Disorder Induced Quantum Phase Transition in Random-Exchange Spin-1/2 Chains

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We investigate the effect of quenched bond disorder on the anisotropic antiferromagnetic spin-1/2 (XXZ) chain as a model for disorder-induced quantum phase transitions. We find nonuniversal behavior of the average correlation functions for weak disorder, followed by a quantum phase transition into a strongly disordered phase with only short-range xy correlations. We find no evidence for the universal strong-disorder fixed point predicted by the real-space renormalization group, suggesting a qualitatively different view of the relationship between quantum fluctuations and disorder.

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The existence and nature of quantum phase transitions (QPTs) [1–3] has in recent years emerged as one of the most interesting aspects of low-dimensional quantum systems. QPTs arise from the subtle interplay between short-range interactions on one hand and quantum fluctuations on the other [4]. Since the latter are particularly strong in one dimension, quantum spin chains have emerged as a generic model to investigate QPTs [5–8]. The additional presence of disorder has profound effects on the properties of low-dimensional systems [9,10] as it competes with the subtle effects of quantum fluctuations. Its effect on QPTs has been the subject of recent intense and controversial discussion [7,8,11–18]. Recent experimental advances now permit the investigation of the magnetic properties of nanoscale chains of magnetic atoms ($L \approx 50$) on the steps of metallic surfaces [19].

In one dimension, the strong-disorder renormalization (SDRG) [20,21] group offers potentially exact results for a variety of models. Of particular interest is the prediction of a universal infinite randomness fixed point (IRFP) for disordered antiferromagnetic spin chains. In many systems, SDRG studies suggest a *random-singlet* (RS) phase [22–24] as the ground state for fairly general disorder. In this RS phase, the average spin correlations are predicted to obey a *universal isotropic power-law decay*, $|\overline{\langle S_i^\alpha S_j^\alpha \rangle}| \sim |i-j|^{-2} (\alpha = x, z)$, where the overbar denotes a configurational average over many random chains (replicas). The Luttinger (or spin-liquid) continuum of critical ground states of the ordered chain is thus predicted to collapse to a single point. Numerical results consistent with the RS picture were reported for relatively short ($N \leq 18$) XXZ chains [12] and also for long XX chains ($\Delta = 0$) [13] with couplings uniformly distributed in [0,1]. Recently, some studies suggest the relevance of such a fixed point for the q-state quantum clock model and the quantum Ashkin Teller model [8], while others dispute its existence [6,25].

Recent numerical advances, in particular, the development of the density matrix renormalization group (DMRG) [26], now offer a framework to investigate the relevance of the IRFP to realistic one-dimensional spin systems [27]. In this Letter, we investigate the influence of exchange disorder on the anisotropic spin-1/2 Heisenberg chain (XXZ model), one of the best-known model systems for QPTs in one dimension. We find a qualitatively different scenario for the interplay of quantum fluctuations and disorder. Our results indicate that the spin correlations do *not* obey the universal parameter independent decay law suggested by the RS picture. Instead we find a disorder-induced QPT for finite disorder strength, whose nature can be illustrated by an exactly solvable model.

We present results of a density matrix renormalization group study of antiferromagnetic XXZ chains with randomness in the transverse nearest-neighbor coupling,

$$H = J \sum_{i=1}^{N-1} [\lambda_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + \Delta S_i^z S_{i+1}^z] \qquad (1)$$

($J > 0$), where the anisotropy parameter $\Delta \geq 0$ controls the relative strength of the quantum fluctuations. In the homogeneous system ($\lambda_i \equiv 1$), the ground state of (1) shows long-range order for $\Delta > 1$ (Ising regime), whereas for $\Delta \leq 1$ (critical regime) the spin correlations decay algebraically to zero as $|\langle S_i^\alpha S_j^\alpha \rangle| \sim |i-j|^{-\eta_\alpha}$ with nonuniversal decay exponents [28]:

$$\eta_x = \eta_z^{-1} = 1 - \pi^{-1} \arccos\Delta. \qquad (2)$$

The introduction of quenched randomness brings about subtle changes in the ground state. For reasons of better numerical control of replica averages, we used a bounded probability density $p(\lambda) = \frac{1}{2W}\Theta(W - |\lambda - 1|)$. We investigated chains of length up to $L = 400$ with a finite-size DMRG algorithm and ensured that the ground state and correlations $\langle S_i^\alpha S_j^\alpha \rangle$ could be determined with consistent accuracy for arbitrary choices of λ_i. We noted that for long chains the standard DMRG procedure tends to spontaneously break the local S_z reversal symmetry. We ensured that the resulting data for the correlation functions were nevertheless correct by comparing with explicitly symmetry-adapted high-accuracy DMRG calculations for a number of randomly selected replicas λ_i. We verified the

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accuracy of the correlation functions and energies by comparing with exact data for XX ($\Delta = 0$) chains which can be mapped to noninteracting lattice fermions. For critical systems, we investigated finite-size effects on the estimates of the decay exponents η_x and η_z for $0 \leq \Delta \leq 1$. For ordered chains with periodic boundary conditions, DMRG results for $\langle S_0^z S_{L/2}^z \rangle$ were in good agreement with the known long-range order parameter for $\Delta \geq 1$ [29] until the chain length became significantly shorter than the correlation (or saturation) length [30] of the system. This suggests that chains of length $L = 80$ are sufficient to determine the long-range behavior of the correlation function.

We then performed DMRG calculations for a large number of replicas each for various values of Δ and W. The number of replicas computed varied from 250 for small W, where replica expectation values fluctuate little, to more than 1000 for large W. We have not gathered replica averaged data for the XX model by DMRG as the correlation functions for a small set of replicas showed perfect numerical agreement between DMRG and results from exact diagonalization for chain lengths of up to $L = 160$.

Replica-averaged correlation functions in the critical and Ising regime are shown in Figs. 1 and 2, respectively. The data demonstrate qualitatively different behavior for small and large values of the disorder W. For $\Delta \leq 1$ and $W \leq 1$, both x and z correlation functions decay algebraically with exponents that depend on Δ and W. Fitted to additional exponential components and finite offsets $|\overline{\langle S_i^\alpha S_j^\alpha \rangle}| = A + |i-j|^{-\eta_\alpha} \exp(-\gamma|i-j|)$, the data show negligible inverse correlation lengths γ and offsets A for small W and Δ. The decay of the x correlation accelerates with growing disorder W, whereas that of the z correlation decelerates. The values of the decay exponents η_x and η_z as a function of W are shown in Fig. 3(a), indicating a continuous change of both exponents from their values for ordered chains $W = 0$, in violation of the prediction of the SDRG. To confirm this conclusion, we have computed the replica averaged ($N_{\rm rep} = 100$) xx-correlation function for $W = 0.1$, $\Delta = 0.5$, and $L = 120$, 240, 320, and 400. The correlation functions for the first 75% of the spins for each L are shown in Fig. 4. All data can be fitted with a single power law with exponent $\eta_x = 0.96 \pm 0.02 \neq 2$ consistent with our results for $L = 80$.

For $W > 1$, the x-correlation functions decay exponentially in both the Ising and the critical regimes. The inverse correlation length of the x correlation function is shown in Fig. 3(b). The data is consistent with a crossover to exponential decay at $W = 1$ with significant finite-size effects for $W > 0.8$, in particular, in the Ising regime. In the Ising phase ($\Delta > 1$), the z correlation functions continue to decay to a finite value for large separations [see Fig. 2 (inset)].

The nature of the transition at $W = 1$ is explained by a simple exactly solvable model, defined by the bimodal distribution,

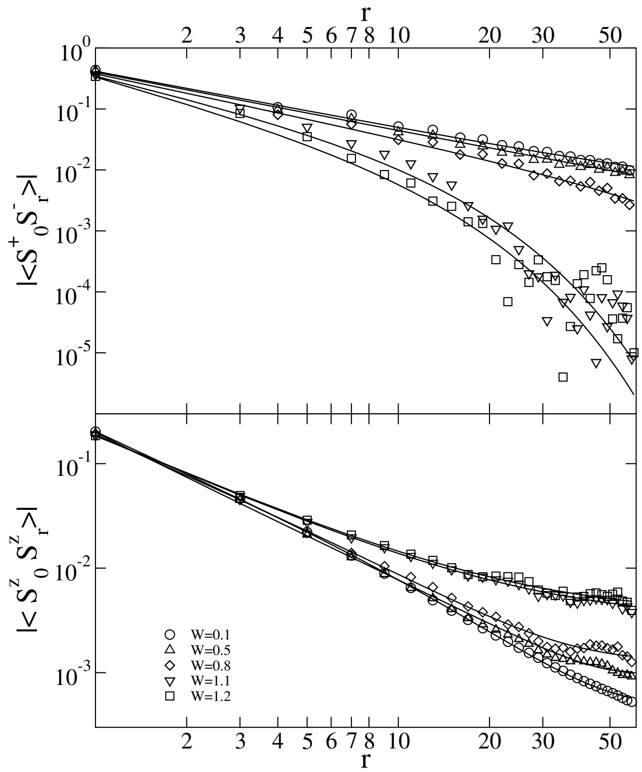

FIG. 1. Doubly logarithmic plots of replica averaged (top) $\overline{\langle S_0^+ S_r^- \rangle}$ and (bottom) $\overline{\langle S_0^z S_r^z \rangle}$ for $\Delta = 0.5$ and various disorder strengths W. The z-correlation functions decay algebraically, the degree of correlation increases with disorder strength, while x correlations decay algebraically for $W < 1$, but exponentially for $W > 1$.

$$p(\lambda) = p\delta(\lambda + 1) + (1 - p)\delta(\lambda - 1), \tag{3}$$

in the general Hamiltonian (1) with $\Delta < 1$. The ground state spin correlations of this model are related to the known correlations [28] of the homogeneous chain ($p = 0$) by a simple gauge transformation [31,32]. Consider a single replica, i.e., one configuration of λ_i drawn from the distribution (3) for an open chain. By a suitable product U of π rotations $\exp(2i\pi S_i^z)$ about the local S_z spin axes, the disorder may be gauged away, i.e., $\tilde{H} = UHU^\dagger$ describes a configuration with $\lambda_i \equiv 1$. As the z spin components are invariant under U, the z correlations of the disordered system are *identical* to those of the homogeneous system. In contrast, a product of two x spin components acquires a string of random signs:

$$U S_i^x S_{i+r}^x U^\dagger = S_i^x S_{i+r}^x \prod_{l=i}^{i+r-1} \lambda_l. \tag{4}$$

The disorder average of (4) simply yields the x correlation of the homogeneous system, multiplied by $(1 - 2p)^r$. The decay of the z correlation thus remains algebraic, whereas the x correlation function is modified by an

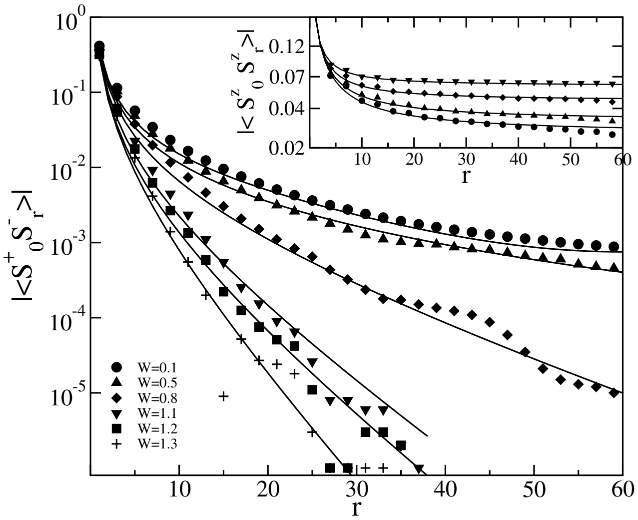

FIG. 2. Logarithmic plots of replica averaged correlation functions in the Ising regime ($\Delta = 1.5$) for various disorder strengths W. The x correlations decay algebraically for $W < 1$ and exponentially for $W > 1$, z-correlation functions saturate at a finite value that increases with the disorder strength (inset).

exponentially decaying factor, with a correlation length diverging with critical exponent equal to unity at the two quantum critical points $p_c = 0, 1$: $\xi_x \sim 1/(2|p - p_c|)$. Applied to the probability density used in the DMRG calculations, this argument yields $p = (W - 1)/(2W)$ and $\xi^{-1} = \ln W$ for $W > 1$ [heavy solid line in Fig. 3(b)]. For $\Delta = 0$, data for larger systems are available [32] and the crossover from $\xi^{-1} = 0$ to $\xi^{-1} = \ln W$ is more clearly visible.

In the limiting cases that are accessible by alternate techniques, our results are in good agreement with both exact data for $W = 0$ and numerical diagonalization results [32] for long ($N \leq 256$) XX chains (see also [13]). The latter also display clear deviations from the IRFP behavior predicted by the SDRG. For the z correlation, an r^{-2} decay with the corresponding finite-size scaling behavior [33] remains perfectly intact from $W = 0$ up to $W = 2$. The static z structure factor is linear in the wave vector q and independent of W. In contrast, the x correlation does not show finite-size scaling, and the static x structure factor is neither linear nor W independent. The x correlation decays progressively faster as W grows. The data may be fitted to a power-law as long as $W < 1$, but with an exponent significantly smaller than the value of 2 predicted for the RS phase. For $W > 1$, the decay is exponential, with an inverse correlation length proportional to the fraction of negative λ (as in the exactly solvable model above).

Combined, these results suggest a qualitative revision of the influence disorder is thought to have on quantum spin chains. No signs of attraction to the IRFP (with universal and isotropic algebraic decay of the spin correlation functions) predicted by the SDRG were observed in our study of finite chains of length up to $L = 400$. Instead, we observe a disorder-driven quantum phase transition at $W = 1$ for $0 \leq \Delta \leq 1$, from a spin-liquid phase with algebraically decaying correlations (with nonuniversal exponents) at $W < 1$ to a different phase with exponential decay of the x correlations. These observations suggest to critically reexamine the applicability of the SDRG and to investigate the possible existence of a crossover length scale beyond which the IRFP emerges as relevant. Recent experiments permit the controlled assembly of finite monoatomic chains of magnetic atoms [19], which may lead to a direct

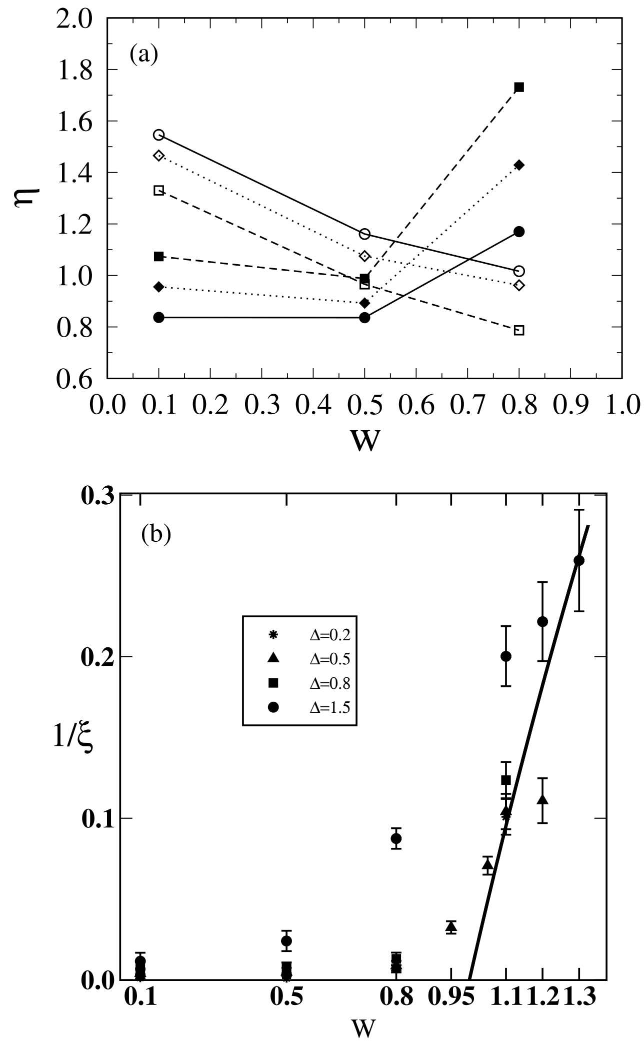

FIG. 3. (a) Exponents η for the algebraic decay of the x and z correlation functions in the critical regime $\Delta < 1$. In contrast to the predictions of the SDRG, the exponents change continuously from their (finite system) values with no disorder. Circles, diamonds, and squares denote $\Delta = 0.2$, 0.5, and 0.8, respectively. Open symbols correspond to η_z and filled symbols to η_x. (b) Inverse correlation length for the decay of the x correlation functions for various Δ as a function of W. For $W > 1$, all data are consistent with the results for the exactly solvable model (heavy line).

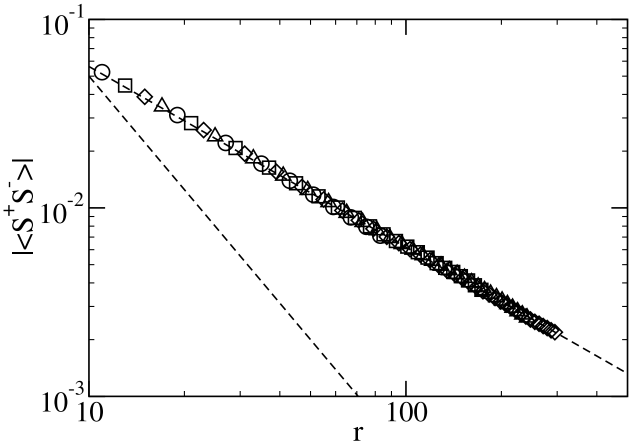

FIG. 4. Doubly logarithmic plots of replica averaged $\overline{\langle S_0^+ S_r^- \rangle}$ for $\Delta = 0.5$ and $W = 0.1$ for $L = 120$ (circles, $\eta_x = 0.994$), $L = 240$ (squares, $\eta_x = 0.958$), $L = 320$ (triangles, $\eta_x = 0.962$), and $L = 400$ (diamonds, $\eta_x = 0.959$) plotted for $10 < r < 0.75L$. The solid line is a fit to the $L = 400$ data, the dashed line the SDRG prediction (prefactor adjusted to match $r = 10$ data). Only one-eighth of each data set is shown for clarity. The exponents of power-law fits for the individual data sets are given above; they are consistent with $\eta_x = 0.96 \pm 0.01$ for $L > 120$.

experimental test of our prediction. We also note that for $L = 400$ the absolute value of the correlation function has dropped by almost 2 orders of magnitude. As a result, a possible crossover to IRFP behavior on larger length scales may be difficult to access experimentally.

For nonbounded disorder, where fluctuating signs of the couplings are present with varying probability for any W, one may anticipate the existence of a crossover length scale where algebraic decay crosses into exponential decay as a function of system size that may be observable by studying long, but finite, chains. DMRG studies for Gaussian disorder, for which replica averages are much more difficult to converge, are presently under way to explore this scenario. The results of the present study are directly applicable to systems where a crystal field or easy plane generates a natural anisotropy. Extrapolating from both limits, they suggest the continued existence of critical behavior for weak isotropic disorder in the isotropic model, a scenario that we will investigate more thoroughly in the future.

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