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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, Lieb, Kennedy, and Tasaki. For the Hamiltonian studied by these authors we can estimate the gap, and prove that it lies between 1/3 and 10/27.

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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 by Affleck, Kennedy, Lieb, and Tasaki [**2**], who demonstrated for a specific nearest-neighbour Hamiltonian of a spin-1 chain the exponential decay of correlations, and the existence of a non-zero spectral gap. We begin by describing an abstract version of Anderson's "valence bond solid" (or "vbs") states [**3**]. 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 $3/10 \leq \gamma \leq 10/27$ for the gap γ in this case. A more extensive study of generalized vbs states on quantum spin chains was undertaken in [**4,5**], where detailed proof of our assertions in this letter can also be found.

So we consider here a chain $\mathbb{Z} = \{\ldots -1, 0, 1, \ldots\}$. At each site of the chain lives a quantum particle described by the $d \times d$ complex matrices $\mathcal{M}_d$. So $A_i \in \mathcal{M}_d$ will denote a 1-particle observable at the site i of the chain. In order to define an expectation or 'state' $\langle\ \rangle$ for the whole chain we need to specify the expectations $\langle A_n \otimes \cdots A_m \rangle$ of all elementary tensor observables. Clearly, these local densities have to satisfy positivity and compatibility requirements such as:

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

where $\mathbb{I}_j$ is the unit matrix at site j. We will moreover restrict our attention to the translation invariant case. Usually states are implicitly given by means of (thermodynamical) limits of finite system expectations. The vbs construction however provides an explicit construction in terms of a few simple finite dimensional ingredients. So let us introduce the following auxilliary objects:

- the Hilbert space $\mathbb{C}^k$
- a unit vector $\varphi \in \mathbb{C}^k \otimes \mathbb{C}^k$
- a linear map W from $\mathbb{C}^k \otimes \mathbb{C}^k$ into $\mathbb{C}^d$.

It is well known that any vector $\varphi \in \mathbb{C}^k \otimes \mathbb{C}^k$ can be written in an essentially unique way as:

$$\varphi = \sum_i \rho_i^{1/2} \overline{\chi_i} \otimes \chi_i \quad ,$$

where the ρ_i are strictly positive, the $\chi_i \in \mathbb{C}^k$ and $\overline{\chi_i} \in \mathbb{C}^k$ are orthonormal sets. In order to avoid trivial degeneracies we will assume that there are exactly k terms in the sum so that the χ_i (and of course also the $\overline{\chi_i}$) form actually a basis of $\mathbb{C}^k$.

Furthermore $\sum_{i=1}^{k} \rho_i = \|\varphi\|^2 = 1$. We will use the notation Φ for:

$$\Phi(A) \equiv \langle \varphi, A\varphi \rangle \qquad A \in \mathcal{M}_k \otimes \mathcal{M}_k \quad .$$

The map W has to match with φ in the following sense:

$$\begin{aligned} \Phi \otimes \Phi(\mathbb{I} \otimes W^*W \otimes B) &= \Phi(\mathbb{I} \otimes B) \\ \Phi \otimes \Phi(A \otimes W^*W \otimes \mathbb{I}) &= \Phi(A \otimes \mathbb{I}) \end{aligned} \qquad (\star)$$

We can now compute the vbs state as follows:

$$\langle A_n \otimes \cdots A_m \rangle = \underbrace{\Phi \otimes \Phi \otimes \cdots \Phi}_{m-n+2 \text{ factors}} (\mathbb{I} \otimes W^* A_n W \otimes \cdots W^* A_m W \otimes \mathbb{I})$$

Remark that SU(2) (or any single site symmetry group whatsoever) does not play any role at all in the construction, though a symmetry will obviously be helpful in actual computations [**6,7,5**]. There is also no reason to assume that W^* is an isometry and so $A \mapsto W^*AW$ is in general not a representation of $\mathcal{M}_d$.

Another way to express condition $(\star)$ is to say that:

$$(\mathrm{id} \otimes \Phi)(W^*W \otimes \mathbb{I}) = \mathbb{I} \quad \text{and} \quad (\Phi \otimes \mathrm{id})(\mathbb{I} \otimes W^*W) = \mathbb{I} \quad .$$

We will in fact assume the stronger condition that there is only one eigenvector of $A \mapsto (\mathrm{id} \otimes \Phi)(W^*AW \otimes \mathbb{I})$ which corresponds to an eigenvalue of modulus 1, namely $\mathbb{I}$. This assumption implies [**4**] that the state is exponentially clustering and that translation symmetry is not broken, i.e. there is no Néel order.

For every $n < m$ the equation

$$(\mathbb{I} \otimes W \otimes W \cdots \mathbb{I})\, \varphi \otimes \varphi \otimes \cdots \varphi = \sum_{i,j} \overline{\chi_i} \otimes (\psi_{\{n,\ldots m\},i,j}) \otimes \chi_j$$

uniquely defines a set of k^2 vectors $\psi_{\{n,\ldots m\},i,j} \in \otimes^{(n-m)} \mathbb{C}^d$. We shall denote the linear span of these vectors by $\mathcal{G}_{\{n,\ldots m\}}$. From the expression for the local expectations it is then immediatly clear that each observable living on the sites $\{n, \ldots m\}$ will have zero expectation as soon as it has no support in the subspace $\mathcal{G}_{\{n,\ldots m\}}$. The local density matrices that define the vbs state hence live on a subspace of dimension at most k^2 independently of n and m. There is in fact a natural 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. It turns out that the subspaces $\mathcal{G}_n$, $n > r$ completely characterize the vbs state:

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

- if a state of the infinite chain is supported by the subspaces $\mathcal{G}_m$, that is if it assigns a zero expectation to all observables that vanish on $\mathcal{G}_m$, then it coincides with the vbs state.

Another way to express this 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

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

as soon as $h_{\{i,\dots i+l\}} \in \otimes^{\ell+1}\mathbb{C}^d$ is non-negative and has support in the orthogonal complement of $\mathcal{G}_{\ell+1}$. Furthermore, if we choose ℓ larger than the interaction length r and $h_{\{i,\dots i+l\}}$ strictly positive on $\mathcal{G}_{\ell+1}^{\perp}$, 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 $h_{\{i,\dots i+l\}} \equiv h_\ell$ is independent of i, we find that any two vbs Hamiltonians H, H', defined by $h_\ell, h'_{\ell'}$ are equivalent in the following sense: if we define the local Hamiltonians for $m \geq n+\ell$ by $H_{\{n,\dots m\}} = \sum_{i=n}^{m-\ell} h_{\{i,\dots i+l\}}$, then there are positive constants $c_\pm$ such that whenever $m-n \geq \ell, \ell'$ we have

$$c_-\, H_{\{n,\dots m\}} \leq H'_{\{n,\dots m\}} \leq c_+\, H_{\{n,\dots m\}} \quad .$$

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 the largest γ such that for all (local) observables X:

$$\langle X^*[H,X]\rangle \geq \gamma\{\langle X^*X\rangle - |\langle X\rangle|^2\} \quad .$$

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

$$\langle X^* H_{\{n,\dots m\}} X\rangle \geq \gamma\{\langle X^*X\rangle - |\langle X\rangle|^2\} \quad ,$$

whenever $\{n,\dots m\}$ 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 take not $\mathcal{M}_d$ as the basic one-site observable algebra, but group together runs of p consecutive sites to obtain a chain with "one-site" observable algebra $\otimes^p \mathcal{M}_d \cong \mathcal{M}_{d^n}$. 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 $k_{\{1,2\}} \in \mathcal{M}_{d^n} \otimes \mathcal{M}_{d^n}$ with

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

This operator is clearly positive, and its support is precisely the complement of $\mathcal{G}_{2p}$. It therefore defines a nearest-neighbour vbs Hamiltonian for the same vbs state as the original Hamiltonian. It is clear from the equivalence of vbs Hamiltonians described above 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

$$k'_{\{1,2\}}k'_{\{2,3\}} + k'_{\{2,3\}}k'_{\{1,2\}} \geq (-\epsilon_p)(k'_{\{1,2\}} + k'_{\{2,3\}})$$

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

$$\left(H'_{\{1,\ldots n\}}\right)^2 \geq (1-2\epsilon_p)H'_{\{1,\ldots n\}} \quad .$$

This means that $H_{\{1,\ldots n\}}$ has a spectral gap at least $(1-2\epsilon_p)$, uniformly in n, which implies the desired result.

Consider now the case of a spin 1 chain ($d = 3$) and choose the auxilliary Hilbert space 2 dimensional ($k = 2$). Let us denote by $\mathcal{D}^{(j)}$ the irreducible spin j representation of SU(2) carried by $\mathbb{C}^{2j+1}$ and choose $\varphi = \frac{1}{\sqrt{2}}\{(+-)-(-+)\} \in \mathbb{C}^2 \otimes \mathbb{C}^2$, where $(+)$ and $(-)$ denote the eigenvectors of S^z in the representation $\mathcal{D}^{(1/2)}$. If we take W^* to be $2/\sqrt{3}$ times the isometry that intertwines $\mathcal{D}^{(1)}$ and $\mathcal{D}^{(1/2)} \otimes \mathcal{D}^{(1/2)}$ then we have all the ingredients to construct a vbs state. The interaction length of this state turns out to be 2 and the space $\mathcal{G}_2$ is the 4 dimensional subspace of $\mathbb{C}^3 \otimes \mathbb{C}^3$ that carries the $\mathcal{D}^{(0)}$ and the $\mathcal{D}^{(1)}$ subrepresentation of $\mathcal{D}^{(1)} \otimes \mathcal{D}^{(1)}$. 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 that has this vbs state as unique ground state.

This nearest-neighbour interaction is the orthogonal projection P_{12} on the orthogonal complement of $\mathcal{G}_2$, which in terms of the usual Heisenberg interaction $\vec{S}_1 \cdot \vec{S}_2$ can be written as $\frac{1}{3} + \frac{1}{2}\vec{S}_1 \cdot \vec{S}_2 + \frac{1}{6}\vec{S}_1 \cdot \vec{S}_2$. The simplest estimate for the gap of this Hamiltonian using the argument of above would be based on the inequality:

$$P_{12}P_{23} + P_{23}P_{12} \geq -\frac{1}{2}(P_{12} + P_{23}).$$

Unfortunately, the constant $-\frac{1}{2}$ (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.

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