Journal of Magnetism and Magnetic Materials 323 (2011) 1855–1859

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

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

Ground state properties of a spin chain within Heisenberg model with a single lacking spin site

M. Mebrouki

Laboratoire de Physique Théorique, École préparatoire sciences et techniques, B.P. 230, 13000 Tlemcen, Algeria

ARTICLE INFO

Article history:
Received 5 August 2010
Received in revised form
9 February 2011
Available online 22 February 2011

Keywords:
Heisenberg model
Next nearest neighbors interactions
Exact diagonalization
Density matrix
Spin impurity

ABSTRACT

The ground state and first excited state energies of an antiferromagnetic spin-$\frac{1}{2}$ chain with and without a single lacking spin site are computed using exact diagonalization method, within the Heisenberg model. In order to keep both parts of a spin chain with a lacking site connected, next nearest neighbors interactions are then introduced. Also, the Density Matrix Renormalization Group (DMRG) method is used, to investigate ground state energies of large system sizes; which permits us to inquire about the effect of large system sizes on energies. Other quantum quantities such as fidelity and correlation functions are also studied and compared in both cases.

1. Introduction

Random effects in low-dimensional antiferromagnetic quantum spin systems have attracted the interest of theoretical and experimental studies in the last decades; see for example [1,2]. Since then, physicists have elaborated theoretical models that capture the essential of physics within a simple fashion. One of the most fundamental and widely studied model, theoretically and later numerically, is the Heisenberg model. In this context, spin chains with random bonds [3–5], frustrated term [6], biquadratic term [7], including all variations that can be explored, are studied. Spin chains with a spin impurity that has a different spin magnitude are also investigated [8]. Spin chains with single [9] as well as randomly distributed [5] impurities and disorder [10,11] are explored. The Kondo model [12] is used to describe a magnetic impurity with spin S interacting locally with a non-interacting conduction electron sea (e.g. rare earth metal alloys and actinide elements).

In the present paper we study a spin chain with a single site non-magnetic atom inserted. It could be also a lacking site. Adding a single non-magnetic impurity to a spin chain compound breaks the chains up to two segments. Our idea is to introduce next nearest neighbors interactions to maintain connection between spin sites at left and right of the "missing" spin. In fact, non-magnetic ions that may be present in a magnetic material serve, among other functions, to stabilize the material and to provide connection to nearby spins with one another [13]. Therefore, the spin-$\frac{1}{2}$ Heisenberg model with next nearest neighbors interactions writes as

$$H=\sum_{i}^{N}[J_1 S_i\cdot S_{i+1}+J_2 S_i\cdot S_{i+2}] \tag{1}$$

where S_i denotes the spin $S=1/2$ operator for lattice site i. Note that for a site with no spin all connection operators with its neighboring sites are omitted in the Hamiltonian.

This model with antiferromagnetic interactions (J_1, $J_2>0$) is well studied [14–17,6]. In fact, the pure spin chain is well known to display a quantum phase transition (Kosterlitz–Thouless transition) [18] from a gapless, translationally invariant state with algebraic spin correlations (the spin fluid phase) to dimer gapful state with exponentially decaying correlations at $\alpha_c\simeq 0.24113$, where $\alpha=J_2/|J_1|$. At $\alpha=0.5$ (the Majumda–Ghosh point) [6], the ground state is exactly solvable. It is a doubly degenerate dimer product of singlet pairs on neighboring sites. In general, the ground state is doubly degenerate for $\alpha>\alpha_c$. For large J_2 ($\alpha>0.5$) an incommensurate phase appears in the ground state phase diagram [17,19].

The major part of our task is to compute ground state and eventually first excited states energies and their corresponding eigenstates of the above Hamiltonian. Physical quantities are then computed through appropriate formulas. Computational physics provides us with a panoply of numerical methods that range from the obvious complete diagonalization to variational methods with more or less accuracy and different areas of excellency. We have

E-mail address: m_mebrouki@yahoo.fr

0304-8853/$ - see front matter © 2011 Elsevier B.V. All rights reserved.
doi:10.1016/j.jmmm.2011.02.022

chosen two of them: exact diagonalization and Density Matrix Renormalization Group (DMRG).

2. Exact diagonalization results

2.1. Ground state energy

The exact diagonalization technique is a direct method that provides us with the whole spectrum of a system Hamiltonian and the corresponding eigenvectors. Unfortunately, the order of matrices to be diagonalized for the Heisenberg model grows as 2^N; with N being the number of sites. Therefore, system sizes treated by such method are very restricted and can go, using different symmetries, to more or less 20 sites; which are far from approaching the thermodynamic limit. Fortunately, the study of such systems do not require the whole spectrum, and generally a set of low-lying states, including the ground state and some few excited states are sufficient to describe their properties. Therefore, numerical methods had been elaborated by physicists to focus on those restricted parts of the spectrum with more or less accuracy; such as the earlier Lanczos method and the recently developed method, the DMRG. Nevertheless, the exact diagonalization still have its relevance, especially for those properties that do not depend on the system size.

Thus, we diagonalize matrices for spin chains with $N=6$, 8, 10, 12 using periodic boundary conditions. The use of these boundaries is governed by the fact that changing the position of the lacking site in the chain does not affect the energy spectrum of a chain with a single lacking site. The value of J_2 goes from 0.05 to 0.55 with a step of 0.05. This is useful to sweep a large interval where the well-known system undergoes quantum phase transitions. This allows us to figure out how the system is affected when a spin site is missed. The value of J_1 is taken to be unity.

Figs. 1 and 2 display the first four lowest energies in function of J_2, for a spin chain without (with) a lacking site, respectively. The chain length is taken to be $N=10$ and J_2 values go from 0.05 to 0.55. The latter interval is thought to contain a critical point of the system [20,18]. In Fig. 1, one can see a nonvanishing gap that appears, as it is the case when $J_2=0.00$. One can also see that the gap is constant until J_2 is around 0.25. Beyond this value the gap is decreasing. Taking into account works that confirm the existence of such a critical point at this value, one can think that the behavior of the gap could be a signature of a spin system that crosses a critical point. In the other hand, Fig. 2 shows that a spin system with a missing site has no gap at all. Actually, the first four low-lying energies including the ground state have the same value. This degeneracy may be due to the frustration of having a short chain (nine sites) with an odd number of spin sites.

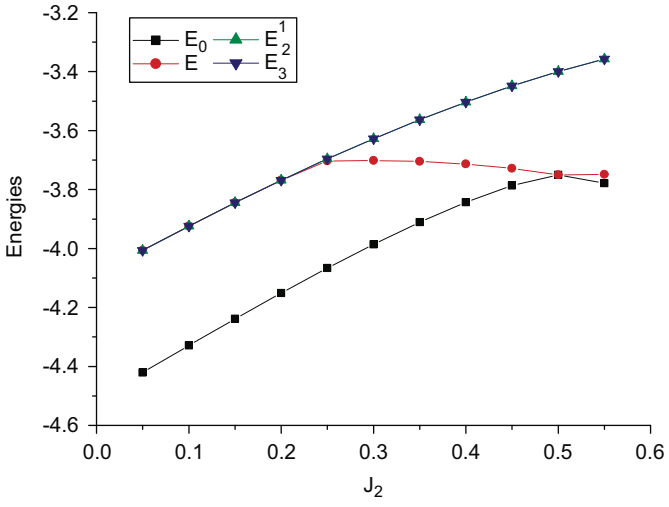

Fig. 1. First four lowest energies as a function of J_2 for a spin chain without a lacking site spin, obtained by exact diagonalization.

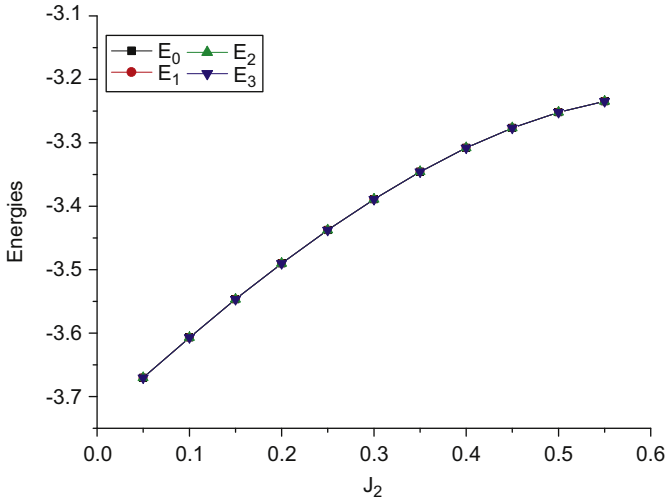

Fig. 2. First four lowest energies as a function of J_2 for a spin chain with a lacking site spin, obtained by exact diagonalization.

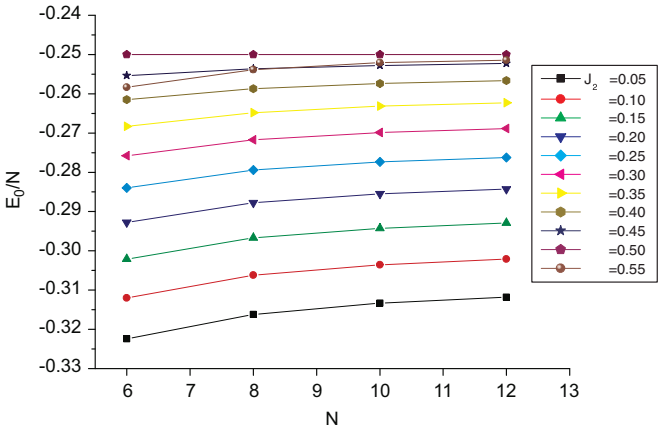

Fig. 3. Exact ground state eigenvalue per site for a spin chain without a lacking site as a function of J_2, obtained by exact diagonalization.

Now, we want to check the variation of the ground state energy per site E_0/N in function of J_2. Thus, Figs. 3 and 4 display E_0/N for spin chains without (with) a lacking site, as J_2 varies from 0.05 to 0.55. Both figures show that, for relative small system sizes (up to 12 sites), the ground state energy per site is increasing (decreasing) as the system size increases. The figures show also that the increasing (decreasing) rate of E_0/N depends on the value of J_2. We remark also that E_0/N increases as J_2 increases to reach a maximum value when $J_2=0.5$ (Majumdar–Gosh point), then it decreases.

As the above results are obtained for small system sizes, this seems to be not so sufficient to make us deciding about the large-N variation of the E_0/N. Therefore, we need to use the DMRG method, which enables us to compute the ground state energy for more long spin chains. This will be explained after we investigate quantum fidelity and correlation functions.