Physica B 403 (2008) 3498–3502

Contents lists available at ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Coupled cluster study of the dimer state of the spin-1/2 alternating Heisenberg chain

Jian-Jun Jiang [a,*], Yong-Jun Liu [b]

[a] Department of Physics, Sanjiang College, No. 10, Long Xi Road, Tiexinqiao, Yuhuatai District, Nanjing, Jiangsu 210012, China
[b] School of Physics Science and Technology, Yangzhou University, Yangzhou 225002, China

ARTICLE INFO

Article history:
Received 14 September 2007
Received in revised form
11 May 2008
Accepted 13 May 2008

PACS:
75.10.Jm
75.50.Ee
03.65.Ca
75.40.Cx

Keywords:
Heisenberg antiferromagnet
Coupled cluster method
Exact diagonalization
LSUB*n* approximation
Ground-state energy
Spin gap

ABSTRACT

We investigate the properties of the spin-1/2 alternating Heisenberg chain using the coupled cluster method accompanied by exact diagonalization up to 24 sites. The ground-state energy per spin e and the spin gap Δ are calculated for a range of α. Our results show that the spin gap opens and the dimerized state dominates the properties of the ground state as $\alpha > 1$. We also study the approach of the ground-state energy per spin e_0 to the uniform spin chain. The results show that the critical behaviour of e_0 is well described by a power law with exponents 1.4307 and 1.4405 obtained by the coupled cluster method and exact diagonalization, respectively.

1. Introduction

The study of low-dimensional gapped quantum antiferromagnets has attracted much experimental and theoretical interest in recent years. Much research activity in this area has been focused on the one-dimensional (1-D) antiferromagnetic Heisenberg (AFH) spin chain with $s = 1$. Haldane [1] argued that the system is gapful and the spin gap has been found in compound $CsNiCl_3$ [2]. There are many studies to investigate Haldane's conjecture. For example, the research on the AKLT [3] model shows that each $s = 1$ spin in the ground state (GS) can be viewed as two $s = 1/2$ spins in the symmetric triplet state. If open boundary condition is considered, two end spins of the AKLT chain are left and form two free $s = 1/2$ objects and all the other two adjacent $s = 1/2$ spins form the RVB state. In article [4], the Haldane problem is studied with a 1-D alternating Heisenberg spin-1/2 chain.

In the present paper, we study a 1-D alternating Heisenberg chain with $s = 1/2$; the exchange couplings between nearest neighbour spins take J and αJ alternatively as shown in Fig. 1. The Hamiltonian is

$$H = J\sum_{i=1}^{N}(S_{2i}S_{2i-1} + \alpha S_{2i}S_{2i+1}) \quad (J > 0,\ \alpha \geqslant 1) \tag{1}$$

The study of the system is important for studies of the magnetic spin-Peierls effect [5] and the property of $Cu(NO_3)_2 \cdot 2.5D_2O$ can be explained with this model [6]. In this paper, we use the coupled cluster method (CCM) accompanied by exact diagonalization (ED) to study this model. The CCM is one of the most universal and powerful methods used in quantum many-body theory. In recent years, the CCM has been applied to different quantum spin systems with much success [7–13].

2. The coupled cluster method applied to the alternating Heisenberg spin chain

2.1. The ground state

The detailed descriptions of the CCM applied to quantum spin systems have been given in Refs. [7,12,13]. Here we apply the method to the alternating Heisenberg spin chain directly. The first

* Corresponding author. Tel.: +86 25 51667506; fax: +86 25 51663485.
E-mail address: jianjunjiang@126.com (J.-J. Jiang).

0921-4526/$ - see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2008.05.012

step of any CCM calculation is to choose a model state and this is often a classical spin state. So we choose the Neel state as the model state in our CCM calculations and the unit cell used in this paper is indicated in Fig. 1. In order to facilitate the following discussion, we divide the model into two sublattices, detonated A and B, and we populate the A sublattice with 'up' spins and the B sublattice with 'down' spins. Then we perform a rotation of the local axes of the spins on the A sublattice by 180° about the y-axis such that all spins in the model state align along the negative z-axis. After this rotation, the Hamiltonian of Eq. (1) can be rewritten as

$$H = -J\sum_{i=1}^{N}\left\{\left[\frac{1}{2}(S_{2i}^{+}S_{2i-1}^{+}+S_{2i}^{-}S_{2i-1}^{-})+S_{2i}^{z}S_{2i-1}^{z}\right]+\alpha\left[\frac{1}{2}(S_{2i}^{+}S_{2i+1}^{+}+S_{2i}^{-}S_{2i+1}^{-})+S_{2i}^{z}S_{2i+1}^{z}\right]\right\} \quad (2)$$

Then the CCM parameterizations of the ket GS and the GS energy are given by [12,13]

$$|\psi\rangle = e^{S}|\Phi\rangle, \quad S=\sum_{l=1}^{2N}\sum_{i_1,i_2,\ldots,i_l} S_{i_1,i_2,\ldots,i_l}s_{i_1}^{+}s_{i_2}^{+}\cdots s_{i_l}^{+} \quad (3)$$

$$E_g = \langle\Phi|e^{-S}He^{S}|\Phi\rangle \quad (4)$$

where $|\Phi\rangle$ is the model state.

The CCM formalism is exact if we consider all spin configurations in the S correlation operator, but it is usually impossible in practice. In this paper, we use a quite general approximation scheme called LSUBn [12,13] to truncate the expansion of the operator S. In the LSUBn approximation, only the configurations including n or fewer correlated spins which span a range of no more than n contiguous lattice sites are retained. The fundamental configurations retained in the LSUBn approximation can be easily found using the lattice symmetry and the restricted condition $S_{\rm tol}^{z}=\Sigma_{i=1}^{2N}S_i^{z}=0$ (because the GS lies in the subspace $S_{\rm tol}^{z}=0$). For example, there are 6 fundamental configurations as shown graphically in Fig. 2(a) retained in the LSUB4 approximation. The number of LSUBn configurations with $n=\{6,8,10\}$ is given in Table 1.

In order to calculate the GS energy, we have to find the correlation coefficients contained in the operator S. Then we need to solve the coupled-ket-state equations, which are obtained by [12,13]

$$\langle\Phi|s_{i_1}^{-}s_{i_2}^{-}\cdots s_{i_l}^{-}e^{-S}He^{S}|\Phi\rangle = 0 \quad (5)$$

For example, the LSUB4 coupled equations are given by

$$J(0.5-0.5S_{2i-1,2i}^{2}+S_{2i-1,2i,2i+1,2i+2}+S_{2i-3,2i}S_{2i,2i+1}) + \alpha J(-S_{2i-1,2i}S_{2i,2i+1}-S_{2i-1,2i}+S_{2i-3,2i}S_{2i,2i+3})=0 \quad (6.1)$$

$$J(-S_{2i-1,2i}S_{2i-3,2i}-S_{2i-3,2i})+\alpha J(-S_{2i-3,2i}S_{2i,2i+1} - S_{2i-3,2i}+0.5S_{2i-1,2i,2i+1,2i+2}+0.5S_{2i-1,2i}^{2})=0 \quad (6.2)$$

$$J(-S_{2i-1,2i}S_{2i,2i+1}-S_{2i,2i+1}+S_{2i-3,2i}S_{2i,2i+3})+\alpha J(0.5 - 0.5S_{2i,2i+1}^{2}+S_{2i,2i+1,2i+2,2i+3}+S_{2i-1,2i}S_{2i,2i+3})=0 \quad (6.3)$$

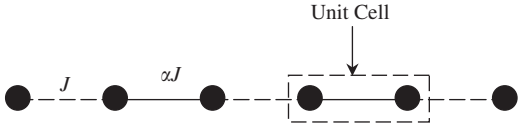

Fig. 1. The structure of the alternating Heisenberg chain. The unit cell is also indicated in this figure.

Table 1
Number of fundamental configurations of the LSUBn approximation with $n=\{6,8,10\}$

	N_F	N_{Fe}
LSUB6	17	15
LSUB8	50	56
LSUB10	157	210

N_F denotes the number of the fundamental configurations for the ground state, and N_{Fe} denotes the number of the fundamental configurations for the excited state.

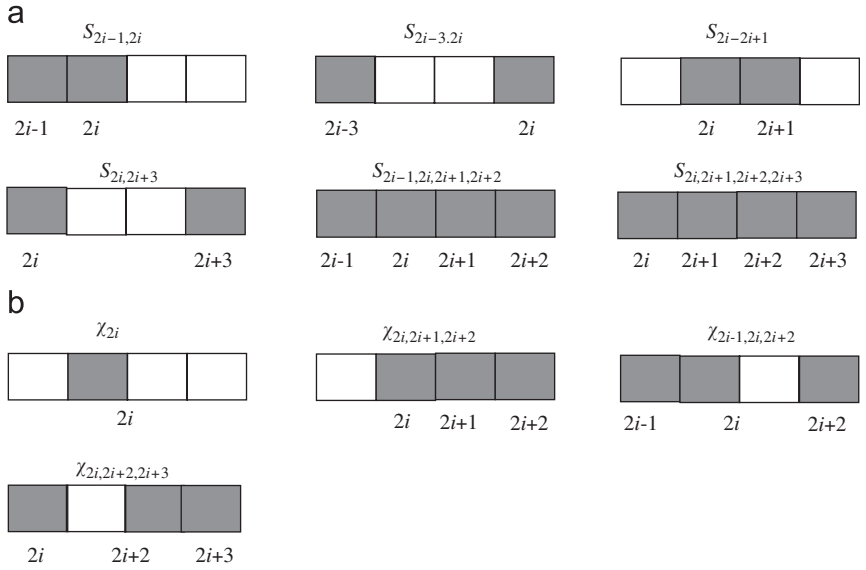

Fig. 2. The fundamental LSUB4 configurations for the ground and the excited state are given by diagrams a and b, separately. The centers of the shaded squares mark the flipped spins with respect to the model Neel state. Note that the configurations are independent of the index i by the lattice symmetry.