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Spin-Spin Correlations in the One-Dimensional Spin-1/2 Antiferromagnetic Heisenberg Chain

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We have calculated the spin-spin correlations in the ground state of spin-1/2, one-dimensional, antiferromagnetic Heisenberg chain numerically. Using improved algorithms, we have been able to perform exact diagonalizations for lattices up to 30 sites and quantum Monte Carlo simulations for lattices up to 512 sites. This extensive range allows us to investigate the logarithmic dependence of spin-spin correlations. We present our results and discuss their implications.

In this paper, we report our numerical studies of spin-spin correlations for the spin-1/2 antiferromagnetic Heisenberg (AFH) model in one dimension. The model, defined by,

$$H = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} \quad (1)$$

has been studied for a long time. The ground state energy and the energy spectrum can be obtained by Bethe Ansatz analytically.¹⁻³ However, the values of spin-spin correlations, except for the nearest¹ and next-nearest neighbors,⁴ are still unknown. Using field theory techniques, Luther and Peschel⁵ proposed that the spin-spin correlation

functions, $S^\alpha(r) \equiv \langle S_0^\alpha S_r^\alpha \rangle$, where $\alpha = x, y, z$, which by spin isotropy should be independent of α , should decay as function of distance as $S^\alpha(r) \equiv S(r)$, where

$$S(r) \approx \frac{(-1)^r}{r} \quad (2)$$

However, it has been speculated for some time that there should be a logarithmic correction to Eq. (2). Recently, Kaplan et. al.^{6,7} showed that, based on their finite lattice calculations, the spin-spin correlation functions behave as

$$S(r) \approx \frac{(-1)^r \ln^\sigma(r)}{r}, \quad (3)$$

and they found that $0.2 < \sigma < 0.3$.

In view of the fairly small systems sizes studied in ^{6,7} -- exact diagonalization results for lattices up to 20 sites and Monte Carlo results for lattices up to 40 sites -- there remains some uncertainty as to the validity of this result. In particular, a recent Monte Carlo study by Liang⁸ of the spin-spin correlations for lattices up to 128 sites found that $\sigma \approx 0$. Thus it seems that a further investigation of this issue is warranted.

To begin we show some of our results for exact diagonalizations of the antiferromagnetic Heisenberg model in one dimension. Recently, we have developed a novel means of implementing the Lanczos method for exact diagonalization of quantum spin models which enables us to carry out numerical studies on substantially larger lattices than previously studied.⁹ For the spin-1/2 rings (i.e., one dimensional lattices with periodic boundary conditions) we were able to calculate a few low-lying excited state energies and the spin-spin correlations for lattices up to 30 sites. We list results for N

= 24, 26, 28, and 30 in Table I. As shown in Table I, the spin-spin correlations, as function of distance, show an oscillation of odd and even sites. Such oscillation is absent for free boundary conditions. We have used the rotational invariant symmetry in spin space to check our results and find the required symmetry. To obtain results for the infinite lattice, we have used the scaling relation, proposed by Kaplan et. al.^{6,7}, that for sufficiently large r and N ,

$$S(r, N) = S(r, \infty) f(r/N) \quad (4)$$

where,

$$f(y) = [1 + 0.28822 \sinh^2(1.6730y)]^{1.75} \quad (5)$$

We have done a few checks on this scaling relation -- such as $S(r, N)/S(r, 2N) = S(2r, 2N)/S(2r, 4N)$, etc. -- and we found that the checks are consistent with our data to four digits. From the scaling relation of Eq. (4), we can obtain the estimates for the infinite chain from each finite lattice data. We then try to fit the data to $a + \frac{b}{N^\alpha}$ by the least square approximations. Comparing with the known exact results for the nearest and next nearest neighbor correlations, $S(1, \infty) = -0.147716^1$ and $S(2, \infty) = 0.060680^4$, we found that $\alpha = 2$ gives a good fit. The spin-spin correlations for the infinite lattice estimated by such a procedure are listed in the last column of Table I.

Another quantity of interest is the the structure factor $S(\pi)$, defined by,

$$S(\pi) \equiv \sum_{r=0}^N (-1)^r \langle S_0^z S_r^z \rangle \quad (6)$$

We also list its values in Table I.

To test for logarithmic corrections to the power law decay of the spin-spin correlations, it is not sufficient to use data for lattices no larger than 30 sites. The maximum separation distance one can get is only 15 sites (because of periodic boundary conditions), and it is impossible to reach any firm conclusion concerning the existence of logarithmic corrections based on results from such short distances. Studies of the spin-spin correlations for larger systems are needed in order to have more convincing answers. Limitations on the sizes of matrices that can be diagonalized prevents us from undertaking diagonalization studies for $N > 30$. Hence we turn to the world line Monte Carlo simulation method.¹⁰, which as we shall see permits us to study very large systems ($N = 512$ sites). According to the well-known Jordan-Wigner transformation,¹¹ the 1-D XXZ model, defined by,

$$H_{xxz} = \sum_i [-2t (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + V S_i^z S_{i+1}^z], \quad (7)$$

can be mapped into a spinless fermion model, defined by,

$$H_{spinless} = \sum_i [-t (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + V (n_i - \frac{1}{2}) (n_{i+1} - \frac{1}{2})], \quad (8)$$

where $c_i^\dagger$ creates an spinless fermion on site i , $n_i = c_i^\dagger c_i$, and S_i^m is the m th component of the spin operator on site i . The interaction consider here is only a nearest neighbor one. This mapping is an exact one if one uses open boundary. For the 1-D rings, the two Hamiltonians differ by a boundary term which causes an error of order $1/N$, where N is the length of the 1-D lattice. Here we consider only the isotropic case, $V = 2t$, which corresponding to the antiferromagnetic Heisenberg model.

Using the path integral formulation we can write the partition function as

$$Z = \text{Tr} e^{-\beta H} = \sum_{i_1, \dots, i_L} \langle i_1 | e^{-\Delta\tau H} | i_L \rangle \langle i_L | e^{-\Delta\tau H} | i_{L-1} \rangle \cdots \langle i_2 | e^{-\Delta\tau H} | i_1 \rangle, \quad (10)$$

where $\{i_1, \dots, i_L\}$ are a set of complete basis states, and we have divided the imaginary-time interval $0 < \tau < \beta$ into L subintervals of width $\Delta\tau = \beta/L$. To calculate the matrix elements in Eq. (10) we use checkboard break up to write $H = H_1 + H_2$, where $H_{1(2)}$ are the sums of Eq. (8) for $i = \text{odd}(\text{even})$, and use the fact that for small $\Delta\tau$,

$$e^{\Delta\tau H} = e^{\Delta\tau H_1} e^{\Delta\tau H_2} [1 + O(\Delta\tau^2)]. \quad (11)$$

The summations over all complete sets of states are done by the heat-bath algorithm. To test our approach we have done Monte Carlo simulations for smaller size of rings ($N = 24, 28$), as listed in Table II. Comparison with the exact values in Table I., makes clear that the agreement is quite good, although not perfect.

The sources of the discrepancies between Table I and Table II arise from several features of the world line Monte Carlo method: nonzero temperature due to finite β values in Eq. (9) and (10), discreteness effects in the imaginary time variable ($\Delta\tau$), the extra boundary term mentioned above, our restriction to the zero winding number sector in the fermion world lines¹⁰, and the statistical errors inherent in the Monte Carlo method. We have analyzed each source of error independently. Both the finite β and $\Delta\tau$ effects can be corrected by straightforward extrapolations. To examine the effect

of the extra boundary term discussed above we have compared the two models (spin and fermion) with fixed boundary conditions for small lattice and found good agreement. The reasons that we did not do exact diagonalization studies or Monte Carlo simulations for lattices larger than 24 sites with fixed boundary conditions is that we have to use the ring symmetry to (1) reduce computer memory requirements for exact diagonalizations and (2) permit vectorization of the Monte Carlo code. Concerning the error introduced by performing the Monte Carlo simulation in zero winding number sector, we note that Hirsch et. al.¹⁰ have shown that nonzero winding number sectors contribute substantially only for small lattices; for large lattices, this error is negligible.

In the end we find that all the systematic errors are small and can in principle be corrected by various scaling methods. However, the Monte Carlo statistical error, even though only 1 percent or smaller, prevents an accurate extrapolation of spin-spin correlations for an infinite lattice at zero temperature. We believe it is inadequate to use our raw Monte Carlo data to obtain the ground state spin-spin correlations and hence to test directly for logarithmic corrections to Eq. (2). However, there is an alternate way of testing the behavior of ground state spin-spin correlations which suppresses these statistical effects. Specifically, if the spin-spin correlations behaves as in Eq. (4), then the structure factor at wave vector π , $S(\pi)$, will behave, as a function of lattice size N , as

$$S(\pi) = \sum_{r=1}^N \frac{\ln^{\sigma} r}{r} \approx \ln^{1+\sigma}(N) . \quad (12)$$

Note that the errors in $S(\pi)$ are small enough to give quite an accurate estimate of the

value of σ . We have calculated $S(\pi)$ for $N < 30$ by using Monte Carlo simulations, as listed in Table II., and they agree with the results obtained by exact diagonalization within statistical error of 1 percent. In Fig. 1 we plot $S(\pi)$ versus $\ln(N)$ for lattices up to 512 sites and it shows a linear behavior, suggesting that $\sigma = 0$, as predicted by Luther and Peschel.⁵ and consistent with the recent results of Liang⁸ but in disagreement with the earlier value ($0.2 < \sigma < 0.3$) obtained by Kaplan et al.^{6,7}. We believe that the discrepancy arises from the small sizes of the lattices studied by this last group.

In summary, we have studied the spin-spin correlations of one dimensional anti-ferromagnetic Heisenberg model by exact diagonalization method for lattices up to 30 sites and by the world line Monte Carlo simulation method for lattices up to 512 sites. We have used the scaling relation proposed by Kaplan et. al.^{6,7} to obtain the estimates of the spin-spin correlations for the infinite lattice. By studying the behavior of the structure factor $S(\pi)$, we found that the original Luther and Peschel prediction⁵ of a power law decay of $S(r)$ as function of distance is consistent with our data.

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Table Captions

Table I.: Spin-spin correlations and structure factor $S(\pi)$ (Eq. (6)) of the one dimensional spin-1/2 antiferromagnetic Heisenberg model for $N = 24, 26, 28$, and 30 . Data obtained by exact diagonalization method.

Table II.: Spin-spin correlations and structure factor $S(\pi)$ (Eq. (6)) of the one dimensional spin-1/2 antiferromagnetic Heisenberg model for $N = 24$, and 28 . Data obtained by world line Monte Carlo simulation method. Numbers appear in parentheses are statistical errors.

Figure Captions

Fig.1: Structure factor $S(\pi)$, defined by Eq. (6), versus $\ln(N)$ for $4 \leq N \leq 512$. It shows a linear behavior.

Table I

	N = 24	N = 26	N = 28	N = 30	N = ∞
$\langle S_0^\alpha S_1^\alpha \rangle$	-0.148195	-0.148124	-0.148067	-0.148022	-0.147715
$\langle S_0^\alpha S_2^\alpha \rangle$	0.061142	0.061072	0.061018	0.060973	0.060676
$\langle S_0^\alpha S_3^\alpha \rangle$	-0.051416	-0.051239	-0.051100	-0.050988	-0.050242
$\langle S_0^\alpha S_4^\alpha \rangle$	0.035917	0.035723	0.035571	0.035450	0.034647
$\langle S_0^\alpha S_5^\alpha \rangle$	-0.032947	-0.032627	-0.032377	-0.032177	-0.030880
$\langle S_0^\alpha S_6^\alpha \rangle$	0.026657	0.026308	0.026037	0.025821	0.024443
$\langle S_0^\alpha S_7^\alpha \rangle$	-0.025611	-0.025106	-0.024716	-0.024409	-0.02040
$\langle S_0^\alpha S_8^\alpha \rangle$	0.022301	0.021752	0.021331	0.021000	0.018976
$\langle S_0^\alpha S_9^\alpha \rangle$	-0.022165	-0.021412	-0.020842	-0.020400	-0.017753
$\langle S_0^\alpha S_{10}^\alpha \rangle$	0.020238	0.019415	0.018798	0.018322	0.015551
$\langle S_0^\alpha S_{11}^\alpha \rangle$	-0.020731	-0.019624	-0.018809	-0.018189	-0.014677
$\langle S_0^\alpha S_{12}^\alpha \rangle$	0.019621	0.018402	0.017514	0.016844	0.013166
$\langle S_0^\alpha S_{13}^\alpha \rangle$		-0.019084	-0.017916	-0.017053	-0.012494
$\langle S_0^\alpha S_{14}^\alpha \rangle$			0.017119	0.016179	0.011418
$\langle S_0^\alpha S_{15}^\alpha \rangle$				-0.016701	-0.011249
$S(\pi)$	1.204260	1.230689	1.255309	1.278358	

Table II.

	N = 24	N = 28
$\langle S_0^\alpha S_1^\alpha \rangle$	-0.149(1)	-0.149(1)
$\langle S_0^\alpha S_2^\alpha \rangle$	0.063(2)	0.062(2)
$\langle S_0^\alpha S_3^\alpha \rangle$	-0.051(2)	-0.052(2)
$\langle S_0^\alpha S_4^\alpha \rangle$	0.035(1)	0.036(1)
$\langle S_0^\alpha S_5^\alpha \rangle$	-0.032(1)	-0.033(1)
$\langle S_0^\alpha S_6^\alpha \rangle$	0.026(1)	0.027(1)
$\langle S_0^\alpha S_7^\alpha \rangle$	-0.025(1)	-0.025(1)
$\langle S_0^\alpha S_8^\alpha \rangle$	0.021(1)	0.022(1)
$\langle S_0^\alpha S_9^\alpha \rangle$	-0.021(1)	-0.021(1)
$\langle S_0^\alpha S_{10}^\alpha \rangle$	0.019(1)	0.019(1)
$\langle S_0^\alpha S_{11}^\alpha \rangle$	-0.018(2)	-0.019(1)
$\langle S_0^\alpha S_{12}^\alpha \rangle$	0.017(2)	0.018(1)
$\langle S_0^\alpha S_{13}^\alpha \rangle$		-0.018(1)
$\langle S_0^\alpha S_{14}^\alpha \rangle$		0.017(1)
$S(\pi)$	1.214(11)	1.268(16)

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