Spin correlations functions in random-exchange $s=1/2$ XXZ chains

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The decay of (disorder-averaged) static spin correlation functions at $T=0$ for the one-dimensional spin-1/2 XXZ antiferromagnet with uniform longitudinal coupling $J_\lambda$ and random transverse coupling $J_{\lambda,i}$ is investigated by numerical calculations for ensembles of finite chains. At $\Delta=0$ (XX model) the calculation is based on the Jordan-Wigner mapping to free lattice fermions for chains with up to $N=100$ sites. At $\Delta \neq 0$ Lanczos diagonalizations are carried out for chains with up to $N=22$ sites. The longitudinal correlation function $\langle S_{0}^{z}S_{i}^{z} \rangle$ is found to exhibit a power-law decay with an exponent that varies with $\Delta$ and, for nonzero $\Delta$, also with the width of the $\lambda _{i}$-distribution. The results for the transverse correlation function $\langle S_{0}^{x}S_{i}^{x} \rangle$ show a crossover from power-law decay to exponential decay as the exchange disorder is turned on. © 1996 American Institute of Physics.

$\eta_1 = 1/\eta_z = 1 -(1/\pi)\arccos \Delta$. (3)

The RSRG study further predicts that this exponent value is $\eta_1=\eta_z=2$, independent of the longitudinal coupling $\Delta$ and the disorder strength $\sigma$, provided the latter is not too small. It is indeed quite unusual that the anisotropic randomization of an anisotropic exchange interaction should effectively remove the effects of anisotropy in the spin correlations.

We report results of finite-chain studies which goes significantly beyond that of Ref. 5 in statistics and system sizes. For the XX model ($\Delta = 0$), we carried out the computation in the (free-) fermion representation, which allows us to handle chains with up to $N=100$ spins and beyond. For $\Delta \neq 0$ we must resort to Lanczos diagonalizations. Here the largest system for which we can perform the computation with reasonable statistics has $N=22$ sites. For graphical purposes we shall consider, henceforth, the absolute value, $|\langle S_{0}^{x}S_{i}^{x} \rangle|$, of the spin pair correlations.

We first consider the case $\Delta = 0$ (XX model). If the longitudinal correlation function does exhibit power-law decay, $|\langle S_{0}^{x}S_{N/2}^{x} \rangle| \sim r^{-\eta_1}$, as predicted, then the exponent $\eta_1$ also governs the $N$-dependence of the function $|\langle S_{0}^{x}S_{N/2}^{x} \rangle|$ in a cyclic chain of $N$ sites. We have evaluated this quantity for systems with $N=100$ sites and for disorder strengths $\sigma=2$, all with ensemble averages over up to $10^5$ configurations.

The data analysis yields $\eta_1=2$ independent of $\sigma$. This is consistent with the RSRG prediction$^{2,3}$ but in contradiction to the earlier finite-size study,$^5$ where a significant $\sigma$-dependence of $\eta_1$ was observed. Our data also confirm that the disorder-averaged logarithm of $|\langle S_{0}^{x}S_{N/2}^{x} \rangle|$ exhibits the decay law $\sim r^{-1/2}$ as predicted in Ref. 3.

The decay of the transverse correlation function $\langle S_{0}^{x}S_{i}^{x} \rangle$ is much more sensitive to the presence of exchange disorder, as is demonstrated by the data shown in Figs. 1 and 2. In the main diagram of Fig. 1 we show the function $|\langle S_{0}^{x}S_{N/2}^{x} \rangle|$ versus $r$ in a logarithmic plot for ensembles with different disorder strengths. Turning on the exchange disorder with gradually.

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The combination of randomness and quantum fluctuations is well known to be a fertile ground for interesting physical phenomena including Anderson localization. In one-dimensional (1D) tight-binding systems the rule is that disorder always leads to localization. However, if the randomness is purely off-diagonal, the localization length diverges at the band center, which is bound to affect the decay law of correlation functions. One particular off-diagonally disordered fermion model, the 1D half-filled tight-binding model with random hopping, is equivalent to the special case of that phase would imply that the characteristic exponent $\eta_\alpha$ assumes the same value in the longitudinal ($z$) and transverse ($x$) correlation functions, in marked contrast to the case with no exchange disorder ($\sigma=0$), for which we know the exact result$^8$

\[ \langle S_{0}^{x}S_{i}^{x} \rangle \sim (-1)^i r^{-\eta_\alpha}, \quad \alpha = x, z. \] (2)

The singlet nature of that phase would imply that the characteristic exponent $\eta_\alpha$ assumes the same value in the longitudinal ($z$) and transverse ($x$) correlation functions, in marked contrast to the case with no exchange disorder ($\sigma=0$), for which we know the exact result$^8$

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The RSRG study further predicts that this exponent value is $\eta_1=\eta_z=2$, independent of the longitudinal coupling $\Delta$ and the disorder strength $\sigma$, provided the latter is not too small. It is indeed quite unusual that the anisotropic randomization of an anisotropic exchange interaction should effectively remove the effects of anisotropy in the spin correlations.

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The uniform longitudinal spin coupling corresponds to a fermion interaction. Here we consider the range $0 \leq \Delta \leq 1$, use periodic boundary conditions, and take the random transverse coupling $J_{\lambda,i}$ to be described by a Gaussian distribution with $\lambda_{i} = 1, \lambda_{i} = 1 + 1/2 \delta_{ij}$. The spin correlations at $T=0$ of this model were recently investigated by means of a real-space renormalization group (RSRG) method$^{2,3}$ based in part on ideas from earlier work,$^4$ and by means of a finite-chain study.$^5$

One interesting proposition made in the context of the RSRG study is the existence of a random-singlet phase with algebraically decaying spin pair correlations.$^{2,3}$

\[ \langle S_{0}^{x}S_{i}^{x} \rangle \sim (-1)^i r^{-\eta_\alpha}, \quad \alpha = x, z. \] (2)

The singlet nature of that phase would imply that the characteristic exponent $\eta_\alpha$ assumes the same value in the longitudinal ($z$) and transverse ($x$) correlation functions, in marked contrast to the case with no exchange disorder ($\sigma=0$), for which we know the exact result$^8$
The slope of that line determines the exponent $\eta_1$, as a function of the disorder strength $\sigma$.

Increasing $\sigma$ causes the transverse correlations to decay more and more rapidly as one might expect.\(^8\)

For $0 \leq \sigma \leq 0.5$ the data describe a power-law behavior. This is also evident in the bundle of curves near the top of Fig. 2, which shows the $r$-dependence of the function $|\langle S^z_0 S^z_{N/2} \rangle|$ semi-logarithmically at $\sigma = 0.4$ for various system sizes. The values $|\langle S^z_0 S^z_{N/2} \rangle|$ at the endpoints of these curves plotted vs $N/2$ in a log-log graph fall onto a straight line, and the slope of that line determines the exponent $\eta_1$. This is illustrated by the full squares in the inset to Fig. 2.

The $\sigma$-dependence of $\eta_1$ as obtained from this procedure is shown in the inset to Fig. 1. For the system without exchange disorder we reproduce the exactly known value $\eta_1 = 1/2$,\(^8\) which is a special case of (3). As $\sigma$ increases from zero, $\eta_1$ grows gradually and monotonically, at first slowly, then more and more rapidly.

For $\sigma \geq 0.5$ the curves in Fig. 1 suggest the occurrence of a crossover from algebraic decay to exponential decay, $|\langle S^z_0 S^z_{N/2} \rangle| \sim \exp(-r/\xi)$, in the range of $r$ for which we have data. The exponential character of the decay is more strikingly manifest in the lower bundle of data shown in the main plot of Fig. 2, representing the function $|\langle S^z_0 S^z_{N/2} \rangle|$ at $\sigma = 1$ for various system sizes.\(^8\) The smallest expectation values are known only with considerable (relative) uncertainty despite the augmented statistics.

The triangles, which represent the values $|\langle S^z_0 S^z_{N/2} \rangle|$ vs $N/2$ in this semi-logarithmic plot, are consistent with a straight line. Its slope determines the disorder-induced correlation length $\xi$. Over the range of disorder strengths, where our data suggest exponential decay of $|\langle S^z_0 S^z_{N/2} \rangle|$, $\xi$ thus determined decreases monotonically with increasing $\sigma$.

Our data for the exchange disordered XX model are consistent with two alternative scenarios, which are equally interesting:

(i) There exists a transition at some nonzero value of the disorder strength $\sigma_c \approx 0.5$, from algebraically to exponentially decaying transverse spin correlations.

(ii) A transition of the same nature occurs at $\sigma_c = 0$ instead, which produces very similar crossover effects in the finite-chain data.

A more extensive study for longer chains and with better statistics will be necessary to discriminate with confidence between the two scenarios.\(^9\) The data are definitely incompatible with a persistent power-law decay as predicted by RSRG.

Now we turn to one case, $\Delta = 0.75$, with fermion interaction (XXZ model). Since the computations are much more involved, the available data are limited by comparison with the case $\Delta = 0$. At $\Delta \neq 0$ neither our data for the longitudinal correlations nor those for the transverse correlations are compatible with the RSRG predictions.

The function $|\langle S^x_0 S^x_{N/2} \rangle|$ for various system sizes and $\sigma = 1.5$ is shown logarithmically in Fig. 3. The endpoint data $(r = N/2)$, which fall neatly onto a straight line, describe a power-law decay with $\eta_x = 1.26$. The exponent values obtained for two smaller disorder strengths are $\eta_x = 1.17$ ($\sigma = 0.5$) and $\eta_x = 1.31$ ($\sigma = 0.25$). The exact result (3) for $\sigma = 0$ assumes the value $\eta_x = 1.298 \ldots$.

All combined, the data suggest that the function $|\langle S^z_0 S^z \rangle|$ is governed by a power-law which persists in the presence of randomness. The $\sigma$-dependence of the exponent...
$\eta_2$ appears to go through a minimum of considerable depth at $\sigma \neq 0$ which implies the curious phenomenon that the longitudinal correlations are enhanced by a small amount of transverse exchange disorder relative to the correlations in the uniform-exchange system.

The data for the transverse correlations $\langle S^z_0 S^z_r \rangle$ at $\Delta = 0.75$ exhibit properties very similar to what we have observed and described for the free-fermion case ($\Delta = 0$). For not too large disorder strengths ($\sigma \leq 0.5$), we see a power-law behavior with an exponent that increases monotonically from the exactly known value $\eta_3 = 0.769 \ldots$ at $\sigma = 0$, as given by expression (3), to $\eta_3 = 1.00$ at $\sigma = 0.25$ and $\eta_3 = 1.49$ at $\sigma = 0.5$, at which point a crossover to exponential behavior makes itself felt. The exponential decay law at $\sigma = 1.5$ is quite evident in the semi-logarithmic plot of Fig. 4.

The discrepancies between our results and the RSRG predictions of Refs. 2, 3 call for an explanation in future studies. Possibly, the strongly anisotropic nature of the exchange in the model system (1) – even for $\Delta = 1$ – is not adequately taken into account by the RSRG procedure, which derives from a method originally developed for a model with isotropic exchange.\(^5\)

In order to gain further insight into the properties of the XXZ chain with random exchange, we plan to investigate the nature of low-lying excitations and the properties of dynamic correlation functions. At $\Delta = 0$ the Jordan-Wigner mapping to free fermions will make it possible to carry out these calculations for large systems. At $\Delta \neq 0$ the KPM method developed recently\(^{12}\) promises to be an adequate calculational instrument.

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\(^{7}\) See Fig. 2 of Ref. 5.
\(^{8}\) The upward curvature in the vicinity of $r = N/2$ is an obvious finite-size effect attributable to periodic boundary conditions.
\(^{9}\) B. M. McCoy, Phys. Rev. 173, 531 (1968).
\(^{10}\) Preliminary results for chains with up to $N = 200$ sites indicate that scenario (ii) is more likely.
\(^{11}\) The same effect had previously been observed in Ref. 5, also for the case $\Delta = 0$, where it is absent in our data.