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LETTER TO THE EDITOR

Valence bond states on quantum spin chains as ground states with spectral gap

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Abstract. We show that every translation invariant valence bond state on a one-dimensional quantum spin chain arises as the unique ground state of a certain family of finite-range interactions. For each interaction in this family we show the existence of a non-zero spectral gap above the ground state energy. A special example of this structure is a state recently studied by Affleck *et al.* For the Hamiltonian studied by these authors we can estimate the gap, and prove that it lies between 1/3 and 10/27.

It is well known that, even for nearest-neighbour interactions on a one-dimensional quantum spin chain, determining ground state properties such as degeneracy, symmetry breaking, exponential clustering, existence of a gap, etc, is a very hard problem. Some progress on the uniqueness problem was made recently in [1]. We are concerned here with an extension of recent work [2] which demonstrated for a specific nearest-neighbour Hamiltonian of a spin-1 chain the uniqueness of the ground state, the exponential decay of correlations, and the existence of a non-zero spectral gap. Estimates for the gap in this and some other models have also been given in [3]. Starting from this example, we will develop an abstract version of 'valence bond solid' (or VBS) states [4, 5]. We then show that for each VBS state there is a family of Hamiltonians, for which this state is a ground state with non-zero spectral gap. The example of [2] falls into this class, and we obtain a bound $3/10 \leqslant \gamma \leqslant 10/27$ for the gap γ in this case. The techniques of [2] make explicit use of the rotation invariance of the ground state. In contrast, no such symmetry is needed in our approach so that, e.g., the state of [2] is embedded into a 19-dimensional manifold of less symmetrical states, all of which are ground states of perturbations of the Hamiltonian in [2]. Although a general perturbation will destroy the VBS nature of the Hamiltonian and its ground state, this shows that VBS ground states are a much less singular occurrence than was apparent from the previous literature. A more extensive study of generalized VBS states on quantum spin chains was undertaken in [6, 7], where detailed proof of our assertions in this letter can also be found.

The state considered in [2] is the unique ground state of the Hamiltonian

$$H = \sum_i \{\tfrac{1}{2}\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} + \tfrac{1}{6}(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2 + \tfrac{1}{3}\} \tag{1}$$

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where $\boldsymbol{S}_i$ denotes the spin operators of a spin-1 at site i. The expression in braces is nothing but the projection onto the spin-2 subspace in the decomposition of the tensor product of the two spin-1 representations at sites i and $(i+1)$. The state is constructed as follows. The spin-1 state space ($\mathbb{C}^3$) at any site i is considered as the triplet subspace in a pair of two spin-$\frac{1}{2}$ degrees of freedom. Let us call these two spin-$\frac{1}{2}$ systems the right and left radical at site i. The valence bond is formed by combining the right radical at site i with the left radical at site $(i+1)$, and specifying a state φ for this pair. Since the ground state is to be translation invariant, φ will be the same for every bond. In the example it is just the singlet state for the composition of the two spin-$\frac{1}{2}$ systems. We thus have an auxiliary chain, whose sites correspond to the bonds of the original spin-1 chain, and we have a state vector for any finite segment of this auxiliary chain, which is just the product of the φ-vectors for each bond. Note that an observable, living at one site of the original chain, can also be considered as an observable of this auxiliary chain: any operator on $\mathbb{C}^3$ (which we identified with the triplet subspace of the two spin-$\frac{1}{2}$ radicals) is extended to the whole product space $\mathbb{C}^2\otimes\mathbb{C}^2$ of the radicals by defining it as zero on the singlet state. Thereby, such an observable becomes an observable of the auxiliary chain, and we can compute its expectation value, and the expectation values of any product of such observables, in the product state built from φ. By definition, these are the expectations of the valence bond state on the original spin-1 chain. To summarize, a valence bond state is a restriction of a product state, after the latter has been shifted by half a lattice step.

The generalization of this scheme is now straightforward. At each site of the chain, labelled by $i\in\{\ldots,-1,0,1,\ldots\}$ we consider a quantum system described in a d-dimensional Hilbert space. Thus $A_i\in\mathcal{M}_d$ will denote a 1-particle observable at the site i of the chain, where we use $\mathcal{M}_d$ to denote the complex $d\times d$-matrices. We replace the spin-$\frac{1}{2}$ systems in the example by an arbitrary quantum system with Hilbert space $\mathbb{C}^k$ with finite k. The state of the bonds will be given by a unit vector $\varphi\in\mathbb{C}^k\otimes\mathbb{C}^k$. The next ingredient is the identification of observables $A_i\in\mathcal{M}_d$ with observables of the auxiliary chain. Here we allow some more freedom than just an identification of $\mathbb{C}^d$ with a subspace of $\mathbb{C}^k\otimes\mathbb{C}^k$: this identification will be of the form $A_i\mapsto W^*AW$, with a fixed linear operator W: $\mathbb{C}^k\otimes\mathbb{C}^k\to\mathbb{C}^d$. The expectation of an observable $A_n\otimes\ldots\otimes A_m$ living on sites $n,\ldots,m$ in the valence bond state is then

$$\langle A_n\otimes\ldots\otimes A_m\rangle=\langle\Phi_{nm}\,|\,(\mathbb{1}\otimes W^*A_nW\otimes\ldots\otimes W^*A_mW\otimes\mathbb{1})\Phi_{nm}\rangle \tag{2}$$

where the scalar product on the right is taken in the $2(m-n+2)$-fold tensor product of $\mathbb{C}^k$ with itself, and $\Phi_{nm}=\varphi\otimes\varphi\otimes\ldots\otimes\varphi$ with $(m-n+2)$ factors. With a suitable normalization of W this equation clearly defines a state on the set of observables on the specified sites, i.e. there is a density matrix ρ_{nm} on the $(n-m+1)$-fold tensor product of $\mathbb{C}^d$ with itself such that

$$\langle A_n\otimes\ldots\otimes A_m\rangle=\mathrm{tr}(\rho_{nm}A_n\otimes\ldots\otimes A_m). \tag{3}$$

Apart from the normalization condition $\langle\mathbb{1}\rangle=1$, a state on the chain also has to satisfy the consistency conditions

$$\langle\mathbb{1}_{n-1}\otimes A_n\otimes\ldots\otimes A_m\rangle=\langle A_n\otimes\ldots\otimes A_m\otimes\mathbb{1}_{m+1}\rangle=\langle A_n\otimes\ldots\otimes A_m\rangle$$

where $\mathbb{1}_i$ denotes the unit operator at site i. In terms of φ and W these are easily seen to be equivalent to

$$\begin{aligned}\langle\varphi\otimes\varphi\,|\,(\mathbb{1}\otimes W^*W\otimes B)\varphi\otimes\varphi\rangle&=\langle\varphi\,|\,(\mathbb{1}\otimes B)\varphi\rangle\\ \langle\varphi\otimes\varphi\,|\,(A\otimes W^*W\otimes\mathbb{1})\varphi\otimes\varphi\rangle&=\langle\varphi\,|\,(A\otimes\mathbb{1})\varphi\rangle\end{aligned} \tag{4}$$

for arbitrary $A, B \in \mathcal{M}_k$. With this condition our construction of generalized valence bond states is complete. Note that no group representations or symmetry conditions were necessary. However, if both $\mathbb{C}^d$ and $\mathbb{C}^k$ carry an irreducible representation of SU(2) of spin $(d-1)/2$ and $(k-1)/2$, respectively, it is easy to get a rotation invariant state $\langle\cdot\rangle$ from this construction: we simply take φ as the unique rotation invariant vector in $\mathbb{C}^k \otimes \mathbb{C}^k$, and take W as an intertwining operator from $\mathbb{C}^k \otimes \mathbb{C}^k$ to $\mathbb{C}^d$. Such an operator exists iff d is odd and $(d-1)/2 \leqslant (k-1)$, i.e. $d \leqslant (2k-1)$, in which case W is unique up to a factor. It is easy to see that equation (4) can then be satisfied by a suitable choice of this factor. Both φ and W can be written out explicitly in terms of Clebsch–Gordan coefficients. The state of [2] is the simplest non-trivial case of this $(d=3, k=2)$; the other states have been studied in [7].

In the theory of valence bond states developed in [6] a central role is played by the operator $\hat{\mathbb{E}}: \mathcal{M}_k \to \mathcal{M}_k$ defined by

$$\langle \chi | \hat{\mathbb{E}}(B) \chi' \rangle = \langle \chi \otimes \varphi | (W^* W \otimes B) \chi' \otimes \varphi \rangle. \tag{5}$$

The first consistency condition (4) can then be stated as $\hat{\mathbb{E}}(\mathbb{1}) = \mathbb{1}$. $\hat{\mathbb{E}}$ is analogous to a transfer matrix. Its powers determine all the correlation functions of the VBS state, which hence decay exponentially like the powers of the eigenvalues of $\hat{\mathbb{E}}$. It is shown in [6] that the translation symmetry is unbroken in the VBS state, i.e. that the state allows no convex decomposition into periodic states, if and only if $\mathbb{1}$ is the only eigenvector of $\hat{\mathbb{E}}$ with an eigenvalue of modulus 1, or equivalently, if $\hat{\mathbb{E}}^n$ converges to the eigenprojection of 1 as $n \to \infty$. We shall assume this condition from now on.

For every $n < m$ and any basis $\{\chi_i\}_{i=1}^k \subset \mathbb{C}^k$ the equation

$$(\mathbb{1} \otimes W \otimes W \ldots \otimes \mathbb{1}) \varphi \otimes \varphi \otimes \ldots \otimes \varphi = \sum_{i,j} \chi_i \otimes (\psi_{\{n,\ldots,m\},i,j}) \otimes \chi_j \tag{6}$$

uniquely defines a set of k^2 vectors $\psi_{\{n,\ldots,m\},i,j} \in \bigotimes^{(n-m+1)} \mathbb{C}^d$. We shall denote the linear span of these vectors by $\mathcal{G}_{\{n,\ldots,m\}}$. From the expressions (2), (3) for the local expectations it is then immediately clear that the local density matrix ρ_{nm} will be supported by $\mathcal{G}_{\{n,\ldots,m\}}$, i.e. that the eigenvectors of ρ_{nm} with positive eigenvalues must be contained in $\mathcal{G}_{\{n,\ldots,m\}}$. We shall therefore call this space the space of 'valence bond vectors' over the sites $n, \ldots, m$. Note that this space has dimension at most k^2 independently of n and m. There is in fact a finite 'interaction length' r given by the smallest interval $\{1, \ldots, r\}$ such that $\mathcal{G}_r \equiv \mathcal{G}_{\{1,\ldots,r\}}$ has exactly dimension k^2.

A crucial property of the valence bond vectors, which is closely related to the exponential clustering of the VBS state, is that for sufficiently long chains any valence bond vector represents the VBS state. More precisely, for any finite segment $\{n, \ldots, m\}$ and $\varepsilon > 0$ we can find some L such that

$$|\langle \Psi | A \Psi \rangle - \langle A \rangle| \leqslant \varepsilon \| A \| \tag{7}$$

where Ψ is any unit vector in $\mathcal{G}_{\{n-L,\ldots,m+L\}}$, and A is an observable living on the segment $\{n, \ldots, m\}$. It immediately follows from this property that any state, whose local density matrices are supported by the subspaces $\mathcal{G}_{\{m,\ldots,n\}}$ must coincide with the VBS state. In other words, this state is uniquely characterized by the property that any observable A on a segment $\{n, \ldots, m\}$ which vanishes on $\mathcal{G}_{\{n,\ldots,m\}}$ has zero expectation.

The second fundamental property of VBS vectors is that if a vector has VBS form on two segments with sufficiently large overlap, then it is a VBS vector on the union of the segments. More precisely, if $n > r$ the conditions $\Psi \in \mathbb{C}^d \otimes \mathcal{G}_n$ and $\Psi \in \mathcal{G}_n \otimes \mathbb{C}^d$ imply $\Psi \in \mathcal{G}_{n+1}$. The proof relies on comparing the two expansions of Ψ in terms of

VBS vectors. By induction we get from this the stronger result

$$\mathscr{G}_m = \bigcap_{i=0}^{m-n} \otimes^i \mathbb{C}^d \otimes \mathscr{G}_n \otimes \otimes^{(m-n-i)} \mathbb{C}^d \tag{8}$$

for all $m \geqslant n > r$.

Another way to express the properties (7) and (8) of VBS vectors is to turn the VBS state into a ground state of a translation invariant finite range Hamiltonian. Indeed, the VBS state $\langle\,\rangle$ is clearly a ground state of

$$H \equiv \sum_{i \in \mathbb{Z}} h_{\{i,\ldots,i+l\}}$$

as soon as $h_{\{i,\ldots,i+l\}} \in \otimes^{l+1} \mathscr{M}_d$ is non-negative and has support in the orthogonal complement of $\mathscr{G}_{l+1}$. Furthermore, if we choose l larger than the interaction length r and $h_{\{i,\ldots,i+l\}}$ strictly positive on $\mathscr{G}_{l+1}^{\perp}$, H will have the VBS state $\langle\,\rangle$ as unique ground state by virtue of the above result. A Hamiltonian with this property will be called a VBS Hamiltonian for the VBS state $\langle\,\rangle$. There are many such Hamiltonians associated with each VBS state, varying also in the range l. However, restricting to the translation invariant case, where $h_{\{i,\ldots,i+l\}} \equiv h_l$ is independent of i, we find that any two VBS Hamiltonians H, H', defined by $h_l, h_{l'}'$ are equivalent in the following sense: if we define the local Hamiltonians for $m \geqslant n+l$ by $H_{\{n,\ldots,m\}} = \sum_{i=n}^{m-l} h_{\{i,\ldots,i+l\}}$, then there are positive constants $c_{\pm}$ such that whenever $m - n \geqslant l, l'$ we have

$$c_- H_{\{n,\ldots,m\}} \leqslant H'_{\{n,\ldots,m\}} \leqslant c_+ H_{\{n,\ldots,m\}}. \tag{9}$$

This follows easily from translation invariance, and from the fact that the operators in this inequality have the same null spaces.

The ground state energy gap γ of the Hamiltonian H is defined as the largest γ such that for all (local) observables X:

$$\langle X^*[H, X]\rangle \geqslant \gamma\{\langle X^* X\rangle - |\langle X\rangle|^2\}. \tag{10}$$

Since we are considering states for which the positive operator $H_{\{n,\ldots,m\}}$ has zero expectation, we may omit the commutator in this definition, and have to show instead that

$$\langle X^* H_{\{n,\ldots,m\}} X\rangle \geqslant \gamma\{\langle X^* X\rangle - |\langle X\rangle|^2\}$$

whenever $\{n, \ldots, m\}$ is much larger than the area of localization of X. Our strategy for proving this inequality for some strictly positive γ is the following. First of all, neither the existence of the gap, nor even the value of γ changes when we do not take $\mathscr{M}_d$ as the basic one-site observable algebra, but group together runs of p consecutive sites to obtain a chain with 'one-site' observable algebra $\otimes^p \mathscr{M}_d \cong \mathscr{M}_{d^p}$. This grouping does not change the VBS property of the state under consideration. If we choose p larger than l, we may now consider the given Hamiltonian as a nearest-neighbour interaction $k_{\{1,2\}} \in \mathscr{M}_{d^p} \otimes \mathscr{M}_{d^p}$ with

$$k_{\{1,2\}} \equiv \tfrac{1}{2} \sum_{i=1}^{p-r} h_{\{i,\ldots,i+l\}} + \sum_{i=p-r+1}^{p} h_{\{i,\ldots,i+l\}} + \tfrac{1}{2} \sum_{i=p+1}^{2p-r} h_{\{i,\ldots,i+l\}}.$$

This operator is clearly positive, and its support is precisely the complement of $\mathscr{G}_{2p}$. It therefore defines a nearest-neighbour VBS Hamiltonian for the same VBS state as the original Hamiltonian. It is clear from the equivalence (9) of VBS Hamiltonians that the interaction $k_{\{1,2\}}$ defines a Hamiltonian with gap, if and only if any other operator

with the same support has this property. The most convenient choice is to replace $k_{\{1,2\}}$ by its support projection, i.e. by the projection onto the orthogonal complement of $\mathcal{G}_{2p}$. Let us denote this projection by $k'_{\{1,2\}}$. Then a crucial step in the proof is to use the cluster properties of VBS states to show that, provided p was chosen large enough, $k'_{\{1,2\}}$ and $k'_{\{2,3\}}$ nearly commute, and

$$k'_{\{1,2\}}k'_{\{2,3\}}+k'_{\{2,3\}}k'_{\{1,2\}} \geqslant (-\varepsilon_p)(k'_{\{1,2\}}+k'_{\{2,3\}})$$

for some $\varepsilon_p > 0$, which becomes small for large p. From this, and the fact that $k'_{\{i,i+1\}}$ and $k'_{\{j,j+1\}}$ commute for $|i-j| \geqslant 2$, it is easy to see that

$$(H'_{\{1,\ldots,n\}})^2 \geqslant (1-2\varepsilon_p)H'_{\{1,\ldots,n\}}. \tag{11}$$

This means that $H'_{\{1,\ldots,n\}}$ has a spectral gap at least $(1-2\varepsilon_p)$, uniformly in n, which implies the desired result. We mention that the idea of establishing a gap by proving an inequality like (11) for the square of the local Hamiltonian has also been used by Knabe [3].

Now consider again the state on the spin-1 chain of our first example. The interaction length of this state turns out to be $r=2$, which is expected, because $k^2=4$ vectors in a space of dimension $d^r=3^2$ are generically independent. $\mathcal{G}_2$ is the four-dimensional subspace of $\mathbb{C}^3\otimes\mathbb{C}^3$ that carries the spin-0 and spin-1 subrepresentations in the product of two spin-1 representations. In this case we have, moreover, that $\mathcal{G}_3 = \mathcal{G}_2\otimes\mathbb{C}^3 \cap \mathbb{C}^3\otimes \mathcal{G}_2$. This means that, while the general structure outlined above guarantees only the existence of a next-nearest-neighbour VBS Hamiltonian, there is already a nearest-neighbour Hamiltonian which has this VBS state as its unique ground state. For example, we can take the Hamiltonian (1), where this nearest-neighbour interaction is the orthogonal projection P_{12} on the orthogonal complement of $\mathcal{G}_2$. The simplest estimate for the gap of this Hamiltonian using the above argument would be based on the inequality:

$$P_{12}P_{23}+P_{23}P_{12} \geqslant -\varepsilon(P_{12}+P_{23}).$$

Unfortunately, the constant $\varepsilon = 1/2$ (which is optimal) is not good enough to lead to a non-zero lower bound for the gap. We should therefore regroup the chain as outlined above, which considerably complicates explicit computations. A careful analysis based on the explicit form of the state leads to a lower bound of 3/10 for the gap which is reasonably close to the easily obtained upper bound of 10/27 (see e.g. [8]).

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