Breakdown of the perturbative renormalization group for $S \geqslant 1$ random antiferromagnetic spin chains

A. Saguia, Beatriz Boechat, and M. A. Continentino
Instituto de Física, Universidade Federal Fluminense, 24210-130, Niterói, RJ, Brazil

O. F. de Alcantara Bonfim
Department of Physics, Reed College, Portland, Oregon 97202

(Received 24 October 2000; published 12 January 2001)

We investigate the application of a perturbative renormalization group (RG) method to random antiferromagnetic Heisenberg chains with arbitrary spin size. At zero temperature we observe that initial arbitrary probability distributions develop a singularity at $J=0$, for all values of spin S. When the RG method is extended to finite temperatures, without any additional assumptions, we find anomalous results for $S \geqslant 1$. These results lead us to conclude that the perturbative scheme is not adequate to study random chains with $S \geqslant 1$. Therefore a random singlet phase in its more restrictive definition is only assured for spin-1/2 chains.

DOI: 10.1103/PhysRevB.63.052414 PACS number(s): 75.10.Hk, 64.60.Ak, 64.60.Cn

Low-dimensional random quantum magnetic systems have become an object of increasing interest in recent years. Despite the apparent simplicity, quantum spin chains show a wealth of physical properties which have attracted the attention of both theoretical and experimental physicists. It is generally accepted that quantum antiferromagnetic spin-1/2 chains in the presence of disorder exhibit, at low temperatures, a random singlet (RS) phase characterized by power law behavior of thermodynamic quantities.[1,2] This has, in fact, been observed in several experiments.[3–7] Theoretically, the phase was revealed by a real space renormalization group (MDH) approach.[1] These results have motivated many authors to study the physical properties of other random antiferromagnetic quantum (RAQ) chains with $S \geqslant 1$. In this case there are additional problems, as for example, what happens to the Haldane gap of integer spins chains[8] in the presence of disorder. In fact, the possibility of the energy gap being suppressed by disorder, driving the system to a RS phase has become a very attractive matter for investigation. In particular, the $S=1$ RAQ chains has been exhaustively studied by several methods.[9–16] Many authors have employed extended versions of the MDH scheme to explore the ground state properties of the model. In the course of these investigations, some authors suggested the existence of random singlet phase in the spin-1 chain in the strong disorder regime.[9–13] On the other hand, studies based on exact diagonalization,[14] quantum Monte Carlo (MC) simulation,[15] and density matrix renormalization group (DMRG) techniques[16] found that the Haldane phase is quite robust against randomness.

In view of these controversial results and the fact that most calculations for spin-1 chains have been done at $T=0$, we were motivated to extend the MDH analysis to finite temperature. Our goal was to generalize the MDH recursion relations to study the thermodynamic behavior of chains with arbitrary spin size. We performed careful numerical procedures to iterate our generalized MDH equations at finite temperature. The anomalous results we have obtained for the free energy and are presented in this communication indicate that the MDH approach breaks down for chains with $S \geqslant 1$. Therefore, we argue that it is impossible to conclude on the existence or not of the RS phase in the $S \geqslant 1$ RAQ chains, as proposed in previous zero temperature studies using the MDH method.[9–13] Actually, within the MDH approximation the existence of the RS phase is assured only for the spin-1/2 chains.

The random magnetic systems are described by the Heisenberg Hamiltonian:

$$H = \sum_{i=1}^{L-1} J_i \vec{S}_i . \vec{S}_{i+1}, \tag{1}$$

where $J_i > 0$ is the nearest neighbor antiferromagnetic interaction and $\vec{S}_i$ are quantum spin operators. The exchange couplings are random variables distributed according to a given probability distribution $P_J(J_i, \Omega)$, with a cutoff Ω. The MDH method consists in eliminating the pair of spins with the strongest coupling ($J_2 = \Omega$) in the random chain by considering the interaction (J_1 and J_3) with the neighboring spins of this pair as a perturbation (see Fig. 1).

The Hamiltonian for the strongly coupled pair of spins $\vec{S}_2$ and $\vec{S}_3$ is given by

$$H_0 = J_2 \vec{S}_2 . \vec{S}_3 . \tag{2}$$

These spins are weakly coupled to the neighbors via

$$H_1 = J_1 \vec{S}_1 . \vec{S}_2 + J_3 \vec{S}_3 . \vec{S}_4 . \tag{3}$$

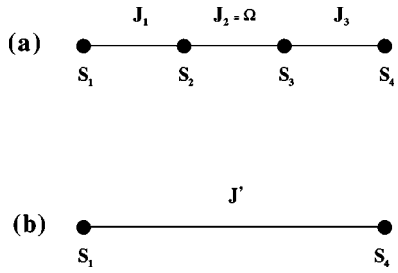

FIG. 1. Spins and coupling constants involved in the elimination transformation (a) to (b).

We calculate the free energy of the system formed by $\vec{S}_1$, $\vec{S}_2$, $\vec{S}_3$, and $\vec{S}_4$ through perturbation theory in second order of H_1 (see Ref. 1). After some simple but extensive calculations we come with the results:

$$F' = F_0 - \frac{1}{3\Omega}[S(S+1)]^2(J_1^2+J_3^2)V_s(\beta\Omega) \tag{4}$$

with

$$F_0 = -S(S+1)\Omega - \frac{1}{\beta}\ln\sum_{i=0}^{2S}(2i+1)\exp\left[-\frac{1}{2}i(i+1)\beta\Omega\right] \tag{5}$$

and

$$J' = \frac{2}{3}S(S+1)\frac{J_1J_3}{\Omega}W_s(\beta\Omega), \tag{6}$$

where $\beta = 1/k_BT$ and the functions V and W are given by

$$V_s(y) = \frac{(2S+1)^2 - \sum_{i=0}^{2S}(2i+1)e^{-(1/2)i(i+1)y}\left[1-\frac{1}{2}i(i+1)y\right]}{4S(S+1)\sum_{i=0}^{2S}(2i+1)e^{-(1/2)i(i+1)y}} \tag{7}$$

and

$$W_s(y) = \frac{(2S+1)^2 - \sum_{i=0}^{2S}(2i+1)e^{-(1/2)i(i+1)y}\left[1+\frac{1}{2}i(i+1)y\right]}{4S(S+1)\sum_{i=0}^{2S}(2i+1)e^{-(1/2)i(i+1)y}}. \tag{8}$$

Equations (4)–(8) are the generalization of the MDH equations for the thermodynamic properties of RAQ chains with arbitrary spin size. For S=1/2 we recover the original MDH recursion relations.[1] The S=1 case has already been studied in the limit of very low temperatures.[10]

When the decimation process is carried out for a spin-1/2 chain the distribution $P_J(J_i,\Omega)$, independently of the form of the original distribution of antiferromagnetic bonds, rather quickly approaches a fixed form singular at $J=0$,[2]

$$P_J(J_i,\Omega) \approx \frac{\alpha}{\Omega}\left(\frac{J_i}{\Omega}\right)^{-1+\alpha}\Theta(\Omega - J_i) \tag{9}$$

with

$$\alpha = -\frac{1}{\ln\Omega}. \tag{10}$$

The fixed form of $P_J(J_i,\Omega)$ determines the low-temperature behavior of the thermodynamic quantities. The exponent α gives rise to logarithmic corrections in the thermodynamic functions.

The great merit and the reason for the success of the MDH theory[1] was to show that the characteristic RS phase behavior of spin-1/2 chain is universal. More specifically, it is independent of the original distribution of exchange couplings. The MDH approach represented a considerable progress with respect to previous methods[5,6,17] which required an initial distribution of bonds with a particular form. Actually, in order to reproduce the power law dependence of the low temperature thermodynamic quantities observed experimentally, the previous models required an initial distribution already with a power law behavior.[6,17]

We turn now to the numerical simulation of chains with spins $S=1$ and $S=3/2$. Each chain is composed of N spin-S objects with periodic boundary conditions (with $N=50{,}000$). We carried out the averages over ten different configurations for each $P_J(J_i,\Omega)$ to obtain the free energy of the system. We start by choosing the exchange coupling from an uniform distribution $P_J(J_i,\Omega)$ given by

$$P_J(J_i,\Omega) = \begin{cases} \dfrac{1}{1-\Delta} & \text{for } \Delta \leqslant J_i \leqslant 1 \\ 0 & \text{otherwise.} \end{cases} \tag{11}$$

The parameter Δ represents the strength of the initial disorder of the couplings. The case $\Delta=0$ represents the strong disorder limit because the distribution becomes extremely broad in a logarithmic scale; namely, infinitesimally weak bonds appear. The weak disorder regime is represented by finite values of Δ. The distribution, in this case, presents a gap Δ.

We have studied the flow of the initial coupling distribution, Eq. (11), for the spin-1 chain for the following cases: $\Delta=0$, $\Delta=0.05$, $\Delta=0.1$, and $\Delta=0.2$. We found that for any Δ, successive elimination transformations give rise to weaker and weaker couplings as the cutoff Ω decreases, *independently of the temperature*. For sufficiently small Ω, i.e., after a sufficient number of eliminations, the distribution $P_J(J_i,\Omega)$ becomes peaked at $J_i=0$ and, as in the T=0 case,[10–13] can be approximated by a power law. We should point out that the convergence to a power law depends on the value of Δ. It is faster in the case of the gapless ($\Delta=0$) initial distribution. As in the case of spin-1/2 chains[1] the power-law exponent obtained for the $S=1$ chain is nonuniversal: it depends on temperature and cutoff, although weakly. In Fig. 2 we present, for completeness, the power-law behavior of $P_J(J_i,\Omega)$ with exponent $\alpha=0.38$ obtained from an initial distribution with $\Delta=0$, at a fixed temperature $k_BT=0.10\Omega$.

Now we focus on the free energy per spin and the specific heat of the spin-1 chain. In Fig. 3 we show the plot of the specific heat versus temperature (given in units of Ω). Despite the power-law dependence of $P_J(J_i,\Omega)$ at low energies described above, we find a nonphysical behavior in the free energy of the system. For intermediate temperatures, the free energy gives rise to a negative specific heat (see Fig. 3).

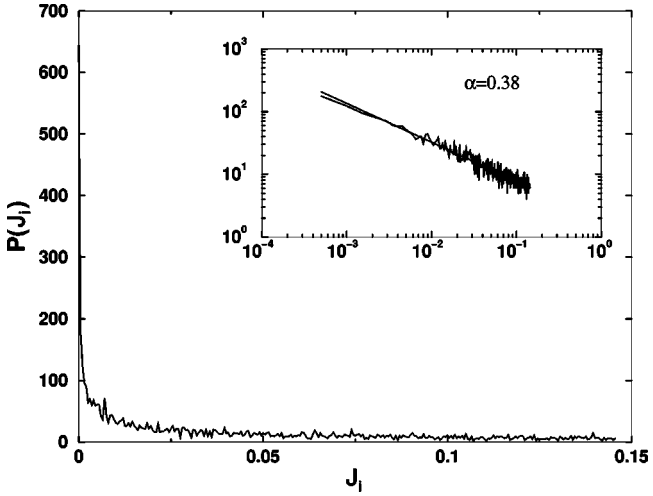

FIG. 2. Power-law behavior of $P_J(J_i,\Omega)$ in the low-energy limit, at $k_BT=0.10\Omega$. Inset: the Log-log plot of $P_J(J_i,\Omega)$ yields the exponent $\alpha=0.38$.

Nonetheless, at very low temperatures the free energy and thus the specific heat is well-behaved, being described by a power law (see inset of Fig. 3). These very low temperature features are similar to the random singlet phase of the disordered spin-1/2 chain.[1] Moreover, at higher temperatures, the free energy curve is again well-behaved and gives rise to a physically meaningful specific heat.

The presence of the factor $2S(S+1)/3$ in Eq. (6), which defines the renormalized coupling J', plays an important role in our discussion. In the case of the spin-1 chain it is 4/3. At low temperatures ($k_BT<0.37\Omega$), the function $W_1(\beta\Omega)$ is larger than 3/4, consequently, when the couplings neighboring the cutoff Ω are not small enough, couplings larger than those eliminated may be generated [see Eqs. (6) and (8)]. In this low temperature regime, although the cutoff decreases rapidly, large couplings are generated with non-negligible probability. When the couplings between the strongly coupled pair of spins and its neighbors are not sufficiently weak, the perturbative scheme fails, giving rise to the spurious result observed in the free energy. At higher temperatures ($k_BT>0.37\Omega$) the MDH method gives correct results for the thermodynamic properties.[10] There the function $W_1(\beta\Omega)<3/4$ cancel the coefficient 4/3 of J_1' [see Eq. (8)], thus validating the present approach, independently of the starting distribution. In addition, when one considers distributions with a finite gap (weakly disordered distributions), the breakdown of the MDH formalism is most pronounced. The probability of obtaining, at low temperatures, the product $J_1\ J_3<3/4\Omega^2$ depends on the value of the gap. By increasing Δ, the initial distribution will not generate infinitesimally weak couplings to ensure that the product is sufficiently small.

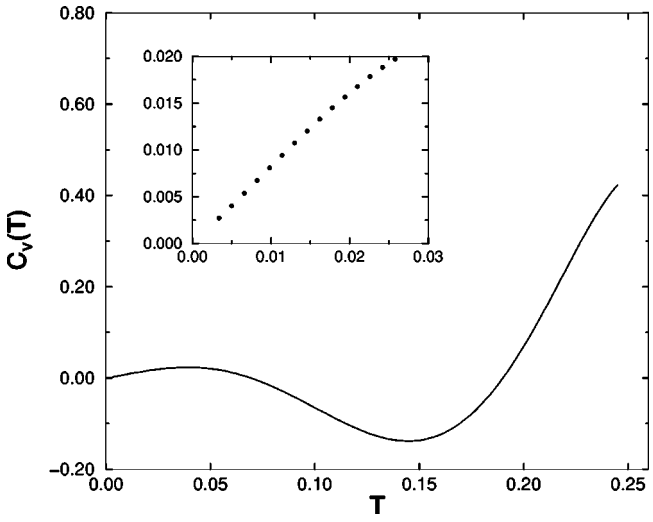

FIG. 3. Low temperature behavior of the specific heat of the random spin-1 chain for $\Delta=0$. Inset: the power-law behavior with exponent equal to 0.77.

TABLE I. Renormalized coupling for chains with $S=1/2$ and $S=1$ obtained with clusters of size 2, 4, 6, and 8. We have taken $J_i=\Omega=1$.

Cluster size	Spin-1/2	Spin-1
2	0.500 000	1.333333
4	0.377 992	1.881373
6	0.312 648	2.597776
8	0.270 240	

In the spin-3/2 chain we performed the decimation process by starting with a uniform gapless probability distribution. Despite the larger coefficient in Eq. (6), $P_J(J_i,\Omega)$ still develops a power-law behavior as the cutoff Ω becomes sufficiently small. However, this convergence is much slower than that for a spin-1 chain. Now the couplings J' which are larger than the decimated out coupling Ω are statistically predominant. The effect of the breakdown of the MDH method in the free energy of the $S=3/2$ chain is more dramatic yielding a negative specific heat even in the very low temperature limit.

These results has led us to try to improve the MDH transformation in two directions: first we considered the decimation of larger spin clusters. In order to gain an insight on whether or not this procedure would work, it was sufficient to carry out the decimation at zero temperature. The intent was to investigate whether the perturbation scheme, using larger clusters, would decrease the factor appearing in the expression for the new coupling J'. We have carried out numerically the decimation process for RAQ chains with both spin $S=1/2$ and $S=1$, considering clusters with 2, 4, 6, and 8 spins. In our numerical calculations we considered, for simplicity, $J_i=\Omega=1$, where the J_i's stand for the bonds between neighboring spins in the cluster. The results for the case of a cluster with only two spins can be directly compared with the value 1/2 and 4/3 of the original MDH procedure [see Eq. (6)] in the $S=1/2$ and $S=1$ RAQ chains, respectively. We list the results in Table I. In the case of a spin-1/2 chain the results indicate that the MDH scheme is always improved. However, the resulting values for larger clusters in the spin-1 chain makes clear that the problem remains unsolved.

We also tried to improve the MDH scheme by consider-

ing terms of higher order in the perturbation expansion, at zero temperature. In that case, our purpose was to investigate whether the higher order corrections would decrease the factor $2S(S+1)/3$ in Eq. (6). We have thus calculated the $T=0$ renormalized coupling, for the spin-1 chain, up to third order in Ω, which is given by

$$J' = \frac{4}{3\Omega} J_1 J_3 + \frac{1}{\Omega^2}(J_1^2 J_3 + J_1 J_3^2). \tag{12}$$

Once again, we come upon a result which reinforces that the MDH formalism is not suitable to describe the low temperature properties of the RAQ chains with $S \geqslant 1$ [defined in Eq. (1)]. Moreover, in the fourth-order correction to the renormalized bond biquadratic exchange couplings are generated. In this case we should consider these interactions already from the beginning in the Hamiltonian model. Finally we call attention that starting with a power law distribution, the MDH procedure works very well. In this case, only pairs of spins weakly coupled are present in the chain and the probability of the generated coupling being larger than the one eliminated is statistically negligible. The singular form of $P_J(J_i,\Omega)$ dominates the thermodynamic properties which are also described by power laws. Of course this is in strong contrast with the robust and universal character of the RS phase for the spin-1/2 chain, which is indeed a new fixed point.[1,2]

In summary, at zero temperature there is not a safe criterion to discuss the possibility of the occurrence of the RS phase in the RAQ chains. In fact, it was necessary to extend the MDH scheme, for $S \geqslant 1$, to finite temperature to establish the failure of the perturbative approach. In view of the results we have obtained, we strongly claim that the MDH procedure is not adequate to study the RAQ chains with $S \geqslant 1$ defined in Eq. (1). Moreover, the existence of a RS phase at low temperature is a property assured only for spin-1/2 RAQ chains.

The authors are grateful to the Brazilian agencies FAPERJ and CNPq for financial support.

[1] S. K. Ma, C. Dasgupta, and C. K. Hu, Phys. Rev. Lett. **43**, 1434 (1979); C. Dasgupta, and S. K. Ma, Phys. Rev. B **22**, 1305 (1980).
[2] D. S. Fisher, Phys. Rev. B **50**, 3799 (1994); **51**, 6411 (1995).
[3] J. C. Scott, A. F. Garito, A. J. Heeger, P. Nannelli, and H. D. Gilman, Phys. Rev. B **12**, 356 (1975).
[4] Y. Endoh, G. Shirane, R. J. Birgeneau, and Y. Ajiro, Phys. Rev. B **19**, 1476 (1979).
[5] L. N. Bulaevskii, A. V. Zvarykina, Yu S. Karimov, R. B. Lyubovskii, and I. F. Shchegolev, Zh. Éksp. Teor. Fiz. **62**, 725 (1972) [Sov. Phys. JETP **35**, 384 (1972)].
[6] G. Theodorou and M. H. Cohen, Phys. Rev. Lett. **37**, 1014 (1976).
[7] J. C. Fernandes, R. B. Guimarães, M. A. Continentino, H. A. Borges, J. V. Valarelli, and A. Lacerda, Phys. Rev. B **50**, 16 754 (1994).
[8] F. D. M. Haldane, Phys. Rev. Lett. **50**, 1153 (1983).
[9] M. A. Continentino, J. C. Fernandes, R. B. Guimarães, B. Boechat, H. A. Borges, J. V. Valarelli, E. Hanapel, Alex Lacerda, and P. R. J. Silva, Philos. Mag. B **73**, 601 (1996).
[10] B. Boechat, A. Saguia, and M. A. Continentino, Solid State Commun. **98**, 411 (1996).
[11] R. A. Hyman and Kun Yang, Phys. Rev. Lett. **78**, 1783 (1997).
[12] C. Monthus, O. Golinelli, and Th. Jolicoeur, Phys. Rev. Lett. **79**, 3254 (1997); C. Monthus, O. Golinelli, and Th. Jolicoeur, Phys. Rev. B **58**, 805 (1998).
[13] A. Saguia, Beatriz Boechat, and M. A. Continentino, Phys. Rev. B **58**, 58 (1998); **62**, 5541 (2000).
[14] Y. Nishiyama, Physica A **252**, 35 (1998); Erratum, *ibid.* **258**, 499 (1998).
[15] Y. Nishiyama, Eur. Phys. J. B **6**, 335 (1998).
[16] K. Hida, Phys. Rev. Lett. **83**, 3297 (1999).
[17] G. Theodorou, Phys. Rev. B **16**, 2264 (1977); **16**, 2273 (1977).