Disorder-induced phases in the S=1 antiferromagnetic Heisenberg chain

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We use extensive density matrix renormalization group (DMRG) calculations to explore the phase diagram of the random S=1 antiferromagnetic Heisenberg chain with a power-law distribution of the exchange couplings. We use open chains and monitor the lowest gaps, the end-to-end correlation function and the string order parameter. For this distribution at weak disorder, the system is in the gapless Haldane phase with a disorder dependent dynamical exponent, z, and z=1 signals the border between the nonsingular and singular regions of the local susceptibility. For strong enough disorder, which approximately corresponds to a uniform distribution, a transition into the random singlet phase is detected, at which the string order parameter as well as the average end-to-end correlation function are vanishing and at the same time the dynamical exponent is divergent. Singularities of physical quantities are found to be somewhat different in the random singlet phase and in the critical point.

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I. INTRODUCTION

The S=1 spin antiferromagnetic Heisenberg chain has received much attention, both experimentally and theoretically, since Haldane¹ conjectured that its low-energy properties are qualitatively different from that of the exactly solved S=1/2 model. The S=1 chain (together with all other integer spin chains) has a finite gap in the excitation spectrum and hidden topological order in the ground state, which is characterized by the string correlation function.² On the other hand, the bulk spin-spin correlation length, ξ . In an open chain of length L, there are spin S=1/2 degrees of freedom at each edge and the end-to-end correlations approach a finite value in an exponential fashion, having the same characteristic length scale, ξ , as bulk correlations.³

Quenched disorder, which is realized by random couplings, also has different effects for S=1/2 and S=1. In the former case any amount of disorder is enough to drive the system into a new type of fixed point,⁴ whereas for the *S* =1 chain, weak disorder is irrelevant and the properties of the weakly random chain are the same as that of the pure one.⁵ For stronger disorder, however, the low-energy properties of the system are changed and detailed analytical and numerical investigations were devoted to clarify the properties of the new random fixed points.

The analytical studies of the random chain are made by variants of the strong disorder renormalization group (RG) method, which has been introduced for the S=1/2 chain by Ma, Dasgupta, and Hu⁶ and has been analyzed in great detail by Fisher.⁴ This strong disorder RG method has been used afterwards for a large variety of random quantum and classical systems (for a review, see Ref. 7). For the S=1 chain, extensions of the original Ma-Dasgupta rules are necessary^{8,9} to describe the disorder induced phases in the system, which include a gapless Haldane (GH) phase, for intermediate dis-

order, and a random singlet (RS) phase, for stronger disorder.

Numerical studies of the random S=1 chain have been made by exact diagonalization¹⁰ of the density matrix renormalization¹¹ (DMRG), by quantum Monte Carlo (QMC) methods,^{12,13} and by numerical implementations of the strong disorder RG method.¹⁴ Despite considerable numerical effort, several aspects of the low-energy properties of the random S=1 chain are still unclear and some numerical results are conflicting. In the numerical calculations mainly boxlike distribution of disorder is considered, which, as noted in Ref. 15, represent only a limited strength of randomness. In numerical RG studies both the GH and the RS phases are identified; however, the transition point between these phases is rather approximate. In DMRG calculation (see also Ref. 10), Hida¹¹ has identified only the GH phase, and conjectured that the RS phase is not accessible for any finite strength of disorder. In a comment to Hida's work,¹¹ Yang and Hyman¹⁵ have predicted the appearance of the RS phase for some type of power-law distribution of the disorder. Another numerical work by QMC simulations¹² has shown the existence of the RS phase even for the boxlike distribution and these results are confirmed by independent QMC simulations.¹³ In the QMC calculations, some properties of the RS phase are verified (cf. scaling relation between length and time, decay of the string correlation function), but results about the spin-spin correlation function are different from the RG predictions. At the critical point no numerical estimates are available to check analytical RG predictions. We note on recent studies of Griffiths effects¹⁶ in the system with enforced dimerization^{17,18} and related work on the random S=3/2 and higher spin chains.^{19–21}

In this paper, our aim is to study the low-energy properties of the random S=1 chain by the DMRG method.²² The features of our study are the following: (i) We consider a more general (power-law) distribution of disorder, which allows us to enter more deeply into the RS phase, thus to obtain convincing evidence of its existence. (ii) We calculate a different physical quantity, the end-to-end correlation function, which carries important information about the phases of the system. The average end-to-end correlation function has a finite limiting value in the GH phase and vanishes in the RS phase. Furthermore, in the GH phase from the low-value tail of its distribution, independent estimates about the dynamical exponent are obtained. (iii) We try to perform a comparative analysis between the properties of the system at the critical point and in the RS phase and to check the available RG predictions.

The structure of our paper is the following. The model, the basic ingredients of the strong disorder RG methods, and the conjectured phases are given in Sec. II. Results of our DMRG studies are presented in Sec. III and discussed in Sec. IV.

II. THE MODEL AND THE STRONG DISORDER RG RESULTS

A. Model

We consider the spin S=1 random antiferromagnetic Heisenberg chain with the Hamiltonian

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

where the $J_i > 0$ are independent and identically distributed random variables. Here, we use the following power-law distribution

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

where $\delta^2 = var[\ln J]$ measures the strength of disorder. In previous numerical work, a boxlike distribution was used,

$$P_{W}(J) = \begin{cases} 1/W & \text{for } 1 - W/2 < J < 1 + W/2 \\ 0 & \text{otherwise,} \end{cases}$$
(3)

in which the strength of disorder grows with *W*. Note that the possible maximal value, W=2, corresponds to the uniform distribution, which can be obtained from Eq. (2) with $\delta=1$ and having a prefactor, 1/2, and a range $0 \le J \le 2$. Consequently, the power-law distribution for $\delta > 1$ represents a disorder, which is stronger than any boxlike disorder.

The low-energy behavior of the system of size, L, is encoded in the distribution of the lowest gap, Δ , denoted by $P_L(\Delta)$. We note that for an open chain the first gap corresponds to the localized edge states; therefore, one should study the second (not localized) gap. The average spin-spin correlation function is denoted by

$$C(i,j) = \left[\langle S_i^z S_j^z \rangle \right]_{\text{av}},\tag{4}$$

where $[\cdots]_{av}$ stands for averaging over quenched disorder. For bulk correlations with $|j-i| \leq i, j = O(L)$, we have $C(i,j) = C_b(|j-i|)$, whereas for end-to-end correlations, $C(1,L) \equiv C_1(L)$. The string correlation function of the model is defined by²

$$O^{z}(r) = -\langle S_{l}^{z} \exp[i\pi(S_{l+1}^{z} + S_{l+2}^{z} + \dots + S_{l+r-1}^{z})]S_{l+r}^{z}\rangle, \quad (5)$$

and its large r limiting value is the string order parameter. For several quantities it turned out useful to consider the average of its inverse. More precisely, for a physical observable, f, we denote by f^{iv} the following quantity:

$$f^{\rm iv} = \frac{1}{[f^{-1}]_{\rm av}},\tag{6}$$

what we shall call as inverse average.

B. Weak disorder limit—Haldane phase

In absence of randomness $(J_i=J)$ the spectrum is gapped,¹ and bulk spin-spin correlations are short ranged, $C_b(r) \sim \exp(-r/\xi)$ with $\xi=6.03^3$. On the contrary, end-to-end spinspin correlations and the string correlation function have a finite limiting value. For weak disorder, when the distribution of J is sufficiently narrow, the Haldane gap is robust and the system stays in the Haldane phase.⁵ The border of the Haldane phase can be estimated by noting that the Haldane gap is robust against enforced dimerization,²³ when even and odd couplings are different, so that

$$J_i = J(1 + D(-1)^i) \exp(\delta \zeta_i), \tag{7}$$

where ζ_i are random numbers of mean zero and variance unity. The pure system (δ =0) for D < 0.25 stays in the Haldane phase²⁴ and at the phase transition point the coupling at an odd bond, J_o , and that at an even bond, J_e , are related as $J_o=0.6J_e$. We expect that in the presence of disorder the Haldane gap stays finite, if the maximum (J_{max}) and the minimum (J_{min}) values of the couplings satisfy $J_{min}/J_{max} > 0.6$. From this argument we obtain for the border of the Haldane phase for the box distribution $W_G \approx 0.5$. On the other hand, for the power-law distribution in Eq. (2) $J_{min}=0$; therefore, for any δ >0 the Haldane phase is expected to be destroyed.

C. Strong disorder limit—RG approach

For strong disorder the low-energy properties of the system are explored by variants of the strong disorder RG approach. In the standard Ma-Dasgupta-type RG approach, the couplings of the random antiferromagnetic Heisenberg chain are put in descending order and the largest coupling defines the energy scale, Ω , in the system. During renormalization the pair of spins with the largest coupling, say $J_i=\Omega$, are replaced by a singlet and decimated out. At the same time a new coupling is generated between the spins at the two sides of the singlet, which is given in a perturbation calculation as

$$\tilde{J} = \frac{4}{3} \frac{J_{i-1}J_{i+1}}{J_i}.$$
(8)

As noticed by Boechat, Saguia, and Continentino²⁵ for weak disorder some of the generated new couplings can be larger than the energy scale, Ω . Therefore, the standard strong disorder RG approach works only for strong enough disorder and describes only the RS phase of the system.

To cure this problem, different types of RG approaches are proposed. Monthus *et al.*⁹ suggested to replace the pair of spin S=1 connected by the strongest bond by a pair of S=1/2. In this case the renormalized system consists of a set of spin S=1 and S=1/2 degrees of freedom, having both antiferromagnetic and ferromagnetic couplings. The renormalized couplings, which are calculated perturbatively, are all smaller than Ω . This RG approach, during which no spin larger than S=1 is generated, can be used to describe both the gapless Haldane and the RS phases and provides precise numerical estimates about the critical exponents.

In another modified RG approach, Saguia *et al.*¹⁴ use the standard perturbative approach in Eq. (8), provided $\max(J_{i-1}, J_{i+1}) < 3\Omega/4$. Otherwise the triplet of spins with couplings, $\max(J_{i-1}, J_{i+1})$, and Ω is replaced by a single spin. Also in this method the variation of the energy scale is monotonic: the generated two new couplings are both smaller than Ω .

Recently, a variant of the strong disorder RG method was proposed by one of us,²⁶ in which the pair of spins with the strongest coupling is decimated out, but—and this is a feature of our current method—the new coupling between the remaining spins is calculated nonperturbatively. The four spins with couplings J_{i-1} , J_i , and J_{i+1} are replaced by two spins and during decimation the lowest gap in the two systems remains the same. It is easy to see that the rule we use is somewhat similar to the approach by Saguia *et al.*¹⁴ However, this method has no discontinuity in the approximation, which could be important in the vicinity of the critical point, where a crossover takes place between the different decimation regimes.

D. Disorder induced phases

Based on a modified strong disorder RG approach^{8,9,14} and different numerical calculations,^{11–13} the following scenario of the phase transition in the model is conjectured with increasing strength of disorder.

1. Gapless Haldane phase

For sufficiently strong disorder ($\delta > \delta_G$ or $W > W_G$), the gap in the Haldane phase is closed and one arrives to the gapless Haldane phase. As we have argued in Sec. II B, $\delta_G = 0$ and $W_G \approx 0.5$. The GH phase is a quantum Griffiths phase,¹⁶ in which the correlation length, $\xi(\delta)$, is finite, whereas the typical time scale, $t_r \sim \Delta^{-1}$, is divergent. Relation between the size of the system, *L*, and the smallest gap is given by

$$\Delta \sim L^{-z},\tag{9}$$

where z is the disorder induced dynamical exponent. The distribution of the lowest gap is given by

$$P_L(\Delta)d\Delta = L^{-z}\widetilde{P}\left[\frac{\Delta}{L^z}\right]d\Delta,$$
 (10)

and $\tilde{P}(x) \sim x^{-1+1/z}$ for small *x*, so that from the low-energy tail *z* can be calculated. Similarly the distribution of the end-to-end correlation function has a vanishing tail, which be-

haves as²⁷ $P(C_1) \sim C_1^{-1+1/z}$, which gives an independent way to calculate the dynamical exponent. Some thermodynamical quantities such as the local susceptibility, χ , and the specific heat, c_v , are singular at low temperature,⁷

$$\chi(T) \sim T^{-1+1/z}, \quad c_v(T) \sim T^{1/z}.$$
 (11)

The limit of divergence of $\chi(T)$ is signaled by z=1, and the corresponding disorder is denoted by $\delta_1(W_1)$. The separation of the two parts of the GH phase with z < 1 and z > 1 can be located by considering the inverse average of the gap, Δ^{iv} , and the inverse average of the end-to-end correlation function, C_1^{iv} . In the nonsingular region, z < 1, both Δ^{iv} and C_1^{iv} are finite, whereas in the singular region, z > 1, both are vanishing.

To see this, we consider the inverse average of the gap

$$\Delta^{\mathrm{iv}} \sim \left[\int_{\Delta_{\mathrm{min}}}^{\Delta_{\mathrm{max}}} \Delta^{-2+1/z} \mathrm{d}\Delta \right]^{-1} \sim \frac{z-1}{\Delta_{\mathrm{min}}^{-1+1/z} - \Delta_{\mathrm{max}}^{-1+1/z}}, \quad (12)$$

which indeed tends to zero, if z > 1 and $\Delta_{\min} \rightarrow 0$. On the other hand, for the vanishing of the average gap, one needs $\Delta_{\max} \rightarrow 0$. One can use a similar reasoning for the end-to-end correlation function, for which the upper limit of the distribution, $C_1^{\max} > 0$, thus $[C_1]_{iv} > 0$, in the whole region, $\delta < \delta_1$.

In a static sense, the gapless Haldane phase is noncritical: the average end-to-end correlation function, as well as the string order parameter, is finite in the complete GH phase.

2. Critical point

Increasing the strength of disorder over a critical value $(\delta_C \text{ or } W_C)$, the system arrives at the random singlet phase. As the critical strength of disorder is approached, the correlation length diverges: $\xi \sim (\delta_C - \delta)^{-\nu}$, with $\nu = (1 + \sqrt{13})/2$, and the string order parameter vanishes as^{8,9} $O^z(\delta) \sim (\delta_C - \delta)^{2\beta}$, with $\beta = 2[(3 - \sqrt{5})/(\sqrt{13} - 1)]$. At the critical point the string order-parameter decays algebraically, $O^z(r) \sim r^{-\eta^{\text{st}}}$, with $\eta^{\text{st}} = 2\beta/\nu$. The end-to-end correlation function goes to zero algebraically, too, $C_1(L) \sim L^{-\eta_1}$, similarly to the bulk spin-spin correlation function, $C_b(r) \sim r^{-\eta}$. Here, however, there are no theoretical conjectures about the exponents η_1 and η . The relation at the critical point between the correlation length and the relaxation time is strongly anisotropic,

$$\ln t_r \sim \xi^{\psi},\tag{13}$$

with $\psi = 1/3$; thus, the dynamical exponent, *z*, is formally infinity. This type of infinite disorder scaling is seen in the distribution of the gaps, which is given by

$$P_L(\Delta)d\Delta = L^{-\psi}\widetilde{P}\left[\frac{\ln\Delta}{L^{\psi}}\right]d\ln\Delta.$$
(14)

In the space of variables, dimerization (*D*) and disorder (δ), the critical point of the system, represent a multicritical point in which three Griffiths phases with different symmetry meet.¹⁷ The corresponding exponents follow by permutation symmetry and the calculation can be generalized for higher values of *S*.¹⁷

	$\eta^{ m st}$	β	ν	ψ	η	η_1
RS CP	0.382 [0.41(4)] 0.509 [0.39(3)]	0.586	2 2.30	1/2 [0.45(5)] 1/3 [0.35(5)]	2	1 [0.86(6)] [0.69(5)]

TABLE I. Theoretical predictions for the critical exponents in the random singlet (RS) phase and at the critical point (CP). Values obtained in this paper are given in square brackets.

3. Random singlet phase

For a disorder $\delta > \delta_C (W > W_C)$, the low-energy behavior of the system is controlled by an infinite disorder fixed point and the system is in the RS phase. The RS phase is a critical phase, both ξ and t_r are divergent, and its properties are assumed to be identical to the RS phase of the random S =1/2 chain. This latter system is studied in great detail by Fisher⁴ with the asymptotically exact strong disorder RG method and these results have been confronted with detailed numerical investigations.²⁸⁻³⁰ Here we repeat that in the RS phase there is infinite disorder scaling, so that relations in Eqs. (13) and (14) are valid with an exponent, $\psi = 1/2$. The RS phase is unstable against enforced dimerization, as given in Eq. (7), and the correlation length behaves as $\xi(D) \sim D^{-\nu}$, with $\nu=2$. In the RS phase the bulk and end-to-end correlation functions decay algebraically. In Table I we collected the conjectured values of the critical exponents both in the random singlet phase and at the critical point and compared these values with the estimates obtained in this paper.

E. Summary of the existing numerical results

In previous numerical studies the box distribution in Eq. (3) has been used. In Table II we present the estimates of the borders of the different phases obtained by different numerical methods, such as by numerical implementation of the strong disorder RG, by DMRG, and by QMC. We note that for the power-law disorder in Eq. (2) the critical disorder is estimated¹⁵ as $\delta_C \approx 1.5$. Using variants of the strong disorder RG method,^{9,14} the calculated critical exponents in the RS phase—within numerical precision—correspond to the predicted, analytical values. To reach the asymptotic region, however, one often needs to treat very long chains of length $L=10^4-10^6$, see Ref. 9. The DMRG and QMC investigations

TABLE II. Numerical estimates for the borders of the different phases of the random S=1 chain with boxlike disorder, see Eq. (3). The different phases are defined by $W < W_G$, Haldane phase; $W_G < W < W_1$, GH phase with nondivergent local susceptibility; $W_1 < W < W_C$, GH phase with divergent local susceptibility; and $W > W_C$, RS phase.

	W_G	W_1	W _C
RG(9)			1.48
RG(14)		0.76	2.
DMRG(11)		1.8	no
QMC(12)	1.37	1.7	1.8
QMC(13)			<2

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have led to different conclusions for the strongest box disorder, with W=2. No RS phase is found by DMRG,¹¹ whereas by QMC infinite disorder scaling is detected.^{12,13} The average string correlation function was shown to decay algebraically with¹³ $\eta_{st}=0.378(6)$, close to the theoretical result in Table I. On the other hand, the average spin-spin correlation function was found to have an exponent,¹³ $\eta=1$, which greatly differs from the theoretical value of $\eta=2$.

III. NUMERICAL INVESTIGATIONS

A. The DMRG method

Most of our numerical results are based on DMRG calculations. In this case we used open chains up to length L=64, for weak disorder and up to L=32 for strong disorder and calculated the lowest two gaps, the end-to-end correlation function and the string order parameter. This latter quantity is calculated for open chains between points i=L/4 and j=3L/4. Note that for an open chain the first gap is related to the surface degrees of freedom and goes to zero exponentially with L. The characteristic bulk excitations are given by the second gap and we studied this quantity. In the numerical calculation we have retained up to m=180 states in the DMRG and checked that convergence of the numerical results is reached. We used the power-law distribution of disorder in Eq. (2) in the canonical ensemble, i.e., there was no constraint to the value of the sum of the odd and even couplings. In this way there is a nonzero residual dimerization, which could be the source of some error for small systems. However, using the microcanonical ensemble, in which the sum of the odd couplings is the same as that of the even couplings, could lead to different finite-size exponents for the end-to-end correlation function, which is known for the random transverse-field Ising chain.³¹⁻³³ We have calculated typically 10 000 independent disorder realizations in each case.

B. Gapless Haldane phase

1. Nonsingular region: z < 1

We have calculated the distribution of the (second) gap and determined its inverse average, Δ^{iv} , which is presented in Fig. 1 as a function of the inverse size, L^{-1} , for different values of δ . The limiting value as $L \rightarrow \infty$ is monotonously decreasing with δ and Δ^{iv} seems to approach zero at a limiting disorder $\delta_1 \approx 0.45 - 0.5$. A similar conclusion is obtained from the behavior of the inverse average of the endto-end correlation function, $C_1^{iv}(L)$, which is shown in the inset of Fig. 1.



FIG. 1. The inverse average gap, Δ^{iv} , as a function of the inverse size of the system for different strengths of disorder, δ =0.1, 0.2, 0.3, 0.4, and 0.5 from the top to the bottom, respectively. Δ^{iv} seems to vanish around $\delta \approx 0.5$. Inset: the inverse average end-toend correlation function as a function of inverse size, with the same values of disorder, as in the main panel. Note that for weak disorder the size dependence of C_1^{iv} is nonmonotonic, which is due to a finite correlation length in the system.

Note, however, that the average end-to-end correlation function, as shown in Fig. 3 is finite at δ_1 . The extrapolated values of Δ^{iv} and $C_1^{iv}(L)$ are shown in Fig. 2. Close to δ_1 , both curves are compatible with an approximately linear variation with $\delta_1 - \delta$. At the boundary point, $\delta_1 = \delta$, the size dependences of Δ^{iv} and $C_1^{iv}(L)$ are shown in the inset of Fig. 2. Both are linear in L^{-1} , in accordance with the criterion that at δ_1 the disorder induced dynamical exponent is $z(\delta_1)=1$.



FIG. 2. Extrapolated values of the inverse average gap and the inverse average end-to-end correlation function as a function of the strength of disorder. At δ =0 we obtain estimates for the nonrandom model, Δ =0.4105(3) and C_1 =0.283(1). Inset: Size dependence of the inverse average gap and the inverse average end-to-end correlation function in a log-log plot at the boundary of the gapless Haldane phase. Both lines have an approximate slope, z=1, denoted by broken lines. The typical value of the error is indicated; otherwise, the error is smaller than the size of the symbol.



FIG. 3. The average string order parameter, O^z , the average end-to-end correlation function, $C_1(L)$, and the disorder induced dynamical exponent, 1/z, as a function of the strength of disorder. Inset: finite-size dependence of the string order parameter and the average end-to-end correlation function at the critical point (δ_c =1, open symbols) and in the RS phase (δ_c =1.5, full symbols) in a log-log plot. The slope of the broken lines representing the critical exponents are \bigcirc , $0.39\pm0.03[0.509]$; \spadesuit , $0.41\pm0.04[0.382]$; \diamondsuit , 0.69 ± 0.05 ; and \blacklozenge , $0.86\pm0.06[1.0]$, where in the brackets we presented the theoretical RG results; see Table I. Typical values of the error are indicated; otherwise, the error is smaller than the size of the symbol.

2. Singular region: z > 1

We have calculated the average string order parameter and the average end-to-end correlation function for different sizes L. Also we have determined the disorder induced dynamical exponent, z, which is deduced from the low-energy tail of the gap distribution [see Eq. (10)]. The extrapolated values of O^z and C_1 , as well as 1/z are plotted in Fig. 3 for different strengths of disorder. All these three quantities tend to zero around the same limiting value of disorder and the border of the Griffiths phase, i.e., the location of the critical point can be determined as $\delta_c = 1.0(1)$. In the extrapolation procedure we have made use of the finite-size dependence of $O^{z}(L) \sim L^{-\eta_{st}}$ and $C_{1}(L) \sim L^{-\eta_{1}}$ at the critical point, which is shown in the inset of Fig. 3. For weaker disorder, δ $< \delta_c, O^z$ tends to a finite limiting value, which is illustrated in Fig. 4 using a scale $L^{-\eta_{st}}$. A similar conclusion is obtained for the average end-to-end correlation function, which is presented in the inset of Fig. 4.

C. Critical point and the RS phase

Our aim with the numerical investigations in this subsection is twofold: first, to check the properties of the RS phase, thus to present numerical evidences, and second, and this is numerically more demanding, to try to discriminate between the properties in RS phase and at the critical point. We start to analyze the finite-size dependence of the average string order parameter and that of the average end-to-end correlation function, which is shown in the inset of Fig. 3 at two values of the disorder, $\delta=1$ and $\delta=1.5$. The first value should



FIG. 4. The average string order-parameter as a function of $L^{-\eta_{st}}$, with η_{st} =0.39 as obtained in the inset of Fig. 3, for disorder, δ =0.3, 0.5, 0.8, 1.0, and 1.5 from the top to the bottom. Inset: the average end-to-end correlation function as a function of $L^{-\eta_1}$, η_1 =0.69 being the critical decay exponent, for the same values of disorder as in the main panel. Solid straight lines over the δ =1.0 points are guides to the eyes.

be close to the critical point (see Fig. 3); however, there is certainly some uncertainty, see the values of W_G in Table II. The second value of disorder, δ =1.5, should be deeply in the RS phase; however, see the RG estimates in Ref. 15.

At $\delta = 1.5$ the decay of the average string order-parameter, as well as that of the end-to-end correlation function is algebraic, and the decay exponents of both quantities are in agreement with the theoretical prediction in the RS phase, as given in Table I. For the average end-to-end correlation function we have somewhat less accuracy, which could be due to similar crossover effects as noted for the bulk spin-spin correlation function in Ref. 13. The same type of analysis of the results at $\delta = 1$ give somewhat different results. The decay of the average end-to-end correlation function is characterized by an exponent, $\eta_1 = 0.69$, which differs considerably from the value in the RS phase. On the other hand, the decay exponent of the average string order parameter, within the error of the calculation, agrees with the value found in the RS phase. We note that at the same disorder in the OMC simulation¹³ also the exponent in the RS phase is observed. One possible explanation is that $\delta = 1$ is already in the RS phase and therefore we find the corresponding exponent. Anyway, even at the critical point one expects strong crossover effects due to the vicinity of the RS fixed point, so that probably much larger systems are needed to observe the true asymptotic behavior.

Finally, we compare in Fig. 5 the distribution of the gaps at the critical point (a) and in the RS phase (b). For both cases the distribution is broadened with increasing L, which is a clear signal of infinite disorder scaling. Indeed, one can obtain a good scaling collapse using the form in Eq. (14). In the insets we have illustrated this type of behavior by using the theoretical predictions, $\psi=1/3$ at the critical point and $\psi=1/2$ in the RS phase, respectively. The estimated exponents obtained from the optimal scaling collapse are shown in Table I.



FIG. 5. (Color online) Distribution of the gaps in finite systems at the critical point, $\delta = 1$ (a) and in the RS phase, $\delta = 1.4$ (b). In the insets scaling collapse with Eq. (14) is shown with $\psi = 1/3$ (a) and $\psi = 1/2$ (b).

IV. CONCLUSION

The random antiferromagnetic S=1 chain is a paradigm of disorder induced phase transition phenomena (see also Ref. 34) for which detailed strong disorder RG predictions are available. These predictions, however, have only been partially verified by numerical calculations and even the numerical results are somewhat conflicting. In this paper we have used extensive DMRG calculations with the aim to clarify the low-energy properties of the system with varying strengths of disorder. The sizes of the systems we used in the calculation are comparable with those in previous DMRG studies;¹¹ however, we used a power-law distribution of the couplings in Eq. (2), which can be more random, than the box distribution in Eq. (3) used previously. We have also calculated a quantity, the end-to-end spin-spin correlation function, which can be used to locate the borders of the different phases in the system and to obtain an independent estimate of the dynamical exponent. Our calculations gave further numerical support of the phase diagram predicted by the strong disorder RG method and our results are basically in agreement with the scenario of disorder induced phase transitions. In the RS phase we made calculations far from the critical point, which is not possible with boxlike distribution of couplings as given in Eq. (3) and obtained estimates for the critical exponents which are compatible with the RG predictions. Our results at the critical point are less conclusive, which is probably due to crossover effects and the inaccurate location of this point. For the critical exponent of the end-to-end correlation function, η_1 , and that of the gap scaling, ψ , numerical estimates at the critical point are clearly different from that in the RS phase, which are in accordance with the RG results. On the other hand, for the average string correlation function our numerical results are in conflict with the RG prediction. We believe that at this point much larger finite systems are necessary to obtain a precise numerical estimate and thus to be able to test the results of RG predictions.

We close our paper by mentioning that the present day numerical possibilities to explore the properties of the random S=1 chain seem to be exhausted, as far as DMRG or QMC methods are considered. Some independent and probably more accurate results can be expected, however, by the numerical application of different variants of the strong disorder RG method, in particular in the vicinity of the critical point and in the RS phase. Results obtained in this direction will be published in the future.²⁶

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