Physics Letters A ••• (••••) •••–•••

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Physics Letters A

www.elsevier.com/locate/pla

Variational model for one-dimensional quantum magnets

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ARTICLE INFO

Article history:
Received 1 February 2018
Received in revised form 21 February 2018
Accepted 23 February 2018
Available online xxxx
Communicated by M. Wu

Keywords:
1D quantum magnet
Staggered magnetic field
Jordan–Wigner transformation
Trial wave function
Ground state energy
Correlation function

ABSTRACT

A new variational technique for investigation of the ground state and correlation functions in 1D quantum magnets is proposed. A spin Hamiltonian is reduced to a fermionic representation by the Jordan–Wigner transformation. The ground state is described by a new non-local trial wave function, and the total energy is calculated in an analytic form as a function of two variational parameters. This approach is demonstrated with an example of the XXZ-chain of spin-1/2 under a staggered magnetic field. Generalizations and applications of the variational technique for low-dimensional magnetic systems are discussed.

1. Introduction

One-dimensional magnetic systems, both a simple chain and complex ones like decorated chains, zig-zag and ladder structures, are drawn a considerable attention of theoreticians and experimentalists [1–3]. It is related to recent progress in the synthesis of one-dimensional molecular magnets [4] and quasi-one-dimensional magnetic structures in crystalline substances [5].

A Heisenberg chain of spin-1/2 is one of the most fundamental and thoroughly investigated models of magnetism [1]. Nevertheless, a few exotic phases were recently revealed: the ground state with E8 symmetry under a transverse magnetic field in $CoNb_2O_6$ [6], Bose glass in $(Yb_{1-x}Lu_x)_4As_3$ [7], and etc.

Analytic solutions for the Heisenberg antiferromagnetic (AFM) chain with magnetic field directed along the quantization axis are well-known, namely the ground state energy [1,2,8] and excitation spectrum [9–11] which is gapless at magnetic fields below the critical value [12]. At the same time, a spin gap is observed in various one- and quasi-one-dimensional magnets [5]. In some cases the gap stems from a staggered magnetic field appeared due to the Dzyaloshinskii–Moriya interaction [13] or an effect of the transverse magnetic field on an anisotropic zig-zag chain [4].

There are no analytic solutions for the Heisenberg chain under the staggered magnetic field. An asymptotic solution for the isotropic chain in the limit of weak staggered field ($h_{st} \to 0$) was obtained by transformation to the sine-Gordon model [14]. It is valid within a very narrow region in the vicinity of $h_{st} = 0$. The finite-temperature density-matrix renormalization group (DMRG) theory allowed resolving the problem at wider range of finite staggered field [15]. Recently the XXZ-chain with staggered magnetic field was thoroughly investigated using the mean-field approach with fluctuation corrections up to the second order and the exact diagonalization on finite clusters [16]. The Heisenberg Hamiltonian was preliminarily mapped onto a fermionic representation by the Jordan–Wigner transformation [17]. It was shown that the mean-field approximation with the corrections in a number of cases gives unsatisfactory results. In particular, in the limit $h_{st} \to 0$ it leads to a divergence of the ground state energy for the XY-chain and an unphysical behavior of the spin gap for the isotropic Heisenberg chain [16].

On the other hand, the mapping on the fermionic representation by means of the Jordan–Wigner transformation makes possible applying well-developed techniques of strongly correlated Fermi systems theory. In particular, a variational Gutzwiller approach [18] has allowed calculating the ground state energy of the Hubbard model for the infinite-dimensional lattice. It was also successively applied to low dimensional lattices up to one-dimensional chain [19]. The Gutzwiller trial wave function had

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https://doi.org/10.1016/j.physleta.2018.02.031
0375-9601/

been intended for control of intrasite correlations, its generalization enabled to include non-local correlations between the nearest neighbors [20]. It was shown that this trial wave function produces a good approximation of the ground state for the Hubbard model even in the one-dimensional case. Since the fermionic representation for Heisenberg chain contains interactions between the nearest-neighboring sites, the generalized non-local trial wave function seems to be a promising candidate for its ground state description.

In the present Letter, we propose a new variational approach to one-dimensional quantum magnets and illustrate it by example of the Heisenberg XXZ-chain with the staggered magnetic field. The procedure includes the follow steps: (i) the transition to the fermionic representation by means of the Jordan–Wigner transformation, (ii) development of the trial wave function for spinless fermions, (iii) calculation of the ground state energy, correlation functions, and other characteristics with the trial wave function.

2. Jordan–Wigner transformation

The Hamiltonian of spin-1/2 Heisenberg XXZ chain under the staggered magnetic field has the following form [16]

$$\hat{H} = \hat{H}_{xy} + \hat{H}_{zz} + \hat{H}_{st} \tag{1}$$

where $\hat{H}_{xy} = \frac{J}{2}\sum_i^N \left(\hat{S}_i^+\hat{S}_{i+1}^- + \hat{S}_i^-\hat{S}_{i+1}^+\right)$ and $\hat{H}_{zz} = J\Delta\sum_i^N \hat{S}_i^z\hat{S}_{i+1}^z$ are the xy- and zz-terms of the Hamiltonian, $\hat{H}_{st} = h_{st}\sum_i^N (-1)^i \hat{S}_i^z$ is the contribution of the staggered magnetic field h_{st}, $\hat{S}_i^+\left(\hat{S}_i^-\right)$ and $\hat{S}_i^z$ are the operators of spin raising (lowering) and its component along the z-axis. The constant J is assumed to be positive. Below we discuss mainly behavior of the anisotropic AFM chain ($\Delta \geq 0$), however the results remain valid for the ferromagnetic (FM) chain also ($\Delta < 0$).

The Jordan–Wigner transformation allows representing the spin operators through creation (annihilation) operators for spinless fermions at the i-th chain site $\hat{c}_i^\dagger$ ($\hat{c}_i$) [17]:

$$\begin{aligned}
\hat{S}_i^+ &= \hat{c}_i^\dagger \exp\left(i\pi\sum_{j=1}^{i-1}\hat{n}_j\right),\\
\hat{S}_i^- &= \exp\left(-i\pi\sum_{j=1}^{i-1}\hat{n}_j\right)\hat{c}_i,\\
\hat{S}_i^z &= \hat{n}_i - 1/2.
\end{aligned} \tag{2}$$

This reduces the Hamiltonian (1) to a model of fermionic chain [16]:

$$\begin{aligned}
\hat{H} &= \hat{H}_0 + \hat{H}_1, \qquad (3)\\
\hat{H}_0 &= \sum_j^{N/2}\Big[\frac{J}{2}\left(\hat{a}_j^\dagger\hat{b}_j + \hat{a}_{j+1}^\dagger\hat{b}_j + h.c.\right)\\
&\quad + h_{st}\left(\hat{a}_j^\dagger\hat{a}_j - \hat{b}_j^\dagger\hat{b}_j\right)\Big],\\
\hat{H}_1 &= J\Delta\sum_j^{N/2}\Big[\left(\hat{a}_j^\dagger\hat{a}_j - \frac{1}{2}\right)\left(\hat{b}_j^\dagger\hat{b}_j - \frac{1}{2}\right)\\
&\quad + \left(\hat{b}_j^\dagger\hat{b}_j - \frac{1}{2}\right)\cdot\left(\hat{a}_{j+1}^\dagger\hat{a}_{j+1} - \frac{1}{2}\right)\Big],
\end{aligned}$$

where $\hat{a}_i^\dagger$ and $\hat{b}_i^\dagger$ are the creation operators for spinless fermions at the A and B sublattices correspondingly, that is, $\hat{a}_i^\dagger \equiv \hat{c}_i^\dagger$ ($i \in A$) and $\hat{b}_j^\dagger \equiv \hat{c}_j^\dagger$ ($j \in B$). The Hamiltonian (3) contains quadratic ($\hat{H}_0$) and biquadratic ($\hat{H}_1$) parts. The first one corresponds to the kinetic energy of a tight-binding model, and the second represents an interaction between the fermions at the nearest-neighboring chain sites.

The quadratic part of the Hamiltonian $\hat{H}_0$ is diagonalized by a unitary transformation [16]

$$\hat{H}_{0d} = U\hat{H}_0U^{-1} = \sum_k \varepsilon_k\left(\hat{\alpha}_k^\dagger\hat{\alpha}_k - \hat{\beta}_k^\dagger\hat{\beta}_k\right) \tag{4}$$

where $\varepsilon_k = \sqrt{J^2\cos^2(k/2) + h_{st}^2}$. Hereinafter we use a reduced Brillouin zone corresponding to the doubled chain period, that is, $k/2 \to k$. It should be mentioned that $\hat{H}_{0d}$ corresponds to the XY-model with the staggered magnetic field. In the ground state, the branch with the negative eigenvalues is fully filled up ($n_{\beta k} = \hat{\beta}_k^\dagger\hat{\beta}_k = 1$), and that with the positive ones is empty ($n_{\alpha k} = \hat{\alpha}_k^\dagger\hat{\alpha}_k = 0$). Thus the ground state of the XY-chain in the staggered magnetic field is determined exactly:

$$|\tilde{\varphi}\rangle = \prod_k \beta_k^\dagger|0\rangle. \tag{5}$$

For the sake of convenience, below we apply a representation of the operators $\hat{a}_i^\dagger$ and $\hat{b}_i^\dagger$ expressed in terms of the diagonal operators $\hat{\alpha}_k^\dagger$ and $\hat{\beta}_k^\dagger$ by means of the inverse transformation $|\varphi\rangle = U^{-1}|\tilde{\varphi}\rangle$.

3. Trail wave function

To generate a non-local trial wave function one should define projection operators on all possible configurations of the nearest neighboring pairs of sites in the chain [20]. There are four such configurations for spinless fermions

$$\begin{aligned}
\hat{Y}_1 &= \sum_{<i,j>}\left(1-\hat{n}_i^A\right)\left(1-\hat{n}_j^B\right),\\
\hat{Y}_2 &= \sum_{<i,j>}\hat{n}_i^A\left(1-\hat{n}_j^B\right),\\
\hat{Y}_3 &= \sum_{<i,j>}\left(1-\hat{n}_i^A\right)\hat{n}_j^B,\\
\hat{Y}_4 &= \sum_{<i,j>}\hat{n}_i^A\hat{n}_j^B
\end{aligned} \tag{6}$$

where $<\ldots>$ denotes a sum over all the pairs of the nearest neighbors. The sites in the pairs belong to different sublattices: ($i \in A$) and ($j \in B$).

It is worth noticing that the operators $\hat{Y}_k$ are not completely independent [20]. Thus, let us consider expectation values of the operators $y_k = L^{-1} < \hat{Y}_k >$. They can be interpreted as probabilities of the corresponding pairs configurations. One can see that y_k are related to one another by conditions of normalization ($\sum_k y_k = 1$) and half-band filling ($y_2 + y_3 + 2y_4 = 1$). Then it is convenient to introduce a pair of independent symmetrized operators $\hat{M} = \hat{Y}_3 - \hat{Y}_2$ and $\hat{P} = \hat{Y}_3 + \hat{Y}_2$. Their physical meaning can be clarified by the averages $m = L^{-1} < \hat{M} >$ and $p = L^{-1} < \hat{P} >$: the limiting value $m = 1$ corresponds to the chain state when all the site of the B sublattice are filled up ($n_B = 1$) and all the sites of the A sublattice are empty ($n_A = 0$), and in the opposite limit ($m = -1$) vice versa ($n_A = 1$ and $n_B = 0$). That is why, m denotes the AFM magne-

Please cite this article in press as: Yu.B. Kudasov, R.V. Kozabaranov, Variational model for one-dimensional quantum magnets, Phys. Lett. A (2018), https://doi.org/10.1016/j.physleta.2018.02.031