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2003 J. Phys. A: Math. Gen. 36 L599

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INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **36** (2003) L599–L604 PII: S0305-4470(03)67085-X

LETTER TO THE EDITOR

The possibility of gapless excitations in antiferromagnetic spin chains with long-range interactions

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Received 5 August 2003, in final form 1 October 2003
Published 12 November 2003
Online at stacks.iop.org/JPhysA/36/L599

Abstract

The Lieb–Shultz–Mattis theorem is extended to Heisenberg chains with long-range interactions. We prove that the half-integer spin chain has no gap, if it possesses *unique* ground state and the exchange decays faster than the *inverse-square* of distance between spins. The results can be extended to a wide class of one-dimensional models.

PACS numbers: 75.10.Jm, 75.50.Ee, 71.10.−w, 68.35.Rh, 05.50.+q, 02.30.Ik

The zero-temperature ground-state properties of one-dimensional antiferromagnets have been studied intensively over a long period. There are various numerical and field theoretical approaches to the problem. At the same time there are just a few exact non-perturbative methods. The spin $S = 1/2$ antiferromagnetic (AF) Heisenberg spin chain with nearest-neighbour (n.n.) interactions was solved exactly by Bethe [1]. Bethe's ansatz was applied later to peculiar higher spin chains with polynomial spin exchange [2].

Lieb *et al* [3] offered another non-perturbative approach. They proved that $S = 1/2$ even length L AF n.n. Heisenberg chain with periodic boundary conditions has at least one *low-energy*, $O(1/L)$ excitation above the *unique* ground state. Later Haldane [4], using the σ-model description, argued that the AF n.n. *integer* spin Heisenberg chains have a *gap* between the ground state and the first excited state, whereas the *half-integer* spin chains have *no gap*. The part of Haldane's conjecture was proved for the *half-integer* spin chains [5, 6] by means of extension of the Lieb–Schultz–Mattis (LSM) theorem. Namely, the half-integer spin chains are gapless if they have a unique ground state in the thermodynamic limit.

The LSM theorem was also extended to the case with an applied magnetic field [7]. It was generalized to Heisenberg chains with $SU(n)$ [6] and other [8] symmetries, to fermionic chains [9], to spin [10] and fermionic [11] models on ladders, etc. Very recently, its extension to higher dimensions has been discussed [12–14] applying the arguments used by Laughlin in the quantum Hall effect [15].

This letter is devoted to the extension of LSM theorem to AF Heisenberg chains with *long-range* interactions. The $S = 1/2$ chain with the spin exchange decaying as $1/r^2$, where r is the distance between spins, has been extensively investigated since it was solved exactly by Haldane and Shastry [16]. The integrability is a consequence of an infinite symmetry of this model [17]. Despite the presence of long-range interactions, its low-energy properties are similar to those of the chain with n.n. interactions: both models are gapless and belong to the same universality class. Here we discuss the zero-temperature ground-state properties of the *translationally* invariant AF *half-integer* spin chain with *arbitrary* exchange coupling. We will prove that, in the thermodynamic limit, it either has *gapless* excitations or *degenerate* ground states, provided that the coupling decays faster than $1/r^2$.

The Hamiltonian of a Heisenberg chain with long-range interactions, which is studied here, is

$$\mathcal{H}_L = \sum_{r=1}^{L'} \sum_{i=0}^{L-1} J(r) \vec{S}_i \cdot \vec{S}_{i+r} \qquad L' = (L-1)/2 \tag{1}$$

where the chain length L is chosen to be *even*. We see that the sum over r is taken up to the half-size L' of the chain. Note that the spin exchange coupling $J(r)$ depends on the distance between the spins only. Periodic boundary conditions are assumed: $\vec{S}_i = \vec{S}_{i+L}$. The last two conditions imply the translational invariance of (1).

Let us consider the nonlocal unitary operator

$$U = \mathrm{e}^{\mathcal{A}} \qquad \mathcal{A} = \frac{2\pi \mathrm{i}}{L} \sum_{k=1}^{L} k S_k^z. \tag{2}$$

It rotates the spins around the z-axis with the relative angle $2\pi/L$ between the neighbouring spins. We are interested in formal algebraic properties of U. However, as was shown recently, it has a clear physical meaning too. In spin chains and ladders, the ground-state expectation value of U can be treated as an order parameter, which characterizes various valence-bond-solid ground states [18]. In sine-Gordon theory, it is related to expectation values of vertex operators [19].

It is well known that the action of (2) on the ground state of the Heisenberg chains with *short-range* interactions gives rise to the state with an energy which approaches the energy of the ground state in the thermodynamic limit $L \to \infty$ [3, 6]. Below we will discuss the possibility of extending this property to the Hamiltonian (1) with *long-range* interactions.

In this letter, for the sake of simplicity, we assume the *uniqueness* of the ground state $|\Omega\rangle$ of a finite chain. Note that in this case $|\Omega\rangle$ is a spin-*singlet*. Our assumption is fulfilled for a wide class of models on even length chains. In the case of alternating couplings, i.e. $J(2r-1) > 0, J(2r) \leqslant 0$, it can be proved *exactly* using Perron–Frobenius-type arguments [6].

It is convenient to rewrite $\mathcal{H}_L$ in the following form:

$$\mathcal{H}_L = \sum_{r=1}^{L'} J(r) \mathcal{H}_L^r \qquad \text{where} \quad \mathcal{H}_L^r = \sum_{i=0}^{L-1} \vec{S}_i \cdot \vec{S}_{i+r}.$$

Then the energy gap between the ground state $|\Omega\rangle$ and the shifted state $U|\Omega\rangle$ is

$$\Delta E_L = \sum_{r=1}^{L'} \Delta E_L^r \qquad \text{where} \quad \Delta E_L^r = \langle\Omega|U^+ \mathcal{H}_L^r U|\Omega\rangle - \langle\Omega|\mathcal{H}_L^r|\Omega\rangle. \tag{3}$$

The straightforward calculations show that

$$U^{+}\mathcal{H}_{L}^{r}U-\mathcal{H}_{L}^{r}=\sum_{i=0}^{L-1}\left\{\mathcal{K}(r/L)S_{i}^{+}S_{i+r}^{-}+\text{h.c.}\right\}+[\mathcal{H}_{L}^{r},\mathcal{A}] \tag{4}$$

where

$$\mathcal{K}(\phi)=\tfrac{1}{2}\{\exp(2\pi\mathrm{i}\phi)-(1+2\pi\mathrm{i}\phi)\}\quad\text{and}\quad S_{i}^{\pm}=S_{i}^{x}\pm\mathrm{i}S_{i}^{y}.$$

Note that the coefficients in front of spin operators do not depend on the absolute positions of the spins, but depend on their distance. Taking the sum of (4) over r, we obtain

$$U^{+}\mathcal{H}_{L}U-\mathcal{H}_{L}=\sum_{r=1}^{L'}J(r)\left\{\mathcal{K}(r/L)\mathcal{H}_{L}^{r+}+\text{h.c.}\right\}+[\mathcal{H}_{L},\mathcal{A}]\qquad\text{where}\quad\mathcal{H}_{L}^{r\,\pm}=\sum_{i=0}^{L-1}S_{i}^{\pm}S_{i+r}^{\mp}. \tag{5}$$

The mean value of the commutator $[\mathcal{H}_L,\mathcal{A}]$ vanishes on $|\Omega\rangle$, because $|\Omega\rangle$ is an eigenstate of $\mathcal{H}_L$. The mean value of $\mathcal{H}_L^{r\,\pm}$ is of the order of L:

$$|\langle\Omega|\mathcal{H}_{L}^{r\,\pm}|\Omega\rangle|\leqslant 1/4L. \tag{6}$$

Now, using (3), (5) and (6), we can estimate the upper bound of the gap:

$$|\Delta E_{L}|\leqslant\frac{L}{2}\sum_{r=1}^{L'}J(r)|\mathcal{K}(r/L)|=\frac{1}{L}\sum_{r=1}^{L'}r^{2}J(r)\frac{|\mathcal{K}(r/L)|}{2(r/L)^{2}}. \tag{7}$$

The function $|\mathcal{K}(\phi)|/(2\phi^2)$ is continuous on the unit interval $0\leqslant\phi\leqslant 1$ (see the definition in (4)). So, it can be replaced in (7) by its maximal value C and we obtain

$$|\Delta E_{L}|\leqslant\frac{C}{L}\sum_{r=1}^{L'}r^{2}J(r). \tag{8}$$

We conclude that the energy gap between the ground state and the shifted state $U|\Omega\rangle$ vanishes in the thermodynamic limit, provided that

$$\lim_{L\to\infty}\frac{1}{L}\sum_{r=1}^{L'}r^{2}J(r)=0.$$

Any function, obeying

$$\lim_{r\to\infty}r^{2}J(r)=0 \tag{9}$$

satisfies this condition. Note that up to now we have not distinguished between the integer and the half-integer spin chains.

In order to prove that $U|\Omega\rangle$ is a real excitation, i.e. it does not coincide with the ground state $|\Omega\rangle$ and does not approach it in the thermodynamic limit, it is sufficient to show that both states are orthogonal [3, 6]. We use the translation T by one lattice site to demonstrate this. The ground state is an eigenstate of T, because T commutes with the Hamiltonian (1): $T|\Omega\rangle=\mathrm{e}^{\mathrm{i}p}|\Omega\rangle$, where $p=0,\pi$ due to the reflection symmetry. The shift operator (2) transforms as: $T^{-1}UT=U\exp\left(2\pi\mathrm{i}S_1^z\right)\exp\left(-2\pi\mathrm{i}\mathcal{S}^z/L\right)$, where $\mathcal{S}^z=\sum_{i=0}^{L-1}S_i^z$ is the z-component of the total spin $\vec{\mathcal{S}}$. We have $\mathcal{S}^z|\Omega\rangle=0$, because $|\Omega\rangle$ is a singlet. Using the equations above, we obtain: $TU|\Omega\rangle=\mathrm{e}^{-2\pi\mathrm{i}S}\,\mathrm{e}^{\mathrm{i}p}U|\Omega\rangle$. We see that the eigenvalues of T on $|\Omega\rangle$ and $U|\Omega\rangle$ differ for *half-integer S* only. So, in this case the two states are orthogonal. Then, in the $L\to\infty$ limit, either (i) $U|\Omega\rangle$ generates another ground state(s) or (ii) $|\Omega\rangle$ remains a unique ground state with gapless excitations, created by $U|\Omega\rangle$. In the second case, of course, the ground state should be a spin-*singlet*.

We come to the conclusion that:

The translationally invariant AF Heisenberg half-integer spin chain is gapless if it has unique ground state and the exchange coupling of interacting spins decays faster than the inverse-square of their distance.

This is the main result of this letter. Below we will discuss it and compare with some known models.

The examples of $J(r)$, which satisfy the conditions above, are

(a) $1/(r^2\log(r))$ (b) $1/r^\alpha \quad \alpha > 2$ (c) $r^n\exp(-r/a) \quad a > 0$.

The last case is a short-range interaction effectively.

Note that the resulting statement excludes the *coexistence* of a gap and a unique ground state under the aforementioned conditions. For finite even values of L the uniqueness of the ground state can be proved for a wide class of the chains, as was mentioned above. In the thermodynamic limit, however, the low-energy state can generate either a continuum of gapless excitation or spontaneously broken translation symmetry. In the last case, the chain can have a gap. The simplest example, which demonstrates both types of behaviour, is related to the short-range interaction case. It is the well-known chain with nearest-neighbour $J(1) = J_1 > 0$ and next-nearest-neighbour $J(2) = J_2 > 0$ interactions ($J(r) = 0$ for $r > 2$) [20]. For $J_2 = 0$ (the *XXX* model) this chain is exactly solvable and gapless with a unique ground state, as was mentioned above. At the Majumdar–Ghosh point $J_2 = 0.5J_1$ it has a gap and two different ground states, consisting of nearest-neighbour dimers [21]. Although there are no exact results for the ground state behaviour between these two exactly solvable points, the conformal field theory approach predicts that for small values of J_2 the chain still remains gapless with a unique ground state [20], whereas for small values of J_1 it has a gap and twofold degenerate ground states [22]. The critical point $J_2^c \approx 0.241J_1$ [23], which has been calculated with high precision [24], separates the two different phases.

Our result gives only the *sufficient* condition for the chain to be gapless or to have degenerate ground states in the thermodynamic limit. The integer spin chains or chains with exchange coupling decay slower than $1/r^2$ can have a gap and a unique ground state simultaneously. They can also be gapless. For example, the $S = 1$ chain with the alternating exchange $J(r) = (-1)^r/r^\alpha$, $1 < \alpha < 3$ exhibits gapless behaviour [25]. However, the same chain with $J(r) = 1/r^2$ has a gap, as was shown numerically in [26]. Its ground-state properties are similar to those of a Haldane chain with n.n. interactions [4]. Another simple example is the case when the spin exchange coupling does not depend on the distance: $J(r) = J$ for all r. This is an exactly solvable model with the energy levels up to an additive constant proportional to $\mathcal{S}(\mathcal{S}+1)$, where $\mathcal{S} = 0, 1, \ldots, SL$ is the total spin of the chain. They are highly degenerate due to the additional permutation group symmetry. The ground-state subspace consists of all singlets and there is a gap between them and the lowest $\mathcal{S} = 1$ excitations. Note that this property cannot be considered as a consequence of the statement proved in this letter, because the coupling $J(r) = J$ does not satisfy the required condition.

As we have mentioned before, the $S = 1/2$ chain with $J(r) = 1/r^2$ corresponds to the Haldane–Shastry integrable model. In the case of the *periodic* boundary conditions the coupling is slightly modified[1]: $J_L^{\mathrm{Hsh}}(r) = ((L/\pi)\sin(\pi r/L))^{-2}$. For $J(r) = J_L^{\mathrm{HSh}}(r)$ the

[1] Of course, we have: $\lim_{L\to\infty} J_L^{\mathrm{HSh}}(r) = 1/r^2$. Note that the dependence on the chain length does not change anything in the final result (7), where we can impose $J(r) = J_L(r)$.

upper bound of the gap in (7) is nonzero. This fact does not guarantee the existence of a low-energy state[2]. Nevertheless, the exact solution shows that this model has gapless excitations.

Acknowledgments

The author is grateful to Professor R Flume for hospitality during his visit to Physikalisches Institut, Universität Bonn. He thanks R Flume, R Poghossian and D Karakhanyan for stimulating discussions. This work is supported by Volkswagen Foundation of Germany, by grants INTAS #00-561 and INTAS #99-01459 and Swiss SCOPE grant.

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$$\frac{\pi^2}{2}\int_0^{1/2} \frac{|\mathcal{K}(\phi)|}{\sin^2(\pi\phi)}\,\mathrm{d}\phi.$$

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