Exact symmetry breaking ground states for quantum spin chains

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We introduce a family of spin-1/2 quantum chains, and show that their exact ground states break the rotational and translational symmetries of the original Hamiltonian. We also show how one can use projection to construct a spin-3/2 quantum chain with nearest neighbor interaction, whose exact ground states break the rotational symmetry of the Hamiltonian. Correlation functions of both models are determined in closed form. Although we confine ourselves to examples, the method can easily be adapted to encompass more general models.

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The question of exact ground state of a given quantum many body system, i.e. a quantum spin chain, has always been fascinating and of great importance to physicists in all fields, from condensed matter physics and statistical mechanics to mathematical physics and quantum field theory \cite{1-3}. Besides their inherent interest as theoretical laboratory, where the phenomenon of quantum phase transition \cite{4} can be studied in detail and in analytical form, quantum spin chains provide an important link with classical statistical mechanics on two dimensional lattice models, the latter is a subject with a rich and fascinating variety of cooperative and critical phenomena affording insights into many properties of real physical, chemical and biological systems.

As prototypes of correlated many-body systems, the Hilbert space dimension of quantum spin chains grows exponentially with system size, rendering any numerical treatment of large systems extremely difficult. Therefore any exact solution of a new quantum spin chain, is not only valuable for its own specific characteristics, but may be adapted to encompass more general models.

In this letter, we introduce a new model and technique for constructing exact ground states of quantum spin chains which spontaneously break the symmetries of the parent Hamiltonian. The method is inspired by the original work of Affleck, Kennedy, Lieb and Tasaki who first introduced it for constructing exact invariant ground states for certain quantum chains \cite{5}. Their method, designed in the context of valence bond solids, led in the course of time to the formalism of finitely correlated or matrix product states \cite{6}. The model we introduce is a spin 1/2 quantum system on a ring, with interaction range equal to 4, having both translational and rotational symmetry, nevertheless we show that its exact ground states break both these symmetries. We also find the exact maximum energy state and some of the exact excited states, a progress which has not been reported for any of the models constructed in the AKLT or the matrix product formalism \cite{7-10}. Finally we use this construction to introduce another quantum spin chain, namely a spin 3/2 quantum chain with nearest neighbor interaction, with symmetry breaking ground states. We should stress that although we do this for a specific model with rotational and translational symmetry, our method can be adapted for construction of a broader class of similar models.

Let us first fix our notation: we use $|\pm\rangle$ and $|S\rangle := \frac{1}{\sqrt{2}}(|+, -\rangle - |-, +\rangle)$ to denote respectively the spin up, spin down and a singlet state of two spins. Subscripts indicate the sites of the lattice, thus $|S_{12}, +\rangle$ indicates a singlet on sites 1 and 2 and a spin up state on site 3. Consider the state

$$|\phi_0\rangle := |S_{12}, +\rangle_S |S_{45}, +\rangle_S \cdots |S_{N-2}, +\rangle_S |S_{N-1}, +\rangle_S,$$

shown in figure (1). We require that $|\phi_0\rangle$ be the exact ground state of a spin chain Hamiltonian $H = \sum_{k=1}^{3N} h_{k,k+1,k+2,k+3}$, where we use periodic boundary conditions. To this end, we demand that the local Hamiltonian $h$ be a positive operator and annihilate $|\phi_0\rangle$. A local Hamiltonian $h$ finds four adjacent spins only in one of the mixed states shown in figure (1). Thus, we should have

$$tr[h(|S\rangle \langle S| \otimes |+\rangle \langle +| \otimes I)] = 0,$$

$$\langle +|s|S\rangle = 0,$$

$$tr[h(I \otimes |+\rangle \langle +| \otimes |S\rangle \langle S|)] = 0.$$  \hspace{1cm} (2)

Since $|S\rangle$ is a singlet, the state $|+\rangle|S\rangle$, can be written as a linear combination of states with total spin 0 and 1. Therefore a projector $P_2$ which projects the product of four adjacent spins on the the sector with total spin 2, automatically satisfies equations (2). However there is one other projector which satisfies equations (2), and its annihilation of these states is quite nontrivial. This is the projector $P_0 := |\chi\rangle \langle \chi|$, where $|\chi\rangle$ (or its embedding on sites 1,2,3 and 4) is a singlet of four spins constructed as follows:

$$|\chi\rangle = |S_{14}, S_{23}\rangle + |S_{13}, S_{24}\rangle.$$ \hspace{1cm} (3)

To show this we use the simple fact that

$$|\chi\rangle = |S_{14}, S_{23}\rangle + |S_{13}, S_{24}|
Similarly one finds that the last equations of (2) are satisfied. For the second relation we note that

\[ \langle +1 | S_{12} \rangle = \frac{1}{\sqrt{2}} | -2 \rangle, \quad \langle -1 | S_{12} \rangle = -\frac{1}{\sqrt{2}} | +2 \rangle, \]

to arrive at the identity

\[ \langle S_{23} | S_{12}, S_{34} \rangle = -\frac{1}{2} | S_{14} \rangle, \]

where 1, 2, 3 and 4 are any four different indices. From this identity one can easily derive other identities simply by permuting indices in an appropriate way, namely

\[ \langle S_{14} | S_{12}, S_{34} \rangle = \frac{1}{2} | S_{12} \rangle, \quad \langle S_{34} | S_{13}, S_{24} \rangle = \frac{1}{2} | S_{12} \rangle. \]

These two identities, immediately imply that \( \langle S_{14} | \chi \rangle = 0 \). Similarly one finds \( \langle S_{12} | \chi \rangle = 0 \), hence the first and the last equations of (2) are satisfied. For the second relation of equation (2) we note that

\[ \langle \chi | S_{23} \rangle = \langle S_{14}, S_{23} | S_{23} \rangle + \langle S_{13}, S_{24} | S_{23} \rangle = \frac{3}{2} | S_{14} \rangle, \]

hence

\[ \langle \chi | +1, S_{23}, +4 \rangle = \frac{3}{2} | S_{14} | +1, +4 \rangle = 0. \]

This proves the assertion that \( P_0 \) annihilates all three kinds of local states. Thus, we find that the local Hamiltonian can be of the form \( h = 2 J P_2 + P_0 \), where \( J \) is a positive but arbitrary coupling constant, the factor of 2 is for convenience and one of the couplings, the coefficient of \( P_0 \), has been re-scaled to unity. The final form of the Hamiltonian in terms of spin operators can be found as follows. First we note that \( \frac{3}{2} \otimes 4 = 2 \oplus 1 \oplus 0 \) where the exponents indicate the multiplicities and \( P_0 \) is the projector to one of the above two zeros. Let us denote the sum of spin-\( j \) projectors in the above decomposition by \( P_j \). Then, from \( S \cdot S = \sum_j j(j + 1) P_j \), where \( S \) is the spin operator of four consecutive sites, we have

\[ I = P_0 + P_1 + P_2, \]
\[ S \cdot S = 2 P_1 + 6 P_2, \]
\[ (S \cdot S)^2 = 4 P_1 + 36 P_2, \]

from which we obtain

\[ P_0 = 1 - \frac{2}{3} S \cdot S + \frac{1}{12} (S \cdot S)^2, \]
\[ P_2 = -\frac{1}{12} S \cdot S + \frac{1}{24} (S \cdot S)^2. \]

This readily gives \( P_2 = (P_2) \) in terms of spin operators. However, the individual projector \( P_0 \) can not be obtained in this way. Direct calculation from (3) is notoriously tedious. We can circumvent this problem by calculating the other projector \( P'_0 = | \chi^{+} \rangle \langle \chi^{+} | \) and subtract it from \( P_0 \) to obtain \( P_0 \). It is straightforward to check from (4) that the other singlet which should be perpendicular to \( | \chi \rangle \) is the following

\[ | \chi^{+} \rangle = | S_{12}, S_{34} \rangle. \]

This readily gives

\[ P_0 = P_0 - | \chi^{+} \rangle \langle \chi^{+} | = P_0 - \left( \frac{1}{4} - s_1 \cdot s_2 \right) \left( \frac{1}{4} - s_3 \cdot s_4 \right). \]

Putting all these together, and discarding overal constants, we find

\[ H = \sum_{i=1}^{3N} s_i \cdot s_{i+1} (1 - 2 s_{i+2} \cdot s_{i+3}) \]
\[ - \frac{4 + J}{3} s_1 \cdot s_4 + \frac{1 + J}{6} \right( s_1 \cdot s_4 \right)^2, \]

where \( s_i \) is the spin operator of one site and \( S_i \) is the spin operator of a block of four spins at sites \( i, i+1, i+2, i+3 \). Note that the relative strength of consecutive couplings are approximately 1: 0.48: 0.06.

The state \( | \phi_0 \rangle \) is the exact ground state of \( H \) which breaks translational and rotational symmetry of the Hamiltonian. Clearly, it is not invariant under rotation, it is the top state of the total spin-\( \frac{N}{2} \) sector, other states which are degenerate with it in energy, are obtained by acting with total \( L_z = \sum_{k=1}^{3N} \sigma_k^z \) operator, which does not affects the singlets but flips the up spins. None of these \( N + 1 \) states, are invariant under translation. Thus the ground state has a \( 3(N + 1) \) fold degeneracy, generated by the broken symmetries of the Hamiltonian, namely the continuous \( so(3) \) symmetry and the discrete translational symmetry. To find translational invariant states, we form the states \( | \Psi^j \rangle, j = 0, 1, 2 \) as follows:

\[ | \Psi^j \rangle := \frac{1}{\sqrt{3}} (| \phi_0 \rangle + \omega^j | \phi_1 \rangle + \omega^{2j} | \phi_2 \rangle), \]

where \( \omega^3 = 1 \), and \( | \phi_i \rangle = T | \phi_{i-1} \rangle \), where \( T \) is the one-site translation operator, figure (2). These states are eigenstates of \( T \), with eigenvalues 1, \( \omega \) and \( \omega^2 \) respectively.
One can readily show that for \( i \neq j \),
\[
\langle \phi_i | \phi_j \rangle = ((+, S | S_i +))^N = \left( \frac{-1}{2} \right)^N,
\]
from which we find the states \(| \Psi^j \rangle \) are normalized in the thermodynamic limit. In this same limit, the correlation functions are easy to find. First the magnetization turns out to be
\[
\langle \Psi^j | S^z | \Psi^j \rangle = \frac{1}{6}, \quad \forall \ j.
\]
and the two-point correlation function becomes
\[
\langle \Psi^j | S_i^z S_j^z | \Psi^j \rangle = \frac{1}{12} \delta_{r,2} - \sum_{n=1}^{N} \delta_{r,3n+1},
\]
\[
\langle \Psi^j | S_i^x S_j^x | \Psi^j \rangle = -\frac{1}{12} \delta_{r,2}, \quad \forall j.
\]
We now ask if it is possible to find some of the exact excited states of the Hamiltonian. We will show that this is indeed possible, although the states thus found are not the low-lying states of the energy spectrum. To proceed, we note that the state
\[
| \Omega \rangle := | +, +, +, \cdots, +, + \rangle,
\]
is an exact energy eigenstate, indeed the maximum energy eigenstate with \( E_{\text{max}} = 6NJ \) (here we are working with \( h = 2JP_2 + P_0 \) and not with (10), in which multiplicative and additive constants have been ignored). To see this note that \( P_0 | \Omega \rangle = 0 \) and \( P_2 | \Omega \rangle = | \Omega \rangle \). The maximality of the energy is found by taking \( J \) very large and noting the continuity of the energy with respect to \( J \). Consider now the one "hole" state of the form
\[
| n \rangle = | +, +, \cdots, -, \cdots, +, + \rangle,
\]
where the state in the \( n - th \) position has been flipped. A general one-hole state is of the form
\[
| \psi^r \rangle = \sum_{n=1}^{3N} \psi_n^r | n \rangle.
\]
It is obvious that \( P_0 | n \rangle = 0 \), for any embedding of projection \( P_0 \) on four consecutive sites. To see this, note that the total \( z \) component of each four consecutive spins is either 2 or 1. Also from the explicit form of the spin-2 states, one can check that \( P_2 \) does not take a state \(| n \rangle \) outside the one-hole sector. In fact, a simple calculation shows that
\[
H | n \rangle = 6J(N - 1) | n \rangle + \frac{J}{2} \sum_{k=1}^{3} (4 - k)(| n + k \rangle + | n - k \rangle).
\]
Inserting this in the eigenvalue equation \( H | \psi^r \rangle = E_r | \psi^r \rangle \), gives
\[
(E_{\text{max}} - E_r)/BJ = \frac{1}{2} \sum_{i=1}^{N} \frac{81}{8} S_i \cdot S_{i+1} + \frac{29}{6} (S_i \cdot S_{i+1})^2 + \frac{2}{3} (S_i \cdot S_{i+1})^3,
\]
where $C = \frac{165}{142} N$. In this way, we construct a rotationally invariant Hamiltonian whose exact ground state breaks this rotational symmetry. The remarkable point is that we can also obtain the explicit form of this state, beyond the construction shown in figure (4). With this explicit expression one can then determine the correlations in this state which are no longer restricted to nearest neighbor sites. To achieve this, let us first construct a Matrix Product (MP) representation for the parent (upper) dimer state in figure (4). In view of the MP representation [10] of dimerized Majumdar-Ghosh state [11], this state has the following representation:

$$|\phi_0\rangle = tr(A_{i_1} A_{i_2} B_{i_3} A_{i_4} A_{i_5} B_{i_6} \cdots |i_1, i_2, i_3, i_4, i_5, i_6, \cdots\rangle)$$

where

$$A_+ = |+\rangle\langle 0 | + |0\rangle\langle -|,$$

$$A_- = |-\rangle\langle 0 | - |0\rangle\langle +|,$$

$$B_+ = |0\rangle\langle 0 |,$$

$$B_- = 0,$$

and $|+, -\rangle$ and $|0\rangle$ are three orthonormal states. Using the Clebsh-Gordon coefficients to decompose the product of three states in a bulk of the upper chain in figure (4) and noting that $B_- = 0$, we find the following matrices corresponding to the states of a single spin 3/2 site on the lower chain:

$$A_{3/2} = A_+ B_+ A_+,$$

$$A_{1/2} = \frac{1}{\sqrt{3}}(A_+ B_+ A_+ + A_+ B_+ A_-),$$

$$A_{-3/2} = 0,$$

$$A_{-1/2} = \frac{1}{\sqrt{3}}A_+ B_+ A_-,$$

leading to

$$A_{3/2} = \sigma^+, \quad A_{1/2} = -\frac{1}{\sqrt{3}}\sigma_z, \quad A_{-1/2} = -\frac{1}{\sqrt{3}}\sigma_z, \quad A_{-3/2} = 0.$$

The state of the lower chain is now given by a matrix product state, with the above matrices. The ground state is a multiplet with total spin $\frac{3}{2}$.

$$\langle S^2 \rangle = \frac{5}{4} - u, \quad \langle S^x \rangle = \langle S^y \rangle = 0,$$

where $u := \frac{1}{2(2+\sqrt{3})}$. With the notation $G^a(1, r) := \langle S^a S^a_r \rangle - \langle S^a \rangle \langle S^a_r \rangle$, we have

$$G^2(1, r) = A_t(-1)^{r-1} e^{-\frac{v}{2}}, \quad G^4(1, r) = A_t(-1)^{r-1} e^{-\frac{v}{2}},$$

where

$$A_t := \frac{12 + 6\sqrt{3}}{4}, \quad A_v := \frac{12 + 7\sqrt{3}}{4}$$

and

$$\xi_t = \frac{1}{\ln(2 + \sqrt{3})}, \quad \xi_t = \frac{1}{\ln(2 + \sqrt{3})}$$

The correlation functions for other states in the ground state multiplet can be determined by the application of rotational symmetry. In summary, we have introduced a one-parameter family of isotropic spin 1/2 quantum chains, whose exact ground states break the translational and rotational symmetry of the Hamiltonian. The totality of degenerate vacua of these models are generated by the application of rotation and translation operators. Besides the ground state, the maximum energy state and some of the lower energy states have also been derived in closed analytical form. A related spin 3/2 quantum chain with nearest neighbor interactions has also been constructed, the exact ground state of which has an MP representation. The method presented in this letter can be pursued further, to make other spin models whose ground state break the rotational symmetry of the Hamiltonian. There is also an interesting un-answered question which deserve further investigation: Is there a singlet state which is invariant under rotation and has a higher energy than the degenerate ground states [13]? V. K. would like to thank Laleh Memarzadeh for very valuable and constructive discussions. S. A. and S.B. would also thank Ali Rezakhani for valuable discussions.

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[13] Direct and lengthy calculation shows that for a ring of size 4, \( |\alpha\rangle := |S_{14}, S_{23}\rangle - |S_{12}, S_{34}\rangle \) and \( |\beta\rangle := |S_{13}, S_{24}\rangle \) are eigenstates with energies 1 and 3 resp. and for a ring of size 6, \( |\gamma\rangle = |S_{16}, S_{25}, S_{34}\rangle - 2|S_{12}, S_{36}, S_{45}\rangle + |S_{14}, S_{23}, S_{56}\rangle \) is an eigenstate with energy 2.