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Néel order in the ground state of Heisenberg antiferromagnetic chains with long-range interactions

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Abstract. We consider the ground state of one-dimensional antiferromagnets with long-range interactions with Hamiltonian given by

$$H = -\sum_x \sum_n (-1)^n J(n) \boldsymbol{S}_x \cdot \boldsymbol{S}_{x+n}$$

where $J(n) = Jn^{-\alpha}$, with $J > 0$. We prove Néel order for all $1 < \alpha < 3$ if the spin s is sufficiently large. We also prove the absence of long-range order when $\alpha > 3$ for any spin value.

1. Introduction

The antiferromagnetic Heisenberg model with long-range staggered interactions is defined by the Hamiltonian

$$\mathcal{H}_\Lambda = -\sum_{x\in\Lambda} \sum_{n=1}^{L} (-1)^n J(n) \boldsymbol{S} \tag{1}$$

where

$$\Lambda = \{0, 1, \ldots, L\} \subset \mathbb{Z}$$

and L is an odd integer number, in order to avoid frustration when periodic boundary conditions are chosen. We also define

$$J(n) = Jn^{-\alpha} \qquad J > 0, \alpha > 0.$$

The $\boldsymbol{S}_x$ variables are usual spin operators at site x such that $\boldsymbol{S}^2 = s(s+1)$, obeying the canonical commutation relations

$$[S_x^i, S_y^j] = \mathrm{i}\epsilon_{ijk} S_x^k \delta_{xy}.$$

This is exactly the model first discussed by Fröhlich *et al* in [1], where they proved that, at $T > 0$, this system with $1 < \alpha < 2$ presents Néel order for suffficiently large spins.

In this paper we show that, for this same model, long-range order (LRO) will be present in the ground state, for a sufficiently large spin, when $1 < \alpha < 3$. To obtain this result we use infrared bounds [2] adapted for the study of ground states [3].

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We also show that this result is the best possible, since we prove that, if $\alpha > 3$, LRO is impossible in the ground state for any spin value. This result can be achieved by mimicking the proof of the Mermin–Wagner theorem [4] which shows the absence of spontaneous magnetization in models with continuous symmetry if $d < 2$. This can be done with the use of an inequality proposed by Shastry [5] which plays the role of the Bogoliubov inequality in the ground state.

The discussion about the energy gap between the ground state and the first excited states in these systems is carried on elsewhere [6].

2. Definitions and notation

We first introduce the Fourier transform of an arbitrary function f by

$$\hat{f}(k) = \frac{1}{\sqrt{\Lambda}} \sum_{x\in\Lambda} f(x)\,\mathrm{e}^{-\mathrm{i}kx}$$

where $k \in \Lambda^* \equiv \{k = (2\pi/L)q; q = 0, 1, \ldots, L\}$. Applying this definition to the Hamiltonian (1) with periodic boundary conditions, we obtain

$$\widehat{\mathcal{H}}_\Lambda = \sum_{k\in\Lambda^*} \sum_n \frac{J(n)}{2}[1 - (-1)^n \cos kn]\widehat{S}_k^* \cdot \widehat{S}_k. \tag{2}$$

In fact, the Hamiltonian (2) is not equal to (1), since both operators differ by an additive constant. This constant, however, will play no role in the subsequent analysis.

We also introduce the usual two-point function

$$\widehat{g}_k^i = \langle \widehat{S}_k^i \widehat{S}_{-k}^i \rangle$$

where the expectation value of an observable A in the Gibbs ensemble is defined in the standard way:

$$\langle A \rangle = \frac{\mathrm{Tr}(A)\exp\{-\beta\mathcal{H}\}}{\mathrm{Tr}\exp\{-\beta\mathcal{H}\}}.$$

The Duhamel two-point function, denoted by (A, B), is given by

$$(A, B) = \frac{1}{\mathrm{Tr}\exp\{-\beta\mathcal{H}\}} \int_0^1 \mathrm{d}x\ \mathrm{Tr}[\exp\{-x\beta\mathcal{H}\}A\exp\{-(1-x)\beta\mathcal{H}\}B].$$

From now on, whenever ambiguities are absent we shall represent $\widehat{S}_k$ by S_k.

3. Existence of LRO for $1 < \alpha < 3$

The first condition to be imposed on the exchange function in (1) is due to the thermodynamic stability of the system. We need $\sum_n J(n) < \infty \Rightarrow \alpha > 1$.

The property of reflection positivity for the model defined by (1) was proved in [1]. For systems satisfying this property it is possible to derive the infrared bound, which is an upper bound for the two-point function based on the Duhamel inequality [2]:

$$g_k^i \leqslant \frac{1}{2}\left[\left(\sum_{i=1}^3 B_k^i\right)\left(\sum_{i=1}^3 C_k^i\right)\right]^{\frac{1}{2}} \coth\left[\frac{\beta}{2}\left(\frac{\sum_{i=1}^3 C_k^i}{\sum_{i=1}^3 B_k^i}\right)^{\frac{1}{2}}\right] = G_k.$$

Here,

$$B_k = \sum_{i=1}^3 B_k^i = \frac{3}{\sum_n J(n)[1 - (-1)^n \cos kn]}$$

so that the Duhamel two-point function is bounded by

$$(S_k^i, S_{-k}^i) \leqslant \frac{B_k^i}{2\beta}. \tag{3}$$

This Gaussian domination result can be derived by performing chessboard estimates over a model which is defined by a reflection positive Gibbs measure (for more details on this subject the reader is referred to [1]).

The term $\sum_{i=1}^3 C_k^i = C_k$ is an upper bound to the expected value of the double commutator $\sum_{i=1}^3 [S_k^i, [\widehat{\mathcal{H}}_\Lambda, S_{-k}^i]]$. This double commutator can be evaluated explicitly

$$\sum_{i=1}^3 [S_k^i, [\widehat{\mathcal{H}}_\Lambda, S_{-k}^i]] = -\frac{4}{\Lambda} \sum_x \sum_n \frac{J(n)}{2} (-1)^n (1 - \cos kn) \boldsymbol{S}_x \cdot \boldsymbol{S}_{x+n}$$

leading to the operator inequality:

$$\sum_{i=1}^3 [S_k^i, [\widehat{\mathcal{H}}_\Lambda, S_{-k}^i]] \leqslant -4 \left[\sum_n \frac{J(n)}{2} (-1)^n (1 - \cos kn) \right] s(s+1) = C_k.$$

The sum rule

$$\frac{1}{\Lambda} \sum_{k \in \Lambda^*} \sum_{i=1}^3 g_k^i = s(s+1)$$

follows from $\boldsymbol{S}^2 = s(s+1)$ so that

$$\frac{1}{\Lambda} \sum_{i=1}^3 g_{k=\pi}^i = s\,(s+1) - \frac{1}{\Lambda} \sum_{k \neq \pi} G_k.$$

We want to study the ground state of the system and so we first take the limit $\beta \to \infty$ with fixed Λ, and then the limit $L \to \infty$. Taking into account the inequality $\coth x \leqslant 1 + 1/x$, we obtain [3]

$$\lim_{L \to \infty} \frac{1}{\Lambda} \sum_{i=1}^3 g_\pi^i \geqslant D - \frac{1}{4\pi} \int_{-\pi}^{+\pi} \mathrm{d}k \left[\left(\sum_{i=1}^3 B_k^i \right) \left(\sum_{i=1}^3 C_k^i \right) \right]^{\frac{1}{2}}.$$

Therefore, a sufficient condition for long-range Néel order is that the right-hand side is positive. It turns out that this condition leads to

$$[s(s+1)]^{\frac{1}{2}} > \frac{1}{2\pi} \int_0^{+\pi} \mathrm{d}k \left\{ \frac{-6 \sum_n J(n)(-1)^n (1 - \cos kn)}{\sum_n J(n)[1 - (-1)^n \cos kn]} \right\}^{\frac{1}{2}} = I.$$

We are now in the position to state the following theorem.

Theorem 1. For the model described above, with $J(n) = Jn^{-\alpha}$ for every $1 < \alpha < 3$, there exists $s(\alpha) < \infty$ such that the system will show LRO at zero temperature if $s > s(\alpha)$.

Proof. We must show that for a certain interval of values of α there exists $\mathcal{I}$ such that $I < \mathcal{I} < \infty$.

The numerator can be bounded by

$$\sum_n n^{-\alpha} (-1)^n (1 - \cos kn) \leqslant 2 \sum_n n^{-\alpha} (-1)^n = 2A(\alpha).$$

Then making $k \to k + \pi$ in I, we establish the inequality

$$I \leqslant 2\sqrt{-12A(\alpha)} \int_0^\pi \mathrm{d}k \frac{1}{[\sum_n n^{-\alpha}(1 - \cos kn)]^{1/2}}.$$

We also have

$$\sum_n n^{-\alpha}(1 - \cos kn) \geqslant \sum_{n=1}^{[\pi/k]} n^{-\alpha}(1 - \cos kn)$$

where $[\pi/k]$ is the least integer smaller or equal to π/k.

The function $(1 - \cos kn)$ that appears above is now substituted by a quadratic function that contains its limits in $kn = 0$ and $kn = \pi$, producing

$$\sum_{n=1}^{[\pi/k]} n^{-\alpha}(1 - \cos kn) \geqslant 2\frac{k^2}{\pi^2} \sum_{n=1}^{[\pi/k]} n^{2-\alpha}. \tag{4}$$

Two distinct estimations can now be performed, according to the fact that $\alpha \leqslant 2$ or $\alpha \geqslant 2$. If $1 < \alpha \leqslant 2$,

$$2\frac{k^2}{\pi^2} \sum_{n=1}^{[\pi/k]} n^{2-\alpha} \geqslant 2\frac{k^2}{\pi^2}\left[\frac{\pi}{k}\right] = f_{\alpha\leqslant 2}(k).$$

If $\alpha \geqslant 2$ we then have

$$\frac{k^2}{\pi^2} \sum_{n=1}^{[\pi/k]} n^{2-\alpha} \geqslant 2\frac{\pi^{(1-\alpha)}}{k^{(1-\alpha)}} = f_{\alpha\geqslant 2}(k).$$

At this point we obtain

(i) $1 < \alpha \leqslant 2$,

$$I \leqslant \mathcal{I} = \sqrt{-12A(\alpha)} \int_0^\pi \mathrm{d}k \frac{1}{\sqrt{f_{\alpha\leqslant 2}(k)}} < \infty$$

for any α in the given interval;

(ii) $\alpha \geqslant 2$,

$$I \leqslant \mathcal{I} = \sqrt{-12A(\alpha)} \int_0^\pi \mathrm{d}k \frac{1}{\sqrt{f_{\alpha\geqslant 2}(k)}}$$

so that the above integral is finite whenever $(1-\alpha)/2 > -1$, implying $\alpha < 3$. The condition for LRO can then be restated as

$$[s(s+1)]^{\frac{1}{2}} > \mathcal{I}$$

which can always be made true for $\alpha < 3$ and s sufficiently large. $\square$

4. Absence of order for $\alpha > 3$

It is now convenient to redefine the Hamiltonian by

$$\widetilde{\mathcal{H}}_\Lambda = h \sum_{x\in\Lambda} (-1)^x S_x^3 + \left(\sum_{n=1}^{L} (-1)^n J(n) \boldsymbol{S}_x \cdot \boldsymbol{S}_{x+n} \right) = \mathcal{H}_\Lambda + h\sqrt{|\Lambda|}\hat{S}_\pi$$

where h represents an external field that will later be taken in the limit $h \to 0$. We now define the spontaneous magnetization as

$$\sigma(h) = \lim_{|\Lambda|\to\infty} \frac{1}{|\Lambda|} \left\langle \sum_{x\in\Lambda} S_x^3 \,\mathrm{e}^{\mathrm{i}\pi x} \right\rangle_\Lambda$$

and state the following.

Theorem 2. If $\alpha > 3$ we have

$$\lim_{h\to 0} \sigma(h) = 0.$$

Proof. Our proof follows from the following inequality [5],

$$\langle\{b^\dagger, b\}\rangle\sqrt{\langle[[a^\dagger, \widetilde{\mathcal{H}}_\Lambda], a]\rangle(a^\dagger, a)\beta} \geqslant |\langle[a^\dagger, b]\rangle|^2 \tag{5}$$

where a, b are self-adjoint operators. The problem is now reduced to performing a convenient choice of the operators a and b. We shall take

$$a^\dagger = S^-_{-k} \qquad \text{and} \qquad b = S^+_{k+\pi}.$$

Here $S^\pm_k$ are the Fourier transforms of the operators $S^\pm_x = S^1_x \pm \mathrm{i}S^2_x$.

We then have, on the right-hand side of (5),

$$\langle[a^\dagger, b]\rangle = \langle[S^-_{-k}\ , S^+_{k+\pi}]\rangle = 2\sigma(h).$$

The anticommutator on the left-hand side is given by

$$\langle\{b^\dagger, b\}\rangle = \frac{1}{|\Lambda|}\sum_{x,y}\langle S^-_x S^+_y\,\mathrm{e}^{-\mathrm{i}\pi(y-x)}\,\mathrm{e}^{-\mathrm{i}k(y-x)} + S^+_x S^-_y\,\mathrm{e}^{-\mathrm{i}\pi(x-y)}\,\mathrm{e}^{-\mathrm{i}k(x-y)}\rangle$$

so that summing both sides over k we obtain the inequality

$$\sum_{k\in\Lambda^*}\langle\{b^\dagger, b\}\rangle \leqslant |\Lambda| s(s+1)$$

by using the translation invariance of the expected value followed by an estimation in the norm. The double commutator in (5) can also be estimated in the norm after an explicit calculation

$$\langle[[a^\dagger, \widetilde{\mathcal{H}}_\Lambda], a]\rangle \leqslant 4\sum_{n=1}^{\infty}\{(1-\cos kn)n^{-\alpha}s(s+1) + |h\sigma(h)|\}.$$

The Duhamel two-point function can be bounded in the following way

$$(a^\dagger, a) = (S^1_{-k}, S^1_k) + (S^2_{-k}, S^2_k) + 2\mathrm{i}(S^2_k, S^1_k)$$

where we used the reality of the operator S^1 and the fact that $S^2_k = -S^2_{-k}$. By applying the Schwarz inequality to estimate the modulus of the imaginary term above we obtain

$$(a^\dagger, a) \leqslant (S^1_{-k}, S^1_k) + (S^2_{-k}, S^2_k) + 2\sqrt{(S^1_{-k}, S^1_k)(S^2_{-k}, S^2_k)}$$

so that the infrared bound (3) produces

$$(a^\dagger, a) \leqslant \frac{2}{\beta E_k} \qquad k \neq \pi$$

where $E_k = \sum_n[1-(-1)^n\cos kn]n^{-\alpha}$.

Putting it all together, summing both sides over k and using the parity of the integrand, we have when $L \to \infty$

$$\begin{aligned} s(s+1) &\geqslant \frac{2\sigma(h)^2}{\pi}\int_0^\pi \mathrm{d}k\left\{\frac{E_k}{2[\sum_n(1-\cos kn)n^{-\alpha}s(s+1) + |h\sigma(h)|]}\right\}^{1/2} \\ &= 2\sigma(h)^2 I(\alpha, h). \end{aligned}$$

We must now search for $\mathcal{I}(\alpha, h) \leqslant I(\alpha, h)$ such that $\lim_{h\to 0} \mathcal{I}(\alpha, h) \to \infty$, in which case $\lim_{h\to 0} \sigma(h) = 0$. We first look at the denominator of the integrand, where we use the inequality $1 - \cos kn \leqslant k^2n^2/2$:

$$I(\alpha, h) \geqslant \frac{2}{\pi}\int_0^\pi \mathrm{d}k \left\{ \frac{E_k}{2[\sum_n k^2 n^{2-\alpha} s(s+1) + |h\sigma(h)|]} \right\}^{1/2}.$$

The numerator can be bounded in the following way (4):

$$\sum_n [1 - (-1)^n \cos kn] n^{-\alpha} = \sum_n [1 - \cos(k+\pi)n] n^{-\alpha}$$

$$\geqslant \frac{2(k+\pi)^2}{\pi^2} \sum_n n^{2-\alpha} = \frac{2(k+\pi)^2}{\pi^2} R(\alpha)$$

and we notice that $R(\alpha) < \infty$ if $\alpha > 3$.

Now we have $\mathcal{I}(\alpha, h) = \mathcal{I}_1(\alpha, h) + \mathcal{I}_2(\alpha, h)$, where

$$\mathcal{I}_1(\alpha, h) = \frac{2\sqrt{2R(\alpha)}}{\pi^2} \int_0^\pi \mathrm{d}k \frac{k}{\{2[\sum_n k^2 n^{2-\alpha} s(s+1) + |h\sigma(h)|]\}^{1/2}}$$

which is finite for $\alpha > 3$ in the limit $h \to 0$, and

$$\mathcal{I}_2(\alpha, h) = \frac{2\sqrt{2R(\alpha)}}{\pi^2} \int_0^\pi \mathrm{d}k \frac{\pi}{\{2[\sum_n k^2 n^{2-\alpha} s(s+1) + |h\sigma(h)|]\}^{1/2}}$$

which has a logarithmic divergence when $h \to 0$, indicating that LRO does not occur if $\alpha > 3$. $\square$

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