Quantum Monte Carlo simulation method for spin systems

Anders W. Sandvik* and Juhani Kurkijärvi
Department of Physics, Åbo Akademi, Porthansgatan 3-5, SF-20500 Åbo, Finland
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A quantum Monte Carlo simulation scheme for spin systems is presented. The method is a generalization of Handscomb's method but applicable to any length of the spin, i.e., when the spin traces cannot be evaluated analytically. The Monte Carlo sampling is extended to the space of spin vectors in addition to the usual operator-index sequences. An important technical point is that the index sequences are augmented with the aid of unit operators to a constant, self-consistently determined length. The scheme is applied to the one-dimensional antiferromagnetic spin-S Heisenberg model. Results at low temperatures are reported for $S=1$ and $S=\frac{3}{2}$ and system sizes up to $N=64$. The computed magnetic structure factor in the $S=1$ chain is in agreement with earlier ground-state calculations. For $S=\frac{3}{2}$ we find the exponent $\bar{\gamma}=0.49\pm0.04$ for the divergence of the antiferromagnetic structure factor. Further, the susceptibility as a function of the wave number is computed. For $S=1$ the staggered susceptibility $\chi(\pi)$ at $T=0$ is found to take the value 20.0 ± 1.5 in units such that $\chi(q)\rightarrow T^{-1}$ at high temperatures (with the temperature scale defined by $k_B=1$). For $S=\frac{3}{2}$ we obtain the exponent $\gamma=1.45\pm0.05$ for the divergence of the staggered susceptibility.

I. INTRODUCTION

Quantum Monte Carlo simulation is an important tool in nonperturbative investigations of spin systems at finite temperatures. The problem is calculating the quantum-mechanical thermal expectation value of an observable $\hat{A}$,

$$\langle \hat{A} \rangle = \frac{1}{Z}\mathrm{Tr}\{\hat{A}e^{-\beta\hat{H}}\} , \tag{1.1}$$

where β is the inverse temperature and Z the partition function,

$$Z=\mathrm{Tr}\{e^{-\beta\hat{H}}\} . \tag{1.2}$$

As the Hamiltonian generally consists of noncommuting terms,

$$\hat{H}=\sum_{i=1}^{M}\hat{H}_i , \quad [\hat{H}_i,\hat{H}_j]\neq 0 \ \text{ for some } i,j, \tag{1.3}$$

direct evaluation of $e^{-\beta\hat{H}}$ is impossible, except for small systems for which the Hamiltonian can be diagonalized numerically.

Several Monte Carlo algorithms for (1.1) have been proposed. Early simulations of the ferromagnetic spin-$\frac{1}{2}$ Heisenberg model were performed by Handscomb[1] in the 1960's, with a method based on the Taylor expansion of $e^{-\beta\hat{H}}$. Writing the Hamiltonian in terms of spin permutation operators, the Monte Carlo simulation is carried out in a space of index sequences corresponding to strings of permutation operators, the traces of which are easily calculated. Over the past decade most progress in the field has been made along the lines of the Suzuki-Trotter approach.[2–4] There the generalized Trotter formula is used to map the quantum system onto a classical system with an additional "imaginary time" dimension. The spin-$\frac{1}{2}$ Heisenberg model on various lattices has been extensively studied with this method.[5–10] A number of computations on higher spins have also been carried out.[11–15]

Lately several improvements of Handscomb's scheme have been reported. Simulations have been performed on the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model on different lattices,[16–19] the XY model,[20] and the spin-S exchange model.[21] The basic limitation of the method, i.e., that the traces of the products of terms of the Hamiltonian must be known, has not been removed, however. A scheme, which overcomes this problem, is presented in this paper. Writing out the traces as sums over diagonal matrix elements in a suitably chosen representation, the Monte Carlo simulation is carried out in a combined space of spin states and index sequences. The method is applicable to any spin and any spatial dimensionality. A fast algorithm for performing a random walk in the configuration space is presented for the spin-S Heisenberg model.

The plan of the paper is as follows. In Sec. II we briefly review Handscomb's scheme and give a general outline of our new method without making assumptions relating to specific models. In Sec. III the scheme is applied to the one-dimensional antiferromagnetic spin-S Heisenberg model. The simulation algorithm is described and tests on small systems are compared with exact data. In Sec. IV results on the magnetic properties of the spin-1 and spin-$\frac{3}{2}$ models are reported for lattice sizes up to $N=64$. The last section is devoted to discussion.

II. OUTLINE OF THE METHOD

In the first part of this section we review Handscomb's simulation scheme. In the second part we formulate a new method also based on the Taylor expansion of $e^{-\beta\hat{H}}$, but relying on Monte Carlo sampling of both operator

strings and spin states. Unlike in the work on Handscomb's method, the Taylor series is cut at an adequate length, and the space of operator strings is extended to allow for unit operators. In this way operator averages are written as sums over diagonal matrix elements of operator strings of a fixed length, which considerably simplifies the construction of a fast simulation algorithm. We show that there are "cycles" of terms of equal contribution to the partition function. A configuration space is defined in which a configuration corresponds to such a cycle of matrix elements. Expressions for observables are derived and an algorithm of generating configurations is described without referring to any specific model.

The suggestion of Handscomb[1] is to expand $e^{-\beta\hat{H}}$ in a Taylor series and write all powers of $\hat{H}$ as sums of products of the operators $\hat{H}_i$ in (1.3). The partition function is then

$$Z=\sum_{n=0}^{\infty}\sum_{\{C_n\}}\frac{(-\beta)^n}{n!}\mathrm{Tr}\left\{\prod_{j=1}^{n}\hat{H}_{l_j}\right\}, \tag{2.1}$$

where C_n denotes a sequence of indices $(l_1,l_2,\ldots,l_n)$ with $1\le l_j\le M$, where M is the number of the operators $\hat{H}_i$ as a sum of which the Hamiltonian is written. For an operator $\hat{A}$, satisfying

$$\mathrm{Tr}\left\{\hat{A}\prod_{j=1}^{n}\hat{H}_{l_j}\right\}=0\ ,\quad \text{if } \mathrm{Tr}\left\{\prod_{j=1}^{n}\hat{H}_{l_j}\right\}=0\ , \tag{2.2}$$

the thermal expectation value can be written as

$$\langle\hat{A}\rangle=\sum_{n=0}^{\infty}\sum_{\{C_n\}}A(C_n)W(C_n)\ , \tag{2.3}$$

where

$$W(C_n)=\frac{1}{Z}\frac{(-\beta)^n}{n!}\mathrm{Tr}\left\{\prod_{j=1}^{n}\hat{H}_{l_j}\right\} \tag{2.4}$$

and

$$A(C_n)=\begin{cases}\mathrm{Tr}\left\{\hat{A}\prod_{j=1}^{n}\hat{H}_{l_j}\right\}\Big/\mathrm{Tr}\left\{\prod_{j=1}^{n}\hat{H}_{l_j}\right\} & \text{if } W(C_n)\neq 0,\\ 0, & \text{if } W(C_n)=0\ .\end{cases} \tag{2.5}$$

If all the traces in (2.4) and (2.5) can be handily evaluated, the average can be estimated using importance sampling in the space of index sequences of all lengths. If the "weight factors" $W(C_n)$ are positive for all C_n, the thermal expectation value is the arithmetic mean of the function $A(C_n)$ in a random walk with the probability distribution $W(C_n)$:

$$\langle\hat{A}\rangle=\langle A(C_n)\rangle_W\ . \tag{2.6}$$

Several algorithms for generating sequences have been proposed.[1,16–18] If there are both positive and negative weight factors, $|W(C_n)|$ can be taken for the distribution, and the expectation value is

$$\langle\hat{A}\rangle=\frac{\langle\mathrm{sgn}[W(C_n)]A(C_n)\rangle_{|W|}}{\langle\mathrm{sgn}[W(C_n)]\rangle_{|W|}}\ , \tag{2.7}$$

where sgn is the sign function. A small value of the "mean of the signs," $\langle\mathrm{sgn}[W(C_n)]\rangle$, leads to large statistical fluctuations in the Monte Carlo average (2.7). This "sign problem" also occurs in the context of the Suzuki-Trotter scheme.[6,22] Fortunately many models of interest can be written in a form where all weight factors are positive.

A severe limitation of Handscomb's method is that the traces of the operator strings are not easy to evaluate in general. For the spin-$\frac{1}{2}$ Heisenberg model, the Hamiltonian can be written in terms of operators such that the trace of any string can easily be calculated analytically. For higher spins this is not possible, however, and the original formulation of Handscomb's method cannot be used. Below we outline a simulation scheme, closely related to Handscomb's, which avoids this impasse. By writing the traces in (2.4) and (2.5) as sums over diagonal matrix elements, we construct a simulation scheme in principle applicable to any spin system.

Consider a Hamiltonian written in the form (1.3) with the operators $\hat{H}_i$ satisfying the following requirement. In a suitably chosen representation with the basis vectors $\mathcal{B}_\alpha=\{|\alpha\rangle\}$, $\hat{H}_i$ operating on a basis vector gives either zero or a vector proportional to a basis vector, i.e.,

$$\hat{H}_i|\alpha\rangle\propto|\alpha'\rangle\ ,\quad |\alpha\rangle,|\alpha'\rangle\in\mathcal{B}_\alpha\ . \tag{2.8}$$

For definiteness we now choose the eigenstates of the z components $\hat{S}^z_j, j=1,\ldots,N$, of the spin-$S$ operators on a lattice of N sites,

$$|\alpha\rangle=|S_1,S_2,\ldots,S_N\rangle\ , \tag{2.9}$$

where S_j is an eigenvalue of $\hat{S}^z_j$. In order to satisfy (2.8), the operators $\hat{H}_i$ can be chosen as products of $\hat{S}^z_j$'s and ladder operators $\hat{S}^+_j$ and $\hat{S}^-_j, j=1,\ldots,N$.

Following Handscomb we expand $e^{-\beta\hat{H}}$ in a Taylor series. The series is cut at the Lth term with L chosen large enough to reduce the truncation error below the statistical error of the Monte Carlo simulation. Further along in this section, an algorithm of finding an optimum value of L will be described. The traces over the spin configurations are written out as sums over diagonal matrix elements. The thermal average of an operator $\hat{A}$ is

$$\langle\hat{A}\rangle=\frac{1}{Z}\sum_{\alpha}\sum_{n=0}^{L}\sum_{\{C_n\}}\frac{(-\beta)^n}{n!}\langle\alpha|\hat{A}\prod_{j=1}^{n}\hat{H}_{l_j}|\alpha\rangle\ , \tag{2.10}$$

where C_n, as before, denotes a sequence of indices $(l_1,l_2,\ldots,l_n)$ of length n with each l_j varying according to $1\le l_j\le M$, M being the number of terms in the Hamiltonian. Our intention is to estimate the average using importance sampling in a combined space of spin vectors and index sequences. In order to simplify the construction of a fast Monte Carlo simulation algorithm, we insert $L-n$ unit operators in every operator string of length $n<L$ and define $\hat{H}_0=\hat{I}$. The Taylor expansion up to order L will then be taken care of by a summation over all index sequences C_L of length L with zero added into the range of the indices l_j in C_L, i.e., $0\le l_j\le M$. There are $\binom{L}{n}$ such extended index sequences corresponding to each original index sequence of length n arising from all

the choices of the positions of the unit operators in the string. A factor $\binom{L}{n}^{-1}$ must therefore be included in each term of the Taylor series. We get

$$\langle \hat{A} \rangle = \frac{1}{Z} \sum_{\alpha} \sum_{\{C_L\}} \frac{(-\beta)^{n(C_L)}[L-n(C_L)]!}{L!} \times \langle \alpha | \hat{A} \prod_{j=1}^{L} \hat{H}_{l_j} | \alpha \rangle , \tag{2.11}$$

where $n(C_L)$ is the number of nonzero indices in the sequence C_L. Provided that a function $A(\alpha, C_L)$ can be found such that (2.11) is equal to

$$\langle \hat{A} \rangle = \sum_{\alpha} \sum_{C_L} A(\alpha, C_L) W(\alpha, C_L) , \tag{2.12}$$

with the weight factor

$$W(\alpha, C_L) = \frac{1}{Z} \frac{(-\beta)^{n(C_L)}[L-n(C_L)]!}{L!} \langle \alpha | \prod_{j=1}^{L} \hat{H}_{l_j} | \alpha \rangle , \tag{2.13}$$

the average can be calculated using importance sampling over spin vectors $|\alpha\rangle \in \mathcal{B}_\alpha$ and index sequences C_L of length L. We will now show that terms contributing to (2.12) come in sets of terms of equal weight factor and that each such set can be generated out of the spin vector and the index sequence of any single term of the set. We define binary counterparts $\hat{H}'_i$ to the operators $\hat{H}_i$ according to

$$\langle \alpha' | \hat{H}'_i | \alpha \rangle = \begin{cases} 1, & \text{if } \langle \alpha' | \hat{H}_i | \alpha \rangle \neq 0 \\ 0 & \text{if } \langle \alpha' | \hat{H}_i | \alpha, \rangle = 0 \end{cases} \quad |\alpha\rangle, |\alpha'\rangle \in \mathcal{B}_\alpha , \tag{2.14}$$

i.e., on acting on a basis vector, $\hat{H}'_i$ either delivers zero or a basis vector. Consider (α, C_L) for which $W(\alpha, C_L) \neq 0$. One can easily see that the following equality holds:

$$\langle \alpha | \hat{H}_{l_L} \cdots \hat{H}_{l_2} \hat{H}_{l_1} | \alpha \rangle = \langle \alpha | \hat{H}'^{\dagger}_{l_1} \hat{H}_{l_1} \hat{H}_{l_L} \cdots \hat{H}_{l_2} \hat{H}'_{l_1} | \alpha \rangle , \tag{2.15}$$

where $H'^{\dagger}_{l_1}$ is the adjoint of $\hat{H}'_{l_1}$. We write (2.15) as

$$\langle \alpha | \hat{H}_{l_L} \cdots \hat{H}_{l_2} \hat{H}_{l_1} | \alpha = \langle \alpha(1) | \hat{H}_{l_1} \hat{H}_{l_L} \cdots \hat{H}_{l_2} | \alpha(1) \rangle , \tag{2.16}$$

where $|\alpha(1)\rangle$ is a propagated state $\hat{H}'_{l_1} |\alpha\rangle$, which is one of the basis vectors. Thus $W(\alpha, C_L) = W[\alpha(1), C_L(1)]$, where $C_L(1)$ denotes the index sequence obtained by cyclically permuting the sequence C_L once. In general we have

$$W(\alpha, C_L) = W[\alpha(p), C_L(p)] , \tag{2.17}$$

where $|\alpha(p)\rangle$ is the pth propagated state

$$|\alpha(p)\rangle = \prod_{j=1}^{p} \hat{H}'_{l_j} |\alpha\rangle , \tag{2.18}$$

and $C_L(p)$ denotes the index sequence $(l_{p+1}, \ldots, l_L, l_1, \ldots, l_p)$ obtained by cyclically permuting the sequence $C_L = (l_1, l_2, \ldots, l_L)$ p times. The propagated states satisfy the boundary condition $|\alpha(L)\rangle = |\alpha(0)\rangle = |\alpha\rangle$. Although all the combinations $[\alpha(p), C_L(p)]$, $P = 0, \ldots, L-1$, give terms of equal weight factor in (2.12), the functions $A[\alpha(p), C_L(p)]$ need not be the same for every p. The Monte Carlo simulation is formulated so as to sample the cycle average, $(1/L) \sum_{p=0}^{L-1} A[\alpha(p), C_L(p)]$.

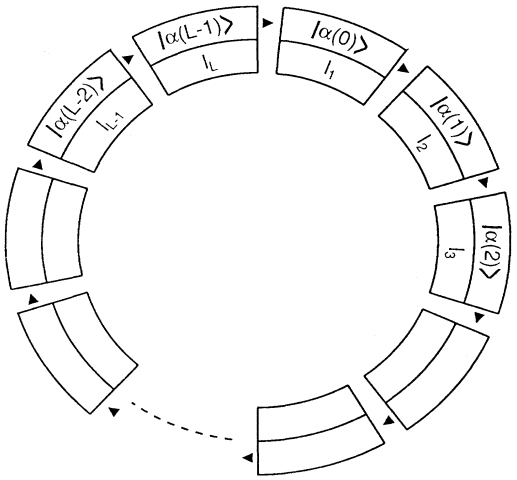

FIG. 1. Symbolical representation of a cycle of spin states with the evolution determined by the operators corresponding to the index sequence $(l_1, \ldots, l_L)$.

We define a configuration space $\{\mathcal{C}\}$ in which each configuration $\mathcal{C}$ is specified by a cycle of spin states $|\alpha(0)\rangle, \ldots, |\alpha(L-1)\rangle$ with the boundary condition $|\alpha(L)\rangle = |\alpha(0)\rangle$, and an index sequence $C_L = (l_1, l_2, \ldots, l_L)$ such that $\hat{H}'_{l_p} |\alpha(p-1)\rangle = |\alpha(p)\rangle$, as depicted in Fig. 1. Assuming that all weight factors are positive, we define

$$f(\mathcal{C}) = \ln \left[\frac{\beta^{n(C_L)}[L-n(C_L)]!}{L!} \right] \tag{2.19}$$

and

$$g_p(\mathcal{C}) = \ln(|\langle \alpha(p) | \hat{H}_{l_p} | \alpha(p-1) \rangle|), \quad p = 1, \ldots, L . \tag{2.20}$$

The weight factor of a configuration is then

$$W(\mathcal{C}) = \frac{1}{Z} \exp \left[f(\mathcal{C}) + \sum_{p=1}^{L} g_p(\mathcal{C}) \right] \tag{2.21}$$

and the thermal expectation value (2.12) is obtained as the average of a function $A(\mathcal{C})$ over configurations with the probability distribution $W(\mathcal{C})$:

$$\langle \hat{A} \rangle = \langle A(\mathcal{C}) \rangle_W . \tag{2.22}$$

We now consider the function $A(\mathcal{C})$ corresponding to some observables of interest. If $\hat{A}$ is diagonal we clearly have

$$A(\mathcal{C})=\frac{1}{L}\sum_{p=0}^{L-1}\langle\alpha_k(p)|\hat{A}|\alpha_k(p)\rangle\ . \tag{2.23}$$

Defining

$$S_j(p)=\langle\alpha_k(p)|\hat{S}^z_j|\alpha_k(p)\rangle\ , \tag{2.24}$$

a spin correlation function is

$$C(i,j)=\langle\hat{S}^z_i\hat{S}^z_j\rangle=\left\langle\frac{1}{L}\sum_{p=0}^{L-1}S_i(p)S_j(p)\right\rangle_W\ . \tag{2.25}$$

Consider the response function $G(i,j)$ of spin i to a field $\mathcal{H}_j$ in the z direction which couples only to spin j. The susceptibility at wave vector $\mathbf{q}$ can be evaluated according to

$$\chi(\mathbf{q})=\frac{1}{N}\sum_{ij}e^{-i\mathbf{q}\cdot(\mathbf{r}_i-\mathbf{r}_j)}G(i,j)\ , \tag{2.26}$$

where r_i is the position of the ith lattice point. The single-spin response function at zero field is

$$\begin{aligned}G(i,j)&=\frac{\partial\langle\hat{S}^z_i\rangle}{\partial\mathcal{H}_j}\Big/_{\mathcal{H}_j=0}\\&=\frac{1}{Z}\frac{\partial}{\partial\mathcal{H}_j}\mathrm{Tr}\{\hat{S}^z_i e^{-\beta(\hat{H}-\mathcal{H}_j\hat{S}^z_j)}\}\Big/_{\mathcal{H}_j=0}\\&\quad-\langle\hat{S}^z_i\rangle\frac{1}{Z}\frac{\partial Z}{\partial\mathcal{H}_j}\Big/_{\mathcal{H}_j=0}\ ,\end{aligned} \tag{2.27}$$

which yields

$$\begin{aligned}G(i,j)=&\frac{1}{Z}\sum_{\alpha}\sum_{n=0}^{\infty}\sum_{m=0}^{n}\frac{\beta(-\beta)^n}{(n+1)!}\langle\alpha|\hat{S}^z_i\hat{H}^m\hat{S}^z_j\hat{H}^{n-m}|\alpha\rangle\\&-\langle\hat{S}^z_i\rangle\langle\hat{S}^z_j\rangle\ .\end{aligned} \tag{2.28}$$

Cutting the sum over n at $n=L$ and assuming $\langle\hat{S}^z_i\rangle=0$, this can be written as a sum over index sequences C_L:

$$\begin{aligned}G(i,j)=&\frac{1}{Z}\sum_{\alpha}\sum_{\{C_L\}}\sum_{p=0}^{L}\frac{\beta(-\beta)^{n(C_L)}[L-n(C_L)]!}{(L+1)!}\\&\times S_i(0)S_j(p)\langle\alpha|\prod_{k=0}^{L}\hat{H}_{l_k}|\alpha\rangle\ ,\end{aligned} \tag{2.29}$$

where $S_i(p)$ is the matrix element defined in (2.24). Writing (2.29) as a sum over the configuration space $\{\mathcal{C}\}$ gives

$$G(i,j)=\sum_{\{\mathcal{C}\}}\sum_{p=0}^{L}\frac{\beta}{L+1}S_i(0)S_j(p)W(\mathcal{C}) \tag{2.30}$$

or, with the average of $S_p(m)S_j(m+p)$ over all positions m of the state cycle in the place of $S_i(0)S_j(p)$,

$$G(i,j)=\sum_{\{C\}}\sum_{p=0}^{L}\sum_{m=0}^{L-1}\frac{\beta}{L(L+1)}S_i(m)S_j(m+p)W(\mathcal{C})\ . \tag{2.31}$$

With the boundary condition $S_j(L)=S_j(0)$, the Monte Carlo average emerges as

$$\begin{aligned}G(i,j)=\left\langle\frac{\beta}{L(L+1)}\right.&\left[\left[\sum_{p=0}^{L-1}S_i(p)\right]\left[\sum_{p=0}^{L-1}S_j(p)\right]\right.\\&\left.\left.+\sum_{p=0}^{L-1}S_i(p)S_j(p)\right]\right\rangle_W\ .\end{aligned} \tag{2.32}$$

The energy and the heat capacity can be found from the well-known formulas

$$\langle\hat{E}\rangle=-\frac{\partial}{\partial\beta}\ln Z\ ,\quad\langle\hat{C}\rangle=\beta^2\frac{\partial^2}{\partial\beta^2}\ln Z\ . \tag{2.33}$$

The results are formally equivalent to those obtained in the context of Handscomb's method,

$$\begin{aligned}&\langle\hat{E}\rangle=-\frac{1}{\beta}\langle n(C_L)\rangle_W\ ,\\&\langle\hat{C}\rangle=\langle n(C_L)^2\rangle_W-\langle n(C_L)\rangle^2_W-\langle n(C_L)\rangle_W\ .\end{aligned} \tag{2.34}$$

The Monte Carlo simulation requires a fast algorithm of generating configurations according to the probability distribution $W(\mathcal{C})$. Starting with an arbitrary configuration, small changes are made in the spin states and/or in the index sequence. The changes must be chosen such that any configuration can be reached by a series of them. The probability of a change is determined so as to satisfy the detailed balance principle,

$$W(\mathcal{C})P(\mathcal{C}\to\mathcal{C}')=W(\mathcal{C}')P(\mathcal{C}'-\mathcal{C})\ , \tag{2.35}$$

where $P(\mathcal{C}\to\mathcal{C}')$ is the probability of a transition from configuration $\mathcal{C}$ to $\mathcal{C}'$. Let Δ denote a change that takes the configuration $\mathcal{C}$ into $\mathcal{C}'$ and $-\Delta$ its reverse:

$$\begin{aligned}&\mathcal{C}\xrightarrow{\Delta}\mathcal{C}'\ ,\\&\mathcal{C}'\xrightarrow{-\Delta}\mathcal{C}\ .\end{aligned} \tag{2.36}$$

The transition probability $P(\mathcal{C}\to\mathcal{C}')$ can be viewed as a product of two probabilities:

$$P(\mathcal{C}\to\mathcal{C}')=P_c(\mathcal{C},\Delta)P_a(\mathcal{C},\mathcal{C}')\ , \tag{2.37}$$

$P_c(\mathcal{C},\Delta)$ being the probability of picking the change Δ and $P_a(\mathcal{C},\mathcal{C}')$ the probability of accepting the new configuration $\mathcal{C}'$. If $P_c(\mathcal{C},\Delta)$ satisfies

$$P_c(\mathcal{C},\Delta)=P_c(\mathcal{C}',-\Delta)\ , \tag{2.38}$$

the probability of accepting the transition is given by the Metropolis algorithm,[23]

$$P_a(\mathcal{C},\mathcal{C}')=\begin{cases}W(\mathcal{C}')/W(\mathcal{C}), & \text{if } W(\mathcal{C}')<W(\mathcal{C})\\1, & \text{if } W(\mathcal{C}')\geq W(\mathcal{C})\ .\end{cases} \tag{2.39}$$

Contrary to most classical Monte Carlo simulations, the balance requirement (2.38) is not trivially satisfied here for all types of changes. $P_c(\mathcal{C},\Delta)$ must therefore be explicitly constructed in general. In the next section an algorithm for the Heisenberg model will be presented where most of the changes required indeed satisfy (2.38) trivially. Only one type of change needs an additional acceptance criterion which turns out relatively simple however.

During the simulation all the spins $S_j(p)$, with $j=1,\ldots,N$ and $p=0,\ldots,L-1$, defining a cycle of states $|\alpha(0)\rangle,\ldots,|\alpha(L-1)\rangle$, are stored along with the index sequence C_L. The random walk can be started from an arbitrary configuration. The types of changes that guarantee ergodicity are model dependent. Below we introduce the concepts of global and local changes, which will be exemplified in the next section.

A change will be called global if all the spin states of the configuration $\mathcal{C}$ are affected, the index sequence remaining the same. A lattice site j is randomly selected, and the spins $S_j(p), p=0,\ldots,L-1$, are flipped according to

$$S_j'(p)=S_j(p)+\Delta_j, \quad p=0,\ldots,L-1 . \tag{2.40}$$

If all Δ_j which leave all $S_j'(p)$ within the range $-S,-S+1,\ldots,S$ are chosen with the same probability, (2.38) is trivially satisfied, and the probability of accepting the transition to the new configuration $\mathcal{C}'$ is given by (2.39) with

$$\frac{W(\mathcal{C}')}{W(\mathcal{C})}=\exp\left[\sum_{p=1}^{L}[g_p(\mathcal{C}')-g_p(\mathcal{C})]\right], \tag{2.41}$$

with the functions g_p defined in (2.20).

A change in the index sequence is a local change. A set of indices within a limited range $[p_1,p_2]$ (or $[p_1,L]$ and $[1,p_2]$ for $p_1>p_2$) of the sequence are replaced with a new set of indices in such a way that only the spin states within the corresponding range are affected. Given that a probability $P_c(\mathcal{C},\Delta)$ of selecting the change Δ is defined so as to satisfy (2.38), the probability of accepting a local change is given by (2.39) with

$$\frac{W(\mathcal{C}')}{W(\mathcal{C})}=\begin{cases}\exp\left[f(\mathcal{C}')-f(\mathcal{C})+\sum_{p=p_1}^{p_2}[g_p(\mathcal{C}')-g_p(\mathcal{C})]\right], \\ \exp\left[f(\mathcal{C}')-f(\mathcal{C})+\sum_{p=p_1}^{L}[g_p(\mathcal{C}')-g_p(\mathcal{C})]+\sum_{p=1}^{p_2}[g_p(\mathcal{C}')-g_p(\mathcal{C})]\right].\end{cases} \tag{2.42}$$

If the Hamiltonian conserves the magnetization, all the states in the cycle have the same total spin-z component which therefore can only be altered globally. This opens the possibility of investigating subspaces of different z components of the total spin by allowing only such global changes as preserve the total magnetization.

We now turn to the question of determining L. It is clearly desirable to choose L as small as possible without compromising the accuracy of the calculation. This can be done by starting the simulation with a small L and continually monitoring the number of indices zero in the sequence. If this number becomes smaller than some low number, L is increased by adding zeros to the index sequence and correspondingly states to the state cycle. This process is continued until equilibrium is reached. The actual simulation is then carried out with the value of L thus obtained. If, at the end of the simulation, the number of nonzero indices has not reached L, one can conclude that the finite L has not degraded the outcome.

III. APPLICATION TO THE SPIN-S ONE-DIMENSIONAL ANTIFERROMAGNETIC HEISENBERG MODEL

In this section the simulation scheme is applied to the spin-S one-dimensional antiferromagnetic Heisenberg model. The algorithm is described and results of test runs on small systems are compared with exact data.

The Heisenberg Hamiltonian is

$$\hat{H}=J\sum_{i=1}^{N}\hat{S}_i\cdot\hat{S}_{i+1} , \tag{3.1}$$

where $\hat{S}_i$ is the spin-S operator on site i of a lattice of N sites, and $\hat{S}_{N+1}=\hat{S}_1$ for periodic boundary conditions. In the antiferromagnetic case $J>0$. We define the operators

$$\begin{aligned}\hat{H}_{1b}&=J\hat{S}_b^z\hat{S}_{b+1}^z+c ,\\ \hat{H}_{2b}&=\frac{J}{2}\hat{S}_b^+\hat{S}_{b+1}^- ,\\ \hat{H}_{3b}&=\frac{J}{2}\hat{S}_b^-\hat{S}_{b+1}^+ ,\end{aligned} \tag{3.2}$$

where c is a constant chosen as described later and included in order to make all the weight factors positive. In terms of these operators the Hamiltonian reads

$$\hat{H}=\sum_{b=1}^{N}\sum_{t=1}^{3}\hat{H}_{tb}-Nc . \tag{3.3}$$

The constant Nc in the Hamiltonian only sets the zero level of the energy and will be dropped hereafter. In the representation chosen in the previous section, the operators H_{tb} satisfy the condition (2.8) with

$$\begin{aligned}\hat{H}_{1b}|\ldots,S_b,S_{b+1},\ldots\rangle&=h_1(S_b,S_{b+1})|\ldots,S_b,S_{b+1},\ldots\rangle ,\\ \hat{H}_{2b}|\ldots,S_b,S_{b+1},\ldots\rangle&=h_2(S_b,S_{b+1})|\ldots,S_b+1,S_{b+1}-1,\ldots\rangle ,\\ \hat{H}_{3b}|\ldots,S_b,S_{b+1},\ldots\rangle&=h_3(S_b,S_{b+1})|\ldots,S_b-1,S_{b+1}+1,\ldots\rangle ,\end{aligned} \tag{3.4}$$

where

$$h_1(S_a,S_b)=JS_aS_b+c\ ,$$
$$h_2(S_a,S_b)=\frac{J}{2}\sqrt{[S(S+1)-S_a(S_a+1)][S(S+1)-S_b(S_b-1)]}\ , \tag{3.5}$$
$$h_3(S_a,S_b)=h_2(S_b,S_a)\ .$$

For $S=\frac{1}{2}$, also the sums $\hat{H}_{2b}+\hat{H}_{3b}$ satisfy (2.8), which means that only two types of operators are needed in the sum (3.3). We will describe the algorithm for the general spin, however, as the simplifications for $S=\frac{1}{2}$ are obvious. Binary counterparts $\hat{H}'_{tb}$ to the operators $\hat{H}_{tb}$ are defined according to (2.14). $\hat{H}'_{00}=\hat{H}_{00}$ is the unit operator. C_L now denotes a sequence of index pairs $\binom{t_1}{b_1},\binom{t_2}{b_2},\ldots,\binom{t_L}{b_L}$, where $t_i=1,2,3$ and $b_i=1,2,\ldots,N$ or $t_i=b_i=0$. The number of index pairs not equal to $\binom{0}{0}$ is denoted by $n(C_L)$. A configuration in the space $\{\mathcal{C}\}$ is defined as a sequence of index pairs referring to an operator string together with a cycle of spin states $|\alpha(0)\rangle,\ldots,|\alpha(L-1)\rangle$ satisfying $\hat{H}'_{t_pb_p}|\alpha(p-1)\rangle=|\alpha(p)\rangle$ and the boundary condition $|\alpha(L)\rangle=|\alpha(0)\rangle$. The weight factor of a configuration is

$$W(\mathcal{C})=\frac{1}{Z}\frac{(-\beta)^{n(C_L)}[L-n(C_L)]!}{L!}\times\langle\alpha(0)|\prod_{i=1}^{L}\hat{H}_{t_ib_i}|\alpha(0)\rangle\ . \tag{3.6}$$

The operator string must contain the same number of raising and lowering operators for every spin. Think of the index pair $\binom{2}{b}$ as creating a directed link from site b to site $b+1$ (or from N to 1 if $b=N$) and the pair $\binom{3}{b}$ as creating one from site $b+1$ to b (or from 1 to N). The links created by the whole sequence must then form closed loops on the lattice in order for each site to have as many inward as outward directed links. On a chain with open boundaries, all such closed loops can be built out of 2-link loops of the type shown in Fig. 2(a). For periodic boundary conditions, additional "ring-loops" as depicted in Fig. 2(b) are required. For a chain with open boundaries and for a ring with an even number of sites, all closed loops contain an even number of links, which means that the total number of operators H_{2b} and H_{3b} is even. If the constant c in (3.2) is chosen to satisfy $JS^2+c<0$, all weight factors will be positive. This applies to any lattice where all closed loops connecting interacting neighbors contain an even number of bonds. With c chosen as above there are no restrictions on the type $\binom{1}{b}$ index pairs.

Assuming that the constant c is chosen so as to make all the weight factors positive, the functions g_p defined in (2.20) are

$$g_p(\mathcal{C})=\begin{cases}0, & \text{if } t_p=0\ ,\\ \log[-h_1(S_{b_p}(p-1),S_{b_p+1}(p-1))], & \text{if } t_p=1\ ,\\ \log[h_{t_p}(S_{b_p}(p-1),S_{b_p+1}(p-1))], & \text{if } t_p=2,3\ .\end{cases} \tag{3.7}$$

A random walk in the configuration space $\{\mathcal{C}\}$ consists of global and local changes as described in the previous section. Global changes are made according to (2.40). In the evaluation of the ratio of the new and old weight factors (2.41), only the matrix elements of operators acting on the flipped spin j have to be taken into account. Defining as $\{p_j\}$ the subset of positions whose index pairs $\binom{t_{p_j}}{b_{p_j}}$ contain a bond b_{p_j} with the flipped spin j, the ratio is

$$\frac{W(\mathcal{C}')}{W(\mathcal{C})}=\exp\left[\sum_{p\in\{p_j\}}[g_p(\mathcal{C}')-g_p(\mathcal{C})]\right]\ . \tag{3.8}$$

If both the values $\pm S$ appear among the spins $S_j(p)$, $p=0,\ldots,L-1$, the spins of the jth row cannot be flipped globally. In order to rapidly find the spins that can be flipped, the distributions of the spins in the different states $-S,-S+1,\ldots,S$ are continually recorded for every j.

The following types of local changes are made.

(1) A single index pair can be replaced by another if both the original and the new pair belong to the subset $\{\binom{0}{0},\binom{1}{1},\ldots,\binom{1}{N}\}$. A position p is randomly chosen in the current sequence. If the corresponding index pair does not belong to the subset above, the change trial is canceled. Otherwise a new index pair is chosen from the subset and the weight factor ratio is calculated as

$$\frac{W(\mathcal{C}')}{W(\mathcal{C})}=\exp[f(\mathcal{C}')-f(\mathcal{C})+g_p(\mathcal{C}')-g_p(\mathcal{C})]\ . \tag{3.9}$$

The requirement (2.38) is trivially satisfied.

(2) Two-pair changes are needed in order to insert and delete index pairs of type $\binom{2}{b}$ and $\binom{3}{b}$. Two positions p_1 and p_2 with $p_1<p_2$ are randomly chosen and their index pairs are replaced with two new pairs such that the new

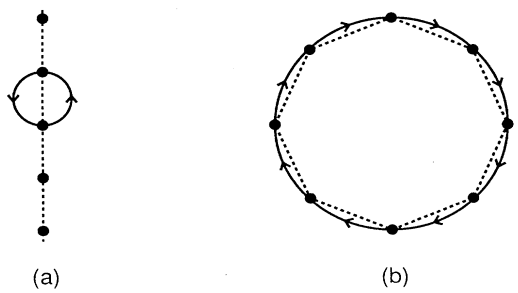

FIG. 2. "Elementary loops" of which all closed loops on a one-dimensional lattice can be built: (a) for open boundaries, (b) one of the additional ring loops required with periodic boundary conditions.

index sequence gives only closed loops of links on the lattice as described above. The possible new pairs belong to a subset of two-pair combinations where each combination can be exchanged for another. These subsets are

$$
\begin{aligned}
&\{\binom{0}{0}\binom{0}{0},\ \binom{1}{m}\binom{0}{0},\ \binom{0}{0}\binom{1}{m},\ \binom{1}{m}\binom{1}{n},\ \binom{2}{m}\binom{3}{m},\ \binom{3}{m}\binom{2}{m}\},\\
&\{\binom{2}{b}\binom{0}{0},\ \binom{0}{0}\binom{2}{b},\ \binom{2}{b}\binom{1}{m},\ \binom{1}{m}\binom{2}{b}\},\\
&\{\binom{3}{b}\binom{0}{0},\ \binom{0}{0}\binom{3}{b},\ \binom{3}{b}\binom{1}{m},\ \binom{1}{m}\binom{3}{b}\},\\
&\{\binom{2}{a}\binom{3}{b},\ \binom{3}{b}\binom{2}{a}\},\quad a\neq b\\
&\{\binom{2}{a}\binom{2}{b},\ \binom{2}{b}\binom{2}{a}\},\\
&\{\binom{3}{a}\binom{3}{b},\ \binom{3}{b}\binom{3}{a}\},
\end{aligned}
\tag{3.10}
$$

in a short-hand notation where the subsets with the indices m and n actually contain all combinations of $m,n=1,\ldots,N$, but each choice of the indices a and b constitutes a separate subset. If every new combination in the appropriate subset is chosen with equal probability, the balance condition (2.38) is satisfied. If neither the old two-pair combination nor the new one contains an index pair of the type $\binom{2}{b}$ or $\binom{3}{b}$, the weight factor ratio is

$$
\frac{W(\mathcal{C}')}{W(\mathcal{C})}=\exp[f(\mathcal{C}')-f(\mathcal{C})+g_{p_1}(\mathcal{C}')+g_{p_2}(\mathcal{C}')-g_{p_1}(\mathcal{C})-g_{p_2}(\mathcal{C})]\ . \tag{3.11}
$$

Otherwise the new index sequence may flip spins outside the allowed range, which would correspond to a "forbidden" state cycle. The spin states to be affected can be chosen either in the interval $[p_1,p_2-1]$ or $[p_2,L-1]$ and $[0,p_1-1]$. The effect of the change on the states in the interval chosen is checked. If the new cycle is forbidden the change is cancelled. If not, the change is accepted or rejected according to (2.39) with the ratio of the new to the old weight factor calculated according to (2.42).

(3) In order to create the ring loops of Fig. 2(b), which appear with periodic boundary conditions, we apply "half-ring" changes of the type graphically depicted in Fig. 3. A set of index pairs corresponding to a half-ring of links of one type are replaced with the set of indices corresponding to the "missing" half-ring of oppositely directed links. In this type of change, requirement (2.38) is not trivially satisfied as the total number of ways of constructing half-rings is not the same in both directions. The following algorithm is applied in order to satisfy (2.38). A set of $N/2$ index pairs $R=\{\binom{t}{b_1},\ldots,\binom{t}{b_{N/2}}\}$ with $t=2$ or 3 and $b_i\neq b_j$ for $i\neq j$ are randomly selected. The number of ways of forming a half-ring made up of these index pairs is

$$
N_R=\prod_{i=1}^{N/2} n(t,b_i)\ , \tag{3.12}
$$

where $n(t,b_i)$ is the number of index pairs $\binom{t}{b_i}$ in the current sequence. These numbers are continually recorded. The number of ways of restoring the original pattern of links from the sequence after a change is

$$
N_{R'}=\prod_{i=1}^{N/2}[n(t',b_i')+1]\ , \tag{3.13}
$$

where $t'=2$ if $t=3$ and vice versa and b_i' is an index not appearing among the b_i's in R. To satisfy (2.38) the change should be canceled with the probability

$$
P_{\text{cancel}}=1-\frac{N_R}{N_R+N_{R'}}\ . \tag{3.14}
$$

If the change is not canceled, one of each of the index pairs $\binom{t}{b_i}$ in the sequence is picked at random and replaced by one of the $\binom{t'}{b_i}$'s. After checking that the resulting new state cycle is not forbidden, the ratio of the weight factors is calculated according to (2.42).

We define a Monte Carlo step (MC step) as a random sequence of L two-pair changes, L single-pair changes, L half-ring changes, and N global changes. The simulation is started with all index pairs at $\binom{0}{0}$ and with a random spin configuration. The length of the cycles is extended according to the process described in the previous section until L has remained constant for I_1 MC steps with I_1 typically on the order of 10^4. For this process, the temperature is set slightly lower than the actual simulation temperature in order to ensure a large enough L. After raising the temperature, the system is again thermalized in I_2 MC steps, with typically $I_2=2I_1$. After these preliminaries, data for averages is collected every fifth MC step. The run is divided into ≈ 10 bins of $\approx 10^4$ MC steps each. The statistical error is obtained as the standard deviation of the average of the bin averages.

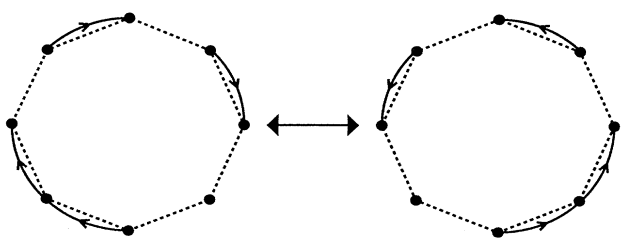

FIG. 3. Graphical representation of a typical half-ring change, where a set of $N/2$ links are replaced with oppositely directed links such that the number of inward and outward directed links is preserved at all sites.

Observables are calculated according to Sec. II. The correlation functions are normalized according to

$$C(k,l)=\frac{3}{S(S+1)}\langle S_k^z S_l^z\rangle \ , \tag{3.15}$$

which gives $C(k,k)=1$ as the interaction is isotropic. The magnetic structure factor at wave number q is

$$S(q)=\frac{1}{N}\sum_{kl} e^{i(k-l)q}C(k,l) \ . \tag{3.16}$$

The susceptibility at wave number q is calculated according to

$$\chi(q)=\frac{3}{S(S+1)}\frac{1}{N}\sum_{kl} e^{i(k-l)q}G(k,l) \ , \tag{3.17}$$

which gives $\chi(q)\rightarrow\beta$ at higher temperatures for all S. We choose the coupling constant J in (3.1) as

$$J=\frac{3}{S(S+1)} \ , \tag{3.18}$$

which gives the energy scale normally used for $S=\frac{1}{2}$. The energy is calculated both according to (2.34) and according to

$$\frac{E}{N}=3C(k,k+1) \ , \tag{3.19}$$

which holds for the isotropic interaction. The energy calculated in two different ways provides a good check on the simulation, as does the required value unity for $C(k,k)$.

A program for general S was constructed and another taking advantage of the simplifications with $S=\frac{1}{2}$. In order to check the programs, tests were run on small systems for which exact data for comparison were computed by exact diagonalization. The tests consisted of 2×10^4 MC steps for fixing L, 4×10^4 steps for thermalization, and 10 bins for data taking, 2×10^4 steps each. The results presented are for $S=\frac{1}{2}$, 1, $\frac{3}{2}$, and system sizes $N=10$, 8, and 6, respectively. Periodic boundary conditions were implemented. Figure 4 displays the antiferromagnetic structure factors and Fig. 5 the staggered susceptibilities. The Monte Carlo results agree with the exact data down to temperatures where the systems are effectively in the ground state. In all figures $T=\beta^{-1}$ without any factors [see Eqs. (1.1), (3.1), and (3.18)], i.e., the temperature scale is defined by $k_B=1$.

For the system with $S=1$ and $N=8$, the order of the Taylor expansion, L, ranged from 42 at $T=3.0$ to 398 at $T=0.1$. The acceptance ratio for single-pair changes is around 50%. For two pair changes it varies between 30% and 50%. At high temperatures the acceptance rate of global changes lies around 50% and approaches zero as the temperature decreases. For ground-state properties, no global changes are needed if the initial state vectors are in the total $S^z=0$ subspace and β is chosen large. The probability of half-ring changes approaches zero as

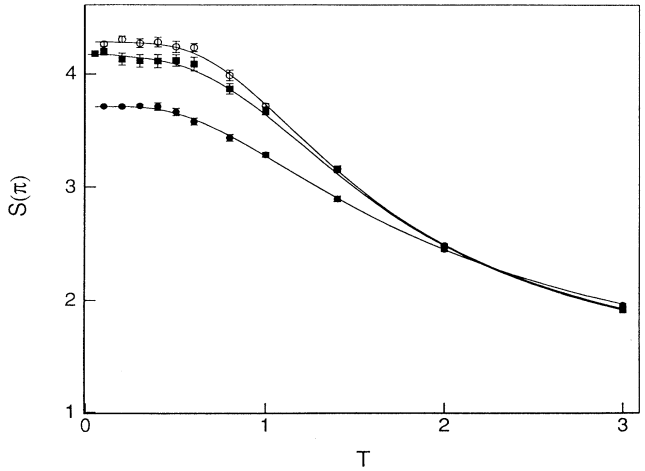

FIG. 4. Antiferromagnetic structure factor for $S=\frac{1}{2}$, $N=10$ (solid circles), $S=1$, $N=8$ (open circles), and $S=\frac{3}{2}$, $N=6$ (solid squares). The solid curves are the corresponding exact results.

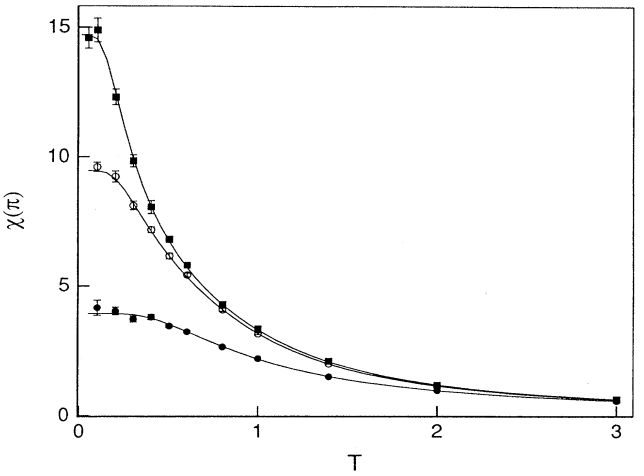

FIG. 5. Staggered susceptibility for $S=\frac{1}{2}$, $N=10$ (solid circles), $S=1$, $N=8$ (open circles), and $S=\frac{3}{2}$, $N=6$ (solid squares), along with the exact results (solid curves).

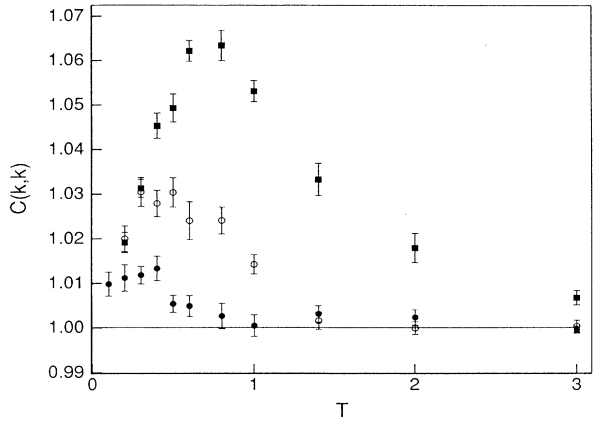

FIG. 6. Correlation function $C(k,k)$ as calculated in a run with no half-ring changes for $S=1$, $N=4$ (solid squares), $N=8$ (open circles), and $N=12$ (solid circles). For the isotropic interaction, $C(k,k)$ should equal unity.

the system size increases. If no half-ring changes are made, only the subspace with identical numbers of ring loops in both directions is sampled. This introduces nonuniformity as only the xy part of the interaction is affected. The importance of the subspace with an excess of ring loops in one direction seems to decrease for large systems, which is as expected since effects of the boundary conditions should diminish as the system grows. Figure 6 shows the correlation function $C(k,k)$ calculated without half-ring changes in the subspace of identical numbers of ring loops in both directions for $S=1$ and $N=4$, 8, and 12. The nonuniformity vanishes rapidly as the system grows, and the temperature range in which it appears becomes narrower. Other calculated quantities agree with the exact results in the same temperature ranges as $C(k,k)$. It should be safe, therefore, to leave out the half-ring changes for large systems.

IV. RESULTS

In order to demonstrate the power of the new method, we carried out simulations on systems up to $N=64$ for $S=1$ and $S=\frac{3}{2}$. An integer and a half-integer spin were chosen in view of Haldane's conjecture[24] suggesting that essentially different behaviors would be found. Although numerical investigations have been carried out before, there still seem to be unclear points left, particularly with $S>\frac{1}{2}$. Our simulations consisted of $(2-4)\times 10^5$ MC steps, in some cases divided into several independent runs. Although no half-ring changes were made for $N\geq 32$, the correlation function $C(k,k)$ did not stray outside the range of the statistical error from unity at any temperature.

We computed the energy per spin and the magnetic structure factors at several temperatures. The exponent of the divergence of the antiferromagnetic structure factor was determined. Further, the q-dependent static susceptibility was studied, the staggered susceptibility in particular. We find a finite value for the $S=1$ staggered susceptibility at $T=0$ and determine the exponent of the divergence in the $S=\frac{3}{2}$ case.

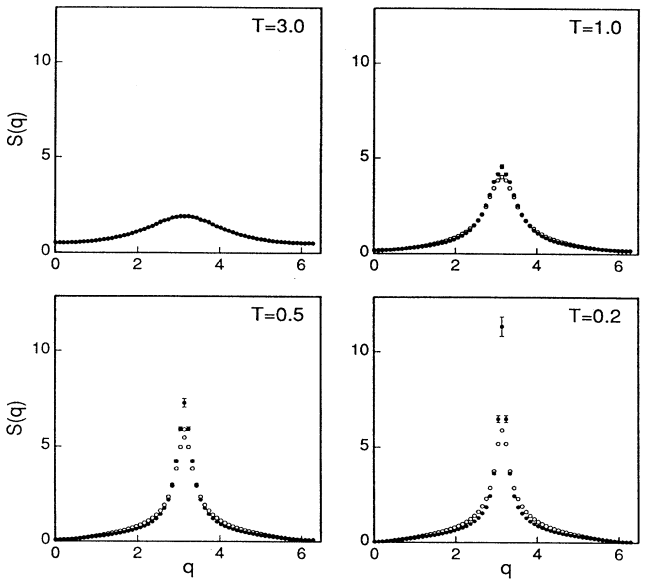

FIG. 8. Magnetic structure factors as functions of the wave number for $N=64$ at different temperatures (open circles for $S=1$, solid circles for $S=\frac{3}{2}$). For $S=1$ the $T=0.1$ results (not shown) does not differ from the $T=0.2$ data within the statistical error.

Figure 7 displays energies per spin in systems with $N=64$. Within the statistical error, no differences can be seen between system sizes $N=32$ and $N=64$ with either $S=1$ or $S=\frac{3}{2}$. The energies of Fig. 7 should therefore be good estimates for the infinite systems. The low-temperature results are consistent with the ground-state energies reported by Liang.[25]

In Fig. 8 we plot the magnetic structure factors $S(q)$ at different temperatures for $S=1$ and $S=\frac{3}{2}$. For $S=1$, the spin correlation function decays exponentially even in the ground state,[15,24,25] which implies a finite structure factor for all q. Our low-temperature results, corrected for the

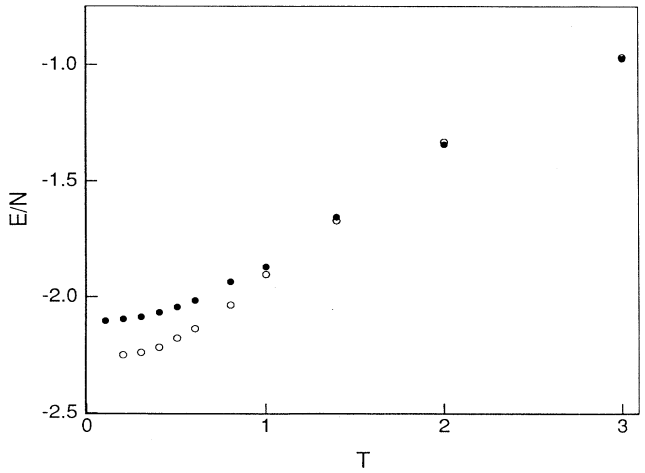

FIG. 7. Energy per spin for $N=64$ with $S=1$ (solid circles) and $S=\frac{3}{2}$ (open circles). Statistical errors are less than the size of the symbols.

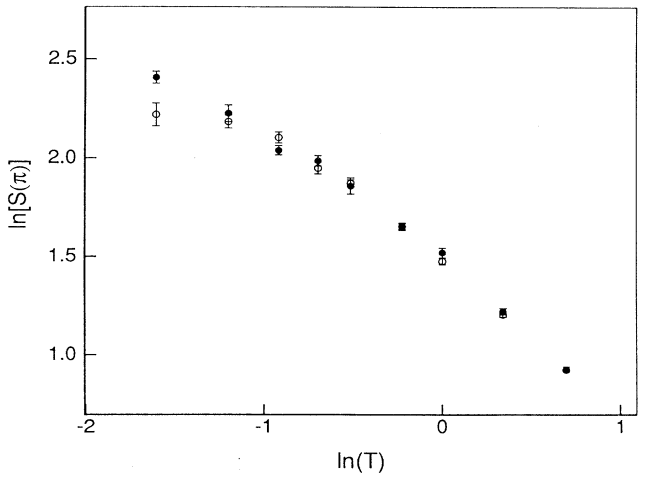

FIG. 9. $\ln[S(\pi)]$ vs $\ln(T)$ for $S=\frac{3}{2}$. Open circles are for $N=32$ and solid circles for $N=64$.

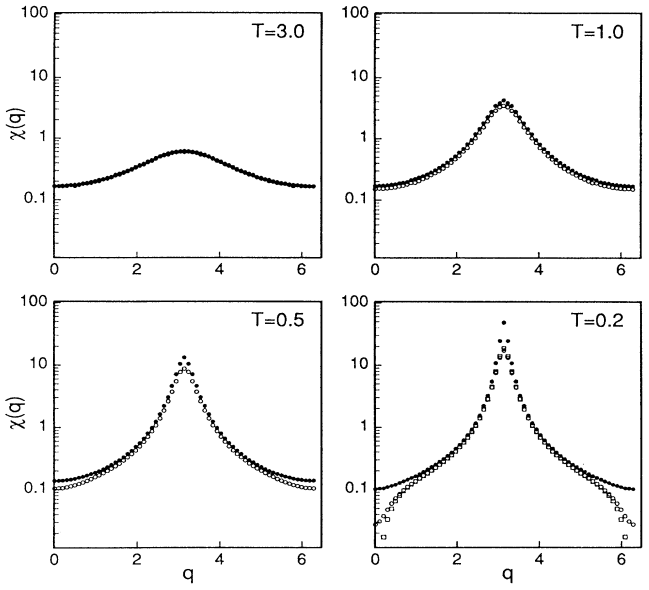

FIG. 10. Static susceptibilities at different temperatures for $N=64$ as functions of the wave number (open circles for $S=1$, solid circles for $S=\frac{3}{2}$). In the $T=0.2$-graph data for $S=1$, $T=0.1$ are included (open squares).

factor $\frac{3}{2}$ in units, agree with the ground-state structure factors reported in Ref. 15. For $S=\frac{3}{2}$, there is strong evidence pointing to a diverging antiferromagnetic structure factor at $T=0$.[13,25] Figure 9 displays $\ln[S(\pi)]$ against $\ln(T)$ for $N=32$ and $N=64$. Except for the lowest temperature ($T=0.2$), no size dependence can be seen within the statistical error. A straight-line fit through the five lowest temperature points of the $N=64$ data delivers the exponent $\bar{\gamma}=0.49\pm0.04$ for the divergence of $S(\pi)$. This value differs considerably from the value 0.70 ± 0.07 reported in Ref. 13.

Figure 10 shows the static susceptibilities as functions of the wave number at different temperatures for $N=64$. As the temperature decreases, the peaks emerging at $q=\pi$ initially look the same for $S=1$ and $S=\frac{3}{2}$, in spite

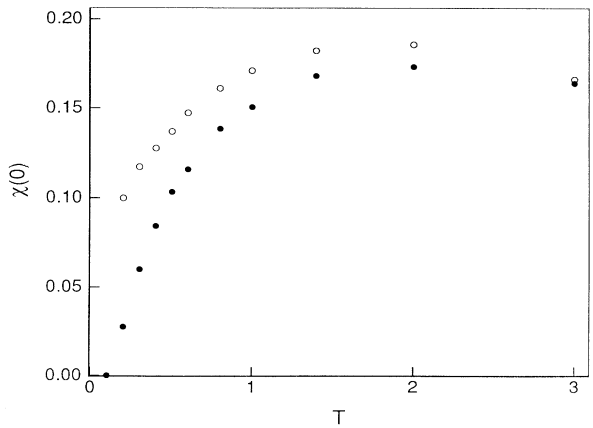

FIG. 11. Uniform susceptibility for $S=1$ (solid circles) and $S=\frac{3}{2}$ (open circles). The lattice size is $N=64$. Statistical errors are at most the size of the symbols.

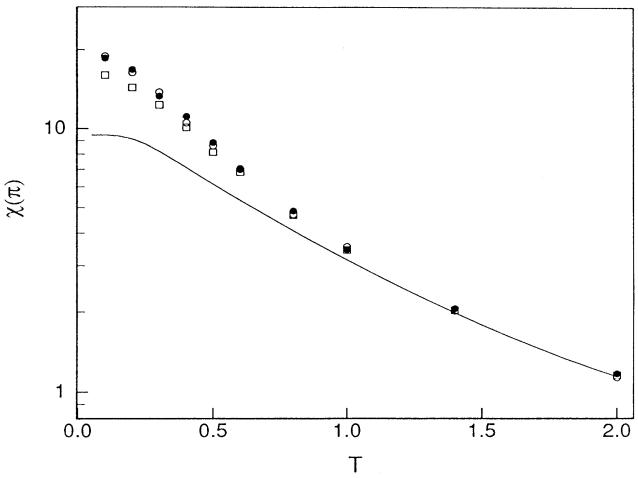

FIG. 12. Staggered susceptibilities for $S=1$. The solid line is the exact result for $N=8$. The Monte Carlo results are for $N=16$ (open squares), $N=32$ (open circles), and $N=64$ (solid circles). Statistical errors are on the order of the size of the symbols.

of the eventual divergence at $T=0$ with $S=\frac{3}{2}$. At $T=0$, the uniform ($q=0$) susceptibility vanishes even in the thermodynamic limit for $S=1$ as there is an excitation gap, and the ground state is a singlet.[24,26] For the gapless $S=\frac{3}{2}$ chain, one expects the same behavior as with $S=\frac{1}{2}$ where the uniform susceptibility takes a nonzero value at $T=0$.[27] Figure 11 displays the two $\chi(0)$ as functions of the temperature for $N=64$. In both cases, the $N=32$ and the $N=64$ data agree within the statistical error. We do not have enough low-temperature data in order to determine $\chi(0)$ at $T=0$ for $S=\frac{3}{2}$.

On account of the gap in the $S=1$ chain, one expects the staggered susceptibility to take a finite value at $T=0$. Figure 12 is a plot of $\chi(\pi)$ as a function of T. Again, at the temperatures studied, no differences can be seen between $N=32$ and $N=64$. Assume that the thermodynamic limit is within the statistical error of the $N=64$ data. Then a linear extrapolation of the $T=0.2$ and $T=0.1$ results gives $\chi(\pi)=20.0\pm1.5$ at $T=0$. For $S=\frac{3}{2}$ the staggered susceptibility diverges. In Fig. 13, $\ln[\chi(\pi)]$ is displayed against $\ln(T)$. A straight-line fit to the five lowest temperature points of the $N=64$ data delivers the exponent $\gamma=1.45\pm0.05$ which also differs from the value reported in Ref. 13 (1.70 ± 0.06). It is not clear that the exponents $\bar{\gamma}$ and γ should not change slightly going to even lower temperatures. Figures 9 and 13 show that they obviously evolve within the range studied here. Within the statistical error, our indices satisfy the relation $\gamma-\bar{\gamma}=1$.[13]

Most of the computations were carried out on a VAX-8800 and a VAX-3100 work station. We also used the CRAY X-MP EA/432 at the Centre for Scientific Computing in Helsinki. On the average the program running on the VAX-8800 with $S=1$ and $N=64$ requires 0.1 s per MC step at $T=1.0$ ($L=348$), 0.3 s at $T=0.5$ ($L=620$), and 0.9 s at $T=0.2$ ($L=1370$). At $T=0.1$ ($L=2594$) 1.1 s per MC step is required when no global

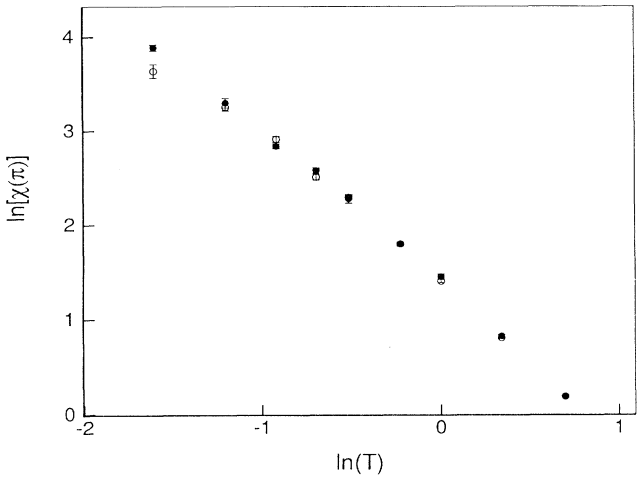

FIG. 13. $\ln[\chi(\pi)]$ vs $\ln(T)$ for $S=\frac{3}{2}$. Open circles are for $N=32$ and solid circles for $N=64$.

changes are made. Data collection for observables at every fifth MC step is included in the average. With $S=\frac{3}{2}$ slightly more time is required. Since most of the code cannot be vectorized, the gain in speed with the CRAY is only a factor of roughly 7.

V. DISCUSSION

The simulation algorithm described here is easily generalized to lattices of higher spatial dimensions. Two-pair changes can generate index sequences corresponding to any closed loop on a two-dimensional quadratic lattice with open boundaries. Only the last three subsets of (3.10) have to be modified in order to allow for the types of changes graphically depicted in Fig. 14. The one-dimensional half-ring changes can be trivially generalized to two-dimensional periodic lattices.

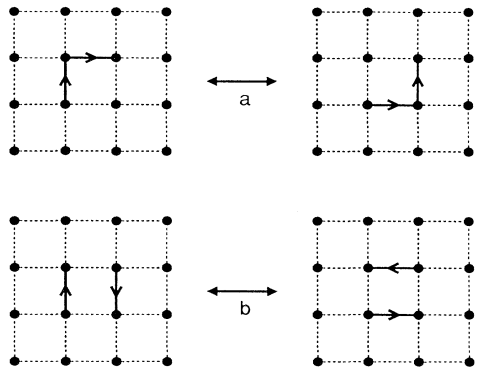

FIG. 14. Graphical representation of the additional loop changes required in the case of a two-dimensional lattice.

In conclusion, a new quantum Monte Carlo simulation algorithm applicable for any S and for any spatial dimensionality has been constructed. The usefulness of the method was demonstrated applying it to the one-dimensional antiferromagnetic spin-S Heisenberg model. Simulation results confirm earlier calculations of the magnetic structure factor in the $S=1$ chain. For $S=\frac{3}{2}$ we find the exponent $\bar{\gamma}=0.49\pm0.04$ for the divergence of the antiferromagnetic structure factor. Our results for the $S=1$ staggered susceptibility suggest the finite value $\chi(\pi)=20.0\pm1.5$ at $T=0$. For $S=\frac{3}{2}$, the present calculation gives the exponent $\gamma=1.45\pm0.05$ for the divergence of $\chi(\pi)$.

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*Present address: Department of Physics, University of California, Santa Barbara, CA 93106.

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