

Linear energy bounds for Heisenberg spin systems

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Abstract. Recently obtained results on linear energy bounds are generalized to arbitrary spin quantum numbers and coupling schemes. Thereby the class of so-called independent magnon states, for which the relative ground-state property can be rigorously established, is considerably enlarged. We still require that the matrix of exchange parameters has constant row sums, but this can be achieved by means of a suitable gauge and need not be considered as a physical restriction.

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1. Introduction

For ferromagnetic spin systems the ground-state $|\uparrow\uparrow \dots \uparrow\rangle$ and the first few excited states, called magnon states, are well-known and extensively investigated, see e. g. [1]. For anti-ferromagnetic (AF) coupling the state $|\uparrow\uparrow \dots \uparrow\rangle$ will be the state of highest energy, and could be called the "anti-ground-state". Also the magnon states which have a large total spin quantum number S are still eigenstates of the Heisenberg Hamiltonian, but seem to be of less physical importance at first glance, since in thermal equilibrium they are dominated by the low-lying eigenstates. However, these states will become ground-states if a sufficient strong magnetic field \mathbf{H} is applied, since the Zeeman term in the Hamiltonian will give rise to a maximal energy shift of $-\mu_B g S H$. Hence the magnon states are yet important for the magnetization curve $\mathcal{M}(\mathbf{H})$, especially at low temperatures.

What can then be said about the energies of the magnon states in general? The anti-ground state (or "magnon vacuum") has the energy $E_0 = J s^2$ and the total magnetic quantum number $M = N s$. Here N denotes the number of spins with individual spin quantum number s and J denotes the sum of all exchange parameters of the spin system, see section 2 for details. The 1-magnon states ly in the subspace with $M = N s - 1$. Their energies can be calculated, up to a constant shift and a factor $2s$, as the eigenvalues of the symmetric $N \times N$ -matrix of exchange parameters, which can be done exactly in most cases. Let E_1^{\min} denote the smallest of these energies. More generally, we will write E_a^{\min} for the minimal energy within the subspace with total magnetic quantum number $M = N s - a$. It turns out that typically the graph of $a \mapsto E_a^{\min}$ will be an approximate parabola with positive curvature, see [2][3]. However, there are exceptions to this rule, see [4][5], one exception being given by the recently discovered "independent magnon states" [6][7]. Here, for some small values of a , we have

$$E_a^{\min} = (1 - a)E_0 + aE_1^{\min}, \quad (1)$$

i. e. $a \mapsto E_a^{\min}$ is locally an affine function. The existence of states satisfying (1) is not just a curiosity but has interesting physical consequences with respect to magnetization: Since the Zeeman term is also linear in a , the independent magnon states simultaneously become ground-states at the saturation value of the applied magnetic field. One would hence observe a marked jump in the magnetization curve $\mathcal{M}(\mathbf{H})$ at zero temperature, see the discussion in [6]. Other examples of spin systems exhibiting jumps in the magnetization curve due to linear parts of the energy spectrum are known, see [8][9][10][11][12] and [13].

The independent magnon states which satisfy (1) can be analytically calculated. In order to rigorously prove that their energy eigenvalues are minimal within the subspaces with $M = N s - a$, one could try to prove a general inequality of the form

$$E_a^{\min} \geq (1 - a)E_0 + aE_1^{\min} \quad (2)$$

for all $a = 0, \dots, 2Ns$ and AF-coupling. Geometrically, (2) means that energies in the plot of E versus a ly on or above the line joining the first two points with E_0 and E_1 .

A proof of (2) is given in [6] only for the special case of $s = \frac{1}{2}$ and certain homogeneous coupling schemes. This is an unsatisfying situation since the independent magnon states constructed in [6][7] can be defined for any s and their minimal energy property is numerically established without any doubt.

Thus this article is devoted to the generalization of the quoted proof to arbitrary s and coupling schemes. The only assumption we need is that the exchange parameters $J_{\mu\nu}$ have equal signs. For AF-coupling, i. e. $J_{\mu\nu} \geq 0$, we obtain (2). The ferromagnetic case $J_{\mu\nu} \leq 0$ is completely analogous and yields

$$E_a^{\max} \leq (1 - a)E_0 + aE_1^{\max}, \quad (3)$$

with self-explaining notation. Hence it will not be necessary to consider the ferromagnetic case separately in the rest of this article.

As remarked before, it is an obvious benefit of the generalisation of the quoted proof to rigorously establish the minimal energy property of the independent magnon states for arbitrary s . Moreover, it is now easy to extend the construction of independent magnon states to coupling schemes with different exchange parameters. For example, one could consider a cuboctahedron with two different exchange constants: $J_1 > 0$ for the bonds within two opposing squares and J_2 satisfying $0 < J_2 < J_1$ for the remaining bonds. This coupling scheme would admit the same independent magnon states as those considered in [6].

The technique of the proof of the generalized inequality is essentially the same as that of the old one. The generalization to arbitrary s is achieved by replacing every spin s by a group of $2s$ spins $\frac{1}{2}$ and the coupling between two spins by a uniform coupling between the corresponding groups. The energy eigenvalues of the new system include the eigenvalues of the old one. In this way the proof can be reduced to the case of $s = \frac{1}{2}$. In the next step we embed the Hilbert space of the spin $\frac{1}{2}$ system into some sort of bosonic Fock space for magnons and compare the Heisenberg Hamiltonian with that for the ideal magnon gas. The difference of these two Hamiltonians has two components of different origin: First, there occurs some (positive definite) term due to a kind of "repulsion" between magnons. Only here the AF-coupling assumption is needed. Second, the "kinetic energy" part (or XY-part) of the magnon gas Hamiltonian produces some unphysical states, due to the fact that the magnon picture is only an approximation of the real situation. The necessary projection onto the physical states further increases the ground state energy. Both components introduce a $>$ -sign in (2). As far as the Heisenberg spin system can be *exactly* viewed as an ideal magnon gas, we have an $=$ -sign in (2) as for independent magnons. The analogy of a antiferromagnet in a strong magnetic field with a repulsive Bose gas is well-known, see for example [14][15][16].

The paper is organized as follows: Section 2 contains the pertinent notation and definitions, section 3 the main theorem together with its proof in two steps (sections 3.1 and 3.2) and section 4 a short discussion.

2. Notation and Definitions

We consider systems with N spin sites, individual spin quantum number s and Heisenberg Hamiltonian

$$H = \sum_{\mu, \nu=1}^N J_{\mu\nu} \mathbf{s}_\mu \cdot \mathbf{s}_\nu. \quad (4)$$

Here $\mathbf{s}_\mu = (\mathbf{s}_\mu^{(1)}, \mathbf{s}_\mu^{(2)}, \mathbf{s}_\mu^{(3)})$ is the (vector) spin operator at site μ and $J_{\mu\nu}$ is the exchange parameter determining the strength of the coupling between sites μ and ν . $J_{\mu\nu}$ will be considered as the entries of a real $N \times N$ -matrix \mathbf{J} . As usual,

$$\mathbf{S}^{(i)} \equiv \sum_{\mu} \mathbf{s}_\mu^{(i)} \quad (i = 1, 2, 3) \quad (5)$$

and

$$\mathbf{s}_\mu^\pm \equiv \mathbf{s}_\mu^{(1)} \pm i\mathbf{s}_\mu^{(2)}, \quad \mu = 1, \dots, N. \quad (6)$$

The Hilbert space which is the domain of definition of the various operators considered will be denoted by $\mathcal{H}(N, s)$. It can be identified with the N -fold tensor product

$$\mathcal{H}(N, s) = \bigotimes_{i=1}^N \mathcal{H}(1, s). \quad (7)$$

Note that the exchange parameters $J_{\mu\nu}$ are not uniquely determined by the Hamiltonian H via (4). Different choices of the $J_{\mu\nu}$ leading to the same H will be referred to as different “gauges”.

First, the anti-symmetric part of \mathbf{J} does not enter into (4) and could be chosen arbitrarily. However, throughout this article we will choose $J_{\mu\nu} = J_{\nu\mu}$, i. e. consider \mathbf{J} as a symmetric matrix. Second, the diagonal part of \mathbf{J} is not fixed by (4). Since $\mathbf{s}_\mu \cdot \mathbf{s}_\mu = s(s+1)\mathbf{1}$ we may choose arbitrary diagonal elements $J_{\mu\mu}$ without changing H , as long as their sum vanishes, $\text{Tr}\mathbf{J} = 0$. The usual gauge chosen throughout the literature is $J_{\mu\mu} = 0$, $\mu = 1, \dots, N$, which will be called the “zero gauge”. In this article, however, we will choose another gauge, called “homogeneous gauge”, which is defined by the condition that the row sums

$$J_\mu \equiv \sum_{\nu} J_{\mu\nu} \quad (8)$$

will be independent of μ . Of course, there exist spin systems which admit both gauges simultaneously, e. g. homogeneous spin rings. These systems will be called “weakly homogeneous”. We will see that the condition of weak homogeneity used in previous articles [3] [6] is largely superfluous and can be replaced by the homogeneous gauge (but see section 4).

Note that the eigenvalues of \mathbf{J} may non-trivially depend on the gauge. The homogeneous gauge has the advantage that energy eigenvalues in the 1-magnon-sector are simple functions of the eigenvalues of \mathbf{J} , see below. The quantity

$$J \equiv \sum_{\mu\nu} J_{\mu\nu} \quad (9)$$

is gauge-independent. If exchange parameters satisfying $\tilde{J}_{\mu\nu} = \tilde{J}_{\nu\mu}$ are given in the zero gauge, the corresponding parameters $J_{\mu\nu}$ in the homogeneous gauge are obtained as follows:

$$J_{\mu\nu} \equiv \tilde{J}_{\mu\nu} \text{ for } \mu \neq \nu, \quad (10)$$

$$J_{\mu\mu} \equiv \frac{1}{N} J - \tilde{J}_{\mu}. \quad (11)$$

It follows that

$$j \equiv J_{\mu} = \sum_{\nu} \tilde{J}_{\mu\nu} + J_{\mu\mu} = \frac{J}{N}. \quad (12)$$

Since H commutes with $\mathbf{S}^{(3)}$, the eigenspaces \mathcal{H}_a of $\mathbf{S}^{(3)}$ with eigenvalues $M = Ns - a$, $a = 0, 1, \dots, 2Ns$, are invariant under the action of H . \mathcal{H}_a will be called the a -magnon-sector. Let \mathcal{P}_a denote the projection onto \mathcal{H}_a and

$$H_a \equiv \mathcal{P}_a H \mathcal{P}_a. \quad (13)$$

An orthonormal basis of \mathcal{H}_a is given by the product states $\|m_1, m_2, \dots, m_N\rangle\rangle$ satisfying

$$\mathbf{s}_{\mu}^{(3)} \|m_1, m_2, \dots, m_N\rangle\rangle = m_{\mu} \|m_1, m_2, \dots, m_N\rangle\rangle, \quad (14)$$

where m_{μ} can assume the $2s$ values

$$m_{\mu} = s, s-1, \dots, -s. \quad (15)$$

In the case of $s = \frac{1}{2}$, $m_{\mu} \in \{\frac{1}{2}, -\frac{1}{2}\} \equiv \{\uparrow, \downarrow\}$ and the state (14) can be uniquely specified by the ordered set $|n_1, \dots, n_a\rangle$ of a spin sites μ with $m_{\mu} = -\frac{1}{2}$. We will use both notations equivalently:

$$|n_1, \dots, n_a\rangle \equiv \|m_1, m_2, \dots, m_N\rangle\rangle. \quad (16)$$

For example,

$$|1, 3, 4\rangle = \|\downarrow\uparrow\downarrow\uparrow\uparrow\rangle\rangle, \quad a = 3, \quad N = 5. \quad (17)$$

We now consider again arbitrary s . The subspace \mathcal{H}_1 is N -dimensional and, similarly as above, its basis vectors $\|m_1, m_2, \dots, m_N\rangle\rangle$ may be denoted by $|n\rangle$, $n = 1, \dots, N$, if n denotes the site with lowered spin, i. e. $m_{\mu} = s - \delta_{\mu n}$, $\mu = 1, \dots, N$.

Consider

$$H_1 = \mathcal{P}_1 \left(\sum_{\mu\nu} J_{\mu\nu} \mathbf{s}_{\mu}^{(3)} \mathbf{s}_{\nu}^{(3)} + \frac{1}{2} \sum_{\mu\nu} J_{\mu\nu} (\mathbf{s}_{\mu}^+ \mathbf{s}_{\nu}^- + \mathbf{s}_{\mu}^- \mathbf{s}_{\nu}^+) \right) \mathcal{P}_1 \quad (18)$$

$$\equiv H_1^Z + H_1^{XY}, \quad (19)$$

and

$$H_1^Z |n\rangle = \left(\sum_{\mu\nu} J_{\mu\nu} (s - \delta_{\mu n})(s - \delta_{\nu n}) \right) |n\rangle \quad (20)$$

$$= (s^2 N j - 2s j + J_{nn}) |n\rangle. \quad (21)$$

Similarly, we obtain after some calculation

$$H_1^{XY}|n\rangle = 2s \sum_{m, m \neq n} J_{nm}|m\rangle + (2s-1)J_{nn}|n\rangle. \quad (22)$$

Hence

$$H_1 = (s^2 N j - 2s j) \mathbb{1}_{\mathcal{H}_a} + 2s \mathbf{J} \quad (23)$$

and the eigenvalues of H_1 are

$$E_\alpha = s^2 N j + 2s(j_\alpha - j), \quad (24)$$

if j_α , $\alpha = 1, \dots, N$, are the eigenvalues of \mathbf{J} . This simple relation between H_1 and \mathbf{J} only holds in the homogeneous gauge. Note further that, due to the homogeneous gauge, j is one of the eigenvalues of \mathbf{J} , the corresponding eigenvector having constant entries.

We denote by j_{\min} the minimal eigenvalue of \mathbf{J} and by E_1^{\min} the corresponding minimal eigenvalue of H_1 .

3. The Main Result

Theorem 1 *Consider a spin system with AF-Heisenberg coupling scheme and homogeneous gauge, i. e.*

$$j \equiv \sum_{\nu} J_{\mu\nu} \quad (25)$$

being independent of μ and

$$J_{\mu\nu} \geq 0 \text{ for } \mu \neq \nu. \quad (26)$$

Then the following operator inequality holds:

$$H_a \geq (Njs^2 - 2sa(j - j_{\min})) \mathbb{1}_{\mathcal{H}_a} \quad (27)$$

for all $a = 0, 1, \dots, 2Ns$.

The rest of this section is devoted to the proof of this theorem.

3.1. Reduction to the case $s = \frac{1}{2}$

We will construct another Hamiltonian

$$\widehat{H} = \sum_{\alpha, \beta=1}^{\widehat{N}} \widehat{J}_{\alpha\beta} \widehat{\mathbf{s}}_\alpha \cdot \widehat{\mathbf{s}}_\beta \quad (28)$$

acting on the Hilbert space $\widehat{\mathcal{H}} = \mathcal{H}(2Ns, \frac{1}{2})$, i. e. $\widehat{N} = 2Ns$ and $\widehat{s} = \frac{1}{2}$. Intuitively, every spin site with spin s is replaced by a group of $2s$ spin sites with spin $\frac{1}{2}$ and the coupling between spin sites is extended to a uniform coupling between groups, see figure 1.

Formally, we set

$$\alpha \equiv (\mu, i), \quad i = 1, \dots, 2s \quad (29)$$

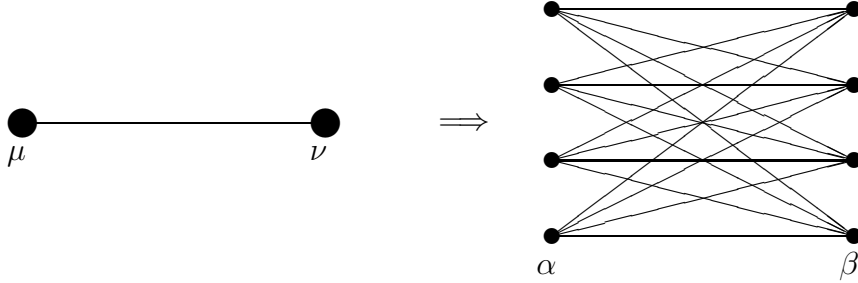


Figure 1. Reduction to the case $s = \frac{1}{2}$ by replacing single spins by groups of $2s$ spins $\frac{1}{2}$.

and

$$\widehat{J}_{\alpha\beta} = \widehat{J}_{(\mu,i)(\nu,j)} \equiv J_{\mu\nu}, \quad i, j = 1, \dots, 2s. \quad (30)$$

The new matrix $\widehat{\mathbf{J}}$ satisfies the homogeneous gauge condition if \mathbf{J} does.

According to the well-known theory of the coupling of angular momenta or spins the tensor product spaces

$$\mathcal{H}(2s, \frac{1}{2}) = \bigotimes_{i=1}^{2s} \mathcal{H}(1, \frac{1}{2}) \quad (31)$$

can be decomposed into eigenspaces of $(\sum_{i=1}^{2s} \mathbf{s}_i)^2$ with eigenvalues

$$S(S+1), \quad S = s, s-1, \dots, \begin{cases} 0 & \text{if } 2s \text{ even} \\ \frac{1}{2} & \text{if } 2s \text{ odd} \end{cases} \quad \text{The eigenspace with the maximal } S = s$$

will be denoted by \mathcal{K}_s and the projector onto this eigenspace by \mathbf{P}_s . \mathcal{K}_s is isomorphic to $\mathcal{H}(1, s)$. This isomorphism can be chosen such that the following isometric embedding

$$\mathbf{j}_s : \mathcal{H}(1, s) \longrightarrow \mathcal{K}_s \hookrightarrow \mathcal{H}(2s, \frac{1}{2}) \quad (32)$$

satisfies

$$\mathbf{j}_s \mathbf{s} \mathbf{j}_s^* = \mathbf{P}_s \left(\sum_{i=1}^{2s} \mathbf{s}_i \right) \mathbf{P}_s. \quad (33)$$

Let \mathbf{j} denote the tensor product of the \mathbf{j}_s

$$\mathbf{j} : \mathcal{H}(N, s) \longrightarrow \mathcal{H}(2Ns, \frac{1}{2}) \quad (34)$$

and $\mathbf{P} = \bigotimes_{\nu=1}^N \mathbf{P}_s$ the corresponding projector onto $\bigotimes_{\nu=1}^N \mathcal{K}_s$ which commutes with \widehat{H} . Then it follows from (33) that

$$\mathbf{j} H \mathbf{j}^* = \mathbf{P} \widehat{H} \mathbf{P}. \quad (35)$$

In other words, H may be viewed as the restriction of \widehat{H} onto the subspace of states with maximal spin $S = s$ within the groups. The eigenvalues of H form a subset of the

eigenvalues of \widehat{H} .

The relation (30) between the exchange parameters may be written in matrix form as

$$\widehat{\mathbf{J}} = \mathbf{J} \otimes \mathbf{E}, \quad (36)$$

where \mathbf{E} is the $2s \times 2s$ -matrix completely filled with 1's. The eigenvalues of \mathbf{E} are $2s$ and 0 , the latter being $(2s - 1)$ -fold degenerate, hence the eigenvalues of the $\widehat{\mathbf{J}}$ -matrix satisfy

$$\widehat{j}_\alpha = 2sj_\alpha \text{ or } 0. \quad (37)$$

It will be illustrative to check the spectral inclusion property for some known eigenvalues of Heisenberg Hamiltonians.

The eigenvalue of H for the magnon vacuum state $|\uparrow\uparrow \dots \uparrow\rangle$ is

$$E_0 = Njs^2. \quad (38)$$

For \widehat{H} we analogously have

$$\widehat{E}_0 = (2sN)\widehat{j}(\frac{1}{2})^2, \quad (39)$$

which is identical with (38) by $\widehat{j} = 2sj$. Similarly, the eigenvalues of H in the 1-magnon-sector $M = Ns - 1$ are

$$E_\alpha = jNs^2 + 2s(j_\alpha - j), \quad (40)$$

cf. (24), hence

$$\widehat{E}_\alpha = \widehat{j} \cdot 2sN \cdot \frac{1}{4} + 2\frac{1}{2}(\widehat{j}_\alpha - \widehat{j}), \quad (41)$$

which is identical with (40) because of (37).

Analogously to the cases considered it is easy to see that the bounds of the *rhs* of (27) are the same for H and \widehat{H} : Since \widehat{j} and \widehat{j}_{\min} cannot be zero, they must satisfy

$$\widehat{j} = 2sj, \quad \widehat{j}_{\min} = 2sj_{\min}, \quad (42)$$

according to (37).

Further, the spectrum of H_a is contained in the spectrum of \widehat{H}_a . Thus it suffices to prove (27) for \widehat{H} , i. e. $s = \frac{1}{2}$.

3.2. Embedding into the magnon Fock space

Throughout this section we set $s = \frac{1}{2}$. Recall that

$$\mathcal{H}(N, \frac{1}{2}) = \bigoplus_{a=0}^N \mathcal{H}_a \quad (43)$$

denotes the decomposition of the Hilbert space of the system into eigenspaces of $\mathbf{S}^{(3)}$ with eigenvalues $M = \frac{1}{2}N - a$.

Let

$$\mathcal{B}_a(\mathcal{H}_1) \subset \bigotimes_{i=1}^a \mathcal{H}_1 \quad (44)$$

denote the completely symmetric subspace of the a -fold tensor product of 1-magnon-spaces and

$$\mathcal{B}_a(T) : \mathcal{B}_a(\mathcal{H}_1) \longrightarrow \mathcal{B}_a(\mathcal{H}_1) \quad (45)$$

be the corresponding restriction of $T \otimes \mathbf{1} \otimes \dots \otimes \mathbf{1} + \dots + \mathbf{1} \otimes \dots \otimes \mathbf{1} \otimes T$ if $T : \mathcal{H}_1 \longrightarrow \mathcal{H}_1$ is any linear operator.

Recall that a basis of \mathcal{H}_a is given by the states

$$|n_1, n_2, \dots, n_a\rangle, \quad 1 \leq n_1 < n_2 < \dots < n_a \leq N \quad (46)$$

where the n_i denote the lowered spin sites. Let

$$\mathcal{S}_a : \bigotimes_{i=1}^a \mathcal{H}_1 \longrightarrow \mathcal{B}_a(\mathcal{H}_1) \quad (47)$$

denote the ‘‘symmetrizer’’, i. e. the sum over all permuted states divided by the square root of its number. The assignement

$$|n_1, n_2, \dots, n_a\rangle \mapsto \mathcal{S}_a |n_1\rangle \otimes |n_2\rangle \otimes \dots \otimes |n_a\rangle \quad (48)$$

can be extended to an isometric embedding denoted by

$$\mathcal{J}_a : \mathcal{H}_a \longrightarrow \mathcal{B}_a(\mathcal{H}_1). \quad (49)$$

It satisfies $\mathcal{J}_a^* \mathcal{J}_a = \mathbf{1}_{\mathcal{H}_a}$. Hence $\mathbf{P}_a \equiv \mathcal{J}_a^* \mathcal{J}_a$ will be a projector onto a subspace of $\mathcal{B}_a(\mathcal{H}_1)$ denoted by $\mathcal{I}_a(\mathcal{H}_1)$. Obviously,

$$\mathcal{J}_a^* = \mathcal{J}_a^* \mathbf{P}_a. \quad (50)$$

The states contained in $\mathcal{I}_a(\mathcal{H}_1)$ are called ‘‘physical states’’ since they are in 1 : 1-correspondence with the states in \mathcal{H}_a . The orthogonal complement of $\mathcal{I}_a(\mathcal{H}_1)$ contains ‘‘unphysical states’’ like $|n\rangle \otimes |n\rangle$. More general, it is easy to see that any superposition of product states is orthogonal to $\mathcal{I}_a(\mathcal{H}_1)$ iff all product states of the superposition contain at least one factor twice or more.

We define

$$\tilde{H}_a \equiv \mathcal{J}_a^* \mathcal{B}_a(\mathcal{H}_1) \mathcal{J}_a. \quad (51)$$

Recall that \mathcal{H}_1 was defined as the Hamiltonian in the 1-magnon sector.

The main part of the remaining proof will consist of comparing \tilde{H}_a with H_a . To this end, H will be split into a ‘‘Z-part’’ and an ‘‘XY-part’’ according to

$$H = \sum_{\mu\nu} J_{\mu\nu} \mathbf{s}_\mu^{(3)} \mathbf{s}_\nu^{(3)} + \frac{1}{2} \sum_{\mu\nu} J_{\mu\nu} (\mathbf{s}_\mu^+ \mathbf{s}_\nu^- + \mathbf{s}_\mu^- \mathbf{s}_\nu^+) \quad (52)$$

$$\equiv H^Z + H^{XY}, \quad (53)$$

and, analogously, $H_a = H_a^Z + H_a^{XY}$ and $\tilde{H}_a = \tilde{H}_a^Z + \tilde{H}_a^{XY}$.

Proposition 1

$$H_a^{XY} = \tilde{H}_a^{XY}. \quad (54)$$

Proof: Let $|n_1, n_2, \dots, n_a\rangle$ be an arbitrary basis vector of \mathcal{H}_a . It suffices to consider a Hamiltonian of the form

$$H^{XY} = \frac{1}{2}(\mathbf{s}_\mu^+ \mathbf{s}_\nu^- + \mathbf{s}_\mu^- \mathbf{s}_\nu^+). \quad (55)$$

Moreover we need only consider the case $\mu < \nu$ since for $\mu = \nu$ the basis vectors are eigenvectors both of H_a^{XY} and \tilde{H}_a^{XY} with eigenvalues $\frac{1}{2}$. We have to distinguish between four cases:

(i) $\mu, \nu \notin \{n_1, n_2, \dots, n_a\}$:

$$H_a^{XY} |n_1, n_2, \dots, n_a\rangle = \frac{1}{2}(\mathbf{s}_\mu^+ \mathbf{s}_\nu^- + \mathbf{s}_\mu^- \mathbf{s}_\nu^+) |n_1, n_2, \dots, n_a\rangle \quad (56)$$

$$= 0 \quad (57)$$

$$= \tilde{H}_a^{XY} |n_1, n_2, \dots, n_a\rangle, \quad (58)$$

since $|n_1, n_2, \dots, n_a\rangle$ is annihilated by \mathbf{s}_μ^+ and \mathbf{s}_ν^+ .

(ii) $\mu \in \{n_1, n_2, \dots, n_a\}$, but $\nu \notin \{n_1, n_2, \dots, n_a\}$:

$$\begin{aligned} H_a^{XY} |n_1, \dots, \mu, \dots, n_a\rangle &= \frac{1}{2} \mathbf{s}_\mu^+ \mathbf{s}_\nu^- |n_1, \dots, \mu, \dots, n_a\rangle \\ &= \frac{1}{2} \text{Sort} |n_1, \dots, \nu, \dots, n_a\rangle. \end{aligned} \quad (59)$$

$$\begin{aligned} \tilde{H}_a^{XY} |n_1, \dots, \mu, \dots, n_a\rangle &= \mathcal{J}_a^* \mathcal{B}_a(H_1^{XY}) \mathcal{J}_a |n_1, \dots, \mu, \dots, n_a\rangle \\ &= \mathcal{J}_a^* \mathcal{B}_a(H_1^{XY}) \mathcal{S}_a |n_1\rangle \otimes \dots \otimes |n_a\rangle \\ &= \frac{1}{2} \mathcal{J}_a^* \mathcal{S}_a (\mathbf{s}_\mu^+ \mathbf{s}_\nu^- |n_1\rangle \otimes \dots \otimes |n_a\rangle \\ &\quad + \dots + |n_1\rangle \otimes \dots \otimes \mathbf{s}_\mu^+ \mathbf{s}_\nu^- |\mu\rangle \otimes \dots \otimes |n_a\rangle \\ &\quad + \dots + |n_1\rangle \otimes \dots \otimes \mathbf{s}_\mu^+ \mathbf{s}_\nu^- |n_a\rangle) \\ &= \frac{1}{2} \mathcal{J}_a^* \mathcal{S}_a |n_1\rangle \otimes \dots \otimes |\nu\rangle \otimes \dots \otimes |n_a\rangle \\ &= \frac{1}{2} \text{Sort} |n_1, \dots, \nu, \dots, n_a\rangle. \end{aligned} \quad (60)$$

Hence $H_a^{XY} |n_1, \dots, \mu, \dots, n_a\rangle = \tilde{H}_a^{XY} |n_1, \dots, \mu, \dots, n_a\rangle$.

(iii) The case $\nu \in \{n_1, n_2, \dots, n_a\}$, but $\mu \notin \{n_1, n_2, \dots, n_a\}$ is completely analogous.

(iv) $\mu, \nu \in \{n_1, n_2, \dots, n_a\}$:

In this case $H_a^{XY} |n_1, \dots, \mu, \dots, \nu, \dots, n_a\rangle = 0$, since the state is annihilated by \mathbf{s}_μ^- as well as by \mathbf{s}_ν^- . On the other side $\tilde{H}_a^{XY} =$

$\frac{1}{2} \mathcal{J}_a^* \mathcal{S}_a (|n_1\rangle \otimes \dots \otimes |\nu\rangle \otimes \dots \otimes |\nu\rangle \otimes \dots \otimes |n_a\rangle + |n_1\rangle \otimes \dots \otimes |\mu\rangle \otimes \dots \otimes |\mu\rangle \otimes \dots \otimes |n_a\rangle) = 0$, since $\mathcal{J}_a^* = \mathcal{J}_a^* \mathcal{P}_a$ and $\mathcal{S}_a(\dots)$ is orthogonal to the subspace $\mathcal{I}_a(\mathcal{H}_1)$, see the remark after (50).

■

Proposition 2

$$H_a^Z \geq \tilde{H}_a^Z + \frac{1-a}{4} Nj. \quad (61)$$

Proof: It turns out that the $|n_1, \dots, n_a\rangle$ are simultaneous eigenvectors for H_a^Z and \tilde{H}_a^Z : First consider H_a^Z and rewrite $|n_1, \dots, n_a\rangle$ in the form $\|m_1, \dots, m_N\rangle\rangle$ satisfying

$$\mathbf{S}_\mu^{(3)}\|m_1, \dots, m_N\rangle\rangle = m_\mu\|m_1, \dots, m_N\rangle\rangle. \quad (62)$$

It follows that

$$H_a^Z\|m_1, \dots, m_N\rangle\rangle = \sum_{\mu\nu} J_{\mu\nu} m_\mu m_\nu \|m_1, \dots, m_N\rangle\rangle \quad (63)$$

$$\equiv \epsilon\|m_1, \dots, m_N\rangle\rangle. \quad (64)$$

We set

$$a_\mu \equiv \frac{1}{2} - m_\mu \in \{0, 1\} \quad (65)$$

and obtain

$$\epsilon = \sum_{\mu\nu} J_{\mu\nu} m_\mu m_\nu \quad (66)$$

$$= \frac{1}{4} \left(\sum_{\mu\nu} J_{\mu\nu} \right) - \sum_{\mu\nu} J_{\mu\nu} a_\nu + \sum_{\mu \neq \nu} J_{\mu\nu} a_\mu a_\nu + \sum_{\mu} J_{\mu\mu} (a_\mu)^2 \quad (67)$$

$$= \frac{1}{4} Nj - ja + \sum_{\mu}' J_{\mu\mu} + \alpha, \quad (68)$$

where

$$\alpha \equiv \sum_{\mu \neq \nu} J_{\mu\nu} a_\mu a_\nu \geq 0, \quad (69)$$

since $J_{\mu\nu} \geq 0$ for $\mu \neq \nu$ by the assumption of AF-coupling. \sum_{μ}' denotes the summation over all μ with $a_\mu = 1$.

Now consider

$$\tilde{H}_a^Z\|m_1, \dots, m_N\rangle\rangle = \tilde{H}_a^Z|n_1, \dots, n_a\rangle \quad (70)$$

$$= \mathcal{J}_a^* \mathcal{S}_a (H_1^Z|n_1\rangle \otimes |n_2\rangle \otimes \dots \otimes |n_a\rangle + \dots \\ + |n_1\rangle \otimes |n_2\rangle \otimes \dots \otimes H_1^Z|n_a\rangle). \quad (71)$$

The terms $H_1^Z|n_i\rangle$ are special cases of (63),(66) for $a = 1$, hence

$$H_1^Z|n_i\rangle = \frac{1}{4} Nj - j + J_{n_i, n_i}, \quad (72)$$

since $\alpha = 0$ in this case. We conclude

$$\tilde{H}_a^Z\|m_1, \dots, m_N\rangle\rangle = \left(aj \left(\frac{N}{4} - 1 \right) + \sum_{\mu}' J_{\mu\mu} \right) \|m_1, \dots, m_N\rangle\rangle \quad (73)$$

$$\equiv \delta\|m_1, \dots, m_N\rangle\rangle. \quad (74)$$

Combining (63),(66) and (73) yields

$$\epsilon - \delta = \frac{1-a}{4} Nj + \alpha \geq \frac{1-a}{4} Nj \quad (75)$$

or

$$H_a^Z - \tilde{H}_a^Z \geq \frac{1-a}{4} Nj \mathbf{1} \quad (76)$$

■

The rest of the proof is straight forward. Combining proposition 1 and 2 we obtain

$$H_a \geq \tilde{H}_a + \frac{1-a}{4} Nj \mathbf{1} \quad (77)$$

Let Φ be a normalized eigenvector of \tilde{H}_a with minimal eigenvalue \tilde{E}_a . Then

$$\tilde{E}_a = \langle \Phi | \tilde{H}_a | \Phi \rangle = \langle \mathcal{J}_a \Phi | \mathcal{B}_a(H_1) | \mathcal{J}_a \Phi \rangle \geq \tilde{E}_a, \quad (78)$$

where \bar{E}_a is the minimal eigenvalue of $\mathcal{B}_a(H_1)$. Since the ground state energy of non-interacting bosons is additive, we obtain further

$$\bar{E}_a = aE_{min}(1) = a(\frac{1}{4}jN + j_{min} - j) \quad (79)$$

and

$$\tilde{H}_a \geq \tilde{E}_a \mathbf{1} \geq a(\frac{1}{4}jN + j_{min} - j) \mathbf{1}. \quad (80)$$

Using (77) the final result is

$$H_a \geq (\frac{1}{4}Nj - a(j - j_{min})) \mathbf{1}. \quad (81)$$

4. Discussion

In the above proof the two parts of the Hamiltonian according to $H = H^Z + H^{XY}$ are considered separately. Thus this part of the proof could be immediately generalized to the XXZ -model given by

$$H(\Delta) = \Delta H^Z + H^{XY}, \quad \Delta > 0, \quad (82)$$

similarly as in [6]. However, the considerations in section 2 concerning the homogeneous gauge and in section 3.1 concerning the reduction to the case $s = \frac{1}{2}$ presuppose an isotropic Hamiltonian. Hence an immediate generalisation to the XXZ -model on the basis of the above proof is only possible for weakly homogeneous systems and $s = \frac{1}{2}$. Compared with the result in [6] this means that the condition $J_{\mu\nu} \in \{0, J\}$, $J > 0$ appearing in [6] can be weakened to $J_{\mu\nu} \geq 0$.

As already pointed out, the above inequality (81) is intended to apply for small values of a , i. e. large values of $M = Ns - a$. For small M much better estimates are known [3]. However, for small a the inequality cannot be improved since there are examples where equality holds in (81) for a couple of values of a , e. g. $a = 0, \dots, \frac{N}{9}$, see [6] and [7].

Notwithstanding the construction of independent magnon states in particular examples, the proof of (27) anew establishes that the Heisenberg Hamiltonian is only equivalent to the Hamiltonian of a Bose gas of magnons if additional interaction terms are considered, see also [14]. Apart from the repulsion term (69) in the case of AF-coupling an infinite repulsion term would have to be introduced which guarantees that no site is occupied by more than one magnon (in the case $s = \frac{1}{2}$). Thus magnons appear as bosons additionally satisfying the Pauli exclusion principle. The reader may ask why magnons are not rather considered as fermions, for which the exclusion principle is automatically satisfied. The reason not to do this is that the interchange of fermions at different sites would sometimes produce factors of -1 which cannot be controlled, at least generally. For special topologies, e. g. spin rings or chains the independent fermion concept works well and yields the exact solution of the spin $\frac{1}{2}$ XY -model, see [17].

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