Singlet ground states of the bilinear-biquadratic exchange Hamiltonian with reflection symmetry

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Abstract. We apply the Lieb-Schupp method to the isotropic spin-S Hamiltonian with bilinear (\(-J/S^2\)) and biquadratic (\(-J'/S^4\)) exchange interactions on finite lattices with reflection-symmetry to prove that finite volume ground states of the models are spin singlet in the parameter region \(J' \geq 2S^2J, J' \geq 0\).

1. Introduction

Frustration in magnetic systems may arise due to the lattice geometries and competing interactions. Typical models of the geometrically frustrated magnets are antiferromagnetic Heisenberg model on triangular, kagome, or pyrochlore lattice, and one with competing interactions are the axial-next-nearest-neighbor Heisenberg model or the multiple-spin exchange model. These quantum magnets are known to possess interesting phenomena which are quite different from non-frustrated magnetic systems, but the accurate method of theoretical investigations for the properties of frustrated quantum magnets are less limited than non-frustrated and/or classical cases.

The Marshall-Lieb-Mattis theorem is one of the most famous exact results of the quantum spin systems, and it proves ordering energy levels for a large class of the Heisenberg model on finite size bipartite lattices. In the case of antiferromagnetic Heisenberg model this theorem states that the model on a bipartite lattice which contains the same number of sublattice points has a unique spin singlet ground state. But this theorem is not applicable to the model on non-bipartite lattices (frustrated lattices). In 1999 Lieb-Schupp succeeded in a proof of the spin singlet ground states of the model on two dimensional frustrated pyrochlore checkerboard lattice \([1, 2]\). Their method use reflection symmetry of Hamiltonian, on the other hand, the Marshall-Lieb-Mattis theorem is based on the Perron-Frobenius theorem. So their method can be applied to a class of frustrated spin systems satisfying reflection symmetry, but can not conclude the uniqueness of the ground state.

In this study we treat the spin-S isotropic bilinear-biquadratic exchange Hamiltonian:

\[
\mathcal{H} = -\frac{J}{S^2} \sum_{\langle x,y \rangle} \mathbf{S}(x) \cdot \mathbf{S}(y) - \frac{J'}{S^4} \sum_{\langle x,y \rangle} (\mathbf{S}(x) \cdot \mathbf{S}(y))^2
\]

(1)

as one of the models with competing interactions. In the case of Hamiltonian (1) with \(S = 1\) on the linear chain, infinite volume ground state of Hamiltonian (1) in the region \(J' > \pm J > 0\) is
considered to be dimer phase. Competition between bilinear and biquadratic interactions may induce broken translational invariance in spite that Hamiltonian (1) has translational invariance. On the other hand, finite volume ground state in \( J^\prime > J, \ J^\prime \geq 0 \ (J \neq 0) \) including that dimer phase region is proved to be unique spin singlet with the Marshall-Lieb-Mattis type argument [3, 4, 5]. For \( S > 1 \) the same result is established in the region \( 0 \leq J^\prime \leq -SJ/2(S - 1) \) [3].

Our purpose is to show that, with the Lieb-Schupp method, finite volume ground states of Hamiltonian (1) are spin singlet in the region \( J^\prime \geq 2S^2J, \ J^\prime \geq 0 \).

2. Model and its reflection symmetry

Let us consider finite lattices \( \Lambda = \Lambda_L \cup \Lambda_C \cup \Lambda_R \) with reflection symmetry which have an even number of independent sites and the property that it can be split in two equal parts \( \Lambda_L \) and \( \Lambda_R \) that are mirror images of one another about a symmetry plane without sites that cuts bonds \( (x, y) \) with \( x \in \Lambda_L \) and \( y \in \Lambda_R \) which is denoted by \( \Lambda_C \) [2]. With each sites \( x \in \Lambda \), we associate the spin-S operator \( \mathbf{S}(x) = (S_1(x), S_2(x), S_3(x)) \) with \( S(S+1) \) and satisfies the commutation relation \( [S_i(x), S_j(y)] = i\epsilon_{ijk}S_k(x)\delta_{xy} \). Here we use the usual basis in which \( S_3(x) \) is diagonalized, \( S_1(x) \) and \( S_3(x) \) have real matrix elements, and \( S_2(x) \) pure imaginary. In this study we consider that the spin model described by Hamiltonian (1) on \( \Lambda \). The summation in Hamiltonian (1) is all over nearest-neighbor pairs in \( \Lambda \).

For the following discussion let us introduce quadrupole operators:

\[
O_{2,0}(x) = \frac{1}{2} \left( 3S_3^2(x) - S(S+1) \right),
\]

\[
O_{2,\pm 1}(x) = \pm \sqrt{\frac{3}{2}} \left( S_3(x)S_3^\pm(x) + S_3^+(x)S_3(x) \right),
\]

\[
O_{2,\pm 2}(x) = \frac{1}{2} \sqrt{\frac{3}{2}} \left( S_3^\pm(x) \right)^2,
\]

where \( S^+(x) \) and \( S^-(x) \) are the usual spin raising and lowering operators defined by

\[
S^\pm(x) = S_1(x) \pm iS_2(x).
\]

Quadrupole operators satisfy the relation:

\[
\sum_{q=-2}^{2} O_{2,q}(x)O_{2,q}^\dagger(y) = \frac{3}{2} (\mathbf{S}(x) \cdot \mathbf{S}(y))^2 + \frac{3}{4} \mathbf{S}(x) \cdot \mathbf{S}(y) - \frac{1}{2} S^2(S+1)^2,
\]

and then Hamiltonian (1) is written as

\[
\mathcal{H} = J_D \sum_{(x,y)} \mathbf{S}(x) \cdot \mathbf{S}(y) - J_Q \sum_{(x,y)} \sum_{q=-2}^2 O_{2,q}(x)O_{2,q}^\dagger(y)
\]

with

\[
J_D = -\frac{J}{S^2} + \frac{1}{2} J^\prime, \quad J_Q = \frac{2}{3} \frac{J^\prime}{S^4}.
\]

Now we decompose Hamiltonian (7) as follows.

\[
\mathcal{H} = \mathcal{H}_L + \mathcal{H}_R + \mathcal{H}_C.
\]
Here $\mathcal{H}_L$, $\mathcal{H}_R$, and $\mathcal{H}_C$ is a collection of interactions on $(x, y) \in \Lambda_L$, $\Lambda_R$, and $\Lambda_C$, respectively. The right-hand side of equation (9) is unitarily transformed to

$$U^\dagger \mathcal{H} U = \mathcal{H}_L + \mathcal{H}_R - J_D \sum_{(x,y) \in \Lambda_C} \sum_{i=1}^3 T_i(x)T_i(y) - J_Q \sum_{(x,y) \in \Lambda_C} \sum_{q=-2}^2 O_{2,q}(x)O_{2,q}(y)$$

(10)

with

$$U = \exp \left( i\pi \sum_{x \in \Lambda_R} S_2(x) \right)$$

(11)

and $T_1(x) = S_1(x)$, $iT_2(x) = S_2(x)$, $T_3(x) = S_3(x)$, where we have used

$$U^\dagger S_1(x)U = -S_1(x),$$

$$U^\dagger S_2(x)U = S_2(x),$$

$$U^\dagger S_3(x)U = -S_3(x),$$

$$U^\dagger O_{2,q}^\dagger(x)U = O_{2,q}(x),$$

(12)-(15)

for $x \in \Lambda_R$.

Let us write a ground state

$$\psi = \sum_{\alpha, \beta} c_{\alpha \beta} \psi^L_\alpha \otimes \psi^R_\beta$$

(16)

of this Hamiltonian with a coefficient matrix $c_{\alpha \beta}$, where $\psi^L_\alpha$ form a real orthonormal basis of $S_3$ eigenstate for $\mathcal{H}_L$ and $\psi^R_\beta$ is the corresponding state for $\mathcal{H}_R$.

Let us consider the ground state energy of Hamiltonian (10), we have

$$\langle \psi | \mathcal{H} | \psi \rangle = \text{Tr} c^\dagger \mathcal{H}_L + \text{Tr} c^\dagger \mathcal{H}_R - J_D \sum_{(x,y) \in \Lambda_C} \sum_{i=1}^3 \text{Tr} c^\dagger T_i(x)cT_i^\dagger(y) - J_Q \sum_{(x,y) \in \Lambda_C} \sum_{q=-2}^2 \text{Tr} c^\dagger O_{2,q}(x)cO_{2,q}^\dagger(y).$$

(17)

We note that Hamiltonian (10) is left-right symmetric and operators appearing in it have real matrix elements. Then following the arguments in the papers [1, 2, 6, 7], we can see that an eigenstate with Hermite coefficient matrix $c = c^\dagger$ is also a ground state, and the third and forth term in the right-hand side of equation (17) are written as

$$-J_D \sum_{(x,y) \in \Lambda_C} \sum_{i=1}^3 \sum_{k,l} c_k c_l |(T_i(x))_{kl}|^2 - J_Q \sum_{(x,y) \in \Lambda_C} \sum_{q=-2}^2 \sum_{k,l} c_k c_l |(O_{2,q}(x))_{kl}|^2$$

(18)

in the diagonal basis of $c$. This expression is bounded below by

$$-J_D \sum_{(x,y) \in \Lambda_C} \sum_{i=1}^3 \sum_{k,l} |c_k| |c_l| |(T_i(x))_{kl}|^2 - J_Q \sum_{(x,y) \in \Lambda_C} \sum_{q=-2}^2 \sum_{k,l} |c_k| |c_l| |(O_{2,q}(x))_{kl}|^2,$$

(19)

if $J_D \geq 0$, $J_Q \geq 0$. So we confirm that an eigenstate with positive semidefinite coefficient matrix $|c| = \sqrt{c^2}$ is a ground state.
3. Spin singlet ground state

In this section, at first we will prove that a ground state with positive semidefinite coefficient matrix \(|c|\) is spin singlet.

Now we consider a tensor product of spin singlet state

\[
\psi_0 = \bigotimes_{x \in \Lambda_L} \sum_{M=-S}^S (-1)^{S-M} |S, M \rangle_x \otimes |S, -M \rangle_{x'}. \tag{20}
\]

where \(x' \in \Lambda_R\) is the reflection of \(x \in \Lambda_L\) in the symmetry plane on \(\Lambda_C\) and \(M\) is eigenvalue of \(S_3(x)\). We can easily check the overlap of \(\psi_0\) with a ground state with positive semidefinite coefficient matrix \(|c|\) takes non-zero value. Furthermore, since \(\psi_0\) has total spin zero and total spin is a good quantum number of this Hamiltonian, this facts imply that there is at least one ground state with total spin zero in the region \(J_D \geq 0, J_Q \geq 0\).

Next, we will show that all ground states of this model are spin singlet. Let \(b(x)\) be a real valued function on each site \(x\). Then we consider the Hamiltonian in magnetic field of arbitrary amplitude for each site given by

\[
\tilde{H}(b(x)) = -J_D \sum_{(x,y)} \left\{ T_1(x)T_1(y) + T_2(x)T_2(y) + (T_3(x) - b(x))(T_3(y) - b(y)) \right\} + \frac{1}{2} \left[ T_3^2(x) - (T_3(x) - b(x))^2 + T_3^2(y) - (T_3(y) - b(y))^2 \right] \right\} - J_Q \sum_{(x,y)} O_{2,q}(x)O_{2,q}(y). \tag{21}
\]

Following the argument of Kennedy-Lieb-Shastry \[7, 8\], we get inequality

\[
E(b(x)) \geq E(0) \tag{22}
\]

concerning for the ground state energy of \(\tilde{H}(b)\) in \(J_D \geq 0, J_Q \geq 0\).

When we choose

\[
b(x) = \begin{cases} b & x \in \Lambda_L \\ -b & x \in \Lambda_R, \end{cases} \tag{23}
\]

we see

\[
U\tilde{H}(b)U^\dagger = H - 2bJ_D \sum_{x \in \Lambda_C} S_3(x). \tag{24}
\]

Let \(\psi(b)\) be a ground state of \(\tilde{H}(b)\). By the variational principle and inequality (22), we have

\[
\langle \psi(0) | \tilde{H}(b) | \psi(0) \rangle \geq \langle \psi(b) | \tilde{H}(b) | \psi(b) \rangle = E(b) \geq E(0), \tag{25}
\]

which leads to

\[
-2bJ_D \sum_{x \in \Lambda_C} \langle \psi(0) | S_3(x) | \psi(0) \rangle = 0. \tag{26}
\]

This result is independent of value of \(b\). Thus we can conclude \(\sum_{x \in \Lambda_C} \langle \psi(0) | S_3(x) | \psi(0) \rangle = 0\).

We impose a periodic boundary condition in the direction perpendicular to the symmetry plane on \(\Lambda_C\), and then we have \(S_3^{\text{tot}} = \sum_{x \in \Lambda} \langle \psi(0) | S_3(x) | \psi(0) \rangle = 0\). This result also holds for \(S_1^{\text{tot}}\) and \(S_2^{\text{tot}}\). So it implies that all ground states have total spin zero.
4. Summary and Discussions

We have proved that ground states of Hamiltonian (1) on reflection symmetric lattices \( \Lambda \) with a periodic boundary condition in the one direction have total spin zero in the region \( J_D \geq 0, J_Q \geq 0 \) or \( J' \geq 2S^2J, J' \geq 0 \).

For \( S = 1 \) the results of Marshall-Lieb-Mattis type argument based on the Perron-Frobenius theorem state that the ground state is unique spin singlet in the region \( J' > J, J' \geq 0 (J \neq 0) \) \[3, 4, 5\]. Our result can not conclude the uniqueness of the ground state, but these results of previous studies assure it in that parameter region. At \( J' > 0, J = 0 \), there may exist multiple degeneracy on the ground state \[5\]. Our results also conclude that these degenerate ground states are spin singlet.

For \( S > 1 \) the result in reference \[3\] gives that the ground state is unique spin singlet in the region \( 0 \leq J' \leq -SJ/2(S - 1) \). Our results extend the region which one can conclude singlet ground states without uniqueness. In the region \( J > 0, J' > 0 \) the Marshall-Lieb-Mattis type argument can not give any conclusions as far as we know. This argument works well when we can find suitable unitary transformation which leads to signs of off-diagonal matrix elements of irreducible unitarily transformed Hamiltonian satisfying the Perron-Frobenius theorem. But there is no systematic method available to find it so far. The results for \( S = 1 \) in reference \[4, 5\] are established by using special commutation relations between quadrupole operators which hold only for \( S = 1 \). So straightforward extension of the Marshall-Lieb-Mattis type argument to the case of \( S > 1 \) seems to be difficult.

By the variational principle, we can easily check that the ground state becomes saturated ferromagnetic state for \( 0 < J' < SJ \) \[9\]. For \( S > 1 \) in the region \( SJ < J' < 2S^2J \) what types of ground states realize are not clear. Furthermore the Lieb-Schupp method can not conclude the uniqueness of the ground state. We hope that these problems will be resolved by other technique.

Finally we shall comment on the extension of our results to the case of geometrically frustrated lattice. In section 2 we explained the properties of \( \Lambda \), whose typical examples are \( d \)-dimensional hypercubic and honeycomb lattices. Figure 1-(b) without crossing bonds (1/5-depleted lattice) also clearly has reflection symmetry. In this case we can consider a symmetry plane which cuts plaquettes without sites. Our results for Hamiltonian (1) on the reflection symmetric lattices with bipartiteness can be extended to the case of the lattices containing the structure of plaquettes with crossing bond. Spin models on the square lattice with second neighbor interaction which are the so called ‘\( J_1 - J_2 \) model’ and figure 1-(a) is its checkerboard version. Figure 1-(b) is 1/5-depleted lattice with the structure of plaquettes with crossing bond. Here we
set $J_1^D(J_1^Q)$ and $J_2^D(J_2^Q)$ is first and second neighbor dipole (quadrupole) interaction, respectively. Through a similar procedure in section 2 and 3, we can conclude that our results also hold in the region $|J_2^D| \leq J_1^D/2$ and $|J_2^Q| \leq J_1^Q/2$. These conditions originate from the expression of interaction terms on plaquettes with crossing bond satisfying reflection symmetry so as to get a similar lower bound to (19) [1, 2, 10] and a similar inequality to (22) [7, 8, 10].

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