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Non-positive matrix elements for Hamiltonians of spin-1 chains

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Abstract. For a large class of one-dimensional spin-1 Hamiltonians with open boundary conditions, we show that there is a unitary transformation for which the off-diagonal matrix elements of the transformed Hamiltonian are non-positive. We use this to show that the ground state of a finite chain is at most fourfold degenerate, and that the expectation of the string observable of den Nijs and Rommelse in the ground state is bounded below by the expectation of the usual Néel order parameter. (This was proved for a smaller class of Hamiltonians by Kennedy and Tasaki.) The class of Hamiltonians to which our results apply include the general isotropic Hamiltonian $\sum_i [S_i \cdot S_{i+1} - \beta (S_i \cdot S_{i+1})^2]$ for $\beta > -1$. For the usual Heisenberg Hamiltonian the transformed Hamiltonian is $-\sum_i T_i \cdot T_{i+1}$ where the operators $T = (T^x, T^y, T^z)$ satisfy anticommutation relations like $\{T^x, T^y\} = T^z$. We can also use this transformation to obtain variational bounds on the ground-state energy. The transformation used here is closely related to the unitary operator introduced by Kennedy and Tasaki.

The spin-1 chain has been the subject of a great deal of scrutiny since the discovery by Haldane that this chain behaves quite differently from the spin-$\frac{1}{2}$ chain. The Haldane phase of the spin-1 chain is a phase in which there is a unique infinite-volume ground state with exponential decay of the correlations and a gap between the ground-state energy and the rest of the spectrum. Haldane argued that the usual Heisenberg antiferromagnet should be in such a phase [1]. While there is no long-range order in the Haldane phase, there is a hidden order discovered by den Nijs and Rommelse [2]. They introduced a string order parameter to measure this order. Girvin and Arovas [3] numerically evaluated this order parameter and concluded it was non-zero for the usual Heisenberg Hamiltonian. Kennedy and Tasaki [4] introduced a non-local unitary transformation of the spin-1 chain which transforms this non-local order parameter into a simple local order parameter.

In this paper we introduce a closely related unitary transformation of the spin-1 chain which also transforms the hidden order into explicit order and for which the off-diagonal matrix elements of the transformed Hamiltonian are all non-positive. Our results apply to the Hamiltonian

$$H = \sum_i [J_i^x S_i^x S_{i+1}^x + J_i^y S_i^y S_{i+1}^y + J_i^z S_i^z S_{i+1}^z - \beta_i (S_i \cdot S_{i+1})^2] + \sum_i [K_i^x (S_i^x)^2 + K_i^y (S_i^y)^2 + K_i^z (S_i^z)^2] \tag{1}$$

where the parameters satisfy

$$J_i^x, J_i^y, J_i^z > 0 \qquad J_i^x, J_i^y, J_i^z > -\beta_i \tag{2}$$

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and the K_i^α are arbitrary. Throughout this paper we only consider open boundary conditions. For the isotropic Hamiltonian

$$\sum_i [S_i \cdot S_{i+1} - \beta (S_i \cdot S_{i+1})^2] \tag{3}$$

the condition is that $\beta > -1$. This includes the entire interval $-1 < \beta < 1$ in which the model is believed to be in the Haldane phase.

The Perron–Frobenius theorem applies to matrices whose off-diagonal entries are all non-positive. To apply it one must determine which basis vectors are connected in the sense that we can go from one to the other via a sequence of non-zero matrix elements in the transformed Hamiltonian. We find that the set of basis vectors has four connected components. Hence the Perron–Frobenius theorem implies that the ground state is at most fourfold degenerate. For isotropic Hamiltonians this implies that the ground state must either be a singlet or a triplet. Our unitary transformation also yields a trivial proof that the expectation of the string order parameter in the ground state is greater than or equal to the expectation of the usual Néel order parameter. This inequality was proved in [5] for a smaller class of Hamiltonians ($\beta_i = 0$, $J_i^x = J_i^y$ and $K_i^x = K_i^y = 0$). Our transformation also leads to variational bounds on the ground-state energy. For the usual Heisenberg Hamiltonian we find that the energy per site is less than $-1.401\,4625$. Finally, we note that this representation of the Hamiltonian with only non-positive off-diagonal matrix elements makes it possible to perform Monte Carlo simulations for all these Hamiltonians.

The unitary transformation which we will define is somewhat complicated, but its action on the Hamiltonian and the correlation functions is quite simple. So we will defer the definition of the transformation until later and for the moment concentrate on its results. Throughout this paper we will use the basis in which

$$S_i^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad S_i^y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & -\mathrm{i} \\ 0 & \mathrm{i} & 0 \end{pmatrix} \qquad S_i^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

We refer to this basis as the standard basis. Define three operators which act on a single site by

$$T^x = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \qquad T^y = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad T^z = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \tag{4}$$

Let $D_j^\alpha = \exp(\mathrm{i}\pi T_j^\alpha)$. Explicitly, the action of the D_j^α on a single site is given by

$$D^x = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad D^y = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad D^z = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{5}$$

Lemma 1. There is a unitary transformation V such that

$$V S_i^\alpha S_{i+1}^\alpha V^{-1} = -T_i^\alpha T_{i+1}^\alpha \qquad \alpha = x, y, z \tag{6}$$

and

$$V (S_i^\alpha)^2 V^{-1} = (T_i^\alpha)^2 \qquad \alpha = x, y, z. \tag{7}$$

Recall that the string order parameter of den Nijs and Rommelse is given by

$$O^{\alpha}_{\text{string}}(0,l) = -S^{\alpha}_0 \exp\left(i\pi \sum_{j=1}^{l-1} S^{\alpha}_j\right) S^{\alpha}_l.$$

Then

$$\begin{aligned} V O^{\alpha}_{\text{string}}(0,l) V^{-1} &= T^{\alpha}_0 T^{\alpha}_l \\ V S^{\alpha}_0 S^{\alpha}_l V^{-1} &= -T^{\alpha}_0 \prod_{j=1}^{l-1} D^{\alpha}_j T^{\alpha}_l \end{aligned} \tag{8}$$

for $\alpha = x$, y and z. If H is given by (1) and the parameters satisfy (2), then the off-diagonal matrix elements of VHV^{-1} in the standard basis are all non-positive.

Remarks.

1. The lemma says that the unitary operator V transforms $\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1}$ into $-\boldsymbol{T}_i \cdot \boldsymbol{T}_{i+1}$. The operators S^x, S^y, S^z satisfy the usual commutation relations. It is amusing to note that the operators T^x, T^y, T^z satisfy the anticommutation relations $\{T^{\alpha}, T^{\beta}\} = T^{\gamma}$ where α, β, γ is any permutation of x, y, z.

2. The non-positivity of the off-diagonal matrix elements of VHV^{-1} in the standard basis is equivalent to H having non-positive off-diagonal matrix elements in the basis obtained by applying V^{-1} to the standard basis. The resulting basis is not simple, so throughout this paper we find it more convenient to apply the unitary transformation to the Hamiltonian rather than to the standard basis.

Proof. We defer the proofs of (6), (7) and (8) until later. The proof of the last sentence in the lemma is as follows. Equation (6) shows that the off-diagonal matrix elements of $V\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} V^{-1}$ are non-positive and hence the same is true for $V[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \beta(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2]V^{-1}$ if $\beta \geqslant 0$. To show that it is true for $\beta \geqslant -1$ takes a little computation. Define

$$h_i = V[\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1} - \beta(\boldsymbol{S}_i \cdot \boldsymbol{S}_{i+1})^2]V^{-1} = -\boldsymbol{T}_i \cdot \boldsymbol{T}_{i+1} - \beta(\boldsymbol{T}_i \cdot \boldsymbol{T}_{i+1})^2$$

where $\boldsymbol{T}$ is the vector of operators (T^x, T^y, T^z). Then the non-zero matrix elements of h_i are

$$\begin{aligned} \langle AA|h_i|AA\rangle &= -2\beta \qquad \langle AA|h_i|BB\rangle = -1-\beta \\ \langle AB|h_i|AB\rangle &= -\beta \qquad \langle AB|h_i|BA\rangle = -1 \end{aligned} \tag{9}$$

where A and B can be 0, + or − and $A \neq B$. This shows that the off-diagonal elements of h_i are all non-positive if $\beta \geqslant -1$.

The proof of the lemma is completed by noting that the Hamiltonian (1) with the parameters satisfying (2) can be written as a linear combination of h_i, $-T^x_i T^x_{i+1}$, $-T^y_i T^y_{i+1}$, $-T^z_i T^z_{i+1}$, $(T^x_i)^2$, $(T^y_i)^2$ and $(T^z_i)^2$ with all the coefficients non-negative except possibly the coeffecients of the last three operators. The last three operators are diagonal and all the other operators have non-positive off-diagonal matrix elements, so H has non-positive off-diagonal matrix elements. □

Our first application of the 'good signs' of the transformed Hamiltonian is the following.

Theorem 2. The ground state of the Hamiltonian (1) with the parameters satisfying (2) is at most fourfold degenerate. If the Hamiltonian is isotropic ($J_i^x = J_i^y = J_i^z$ and $K_i^\alpha = 0$), then the total spin of the ground state is either 0 or 1 (or both).

Remarks.

1. When $J_i^x = J_i^y$ there is a simple, well known unitary transformation which makes the off-diagonal matrix elements of $J_i^x S_i^x S_{i+1}^x + J_i^y S_i^y S_{i+1}^y + J_i^z S_i^z S_{i+1}^z$ non-positive. Obviously we can include the term $-\beta(S_i \cdot S_{i+1})^2$ and still have non-positive off-diagonal matrix elements if $\beta \geqslant 0$. The Perron–Frobenius theorem applies, but does not say much since the number of connected components of basis vectors grows with the size of the system. A clever argument by Lieb and Mattis shows that in the isotropic case with $\beta \geqslant 0$, the ground state of the Hamiltonian with open boundary conditions is a singlet if the number of lattice sites is even and a triplet if the number is odd [6].

2. The theorem is optimal in the sense that the ground state can indeed be fourfold degenerate. This is the case for the Hamiltonian (3) with $\beta = -\frac{1}{3}$ and open boundary conditions. Generically, we expect that in the Haldane phase the four lowest eigenvalues will be non-degenerate, but the difference between them will be exponentially small in the length of the chain. The Haldane gap would be the difference between these eigenvalues and the fifth eigenvalue. For the isotropic Hamiltonians these four lowest eigenvalues will degenerate into a triplet and a singlet with the difference between them exponentially small in the length of the chain. This scenario is based on the $S = \frac{1}{2}$ degrees of freedom that are localized near the ends of the chain with open boundary conditions [7, 8]. In the isotropic case the above is supported by numerical studies [8], but we should emphasize that none of the above speculations have been proved.

Proof. We have shown that there is a basis in which all of the off-diagonal elements of the Hamiltonian are non-positive. To apply the Perron–Frobenius theorem we need to determine which basis vectors are connected to which basis vectors by a sequence of non-zero matrix elements in the transformed Hamiltonian.

We partition the set of basis vectors into four subsets. B is the set of basis vectors for which the number of $+$s is even and the number of $-$s is even. B_+ is the set for which the number of $+$s is odd and the number of $-$s is even. B_- is defined similarly. B_{+-} is the set for which both the number of $+$s and the number of $-$s is odd. We claim that any element of one of these four sets is connected to any other element in the same set by a sequence of non-zero matrix elements. If the claim is true, then by the Perron–Frobenius theorem the restriction of H to each of the subspaces spanned by these four sets of basis vectors has a unique ground state. So the ground state of H is at most fourfold degenerate. If the Hamiltonian is isotropic, then the ground state may be taken to be an eigenstate of the total spin operator. Since the ground state is at most fourfold degenerate it can only be a singlet or a triplet (or one of each).

Now we turn to the proof of the claim. We first consider B. It contains the basis vector which consists of all 0s. So it suffices to show that we can connect this configuration to any other configuration with an even number of $+$s and an even number of $-$s. The matrix elements $(00) \to (++)$ and $(00) \to (--)$ allow us to introduce the desired number of $+$s and $-$s into the configuration. We can then rearrange them into the desired configuration using the matrix elements of the form $(AB) \to (BA)$ where $A \neq B$. The proof for the other three subsets is similar. □

The next application is a generalization and much simpler proof of a result in [5].

Theorem 3. Let $\langle\ \rangle$ denote expectation in any one of the ground states of H for a finite chain. We assume that the parameters in the Hamiltonian satisfy (2). Then

$$\langle O^{\alpha}_{\text{string}}(0,l)\rangle \geqslant |\langle S^{\alpha}_0 S^{\alpha}_l\rangle|.$$

Proof. By the above calculations, there is a ground state ψ of VHV^{-1} such that

$$\begin{aligned}\langle O^{\alpha}_{\text{string}}(0,l)\rangle &= (\psi, T^{\alpha}_0 T^{\alpha}_l \psi)\\ \langle S^{\alpha}_0 S^{\alpha}_l\rangle &= \left(\psi, -T^{\alpha}_0 \prod_{i=1}^{l-1} D^{\alpha}_i T^{\alpha}_l \psi\right).\end{aligned} \tag{10}$$

We denote a spin configuration for the chain by σ. So σ stands for a string of +s,−s and 0s. Let $\psi(\sigma)$ be the coefficients of the ground state ψ with respect to the standard basis. In other words,

$$\psi = \sum_{\sigma} \psi(\sigma)|\sigma).$$

Since the matrix elements of the Hamiltonian are all real, we may assume $\psi(\sigma)$ is real valued. By the first lemma and the Perron–Frobenius theorem, the sign of $\psi(\sigma)$ is constant on each of the four subspaces B, B_+, B_- and B_{+-}. The operators on the right-hand sides of (10) are block diagonal with respect to these four subspaces, so we can replace $\psi(\sigma)$ by its absolute value and equation (10) will still hold. Thus we can simply assume $\psi(\sigma) \geqslant 0$.

We now have

$$\left(\psi, -T^{\alpha}_0 \prod_{i=1}^{l-1} D^{\alpha}_i T^{\alpha}_l \psi\right) = \sum_{\sigma,\sigma'} \psi(\sigma)\psi(\sigma')\langle\sigma| - T^{\alpha}_0 \prod_{i=1}^{l-1} D^{\alpha}_i T^{\alpha}_l |\sigma').$$

Looking at the matrix elements of D^{α}_i and T^{α}_i we see that

$$\langle\sigma| - T^{\alpha}_0 \prod_{i=1}^{l-1} D^{\alpha}_i T^{\alpha}_l |\sigma'\rangle = \pm\langle\sigma|T^{\alpha}_0 T^{\alpha}_l|\sigma'\rangle$$

and $\langle\sigma|T^{\alpha}_0 T^{\alpha}_l|\sigma'\rangle \geqslant 0$. Hence

$$|\langle S^{\alpha}_0 S^{\alpha}_l\rangle| \leqslant \sum_{\sigma,\sigma'} \psi(\sigma)\psi(\sigma')\langle\sigma|T^{\alpha}_0 T^{\alpha}_l|\sigma'\rangle = \langle O^{\alpha}_{\text{string}}(0,l)\rangle. \qquad \square$$

After applying the unitary operator of [4], the transformed Hamiltonian has a $Z_2 \times Z_2$ symmetry. The Haldane phase corresponds to the full breaking of this symmetry. When we use the transformation V, this symmetry is implemented by the three unitary operators $\prod_i D^{\alpha}_i$, $\alpha = x$, y and z. It is easy to check that each of them leaves the Hamiltonian VHV^{-1} unchanged. (Note that the product of any two of the operators D^{α}_i yields the third operator, so these three operators generate the group $Z_2 \times Z_2$.)

The $Z_2 \times Z_2$ symmetry is present even when we do not have $J^x_i = J^y_i = J^z_i$. When they are all equal and $K^{\alpha}_i = 0$ so that we simply have the isotropic Hamiltonian (3), then the transformed Hamiltonian has another symmetry. Equation (9) shows that the transformed Hamiltonian is left unchanged by any permutation of the three spin states 0, + and −. So we have an additional S_3 symmetry.

We finally turn to the definition of the unitary operator and the proof of lemma 1. The operator V can be written as a product of the non-local unitary operator U of [4] and a second local unitary operator W. A compact representation for the non-local operator was found by Oshikawa [9]:

$$U = \prod_{j<k} \exp(\mathrm{i}\pi S_j^z S_k^x). \tag{11}$$

The transformation for this paper is $V = WU$, where $W = \prod_k W_k$. The operator W_k acts only on the spin at site k and is given by

$$W_k = \begin{pmatrix} 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1 & 0 \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \end{pmatrix}. \tag{12}$$

We now carry out the computations needed to prove lemma 1.

Proof of lemma 1. Lemma 2.1 of [5] says

$$\begin{aligned} US_l^x U^{-1} &= S_l^x \prod_{k>l} \exp(\mathrm{i}\pi S_k^x) \\ US_l^y U^{-1} &= S_l^y \prod_{j<l} \exp(\mathrm{i}\pi S_j^z) \prod_{k>l} \exp(\mathrm{i}\pi S_k^x) \\ US_l^z U^{-1} &= S_l^z \prod_{j<l} \exp(\mathrm{i}\pi S_j^z). \end{aligned} \tag{13}$$

These equations are easily verified using the representation (11). Some simple computation shows

$$W_k S_k^\alpha W_k^{-1} = T_k^\alpha \qquad \alpha = x, z \qquad W_k S_k^y W_k^{-1} = -\mathrm{i} T_k^y D_k^z$$

and hence

$$W_k \exp(\mathrm{i}\pi S_k^\alpha) W_k^{-1} = \exp(\mathrm{i}\pi T_k^\alpha) = D_k^\alpha \qquad \alpha = x, z.$$

So when we apply the unitary operator W to (13) we find

$$\begin{aligned} VS_l^x V^{-1} &= T_l^x \prod_{k>l} D_k^x \\ VS_l^z V^{-1} &= T_l^z \prod_{j<l} D_j^z \\ VS_l^y V^{-1} &= -\mathrm{i} T_l^y \prod_{j\leqslant l} D_j^z \prod_{k>l} D_k^x = -\mathrm{i} \prod_{j<l} D_j^z \prod_{k\geqslant l} D_k^x T_l^y \end{aligned} \tag{14}$$

where the last equality follows from the trivial identity $T_l^y D_l^z = D_l^x T_l^y$. The equations in the lemma follow easily from (14) and the identities

$$T_k^\alpha D_k^\alpha = -T_k^\alpha \qquad \alpha = x, y, z \qquad D_k^x D_k^z = D_k^y. \qquad \square$$

Table 1. Variational bounds on the ground-state energy per site for the usual Heisenberg Hamiltonian. The left column is l, the number of sites in the support of the function f in equation (15).

Number of sites	Number of parameters	Variational energy
2	1	−1.388 6804
3	3	−1.397 5693
4	8	−1.400 0247
5	20	−1.400 8583
6	53	−1.401 1941
7	143	−1.401 3411
8	404	−1.401 4104
9	1160	−1.401 4448
10	3401	−1.401 4625

When $\beta = -\frac{1}{3}$ the ground states of the isotropic Hamiltonian (3) may be found exactly and are known as the VBS states [10]. With open boundary conditions there are four such states. These states are not given by tensor products of states at each site. However, after the unitary transformation of [4], they are simply tensor products. Obviously the same must be true when we use the transformation V. It transforms the VBS subspace into the subspace spanned by the four states $\ldots \phi_k \otimes \phi_k \otimes \phi_k \ldots$ where

$$\phi_1 = |0\rangle + |+\rangle + |-\rangle \qquad \phi_2 = |0\rangle - |+\rangle + |-\rangle$$
$$\phi_3 = |0\rangle + |+\rangle - |-\rangle \qquad \phi_4 = |0\rangle - |+\rangle - |-\rangle.$$

As observed in [10], if one uses the VBS states as variational states for the usual Heisenberg Hamiltonian, $\sum_i S_i \cdot S_{i+1}$, the resulting bound on the energy is better than that obtained using the Néel state as a variational state. If we write the VBS wavefunction $\ldots \phi_1 \otimes \phi_1 \otimes \phi_1 \ldots$ in the form $\sum_\sigma \psi(\sigma)|\sigma\rangle$, then the wavefunction $\psi(\sigma)$ is simply 1, and the spins are uncorrelated. (Here σ ranges over all configurations of +s, −s and 0s.) One can obtain better variational estimates by using wavefunctions with some correlation between the spins. The simplest one is

$$\psi(\sigma) = \exp\left(\alpha \sum_i 1(\sigma_i = \sigma_{i+1})\right)$$

where α is a parameter and $1(\sigma_i = \sigma_{i+1})$ is 1 if $\sigma_i = \sigma_{i+1}$ and is 0 otherwise. Computing the norm of ψ and the expected value of $S_i \cdot S_{i+1}$ reduces to a simple transfer matrix calculation. We then minimize the resulting bound on the energy as a function of α.

More generally we can let

$$\psi(\sigma) = \exp\left(\sum_i f(\sigma_{i+1}, \sigma_{i+2}, \ldots, \sigma_{i+l})\right) \tag{15}$$

where f is any function of l spins. The calculation again reduces to a transfer matrix calculation with the dimension of the transfer matrix growing roughly as 3^l. The number of parameters in the function f also grows like 3^l. The resulting variational bounds are shown in table 1. The most accurate numerical estimate of the ground-state energy is that of White and Huse [11], based on a density matrix formulation of the renormalization group introduced by White [12]. They obtain −1.401 484 038 971(4) for the energy. The best estimate based on extrapolations of finite-chain exact diagonalizations is −1.401 485(2) [13]. Our best variational bound agrees with the numerical values up to the fifth decimal place.

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