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Order Parameters in XXZ-Type Spin $\frac{1}{2}$ Quantum Models with Gibbsian Ground States

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Abstract. A class of general spin $\frac{1}{2}$ lattice models on hyper-cubic lattice Z^d, whose Hamiltonians are sums of two functions depending on the Pauli matrices S^1, S^2 and S^3, respectively, are found, which have Gibbsian eigen (ground) states and two order parameters for two spin components x, z simultaneously for large values of the parameter α playing the role of the inverse temperature. It is shown that the ferromagnetic order in x direction exists for all dimensions $d \geq 1$ for a wide class of considered models (a proof is remarkably simple).

Key words: Gibbsian eigen (ground) states; quantum spin models

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1 Introduction and main result

The existence of several long-range orders (lro's) and order parameters in quantum many-body systems is an important problem which is the first step towards a description of their phase diagrams.

In our previous paper [1] we found a class of quantum spin $\frac{1}{2}$ XZ-type systems on the hyper-cubic lattice $\mathbb{Z}^d$ with a Gibbsian ground state, characterized by the classical spin potential energy $U_0(s_\Lambda)$, in which two lro's can occur for the spin operators S^1 and S^3 in a dimension greater than one. In such the systems there is always the ferromagnetic lro for S^1 even for $d = 1$ if a simple condition for U_0 holds. The Hamiltonians, determined as symmetric matrices in the $2|\Lambda|$ dimensional complex Hilbert space $\mathbb{C}^{2|\Lambda|}$ with the Euclidean scalar product $(\cdot, \cdot)$, were given by

$$H_\Lambda = \sum_{A\subset\Lambda,|A|>0} J_A P_A, \qquad J_A \leq 0, \qquad P_A = S^1_{[A]} - e^{-\frac{\alpha}{2}W_A(S^3_\Lambda)}, \qquad S^1_{[A]} = \prod_{x\in A} S^1_x,$$
$$W_A(S^3_\Lambda) = U_0\big(S^{3A}_\Lambda\big) - U_0\big(S^3_\Lambda\big), \qquad S^{3A}_\Lambda = \big(S^3_{\Lambda\backslash A}, -S^3_A\big). \tag{1}$$

J_A are real numbers, S^1_x, S^3_x, $x \in \mathbb{Z}^d$ are the 'unity' Pauli matrices, $\Lambda \subset \mathbb{Z}^d$ is a hypercube with a finite cardinality $|\Lambda|$ (number of sites). S^1 is diagonal and $S^3_{1,1} = -S^3_{2,2} = 1$. S^1 has zero diagonal elements and $S^1_{1,2} = S^1_{2,1} = 1$. The matrices at different sites commute. $S^l_{[A]}$ is the abbreviated notation for the tensor product of the matrices S^l_x, $x \in A$ and the unity matrices I_x, $x \in \Lambda\backslash A$.

The Gibbsian non-normalized state Ψ_Λ is given by

$$\Psi_\Lambda = \sum_{s_\Lambda} e^{-\frac{\alpha}{2}U_0(s_\Lambda)}\Psi^0_\Lambda(s_\Lambda), \qquad \alpha \in \mathbb{R}^+, \tag{2}$$

where the summation is performed over $(\times(-1,1))^{|\Lambda|}$,

$$\Psi^0_\Lambda(s_\Lambda) = \otimes_{x\in\Lambda}\psi_0(s_x), \qquad \psi_0(1) = (1,0), \qquad \psi_0(-1) = (0,1).$$

These systems differ from the XZ spin $\frac{1}{2}$ systems, which admit Gibbsian ground states considered in [2]. The potential energy of the associated classical Gibbsian system, which generates the ground state, is found there in the form of a perturbation expansion in a small parameter (an analog of α). The authors proved that there is the ferromagnetic lro for S^3 in the ground state in some of their ferromagnetic systems. Our proof of the S^1-lro is a simplified analog of their proof. Uniqueness of a Gibbsian translation invariant ground state is established in the thermodynamic limit for general XZ models with a sufficiently strong magnetic field in [3].

In [4] the classical Gibbsian states are identified with ground states of quantum Potts models. The structure of the considered Hamiltonians are close to the Hamiltonians of XZ spin systems which are represented as a sum of a diagonal and non-diagonal parts.

In this paper we consider the Hamiltonians

$$H_\Lambda = H_{0\Lambda} + V_\Lambda, \qquad H_{0\Lambda} = \sum_{\substack{A,\,A'\subseteq\Lambda,\\ A\cap A'=\varnothing}} \phi_{A,A'} S^1_{[A]} S^2_{[A']}, \tag{3}$$

where $\phi_{A,A'}$ are real valued coefficients, S^2 is the second Pauli matrix with the zero diagonal elements such that $S^2_{1,2} = -S^2_{2,1} = -i$ and V_Λ depends on S^3_Λ. We find the expression for V_Λ which guarantees that Ψ_Λ given by (2) is the eigen (ground) state. This result is a generalization of our previous result since with the help of (6) we reduce our Hamiltonian to the Hamiltonian (1) with J_A depending in S^3_Λ. Our result is summarized in the following theorem

Theorem. *Let V_Λ be given by*

$$V_\Lambda = -\sum_{A\subseteq\Lambda} J_A\big(S^3_A\big) e^{-\frac{\alpha}{2}W_A(S^3_\Lambda)}, \qquad J_A\big(S^3_A\big) = \sum_{A'\subseteq A} (-i)^{|A'|}\phi_{A\setminus A',A'} S^3_{[A']}. \tag{4}$$

Then

I. *Ψ_Λ is an eigenfunction of the Hamiltonian (3);*

II. *Ψ_Λ is its ground state if $\phi_{A,A'} = 0$ for odd $|A'|$ and $J_A \le 0$;*

III. *lro for S^1 occurs in the eigenstate Ψ_Λ if $\lim_{\Lambda\to\mathbb{Z}^d} W_A(s_\Lambda)$ exists for $|A| = 2$ and is uniformly bounded. Moreover, $\langle S^1_{[A]}\rangle_\Lambda \ge a > 0$, where a is a constant independent of Λ if $\lim_{\Lambda\to\mathbb{Z}^d} W_A(s_\Lambda)$ exists and is uniformly bounded.*

IV. *lro occurs for S^3 in the eigenstate Ψ_Λ if lro occurs in the classical spin system with the potential energy U_0.*

If $H_{0\Lambda}$ coincides with the Hamiltonian of the XX Heisenberg model

$$H_{0\Lambda} = \sum_{x,y\in\Lambda} \phi_{x,y}\big(S^1_x S^1_y + S^2_x S^2_y\big),$$

then it can be shown without difficulty, utilizing the equality $\big(S^3\big)^2 = I$, that for the following choice $U_0(s_\Lambda) = \sum_{x\in\Lambda} u_x s_x$ the matrix V_Λ in (4) is given by

$$V_\Lambda = \sum_{x,y\in\Lambda} \phi_{x,y}\left[S^3_x S^3_y \cosh\alpha(u_x - u_y) - (S^3_x - S^3_y)\sinh(\alpha(u_x - u_y)) - \cosh(\alpha(u_x - u_y))\right].$$

If one puts $\phi_{x,y} = \phi_{x-y}$, $\phi_x = \phi_{|x|} = 0$, $|x| \neq 1$, $\phi_1 = J$, $q = e^{\alpha}$ and

$$u_x = x^1 + \cdots + x^d, \qquad x = \left(x^1, \ldots, x^d\right)$$

then the following Hamiltonian of the XXZ Heisenberg model is derived

$$H_\Lambda = J \sum_{\langle x,y\rangle \in \Lambda} \left[S_x^1 S_y^1 + S_x^2 S_y^2 + \frac{q+q^{-1}}{2} S_x^3 S_y^3 \right] - 2J \sum_{\langle x<y\rangle \in \Lambda} \left[\frac{q-q^{-1}}{2}(S_x^3 - S_y^3) + \frac{q+q^{-1}}{2} \right],$$

where the summations are performed over nearest neighbor pairs and "$<$" means lexicographic order. It is remarkable that the term linear in S_x^3 contributes only on the boundary of Λ. These Hamiltonians coincide with the Hamiltonians proposed in [5, 6]. A reader may find out that the Gibbsian ground states of these Hamiltonians are not unique. Gibbsian ground states for a partial case of our Hamiltonians were considered in [7].

If F_A depends on S_A^3, S_A^1 then its expectation value in a state Ψ_Λ is given by

$$\langle F_A \rangle_\Lambda = (\Psi_\Lambda, \Psi_\Lambda)^{-1} \left(\Psi_\Lambda, F_A\left(S_A^1, S_A^3\right)\Psi_\Lambda\right),$$

where $(\cdot,\cdot)$ is the Euclidean scalar product on $\mathbb{C}^{2|\Lambda|}$. Ferromagnetic lro for S^l occurs if

$$\langle S_x^l S_y^l \rangle_\Lambda \geq a_l > 0, \tag{5}$$

where the constants a_l are independent of Λ. It implies that the magnetization M_Λ^l is an order parameter in the thermodynamic limit since

$$\langle (M_\Lambda^l)^2 \rangle_\Lambda \geq a_l > 0, \qquad M_\Lambda^l = |\Lambda|^{-1} \sum_{x\in\Lambda} S_x^l.$$

Besides, the inequality in the statement III of the Theorem for $|A| = 1$ implies that

$$\langle M_\Lambda^1 \rangle_\Lambda \geq a > 0.$$

It is well known that in the classical Ising model with a ferromagnetic short-range potential energy U_0, generated by the nearest neighbor bilinear pair potential, there is the ferromagnetic lro. Hence our quantum systems for such U_0 admit two order parameters M_Λ^l, $l = 1, 3$ in the thermodynamic limit for sufficiently large α since for such U_0 the condition in the statements III–IV of the Theorem is true. For small values of α the magnetization in the third direction vanishes for short-range pair interaction potentials.

The last statement of the theorem follows without difficulty since S^3 is a diagonal matrix and the ground state expectation value $\langle F_A \rangle_\Lambda$ of a function F_A depending on S_A^3 equals the classical Gibbsian expectation value of the same function depending on the classical spins s_A corresponding to the potential energy $U_0(s_\Lambda)$ and the "inverse temperature" α. The orthogonality of the basis

$$(\Psi_\Lambda^0(s_\Lambda), \Psi_\Lambda^0(s'_\Lambda)) = \prod_{x\in\Lambda} \delta_{s_x, s'_x},$$

where $\delta_{s,s'}$ is the Kronecker symbol, has to be applied for proving that.

The proofs of the second statement of the Theorem is based on the proof that H_Λ is positive definite. Its condition implies that the semigroup generated by H_Λ has positive matrix elements. As a result the operator

$$H_\Lambda^+ = e^{\frac{\alpha}{2} U_0(S_\Lambda^3)} H_\Lambda e^{-\frac{\alpha}{2} U_0(S_\Lambda^3)}.$$

generates a Markovian process with a stationary state. We show that it is symmetric and positive definite in the Euclidean scalar product with the operator weight $e^{-\alpha U_0(S^3_\Lambda)}$.

For sufficiently small α and a pair simple ferromagnetic interaction with $\phi_{A,A'}=0$ for $|A'|\neq 0$ lro at non-zero low temperature occurs for S^1 [8].

2 Proof of Theorem

It easy to check that

$$S^2=-iS^3S^1=iS^1S^3. \tag{6}$$

From this equality the following equalities are derived

$$S^2_{[A']}=(-i)^{|A'|}S^3_{[A']}S^1_{[A']},$$
$$H_{0\Lambda}=\sum_{\substack{A,\,A'\subseteq\Lambda,\\ A\cap A'=\varnothing}}(-i)^{|A'|}\phi_{A,A'}S^1_{[A]}S^3_{[A']}S^1_{[A']}=\sum_{\substack{A,\,A'\subseteq\Lambda,\\ A\cap A'=\varnothing}}(-i)^{|A'|}\phi_{A,A'}S^3_{[A']}S^1_{[A\cup A']}.$$

As a result

$$H_{0\Lambda}=\sum_{A\subseteq\Lambda}J_A(S^3_A)S^1_{[A]}. \tag{7}$$

(7) and (4) lead to the following expression for the Hamiltonian (3)

$$H_\Lambda=\sum_{A\subset\Lambda,\,|A|>0}J_A(S^3_A)P_A. \tag{8}$$

Proof of I. S^1 flips spins:

$$S^1_{[A]}\Psi^0_\Lambda(s_\Lambda)=\Psi^0_\Lambda(s^A_\Lambda)=\Psi^0_\Lambda(s_{\Lambda\setminus A},-s_A),\qquad S^3_x\Psi^0_\Lambda(s_\Lambda)=s_x\Psi^0_\Lambda(s_\Lambda).$$

These identities lead to

$$J_A\big(S^3_A\big)P_A\Psi_\Lambda=\sum_{s_\Lambda}\Big(J_A(-s_A)\Psi^0_\Lambda(s_{\Lambda\setminus A},-s_A)-J_A(s_A)e^{-\frac{\alpha}{2}W_A(s_\Lambda)}\Psi^0_\Lambda(s_\Lambda)\Big)\,e^{-\frac{\alpha}{2}U_0(s_\Lambda)}.$$

From the definition of W_A and after changing signs of the spin variables s_A in the first term in the sum it follows that

$$\begin{aligned}J_A\big(S^3_A\big)P_A\Psi_\Lambda&=\sum_{s_\Lambda}\Big[J_A(-s_A)\Psi^0_\Lambda(s_{\Lambda\setminus A},-s_A)e^{-\frac{\alpha}{2}U_0(s_\Lambda)}-J_A(s_A)\Psi^0_\Lambda(s_\Lambda)e^{-\frac{\alpha}{2}U_0(s^A_\Lambda)}\Big]\\ &=\sum_{s_\Lambda}J_A(s_A)\left(e^{-\frac{\alpha}{2}U_0(s^A_\Lambda)}-e^{-\frac{\alpha}{2}U_0(s^A_\Lambda)}\right)\Psi^0_\Lambda(s_\Lambda)=0.\end{aligned}$$

That is, every term in the sum for $H_\Lambda\Psi_\Lambda$ in (8) is equal to zero. This proves the statement.

Proof of II. It is necessary to prove that the Hamiltonian is positive-definite. For that purpose we'll use the operator H^+_Λ introduced in the introduction. It is not difficult to check on the basis Ψ^0_Λ that

$$H^+_\Lambda=\sum_{A\subseteq\Lambda}J_A\big(S^3_A\big)e^{-\frac{\alpha}{2}W_A(S^3_\Lambda)}\big(S^1_{[A]}-I\big),$$

where I is the unity operator. If

$$F = \sum_{s_\Lambda} F(s_\Lambda)\Psi^0_\Lambda(s_\Lambda), \qquad H^+_\Lambda F = \sum_{s_\Lambda} (H^+_\Lambda F)(s_\Lambda)\Psi^0_\Lambda(s_\Lambda)$$

then, taking into account that $J_A(s_A)$ is en even function in s_x, we obtain

$$(H^+_\Lambda F)(s_\Lambda) = -\sum_{A\subseteq\Lambda} J_A(s_A) e^{-\frac{\alpha}{2}W_A(s_\Lambda)}\big(F(s_\Lambda) - F\big(s^A_\Lambda\big)\big).$$

H^+_Λ is symmetric with respect to the new scalar product

$$(F, F')_{U_0} = \big(e^{-\alpha U_0(S^3_\Lambda)}F, F'\big).$$

The check is given by

$$\begin{aligned}(H^+_\Lambda F, F')_{U_0} &= \big(e^{-\alpha U_0(S^3_\Lambda)}H^+_\Lambda F, F'\big) = \sum_{A\subseteq\Lambda}\big(J_A(S^3_A)e^{-\frac{\alpha}{2}[U_0(S^3_\Lambda)+U_0(S^{3A}_\Lambda)]}(S^1_{[A]} - I)F, F'\big)\\ &= \sum_{A\subseteq\Lambda}\big(J_A(S^3_A)e^{-\frac{\alpha}{2}[U_0(S^3_\Lambda)+U_0(S^{3A}_\Lambda)]}F, (S^1_{[A]} - I)F'\big) = (F, H^+_\Lambda F')_{U_0}.\end{aligned}$$

Here we used the equalities

$$e^{-\frac{\alpha}{2}U_0(S^3_\Lambda)}S^1_{[A]} = S^1_{[A]}e^{-\frac{\alpha}{2}U_0(S^{3A}_\Lambda)}, \qquad e^{-\frac{\alpha}{2}U_0(S^{3A}_\Lambda)}S^1_{[A]} = S^1_{[A]}e^{-\frac{\alpha}{2}U_0(S^3_\Lambda)}$$

and the fact that $S^1_{[A]}$ commutes with $J_A(S^3_A)$. From the definitions it follows that

$$(H^+_\Lambda F, F')_{U_0} = \big(H_\Lambda e^{-\frac{\alpha}{2}U_0(S^3_\Lambda)}F, e^{-\frac{\alpha}{2}U_0(S^3_\Lambda)}F'\big). \tag{9}$$

H^+_Λ is positive definite. This is a consequence of the relations

$$\begin{aligned}(H^+_\Lambda F, F)_{U_0} &= -\sum_{A\subseteq\Lambda}\sum_{s_\Lambda} J_A(s_A)e^{-\frac{\alpha}{2}[U_0(s_\Lambda)+U_0(s^A_\Lambda)]}\big(F(s_\Lambda) - F\big(s^A_\Lambda\big)\big)F(s_\Lambda)\\ &= -\frac{1}{2}\sum_{A\subseteq\Lambda}\sum_{s_\Lambda} J_A(s_A)e^{-\frac{\alpha}{2}[U_0(s_\Lambda)+U_0(s^A_\Lambda)]}\big(F(s_\Lambda) - F\big(s^A_\Lambda\big)\big)^2 \geq 0.\end{aligned} \tag{10}$$

Here we took into account that the exponential weight in the sum is invariant under changing signs of spin variables s_A. From (9), (10) it follows that H_Λ is, also, positive definite. Statement is proved.

Proof of III. We have to prove (5) for $l = 1$. From orthogonality of the basis it follows that

$$Z_\Lambda = (\Psi_\Lambda, \Psi_\Lambda) = \sum_{s_\Lambda} e^{-\alpha U_0(s_\Lambda)}$$

and

$$\langle S^1_{[A]}\rangle_\Lambda = Z^{-1}_\Lambda \sum_{s_\Lambda} e^{-\alpha U_0(s_\Lambda)}e^{-\frac{\alpha}{2}W_A(s_\Lambda)} \geq \inf_{s_\Lambda, A} e^{-\frac{\alpha}{2}W_A(s_\Lambda)} \geq e^{-\frac{\alpha}{2}\max\limits_{s_\Lambda, A}|W_A(s_\Lambda)|}.$$

This proves the statement.

3 Discussion

The proposed perturbations V_Λ of the initial Hamiltonian $H_{0\Lambda}$ seem complicated. But it is not always so. If the initial Hamiltonian coincides with the Hamiltonian of the XX Heisenberg model, then in some cases, mentioned in the introduction, the perturbation is very simple and produces an anisotropic quadratic in S_x^3, $x \in \Lambda$ term and a boundary term linear in S_x^3, $x \in \Lambda$ only. A reduction of V_Λ to a simpler form for a quadratic in S_x^3, $x \in \Lambda$ function U_0 can be found in [1]. There is an interesting problem to find out all the cases of the initial Hamiltonians, commuting with the total spin in the third direction, $\phi_{A,A'}$ and U_0 leading to simple anisotropic generalized XXZ models.

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