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Spin correlation 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 $J\Delta$ 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 $\langle S_0^z S_r^z \rangle$ is found to exhibit a power-law decay with an exponent that varies with Δ and, for nonzero Δ, also with the width of the λ_i-distribution. The results for the transverse correlation function $\langle S_0^x S_r^x \rangle$ show a crossover from power-law decay to exponential decay as the exchange disorder is turned on. © *1996 American Institute of Physics.* [S0021-8979(96)00308-3]

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,[1] 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 *XX* case ($\Delta=0$) of the 1D $s=1/2$ *XXZ* model with random transverse exchange coupling, described by the Hamiltonian

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

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 $\overline{\lambda_i}=1$, $\overline{\lambda_i \lambda_j} = 1 + \sigma^2 \delta_{ij}$. 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]

$$\langle S_0^\alpha S_r^\alpha \rangle \sim (-1)^r r^{-\eta_\alpha}, \quad \alpha=x,z. \qquad (2)$$

The singlet nature of that phase would imply that the characteristic exponent η_α 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[6]

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

The RSRG study further predicts that this exponent value is $\eta_x = \eta_z = 2$, independent of the longitudinal coupling Δ and the disorder strength σ, 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.

Here we report results of a finite-chain study which goes significantly beyond that of Ref. 5 in statistics and system sizes. For the *XX* model ($\Delta=0$), we carry out the computation in the (free-) fermion representation, which enables 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, $|\langle S_0^\alpha S_r^\alpha \rangle|$, of the spin pair correlations.

We first consider the case $\Delta=0$ (*XX* model). If the longitudinal correlation function does exhibit power-law decay, $|\langle S_0^z S_r^z \rangle| \sim r^{-\eta_z}$, as predicted, then the exponent η_z also governs the N-dependence of the function $|\langle S_0^z S_{N/2}^z \rangle|$ in a cyclic chain of N sites.[5] We have evaluated this quantity for systems with $N \leq 100$ sites and for disorder strengths $\sigma \leq 2$, all with ensemble averages over up to 10^5 configurations.

The data analysis yields $\eta_z = 2$ independent of σ. This is consistent with the RSRG prediction[2,3] but in contradiction to the earlier finite-size study,[5] where a significant σ-dependence of η_z was observed.[7] Our data also confirm that the disorder-averaged logarithm of $|\langle S_0^z S_r^z \rangle|$ exhibits the decay law $\sim -r^{1/2}$ as predicted in Ref. 3.

The decay of the transverse correlation function $\langle S_0^x S_r^x \rangle$ 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 $|\langle S_0^x S_r^x \rangle|$ versus r in a logarithmic plot for ensembles with different disorder strengths. Turning on the exchange disorder with gradually
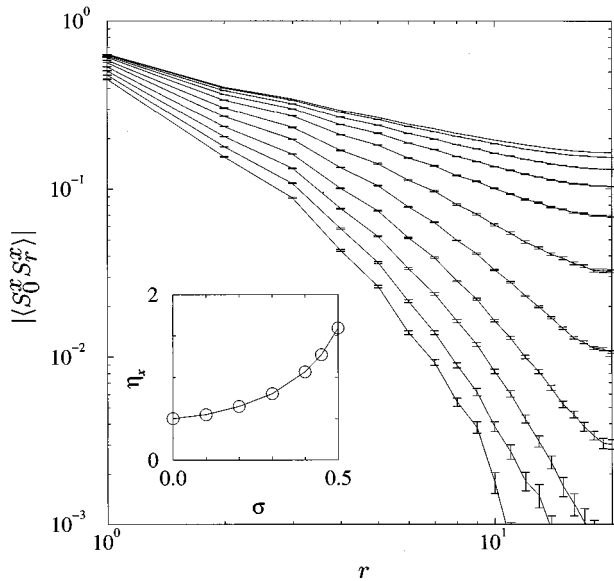
FIG. 1. Log-log plot of $|\langle S_0^x S_r^x \rangle|$ at $T=0$ in the random-exchange XX chain ($\Delta=0$) with $N=40$ spins at disorder strengths $\sigma=0,0.1,\ldots,1$ (top to bottom). For $0<\sigma\leqslant0.5$ the expectation value of $\langle S_0^x S_r^x \rangle$ has been averaged over 10^4 configurations, and for $\sigma>0.5$, over 10^5 configurations. The inset shows the (effective) decay exponent η_x as a function of the disorder strength σ.
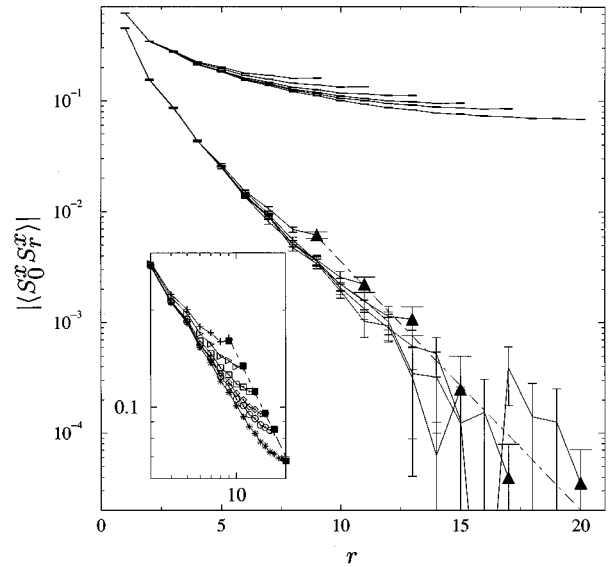

FIG. 2. Semi-logarithmic plot of $|\langle S_0^x S_r^x \rangle|$ with $r\leqslant N/2$ at $T=0$ in the random-exchange XX chain ($\Delta=0$) with $N=18, 22, 26, 30, 34, 40$, for $\sigma=0.4$ (upper set of curves, averaged over 10^4 configurations) and $\sigma=1$ (lower set of curves, averaged over 10^5 configurations). The data points for $\sigma=1$ at maximum distance ($r=N/2$) are marked by full triangles. The straight line which best fits these data points is shown dot-dashed and determines the correlation length ξ. The inset shows the data for $\sigma=0.4$ in a log-log plot. The data points at maximum distance ($r=N/2$) are marked by full squares. The straight line which best fits these data points is shown dot-dashed and determines the correlation exponent η_x.

increasing σ causes the transverse correlations to decay more and more rapidly as one might expect.[8]

For $0\leqslant\sigma\lesssim0.5$ 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 $|\langle S_0^x S_r^x \rangle|$ semi-logarithmically at $\sigma=0.4$ for various system sizes. The values $|\langle S_0^x S_{N/2}^x \rangle|$ 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 η_x. This is illustrated by the full squares in the inset to Fig. 2.

The σ-dependence of η_x 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 $\eta_x=1/2$,[9] which is a special case of (3). As σ increases from zero, η_x grows gradually and monotonically, at first slowly, then more and more rapidly.

For $\sigma\gtrsim0.5$ the curves in Fig. 1 suggest the occurrence of a crossover from algebraic decay to exponential decay, $|\langle S_0^x S_r^x \rangle| \sim \exp(-r/\xi)$, 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 $|\langle S_0^x S_r^x \rangle|$ 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 $|\langle S_0^x S_{N/2}^x \rangle|$ vs $N/2$ in this semi-logarithmic plot, are consistent with a straight line. Its slope determines the disorder-induced correlation length ξ. Over the range of disorder strengths, where our data suggest exponential decay of $|\langle S_0^x S_r^x \rangle|$, ξ thus determined decreases monotonically with increasing σ.

Our data for the exchange disordered XX model are con-

sistent with two alternative scenarios, which are equally interesting:

(i) There exists a transition at some nonzero value of the disorder strength, $\sigma_c\simeq0.5$, 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.[10] 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 $\Delta\neq0$ neither our data for the longitudinal correlations nor those for the transverse correlations are compatible with the RSRG predictions.

The function $|\langle S_0^z S_r^z \rangle|$ 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 $\eta_z=1.26$. The exponent values obtained for two smaller disorder strengths are $\eta_z=1.17$ ($\sigma=0.5$) and $\eta_z=1.31$ ($\sigma=0.25$). The exact result (3) for $\sigma=0$ assumes the value $\eta_z=1.298\ldots$

All combined, the data suggest that the function $|\langle S_0^z S_r^z \rangle|$ is governed by a power-law which persists in the presence of randomness. The σ-dependence of the exponent
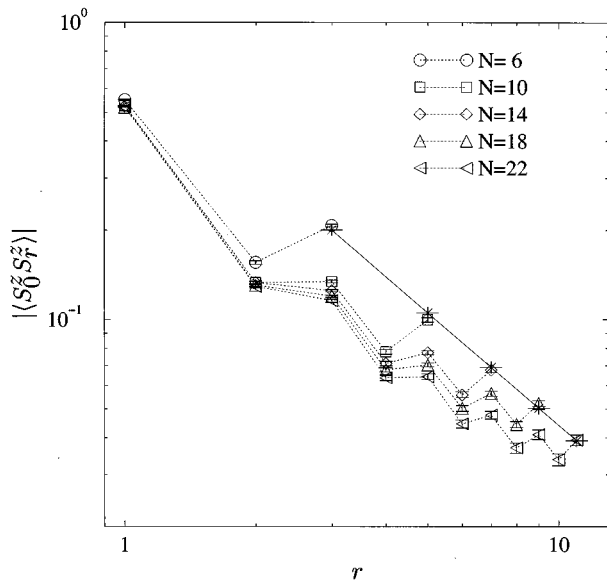
FIG. 3. Log-log plot of $|\langle S_0^z S_r^z \rangle|$ for the *XXZ* model with uniform longitudinal exchange ($\Delta = 0.75$) and random transverse exchange ($\sigma = 1.5$) on chains of various lengths. The data points represent averages over 1000 configurations for $N = 6, \ldots, 18$, and 450 configurations for $N = 22$.
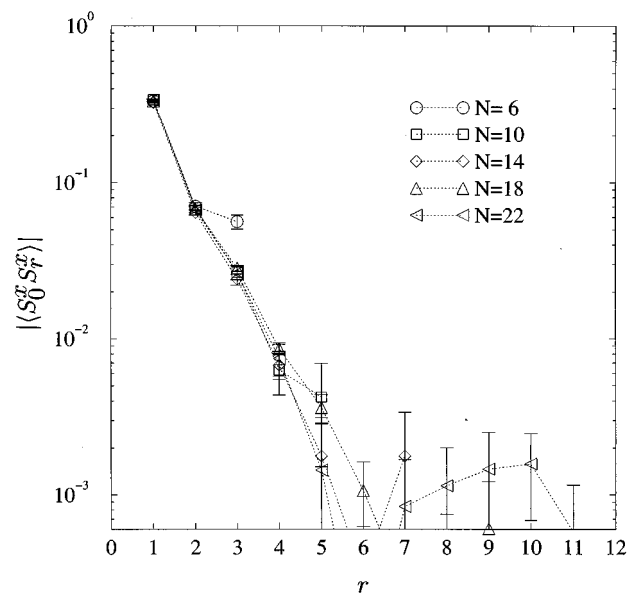

FIG. 4. Semi-logarithmic plot of $|\langle S_0^x S_r^x \rangle|$ for the *XXZ* model with uniform longitudinal exchange ($\Delta = 0.75$) and random transverse exchange ($\sigma = 1.5$) on chains of various lengths. The data points represent averages over 1000 configurations for $N = 6, \ldots, 18$, and 450 configurations for $N = 22$.

η_z appears to go through a minimum of considerable depth at $\sigma \neq 0$,[11] 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 $|\langle S_0^x S_r^x \rangle|$ 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 ($\sigma \lesssim 0.5$), we see a power-law behavior with an exponent that increases monotonically from the exactly known value $\eta_x = 0.769 \ldots$ at $\sigma = 0$, as given by expression (3), to $\eta_x = 1.00$ at $\sigma = 0.25$ and $\eta_x = 1.49$ 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.[4]

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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[8] The upward curvature in the vicinity of $r = N/2$ is an obvious finite-size effect attributable to periodic boundary conditions.

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