Density-matrix renormalization-group simulation of the *SU*(3) antiferromagnetic Heisenberg model

M. Aguado,[1] M. Asorey,[2] E. Ercolessi,[3] F. Ortolani,[3] and S. Pasini[4,*]
[1]*Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Str. 1, D-85748 Garching, Germany*
[2]*Departamento de Física Teórica, Facultad de Ciencias, Universidad de Zaragoza, 50009 Zaragoza, Spain*
[3]*Dipartimento di Fisica, Università di Bologna, Via Irnerio 46, 40127 Bologna, Italy and INFN, Via Irnerio 46, 40127 Bologna, Italy*
[4]*Lehrstuhl für Theoretische Physik I, Universität Dortmund, Otto-Hahn Straße 4, 44221 Dortmund, Germany*
(Received 25 September 2008; published 26 January 2009)

We analyze the antiferromagnetic *SU*(3) Heisenberg chain by means of the density-matrix renormalization group. The results confirm that the model is critical and the computation of its central charge and the scaling dimensions of the first-excited states show that the underlying low-energy conformal field theory is the $SU(3)_1$ Wess-Zumino-Novikov-Witten model.

DOI: 10.1103/PhysRevB.79.012408 PACS number(s): 64.60.F−, 64.60.ae, 11.25.Hf, 89.70.Cf

I. INTRODUCTION

In recent years, a renewed interest in models of condensed matter with a symmetry larger than *SU*(2) has arisen. This is because these models represent not only challenging theoretical problems but also can be effectively experimentally implemented. In particular *SU*(4) systems can be realized in laboratories in transition-metal oxides[1] where the electron spin is coupled to the orbital degrees of freedom. A possible realization of *SU*(3) antiferromagnetic (AFM) spin chains in systems of ultracold atoms in optical lattices has been recently proposed.[2] In this case the spin would be related to the *SU*(3) rotation in an internal space spanned by the three available atomic states [colors, in the *SU*(3) language], with the condition that the number of particles of each color is conserved. Other examples involve the *SU*(3) trimer state in a spin tetrahedron chain[3,4] or the spin tube models in a magnetic field,[5] where the low-energy effective Hamiltonian can be identified with a particular anisotropic *SU*(3) spin chain.

From a theoretical point of view, the *SU*(3) spin model has also been studied from different viewpoints. In recent years the interest on ferromagnetic *SU*(*N*) spin chains has been boosted by their implication in the anti–de Sitter/conformal field theory (AdS/CFT) correspondence.[6,7] On the other side the family of integrable spin chains include some models with *SU*(3) symmetry, as first shown by Sutherland,[8] who generalized the Bethe ansatz to multiple component systems which include the *SU*(3) spin chain, showing that it is gapless. Also the *SU*(3) Heisenberg model can be directly related to a particular *SU*(3)-symmetric bilinear biquadratic spin-1 chain, the Lai-Sutherland (LS) model, which is also known to be critical.[9,10] In terms of CFT the LS model and the *SU*(3) spin chain should belong to the same universality class, that of the $SU(3)_1$ Wess-Zumino-Novikov-Witten (WZNW) model.[11,12]

In this paper we present a numerical analysis of the *SU*(3) spin chain by means of the density-matrix renormalization group (DMRG). After a short description of the model and its mathematical framework (Sec. II), we present our new results (Sec. III) which confirm the criticality of the model as well as its correspondence to the Lai-Sutherland model. In particular, due to the ability of our program to provide the quantum numbers for each state, we can show that the excited states of the spin chain have the same quantum numbers as the irreducible representations (IR) of *SU*(3). We compute the scaling dimensions of the first excitations, which turn out to agree with those of the $SU(3)_1$ WZNW model, which corresponds to the low-energy effective-field theory descriptions of our spin chain. The results are further confirmed by the computation of the central charge by means of the vacuum entanglement entropy.

II. *SU*(3) MODEL

We consider the following Heisenberg model

$$H = J\sum_{i=1}^{L} \mathbf{S}_i \cdot \mathbf{S}_{i+1}, \qquad (1)$$

where the spin variables are expressed in terms of the generators of *SU*(3) in the fundamental representation: $\mathbf{S}_i^a = \frac{1}{2}\lambda_i^a$, with $a=1,\ldots,8$ and λ_a being the eight Gell-Mann matrices. The sign of J selects an antiferromagnetic spin chain ($J>0$) or a ferromagnetic (FM) one ($J<0$). In the following we shall concentrate only on the AFM case, which has been partially considered also in Refs. 13 and 14.

In terms of the following ladder operators, $T^{\pm}=\lambda^1 \pm i\lambda^2$, $V^{\pm}=\lambda^4 \pm i\lambda^5$, and $U^{\pm}=\lambda^6 \pm i\lambda^7$, Hamiltonian (1) becomes

$$H = \frac{J}{2}\sum_{i=1}^{L}\left\{\frac{1}{4}(T_i^+T_{i+1}^- + V_i^+V_{i+1}^- + U_i^+U_{i+1}^- + \text{H.c.}) + \frac{1}{2}\lambda_i^3\lambda_{i+1}^3 + \frac{1}{2}\lambda_i^8\lambda_{i+1}^8\right\}. \qquad (2)$$

This makes easier to identify two operators, S_z and Q_z, given by the sums of the two diagonal Gell-Mann matrices

$$S_z = \sum_i \frac{1}{2}\lambda_i^3, \quad Q_z = \sum_i \frac{\sqrt{3}}{2}\lambda_i^8 \qquad (3)$$

that commute with the Hamiltonian and correspond to conserved quantities (isospin and hypercharge). The corresponding quantum numbers label the different eigenstates of Eq. (1).

The Lai-Sutherland model is defined as the bilinear biquadratic spin-1 chain

$$H = J' \sum_{i=1}^{L} [\tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_{i+1} + (\tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_{i+1})^2] \tag{4}$$

and characterized by an $SU(3)$ symmetry. Model (4) and the $SU(3)$ spin chain can be mapped one onto the other by means of the following identity[15]

$$\tilde{\mathbf{S}}_i \tilde{\mathbf{S}}_{i+1} + (\tilde{\mathbf{S}}_i \tilde{\mathbf{S}}_{i+1})^2 - 1 = \frac{1}{3} + \frac{1}{2} \sum_{a=1}^{8} \lambda_i^a \lambda_{i+1}^a. \tag{5}$$

We have already mentioned in Sec. I that the LS model is known to be gapless and to belong to the same universality class of the $SU(3)$ level-1 Wess-Zumino-Novikov-Witten model with central charge $c=2$. Due to the correspondence between the two models, the $SU(3)_1$ WZNW model has to be the low-energy effective critical-field theory also for the $SU(3)$ spin chain. We shall numerically show that the $SU(3)$ Heisenberg chain is critical, and from the energy state obtained from the DMRG, we shall compute the central charge and the scaling dimensions of Eq. (1) and compare them to the values predicted for the $SU(3)_1$ WZNW model.

The states of the spin chain can be organized according to the irreducible representations of the affine (Kac-Moody) Lie algebra associated to $SU(3)$. Let us recall[16] that a useful way of representing the IR's of the Lie algebra $su(3)$ is through the Young Tableau (YT), which can be labeled by two positive integer numbers (p,q). Once p and q are known, one can easily compute the dimension d of the representation and the quantum numbers associated to the isospin S_z and the hypercharge Q_z according to[17,16]

$$d = \frac{1}{2}(p+1)(q+1)(p+q+2) \tag{6}$$

and

$$S_z = -I, -I+1, \ldots, I-1, I, \quad Q_z = \frac{3}{2}Y, \tag{7}$$

where $I=\frac{1}{2}(r+s)$ and $Y=(r-s)-\frac{2}{3}(p-q)$, with $0 \leq r \leq p, 0 \leq s \leq q$. In particular, the cases (1,0) and (0,1) give, respectively, the fundamental (**3**) and the antifundamental ($\bar{\mathbf{3}}$) IR, while the singlet representation (**1**) corresponds to (0,0).

It has been proved[18] that, in analogy with the $SU(2)$ case, the ground state (GS) of the AFM $SU(3)$ Hamiltonian is a singlet, and since it is made of particles u, d, and s in equal number, it can be obtained in finite chains having only a number of sites which is a multiple of three, $L=3M$. As for the excited states, we expect them to be in correspondence with the tower of conformal states of the corresponding $SU(3)$ WZNW model. The primary states of this theory are a finite number and are given[16] by fields $\Phi_{\lambda,\bar{\lambda}}$, whose holomorphic (antiholomorphic) part transforms according to a representation $\lambda=(p,q)$ $[\bar{\lambda}=(p',q')]$ with the values of p,q (and similarly of p',q') satisfying the condition: $p+q \leq k$, where k is the level. The conformal dimension of the primary field is then $x_{\lambda,\bar{\lambda}}=x_{(p,q)}+x_{(p',q')}$ with

$$x_{(p,q)} = \frac{1}{3(k+3)}(p^2+q^2+pq+3p+3q), \tag{8}$$

and a similar expression for $x_{(p',q')}$. For future reference, the values of $x_{\lambda,\bar{\lambda}}$ for some primary fields in the case of $k=1$ are reported in Table I.

TABLE I. Quantum numbers and scaling dimensions for some of the primary fields $\Phi_{\lambda,\bar{\lambda}}$ of the $SU(3)_1$ WZNW model.

λ	$\bar{\lambda}$	(S_z,Q_z)	$x_{\lambda,\bar{\lambda}}$
(**1**)	(**1**)	(0,0)	0
(**3**)	(**1**)	$(\pm 1/2, 1/2)$; $(0,-1)$	1/3
($\bar{\mathbf{3}}$)	(**1**)	$(\pm 1/2, -1/2)$; $(0,1)$	1/3
(**3**)	($\bar{\mathbf{3}}$)	$(\pm 1/2, \pm 3/2)$; (0,0)(3 times); $(\pm 1, 0)$	2/3

To end up this section, we notice that in a finite chain of length L not all quantum numbers, i.e., states, may be realized. For example, working with periodic boundary conditions and with an even number of sites, the singlet $(\mathbf{1})\times(\mathbf{1})$ (ground) state, with $x=0$, appears only for chains with $L=6M$ (with M a positive and integer number), while the $(\mathbf{3})\times(\mathbf{1})$ [or the $(\mathbf{1})\times(\bar{\mathbf{3}})$] states are present only if $L=6M+4$ (or $L=6M+2$), both with $x=1/3$.

III. NUMERICAL ANALYSIS

The $SU(3)$ version of the DMRG we have used implements the following Hamiltonian:

$$H = \frac{J}{2} \sum_{i=1}^{L} \left[\frac{1}{4}(k_0 T_i^+ T_{i+1}^- + k_1 V_i^+ V_{i+1}^- + k_2 U_i^+ U_{i+1}^- + \text{H.c.}) + \frac{1}{2}(z_0 \lambda_i^3 \lambda_{i+1}^3 + z_1 \lambda_i^8 \lambda_{i+1}^8) \right], \tag{9}$$

where k_j and z_j are input parameters. Model (9) reproduces the AFM (FM) case when all the k_j's and the z_j's are equal to 1 (-1). By tuning the input parameters k_j and z_j, we can study all the possible anisotropic version of the $SU(3)$ Heisenberg model. A very important feature of this DMRG is that it implements both the quantum numbers S_z and Q_z given in Eq. (3). This implementation considerably reduces the computation time and, on the other hand, once S_z and Q_z are fixed from input, each run of the DMRG yields exclusively the energies of the states within those quantum-number sectors. This is very useful when one needs to classify the excitations according to the values of the isospin and of the hypercharge. By setting $k_1=k_2=z_1=0$, we restrict to the $SU(2)$ sector of $SU(3)$. This has been used as a check to the program; the DMRG in this case reproduces perfectly all the energy states of the $SU(2)$ Heisenberg model.

We study now the isotropic AFM chain with periodic boundary conditions by means of an infinite-size DMRG

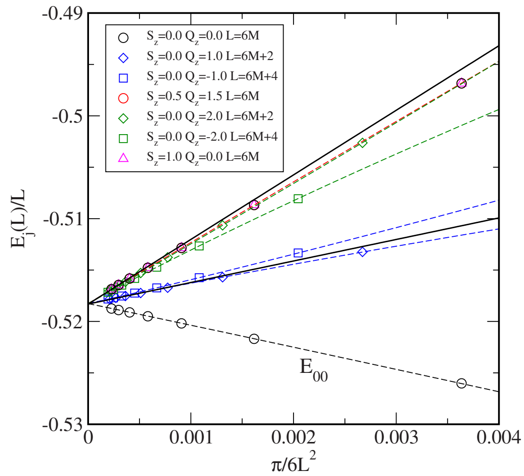

FIG. 1. (Color online) Plot of the ground state E_{00} and first-excited states for chains of different lengths (from $L=12$ up to $L=52$). The solid lines correspond to scaling dimensions $\frac{1}{3}$ and $\frac{2}{3}$ and have been drawn as a guide for the eye. For sake of clarity, not all the degeneracies have been reported.

with up to $m=2200$ states in order to reduce the uncertainty on the energies to the order of magnitude of the truncation error. The data for the ground state and the first-excited states are plotted in Fig. 1.

Let us first concentrate on the *ground state*, which, in agreement with theoretical predictions, it is found only when $L=6M$. The plot of E_{00} as a function of $1/L^2$ shows a good linear behavior; this justifies the fitting of our data by the CFT equations for the GS[19,20]

$$\frac{E_{00}}{L} = e_\infty - \frac{\pi c v}{6L^2}, \tag{10}$$

where e_∞ and the product cv are kept as fitting parameters. We obtain $e_\infty=-0.518\,288$ and $cv=2.044\,19$. In order to derive the value of v we need an independent derivation of c. The central charge for a $SU(N)$ level-k WZNW model is given by[16]

$$c = \frac{k(N^2-1)}{k+N}. \tag{11}$$

If the effective-field theory describing our spin chain is the conformal $SU(3)_1$ WZNW model, the central charge must be $c=2$.

However, it is possible to have a direct numerical derivation of c from the asymptotic behavior of the von Neumann entropy $S_n=-\mathrm{Tr}_n(\rho_n \log_2 \rho_n)$ of the reduced density matrix $\rho_n=\mathrm{Tr}_{i>n}\,\rho$ of a subchain with n spins of a critical system of length L, as a function of n and L, where ρ is the density matrix associated to the ground state of the chain. Indeed, one has[21,22]

$$S_n = \frac{c}{3}\log_2\left[\frac{L}{\pi}\sin\left(\frac{\pi}{L}n\right)\right] + A. \tag{12}$$

As usual c is the central charge while A is a nonuniversal constant. The DMRG computes the density matrix for a block of length n in a chain of length L so that S_n becomes quite simple to calculate. Figure 2 shows the behavior of the von Neumann entropy by using 2000 DMRG states, as a function of the normalized block length n/L in Fig. 2(a) and as a function of $y=\log_2[\frac{L}{\pi}\sin(\frac{\pi}{L}n)]/3$ in Fig. 2(b). As expected,[23,24] the data collapse on the same curve in plot (a) while they confirm the behavior of Eq. (12) in plot (b). In this figure one can observe that in the range for $L\in[18,48]$, and values of the block length n ranging from 8 to $L-8$, the data lie perfectly on a straight line. In these ranges of n and L, the linear regression on all data $S_n=cy+A$ yields the values $A=(1.774\pm0.002)$ and $c=(1.995\pm0.001)$ for the constant and the central charge, respectively. Thus, the theoretical prediction of Eq. (11) is confirmed with very high accuracy. An analogous calculation with only 1000 states in the DMRG run shows qualitatively the same behavior but with evident deviations from a straight line in a plot like Fig. 2(b) for higher values of y. This is the reason why we have performed all calculations keeping 2000 states. Finally, the value of c can be substituted into the product cv derived from the GS to recover the velocity of the excited modes $v=(1{,}0247\pm0.0005)$, which is close to the expected value[8] $\pi/3$.

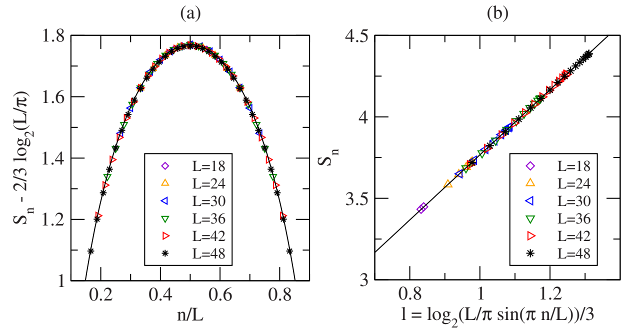

FIG. 2. (Color online) Analysis of the von Neumann entropy using 2000 DMRG states. The figure on the left (a) shows S_n as a function of the block length n for different sizes L of the chain; the figure on the right (b) is the plot of the same data fitted in a logarithmic scale. The linear fit of these data provides the value for the central charge $c=1.995\pm0.001$.

Before proceeding with the analysis of the excited states, let us check the asymptotic value of the energy density e_∞. The theoretical prediction for the ground state of the $S=1$ bilinear biquadratic Heisenberg Hamiltonian (see Ref. 25) is

$$E_{\mathrm{GS}} = -\ln 3 - \frac{\pi}{3\sqrt{3}} + 1, \tag{13}$$

which already takes into account the factor -1 of the left-hand side (l.h.s.) of Eq. (5). Starting from the correspondence between our $SU(3)$ chain and the biquadratic one [Eq. (5)], we can compare the value of e_∞ we obtained with the one predicted by Eq. (13): $E_{\mathrm{GS}}=-0.703212$. The match is exact to the third decimal $(-0.703\,243)$ if one also recalls that the Hamiltonian has a factor 1/4 [due to the definition of the spin variables in terms of the $SU(3)$ generators] so that e_∞ needs to be multiplied by a factor two, and summed to the factor 1/3 of Eq. (5). This is a further numerical proof of the equivalence between the Lai-Sutherland and the $SU(3)$ spin model.

TABLE II. Scaling dimensions of the first (x_1) and the second (x_2) excited states for each L obtained from the DMRG analysis. The mean value (▲) between $L=6M+2$ and $L=6M+4$ for x_1 and x_2 is also provided (see also Fig. 1). For $L=6M$ only the first excitation above the ground state has been considered.

L	x_1	x_2
$6M+2$	0.3414 ± 0.0001	0.6291 ± 0.0003
$6M+4$	0.3406 ± 0.0002	0.6238 ± 0.0003
(▲)	0.3410 ± 0.0002	0.6265 ± 0.0003
$6M$		0.6503 ± 0.0003

Let us study now the *excited states*. With the DMRG code it is possible to fix the quantum numbers S_z and Q_z at every step of the calculation and look for the first low-energy states with given quantum numbers. For every size L of the chain we selected 9 lowest energy states with different values of S_z and Q_z, according to Table I. In this way we can partially verify the degeneracy and the precision of the excited states. In Fig. 1 we have plotted only a subset of the energies for every L since the other values are effectively not distinguishable from the plotted ones (for example, this is the case for the exited states with $S_z=0$ and $Q_z=0$, and $S_z=1/2$ and $Q_z=3/2$, shown in the figure). One immediately sees that the slope of excited states depends on the size L(mod. 6) of the chain. In particular, for $L=6M$ the first excitation scales with a slope which is unmistakably different from the slope of the $L=6M+2$ or $L=6M+4$ data. For small values of L the data corresponding to the same S_z but with opposite Q_z are split by a finite-size correction, while for increasing values of L they tend to overlap and scale to the same asymptotic value. For the excited states CFT predicts that

$$E_j - E_{00} = \frac{2\pi v}{L} x_j, \tag{14}$$

where x_j is the scaling dimension of the jth excitation for a given size L of the chain. We have performed a linear fit on the data of Fig. 1 for $L \in [20,52]$ in order to extract the scaling dimensions. For all values of L, Eq. (10) can be inserted into Eq. (14) with the values of e_∞ and c and v obtained before. The numerical coefficients for the scaling dimensions that one can obtain from the DMRG data for the afore mentioned excited states of Fig. 1 are listed in Table II.

As expected,[14,26,27] the values of the allowed conformal dimensions are very close to the values of 1/3 and 2/3 predicted by a $SU(3)_1$ WZNW model.

IV. CONCLUSIONS

We have provided strong numerical evidence of the criticality of the AFM $SU(3)$ spin chain. Also, we have confirmed that the conformal field theory describing the chain is effectively the $SU(3)_1$ WZNW model by computing the central charge and scaling dimensions of the lowest excited states of the model, which turn out to be organized according to the IR of $SU(3)_1$ Kac-Moody algebra.

There are many interesting generalizations of the above models which deserve further study. In particular, a similar ferromagnetic spin chain is connected with the nonlinear CP^2 sigma mode at $\theta=\pi$ and might be useful to clarify some controversial problems of the model. Another interesting problem is to consider larger $SU(N)$ symmetry groups. In two-dimensional chains, the vacuum state is of Néel type for $N \leq 4$ and of Spin-Peierls type for $N \geq 5$.[28] The analysis by means of DMRG technique might shed some light on the transition mechanism.

ACKNOWLEDGMENTS

We would like to thank G. Morandi, C. Degli Esposti Boschi, M. Roncaglia, and L. Campos Venuti for interesting and helpful discussions. One of the authors (S.P.) would also like to thank S. Rachel, R. Thomale, and A. Läuchli for very constructive discussions. The work of M.A. and E.E. was partially supported by an INFN-CICYT Italian-Spanish Grant No. INFN08-29. The work of E.E. and F.O. was partially supported by Italian MIUR, PRIN project 2007JHLPEZ: "Fisica Statistica dei Sistemi Fortemente Correlati all'Equilibrio e Fuori Equilibrio: Risultati Esatti e Metodi di Teoria dei Campi."

*pasini@fkt.physik.uni-dortmund.de

[1] Y. Tokura and N. Nagaosa, Science **288**, 462 (2000).
[2] M. Greiter *et al.*, Phys. Rev. B **75**, 060401(R) (2007); D. Schuricht and M. Greiter, Europhys. Lett. **71**, 987 (2005).
[3] S. Chen *et al.*, Phys. Rev. B **72**, 214428 (2005).
[4] S. Chen *et al.*, Phys. Rev. B **74**, 174424 (2006).
[5] R. Citro *et al.*, J. Phys.: Condens. Matter **12**, 3041 (2000).
[6] J. A. Minahan and K. Zarembo, J. High Energy Phys. 03 (2003) 013.
[7] N. Beisert and M. Staudacher, Nucl. Phys. B **670**, 439 (2003).
[8] B. Sutherland, Phys. Rev. B **12**, 3795 (1975).
[9] J. K. Lai, J. Math. Phys. **15**, 1675 (1974).
[10] K. Chang *et al.*, J. Phys.: Condens. Matter **1**, 153 (1989).
[11] I. Affleck, Nucl. Phys. B **265**, 409 (1986).
[12] I. Affleck, Nucl. Phys. B **305**, 582 (1988).
[13] C. Itoi and M. H. Kato, Phys. Rev. B **55**, 8295 (1997).
[14] M. Fueheringer *et al.*, arXiv:0806.2563.
[15] A. Schmitt *et al.*, J. Phys. A **29**, 3951 (1996).
[16] P. Di Francesco *et al.*, *Conformal Field Theory* (Springer, Dortmund, 1997).
[17] S. Chaturvedi and N. Mukunda, J. Math. Phys. **43**, 5262 (2002).
[18] T. Hakobyan, Nucl. Phys. B **699**, 575 (2004).
[19] H. W. J. Blöte *et al.*, Phys. Rev. Lett. **56**, 742 (1986).
[20] I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).
[21] C. Holzhey *et al.*, Nucl. Phys. B **424**, 443 (1994).
[22] P. Calabrese and J. Cardy, J. Stat. Mech.: Theory Exp. (2004) P06002.
[23] B. Nienhuis *et al.*, arXiv:0808.2741 (unpublished).
[24] A. M. Läuchli and C. Kollath, J. Stat. Mech.: Theory Exp. (2008) P05018.
[25] G. V. Uimin, JETP Lett. **12**, 225 (1970).
[26] A. Läuchli *et al.*, Phys. Rev. B **74**, 144426 (2006).
[27] P. Corboz *et al.*, Phys. Rev. B **76**, 220404(R) (2007).
[28] K. Harada *et al.*, Phys. Rev. Lett. **90**, 117203 (2003).