Random Exchange Disorder
in the Spin-1/2 XXZ Chain

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Abstract

The one-dimensional XXZ model is studied in the presence of disorder in the Heisenberg Exchange Integral. Recent predictions obtained from renormalization group calculations are investigated numerically using a Lanczos algorithm on chains of up to 18 sites. It is found that in the presence of strong X-Y-symmetric random exchange couplings, a “random singlet” phase with quasi-long-range order in the spin-spin correlations persists. As the planar anisotropy is varied, the full zero-temperature phase diagram is obtained and compared with predictions of Doty and Fisher [Phys. Rev. B 45, 2167 (1992)].

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The study of quantum models in the presence of disorder is an emerging field onto which much attention has been focussed lately. Since all experimentally accessible systems are to some extent affected by randomness in the form of impurities, fields, or couplings, a thorough understanding of disorder effects can help in comparing experimental observations and theoretical predictions. In particular, weakly disordered, low-dimensional quantum spin systems are of interest, since the interplay between randomness and strong quantum fluctuations can be observed. At T=0, phase transitions in quantum spin models are driven by zero-point fluctuations, as opposed to thermal excitations in their classical counterparts. However, when a random potential is introduced, phase transitions can also be driven by random fluctuations. This mechanism is particularly interesting in the case of marginally ordered systems, where the long-range Néel order in the 2D isotropic Heisenberg model has been found to be unstable towards thermal fluctuations and random fields, but not towards randomness in the exchange couplings.

The anisotropic spin-1/2 Antiferromagnetic Heisenberg Chain is a generic model of strongly correlated electrons. It is described by the Hamiltonian,

$$H_0 = J \sum_i (\lambda S^z_i S^z_{i+1} + S^x_i S^x_{i+1} + S^y_i S^y_{i+1}),$$

where the notation is standard. Due to the low dimensionality, quantum fluctuations destroy long-range order in the region $-1 < \lambda \leq 1$, and the spin-spin correlations decay spatially with a power-law. Beyond the Heisenberg point (i.e. $\lambda > 1$), a gap opens in the excitation spectrum and the system develops long-range Néel order with exponentially decaying correlation functions, while for $\lambda \leq -1$ there is a ferromagnetic region with Ising-type long-range order.

Let us now introduce disorder in the form of X-Y symmetric random exchange couplings, i.e. such that the planar symmetry of $H_0$ is not broken by the random potential,

$$H_{\text{random}} = \sum_i \delta_i (S^x_i S^x_{i+1} + S^y_i S^y_{i+1}).$$

The random couplings $\delta_i$ are drawn from a uniform distribution $P(\delta_i) = \theta(\delta_i - \delta_{J_{xy}})\theta(\delta_{J_{xy}} - \delta_i)$, where $\langle \delta_i \rangle = 0$ and $\langle (\delta_i)^2 \rangle = 2(\delta_{J_{xy}})^3/3$. The cut-off parameter $\delta_{J_{xy}}$ serves as a measure...
for the strength of the random potential. The physical properties induced by this distribution are believed to be universal. However, in order to test this idea, we also studied random exchange couplings drawn from a Gaussian distribution, 
\[ P(\delta_i) = \frac{1}{\sqrt{2\pi\sigma_{xy}}} \exp \left( -\frac{\delta_i^2}{2\sigma_{xy}} \right). \]
Here, \( \sigma_{xy} \) serves as a measure of the random strength.

The properties of XXZ chains in the presence of various random potentials have recently been studied by C. A. Doty and D. S. Fisher using renormalization group techniques. It was found that, while random transverse fields destroy the (quasi)-long-range spin order, a power-law decay of the spin correlations may persist in the presence of random exchange couplings as long as the random Hamiltonian does not break the planar symmetry of \( H_0 \). In particular, it was predicted that a quasi-long-range-ordered phase extends from the X-Y regime \((-1 < \lambda \leq 1)\), when \( H_{\text{random}} \) is switched on.

In our study of the above system, we numerically diagonalized chains of up to 18 sites with periodic boundary conditions using a Lanczos algorithm. The observables were obtained from a quenched average, i.e. the ground state \( |\phi_0(j)\rangle \) of a chain was obtained for a given set of random couplings \( j = \{\delta_i\} \), and then the expectation value of some particular operators \( \hat{O} \) were studied. This procedure was repeated for \( m \approx 500 \) different sets of random couplings, and finally the algebraic average over all \( m \) random samples was taken. The quenched average of an operator \( \hat{O} \) is thus defined by
\[
\langle \langle \hat{O} \rangle \rangle = \frac{1}{m} \sum_{j=1}^{m} \langle \phi_0(j)|\hat{O}|\phi_0(j)\rangle. \tag{3}
\]

First, we would like to address the question of whether quasi-long-range order persists in the region \(-1 < \lambda \leq 1\) when the disorder potential \( H_{\text{random}} \) is switched on. The relevant observable is the normalized real-space spin-spin correlation function
\[
\omega^z(l) = \frac{3}{N} \sum_{i=1}^{N} \frac{\langle \langle S_i^z S_{i+l}^z \rangle \rangle}{S(S+1)}, \tag{4}
\]
where \( N \) denotes the number of sites, and \( S = 1/2 \) in our study.

In Fig.1, the spin-spin correlations \( \omega^z(N/2) \) at the maximum separation \( (l = N/2) \) are plotted as a function of the lattice size \( N \) at planar anisotropy \( \lambda = 0.5 \) for a couple of
random strengths $\delta J_{xy}$. If the correlations decay with a power-law $|\omega^z(l)| \propto l^{-\eta_z}$, we expect a straight line with negative slope $\eta_z$ in a double-logarithmic plot. It is found that for all random strengths, $\delta J_{xy}$, a power-law decay (solid line) fits the numerical data much better than an exponential decay (dashed line), e.g. the $\chi^2$-value obtained from least-square fits is typically two orders of magnitude larger when an exponential decay $|\omega^z(l)| \propto \exp (-\xi l)$ is assumed. We observed a similar power-law behavior in a large region of parameter space.

Why does the random potential not destroy quasi-long-range order in this region? According to Doty and Fisher the “random singlet” phase which extends from the X-Y phase of the pure system ($H_0$) can be pictured in terms of randomly distributed tightly coupled singlet pairs of spins. Those spins which are not bound in a singlet pair interact via virtual excitations. It turns out that these “almost-free” spins are anomalously strongly correlated. The probability that “almost-free” spins separated by a distance $R$ interact strongly is proportional to $1/R^2$. This gives rise to the observed power-law behavior in the spin-spin correlations. The decay exponent is found to be $\eta_z = 2$. Note that also, in the exactly solvable X-Y limit ($\lambda = 0$) the system maps into a tight-binding model of free fermions with random nearest-neighbor hopping. In this limit the decay exponent is given by $\eta_z = 2$ if a single characteristic localization length is assumed for the properties of the low-energy wave functions.

In Fig.2, we show $\eta_z$ obtained in our numerical analysis, as a function of the disorder parameter $\delta J_{xy}$ for various anisotropies $\lambda$. The exponent has been extracted using chains of size N=6, 10, 14 and 18. The inset of Fig.2(a) shows the decay exponent $\eta_z$ for the pure system $H_0$ as it has also been obtained in Ref. 6. The exact diagonalization results are in excellent agreement with predictions from conformal invariance and in particular the Heisenberg limit ($|\omega^z(l)| \propto l^{-1}$) and the X-Y limit ($|\omega^z(l)| \propto l^{-2}$) are nicely recovered. For negative anisotropies, ($-1 < \lambda \leq 0$) conformal invariance predicts a constant exponent $\eta_z = 2$, which is also in reasonable agreement with our data, showing that our techniques can reproduce known results very accurately.

On our finite chains and as we depart from the $\delta J_{xy} = 0$ limit, three regions can be
(1) In the regime of small randomness ($\delta J_{xy} < J$) the exponent $\eta_z$ increases slightly as a function of the disorder parameter $\delta J_{xy}$, which is a sign of reduced order.

(2) Around $\delta J_{xy} = J$, there is an area of high competition between the quantum fluctuations of the original Hamiltonian ($J \sum_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y)$) and $H_{\text{random}}$. Locally the random terms can compensate the zero-point fluctuations leading to an antiferromagnetic Ising-like behavior in the correlation functions. As a result, the decay exponent $\eta_z$ has a dent with onset at around $\delta J_{xy} = J$, indicating a crossover into a more ordered Ising-like regime, where correlations decay more slowly than for the uniform system.

(3) For large disorder, ($\delta J_{xy} >> J$) $H_{\text{random}}$ is the dominant term. The dependence of the decay exponent on the planar anisotropy in $H_0$ becomes negligible, and it approaches $\eta_z = 2$ for all values of $\lambda$, as it has been predicted by renormalization group arguments.

In the vicinity of $\lambda = -0.75$ the exponent $\eta_z$ behaves anomalously for small disorder. The observed decay in $\eta_z$ for $\delta J_{xy}$ between $J$ and $2J$ is due to ferromagnetic behavior in the real space spin-spin correlations. This anomaly is observed specially for anisotropies $-1 < \lambda \leq -0.5$. The dent of $\eta_z$ around $\delta J_{xy} = J$ can be understood as a crossover into a phase of higher order. In particular, for $\lambda = -0.75$ we observed a transition into a partially polarized phase indicated by the change of sign in the energy difference $\delta E = E(S^z_{\text{tot}} = 0) - E(S^z_{\text{tot}} = 1)$, where $E(S^z_{\text{tot}} = n)$ is the quenched ground state energy in the subspace with $S^z_{\text{tot}} = n$. The inset of Fig.2(b) shows $\delta E$ as a function of the disorder parameter $\delta J_{xy}$ at anisotropy $\lambda = -0.75$ for a 14-site chain. It can be nicely seen that the transition into the partially polarized phase ($0.55J \leq \delta J_{xy} \leq 3.05J$) corresponds to the dent in $\eta_z$ in the same regime of disorder.

In Fig.3(a), the dependence of the energy on the disorder parameters $\delta J_{xy}$ and $\sigma_{xy}$ at various anisotropies is shown for a 14-site chain. As the random potential becomes dominant, the system is allowed to relax into a ground state of higher entropy. The ground state energy drops proportionally to $\delta J_{xy} \ (\sigma_{xy})$ in this region. In Fig.3(b), we show how
the static structure factor \( S_{zz}(k) = \sum_j \exp(-ikj) \langle 0|S^z_j S^z_{j+1}|0 \rangle \) behaves as a function of the disorder parameters at antiferromagnetic momentum transfer \( k = \pi \) for the 14-site chain. In analogy to Fig.2, three regions can be identified. At low disorder the structure factor remains approximately unchanged. In the region of competition, Néel order is favored for positive anisotropies (\( 0 \leq \lambda \leq 1 \)), resulting in an increase of the antiferromagnetic structure factor especially in the vicinity of \( \lambda \sim 1 \). For negative anisotropies (\( -1 < \lambda \leq 0 \)), the ditch in \( S_{zz}(\pi) \) indicates a crossover into a ferromagnetically polarized region. For large disorder, \( S_{zz}(\pi) \) becomes independent of \( \lambda \), and approaches the X-Y limit for all anisotropies.

The boundary between the long-range-ordered regime and the “random singlet” phase is obtained from the correlations \( \omega^z(N/2) \). In the “random singlet” phase, the spin-spin correlations at distance \( N \) vanish in the bulk limit as \( N \to \infty \). However, as the anisotropy is tuned across the critical value \( \lambda_c \), \( \omega^z(N/2) \) becomes finite, approaching \( |\omega^z(N/2)| = 1 \) in the extreme Ising limit (\( \lambda = \infty \)). At zero disorder the Heisenberg point \( \lambda_c = 1 \) is nicely recovered as the critical point (Fig.3(c)). In Fig.3(d), we see that the transition point between these two phases is reduced to about \( \lambda_c = 0.75 \) at \( \delta J_{xy} = J/\delta J \). As a result of the strong competition effects in the region \( \delta J_{xy} \sim J \), the antiferromagnetic phase bends into the random singlet regime in a “reentrant” transition, indicating a stronger antiferromagnetic order in this region. The whole boundary between “random singlet” and Néel phase is plotted in the phase diagram given in Fig.4.

Both the “random singlet” and the Néel phase lie in the \( S^z_{\text{total}} = 0 \) subspace. On the other hand, as the ferromagnetic limit is approached, there is a transition into a partially polarized phase, i.e. the ground state no longer has \( S^z_{\text{total}} = 0 \). This phase boundary, as well as the transition from the partially into the fully polarized regime, is extracted from comparing the lowest energies of the various \( S^z_{\text{total}} \) subspaces (averaged over the ensemble of random couplings). In the region of competition between quantum fluctuations and the disorder term, the partially polarized phase bends into the “random singlet” regime, in analogy to the effect at the phase boundary between the “random singlet” and the Néel phase, as shown in Fig.4.
For low disorder, our results agree qualitatively with those of Doty and Fisher. However, their study predicts an X-Y-like “mole hill” phase in the region $-1 < \lambda \leq -0.5$, and for small disorder. Numerically, it is hard to distinguish this “mole-hill” from the “random singlet” regime, because both phases show power-law behavior in the correlation functions. However, from our exact diagonalization data we have observed a region (denoted with a question mark in Fig.4) which has power-law decay, and is a member of the $S_{total}^z = 0$ subspace, but does not have any remnant antiferromagnetic correlations, as has been discussed above in the inset of Fig.2(b). We are currently investigating, whether this regime can be identified with the “mole hill” predicted by Doty and Fisher.

In summary, we have presented the first numerical study of the spin-1/2 XXZ chain in the presence of a random exchange potential ($H_{random}$). In contrast to a random field, quasi-long-range order of the zero-disorder X-Y regime $-1 < \lambda \leq 1$ is not destroyed by an X-Y symmetric random exchange. Also, Ising-type long-range order persists in the presence of small random exchange couplings. The power-law behavior in the “random singlet” phase may be due to virtual interactions of “almost-free” spins which are not bound in randomly strong singlet pairs. A complete phase diagram is provided. In addition, we have found an interesting reentrant transition of the ordered phases (in both the ferromagnetic and antiferromagnetic Heisenberg limits) when exchange disorder is included. Such a novel type of behavior (order induced by random couplings) deserves additional study.

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FIGURES

FIG. 1. : Double-logarithmic plot of real-space spin-spin correlations $|\omega^z(l)|$ at maximum separation ($l = N/2$) as a function of lattice size. The squares represent data obtained from exact diagonalizations, the solid lines are fits to power-law decay $|\omega^z(l)| = Al^{-\eta z}$ and the dashed lines are fits to an exponential decay $|\omega^z(l)| = A\exp(-\xi l)$. The size of the squares is comparable to the magnitude of the corresponding error bars.

FIG. 2. : (a) Exponents of the power-law decay $|\omega^z(l)| = Al^{-\eta z}$ as a function of the disorder parameter $\delta J_{xy}$ for various positive planar anisotropies. The inset shows $\eta_z$ as a function of anisotropy in the limit of no disorder. (b) Same as (a) but for negative anisotropies. The inset shows the energy difference $\delta E = E(S_{tot}^z = 0) - E(S_{tot}^z = 1)$ as a function of $\delta J_{xy}$ for the 14-site chain. The change in the sign of $\delta E$ indicates the presence of a partially polarized phase for $0.55J \leq \delta J_{xy} \leq 3.05J$ at anisotropy $\lambda = -0.75$.

FIG. 3. : (a) Ground state energy of the 14-site spin-1/2 XXZ chain as a function of the disorder parameter $\delta J_{xy}$ at various planar anisotropies. The random exchange couplings are drawn from a uniform distribution with cut-off $\delta J_{xy}$. The inset shows the same except when the random exchange couplings are obtained from a Gaussian distribution of width $\sigma_{xy}$. (b) Antiferromagnetic structure factor vs. disorder parameter $\delta J_{xy}$ for the 14-site spin-1/2 XXZ chain. The inset shows the same but when the random exchange couplings are obtained from a Gaussian distribution of width $\sigma_{xy}$. (c) Real space correlation functions at the maximum distance for an $N$ site chain as a function of anisotropy at zero disorder. The bulk limit $N = \infty$ is extracted from a finite size study. (d) Same as (c) at disorder $\delta J_{xy} = J$.

FIG. 4. : Phase diagram of the spin-1/2 XXZ chain in the presence of a random exchange potential. The question mark denotes the “mole hill” phase discussed in the text.