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LETTER TO THE EDITOR

Ground state of XY models of interacting spins in a transverse field

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Abstract. We investigate the ground state of an XY model with a transverse field, characterized by an exchange matrix, whose highest eigenvalue, $\lambda_{\max}$, is supposed to be positive and finite. We prove rigorously that for a spin S the ground state changes at the transverse field value $K_c = S\lambda_{\max}$.

Our model is defined by the Hamiltonian

$$\hat{H} = -\tfrac{1}{2}\sum_{i,j}^{N} J_{ij}(\hat{S}_i^x\hat{S}_j^x + \hat{S}_i^y\hat{S}_j^y) - K\sum_{i}^{N}\hat{S}_i^z \tag{1}$$

where $\hat{S}_i^x$, $\hat{S}_i^y$ and $\hat{S}_i^z$ are the S-spin operators at the site i, N is the number of spins and K is assumed to be positive (for a general review of XY model see [1]). The ground-state properties of the Hamiltonian (1) have attracted some interest, especially for $K = 0$, where the existence of long-range order on hypercubic [2, 3] and triangular [4] lattices was investigated. The effect of the transverse field was examined in [5] for a nearest-neighbour ferromagnetic interaction.

In this paper we will use only two properties of the interaction:

(i) The highest eigenvalue, $\lambda_{\max}$, of the matrix J_{ij} is between zero and infinity

$$0 < \lambda_{\max} < \infty \tag{2}$$

(ii) J_{ij} is symmetric and $J_{ii} = 0, \forall_i$.

With these assumptions our results are more general than those of [5], and can be applied for example, to random interactions.

Introducing the $\hat{S}^{\pm} = \hat{S}^x \pm \hat{S}^y$ operators we rewrite the Hamiltonian (1) in the form

$$\hat{H} = -\tfrac{1}{2}\sum_{i,j}^{N} J_{ij}\hat{S}_i^+\hat{S}_j^- - K\hat{M} \tag{3}$$

where $\hat{M} = \sum_i \hat{S}_i^z$ denotes the total magnetization in the z direction. Let us denote by $|M\rangle$ an eigenstate of $\hat{M}$ with the eigenvalue M. Since $\hat{H}$ and $\hat{M}$ commute, all eigenstates of $\hat{H}$ are characterized by a fixed magnetization M in the z direction. If $M = NS$, then $|NS\rangle$ is the state where all spins are aligned in the z direction; if $M < NS$, $|M\rangle$ denotes an arbitrary element of the subspace where the magnetization in the z direction is M. First we prove that the state $|NS\rangle$ is the ground state for $K > K_c = S\lambda_{max}$. Subsequently, we will show that for $K < K_c$ the ground state is a state with $M < NS$.

The energy E_M of a state $|M\rangle$ with magnetization M is

$$E_M = \langle M|\hat{H}|M\rangle = -KM - \tfrac{1}{2}\sum_{i,j}\langle M|\hat{S}_i^- J_{ij}\hat{S}_j^+|M\rangle. \tag{4}$$

After diagonalizing the second term in equation (4), we have

$$E_M = -KM - \tfrac{1}{2}\sum_{k}^{N}\lambda_k\langle\rho_k|\rho_k\rangle \tag{5}$$

where $|\rho_k\rangle = \sum_j \Theta_{kj}\hat{S}_j^+|M\rangle$ and Θ is the unitary matrix which diagonalizes J_{ij}. Since $\langle\rho_k|\rho_k\rangle$ is a non-negative number, we can estimate E_M as

$$E_M \geqslant -KM - \tfrac{1}{2}\lambda_{max}\rho \tag{6}$$

where

$$\rho = \sum_{k}^{N}\langle\rho_k|\rho_k\rangle = \sum_i\langle M|\hat{S}_i^-\hat{S}_i^+\hat{S}_i^+|M\rangle \geqslant 0. \tag{7}$$

From equation (7) it follows that ρ is zero if $M = NS$. If $\lambda_{max} \leqslant 0$, the right-hand side (RHS) of equation (6) is minimal when $M = NS$ (M maximal, ρ minimal). On the other hand, this minimal value, $E_0 = -KNS$, is exactly the energy of the state $|NS\rangle$, as one can see from equation (4). This means that in the case $\lambda_{max} \leqslant 0$, the ground state is always $|NS\rangle$.

The case $\lambda_{max} > 0$ is more interesting as there is interplay between M and ρ in equation (6). Using the identity $\hat{S}^-\hat{S}^+ = (S-\hat{S}^z)(S+1+\hat{S}^z)$, where $\hat{S}^z$ can take the values $(S, S-1, \ldots, -S)$, we estimate ρ as

$$\rho \leqslant \sum_i\langle M|(S-\hat{S}_i^z)2S|M\rangle = 2S(NS-M). \tag{8}$$

Finally, from equations (6) and (8) we get an inequality

$$E_M \geqslant -NS^2\lambda_{max} - (K - S\lambda_{max})M \tag{9}$$

which gives a lower bound for E_M.

If $K > K_c = S\lambda_{max}$, the RHS of equation (9) is minimal for $M = NS$, giving a lower bound $E_0 = -KNS$ for the energy E_M for any M. As we have seen, the state $|NS\rangle$ has the same energy as this lower bound, $E_0 = E_{NS}$, so we have proved that the ground state is $|NS\rangle$ in this case. From equation (9) we can also estimate the gap between the ground and first excited states to be at least $K - K_c$ (see equation (9) for $M = NS - 1$).

In the second part of the proof, we show that for $K < K_c$ one can construct a state $|\varphi\rangle$ with magnetization $M = NS - 1$, whose energy, E_φ, is smaller than E_0 as follows:

$$|\varphi\rangle = \sum_i^N \frac{c_i}{\sqrt{2S}}\hat{S}_i^-|NS\rangle \tag{10}$$

where $\sum_i |c_i|^2 = 1$, and the set c_i is a solution of the equations

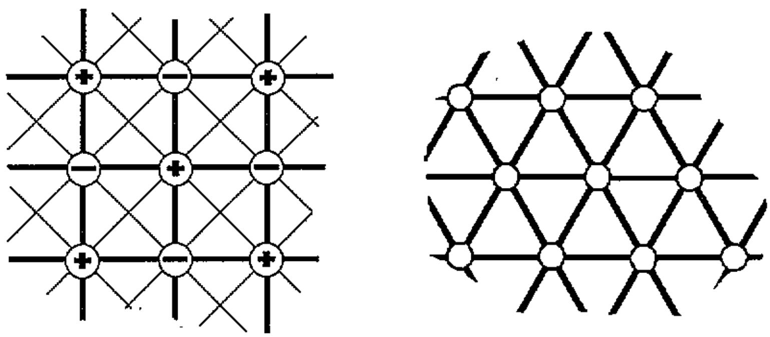
$$\sum_j J_{ij} c_j = \lambda_{\max} c_i \qquad i = 1, \ldots, N. \tag{11}$$

(For the nearest-neighbour ferromagnetic model, $|\varphi\rangle$ is a one-magnon excitation with $k = 0$.) With the help of the relation $\hat{S}_i^+ \hat{S}_j^- |NS\rangle = 2S\delta_{ij}|NS\rangle$, one can easily check that $|\varphi\rangle$ is an eigenstate of $\hat{H}$ (equation (3)):

$$\hat{H}|\varphi\rangle = (-KNS + K - S\lambda_{\max})|\varphi\rangle. \tag{12}$$

Comparing equations (12) and (9) for $M = NS - 1$, we can see that $|\varphi\rangle$ is a state for which the expression (9) holds as an equality. This means that for $K > K_c = S\lambda_{\max}$ the state $|\varphi\rangle$ is an excitation with the smallest possible energy gap, $K - K_c$; for $K < K_c$, the energy of $|\varphi\rangle$ is smaller than E_0, so $|NS\rangle$ cannot be the ground state. This way we have proved that the ground state changes at K_c; for $K < K_c$ the ground state is determined by the details of the interaction matrix.

The value of $\lambda_{\max}$ depends on the structure and on the size of J_{ij}. However, for large enough N and for short-range interactions we expect $\lambda_{\max}$ to be independent of N and determined by the lattice structure. Figure 1 shows two such examples, (For classical spin systems Canning [6] pointed out the important role of the eigensystem of J_{ij}.)



(*a*) (*b*)

Figure 1. (*a*) Example of a non-frustrated lattice. Thick and thin lines denote antiferromagnetic and ferromagnetic interactions, respectively. The sites are marked by the values of ξ_i (see text). (*b*) Frustrated triangular lattice. All interactions are antiferromagnetic. There is no pattern of $\{\xi_i\}$ which would produce only antiferromagnetic interactions.

The first lattice (figure 1(*a*)) is a non-frustrated one with the interaction

$$J_{ij} = \xi_i \xi_j L_{ij} \qquad L_{ij} \geqslant 0 \qquad \xi_i = \pm 1 \tag{13}$$

where L_{ij} is L_1 for nearest neighbours, L_2 for next-nearest neighbours and zero otherwise. In figure 1(*a*) we have chosen a chess board-like $\{\xi_i\}$ pattern giving antiferromagnetic nearest-neighbour and ferromagnetic next-nearest-neighbour interactions, not actually $\lambda_{\max}$ is independent of the choice of $\{\xi_i\}$. For this lattice $z_{\max} = z_i L_1 + z_2 L_2$, where $z_1 = z_2 = 4$.

The second example is the antiferromagnetic triangular lattice with an interaction $-J$ (figure 1(*b*)), where the maximal eigenvalue, $\lambda_{max} = 2J$, is much smaller than it would be for ferromagnetic interactions ($6|J|$), because of the frustration.

For $S = \frac{1}{2}$ the Hamiltonian (3) is equivalent to that of the hard-core Bose gas, via the lattice-gas analogy of Matsubara and Matsuda [7], where K plays the role of the chemical potential, so our result holds equally well for this model.

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