}}\rangle$ can be written as a matrix product state. We will restrict ourselves to the case $n=4$ in the following. A suitable basis for the adjoint representation of $SP(4)$ at lattice site i can be obtained from the bosonic basis of the fundamental representation introduced above as³⁰

$$\begin{aligned} & \frac{1}{\sqrt{2}} b_{1,i}^\dagger b_{1,i}^\dagger |0\rangle_i, \quad \frac{1}{\sqrt{2}} b_{2,i}^\dagger b_{2,i}^\dagger |0\rangle_i, \quad b_{1,i}^\dagger b_{2,i}^\dagger |0\rangle_i, \\ & b_{1,i}^\dagger b_{3,i}^\dagger |0\rangle_i, \quad b_{1,i}^\dagger b_{4,i}^\dagger |0\rangle_i, \quad b_{2,i}^\dagger b_{3,i}^\dagger |0\rangle_i, \quad b_{2,i}^\dagger b_{4,i}^\dagger |0\rangle_i, \\ & \frac{1}{\sqrt{2}} b_{3,i}^\dagger b_{3,i}^\dagger |0\rangle_i, \quad \frac{1}{\sqrt{2}} b_{4,i}^\dagger b_{4,i}^\dagger |0\rangle_i, \quad b_{3,i}^\dagger b_{4,i}^\dagger |0\rangle_i. \end{aligned} \quad (17)$$

We have illustrated these basis states in the weight diagram of the adjoint representation shown in Fig. 4.

In order to derive the matrix product representation we first rewrite the singlet on the bond $(i, i+1)$ as

$$\begin{aligned} & b_{1,i}^\dagger b_{2,i+1}^\dagger - b_{2,i}^\dagger b_{1,i+1}^\dagger + b_{3,i}^\dagger b_{4,i+1}^\dagger - b_{4,i}^\dagger b_{3,i+1}^\dagger \\ & = (b_{1,i}^\dagger, b_{2,i}^\dagger, b_{3,i}^\dagger, b_{4,i}^\dagger) \begin{pmatrix} b_{2,i+1}^\dagger \\ -b_{1,i+1}^\dagger \\ b_{4,i+1}^\dagger \\ -b_{3,i+1}^\dagger \end{pmatrix}. \end{aligned} \quad (18)$$

Second, at each lattice site i we use the outer product to combine the two vectors originating from rewriting Eq. (18) on the bonds $(i-1, i)$ and $(i, i+1)$ into a matrix

$$\begin{aligned} M_i &= \begin{pmatrix} b_{2,i}^\dagger \\ -b_{1,i}^\dagger \\ b_{4,i}^\dagger \\ -b_{3,i}^\dagger \end{pmatrix} (b_{1,i}^\dagger, b_{2,i}^\dagger, b_{3,i}^\dagger, b_{4,i}^\dagger) |0\rangle_i \\ &= \begin{pmatrix} b_{1,i}^\dagger b_{2,i}^\dagger & b_{2,i}^\dagger b_{2,i}^\dagger & b_{2,i}^\dagger b_{3,i}^\dagger & b_{2,i}^\dagger b_{4,i}^\dagger \\ -b_{1,i}^\dagger b_{1,i}^\dagger & -b_{1,i}^\dagger b_{2,i}^\dagger & -b_{1,i}^\dagger b_{3,i}^\dagger & -b_{1,i}^\dagger b_{4,i}^\dagger \\ b_{1,i}^\dagger b_{4,i}^\dagger & b_{2,i}^\dagger b_{4,i}^\dagger & b_{3,i}^\dagger b_{4,i}^\dagger & b_{4,i}^\dagger b_{4,i}^\dagger \\ -b_{1,i}^\dagger b_{3,i}^\dagger & -b_{2,i}^\dagger b_{3,i}^\dagger & -b_{3,i}^\dagger b_{3,i}^\dagger & -b_{3,i}^\dagger b_{4,i}^\dagger \end{pmatrix} |0\rangle_i. \end{aligned} \quad (19)$$

Assuming periodic boundary conditions the VBS state can then be written as the trace of the matrix product

$$|\Psi_{\text{VBS}}\rangle = \text{tr} \left(\prod_{i=1}^N M_i \right). \quad (20)$$

Starting from this representation the static correlation functions in the $SP(4)$ VBS state can be calculated by applying the method introduced by Klümper *et al.*⁸ for the analysis of the q -deformed model. As the first step we calculate the norm of the VBS state. This is done by introducing the complex conjugated matrix \tilde{M} according to $\tilde{M}_{\sigma\sigma'} = M_{\sigma\sigma'}^*$, i.e., by simply taking the complex conjugate of each matrix element in Eq. (19) without transposing the matrix. We then define the 16×16 transfer matrix R at any lattice site as

$$R_{\alpha\beta} = R_{(\sigma\tau),(\sigma'\tau')} = \tilde{M}_{\sigma\sigma'} M_{\tau\tau'}, \quad (21)$$

where we order the indices as $\alpha, \beta = 1, \dots, 16 \leftrightarrow (11), (12), \dots, (44)$. The norm of the VBS state is now given by

$$\langle \Psi_{\text{VBS}} | \Psi_{\text{VBS}} \rangle = \text{tr}(R^N) = 5^N + 10(-1)^N + 5, \quad (22)$$

where we have evaluated the trace by diagonalization of R . In the second step we calculate the expectation value $\langle \Psi_{\text{VBS}} | J_1^3 J_j^3 | \Psi_{\text{VBS}} \rangle$. We introduce the transfer-matrix representation of the spin operators J^3 by

$$\hat{J}_{\alpha\beta} = \hat{J}_{(\sigma\tau),(\sigma'\tau')} = \tilde{M}_{\sigma\sigma'} J^3 M_{\tau\tau'}. \quad (23)$$

Here the operator J^3 acts on the elements of M as

$$J^3 b_1^\dagger = \frac{1}{2} b_1^\dagger, \quad J^3 b_2^\dagger = -\frac{1}{2} b_2^\dagger, \quad J^3 b_3^\dagger = J^3 b_4^\dagger = 0, \quad (24)$$

which implies for example $J^3 b_1^\dagger b_2^\dagger = 0$. This yields

$$\langle \Psi_{\text{VBS}} | J_1^3 J_j^3 | \Psi_{\text{VBS}} \rangle = \text{tr}(J_1 R^{j-2} J_j R^{N-j}), \quad (25)$$

which is easily evaluated by diagonalization of R . As the state $|\Psi_{\text{VBS}}\rangle$ enjoys full $SP(4)$ symmetry, we arrive at

$$\begin{aligned} \langle J_1^a J_j^b \rangle &\equiv \frac{\langle \Psi_{\text{VBS}} | J_1^a J_j^b | \Psi_{\text{VBS}} \rangle}{\langle \Psi_{\text{VBS}} | \Psi_{\text{VBS}} \rangle} \\ &= -\delta_{ab} (-1)^j \frac{9}{10} \frac{5^{-j+1} + \frac{1}{5} \frac{(-1)^N}{5^{N-j}} + \frac{1}{3} \frac{(-1)^N + 1}{5^{N-1}}}{1 + \frac{1}{5^{N-1}} [2(-1)^N + 1]}. \end{aligned} \quad (26)$$

In the general case of $\text{SP}(n)$ the same steps yield in the thermodynamic limit $N \rightarrow \infty$

$$\langle J_1^a J_j^b \rangle \propto \frac{\delta_{ab}}{(n+1)^{j-1}} \sim e^{-j/\xi}. \quad (27)$$

Here the correlation length is given by $\xi = 1/\ln(n+1)$ and vanishes in the limit $n \rightarrow \infty$. We also recover the known result for the AKLT chain.¹

VII. STRING ORDER

It is well known⁶ that there exists a hidden nonlocal topological order or string order in the AKLT model. In fact, this order is found in the whole Haldane phase in the phase diagram of the general spin-1 chain. This string order was further associated with the breaking of a $\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetry in the Haldane phase and the appearance of a fourfold degenerate ground state on the open chain.⁷ We will find a similar behavior in the $\text{SP}(n)$ VBS model.

In analogy to Refs. 6 we define the string operators

$$O_{1j}^{ab} = -J_1^a \exp\left(i\pi \sum_{k=2}^{j-1} \sum_c J_k^c\right) J_j^b, \quad (28)$$

where the second sum is over all c for which J_k^c is diagonal, and J_1^a and J_j^b have to be diagonal as well. In the $\text{SP}(4)$ model the summation is over $c=3, 10$ and we have $a, b \in \{3, 10\}$. Using the transfer-matrix technique we obtain in the thermodynamic limit $N \rightarrow \infty$

$$\begin{aligned} \langle O_{1j}^{33} \rangle &= \langle O_{1j}^{10,10} \rangle = \frac{9}{100} \left(1 + \frac{25}{5^j}\right), \\ \langle O_{1j}^{3,10} \rangle &= \langle O_{1j}^{10,3} \rangle = \frac{9}{100} \left(1 - \frac{25}{5^j}\right), \end{aligned} \quad (29)$$

which remain finite for arbitrary large values of j . In particular, the sum over all four expectation values [Eq. (29)] is independent of j . In analogy to the original AKLT model we expect this hidden string order, as well as the 16-fold degeneracy of the ground state of a chain with open boundary conditions, to be a consequence of the breaking of a discrete symmetry.

We have also calculated the expectation values of the nine string operators [Eq. (28)] in the $\text{SP}(6)$ model. Together with Eq. (29) and the result⁶ for $\text{SU}(2)$ this leads us to the conjecture for general n :

$$\langle O_{1j}^{aa} \rangle = \frac{\left(\frac{n}{2} + 1\right)^2}{\left[\frac{n}{2}(n+1)\right]^2} \left(1 + \frac{\frac{n}{2} - 1}{(n+1)^{j-2}}\right),$$

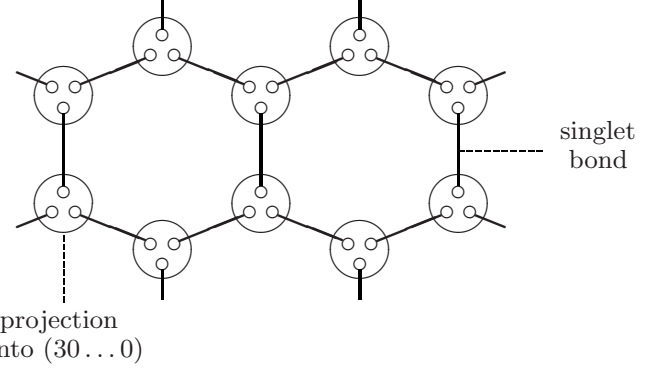


FIG. 5. Graphical representation of the VBS state on a hexagonal lattice. Each small circle represents a fundamental representation $(10\dots 0)$, each line joining two circles for a singlet bond, and each large circle a lattice site on which we project onto the representation $(30\dots 0)$.

$$\langle O_{1j}^{ab} \rangle = \frac{\left(\frac{n}{2} + 1\right)^2}{\left[\frac{n}{2}(n+1)\right]^2} \left[1 - \frac{1}{(n+1)^{j-2}}\right], \quad a \neq b. \quad (30)$$

Although each of the expectation values [Eq. (30)] vanishes in the limit $n \rightarrow \infty$, the number of string operators increases and one obtains

$$\sum_{a,b} \langle O_{1j}^{ab} \rangle = \frac{1}{4} \left(\frac{n+2}{n+1}\right)^2 \rightarrow \frac{1}{4}, \quad n \rightarrow \infty, \quad (31)$$

where the sum is over all a and b for which J^a and J^b are diagonal. We note that Eq. (31) can be written elegantly as a single string operator by replacing J_1^a and J_j^b in Eq. (28) by the sum over all diagonal generators $\sum_c J_{1,j}^c$, respectively.

VIII. TWO-DIMENSIONAL VBS MODEL

Finally we would like to discuss the VBS construction on higher-dimensional lattices. The simplest example is provided by the honeycomb lattice (with coordination number $z=3$) with representations $(30\dots 0)$ on each lattice site. The VBS state is obtained by placing three fundamental representations on each lattice site and projecting onto the representation $(30\dots 0)$, as well as forming a singlet of each one of them with a fundamental representation, on a neighboring site (see Fig. 5). Hence, on each bond we obtain a singlet formed in this way and four uncoupled fundamental representations. The corresponding tensor product decomposes as

$$\begin{aligned} (10\dots 0)^{\otimes 4} &= (40\dots 0) \oplus 3 \cdot (310\dots 0) \oplus 2 \cdot (220\dots 0) \\ &\oplus 3 \cdot (2110\dots 0) \oplus 6 \cdot (20\dots 0) \\ &\oplus (11110\dots 0) \oplus 6 \cdot (110\dots 0) \oplus 3 \cdot (0\dots 0). \end{aligned} \quad (32)$$

Since this tensor product contains in general eight different irreducible representations, the ‘‘projection’’ operator analog to Eq. (11) and hence the Hamiltonian contains the bond operators $(\mathbf{J}_i \mathbf{J}_j)^k$ with a power up to $k=8$. For the cases $n=2, 4$, and 6 , however, some representations on the right-hand side of Eq. (32) do not exist and one obtains powers up

to $k=3, 6$, and 7 , respectively. The explicit construction of the analog $SU(2)$ model with $S=3/2$ spins on the lattice sites can be found in Refs. 1. It is clear from the arguments above that the VBS construction on lattices with larger coordination number or in higher dimensions will lead to a parent Hamiltonian, which contains even higher powers of the bond operators $(\mathbf{J}_i \mathbf{J}_j)^k$.

IX. CONCLUSIONS

In conclusion, we have introduced a spin chain with symplectic symmetry $SP(n)$, which shares all properties of the Haldane scenario for integer-spin quantum antiferromagnets: (i) a unique ground state, (ii) a finite gap in the energy spectrum above the ground state, and (iii) ground-state correlation functions which fall off exponentially. Furthermore we have shown that the ground state possesses string order. We point out that in the limit $n \rightarrow \infty$ the string order remains finite and the correlation length vanishes. The application of the large- n approach to the considered models might be an interesting extension of this work.

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APPENDIX A: EXPLICIT REPRESENTATIONS FOR $SP(4)$

An explicit representation of the generators of $SP(4)$ is provided by

$$\begin{aligned}
 A^1 &= \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, & A^2 &= \begin{pmatrix} 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \\
 A^3 &= \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, & A^4 &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \\
 A^5 &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix}, & A^6 &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \\
 A^7 &= \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \\ -i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}, & A^8 &= \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix},
 \end{aligned}$$

$$A^9 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}, \quad A^{10} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

The normalization is chosen to be

$$\text{tr}(A^a A^b) = 2 \delta_{ab}. \quad (\text{A1})$$

The matrices A^a , $a=1, \dots, 10$, form a basis of $\mathfrak{sp}(4)$, the Lie algebra of $SP(4)$. They satisfy the commutation relations

$$[A^a, A^b] = 2f^{abc} A^c. \quad (\text{A2})$$

The structure constants f^{abc} are totally antisymmetric and obey Jacobi's identity

$$f^{abc} f^{cde} + f^{bcd} f^{cae} + f^{dac} f^{cbe} = 0. \quad (\text{A3})$$

Explicitly, all 84 nonvanishing structure constants are obtained by permutations of the indices from

$$f^{123} = f^{89,10} = i,$$

$$f^{156} = f^{345} = f^{45,10} = f^{478} = f^{568} = f^{579} = f^{67,10} = \frac{i}{2},$$

$$f^{147} = f^{246} = f^{257} = f^{367} = f^{469} = -\frac{i}{2}. \quad (\text{A4})$$

$\mathfrak{sp}(4)$ has rank two, the Cartan subalgebra is spanned by A^3 and A^{10} . We note that $\mathfrak{sp}(2) \cong \mathfrak{su}(2)$ and $\mathfrak{sp}(4) \cong \mathfrak{so}(5)$. A possible matrix representation of the spin operators in the adjoint representation is given by $(J^a)_{bc} = f^{abc}$. However, we stress that these matrices are not the representation matrices in the bosonic basis [Eq. (17)].

APPENDIX B: SOME RESULTS ON THE REPRESENTATION THEORY OF $SP(n)$

In this appendix we review some results on the representation theory of $SP(n)$. First, the dimension of the irreducible representation $(\lambda_1 \dots \lambda_{n/2})$ is given by the formula²⁶

$$\begin{aligned}
 \dim[(\lambda_1 \dots \lambda_{n/2})] &= \prod_{i=1}^{n/2} \frac{\lambda_i + \frac{n}{2} - i + 1}{\frac{n}{2} - i + 1} \prod_{\substack{i,j=1 \\ i < j}}^{n/2} \frac{\lambda_i - \lambda_j + j - i}{j - i} \\
 &\quad \times \frac{\lambda_i + \lambda_j + n + 2 - i - j}{n + 2 - i - j}. \quad (\text{B1})
 \end{aligned}$$

Second, the eigenvalues of the quadratic Casimir operator J^2 were derived by Nwachuku and Rashid³⁶ and read using our conventions

$$J^2 = \frac{1}{8} \sum_{\substack{i=-n/2 \\ i \neq 0}}^{n/2} \kappa_i^2 \frac{\kappa_i - \frac{n}{2} - 1}{\kappa_i - \frac{n}{2} - \frac{1}{2}} \prod_{\substack{j=-n/2 \\ j \neq 0, i}}^{n/2} \left(1 - \frac{1}{\kappa_i - \kappa_j} \right), \quad (\text{B2})$$

where for $1 \leq i \leq n/2$

$$\kappa_i = \frac{n}{2} + i + \lambda_{n/2+1-i}, \quad \kappa_{-i} = n - \kappa_i. \quad (\text{B3})$$

The following special cases allow a closed expression:

$$(\nu 0 \dots 0): \frac{\nu}{4}(n + \nu), \quad (\text{B4})$$

$$\underbrace{(\nu \dots \nu)}_{k \text{ terms}} 0 \dots 0): \frac{\nu k}{4}(n + \nu - k + 1). \quad (\text{B5})$$

The relation to Ref. 36 is obtained by replacing $n \rightarrow n/2$ and rescaling the Casimir operator by a factor of 1/8. For the simplest irreducible representations the formulas (B1)–(B5) easily yield the results stated in Table I.

Finally, we make use of the following results on the decomposition of tensor products into irreducible representations, which is in its general form due to Littellmann³¹ and was specialized to the case we use here by Leung:³²

$$\begin{aligned} & (\mu_1 \mu_2 \dots \mu_{n/2}) \otimes (\nu 0 \dots 0) \\ &= \sum_{\kappa_i} \oplus (\mu_1 + \kappa_1 - \kappa_n, \mu_2 + \kappa_2 - \kappa_{n-1}, \dots, \mu_{n/2} \\ & \quad + \kappa_{n/2} - \kappa_{n/2+1}), \end{aligned} \quad (\text{B6})$$

where the sum is over all integers $\kappa_1, \dots, \kappa_n$ subject to the conditions

$$\begin{aligned} & \kappa_1 + \dots + \kappa_n = \nu, \\ & 0 \leq \kappa_i \leq \mu_{i-1} - \mu_i - \kappa_{n-i+2} + \kappa_{n-i+1}, \\ & 0 \leq \kappa_{n-j} \leq \mu_{j+1} - \mu_{j+2}, \\ & 0 \leq \kappa_{n/2+1} \leq \mu_{n/2}, \end{aligned}$$

where $i=2, 3, \dots, n/2$ and $j=0, 1, \dots, n/2-2$.

APPENDIX C: DERIVATION OF EQ. (14)

In this appendix we will generalize results obtained by Knabe³⁵ on the existence of a gap in SU(2) VBS chains with arbitrary spin. Similar techniques were also used by Fannes *et al.*¹² The main difference of our result as compared to Ref. 35 is that the operators $P_{i,i+1}$ are not assumed to be simple projectors.

Let us start with Eq. (13). The assumption $P_{i,i+1} \leq 1$ yields $P_{i,i+1}^2 \leq P_{i,i+1}$, where inequalities between operators are understood in the sense

$$\langle \psi | P_{i,i+1}^2 | \psi \rangle \leq \langle \psi | P_{i,i+1} | \psi \rangle \leq \langle \psi | \psi \rangle \quad (\text{C1})$$

for all states $|\psi\rangle$. In fact, the most useful results will be obtained if the largest eigenvalue of $P_{i,i+1}$ equals one, which is obtained by multiplication of Eq. (11) with a suitable constant. Using the definitions of Eqs. (13) and (16) one easily finds

$$\begin{aligned} H^2 &= -\frac{1}{m-1} \sum_{i=1}^N P_{i,i+1}^2 + \frac{1}{m-1} \sum_{i=1}^N h_{i,m}^2 + \sum_{\substack{i,j=1 \\ |i-j|>1}}^N P_{i,i+1} P_{j,j+1} \\ & \quad - \frac{1}{m-1} \sum_{i=1}^N \sum_{\substack{k,l=i \\ |k-l|>1}}^{i+m-1} P_{k,k+1} P_{l,l+1}. \end{aligned} \quad (\text{C2})$$

We can now use $P_{i,i+1}^2 \leq P_{i,i+1}$, which implies $-\frac{1}{m-1} \times \sum_i P_{i,i+1}^2 \geq -\frac{1}{m-1} H$, together with the fact that each of the terms $P_{i,i+1} P_{j,j+1}$ appears more often in the third sum than in the fourth sum. Therefore we get the inequality

$$H^2 \geq \frac{1}{m-1} \sum_{i=1}^N h_{i,m}^2 - \frac{1}{m-1} H. \quad (\text{C3})$$

Finally we can use Eq. (15), as well as $\sum_i h_{i,m} = mH$, to obtain Eq. (14) with $\epsilon = m/m-1 (\epsilon_m - 1/m)$.

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