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Spin-$\frac{3}{2}$ random quantum antiferromagnetic chains

A. Saguia
Centro Brasileiro de Pesquisas Físicas Rua Dr. Xavier Sigaud 150—Urca, Rio de Janeiro 22290-180, Rio de Janeiro, Brazil

B. Boechat and M. A. Continentino*
Departamento de Física, Universidade Federal Fluminense, Avenida Litorânea s/n, Niterói, 24210-340, Rio de Janeiro, Brazil

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We use a modified perturbative renormalization group approach to study the random quantum antiferromagnetic spin-$\frac{3}{2}$ chain. We find that in the case of rectangular distributions there is a quantum Griffiths phase, and we obtain the dynamical critical exponent Z as a function of disorder. Only in the case of extreme disorder, characterized by a power-law distribution of exchange couplings, we find evidence that a random singlet phase could be reached. We discuss the differences between our results and those obtained by other approaches.

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The study of random antiferromagnetic chains is an important and actual area in magnetism. Since, by now, many of the physical properties of pure chains are understood, it is natural to include disorder in these systems and look for the modifications it introduces. In the case of spin-$\frac{1}{2}$ random exchange Heisenberg antiferromagnetic chains (REHAC) a perturbative approach introduced by Ma, Dasgupta, and Hu (MDH) was very successful[1] in investigating these systems. This approach turned out to be asymptotically exact and this allowed Fisher[2] to fully characterize the properties of the new disordered phase, for which, the name *random singlet phase* was coined. Unfortunately when generalized to higher spins this method, in its simplest version at least, revealed to be ineffective. The reason is that in the elimination procedure of the strongest bond Ω, the new interaction between the spins, coupled by exchanges J_1 and J_2 to the strongest coupled pair, is given by $J'=(2/3)S(S+1)J_1J_2/\Omega$.[3] For $S\geqslant 1$, the factor $(2/3)S(S+1)>1$ and the problem becomes essentially nonperturbative for arbitrary distributions of exchange interactions. Several approaches have been introduced to circumvent this difficulty,[4–13] which however do not always lead to the same unambiguous results. In this Rapid Communication, we apply a previous method used to treat the random spin-1 chain[13] for the spin-$\frac{3}{2}$ REHAC. This particular chain has been the subject of recent studies[9,11,14] and it would be better to confirm the results obtained in these works using another approach.

As mentioned previously, the method of Ma, Dasgupta, and Hu consists of finding the strongest interaction Ω between pairs of spins in the chain [see Fig. 1(a)] and treating the coupling of this pair with their neighbors (J_1 and J_2) as a perturbation. For a chain of spins $S=3/2$, after elimination of the strongest coupled pair, the new coupling between their neighbors is given by

$$J'=\frac{5}{2}\frac{J_1J_2}{\Omega}. \tag{1}$$

Consider the case $J_1\geqslant J_2$. If $J_1>(2/5)\Omega$, then the new effective interaction J' is necessarily larger than one of those eliminated, in this case, J_2.

Our generalization of the MDH method consists of either of the following procedures shown in Fig. 1. If the largest neighboring interaction to Ω, $J_1<(2/5)\Omega$, then we eliminate the strongest-coupled pair, obtaining an effective interaction between the neighbors to this pair which is given by Eq. 1 [see Fig. 1(a)]. This new effective interaction is always smaller than those eliminated.[15,16] Now suppose $J_1>J_2$ and $J_1>(2/5)\Omega$. In this case, we consider the *trio* of spins $S=\frac{3}{2}$ coupled by the two strongest interactions of the trio, J_1 and Ω, and solve it exactly [see Fig. 1(b)]. The ground state of this trio of spins $S=\frac{3}{2}$ is a degenerate quadruplet. It will be substituted by an effective spin $\frac{3}{2}$ interacting with its neighbors through *new renormalized* interactions obtained by a degenerate perturbation theory acting on the ground state of the trio. This procedure which implies diagonalizing the 64×64 matrix of the trio is carried out *analytically*. This is important for obtaining results on large chains and to deal with the large numbers of initial configurations that we use. These procedures guarantee that we always comply with the criterion of validity of the perturbation theory as shown in Fig. 2. We have considered initial rectangular distributions, $P_0(J)=[1/(\Omega-G)]\Theta(\Omega-J)\Theta(J-G)$ of interactions and even for the weak disorder case, with a gap G as large as $G=0.5$ in the distribution ($\Omega=1$), the method works very well and never an interaction larger than those eliminated is generated (see Fig. 2).

The phase diagram for rectangular original distributions can now be obtained. For a strong disorder, which corresponds to $G=0$, we find a Griffiths phase with a dynamic

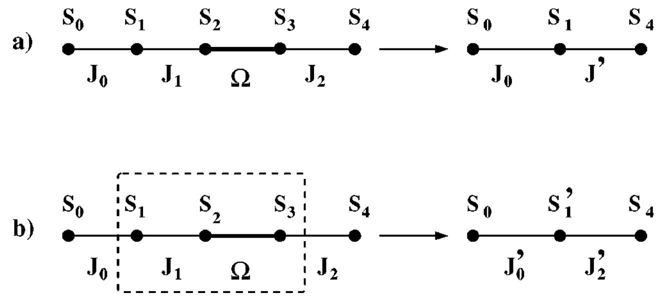

FIG. 1. The two elimination procedures as described in the text ($J_1>J_2$).

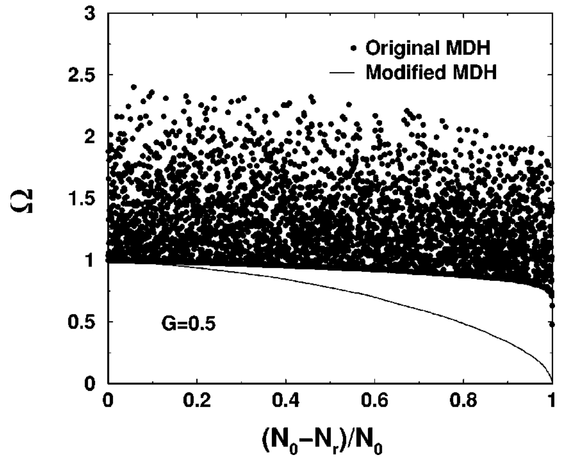

FIG. 2. The evolution of the cutoff, for an initial rectangular distribution with $G=0.5$, along the renormalization process of the spin-$\frac{3}{2}$ REHAC. We show the results for the original MDH and the present (modified) renormalization-group procedures.

exponent $Z \sim 12.7$ as shown in Fig. 3. This phase is characterized by *first-gap distributions*[13] that saturate at low energies in the form $P(-\log_{10}\Delta) \sim \Delta^{1/Z}$ for $\Delta \rightarrow 0$. This is obtained starting from a given configuration of random interactions for a chain of size L and eliminating the spins, as described above, until a single pair remains. The interaction between these remaining spins yields the first gap Δ for excitation. The dynamic exponent Z relates the scales of length and energy through $\Delta \propto L^{-Z}$.

In Fig. 3, we show the first-gap distributions for different degrees of disorder as characterized by different gaps G in the initial distribution of interactions. For all cases, including that of strong disorder $(G=0)$, we find that the first-gap distributions saturate at low energies with the *dynamic exponent* Z independent of L for L sufficiently large. We have to consider large chains in order to observe this effect. We find $Z_\infty \sim 0.43$ and $Z_\infty \sim 1.12$ for $G=0.2$ and $G=0.12$, respectively. From these values of the dynamic exponent we can deduce the existence of a Griffiths phase extending up to $G_c \approx 0.11$ where the dynamic exponent reaches the value $Z=1$. Since, for example, the susceptibility $\chi \propto T^{1-Z}$, a singular low-temperature behavior implies $Z>1$. At G_c there is in fact a significant change in the nature of the thermodynamic behavior of the system.[11] The phase for $G>G_c$ is one with quasilong range order, i.e., with spin correlations decaying algebraically with distance, similar to the zero-temperature phase of the pure chain.[11]

In order to check the existence of a random singlet phase in the spin-$\frac{3}{2}$ chain we consider another class of distributions of exchange couplings associated with *extreme* disorder.[17–21] These distributions are of the form $P(J) \propto J^{-1+1/\delta}$. For $\delta=1$ this reduces to the gapless case of rectangular distribu-

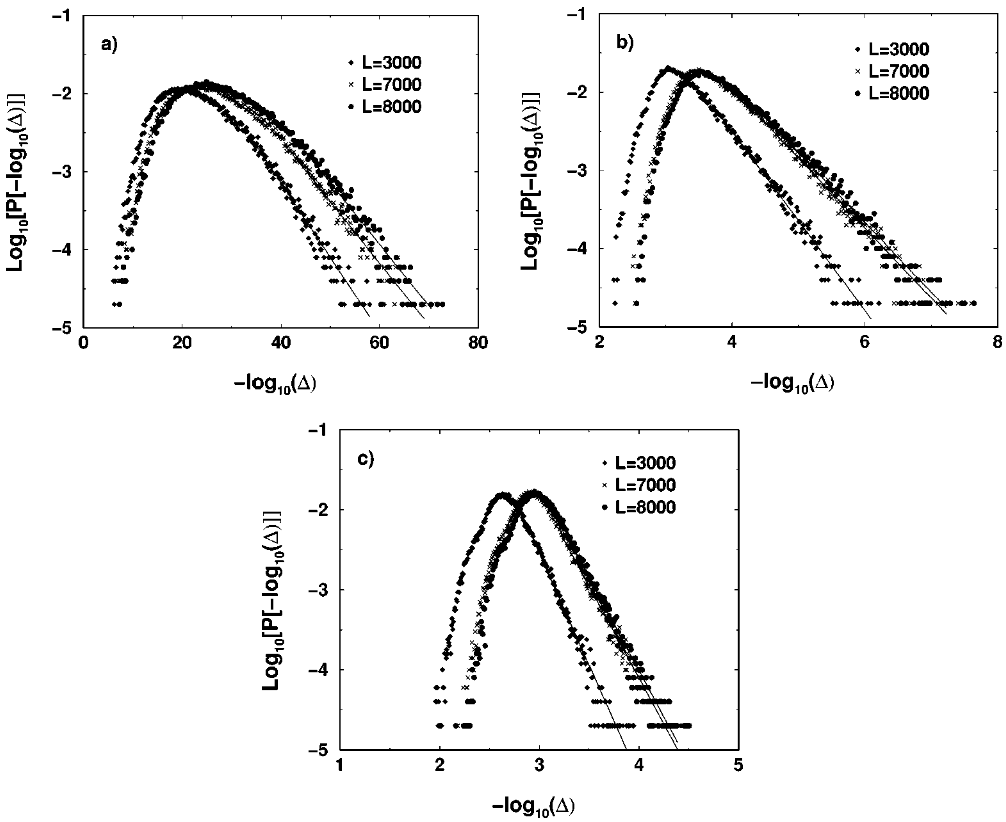

FIG. 3. Probability distributions of first gap for initial rectangular distributions of couplings with gaps G and different systems sizes L. For clarity, not all values of L are shown. The solid lines represent best fits to the form $\log_{10}[P(-\log_{10}\Delta)]=A_L-(1/Z_L)\log_{10}\Delta$. (a) $G=0$, $Z_{3000}=10.51$, $Z_{7000}=12.68$, and $Z_{8000}=12.70$. (b) $G=0.12$, $Z_{3000}=0.87$, $Z_{7000}=1.11$, and $Z_{8000}=1.12$. (c) $G=0.2$, $Z_{3000}=0.35$, $Z_{7000}=0.43$, and $Z_{8000}=0.43$.

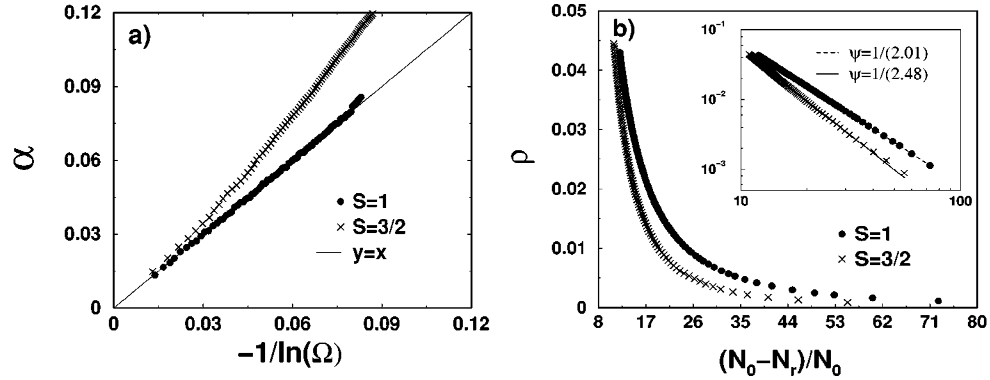

FIG. 4. (a) The exponent α describing the asymptotic low-energy behavior of the renormalized exchange distribution as a function of the scale dependent cutoff. (b) Fraction of active spins as a function of the cutoff. For comparison, we show the results for the spin-1 and spin-$\frac{3}{2}$ REHAC's. In both cases, the starting distribution is extremely disordered with $\delta=20$ (see text).

tions considered previously, and for $\delta>1$ we have the extreme disordered cases. We now report our results for the random spin-$\frac{3}{2}$ chain obtained with the modified renormalization-group procedure[13] for the case of an extremely disordered distribution with $\delta=20$. In a random singlet phase, the fixed-point distribution of interactions, which is attained when the cutoff Ω is sufficiently reduced, takes the form

$$P(J)=\frac{\alpha}{\Omega}\left(\frac{\Omega}{J}\right)^{1-\alpha}. \tag{2}$$

The exponent α is a function of the cutoff Ω and varies as $\alpha=-1/\ln\Omega$. Also for a random singlet phase, the fraction of remaining active spins ρ as a function of the energy scale set by the cutoff Ω[2] is given by

$$\rho=\frac{1}{L}=\frac{1}{|\ln\Omega|^{1/\psi}}. \tag{3}$$

The exponent ψ establishes the connection between the characteristic length L and the energy scale Ω. This is an extension of the usual definition of a dynamic exponent[22] ($\Omega^{-1}\propto\tau\propto L^{z}$) for the case of logarithmic scaling. In Fig. 4(a) we show the exponents α obtained from the asymptotic form of the exchange distributions after the cutoff Ω has been sufficiently reduced. For comparison we show the results for a spin-1 REHAC with the same original extremely disordered distribution for which a random singlet phase is clearly established. We have considered here chains of size as large as $L=4.5\times10^{5}$. In Fig. 4(b) we show the density $\rho=1/L$ of active spins as a function of the cutoff Ω. From this expression we extract the exponent ψ [see Eq. (3)] which takes the value $\psi=1/(2.4)$ close to the value $\psi=1/2$ expected for a random singlet phase.[2] As shown in this figure, for comparison, the spin-1 chain has clearly converged to this phase within the same scale of the cutoffs. Our results suggest that in this case of extreme disorder, the spin-$\frac{3}{2}$ REHAC eventually reaches a random singlet phase, although the convergence is very slow.

Recently, another approach to the spin-$\frac{3}{2}$ chains has predicted the existence of a random singlet phase in these chains, even for weak disorder.[9,14] This is associated with spin-$\frac{1}{2}$ degrees of freedom. These results are quite distinct from those obtained above where a random singlet phase is hardly evident even for extremely disordered original distributions.

The decomposition of a chain of spins S in smaller spins relies on projecting out the highest-energy level of a pair of spins S. However, the remaining excited states are kept in this procedure to maintain the correct number of states. For example, in the case of a pair of spins-1 with a total of nine states, the singlet ground state and the first excited triplet are kept to yield the four states of the relevant antiferromagnetically coupled spin-$\frac{1}{2}$ pair.[5]

The MDH elimination procedure can be generalized for finite temperatures and arbitrary spins S. It is given by

$$J'=\frac{2}{3}S(S+1)\frac{J_1J_2}{\Omega}W_S(\beta\Omega), \tag{4}$$

where

$$W_S(y)=\frac{(2S+1)^2-\sum_{i=0}^{i=2S}(2i+1)e^{-(1/2)i(i+1)y}\left[1+\frac{1}{2}i(i+1)\right]}{4S(S+1)\sum_{i=0}^{i=2S}(2i+1)e^{-(1/2)i(i+1)y}}. \tag{5}$$

Note that for sufficiently high temperatures, the factor $\frac{2}{3}S(S+1)W_S(\beta\Omega)<1$ and the MDH elimination procedure works in this case. A random singlet phase is reached in the sense that the asymptotic distribution of exchange attains the form given by Eq. (2) at these temperatures. However, as T is reduced the problem becomes essentially nonperturbative for spins $S\geqslant1$, as the equation above generates coupling larger than those eliminated. In particular at $T=0$, the excited states which reduce the factor W_S from its value $W_S(T=0)=1$ are now frozen. In fact *none* of the excited states play a role in the problem at zero temperature. Note that in our generalized renormalization scheme, degenerate perturbation theory is applied to the *ground state* of the spin trio. We

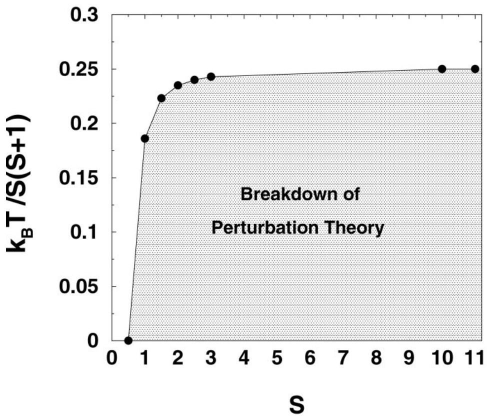

FIG. 5. Temperature T^* below which the MDH perturbation theory breaks down for different values of the spin S. The energy $k_B T^*$ is in units of the cut-off Ω of the original exchange distribution.

believe this is the main reason for the discrepancy between our results and those obtained by the authors of Refs .9 and 14. Consideration of excited states in the problem favors the appearance of an infinite disorder random singlet phase, as it occurs at finite temperatures.

In the limit $S \to \infty$ and $T \to 0$, replacing the sum by an integral and with a proper renormalization of the Hamiltonian, Eqs. (4) and (5) yield $J' = J_1 J_2 / 4 k_B T$, in agreement with the result of Ref. 1 for classical spins. In Fig. 5 we show the temperature T^* below which the simple perturbative approach breaks down for a given value of the spin of the random chain.

Note that for rectangular distributions, the Griffiths phase of the spin-1 REHAC extends up to $G_c = 0.45$ and for spin-$\frac{2}{2}$ up to $G_c = 0.11$. For random classical spin chains, the susceptibility $\chi \propto P(0) |\ln T|$, where $P(0)$ is the finite weight at the origin of the original distribution $P(J)$.[1] This weak logarithmic singularity is similar to that expected for quantum chains at the border of the Griffiths phase ($Z \approx 1$) as if in this case, $G_c = 0$.

We have studied a spin-$\frac{3}{2}$ REHAC using an extension of the renormalization-group procedure introduced by Ma, Dasgupta, and Hu.[1] This method which considers larger clusters of spins eliminates the difficulties associated with the perturbative nature of the MDH procedure for the cases of spins $S \geqslant 1$. The new procedure works very well for the spin-$\frac{3}{2}$ chain and the bonds larger than those eliminated are never generated for the distributions used here. For rectangular distributions, we found that the spin-$\frac{3}{2}$ REHAC presents a Griffiths phase up to a critical value of disorder. We have also considered the case of extreme disorder, where the starting exchange distributions are singular for small values of the coupling. For values of the disorder parameter as large as $\delta = 20$, our results only suggest that a random singlet phase will be asymptotically reached as the cutoff of the distribution $\Omega \to 0$. We have compared our results with those of another approach which predicts a random singlet phase, associated with spin-$\frac{1}{2}$ degrees of freedom, even for weak disorder. We attribute the difference between these results and those we have obtained to the fact that the former approach takes into account excited states which mimic the effects of temperature and favor the appearance of a random singlet phase. Our results however are consistent with those of Igloi *et al.*[11] that find a random singlet phase in spin-$\frac{3}{2}$ chains for the case of extremely disordered distributions.

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*Electronic address: mucio@if.uff.br

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