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Correlation functions in periodic chains

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We present a simple form for the relation between correlation functions on finite periodic one-dimensional systems and the correlation function of the corresponding infinite system. This form is tested on the $S=\frac{1}{2}$ and $S=1$ Heisenberg models. We find good agreement with quantum Monte Carlo results for the spin correlation functions. For $S=\frac{1}{2}$ our results are consistent with the asymptotic form $C(r)\sim\ln(r)^{\sigma}/r$ with $\sigma=\frac{1}{2}$.

Numerical techniques such as exact diagonalization and quantum Monte Carlo can provide exact results for the properties of finite interacting quantum many-particle systems. However, one is limited to relatively small system sizes by available computer resources. Currently, exact diagonalization can be used for on the order of 10–30 particles, whereas quantum Monte Carlo allows for studies of systems roughly an order of magnitude larger. This is still far from the thermodynamic limit, and great care must be taken in extrapolating to infinite system size. For this, the theory of finite-size scaling has been developed.[1] However, for the one-dimensional (1D) $S=\frac{1}{2}$ antiferromagnetic Heisenberg model, attempts to extract the asymptotic form of the spin correlation function from quantum Monte Carlo data have not yielded the form predicted by theory.[3–6] Theoretically, it is now well established that the long-distance correlation function of this model is [3,4]

$$C_{\infty}(r\rightarrow\infty)\sim\ln(r)^{\sigma}/r\ , \tag{1}$$

with $\sigma=\frac{1}{2}$. For the finite-size scaling of the correlation function $C(r,N)$ in a system of N spins, Kaplan *et al.* proposed the relation[2]

$$C(r,N)=C_{\infty}(r)f(r/N)\ . \tag{2}$$

This scaling relation has been used by several authors[5,6] to extrapolate quantum Monte Carlo data for the $S=\frac{1}{2}$ Heisenberg model. The asymptotic form obtained in this way is consistent with the form (1), but with an exponent σ in the log correction which is significantly less than $\frac{1}{2}$, or even 0.[5,6] In this paper, we propose a simple form relating the correlation functions in finite periodic chains to the correlation function of the corresponding infinite system. We test the relation on the $S=\frac{1}{2}$ and $S=1$ antiferromagnetic Heisenberg models, and argue that the reason why previous numerical studies of the $S=\frac{1}{2}$ Heisenberg model have not yielded the correct exponent σ is that the log correction in (1) makes (2) invalid for this model.

Our hypothesis is that in a periodic chain of N sites, the correlation between some quantity at site i and site $i+r$ is built up from correlations between site i and all the images of site $i+r$ due to the periodic boundary conditions. The observed correlation function at distance r is proportional to a sum of correlation functions $C_{\infty}(r')$ of the infinite system at distances $r'=kN+r$ and $r'=(k+1)N-r$, with $k=0,1,2,\ldots$, each term being exponentially damped. The damping is governed by a size- and temperature-dependent correlation length $\xi(T,N)$. We propose that the above mechanism is responsible for the dominant finite-size corrections to the correlation function in periodic chains. In a trivial case, 1D Ising model, the correlation function can be written exactly in the form given by this hypothesis. For the $S=\frac{1}{2}$ and $S=1$ Heisenberg models we find good agreement with exact diagonalization and quantum Monte Carlo results. In particular, for $S=\frac{1}{2}$ our results are consistent with $\sigma=\frac{1}{2}$ in (1).

We now discuss the above hypothesis in detail. First consider models for which the ground-state correlation function $C_{\infty}(r)$ decays slower than exponentially. At finite temperature the correlations are exponentially damped. The hypothesis is then that the long-distance correlation function $C(r,T,N)$ for a periodic system at low temperature is given approximately in terms of the $T=0$ correlation function $C_{\infty}(r)$ of the infinite system, according to

$$C(r,T,N)=A(T,N)\sum_{k=0}^{\infty}\{C_{\infty}(kN+r)e^{-(kN+r)/\xi(T,N)}+C_{\infty}([k+1]N-r)\times e^{-([k+1]N-r)/\xi(T,N)}\}\ . \tag{3}$$

For a system which is critical at $T=0$, such as the spin-S antiferromagnetic Heisenberg model with half-integer S,[7] one expects $\xi(T,N)$ to obey the scaling relation[1]

$$\xi(T,N)=\xi_{\infty}(T)f[\xi_{\infty}(T)/N]\ , \tag{4}$$

where $\xi_{\infty}(T)$ is the correlation length of the infinite system. As $T\rightarrow 0$, this scaling relation implies $\xi(T=0,N)\sim N$. For models with long-range order at $T=0$, such as the 1D Ising model, one expects $\xi(T,N)$ to diverage as $T\rightarrow 0$.

For models with exponentially decaying correlations even at $T=0$, such as the integer-S Heisenberg model,[6–9] the form (3) is not suitable. In this case, where the infinite-N correlation function is a function of a correlation length ξ_∞, we propose the low-temperature form

$$C(r,T,N)=A(T,N)\sum_{k=0}^{\infty}\{C_\infty[kN+r,\xi(T,N)]+C_\infty[k(N+1)-r,\xi(T,N)]\}\ , \tag{5}$$

with $\xi(T,N\to\infty)=\xi_\infty(T)$.

The relations (3) and (5) are constructed so that the modification of the correlation function arising from the periodic boundary conditions described above is taken into account. In particular, it seem natural that in a periodic system, correlations from distances r and $N-r$ should be treated on an equal footing, and when trying to fit numerical data to a theoretical form $C'(r,N)$, one should have $C'(r,N)=C'(N-r,N)$. In the remainder of this paper we present evidence supporting our hypothesis for three specific 1D models.

As a trivial example, we first discuss the 1D Ising model. In a periodic system of N sites the spin correlation function is

$$C^I(r,T,N)=(\Theta^r+\Theta^{N-r})/(1+\Theta^N)\ , \tag{6}$$

where $\Theta=\tanh(J/[k_BT])$, J being the coupling constant. For the infinite system, $C^I_\infty(r,T)=\Theta^r$. Owing to the form of C^I_∞, Eq. (6) can also be written as

$$C^I(r,T,N)=\frac{1-\Theta^N}{1+\Theta^N}\sum_{k=0}^{\infty}(\Theta^{kN+r}+\Theta^{[k+1]N-r})\ . \tag{7}$$

As $T\to 0$, C^I has the form (3) with $\xi(T,N)=\frac{1}{2}e^{2J/(k_BT)}$, independently of N. The form (3) might suggest that only the terms with $k=0$ are needed in (3). However, below we will present results for the $S=\frac{1}{2}$ Heisenberg model, indicating that in this case, terms with $k\neq 0$ are also important.

The 1D antiferromagnetic Heisenberg model is defined by the Hamiltonian

$$H_S=\frac{3J}{S(S+1)}\sum_{i=1}^{N}\mathbf{S}_i\cdot\mathbf{S}_{i+1}\ , \tag{8}$$

with $J>0$. In view of Haldane's conjecture,[7] we expect (3) and (5) to be the relevant relations for half-integer and integer S, respectively. In order to test the validity of our hypothesis, we have calculated the spin correlation function

$$C^{H_S}(r,N)=[3/S(S+1)]\langle S_i^zS_{i+r}^z\rangle \tag{9}$$

in periodic systems for spins $S=\frac{1}{2}$ and $S=1$. We have used a generalization[10] of Handscomb's[11] quantum Monte Carlo technique in the subspace with $\Sigma_iS_i^z=0$, choosing inverse temperatures $\beta=J/(k_BT)$ large enough to obtain ground-state results. There are no approximations in the Monte Carlo method, so all results should be exact within statistical errors.

For $S=\frac{1}{2}$, we have run the simulations at inverse temperatures up to $\beta\approx 1.5\times N$, which is large enough for all measured quantities to be essentially independent of β. Exact diagonalization results for this model are available for N up to 30.[12] Figure 1 shows Monte Carlo results for the correlation function multiplied by $(-1)^rr$ with $N=30$ at $\beta=40$, along with the exact results. The even-odd oscillations are predicted by theory to be due to a term $-1/(\pi r)^2$.[13] In the results to be presented next, we subtract the contribution to the correlation function arising from this term, treating it according to the summation hypothesis (3), with $\xi(T=0,N)=\infty$ and $A(T=0,N)=1$. That is, we subtract

$$C_2(r,N)=-\frac{1}{\pi^2}\sum_{k=0}^{\infty}\left[\frac{1}{(kN+r)^2}+\frac{1}{[(k+1]N-r)^2}\right]. \tag{10}$$

We divide the remainder of the calculated correlation function by the expected asymptotic form (1), so that as $N\to\infty$, results for $1\ll r\ll N$ should approach a constant $A(0,N=\infty)$. Thus we plot

$$D(r,N)=(-1)^r[r/\ln(r)^{1/2}][C^{H_{1/2}}(r,N)-C_2(r,N)]\ . \tag{11}$$

Using the asymptotic form (1) with $\sigma=\frac{1}{2}$ and determining $A(0,N)$ and $\xi(0,N)$ such that the form (3) gives a good fit to the long-distance correlation function, we find the optimum correlation length to be $\xi(0,N)=N$ within less than a percent for all system sizes studied, in agreement with the implication of the scaling law (4). We therefore fix $\xi(0,N)=N$, and are left with the amplitude $A(0,N)$ as the only free parameter. Figure 2 shows exact data for $N=30$[12] and our Monte Carlo results for $N=40,60$, and 80, along with curves given by the relation (3). The agreement is good in the large-r regimes. The even-odd oscillations are almost canceled by the subtraction of $C_2(r)$. We stress that the shapes of the theoretical curves in Fig. 2 are completely determined by (3), once $\xi(0,N)=N$ is fixed; only the amplitudes are chosen to give the best agreement with the numerical data. Treating σ as a free parameter as well, the optimum value of σ is slightly less than $\frac{1}{2}$, but larger than

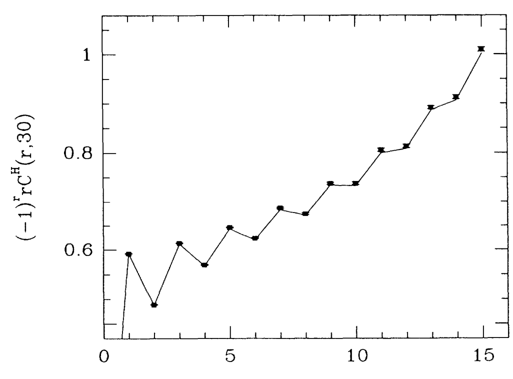

FIG. 1. Exact and Monte Carlo results for the spin correlation function in a periodic spin-$\frac{1}{2}$ Heisenberg chain with 30 spins. The squares are the Monte Carlo results. The solid line goes through the exact results of Ref. 12.

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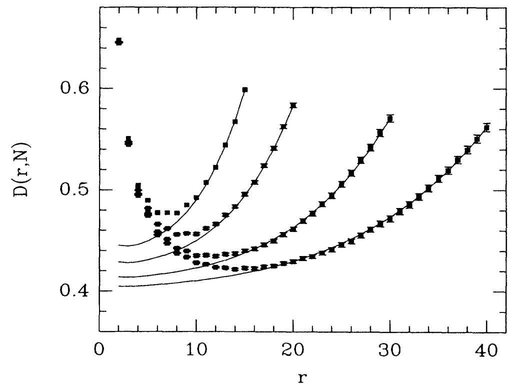

FIG. 2. The correlation function $D(r,N)=(-1)^r[r/\ln(r)^{1/2}][C^{H_{1/2}}(r,N)-C_2(r,N)]$ in systems of 30, 40, 60, and 80 sites (squares), along with the theoretical form (3) (solid curves). The largest r for given N is $N/2$. Here the correlation length is fixed, $\xi(0,N)=N$, and the log exponent $\sigma=\frac{1}{2}$. The only free parameter is the amplitude in (3). The data points for $N=30$ are exact results of Ref. 12. The data points for $N=40$, 60, and 80 are our quantum Monte Carlo results.

0.45 in all the cases studied here. As N grows, the optimum value of the exponent seems to approach $\frac{1}{2}$. Figure 3 shows the $N=60$ and 80 results along with the form (3) with $\sigma=0.4,0.5$, and 0.6. Apparently, $\sigma=0.5$ gives the closest match. In the same figure, we also plot the curves obtained using only the $k=0$ terms in (3) with $\sigma=0.5$. This does not lead to nearly as good an agreement with the Monte Carlo data as using also $k=1,2,\ldots$.

It appears that the spin correlaion function of the spin-$\frac{1}{2}$ Heisenberg model is indeed well described by the form (3), with the asymptotic form (1) having $\sigma=\frac{1}{2}$. Dividing Eq. (3) by the asymptotic form (1), it is clear that the log correction makes the scaling relation (2) invalid if (3) holds in the limit $N\rightarrow\infty$.

We now turn to the case $S=1$ and the proposed relation (5). Haldane conjectured[7] that the integer-S Heisenberg model has a gap between the ground state and the exited states, and that the correlation function decays exponentially. This has been confirmed numerically in several studies of the case $S=1$.[6,8,9] Nomura[9] proposed that the correlation function is actually given by the modified Bessel function $K_0(r/\xi)$, which asymptotically behaves like $e^{-r/\xi}r^{-1/2}$. This form agrees with numerical data for periodic chains,[9] except for $r\approx N/2$. This motivates us to test the relation (5) with $C_\infty=K_0$:

$$C^{H_1}(r,N)=A(N)\sum_{k=0}^{\infty}\left[K_0\left[\frac{(kN+r)}{\xi(N)}\right]+K_0\left[\frac{(kN+N-r)}{\xi(N)}\right]\right]. \qquad (12)$$

For the $S=1$ Heisenberg model exact data are available for N up to 18.[12] Figure 4 shows exact data for $N=16$ and 18,[12] and our Monte Carlo results for $N=32$. The form (12) seems to fit the data very well for $r\geq 4$, even for the smaller systems. We obtain an N-dependent correlation length $\xi(16)=5.8$, $\xi(18)=5.9$, and $\xi(32)=6.5$. The correlation length for $N=32$ is slightly larger than previous Monte Carlo results[6,8,9] ($\xi=6.2$ for $N=64$[6,9]), but agrees with White's result[14] for the correlation length of correlations with a spin-$\frac{1}{2}$ operator at the end of an open chain.

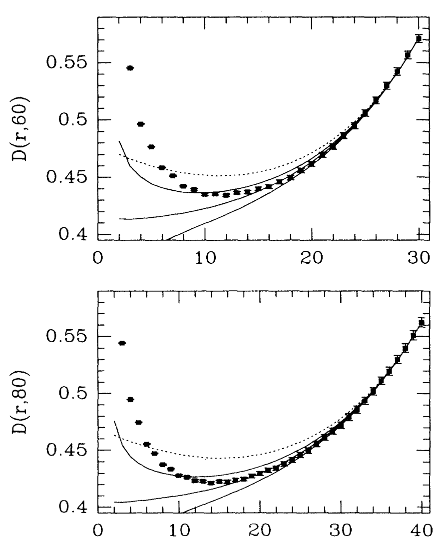

FIG. 3. The correlation functions $D(r,N=60)$ and $D(r,N=80)$ (squares), along with the theoretical form (3) with σ varying. The solid lines are for $\sigma=0.4,0.5$, and 0.6 (top to bottom in each graph). The dotted lines are for $\sigma=0.5$, with only the $k=0$ terms kept in (3).

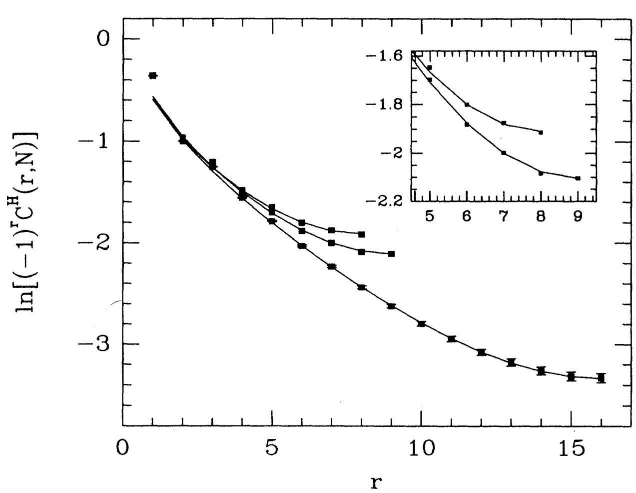

FIG. 4. The logarithm of the spin correlation function in periodic $S=1$ Heisenberg chains with 16, 18, and 32 sites (squares), along with the theoretical form (12) (solid curves). The amplitude and correlation length in (12) are chosen to give the best agreement with the numerical results for each N. Data for 16 and 18 are exact results from Ref. 12, and are shown on a different scale in the inset.

In conclusion, we have presented a hypothesis for the relation between correlation functions in finite periodic chains and the correlation function of the corresponding infinite system. In order to test the hypothesis, we have used a quantum Monte Carlo technique to calculate the spin correlation function of the antiferromagnetic Heisenberg models with $S=\frac{1}{2}$ and 1. We find good agreement with the proposed relations. In particular, our results are consistent with an exponent $\sigma=\frac{1}{2}$ in the log correction of the asymptotic correlation function (1) for $S=\frac{1}{2}$.

We have also tested our hypothesis for the 1D Hubbard model at low temperatures.[15] We find good agreement in this case as well.

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