Quantum phase transition in the random antiferromagnetic spin-1 chain

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We study the random antiferromagnetic spin-1 chain following the evolution of the bond probability distributions under a renormalization group transformation. We use a mapping of the spin-1 chain into an effective spin-1/2 chain with both ferromagnetic (odd bonds) and antiferromagnetic (even and odd bonds) interactions. We obtain a recursion relation for the coupling constants, solving exactly up to a four-spin cluster. Our improved perturbation treatment on these larger clusters shows that the random singlet phase in the spin-1 chain, differently from previous results, is obtained only when 100% of the odd bonds are strong ferromagnetic, i.e., larger than the even antiferromagnetic bonds. Otherwise the ground state is that of a dimerized spin-1/2 chain.

I. INTRODUCTION

In this paper we study the one-dimensional spin-1 quantum Heisenberg antiferromagnetic with randomly distributed interaction strengths. This system is defined by the following Hamiltonian for a chain of L spins:

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

where $\vec{S}_i$ are spin-1 operators and J_i are positive random nearest-neighbor interactions.

The study of low-dimensional disordered magnetic systems has become an important area of research which has attracted the attention of many physicists in recent years.[1–3] Among the various works developed to study random quantum chains, we point out that by Ma, Dasgupta, and Hu (MDH).[1] They studied the properties of random antiferromagnetic Heisenberg chains (RAFCs), with $S=1/2$, using a real-space renormalization group approach (MDH). The MDH scheme has been very successful in explaining the low-temperature thermodynamics of the spin-1/2 RAFC systems which are described by power law behavior and governed by a fixed point with universal properties. Later Fisher[3] solved the MDH renormalization group equations exactly and clarified the structure of the ground-state properties of this new phase which has since been called the random-singlet phase (RSP).

Recently we presented an extensive theoretical and experimental study[4–6] of strongly disordered one-dimensional antiferromagnetic Heisenberg spin-1 systems. Here, strong disorder is defined as very broad bond probability distributions on a logarithmic scale. The main result which has arisen from the magnetic measurements and theoretical calculations is that the strongly disordered spin-1 chain behaves similarly to the spin-1/2 RAFC, with low-temperature power law thermodynamic behavior but weaker singularities. In fact we have generalized the MDH scheme to study spin-1 chains and demonstrated that the Haldane gap[7] present in the pure system is suppressed by strong disorder, being filled by low-energy excitations, in agreement with experimental observations. We pointed out that, although our approach is suitable to describe the system with strong disorder, it fails to describe the weak-disorder regime.

A modified version of the MDH method[8,9] has been proposed to deal with both regimes. It consists in mapping the spin-1 chain to an effective spin-1/2 model with both ferromagnetic and antiferromagnetic bonds.[2] With this mapping the authors of Refs. 8,9 claimed to have obtained a second-order transition separating the RSP from a weak disordered phase.

The effect of randomness on the Haldane phase was also studied by Nishiyama[10,11] who carried out exact diagonalization and quantum Monte Carlo simulations, and by Hida[12] using density matrix renormalization group (DMRG) techniques. They observed that the Haldane phase is quite robust against randomness and found no random-singlet phase even for the case of strong disorder. On the other hand, Todo *et al.*[13] using also a Monte Carlo simulation predicted the possibility of a random-singlet phase for strong enough disorder.

In the present work we use the extended version of the MDH scheme developed in Ref. 8 to study the phase diagram of the disordered spin-1 chain. We have obtained explicit recursion relations for the coupling constants, taking into account up to six-spin clusters, differently from Hyman *et al.*, where only four-spin clusters were considered. By using numerical procedures we carried out our recursion relations directly and followed the evolution of the bond distribution functions. We found no evidence of the unstable fixed point, in the moderate disorder regime, separating a random-singlet phase from a randomly dimerized phase, obtained in Refs. 8 and 9. Our improved perturbation treatment shows that the mapping of the antiferromagnetic spin-1 chain to a random spin-1/2 chain with ferromagnetic and antiferromagnetic bonds gives rise only to the randomly dimerized phase. In order to obtain the random-singlet phase all ferromagnetic bonds should be strong and in this case we are back to the original random spin-1 chain studied previously. Consequently the above mapping does not shed any additional light on the controversy of the existence of the RSP in spin-1 chains.

The remainder of this paper is organized as follows. In Sec. II we outline the formalism and discuss some technical

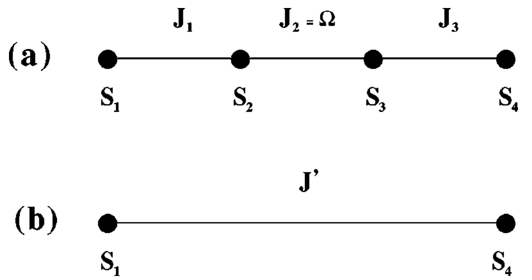

FIG. 1. Spins and couplings constants involved in the elimination transformation of a two-spin cluster, which transforms (a) to (b).

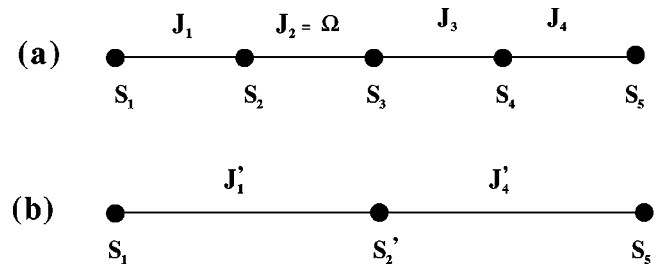

FIG. 2. Spins and couplings constants involved in the elimination transformation of a three-spin cluster, which transforms (a) to (b).

points, in Sec. III we present the results, and in the last section we summarize our main conclusions.

II. FORMALISM

We use the effective spin-one-half (ESH) chain of Hyman and Yang[8] which is a model for the random antiferromagnetic spin-1 chain. Briefly, in this model the chain consists of half spins only. The even bonds are taken from an antiferromagnetic (AF) bond distribution whereas the odd bonds are taken from a distribution containing both antiferromagnetic and ferromagnetic (F) bonds. Hence we can rewrite the model Hamiltonian, Eq. (1), in the form

$$H=\sum_{i=1}^{L-1}(J_{2i-1}\vec{S}_{2i-1}\cdot\vec{S}_{2i}+J_{2i}\vec{S}_{2i}\cdot\vec{S}_{2i+1}), \quad (2)$$

where J_{2i-1} are positive and negative random variables distributed according to a probability distribution $P_{odd}(J_{2i-1})$ and J_{2i} are only positive random variables distributed according to a probability distribution $P_{even}(J_{2i})$. Here $\vec{S}_i$ are spin-1/2 operators and we are interested in the limit $L\to\infty$.

The ESH model can be studied by using an extended MDH method, which properly accounts for strong ferromagnetic bonds. This generalized MDH procedure works in the following way. At any stage of the decimation, the energy scale Ω is set by the strongest antiferromagnetic bond in the system, so that the odd bonds separate into two groups: group A consists of all AF bonds and those F bonds that are weaker than Ω, while group B consists of F bonds that are stronger than Ω. The even bonds are always AF bonds weaker than Ω. After identifying the strongest AF bond, $J_i=\Omega$, we have to distinguish three types of renormalization rules.

(1) If i is odd or if it is even and both neighbors belong to group A, then we directly apply the MDH procedure as originally proposed by Ma, Dasgupta, and Hu.[1] The method consists in eliminating the pair of spins with the strongest antiferromagnetic ($J_2=\Omega$) coupling 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).

We must then solve the spectrum of the unperturbed Hamiltonian for the strongly coupled pair of spins $\vec{S}_2$ and $\vec{S}_3$, which is given by

$$H_0=J_2\vec{S}_2\cdot\vec{S}_3. \quad (3)$$

The ground state $|s\rangle$ for H_0 is a singlet, and there are three excited states $|t\rangle$ forming a triplet. The energies are $E_s=-\frac{3}{4}J$ and $E_t=\frac{1}{4}J$.

The spins $\vec{S}_2$ and $\vec{S}_3$ are weakly coupled to the neighbors via

$$H_1=J_1\vec{S}_1\cdot\vec{S}_2+J_3\vec{S}_3\cdot\vec{S}_4. \quad (4)$$

We next calculate the correction to the H_0 ground-state energy due to the effect of H_1 by perturbation expansion. In second order, E_s is given by

$$E_s+\langle s|H_1|s\rangle+\sum_t\frac{|\langle s|H_1|t\rangle|^2}{E_s-E_t}\equiv E'+J'\vec{S}_1\cdot\vec{S}_4, \quad (5)$$

which provides the following recursion relations:

$$J'=\frac{J_1\cdot J_3}{2\Omega}. \quad (6)$$

(2) If i is even and if one of the neighboring bonds, say, J_{i+1}, belongs to group B, we eliminate the spins S_i, S_{i+1}, S_{i+2} and replace them by a single spin-1/2, $\vec{S}_i'$ (see Fig. 2).

In order to find the modified couplings J_1' and J_4' we first solve the three-spin cluster problem of $\vec{S}_2$, $\vec{S}_3$, $\vec{S}_4$. If we ignore the influence of their neighbors S_1 and S_5, then the Hamiltonian for the trio would be

$$H_0=J_2\vec{S}_2\cdot\vec{S}_3+J_3\vec{S}_3\cdot\vec{S}_4. \quad (7)$$

The ground state $|d\rangle$ for H_0 is a doublet. The energy is

$$E_d=-J_2-J_3-2\sqrt{J_2^2-J_2J_3+J_3^2}. \quad (8)$$

As in the last case, the spins $\vec{S}_1$ and $\vec{S}_5$ are weakly coupled to the neighbors by the following Hamiltonian:

$$H_1=J_1\vec{S}_1\cdot\vec{S}_2+J_4\vec{S}_4\cdot\vec{S}_5. \quad (9)$$

Within the degenerate subspace of the doublet, first-order perturbation theory shifts the ground-state energy of H_0 by

$$\lambda=-A^2(B+1)(BJ_1\vec{S}_1+J_4\vec{S}_5), \quad (10)$$

where

$$B=\frac{-J_3-\sqrt{J_2^2-J_2J_3+J_3^2}}{J_2} \quad (11)$$

and

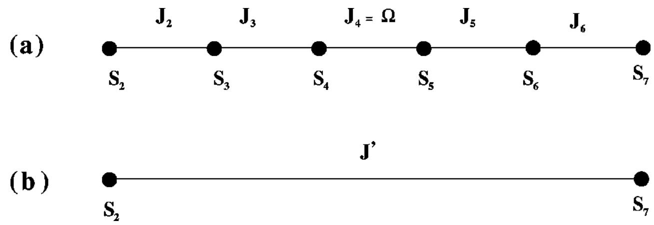

FIG. 3. Spins and couplings constants involved in the elimination transformation of a four-spin cluster, which transforms (a) to (b).

$$A=\frac{1}{\sqrt{2(B^2+B+1)}}. \tag{12}$$

On the other hand, we use the idea that the perturbation H_1 is equivalent to

$$H_1'=J_1'\vec{S}_1\cdot\vec{S}_2'+J_4'\vec{S}_5\cdot\vec{S}_2', \tag{13}$$

where $\vec{S}_2'$ is a single spin-1/2 operator. After calculating, in this last case, the first-order perturbation we obtain

$$\lambda'=\frac{\sqrt{3}}{2}(J_1'\vec{S}_1+J_4'\vec{S}_5). \tag{14}$$

The identification of Eq. (10) with Eq. (14) provides

$$J_1'=\frac{2}{\sqrt{3}}A^2(B+1)BJ_1, \tag{15}$$

$$J_4'=\frac{2}{\sqrt{3}}A^2(B+1)J_4. \tag{16}$$

So we remove the spins $\vec{S}_2$, $\vec{S}_3$, and $\vec{S}_4$, and replace them by another spin 1/2, $\vec{S}_2'$, which couples to the rest of the chain through J_1' and J_4'.

(3) If i is even and both neighbors of J_i belong to group B, we solve the four-spin cluster including spins S_{i-1}, S_i, S_{i+1}, and S_{i+2}. After removing these spins we end up with an effective AF coupling between spins S_{i-2} and S_{i+3} (see Fig. 3).

The Hamiltonian for the six-spin cluster, shown in Fig. 3(a), is given by

$$H=H_0+H_1, \tag{17}$$

where

$$H_0=J_3\vec{S}_3\cdot\vec{S}_4+J_4\vec{S}_4\cdot\vec{S}_5+J_5\vec{S}_5\cdot\vec{S}_6 \tag{18}$$

is the unperturbed Hamiltonian of the four-spin cluster, and

$$H_1=J_2\vec{S}_2\cdot\vec{S}_3+J_6\vec{S}_6\cdot\vec{S}_7 \tag{19}$$

represents a perturbation induced by the presence of neighbor spins $\vec{S}_2$ and $\vec{S}_7$.

The ground state $|s\rangle$ for H_0 is a singlet, and there are 15 excited states which are all obtained. The ground-state energy is given by

$$E_s=-\frac{1}{4}(J_3+J_4+J_5)-\frac{1}{2}(J_3^2+J_4^2+J_5^2-J_3J_4-J_4J_5+2J_3J_5)^{1/2}. \tag{20}$$

The displacement in E_s generated by H_1 is given to second-order perturbation theory by

$$E_s+\langle s|H_1|s\rangle+\sum_{n=1}^{15}\frac{|\langle s|H_1|n\rangle|^2}{E_s-E_n}\equiv E'+J'\vec{S}_2\cdot\vec{S}_7,$$

where the states $|n\rangle$ and energies E_n are, respectively, the eigenvectors and eigenvalues of the unperturbed Hamiltonian H_0. Again, the procedure outlined above easily provides the recursion relation for J' which is too lengthy to be explicitly written here. Formally it can be expressed as

$$J'=f(J_3,J_4,J_5)\cdot J_2J_6 \tag{21}$$

We point out that in the limit $J_3,J_5\to\infty$, $f(J_3,J_4,J_5)\to 4/3J_4$, which recovers our previous result for the original spin-1 chain.[4] The spins $\vec{S}_3$, $\vec{S}_4$, $\vec{S}_5$, and $\vec{S}_6$ are removed, yielding an effective coupling J' between spin $\vec{S}_2$ and $\vec{S}_7$ neighbors of the four-spin cluster. The extended MDH procedure described above keeps the original structure of the system; i.e., even bonds are AF and odd bonds are F or AF. These recursion relations can be iterated by direct numerical simulations. We consider the spins arranged in a line and choose at random the exchange couplings according to probability distributions $P_{even}(J_{2i})$ and $P_{odd}(J_{2i-1})$. We then find the pair of spins with the strongest antiferromagnetic coupling in the chain and address the corresponding renormalization case. As the decimation proceeds, the original probability distributions are modified. Critical points are then evaluated as nontrivial fixed points of these distributions and phases are identified according to the attractor of their points.

III. RESULTS

We have performed extended numerical simulations to iterate the generalized MDH recursion relations. The chain is composed of n spin-1/2 objects with periodic boundary conditions ($n=100\,000$, for example). In this work the starting even exchange coupling distribution $P_{even}(J_{2i})$ is always taken as a uniform distribution with $0\leqslant J_{2i}\leqslant\Omega$ such that $P_{even}(0)\neq 0$. This is the distribution which is considered in most of the studies of random chains and we refer to it as the strongly disordered case. The distribution for the odd couplings, $P_{odd}(J_{2i-1})$, consists of one part P_{odd}' of bonds with $-\Omega\leqslant J_{2i-1}\leqslant\Omega$ and another part $N(J_{2i-1})$ with strong ferromagnetic bonds, i.e., $J_{2i-1}<-\Omega$. The normalization conditions for those distributions are

$$\int_0^{\Omega}P_{even}(J_{2i})dJ=1 \tag{22}$$

and

$$\int_{-\Omega_1}^{-\Omega}N(J_{2i-1})dJ+\int_{-\Omega}^{\Omega}P_{odd}'(J_{2i-1})dJ=1, \tag{23}$$

where $|\Omega_1|>|\Omega|$.

When $P'_{odd}(J_{2i-1})=0$ and all the $J_{2i-1}\to\infty$, the original $S=1$ chain is recovered. For the strongly disordered case corresponding to $P_{even}(J_{2i})$ defined above, successive elimination transformations give rise to weaker and weaker couplings, as the cutoff decreases. For sufficiently small Ω, the distribution $P_{even}(J_{2i})$ becomes peaked at $J_{2i}=0$ approaching the fixed point, power law behavior,

$$P^*(J_{2i},\Omega)\approx\frac{\alpha}{\Omega}\left(\frac{J_{2i}}{\Omega}\right)^{-1+\alpha}, \tag{24}$$

and the Haldane gap present in the pure system is suppressed, being filled by low-energy excitations. The fixed point form $P^*(J_{2i},\Omega)$, Eq. (24), leads to a low-temperature behavior of the thermodynamic quantities described also by power laws,[1,4,5]

$$F\propto T^{1+2\alpha}, \quad C_v\propto T^{\gamma_c} \tag{25}$$

and

$$\chi\propto T^{-1+\gamma_s}, \quad m\propto H^{\gamma_h}, \tag{26}$$

where F is the free energy, C_v is the specific heat, and χ is the susceptibility. H and m are, respectively, the uniform external field and magnetization. The exponents γ_c, γ_s, and γ_h are related to the exponent α of $P^*(J_{2i},\Omega)$ and of the free energy F. Since the power law distribution is not the exact fixed point distribution for the elimination transformation, α and consequently γ_c,γ_s, and γ_h depend on the temperature and cutoff. Thus, the disordered spin-1 chain ground state resembles the disordered spin-1/2 ground state, known as the random-singlet phase, but with weaker singularities.[1,4,5] These are in fact the results we have obtained previously using a direct approach to the spin-1 chain.

Let us now consider more general situations. For convenience we have chosen to study the evolution of the probability distribution $\overline{P}(x_i,\Omega)$ of the variable x_i defined by

$$x_i=\frac{|J_{2i}/J_{2i-1}|}{|J_{2i}/J_{2i-1}|+1}. \tag{27}$$

In order to identify the different phases of the random chain, it is sufficient to follow the flow of the mean value of the $\overline{P}(x_i,\Omega)$ distribution

$$\langle x\rangle=\int_{-\infty}^{+\infty}x\overline{P}(x_i,\Omega)dx. \tag{28}$$

In the random-singlet phase all odd bonds are strong ferromagnetic, i.e., much larger than all antiferromagnetic even bonds. The spin 1/2's are combined into spin-1 objects which eventually form singlets. In this case the mean value $\langle x\rangle$ goes to zero because $J_{2i}/J_{2i-1}\to 0$. On the other hand, in the random dimerized phase the odd bonds (AF or F) become much weaker than the even AF bonds. Only spin 1/2's, weakly coupled, remain in the chain, forming singlets over even bonds (decoupled dimers). In this case the ratio $J_{2i}/J_{2i-1}\to\infty$; hence $\langle x\rangle$ goes to unity. In order to study the competition between these two phases, we have carried out the iteration of the recursion relations, considering two types of initial distributions for $N(J_{2i-1})$: delta and rectangular functions. The important physical ingredient separating the two phases lies on the presence of strong odd ferromagnetic bonds $N(J_{2i-1})$ in the chain. The results we have obtained are the same for both distributions, $N(J_{2i-1})$, indicating that they are insensitive to any specific realization of disorder.

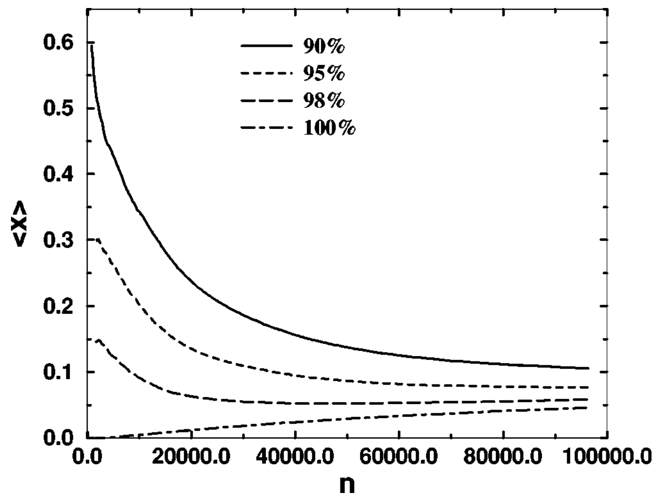

FIG. 4. Evolution of the first moment of the probability distribution, $\overline{P}(x,\Omega)$ as a function of the spin population during the renormalization process. Each curve corresponds to a different initial percentage of strong ferromagnetic odd bonds.

In Fig. 4 we present the results for the delta function case. $P'_{odd}(J_{2i-1})$ is taken as a uniform distribution with $-\Omega\leqslant J_{2i-1}\leqslant\Omega$ and $P_{even}(J_{2i})$ a gapless uniform distribution with $0\leqslant J_{2i}\leqslant\Omega$. The important parameter is the relative weight between strong ferromagnetic bonds and the total number of odd bonds, i.e., the ratio $N/(P'+N)$. The plot shows the evolution of the first moment of the probability distribution, given by Eq. (28), for different values of this ratio. For the two initial distribution of odd bonds, $N(J_{2i-1})$, considered here we have obtained a different flow diagram from the previous study by Hyman and Yang.[8] In their work they find the existence of the random-singlet phase in the chain when 50% or more of the odd bonds are strong ferromagnetic. Our numerical results indicate that the random-singlet phase is only reached when we have 100% of the odd bonds are strong ferromagnetic. Otherwise we are always in the random dimerized phase. The ESH model with 100% of odd bonds strong ferromagnetic just recovers the random spin-1 chain which has been investigated previously.[5] These results show that the mapping of the antiferromagnetic spin-1 chain to a random spin-1/2 chain with both ferromagnetic and antiferromagnetic bonds does not allow any definite conclusion on the crossover from strong to weak disorder in the random spin-1 chain.

For completeness, the random-singlet phase was also characterized by the power law behavior obtained for the probability distribution $P_{even}(J_{2i},\Omega)$ of antiferromagnetic bonds in the low-energy limit [see Eq. (24)]. This is the fixed point form, for which $P_{even}(J_{2i})$ evolves after a sufficiently large number of iterations. Actually this is a characteristic of the random-singlet phase that, independently of the form of the original distribution, it always flows to the power law behavior. Although the exact form of $N(J_{2i-1})$ is not relevant to the overall qualitative features of the phase diagram,

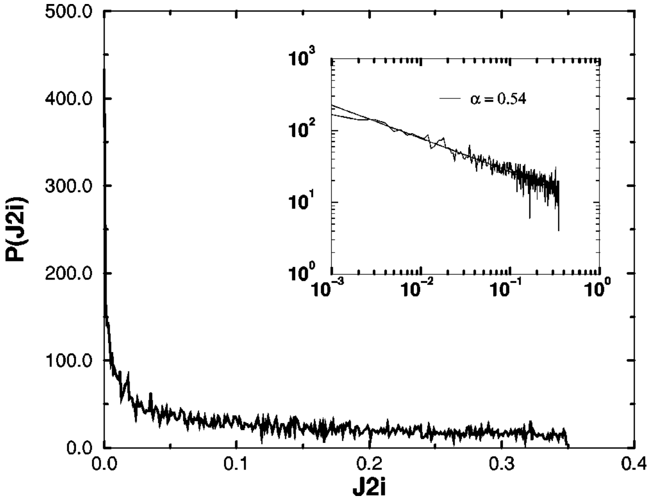

FIG. 5. Power law behavior of the probability distribution $P_{even}(J_{2i},\Omega)$ in the low-energy limit. This plot was obtained for a initial distribution $N(J_{2i-1})=\delta(J_{2i-1}-\Omega_1)$. Inset: the log-log plot of $P_{even}(J_{2i},\Omega)$ yields the exponent $\alpha=0.54$.

this is not the case for the power law exponent of the renormalized $P_{even}(J_{2i})$. We found that although $P_{even}(J_{2i})$ always becomes a power law in the random-singlet phase, the exponent is not universal and depends on the form of the initial distribution $N(J_{2i-1})$. In Fig. 5 we present this power law behavior, with exponent $\alpha=0.54$, obtained for an initial distribution $N(J_{2i-1})=\delta(J_{2i-1}-\Omega_1)$.

IV. SUMMARY

In this work we have investigated the random antiferromagnetic spin-1 chain by means of a real-space renormalization group method. We have obtained explicit recursion relations for the coupling constants of the EHS chain, without any approximation, up to four-spin clusters instead of the two-spin clusters usually considered. Our improved perturbation scheme, applied on larger clusters, allows for a more rigorous treatment of the strong ferromagnetic bonds. We have obtained, differently from previous claims,[8] that only when 100% of the odd bonds of the random spin-1/2 chain, on which we mapped the spin-1 system, are strong ferromagnetic does the random-singlet phase appear. At this point, however, we are back to the original random spin-1 chain investigated previously by us.[4,5] Consequently the mapping of the spin-1 chain into an effective spin-1/2 model does not provide any additional information to that already found in Refs. 4 and 5. In particular it does not shed light on the nature of the crossover from the strong to weak disorder regime. The ground state of the EHS model with less than 100% of odd bonds strong ferromagnetic is that of a random dimerized spin-1/2 chain.

ACKNOWLEDGMENTS

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