Monte Carlo Calculations of the Correlation Functions for Heisenberg Spin Chains at $T=0$

Shoudan Liang
Department of Physics and Materials Research Laboratory, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801
(Received 11 October 1989)

We compute the ground-state spin-spin correlation function for the one-dimensional antiferromagnetic Heisenberg model of spin $\frac{1}{2}$, 1, and $\frac{3}{2}$. The spin-1 chain has a disordered ground state with a correlation length of 6.2 lattice spacings whereas the spin-$\frac{1}{2}$ and the spin-$\frac{3}{2}$ chains both have $[\ln(r)]^{\sigma}/r$ decaying correlation functions. The logarithmic corrections are different for the spin-$\frac{1}{2}$ and the spin-$\frac{3}{2}$ chains. Finite-size scaling is used to analyze the data for chains of up to 128 spins.

PACS numbers: 75.10.Jm, 05.70.Ln, 75.50.Ee

From recent field-theoretical analysis of quantum spin chains,[1] a clear picture has emerged. For the antiferromagnetic Heisenberg model, it is argued using approximate mappings that integer-spin chains have gaps in the excitation spectrum while the half-integer-spin chains do not have gaps. Furthermore, it is shown that the low-energy behaviors of half-integer spin chains all belong to the same universality class described by the O(3) nonlinear σ model with a topological term $\theta=\pi$ (Ref. 2) or equivalently[3] by the Wess-Zumino-Witten (WZW) model with topological coupling $k=1$. The latter model can be exactly solved.[4] The ground-state spin-spin correlation function decays as $(-1)^r/r$. In addition, according to recent developments in conformal field theory,[5] the leading logarithmic correction to this critical behavior is also universal and the correlation function at large distance is given by $(-1)^r[\ln(r)]^{1/2}/r$. It is important to verify this picture by comparing with numerical results on finite chains.

In this Letter, we obtain the ground-state spin-spin correlation functions for the Heisenberg model of spin $\frac{1}{2}$, 1, and $\frac{3}{2}$ for chains. Our calculations show that for the spin-1 chain with 64 spins, the correlation function decays exponentially with a correlation length $\xi=6.2$. For the spin-$\frac{1}{2}$ and the spin-$\frac{3}{2}$ chains of length 128, after a finite-size scaling analysis, the correlation functions are best fitted by the form $(-1)^r[\ln(r)]^{\sigma}/r$. The algebraic decay is in agreement with the Haldane conjecture that the half-integer-spin chains are all in the same universality class. The exponents of the logarithmic correction, however, are different for the spin-$\frac{1}{2}$ ($\sigma=0$) and for the spin-$\frac{3}{2}$ ($\sigma=0.85$) chains. Both exponents are different from the predicted universal value $\frac{1}{2}$.

Using our method discussed below, it is also possible to compute the lowest energy in any total spin sector (the ground state is in the zero total spin sector). From these energies, the zero-temperature magnetic susceptibility can be determined. The susceptibility is related[6] to the topological coupling k in the mapping[7] to the WZW model. Also from the finite-size correction of the ground-state energy, we can obtain the conformal anomaly parameter c which is related to the low-temperature specific heat.[8] In this Letter, however, we will concentrate on the correlation functions.

Our strategy for obtaining the ground-state properties of a finite system is to search first for a good trial wave function, and then project it into the ground state. The trail wave function is expanded in the valence-bond basis[9] which preserves the SU(2) symmetry of the Hamiltonian.

In order to use spin-$\frac{1}{2}$ valence-bond technology for arbitrary spins, we first map the Hamiltonian of a spin-s chain of length L to the one for a spin-$\frac{1}{2}$ system on a $2s\times L$ lattice. For this purpose, a spin-s angular momentum operator is written as $\mathbf{s}=\frac{1}{2}S\sum_{a=1}^{2s}\boldsymbol{\sigma}_a S$, where $\boldsymbol{\sigma}_a$ are Pauli matrices and S is the symmetrization operator $S=[1/(2s)!]\sum_P P$, with the sum over all possible permutations of $2s$ spins. It is easy to show that $[\mathbf{s},S]=0$ and also $S^2=S$. The Heisenberg Hamiltonian becomes

$$H=J\sum_{\langle i,j\rangle}\mathbf{s}_i\cdot\mathbf{s}_j=(J/4)\sum_{a,b}\sum_{\langle i,j\rangle}\boldsymbol{\sigma}_{ia}\cdot\boldsymbol{\sigma}_{jb}S_iS_j\,, \tag{1}$$

where i and j are the nearest neighbors and a and b run from 1 to $2s$. With this Hamiltonian, a spin-s chain of length L is equivalent to a spin-$\frac{1}{2}$ system on a lattice with $2s$ rows and L columns. Since only the states that are totally symmetric in $\boldsymbol{\sigma}_a$ represent the spin-s states, the wave function must be symmetrized for each column.

It is crucial in our method to start with a good trial wave function before projecting to the ground state. We use the spin-$\frac{1}{2}$ valence-bond basis. Since the couplings in (1) are between even and odd sublattices, the ground-state wave function satisfies the Marshall sign convention.[10] In the singlet subspace, we adopt the following approximation:[9]

$$|\phi_{\rm tr}\rangle=\sum_{\substack{\mathbf{i}_a\in\text{ even}\\ \mathbf{j}_a\in\text{ odd}}}h(|\mathbf{i}_1-\mathbf{j}_1|)\cdots h(|\mathbf{i}_n-\mathbf{j}_n|)\times(\mathbf{i}_1,\mathbf{j}_1)\cdots(\mathbf{i}_n,\mathbf{j}_n)\,, \tag{2}$$

where $\mathbf{i}=\{l,a\}$ labels a site at the lth column and the ath

TABLE I. Listed are the best variational parameters $h(l)$ and the corresponding variational energies for the wave function in Eq. (2) for spin $\frac{1}{2}$, 1, and $\frac{3}{2}$. The parametrization is discussed in the text. For comparison, the ground-state energies per site computed by our projection method are also listed. The energies are in the units of J. The numbers in parentheses are the estimated errors. Thus, $-0.4416(1)$ means -0.4416 ± 0.0001.

Spin	L	$h(3)$	$h(5)$	$h(7)$	α	β	Variational energy	Ground-state energy
$\frac{1}{2}$	128	0.207	0.098	0.071	0.157	−0.114	−0.4416(1)	−0.4432(5)
1	64	0.215	0.108	0.048	0.29	−0.29	−1.401(1)	−1.402(1)
$\frac{3}{2}$	128	0.188	0.075	0.045	0.223	−0.202	−2.829(1)	−2.830(5)

row; (i,j) denotes a singlet bond from i to j with i (j) belonging to the even (odd) sublattice; and $h(|\mathbf{i}-\mathbf{j}|)$ is a positive variational parameter for (i,j). The wave function is symmetrized for each column if the weight h depends only on the column label l and not on the row label a. Then permuting spins in each column does not change the wave function.

The wave function in Eq. (2) with $h=1$, independent of the length of a bond, is the Néel state (projected onto the singlet subspace) with long-range correlations and an energy $-Js^2$ per site. We reduce the range of $h(l)$ to optimize the energy using rules for valence-bond states and a Monte Carlo method described in Ref. 9.

In the Monte Carlo calculations, valence-bond configurations are sampled from the multidimensional sum of the wave function according to the positive weight function $h(l)$. The basic process is to choose two sites from next-nearest-neighbor columns at random and attempt an exchange of the bonds connected with the sites. A transition to the new configuration is then made with the probability of the ratio of the weights for the new and the old configurations. The best bond amplitude $h(l)$ is found by the steepest-descent method as the derivatives of the energy can also be computed directly. Since the energy is insensitive to the bond amplitude $h(l)$ at large distances, we set $h(l)=\alpha\exp(-\beta l)$ for $l>l_c$. For smaller l, $h(l)$ are free parameters. Notice that $h(l)=0$ for even l because no bonds are allowed between sites on the same sublattice. Also, setting $h(1)=1$ fixes the normalization constant for the wave function.

The optimized values of $h(l)$ with $l_c=7$ along with the corresponding energies are listed in Table I. For large spins the variational energy is closer to the ground-state energy suggesting that the trial wave function in Eq. (2) is a good description for large s.

After obtaining a good trial wave function, we project it to the ground state. Starting with $|\phi_{\rm tr}\rangle=c_0|E_0\rangle+c_1|E_1\rangle+\cdots$, we define

$$|n\rangle=(H-W)^n|\phi_{\rm tr}\rangle=c_0(E_0-W)^n\{|E_0\rangle+c_1/c_0(E_1-W)^n/(E_0-W)^n|E_1\rangle+\cdots\},$$

where W is a constant. The state $|n\rangle$ approaches the ground state for large n provided that $|(E-W)/(E_0-W)|<1$ for all the states in the energy spectrum. It can be shown that this condition is satisfied for any $W>(E_0+JLs^2)/2$ because the energy spectrum is bounded from both above and below: $E_0<E<JLs^2$, where E_0 $(-JLs^2)$ is the ground state of the antiferromagnetic (ferromagnetic) Heisenberg Hamiltonian.

If W is set equal to JLs^2, we have

$$H-W=J\sum_{\langle i,j\rangle}(\sigma_i\cdot\sigma_j-1)/4=J\sum_{\langle i,j\rangle}Q_{ij},$$

and Q_{ij} is simple to operate on the valence-bond states: $Q_{ij}(i,j)=-(i,j)$ and $Q_{ij}(i,l)(k,j)=-(i,j)(k,l)/2$. Thus after projecting with Q_{ij}, the valence-bond structure is preserved. A Monte Carlo algorithm is similarly implemented except now we also need to sample over the products of Q's coming from expanding $(J\sum_{\langle i,j\rangle}Q_{ij})^n$. In the Monte Carlo calculations, sampling over the wave function and sampling over the products are mixed. Most of the computer time is spent on the latter. We have checked that the final results do not depend on the ratio of the two types of sampling which is typically 16 in our calculations. All the data reported here were averaged over 16 runs with independent starting configurations and random-number seeds. Statistical errors were also estimated from the same set of data.

The correlation functions

$$C_n(r,L)=(-1)^r\frac{\langle n|\mathbf{s}_0\mathbf{s}_r|n\rangle}{\langle n|n\rangle}$$

for the state $|n\rangle$ defined earlier for a chain of length L can be fitted to the formula

$$C_n(r,L)=C(r,L)+\delta(r,L)\exp(-\Delta n) \quad (3)$$

to obtain the ground-state correlation functions $C(r,L)$. Δ is given by $\exp(-\Delta)=|(E_{\rm ext}-W)/(E_0-W)|$, where $E_{\rm ext}$ is the first excitation energy. For a fixed Δ, we determine $C(r,L)$ and $\delta(r,L)$ from the raw data for $C_n(r,L)$ vs n by a linear least χ^2 fit. The best Δ is then determined by minimizing the total error.

Spin 1.—The ground-state correlation function for the spin-1 chain of length 64 is shown in Fig. 1 and is found to decay to zero almost exponentially. Nomura[11] sug-

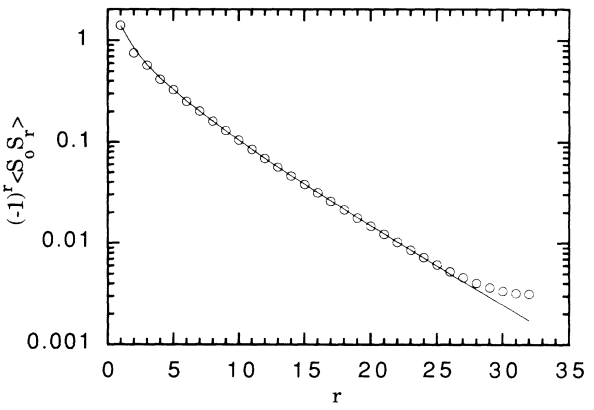

FIG. 1. The circles are the ground-state correlation function for the spin-1 chain of length 64. The line is a fit by the form $a\sqrt{r}\exp(-r/\xi)$. The correlation length ξ is 6.2 ± 0.1. The statistical errors are much smaller than the size of the circles.

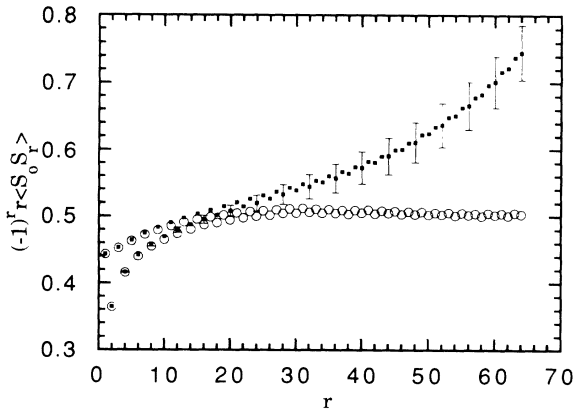

FIG. 2. The solid squares are the ground-state correlation function multiplied by the distance $(-1)^r r\langle s_0 s_r\rangle$ for the spin-$\frac{1}{2}$ Heisenberg chain of length 128. The circles are the correlation function in the thermodynamic limit extracted after a finite-size scaling analysis. The oscillation with even and odd r is consistent with the prediction of conformal field theory. The errors come from two sources with roughly equal magnitudes: statistical error in computing the raw data and the uncertainty in fitting by Eq. (3) which is set to be 3% of $\delta(r,L)$ in Eq. (3).

gested adding a prefactor $\sqrt{r}$ to correct the slight deviation from the pure exponential decay. Fitting by the form $a\sqrt{r}\exp(-r/\xi)$, where a and ξ are constants, we get $\xi=6.2$ which is identical to the value obtained by Nomura.[11] The ground-state energy per site $E_0/LJ=-1.40\pm0.001$ is very close to the previous estimates.[12,13]

The correlation functions were computed from $C_n(r,L)$ with Δn ranging from 1 to 6. Since in this case the best Δ was difficult to determine from the data, we used the known energy gap[12] $E_{\rm ext}-E_0=0.41J$ in the fit.

Spin $\frac{1}{2}$.—The ground-state energy per site calculated for the spin-$\frac{1}{2}$ chain of length 128 is -0.4432 ± 0.0005 which agrees with the exact value from the Bethe *Ansatz* $-\ln2+\frac{1}{4}=-0.4431$.

For a finite system there is a gap to the excited states which goes to zero in the thermodynamic limit. The best energy gap determined using the procedure described above scales with the length of the chain L as $E_{\rm ext}-E_0=41J/L$ for $L=16$, 64, and 128. This, when compared with the energy levels for the zero-momentum singlet excitations of the $k=1$ WZW model,[5] $E_l-E_0=(\pi^2/L)l$ ($l=2,4,\ldots$), shows that the lowest excitation in our trial wave function is very close to the second excited state rather than the first one. This is because the excited state in question must have the same symmetry as the ground state. Thus, the excited state must be not only a singlet with zero momentum[14] but also even under the reflection. Assuming the fitting parameter Δ in Eq. (3) is determined by $E_{\rm ext}-E_0=4\pi^2/L$, we obtain the ground-state correlation functions $C(r,L)$ for $L=64$ and 128 with Δn ranging from 1 to 3 using a linear least χ^2 fit.

To extract the correlation functions in the thermodymamic limit, we assume the following finite-size scaling first proposed by Kaplan, Horsch, and Borysowicz,[15]

$$C(r,L)=C(r,\infty)f(r/L),\quad r,L\to\infty, \tag{4}$$

where $f(x)$ is a smooth function with $f(x)\to1$ for small x. The functions $C(r,\infty)$ and $f(r/L)$ are determined by fitting $C(r,64)$ and $C(r,128)$ by Eq. (4). The finite-size scaling is valid for a system near a critical point. We have checked that for both $s=\frac{1}{2}$ and $\frac{3}{2}$ the correlation functions for a finite chain $C(r,L)$ at $L=32$, 64, and 128 are fitted by Eq. (4) with an accuracy of 1%.

After finite-size correction, $rC(r,\infty)$ is plotted in Fig. 2 along with the raw data $rC(r,128)$. The oscillation of even and odd sites can be fitted by $-0.25/r^2$, in agreement with the conformal field theory.[8] For r smaller than 20, our data $C(r,\infty)$ agree with the previous calculation of Kubo, Kaplan, and Borysowicz[16] who found that the correlation function in that range is described by $[\ln(r)]^\sigma/r$ with $\sigma=0.2$ to 0.3. At larger distances, however, our data suggest a smaller logarithmic correction with $\sigma=0$.

Spin $\frac{3}{2}$.—Using the same procedure as described for the spin-$\frac{1}{2}$ case, an energy gap of $45J/L$ is obtained for chains of length 32, 64, and 128. The energy gap for a finite lattice is slightly larger than the gap for the spin-$\frac{1}{2}$ chain because the logarithmic corrections are stronger.[17] Using the finite-size scaling hypothesis, Eq. (4), we get the correlation function $C(r,\infty)$ from raw data $C(r,64)$ and $C(r,128)$. We have tried to fit the data by both $(-1)^r/r^\eta$ and $(-1)^r[\ln(r)]^\sigma/r$. If one plots $\log[|C(r,\infty)|]$ as a function of $\log(r)$, the absolute value of the slope η grows with the distance r which indicates a poor fit. On the other hand, the form $(-1)^r[\ln(r)]^\sigma/r$ fits the data much better with $\sigma=0.85$ (see Fig. 3). Also, when the correlation functions without finite-size correction $C(L/2,L)$ for $L=32$, 64, and 128 are fitted by this latter

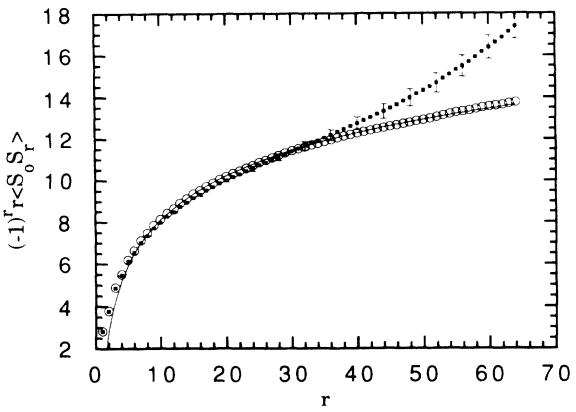

FIG. 3. The solid squares are the ground-state correlation function multiplied by the distance $(-1)^r r\langle s_0 s_r\rangle$ for the spin-$\frac{3}{2}$ chain of length 128. The circles are the correlation function in the thermodynamic limit extracted after a finite-size scaling analysis. The solid line is a fit to $a[\ln(r)]^\sigma/r$ with $\sigma=0.85$. The error bars are determined in the same way as for the spin-$\frac{1}{2}$ case.

form we get $\sigma=0.85$. The $1/r$ decay is consistent with the idea that half-odd-integer-spin chains are all in the same universality class. The exponent for the logarithmic correction σ, however, is somewhat larger than expected.[5]

In conclusion, we have demonstrated the feasibility of computing directly the ground-state correlation functions for a long antiferromagnetic Heisenberg chain with arbitrary spins. For the spin-1 chain, our calculations show that the ground state is disordered with a correlation length equal to 6.2 ± 0.1. On the other hand, for the spin-$\frac{1}{2}$ and the spin-$\frac{3}{2}$ chains, the correlation functions are best fitted by an algebraic form $(-1)^r[\ln(r)]^\sigma/r$. For chains with 128 spins, after a finite-size scaling analysis, we find $\sigma=0$ for the spin-$\frac{1}{2}$ chain and $\sigma=0.85$ for the spin-$\frac{3}{2}$ chain. These results are in agreement with the Haldane conjecture, especially the statement that all the half-odd-integer-spin chains belong to the same universality class.[3] But the leading logarithmic correction disagrees with the predicted value of $\frac{1}{2}$ from conformal field theory.[5]

The computation time for a chain of L spins is proportional to $E_0 sL/\Delta E$, where E_0 is the ground-state energy and ΔE is the energy gap to the first excited state with the same symmetry as the ground state. This method is therefore much easier to apply to systems with a gap in the excitation spectrum. It has also been applied to the spin-$\frac{1}{2}$ Heisenberg model on a square lattice.[18]

I would like to thank I. Affleck, D. Ceperley, E. Fradkin, H. J. Schulz, and B. S. Shastry for helpful discussions. I have also benefitted from communicating with J. Borysowicz and A. Moreo. I am grateful to N. Trivedi for critical comments and a careful reading of the manuscript. This work is supported by NSF-DMR86-12860 through the Materials Research Laboratory. The computing was performed using a iPSC/2 hypercube computer at Cornell University Theory Center's Advanced Computing Facility.

[1]For a review, see for example, I. Affleck, in "Fields, Strings and Critical Phenomena," Proceedings of the Les Houches Summer School, 1989, edited by E. Brezin and J. Zinn-Justin (to be published).

[2]F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983); Phys. Rev. Lett. **50**, 1153 (1983); J. Appl. Phys. **57**, 3359 (1985).

[3]I. Affleck and F. D. M. Haldane, Phys. Rev. B **36**, 5291 (1987).

[4]V. Knizhnik and A. B. Zamolodchikov, Nucl. Phys. **B247**, 83 (1984); A. B. Zamolodchikov and V. A. Fateev, Yad. Fiz. **43**, 1031 (1986) [Sov. J. Nucl. Phys. **43**, 657 (1986)]; D. Gepner and E. Witten, Nucl. Phys. **B278**, 493 (1986).

[5]I. Affleck, D. Gepner, H. J. Schulz, and T. Ziman, J. Phys. A **22**, 511 (1989).

[6]I. Affleck, Phys. Rev. Lett. **56**, 2763 (1986).

[7]I. Affleck, Phys. Rev. Lett. **55**, 1355 (1985); Nucl. Phys. **B265 [FS15]**, 409 (1986).

[8]I. Affleck, Phys. Rev. Lett. **56**, 746 (1986); H. W. Blote, J. L. Cardy, and M. P. Nightingale, *ibid.* **56**, 742 (1986).

[9]S. Liang, B. Doucot, and P. W. Anderson, Phys. Rev. Lett. **61**, 365 (1988).

[10]W. Marshall, Proc. Roy. Soc. London A **232**, 48 (1955).

[11]K. Nomura, Phys. Rev. B **40**, 2421 (1989).

[12]M. P. Nightingale and H. W. Blote, Phys. Rev. B **33**, 659 (1986).

[13]J. B. Parkinson and J. C. Bonner, Phys. Rev. B **32**, 4703 (1985); A. Moreo, Phys. Rev. B **36**, 8582 (1987).

[14]The ground-state crystal momentum can be inferred from the Marshall sign. For an integer-spin chain, the ground-state crystal momentum is zero. For a half-integer-spin chain, it is zero (π) when $L/2$ is even (odd).

[15]T. A. Kaplan, P. Horsch, and J. Borysowicz, Phys. Rev. B **35**, 1877 (1987).

[16]K. Kubo, T. A. Kaplan, and J. Borysowicz, Phys. Rev. B **38**, 11 550 (1988).

[17]T. Ziman and H. J. Schulz, Phys. Rev. Lett. **59**, 140 (1987).

[18]S. Liang, University of Illinois report, 1989 (unpublished).