Energy Gap in Heisenberg Antiferromagnetic Half-Integer Spin Chains with Long-Range Interactions

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Abstract

We show that there is no gap in the excitation spectrum of antiferromagnetic chains with half-integer spins and long-range interactions provided the exchange function has a sufficiently rapid decay.

1 Introduction

The ideas and techniques in this paper, on the problem of a gap in the excitation spectrum of Heisenberg antiferromagnetic chains, share much in common with those in [1] and [2]. In [1] Lieb, Schultz and Mattis proved that the ground state of the model with spin $\frac{1}{2}$ and nearest-neighbor interactions is non-degenerate and has total spin zero. This result was obtained under the assumption of translational invariance and the decomposability of the lattice into two sublattices with antiferromagnetic interactions between them. Under the same assumptions - plus periodic boundary conditions - it was also proved that the energy gap Δ_N between the ground state and the excited states for a finite chain of length N goes to zero as $N \to \infty$. In [2] the results about the uniqueness of the ground state were generalized by Lieb and Mattis: the requirement of translational invariance was dropped, arbitrary spin values were allowed and ferrimagnetic arrays were considered, the antiferromagnetic model being treated as a special case.

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In this note we show that the results of [1] and [2] can be extended to one- dimensional antiferromagnetic chains with periodic boundary conditions, half-integer spins and long range interactions without frustration.

2 The Model

We consider antiferromagnetic chains defined by the Hamiltonian

$$H_N = -J \sum_{x,y \in \Lambda_N} (-1)^{d_{xy}} \left(d_{xy}\right)^{-\alpha} \mathbf{S}_x.\mathbf{S}_y \tag{1}$$

where $J \geq 0$, $\Lambda_N = \{1, 2, ..., N\}$, N even, $\mathbf{S}_x$ are usual spin operators at site $x \in \Lambda_N$ with $\mathbf{S}_x^2 = s(s+1)$ and s is half-integer. The factor $\left(d_{xy}\right)^{-\alpha}$ measures the decay of the interaction with the distance between the spins at sites x and y. We also need periodic boundary conditions, so that $\mathbf{S}_{x+N+1} = \mathbf{S}_x$.

A suitable definition of distance - which takes into account the periodic boundary conditions and the long-range character of the interactions - is the one defined by

$$d_{xy} = \begin{cases} |x-y|\,, \text{if } |x-y| \leq \frac{N}{2} \\ N - |x-y|\,, \text{if } |x-y| > \frac{N}{2} \end{cases}$$

Our result is the following: we prove that the energy gap Δ_N between the unique ground state and the excited states goes to zero as $N \to \infty$ for any $J > 0$ and $\alpha > 2$.

3 Proof of the Result

The model defined by (1) is a translational invariant system which can be decomposed into two sublattices with antiferromagnetic interactions between them. As an immediate consequence we can conclude that the total spin of the ground state is zero.

We now introduce the state $|\Psi_k\rangle$:

$$|\Psi_k\rangle = \mathcal{O}_k \, |\Psi_0\rangle \, ,$$

where $|\Psi_0\rangle$ is the unique ground state of the system and the operator $\mathcal{O}_k$ is given by

$$\mathcal{O}_k = \exp\{ik \sum_{x=1}^{N} x S_x^3\},$$

with $k = \frac{2\pi}{N}$.

As a consequence of translational invariance, we have

$$\langle \Psi_0 \mid \Psi_k \rangle = \left\langle \Psi_0 \mid \mathcal{O}_k \exp\{ikNS_1^3\} \exp\{-ik \sum_{x=1}^{N} S_x^3\} \mid \Psi_0 \right\rangle . \qquad (2)$$

¿From the fact that the ground state is a singlet, it follows that

$$\exp\{-ik \sum_{x=1}^{N} S_x^3\} \left|\Psi_0\right\rangle = \left|\Psi_0\right\rangle ,$$

and since for half-integer spins, in the basis that diagonalize S^3, which shall be used throughout in this paper,

$$\exp\{ikNS_1^3\} = -I,$$

we have the orthogonality relation$\langle \Psi_0 \mid \Psi_k \rangle = - \langle \Psi_0 \mid \Psi_k \rangle = 0$.

Theorem 1 *If $\alpha > 2$ the energy gap Δ_N between the ground state and the excited states goes to zero as $N \to \infty$.*

Proof

We begin by rewritting the Hamiltonian (1) as

$$H_N = -J \sum_{x \in \Lambda_N} \sum_{n=1}^{\frac{N}{2}-1} \left[(-1)^n n^{-\alpha} \mathbf{S}_x . \mathbf{S}_{x+n} + \frac{(-1)^{\frac{N}{2}}}{2} \left(\frac{N}{2}\right)^{-\alpha} \mathbf{S}_x . \mathbf{S}_{x+\frac{N}{2}} \right] , \qquad (3)$$

and then compute the expected value of the energy in the state $\mid \Psi_k \rangle$:

$$E_k \equiv \langle \Psi_k \mid H_N \mid \Psi_k \rangle = \langle \Psi_0 \mid \mathcal{O}_k^{-1} H_N \ \mathcal{O}_k \mid \Psi_0 \rangle .$$

Now we point out that

$$\begin{aligned} \mathcal{O}_k^{-1} H_N \mathcal{O}_k = H_N + J \sum_{x \in \Lambda_N} \sum_{n=1}^{\frac{N}{2}-1} \{ (-1)^n \, n^{-\alpha} [(S_x^1 S_{x+n}^2 - S_x^2 S_{x+n}^1) \sin kn + \\ + (S_x^1 S_{x+n}^1 + S_x^2 S_{x+n}^2) (\cos kn - 1)] + \\ + (-1)^{\frac{N}{2}} \left(\frac{N}{2}\right)^{-\alpha} [(S_x^1 S_{x+\frac{N}{2}}^2 - S_x^2 S_{x+\frac{N}{2}}^1) \sin \frac{kN}{2} + \\ + (S_x^1 S_{x+\frac{N}{2}}^1 + S_x^2 S_{x+\frac{N}{2}}^2) \left(\cos \frac{kN}{2} - 1 \right)] \} , \end{aligned} \qquad (4)$$

where we have used that:

$$\mathcal{O}_k^{-1} S_x^1 \mathcal{O}_k = S_x^1 \cos kx + S_x^2 \sin kx, \qquad (5)$$

$$\mathcal{O}_k^{-1} S_x^2 \mathcal{O}_k = S_x^2 \cos kx - S_x^1 \sin kx, \qquad (6)$$

$$\mathcal{O}_k^{-1} S_x^3 \mathcal{O}_k = S_x^3, \tag{7}$$

It is easy to see that the last two terms on the r. h. s. of (4) equal zero. We also have that

$$J \sum_{x\in\Lambda_N} \sum_{n=1}^{\frac{N}{2}-1} (-1)^n\, n^{-\alpha} \left(S_x^2 S_{x+n}^1 - S_x^1 S_{x+n}^2\right) \sin kn = i \sum_{y\in\Lambda_N} \left[y S_y^3, \widetilde{H}\right],$$

with

$$\widetilde{H} = -J \sum_{x\in\Lambda_N} \sum_{n=1}^{\frac{N}{2}-1} (-1)^n n^{-\alpha-1} \sin kn \mathbf{S}_x . \mathbf{S}_{x+n},$$

so that

$$\langle \Psi_0 \mid i \sum_{y\in\Lambda_N} \left[y S_y^3, \widetilde{H}\right] \mid \Psi_0 \rangle = 0,$$

where the self-adjointness of the operator S^3 was taken into account. The expression in (4) is then reduced to

$$\langle \Psi_0 \mid \mathcal{O}_k^{-1} H_N \ \mathcal{O}_k \mid \Psi_0 \rangle =$$

$$= \langle \Psi_0 \mid H_N + J \sum_{x\in\Lambda_N} \sum_{n=1}^{\frac{N}{2}-1} (-1)^n\, n^{-\alpha} (S_x^1 S_{x+n}^1 + S_x^2 S_{x+n}^2)[\cos kn - 1] \mid \Psi_0 \rangle.$$

It is possible to estimate the sum $(S_x^1 S_{x+n}^1 + S_x^2 S_{x+n}^2)$ by a positive number $\Theta(s)$, which depends only on the value of the spin at each site, $s(s+1) = \mathbf{S}_x^2$, so that:

$$E_k \leq E_0 + J \sum_{x\in\Lambda_N} \sum_{n=1}^{\frac{N}{2}-1} \left|\Theta(s)\,(-1)^n\, n^{-\alpha}[\cos kn - 1]\right|.$$

We have, therefore, for $\Delta E_k \equiv E_k - E_0$, the bound:

$$\Delta E_k \leq J\Theta(s) \sum_{n=1}^{\frac{N}{2}-1} n^{-\alpha}[1 - \cos kn]\mathcal{N}(n).$$

Here $\mathcal{N}(n)$ is the number of pairs of sites at distance n. In the periodic lattice, $\mathcal{N}(n) = N$, so that:

$$\Delta E_k \leq J\Theta(s) \sum_{n=1}^{\frac{N}{2}-1} n^{-\alpha}[1 - \cos kx]N.$$

The sum on the r. h. s. can be estimated for some $c > 0$, by parts, for $1 \leq n \leq \left[\frac{c}{k}\right]$, and $\left[\frac{c}{k}\right] < n \leq N$ - where by $\left[\frac{c}{k}\right]$ we denote the largest integer less or equal than $\frac{c}{k}$ - as follows:

$$J\Theta(s)N \sum_{n<\left[\frac{c}{k}\right]} n^{-\alpha}[1 - \cos kn] \leq \frac{4\pi^2}{N} J\Theta(s) \sum_{n<\left[\frac{c}{k}\right]} n^{2-\alpha},$$

while

$$J\Theta(s) \sum_{N \geq n > \left[\frac{c}{k}\right]} n^{-\alpha}[1 - \cos kn]N \leq 2J\Theta(s)N \sum_{n > \left[\frac{c}{k}\right]} n^{-\alpha} \leq$$

$$\leq 2J\Theta(s)N^2 \left(\frac{c}{k}\right)^{-\alpha},$$

and we obtain for the energy gap Δ_N the following upper bound:

$$\Delta_N \leq \Delta E_{\frac{2\pi}{N}} \leq 2J\Theta(s) \left[N^2 \left(\frac{cN}{2\pi}\right)^{-\alpha} + \frac{\pi^2}{N} \sum_{n < \frac{c}{k}} n^{2-\alpha}\right],$$

which goes to zero if $\alpha > 2$ when $N \to \infty$.End Proof

References

[1] Lieb, E.; Schultz, T.; Mattis, D.; *Ann. Phys.*, **16**, 407 (1961).

[2] Lieb, E.; Mattis, D.; *J. Math. Phys.*, **3**, n. 4, 749 (1961).