

## Disorder-induced phases in higher-spin antiferromagnetic Heisenberg chains

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Extensive density-matrix renormalization-group calculations for spin  $S=1/2$  and  $S=3/2$  disordered antiferromagnetic Heisenberg chains show a rather distinct behavior in the two cases. While at sufficiently strong disorder both systems are in a random singlet phase, we show that weak disorder is an irrelevant perturbation for the  $S=3/2$  chain, contrary to what expected from a naive application of the Harris criterion. The observed irrelevance is attributed to the presence of a new correlation length due to enhanced end-to-end correlations. This phenomenon is expected to occur for all half-integer  $S>1/2$  chains. A possible phase diagram of the chain for generic  $S$  is also discussed.

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### I. INTRODUCTION

A simple model where the effects of the interplay between quantum fluctuations and disorder can be studied in great detail is the spin- $S$  random antiferromagnetic Heisenberg (AFH) chain with Hamiltonian

$$H = \sum_i J_i \vec{S}_i \cdot \vec{S}_{i+1}, \quad (1)$$

where  $J_i > 0$  are quenched random variables.

In the absence of randomness ( $J_i = J$ ) quantum fluctuations lead to qualitatively different behavior for half-integer ( $S=1/2, 3/2, \dots$ ) and integer ( $S=1, 2, \dots$ ) values of the spin.<sup>1</sup> Half-integer spin chains have a gapless spectrum and quasi-long-range order. It is believed that they all belong to the same (bulk) universality class independently on  $S$ .<sup>2</sup> This was explicitly verified numerically for the  $S=3/2$  chain,<sup>3</sup> which was found to have the same bulk decay exponent as for the  $S=1/2$  chain. Integer spin chains are instead gapped and have a hidden topological order.<sup>4</sup>

The effect of quenched randomness on the AFH chains can be studied by the strong disorder renormalization-group (SDRG) method. This technique consists in successively decimating out the strongest bond in the chain.<sup>5</sup> For the  $S=1/2$  chain the SDRG procedure can be carried out in great detail and yields a probability distribution of coupling constants that under renormalization is broadened without limits and in the so-called infinite randomness fixed point the method becomes asymptotically exact. At this fixed point, describing the so-called random singlet (RS) phase,<sup>6</sup> the energy scale  $\Gamma$ , and the length scale  $\xi$  are related via  $\ln \Gamma \sim \xi^\psi$ , which differs from scaling at a conventional (random) fixed point, where  $\Gamma \sim \xi^{-z}$  with a finite dynamical exponent  $z$ . Numerical studies on random spin  $S=1/2$  antiferromagnetic chains generally agree with the SDRG results,<sup>7,8</sup> although some issues are still debated.<sup>9</sup>

For  $S>1/2$  the SDRG procedure requires a higher degree of approximations with respect to the  $S=1/2$  case. A spin  $S$  is represented by a maximally symmetrized combination of  $2S$

identical  $S=1/2$  spins. The SDRG decimation then produces effective spins of magnitudes  $S_{\text{eff}} \leq S$  obtained by linking the spin- $1/2$  objects into correlated singlets. For the  $S=1$  case an SDRG analysis shows that a sufficiently strong randomness induces a RS phase with  $S_{\text{eff}}=1$ , separated from the gapped phase by a gapless region of Griffiths singularities<sup>10</sup> (the gapless Haldane phase<sup>11</sup>) in which the dynamical exponent  $z$  increases with disorder. A recent SDRG study<sup>12</sup> of the disordered AFH chain with  $S=3/2$  indicated the existence of two phases: At strong disorder the relevant degrees of freedom are  $S_{\text{eff}}=3/2$  spins, while at weaker disorder they are of type  $S_{\text{eff}}=1/2$ . Both phases are of RS type with identical critical exponents. A quantum critical point separating them is expected to have specific multicritical exponents.<sup>12,13</sup>

As the SDRG method might fail at weak disorder, its predictions should be tested by means of accurate numerical analysis, which is the aim of the present paper. We will present numerical evidences, supported by theoretical arguments, that the phase diagram for the  $S=3/2$  spin chain differs from what predicted by SDRG.<sup>12</sup> Our numerical results support the existence of a RS phase only for sufficiently strong disorder, while weak disorder appears to be an irrelevant perturbation for the system.

### II. NUMERICAL RESULTS

Here we analyze the critical behavior of the AFH chains with varying degree of disorder by means of density-matrix renormalization-group (DMRG) techniques.<sup>14</sup> Numerical calculations are restricted to the  $S \leq 3/2$  case, and the disorder average is performed on  $10^3$ – $10^4$  samples taken from the distribution

$$p_\delta(J) = \delta^{-1} J^{-1+1/\delta} \quad \text{for } 0 \leq J \leq 1, \quad (2)$$

where  $\delta^2 = \text{var}[\ln J]$  measures the strength of disorder. As usual in DMRG (Ref. 14) we use open boundary conditions and keep typically  $m=80$ – $100$  states in the renormalization procedure. In order to obtain numerically stable results we use the DMRG finite system method performing several “sweeps” ( $\sim 4$ – $5$ ) through the chain,<sup>14</sup> which is an essential

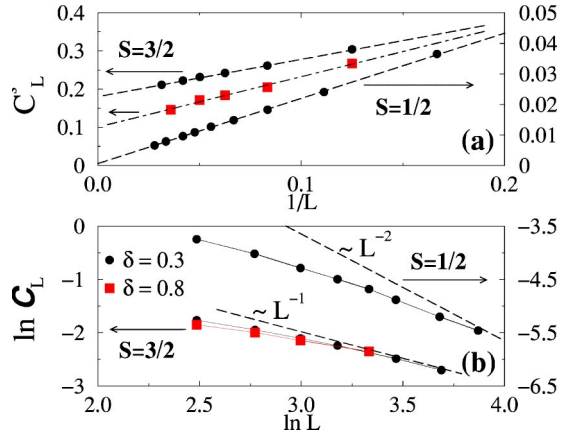


FIG. 1. Average correlations in the random  $S=1/2$  and  $3/2$  chains with disorder strengths  $\delta=0.3$  (circles) and  $\delta=0.8$  (squares). (a) End-to-end correlations; dashed lines are linear fits of the data. (b)  $C_L$  vs  $L$  in a log-log scale. Here the dashed line shows the decay in the pure system ( $1/L$ ) and in a RS phase  $1/L^2$ .

step in the DMRG procedure. The DMRG calculations for the  $S=3/2$  chain have been extended up to  $L=32$  for weak disorder, while at stronger disorder the procedure tends to become less stable and we had to restrict ourselves to shorter chains. However, the physical behavior in the strong disorder regime turns out to be quite well understood, while, in view of the limitations of the SDRG at weak disorder, it is precisely this regime which is physically the most interesting. In the weak disorder regime the DMRG is a rather stable and reliable technique.

### A. Correlation functions

In order to emphasize the differences between the two cases we present together the results for the  $S=3/2$  and  $S=1/2$  chains for the spin-spin correlation function defined as

$$C(i, j) = [\langle S_i^z S_j^z \rangle]_{\text{av}}, \quad (3)$$

where  $[\dots]_{\text{av}}$  denotes the averaging over quenched disorder. The correlation function obviously does not depend on the spin direction.

Figure 1(a) shows a plot of the surface-surface correlation function  $C_L^s \equiv C(1, L)$  plotted as a function of  $1/L$  for  $S=1/2$  ( $\delta=0.3$ ) and  $S=3/2$  ( $\delta=0.3, 0.8$ ). In a RS phase one expects that asymptotically in  $L$  the surface-surface correlation vanishes as  $C_L^s \sim L^{-\eta_{\text{RS}}^s}$  with  $\eta_{\text{RS}}^s = 1$ .<sup>8</sup> This is indeed observed in the case  $S=1/2$ . In the  $S=3/2$  case instead  $C_L^s$  extrapolates to a finite value which indicates the presence of a surface ordering phenomenon or, in other words, a first-order surface transition (formally  $\eta^s = 0$ ). The same type of behavior is observed for the  $S=3/2$  chain in the absence of randomness.<sup>15</sup>

To obtain the bulk exponent  $\eta$  we consider  $C(1, L/2)$  the correlation function between an edge and a spin in the middle of the chain, which decays asymptotically as  $C(1, L/2+1) \sim L^{-(\eta + \eta^s)/2}$ . Thus each point of reference

brings its local scaling dimension,  $\eta/2$  and  $\eta^s/2$ , respectively. In order to eliminate the surface exponent contribution we consider the ratio

$$\mathcal{C}_L \equiv \frac{C(1, L/2+1)C(L/2, L)}{C_L^s}, \quad (4)$$

which decays asymptotically as  $\mathcal{C}_L \sim L^{-\eta}$ . The plot of  $\ln \mathcal{C}_L$  versus  $\ln L$  is shown in Fig. 1(b). In the pure system the bulk exponent is  $\eta=1$ , while in a RS phase one expects  $\eta_{\text{RS}} = 2$ . The numerical data for  $S=3/2$  are quite consistent with a  $1/L$  decay, which seem to be in disagreement with the existence of a RS phase at weak disorder, but rather support the same critical behavior as for the pure system.

In the  $S=1/2$  case the data are not fully consistent with the expected RS exponent  $\eta_{\text{RS}}=2$ , shown as a dashed line, but are characterized by an increasing slope as  $L$  increases in the log-log scale, which is an indication that the asymptotic regime has not yet been reached. This slope in any case is clearly larger than 1. Notice that for the calculation of the bulk exponent we use a combination [see Eq. (4)] of correlation functions between an edge spin and a spin in the middle of the chain. As the distance between these spins is  $L/2$ , it is plausible that  $C_L$  is plagued by stronger finite-size corrections compared to the surface-surface correlation function  $C_L^s$ .

### B. Dynamical exponent

We consider next the dynamical singularities in the system, which are related to the integrated probability distribution  $\Omega(\varepsilon)$  of the smallest energy gap  $\varepsilon$ . This quantity, for small  $\varepsilon$ , behaves as

$$\Omega(\varepsilon) \sim \varepsilon^{1/z'}. \quad (5)$$

If  $z' < 1$  quantum fluctuations dominate and the true dynamical exponent is  $z=1$ , as in the pure system. If  $z' > 1$  the disorder and quantum effects compete and the singular properties of the system are governed by a conventional random fixed point with  $z=z'$ . In the RS phase  $z=z' \rightarrow \infty$ .

Figure 2 shows plots of  $\ln \Omega(\varepsilon)$  versus  $\ln \varepsilon$  for  $S=3/2$  (a) and  $S=1/2$  (b). The different scaling behavior for the two values of the spin can be seen by comparing the data for the same strength of disorder ( $\delta=0.3$ ). In the  $S=1/2$  chain the distribution becomes broader by increasing the chain length, while in the  $S=3/2$  chain  $\ln \Omega(\varepsilon)$  tends to have a finite non-vanishing slope for small  $\varepsilon$ , implying that  $1/z' > 0$ , a conclusion which is at odds with a RS phase.

For sufficiently strong disorder  $\delta=3$ , however, also the  $S=3/2$  spin chains show a broadening gap distribution [Fig. 2(a)]. The inset of Fig. 2 presents a graph of  $\ln \Omega(\varepsilon)$  plotted as a function of the rescaled variable  $\ln \varepsilon/L^\psi$ , with  $\psi=1/2$ , as expected in the RS phase.<sup>16</sup> Similar results were also found at  $\delta=2$ . At such strong values of disorder, due to difficulties in the convergence of the DMRG method, we restricted ourselves to exact diagonalization data of rather short chains  $L$

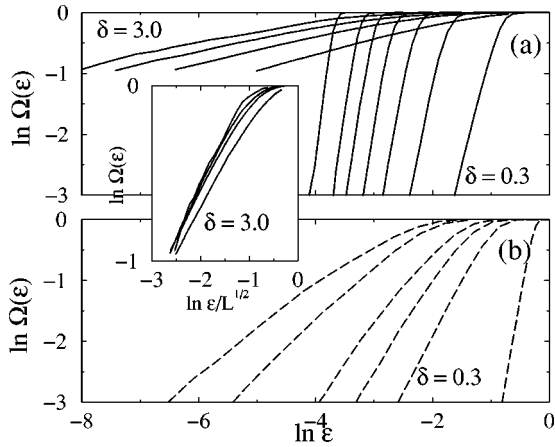


FIG. 2. Integrated probability distribution of the first gap in log-log scale. (a)  $S=3/2$ ,  $\delta=0.3$  ( $L=4, 8, 12, 16, 20, 24, 32$  from left to right) and  $\delta=3$  ( $L=4, 6, 8, 10$ ) shown as solid lines. (b)  $S=1/2$ ,  $\delta=0.3$  ( $L=4, \dots, 24, 32$ ) shown as dashed lines. Inset: Collapse of the data for  $S=3/2$  and  $\delta=3$  as expected in a RS phase ( $L=4, 6, 8, 10$ ).

$\leq 10$ . The asymptotic behavior is, however, reached already for rather small chains, as the good collapse of the data of the inset of Fig. 2 demonstrates.

We have also calculated the dynamical exponent from the distribution of the end-to-end correlation functions  $C_L^s$ , which is expected to scale as<sup>17</sup>

$$P_e(C_L^s) \sim (C_L^s)^{1/z'}. \quad (6)$$

Figure 3 shows a plot of the exponent  $1/z'(L)$  versus  $1/L$ , for  $\delta=0.3$  obtained from the analysis of the gap and of the correlation function [Eqs. (5) and (6)]. Both estimates lead to a finite value  $z' \approx 0.13$ . One may wonder whether this is a genuine effect or just due to a very slow convergence to a possible asymptotic behavior consistent with a RS phase  $1/z'(L) \rightarrow 0$ . On the view of our numerical results we believe that the latter scenario is rather unlikely, as it would require also a nonmonotonic scaling in  $L$  of  $1/z'(L)$  for the data obtained from the gap.

In a similar way we estimated the dynamical exponent for other strengths of disorder. For  $\delta=0.8$  we find  $z'=0.8(2)$ .

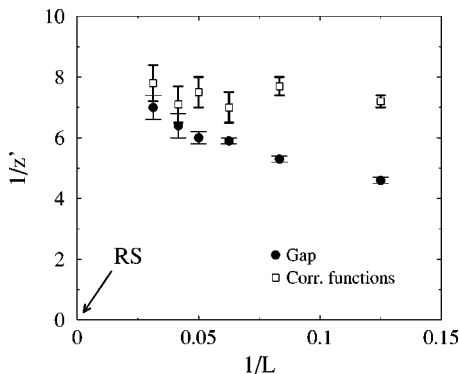


FIG. 3. Finite-size analysis of the inverse dynamical exponent  $1/z'$  as a function of the inverse chain length  $1/L$  for  $S=3/2$  at weak disorder  $\delta=0.3$ . In the RS phase one would expect  $1/z' \rightarrow 0$ .

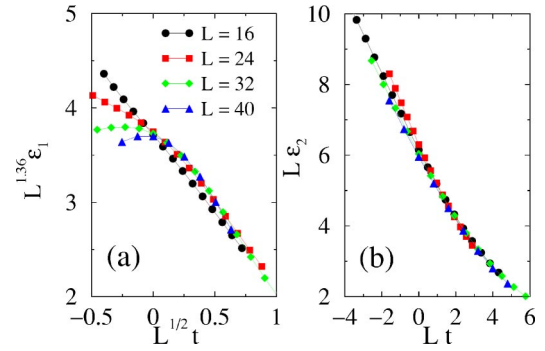


FIG. 4. Finite-size scaling of the first (a) and second (b) gap in the dimerized  $S=3/2$  chain. Data collapse for the first gap is expected to work only in the disordered region ( $t > 0$ ).

At  $\delta=2$  and even stronger disorder the scaling is consistent with a RS behavior. The borderline between the RS phase and the weak disorder phase seems to be located at around  $\delta=1$ .

### C. About the Harris criterion

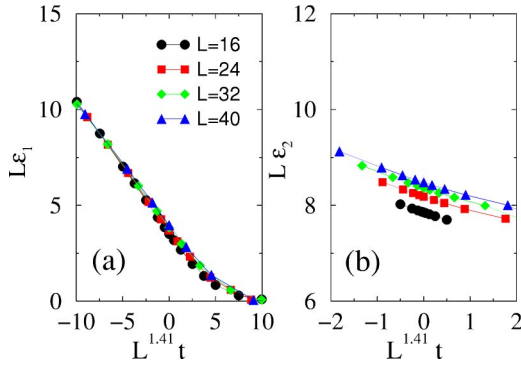
The numerical results for the correlation functions and for the gap distribution strongly suggest that at weak disorder the  $S=3/2$  chain has the same critical properties as in the pure case, i.e., the disorder is *irrelevant*.<sup>18</sup> For sufficiently strong disorder the DMRG results show also that the system is in a RS phase, therefore there is a transition induced by the strength of disorder. The analysis of both the gap and correlation functions indicates that the region of irrelevance extends up to  $\delta=1$ .

According to the Harris criterion<sup>19</sup> disorder is *relevant* if an appropriately defined correlation length<sup>20</sup> in the pure system diverges with an exponent  $\nu$  such that  $2/\nu > d$  (here  $d=1$ ). In the present case, as the disorder is coupled to the local energy operator,  $\tilde{S}_i \cdot \tilde{S}_{i+1}$ , the correlation length  $\xi$  entering in the Harris criterion is that associated to the strength of the dimerization  $t$  defined as the amplitude of the alternated modulation of the coupling constants:  $J_i = 1 + (-1)^i t$ . In the limit  $t \rightarrow 0$  this correlation length diverges as  $\xi \sim |t|^{-\nu}$ . In the  $S=1/2$  case,  $\nu=2/3 < 2$ ,<sup>21</sup> implying relevance of weak disorder.

In the  $S=3/2$  case there is no numerical result available for the critical exponent  $\nu$ , therefore we have analyzed the scaling behavior of the smallest gaps as a function of  $t$ . Scaling plots are given in Fig. 4 and as a comparison the same quantities for the  $S=1/2$  chain are shown in Fig. 5. The gaps are expected to scale as

$$\varepsilon_k(L, t) = L^{-z_k} \tilde{\varepsilon}_k(L^{1/\nu_k} t), \quad (7)$$

with  $\tilde{\varepsilon}_k$  a scaling function and where  $k=1, 2$  label the first and second gaps.<sup>22</sup> As shown above for the  $S=3/2$  at weak disorder and for the pure system the surface is ordered at  $t \leq 0$ , i.e., the correlation function between the edge spins is finite in the limit  $L \rightarrow \infty$  (for  $L$  even). There are several known examples of models with spontaneous surface order,<sup>23</sup> as the one observed in the  $S=3/2$  chain. In these cases one


 FIG. 5. As in Fig. 4 for  $S=1/2$ .

expects a localized low-energy excitation at  $t=0$  with a gap that vanishes faster than  $1/L$  because the ground state is degenerate in the thermodynamic limit, i.e.,  $\varepsilon_1 \sim L^{-z_s}$  with  $z_s > 1$ . Indeed this can be seen in Fig. 4 for the smallest gap in the  $S=3/2$  case,  $\varepsilon_1$ . In the absence of dimerization this quantity scales with an exponent  $z_s \approx 1.36 > 1$ , as shown by the scaling collapse at the point  $t=0$  in Fig. 4(a). The figure also shows that in the surface disordered region  $t > 0$  a reasonably good data collapse for  $\varepsilon_1$  is obtained with the choice  $L^{1/\nu_s}t$  with  $\nu_s=2$ . Notice that in the surface ordered region  $t < 0$  no scaling collapse can be observed. All the other gaps in the  $S=3/2$  are nonlocalized and scale with  $z=1$ , as illustrated in Fig. 4(b) for  $\varepsilon_2$ , and their scaling form involves the bulk correlation length,  $\xi \sim |t|^{-\nu}$ , with  $\nu \approx 1$ . This estimate for  $\nu$  is different from the value  $\nu=2/3$  in the  $S=1/2$  chain. We expect that the origin of this difference is due to the existence of a dangerous irrelevant scaling variable,<sup>24</sup> which is generally observed at first-order surface transitions<sup>23</sup> as in this case.

Our numerical results, summarized above, can be compared with theoretical predictions in Ref. 25. In the resonating valence bond picture the low-energy excitations of the open  $S=3/2$  chain are expected to be described by effective  $S=1/2$  edge-spin degrees of freedom, which are very weakly coupled to the rest of an  $S=1/2$  chain. In the thermodynamic limit the edge spins are expected to be decoupled, the effective coupling being logarithmically small, as  $1/\ln L$ . In this picture the smallest gap (at  $t=0$ ) scales as  $\varepsilon_1 \sim 1/L \ln L$ , whereas the other gaps scale in the same way as for the open  $S=1/2$  chain. Our numerical findings disagree with this prediction at two points. First, the localized gap has a faster size dependence, our numerical results cannot be described by a logarithmic correction. As a matter of fact for sizes we used in the calculation the effective exponent  $z_s$  is monotonously increasing with the size and there is no sign of reversing this tendency. Data of previous numerical calculations in Fig. 5 of Ref. 26 show also strong deviations from a pure logarithmic correction. Our second disagreement concerns the second gap at  $t=0$ , the value of which according to conformal invariance should be

$$\varepsilon_2(L,0)L = \pi v_s x_s \quad (8)$$

in the large  $L$  limit. Here  $v_s=3.87$  is the sound velocity<sup>3</sup> for the  $S=3/2$  chain and  $x_s$  is the surface anomalous dimension,

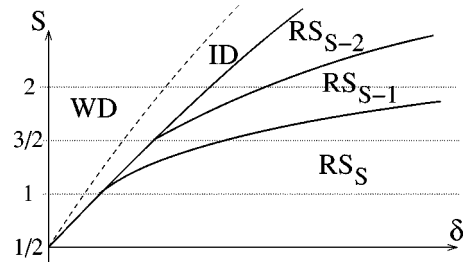


FIG. 6. Schematic phase diagram of the spin  $S$  AFH chain as a function of the strength of disorder  $\delta$ . The  $RS_S$  denotes a random singlet phase where the relevant degrees of freedom are effective  $S$  spins. The WD and ID are the region at weak and intermediate disorders.

which for the  $S=1/2$  chain is<sup>27</sup>  $x_s = \eta^s/2 = 1$ . For the  $S=3/2$  chain the results in Fig. 4 are considerably smaller, our estimate is around  $x_s=1/2$ . Thus there are very probably new operators for the open  $S=3/2$  chain, which are not present in the  $S=1/2$  chain.

As a comparison we plot in Fig. 5 a similar scaling collapse analysis for the first two gaps in the  $S=1/2$  case, using a similar range of system sizes as in Fig. 4. Notice that the best collapse is obtained with a scaling variable  $L^{1.41}t$ , implying  $\nu \approx 0.71$ , not far from the expected value  $\nu=2/3$ , a difference which can be imputed to logarithmic corrections.

The analysis at finite  $t$  reveals that the dimerization couples differently to the  $S=3/2$  chain with respect to the  $S=1/2$  chain. We argue that the appropriate correlation length to be used in the Harris criterion<sup>19,20</sup> for the  $S=3/2$  chain is  $\xi_s$  that associated to the smallest gap and thus with  $\nu_s=2$  the disorder is marginally irrelevant. An accumulation of weak bonds along the chain may result indeed in an effective cut of the system. The resulting scenario is that of weakly interacting segments of finite length in which the relevant length scale is  $\xi_s$ , which is associated to a chain with open boundary conditions. (We note that a similar scenario is used for the renormalization of random  $S=1$  chains, in which the effective coupling between spin-1/2 degrees of freedom is exponentially small.<sup>11</sup>) This scenario therefore provides a plausible explanation for the observed irrelevance of weak disorder for the random  $S=3/2$  chains.

### III. CONCLUSION

We conclude by suggesting a general phase diagram for the spin- $S$  AFH chains as a function of the strength of disorder  $\delta$ . This phase diagram, shown in Fig. 6, is obtained by combining DMRG and SDRG results known for the  $S=1/2$ ,  $S=1$ , and  $S=3/2$  cases with some general arguments for higher  $S$ . First of all, differently from the  $S=1/2$  case, where any amount of disorder is known to lead to a RS phase, we expect that all chains for  $S > 1/2$  have a region of irrelevance, the weak disorder (WD) region, where the system is either critical (half-integer  $S$ ) or gapped (integer  $S$ ). This was already known for  $S$  integer. Our results for the  $S=3/2$  chain suggest that it may be true also for noninteger spin.

At strong enough disorder all  $S$  are in a RS phase com-

posed of effective  $S$  spins, which we indicate as  $RS_S$ . For the  $S=1$  case there is only one such phase ( $RS_1$ ), while a recent SDRG study for  $S=3/2$  (Ref. 12) predicts two distinct phases:  $RS_{3/2}$  and  $RS_{1/2}$ . We found no signatures of this spin reduction transition in our DMRG calculations, which could be anyhow difficult to detect as the  $RS_{1/2}$  and  $RS_{3/2}$  have identical critical exponents. There is also the possibility to have, for higher spins ( $S>3/2$ ), a sequence of multiple RS phases of different nature. Possible phase diagram for higher  $S$  has been recently discussed.<sup>13</sup> We have indicated these transition lines in the phase diagram of Fig. 6, which, for the time being cannot be supported by numerical results. Finally, the WD region may be separated from the RS phase(s) by an intermediate disorder (ID) region where exponents vary continuously with  $\delta$ , as observed in other models.<sup>28</sup> For the gapped (integer  $S$ ) case this would correspond to a region of Griffiths singularities. The qualitative nature of the disorder-induced crossover phenomena for the  $S=1$  chain is still debated (see in Refs. 29 and 30). We will discuss this issue in a future publication.<sup>31</sup>

After this paper was submitted we became aware of a

recent work of Segua *et al.*,<sup>32</sup> who performed a SDRG analysis of the disordered  $S=3/2$  AFH chain. Their calculation differs from that of Ref. 12 as the decimation scheme keeps into account more states, thus it is expected to be more accurate. While the results of Ref. 12 indicated the existence of two RS phases with different effective spins ( $S_{\text{eff}}=1/2$  and  $S_{\text{eff}}=3/2$ ), in the work of Segua *et al.*<sup>32</sup> the renormalization flow indicates that the weak disorder is an irrelevant perturbation of the system. This is in agreement with the conclusion of this paper.

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