

# Finite-size scaling of the ground-state parameters of the two-dimensional Heisenberg model

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The ground-state parameters of the two-dimensional  $S=1/2$  antiferromagnetic Heisenberg model are calculated using the stochastic series expansion quantum Monte Carlo method for  $L \times L$  lattices with  $L$  up to 16. The finite-size results for the energy  $E$ , the sublattice magnetization  $M$ , the long-wavelength susceptibility  $\chi_{\perp}(q=2\pi/L)$ , and the spin stiffness  $\rho_s$ , are extrapolated to the thermodynamic limit using fits to polynomials in  $1/L$ , constrained by scaling forms previously obtained from renormalization-group calculations for the nonlinear  $\sigma$  model and chiral perturbation theory. The results are fully consistent with the predicted leading finite-size corrections, and are of sufficient accuracy for extracting also subleading terms. The subleading energy correction ( $\sim 1/L^4$ ) agrees with chiral perturbation theory to within a statistical error of a few percent, thus providing numerical confirmation of the finite-size scaling forms to this order. The extrapolated ground-state energy per spin is  $E = -0.669437(5)$ . The result from previous Green's function Monte Carlo (GFMC) calculations is slightly higher than this value, most likely due to a small systematic error originating from "population control" bias in GFMC. The other extrapolated parameters are  $M = 0.3070(3)$ ,  $\rho_s = 0.175(2)$ ,  $\chi_{\perp} = 0.0625(9)$ , and the spin-wave velocity  $c = 1.673(7)$ . The statistical errors are comparable with those of previous estimates obtained by fitting loop algorithm quantum Monte Carlo data to finite-temperature scaling forms. Both  $M$  and  $\rho_s$  obtained from the finite- $T$  data are, however, a few error bars higher than the present estimates. It is argued that the  $T=0$  extrapolations performed here are less sensitive to effects of neglected higher-order corrections, and therefore should be more reliable. [S0163-1829(97)01841-9]

## I. INTRODUCTION

In the nonlinear  $\sigma$  model description of the two-dimensional (2D) Heisenberg model,<sup>1</sup> the low-energy and low-temperature properties of the system are completely determined by three ground-state parameters; the sublattice magnetization  $M$ , the spin stiffness constant  $\rho_s$ , and the spin-wave velocity  $c$ . Their values are not given by the theory, however, but have to be determined starting from the microscopic Hamiltonian. A large number of calculations of the ground-state parameters have been carried out. The antiferromagnetically ordered ground state, which has been established rigorously only for  $S > 1/2$ ,<sup>2</sup> was convincingly confirmed also for  $S=1/2$  in a quantum Monte Carlo (QMC) study by Reger and Young.<sup>3</sup> The sublattice magnetization obtained this way,  $M \approx 0.30$  (in units where the Néel state has  $M = 1/2$ ), also indicated that spin-wave theory<sup>4,5</sup> gives a surprisingly good quantitative description of the ground state. The same conclusion was reached by Singh,<sup>6</sup> who carried out a series expansion around the Ising limit, and found  $M \approx 0.30$ ,  $\rho_s \approx 0.18J$ , and  $c \approx 1.7J$  ( $J$  is the nearest-neighbor exchange coupling), all in good agreement with spin-wave theory including the  $1/S$  corrections.<sup>5</sup> Subsequent higher-order spin-wave calculations showed that the  $1/S^2$  corrections to  $M$ ,  $\rho_s$ , and  $c$  indeed are small.<sup>7-9</sup> Several other QMC simulations,<sup>10-19</sup> exact diagonalizations,<sup>20-22</sup> as well as series expansions to higher orders,<sup>23</sup> have confirmed and improved on the accuracy of the above estimates. The presently most accurate calculations<sup>16,18,19,23</sup> indicate that the true values of the ground-state parameters deviate from their  $1/S^2$  spinwave values by only 1–2% or less.

For most practical purposes (such as extracting  $J$  for a system from experimental data), the ground-state parameters

of the 2D Heisenberg model are now known to quite sufficient accuracy. However, there are still reasons to go to even higher precision. One is that the model is one of the basic "prototypic" many-body models in condensed matter physics. It has become a testing ground for various analytical and numerical methods for strongly correlated systems, thus making it important to accurately establish its properties. Another reason is the very detailed predictions that have resulted from field theoretical studies, such as renormalization-group calculations for the nonlinear  $\sigma$  model,<sup>1,24-26</sup> and chiral perturbation theory.<sup>27</sup> Apart from giving the low-energy properties in the thermodynamic limit, these theories also predict the system size dependence of various quantities.<sup>25-27</sup> This is important from the standpoint of numerical calculations such as exact diagonalization and QMC, which are necessarily restricted to relatively small lattices. Finite-size scaling approaches have been very successful in the study of 1D quantum spin systems, having convincingly confirmed various predictions from bosonization and conformal field theory. For example, critical exponents and logarithmic corrections have been extracted from the size dependence of ground-state energies and finite-size gaps,<sup>28</sup> and from correlation functions.<sup>29</sup> With the concrete predictions now available, similar studies show great promise for testing theories also in 2D. For the standard Heisenberg model, finite-size scaling has been used extensively and successfully in extrapolating, e.g., the sublattice magnetization for small lattices to infinite system size,<sup>3,10-14</sup> but only a few studies have so far been accurate enough for reliably addressing the validity of the theoretical predictions for the size corrections.<sup>15,16,18,19</sup>

In one dimension, exact diagonalization, and more recently the density matrix renormalization-group method,<sup>30</sup>

enable highly accurate calculations for systems sufficiently large to approach the limit where the asymptotic scaling forms are valid.<sup>28,29</sup> Calculations with these methods in two dimensions cannot reach linear dimensions large enough to verify the details of the predicted scaling forms, however. Some of the expected leading finite-size behavior has been seen in exact diagonalization studies including systems with up to  $6 \times 6$  spins,<sup>20,21</sup> but constants extracted from the size dependence are typically not consistent with other calculations. For example,  $c$  extracted from the scaling of  $E$  deviates by 15% from other estimates.<sup>20</sup> There are hence clear indications that these small systems are not yet in the regime where only the dominant corrections are important.

QMC can reach significantly larger lattices at the cost of statistical errors which are often relatively large, making it difficult to accurately extract the scaling behavior. Runge carried out Green's function Monte Carlo (GFMC) simulations of  $L \times L$  Heisenberg systems with  $L$  up to 16, and found a reasonable consistency with the leading  $T=0$  size dependence of the energy and the sublattice magnetization.<sup>15,16</sup> He also noted the presence of a subleading correction to the energy,<sup>16</sup> but the accuracy of the GFMC data was not high enough to extract its order, and furthermore  $c$  extracted from the leading correction was sensitive to the subleading one. The extrapolated ground-state energy,  $E = -0.66934(3)$ , is nevertheless the most accurate estimate reported for this quantity.

Chiral perturbation theory has recently enabled calculations of scaling forms for finite size *and* finite temperature for various quantities.<sup>27</sup> Such forms have been used in combination with QMC data in recent work by Wiese and Ying,<sup>18</sup> and Beard and Wiese.<sup>19</sup> Their calculations employed, respectively, methods based on the "loop-cluster algorithm" invented by Evertz *et al.*,<sup>31</sup> and a continuous-time variant of that method developed by Beard and Wiese.<sup>19</sup> These algorithms are based on global flips of loops of spins, and overcome the problems with long autocorrelation times typical of standard Suzuki-Trotter<sup>32,33</sup> or worldline<sup>34</sup> QMC methods (the continuous-time approach furthermore avoids the systematic discretization error of the Trotter approximation). Considerably more accurate finite- $T$  data could therefore be generated, and the leading-order scaling forms of chiral perturbation theory were convincingly verified, both in the "cubic" regime  $T/c \approx 1/L$  (Ref. 18) and the "cylindrical" regime  $T/c \ll 1/L$  (Ref. 19). The extrapolated  $M$ ,  $\rho_s$ , and  $c$  are impressively accurate, although there are some minor discrepancies between the two results for  $M$  (on the border line of what could be expected within statistical errors alone).

In this paper, a finite-size scaling study of  $T=0$  data is reported. Using the stochastic series expansion (SSE) QMC algorithm,<sup>35,36</sup> high-precision energy results are obtained for  $L \times L$  lattices with  $L$  up to 16. The relative statistical errors are as low as  $\approx 10^{-5}$ . Employing a recently suggested data analysis scheme which takes into account covariance among calculated quantities,<sup>37</sup> very accurate results for the sublattice magnetization are also obtained. Furthermore, the spin stiffness and the long-wavelength susceptibility  $\chi(q=2\pi/L)$  are also calculated directly in the simulations.

Assuming for the size dependences polynomials in  $1/L$ , constrained by scaling forms for  $E$  and  $M$  predicted from chiral perturbation theory,<sup>27</sup> all the computed quantities are

included in a coupled  $\chi^2$  fit. The quality of the QMC data for  $E$  and  $M$  is high enough that size corrections *beyond the subleading terms* have to be included. The leading-order corrections are fully consistent with the predictions. From a careful statistical analysis of the fits, bounds for the subleading terms are estimated. The subleading energy correction is found to agree with the prediction of chiral perturbation theory to within a statistical error of 5% (the subleading correction for  $M$  is also estimated, but has not yet been calculated analytically). This is hence a numerical confirmation of chiral perturbation theory to subleading order.

The extrapolated ground-state energy,  $E = -0.669437(5)$ , has a statistical error six times smaller than the GFMC result by Runge,<sup>16</sup> and is slightly lower than his result. Comparing the finite-size data of the two calculations, a clear tendency to overestimation of the energy is seen in the GFMC results. This is likely due to a bias originating from "population control" in GFMC (a small effect of this nature was in fact anticipated by Runge<sup>16</sup>).

The results for the sublattice magnetization,  $M = 0.3070(3)$ , and the spin stiffness,  $\rho_s = 0.175(2)$ , are both slightly lower than the estimates obtained from the finite- $T$  scaling by Beard and Wiese<sup>19</sup> [ $M = 0.3083(2)$  and  $\rho_s = 0.185(2)$ ]. Although it is at this point difficult to definitely conclude which calculation is more reliable, it can again be noted that the high accuracy of the QMC data for  $E$  and  $M$  used in the fits carried out in this paper necessitates the inclusion of size corrections beyond the orders considered by Beard and Wiese.<sup>19</sup> Hence, any remaining effects of neglected corrections of even higher order should be smaller. Quantitative estimates of such effects on the extrapolations performed here support that they are indeed smaller than the statistical errors indicated above. For the spin-wave velocity the two calculations agree, the result obtained here being  $c = 1.673(7)$  and the value reported in Ref. 19 being  $c = 1.68(1)$ .

The outline of the rest of the paper is the following. In Sec. II the SSE algorithm and the covariance error reduction scheme are outlined. The absence of systematic errors are demonstrated in comparisons with exact results for  $4 \times 4$  and  $6 \times 6$  lattices. The fitting procedures and the results of these are discussed in Sec. III. The study is summarized in Sec. IV. Some other problems where the methods applied here should be useful are also mentioned.

## II. NUMERICAL METHODS

The standard 2D Heisenberg model is defined by the Hamiltonian

$$\hat{H} = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j \quad (J > 0), \quad (1)$$

where  $\mathbf{S}_i$  is a spin-1/2 operator at site  $i$  on a square lattice with  $N = L \times L$  sites, and  $\langle i,j \rangle$  denotes a pair of nearest-neighbor sites. Below, in Sec. II A, the SSE approach to QMC simulation of this model is outlined. More details of the algorithm are discussed in Refs. 36 and 38. The SSE method has recently been applied to a variety of spin models,<sup>39–42</sup> as well as 1D Hubbard-type electronic models.<sup>43</sup>

It was recently noted that correlations between measurements of different observables can be used to significantly increase the accuracy of certain quantities calculated in SSE simulations.<sup>37</sup> This covariance scheme for analyzing the data is of crucial importance in the present work, and therefore this method is also described below in Sec. II B. The high accuracy of the procedures is demonstrated by comparing results for  $4 \times 4$  and  $6 \times 6$  lattices with the exact diagonalization data available for these systems.

### A. Stochastic series expansion

Based on the exact power series expansion of  $e^{-\beta\hat{H}}$ , the SSE method<sup>35,36</sup> can be considered a generalization of Handscomb's QMC scheme.<sup>44,45</sup> It is the first "exact" method proposed for QMC simulations of general lattice Hamiltonians at finite temperature (with the usual caveat of being in practice restricted to models for which the sign problem can be avoided). It is not based on a controlled approximation, such as the Trotter formula used in standard worldline methods,<sup>34</sup> and therefore directly gives results accurate to within statistical errors. Despite being formulated at finite  $T$ , temperatures low enough for studying the ground state can easily be reached for moderate-size lattices.

As in Handscomb's method for the  $S=1/2$  antiferromagnet,<sup>45</sup> the SSE approach for this model starts from the Hamiltonian written as ( $J=1$ )

$$\hat{H} = -\frac{1}{2} \sum_{b=1}^{2N} [\hat{H}_{1,b} - \hat{H}_{2,b}] + \frac{N}{2}, \quad (2)$$

where  $b$  is a bond connecting a pair of nearest-neighbor sites  $\langle i(b), j(b) \rangle$ , and the operators  $\hat{H}_{1,b}$  and  $\hat{H}_{2,b}$  are defined as

$$\hat{H}_{1,b} = 2[\frac{1}{4} - S_{i(b)}^z S_{j(b)}^z], \quad (3a)$$

$$\hat{H}_{2,b} = S_{i(b)}^+ S_{j(b)}^- + S_{i(b)}^- S_{j(b)}^+. \quad (3b)$$

An exact expression for an operator expectation value

$$\langle \hat{A} \rangle = \frac{1}{Z} \text{Tr} \{ \hat{A} e^{-\beta\hat{H}} \}, \quad Z = \text{Tr} \{ e^{-\beta\hat{H}} \}, \quad (4)$$

at inverse temperature  $\beta = J/T$ , is obtained by Taylor expanding  $e^{-\beta\hat{H}}$  and writing the traces as sums over diagonal matrix elements in the basis  $\{ |\alpha\rangle = |S_1^z, \dots, S_N^z\rangle \}$ . The partition function is then<sup>35</sup>

$$Z = \sum_{\alpha} \sum_{n=0}^{\infty} \sum_{S_n} \frac{(-1)^{n_2} \beta^n}{n!} \left\langle \alpha \left| \prod_{i=1}^n \hat{H}_{a_i, b_i} \right| \alpha \right\rangle, \quad (5)$$

where  $S_n$  is a sequence of index pairs defining the operator string  $\prod_{i=1}^n \hat{H}_{a_i, b_i}$ ,

$$S_n = [a_1, b_1][a_2, b_2] \dots [a_n, b_n], \quad (6)$$

$$a_i \in \{1, 2\}, b_i \in \{1, \dots, 2N\},$$

and  $n_2$  denotes the total number of index pairs (operators)  $[a_i, b_i]$  with  $a_i = 2$  ( $n = n_1 + n_2$ ). Equation (5) deviates from Handscomb's method,<sup>44,45</sup> which relies on exact evaluation of the traces of the operator sequences and therefore is limited to models for which this is possible.

The Heisenberg model considered here is such a model (one of the very few), but the more general SSE approach of further expanding over a set of basis states is preferable also in this case, for reasons that will be discussed below.

The objective now is to develop a scheme for importance sampling of the terms in the partition function (5). A term, or configuration,  $(\alpha, S_n)$  is specified by a basis state  $|\alpha\rangle$  and an operator sequence  $S_n$ . The operators  $\hat{H}_{1,b}$  and  $\hat{H}_{2,b}$  can act only on states where the spins at sites  $i(b)$  and  $j(b)$  are antiparallel. The diagonal  $\hat{H}_{1,b}$  leaves such a state unchanged, whereas the off-diagonal  $\hat{H}_{2,b}$  flips the spin pair.

### Defining a propagated state

$$|\alpha(p)\rangle = \prod_{i=1}^p \hat{H}_{a_i, b_i} |\alpha\rangle, \quad |\alpha(0)\rangle = |\alpha\rangle, \quad (7)$$

a configuration  $(\alpha, S_n)$  must clearly satisfy the periodicity condition  $|\alpha(n)\rangle = |\alpha(0)\rangle$  in order to contribute to the partition function. For a lattice with  $L \times L$  sites and  $L$  even, this implies that the total number  $n_2$  of the off-diagonal operators must be even, and hence that all terms in Eq. (5) are positive and can be used as relative probabilities in a Monte Carlo importance sampling procedure (this is true for any nonfrustrated system).

For a finite system at finite  $\beta$ , the powers  $n$  contributing significantly to the partition function are restricted to within a well defined regime, and the sampling space is therefore finite in practice. In order to construct an efficient updating scheme for the index sequence it is useful to explicitly truncate the Taylor expansion at some self-consistently chosen upper bound  $n=l$ , high enough to cause only an exponentially small, completely negligible error.<sup>35</sup> One can then define a sampling space where the length of the sequence is *fixed*, by inserting a number  $l-n$  of unit operators, denoted  $\hat{H}_{0,0}$ , in the operator strings. The terms in the partition function (5) are divided by  $\binom{l}{n}$ , in order to compensate for the number of different ways of inserting the unit operators. The summation over  $n$  in Eq. (5) is then implicitly included in the summation over all sequences  $S_l$  of length  $l$ , with  $[a_i, b_i] = [0, 0]$  as an allowed operator. Denoting by  $W(\alpha, S_l)$  the weight of a configuration  $(\alpha, S_l)$ , the partition function is then

$$Z = \sum_{\alpha} \sum_{S_l} W(\alpha, S_l). \quad (8)$$

Since all nonzero matrix elements in Eq. (5) equal one, the weight is (when nonvanishing)

$$W(\alpha, S_l) = \left( \frac{\beta}{2} \right)^n \frac{(l-n)!}{l!}, \quad (9)$$

where  $n$  still is the expansion power of the term, i.e., the number of non-[0,0] operators in  $S_l$ .

The following is only a brief outline of the actual sampling scheme. More details can be found in Refs. 36 and 38. During the simulation,  $S_l$  and one of the states  $|\alpha(p)\rangle$  are stored. Other propagated states are generated as needed. The simulation is started with a randomly generated state  $|\alpha(0)\rangle$ , with an index sequence  $S_l$  containing only [0,0] operators

(unit operators), and with some arbitrary (small)  $l$ . The truncation  $l$  is adjusted as the simulation proceeds, as will be discussed further below.

With the fixed-length scheme, all updates of the operator sequence can be formulated in terms of substitutions of one or several operators. The simplest involves a diagonal operator at a single position;  $[0,0] \leftrightarrow [1,b]$ . This update can be carried out consecutively at all positions  $p$  for which  $a_p \in \{0,1\}$ . In the  $\rightarrow$  direction, the bond index  $b$  is chosen at random and the update is rejected if the spins connected by  $b$  are parallel in the current state  $|\alpha(p-1)\rangle$ . The Metropolis acceptance probabilities<sup>46</sup> required to satisfy detailed balance are obtained from Eq. (9), where the power  $n$  in is changed by  $\pm 1$ . Updates involving the off-diagonal operators  $[2,b]$  are carried out with  $n$  fixed. The simplest is of the type  $[1,b][1,b] \leftrightarrow [2,b][2,b]$ , involving two operators acting on the same bond. These two sequence updates can generate all configurations with spin flips on retracing paths on the lattice, and are the only ones required for a 1D system with open boundary conditions. For a 2D system, configurations associated with spin flips around any closed loop are possible, and an additional type of update is required. It is sufficient to consider substitutions on a plaquette, of the type  $[2,b_1][2,b_2] \leftrightarrow [2,b_3][2,b_4]$ , where  $b_1, \dots, b_4$  is a permutation of the four bonds of a plaquette. For systems with periodic boundary conditions, updates involving cyclic spin flips on loops wrapping around the whole system are required (sampling of different winding number sectors), and cannot be accomplished by the above local sequence alterations. For the square lattice considered here, the winding number can be changed by substituting  $L/2$  operators according to  $[2,b_1] \dots [2,b_{L/2}] \leftrightarrow [2,b_{L/2+1}] \dots [2,b_L]$ , where the set of bonds  $b_1, \dots, b_L$  is a permutation of bonds forming a closed ring around the system in the  $x$  or  $y$  direction.

Updating the operator sequence with the four types of operator substitutions described above suffices for generating all possible configurations within a sector of fixed magnetization,  $m^z = \sum_{i=1}^N S_i^z$ . In the grand canonical ensemble, global spin flips changing the magnetization are also required. Here  $T \rightarrow 0$  will be considered (i.e.,  $T$  is much lower than the finite-size gap), and since the ground state is a singlet<sup>47</sup> the canonical ensemble with  $m^z = 0$  is appropriate. It can be noted that in Handscomb's method the sampling is (in principle) automatically over all magnetization sectors, and therefore a restriction to, e.g.,  $m^z = 0$  is not possible. In practice, this causes problems at low temperatures, and Handscomb's method has therefore been used for the antiferromagnetic Heisenberg model mostly at relatively high temperatures ( $T/J \gtrsim 0.4$  in 2D).<sup>45</sup> The SSE method with the restriction  $m^z = 0$  can be used at arbitrarily low  $T$ .

In order to determine a sufficiently high truncation of the expansion, the fluctuating power  $n$  is monitored during the equilibration part of the simulation. If  $n$  exceeds some threshold  $l - \Delta_l/2$ , the cutoff is increased,  $l \rightarrow l + \Delta_l$ , by inserting additional  $[0,0]$  operators at random positions. In practice  $\Delta_l \approx l/10$  leads to a rapid saturation of  $l$  at a value sufficient to cause no detectable truncation errors. The growth of  $l$  during equilibration is illustrated for a  $4 \times 4$  system in Fig. 1. The distribution of  $n$  during a subsequent

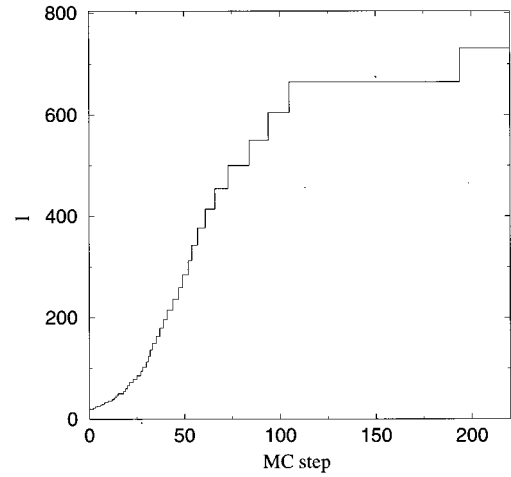


FIG. 1. The operator sequence truncation vs the number of Monte Carlo steps performed for a  $4 \times 4$  lattice at inverse temperature  $\beta = 32$ . The final  $l$  after  $10^5$  MC steps was  $l = 804$  (the last increase occurred after 6674 steps). The increment used was  $\Delta_l = l/10$ .

simulation is shown in Fig. 2, and clearly demonstrates that the truncation of the expansion is no approximation in practice.

A Monte Carlo step (MC step) is defined as a series of the single (diagonal) operator substitutions attempted consecutively at each position in  $S_l$  (where possible), followed by a series of off-diagonal updates carried out on each bond, plaquette, and ring. Due to the locality of the constraints in these updates, the number of operations (the CPU time) per MC step scales linearly with  $N$  and  $\beta$ .<sup>36,38</sup> However, the acceptance rate for the “ring update” that changes the winding number decreases rapidly with increasing system size. It is therefore sometimes useful to increase the number of attempted ring updates with the system size, which then leads to a faster growth of CPU time with  $N$ . The acceptance rate

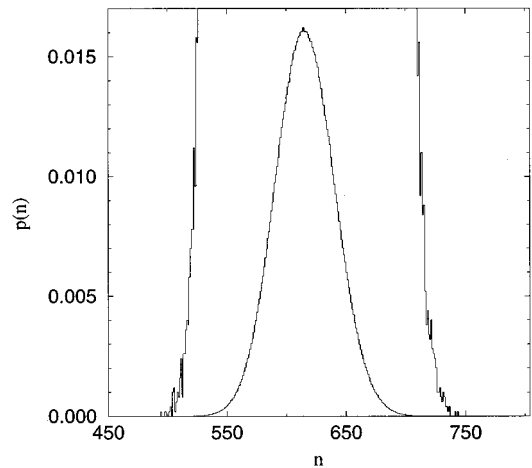


FIG. 2. The distribution of the power  $n$  of the sampled terms in a  $5 \times 10^6$  MC step simulation of  $4 \times 4$  lattice at inverse temperature  $\beta = 32$ , after adjusting  $l$  as shown in Fig. 1. The lower histogram is the full distribution. The higher, only partially visible histogram is the distribution multiplied by a factor 1000. The cutoff was  $l = 804$ , which is significantly larger than the largest  $n$  sampled. Hence, the truncation has not degraded the accuracy of the simulation.

of the ring update currently used becomes too low for  $L \geq 16$ , and simulations of larger systems therefore in practice have to be restricted to the sector with zero winding number. It has recently been noted<sup>48</sup> that in fact exact results are obtained as  $T \rightarrow 0$  even for simulations restricted this way. However, compared to simulations with fluctuating winding numbers, lower temperatures are required for the system observables to saturate at their ground-state values.<sup>48</sup> Here only systems with  $L \leq 16$  are considered, and the update changing the winding number is always included.

Measurements of physical observables are carried out using the index sequences  $S_n$  obtained by omitting the  $[0,0]$  operators in the generated  $S_l$ . These are then, of course, distributed according to the weight function corresponding to Eq. (5).

One can show that the internal energy per spin is simply given by the average of  $n$  [with the constant term in Eq. (2) neglected]:<sup>44,35</sup>

$$E = -\frac{\langle n \rangle}{N\beta}. \quad (10)$$

This expression also shows that the average power, and hence the sequence length  $l$ , scales as  $\beta N$  at low temperatures.

A spin-spin correlation function,

$$C(i, j) = C(\mathbf{r}_i - \mathbf{r}_j) = \langle S_i^z S_j^z \rangle, \quad (11)$$

is obtained averaging the correlations in the propagated states  $|\alpha(p)\rangle$  defined in Eq. (7). Further defining

$$S_i^z[p] = \langle \alpha(p) | S_i^z | \alpha(p) \rangle, \quad (12)$$

the correlation function is given by<sup>35</sup>

$$C(i, j) = \left\langle \frac{1}{n+1} \sum_{p=0}^n S_i^z[p] S_j^z[p] \right\rangle. \quad (13)$$

The corresponding static susceptibility,

$$\chi(i, j) = \int_0^\beta d\tau \langle S_i^z(\tau) S_j^z(0) \rangle, \quad (14)$$

involves correlations between all the propagated states:<sup>36</sup>

$$\begin{aligned} \chi(i, j) = & \left\langle \frac{\beta}{n(n+1)} \left( \sum_{p=0}^{n-1} S_i^z[p] \right) \left( \sum_{p=0}^{n-1} S_j^z[p] \right) \right. \\ & \left. + \frac{\beta}{(n+1)^2} \left( \sum_{p=0}^n S_i^z[p] S_j^z[p] \right) \right\rangle. \end{aligned} \quad (15)$$

Off-diagonal correlation functions can be easily calculated for operators that can be expressed in terms of the spin-flipping operators  $\hat{H}_{2,b}$ , each of which is a sum of two terms;  $\hat{H}_b^+ = S_{i(b)}^+ S_{j(b)}^-$  and  $\hat{H}_b^- = S_{i(b)}^- S_{j(b)}^+$ . The spin stiffness constant, which will be discussed further below, involves a static susceptibility defined in terms of these operators.

Although the simulation scheme is formulated with  $\hat{H}_{2,b} = H_b^+ + H_b^-$ , one can still access the terms individually since only one of them can propagate a given state. One can show that an equal-time correlation function,

$$F_{\sigma\sigma'}(b, b') = \langle \hat{H}_b^\sigma \hat{H}_{b'}^{\sigma'} \rangle, \quad (16)$$

is given by<sup>36</sup>

$$F_{\sigma\sigma'}(b, b') = \left\langle \frac{n-1}{(\beta/2)^2} N(b\sigma; b'\sigma') \right\rangle, \quad (17)$$

where  $N(b\sigma; b'\sigma')$  is the number of times the operators  $\hat{H}_b^\sigma$  and  $\hat{H}_{b'}^{\sigma'}$  appear next to each other in  $S_n$ , in the given order. The corresponding static susceptibility,

$$\chi_{\sigma\sigma'}(b, b') = \int_0^\beta d\tau \langle \hat{H}_b^\sigma(\tau) \hat{H}_{b'}^{\sigma'}(0) \rangle, \quad (18)$$

is given by the remarkably simple formula<sup>36</sup>

$$\chi_{\sigma\sigma'}(b, b') = 4 \langle N(b\sigma) N(b'\sigma') - \delta_{bb'} \delta_{\sigma\sigma'} N(b\sigma) \rangle / \beta, \quad (19)$$

where  $N(b\sigma)$  is the total number of operators  $\hat{H}_b^\sigma$  in  $S_n$ .

Now a direct estimator for the spin stiffness  $\rho_s$  can be constructed. It is defined as the second derivative of the ground-state energy with respect to a twist  $\Phi$  in the boundary condition, around an axis perpendicular to the direction of the broken symmetry. For a finite lattice, where the symmetry is not broken, a factor 3/2 has to be included in order to account for rotational averaging. Distributing the twist equally over all interacting spin pairs  $\langle i, j \rangle_x$  in the  $x$  direction, the finite-size definition for  $\rho_s$  is hence

$$\rho_s = \frac{3}{2} \frac{1}{L^2} \left. \frac{\partial^2 E_0(\phi)}{\partial \phi^2} \right|_{\phi=0}, \quad (20)$$

where  $\phi = \Phi/L$ . An expression which is only dependent on the ground state at  $\phi=0$  is obtained by expanding the Hamiltonian to second order in  $\phi$ . The Hamiltonian in the presence of the twist is

$$\hat{H}(\phi) = \sum_{\langle i, j \rangle_x} \mathbf{S}_i \cdot R(\phi) \mathbf{S}_j + \sum_{\langle i, j \rangle_y} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (21)$$

where  $R(\phi)$  is the rotation matrix

$$R(\phi) = \begin{pmatrix} \cos(\phi) & \sin(\phi) & 0 \\ -\sin(\phi) & \cos(\phi) & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (22)$$

Expanding to second order in  $\phi$  results in

$$\begin{aligned} \hat{H}(\phi) - \hat{H}(0) = & -\frac{1}{2} \sum_{\langle i, j \rangle_x} [\phi^2 (S_i^x S_j^x + S_i^y S_j^y) \\ & + i\phi (S_i^+ S_j^- - S_i^- S_j^+)]. \end{aligned} \quad (23)$$

The first term is proportional to  $\hat{H}(0)$  (for the rotationally invariant case considered here). The expectation value of the second term vanishes, but it gives a contribution quadratic in  $\phi$  in second order perturbation theory. Defining the spin current operator

$$j_s = \frac{i}{2} \sum_{\langle i, j \rangle_x} (S_i^+ S_j^- - S_i^- S_j^+), \quad (24)$$



and the current-current correlation function at Matsubara frequency  $\omega_m = 2\pi mT$ ,

$$\Lambda_s(\omega_m) = \frac{1}{L^2} \int_0^\beta d\tau e^{-i\omega_m \tau} \langle j_s(\tau) j_s(0) \rangle, \quad (25)$$

the stiffness is given by

$$\rho_s = -\frac{3}{2} \left[ \frac{1}{3} E + \Lambda_s(0) \right], \quad (26)$$

where  $E$  is the ground-state energy per spin.

The QMC estimate for the energy is given by Eq. (10). The current-current correlator  $\Lambda_s \equiv \Lambda_s(0)$  is a sum of integrals of the form (18). Denoting by  $N_x^+$  and  $N_x^-$  the number in  $S_n$  of operators  $S_i^+ S_j^-$  and  $S_i^- S_j^+$  with  $\langle i, j \rangle$  a bond in the  $x$  direction, Eqs. (25) and (19) give

$$\rho_s = \frac{3/2}{\beta N} \langle (N_x^+ - N_x^-)^2 \rangle, \quad (27)$$

i.e., the terms linear in  $N_x^+$  and  $N_x^-$  cancel. Defining the winding numbers  $w_x$  and  $w_y$  in the  $x$  and  $y$  direction:

$$w_\alpha = (N_\alpha^+ - N_\alpha^-)/L \quad (\alpha = x, y), \quad (28)$$

the stiffness can also be written as

$$\rho_s = \frac{3}{4} \langle w_x^2 + w_y^2 \rangle / \beta. \quad (29)$$

This definition is clearly valid only for a simulation that samples all winding number sectors. With a restriction to the subspace with  $w_x = w_y = 0$ ,  $\rho_s$  can be calculated using the long-wavelength limit of a current-current correlator involving a twist field with a spatial modulation.<sup>49</sup>

The above method of calculating the stiffness directly from the winding number fluctuations is clearly strongly related to methods used for the superfluid density in simulations of boson models.<sup>50</sup>

### B. Error reduction using covariance

In Monte Carlo simulations, fluctuations (statistical errors) of different physical observables are often correlated with each other. These covariance effects can sometimes be used to obtain improved estimators for certain quantities.<sup>37</sup> In some cases one may have exact knowledge of some quantity independently of the QMC calculation. If there are strong correlations between a known quantity  $A$  and some other, unknown quantity  $B$ , the accuracy of  $B$  can be improved via its covariance with the measured  $A$ , by calculating the average and statistical error under the condition that  $A$  equals its known value. In other cases, it may be possible to calculate a quantity in more than one way in the same simulation. If one of the estimates,  $A_1$ , is more accurate than the other,  $A_2$ , a covariance between  $A_2$  and some other quantity  $B$  can again be used to improve the estimate of  $B$ . With the SSE method the internal energy of the rotationally invariant Heisenberg model can be calculated in two different ways:  $E_1$  from the average power of the series expansion according to Eq. (10), and using the nearest-neighbor correlation function  $C(1,0)$  calculated according to Eq. (13);  $E_2 = 6C(1,0)$ . The manifestly rotationally invariant estimator  $E_1$  is significantly less noisy than  $E_2$ . Results for quantities

with fluctuations correlated to those of  $C(1,0)$ , such as  $C(\mathbf{r})$  with  $r > 1$ , can therefore be improved with the aid of  $E_1$ .

For the purpose of accurately measuring correlations between the fluctuations of two different quantities, the so-called ‘‘bootstrap method’’ is a useful tool.<sup>51</sup> With the simulation data as usually divided into  $M$  ‘‘bin’’ averages, a ‘‘bootstrap sample’’  $\bar{A}_R$  is defined as an average over  $M$  randomly selected bins (i.e., the same number as the total number of bins, allowing, of course, multiple selections of the same bin). With  $r(i)$  denoting the  $i$ th randomly chosen bin,

$$\bar{A}_R = \frac{1}{M} \sum_{i=1}^M A_{r(i)}. \quad (30)$$

The statistical error can be calculated on the basis of  $M_R$  bootstrap samples  $\bar{A}_{R_i}$ , according to<sup>51</sup>

$$\sigma^2 = \frac{1}{M_R} \sum_{i=1}^{M_R} (\bar{A}_{R_i} - \bar{A})^2, \quad (31)$$

where  $\bar{A}$  is the regular average over all bins. Note that Eq. (31) lacks the factor  $(M_R - 1)^{-1}$  present in the conventional expression for the variance of the average calculated on the basis of  $M_R$  bins. The bootstrap method is in general more accurate (due to a better realization of a Gaussian distribution for the bootstrap samples), in particular if  $A$  is not measured directly in the simulation, but is some nonlinear function of measured quantities (in which case  $A$  should be calculated on the basis of bootstrap samples, not individual bins). Sets of bootstrap samples  $\{\bar{A}_{R_i}\}$  and  $\{\bar{B}_{R_i}\}$  generated on the basis of the same randomly selected bins are well suited for evaluating correlations between the statistical fluctuations of  $A$  and  $B$ , and are used in the covariance error reduction scheme described next.

Here this method will be illustrated using simulation results for the staggered structure factor  $S(\pi, \pi)$  and the staggered susceptibility  $\chi(\pi, \pi)$ . These are defined according to

$$S(\pi, \pi) = \frac{1}{N} \sum_{i,j} (-1)^{x_j - x_i + y_j - y_i} C(i, j), \quad (32a)$$

$$\chi(\pi, \pi) = \frac{1}{N} \sum_{i,j} (-1)^{x_j - x_i + y_j - y_i} \chi(i, j), \quad (32b)$$

with  $C(i, j)$  and  $\chi(i, j)$  given by Eqs. (13) and (15). The structure factor is of particular interest, since it defines the sublattice magnetization squared of a finite system. The fluctuations of  $S(\pi, \pi)$  are strongly correlated to those of  $C(1,0)$ , and  $S(\pi, \pi)$  can therefore be calculated to an accuracy significantly higher than if only the direct estimator (13) is used. The susceptibility  $\chi(\pi, \pi)$  is only weakly correlated with  $C(1,0)$ , however, and only a modest gain in accuracy can be achieved for this quantity.

First some results for a  $6 \times 6$  lattice are discussed. This is the largest system for which Lanczos results have been obtained.<sup>21</sup> Comparing with these exact results, the accuracy of the QMC technique and the covariance method can be rigorously checked. The temperature used in the simulation has to be low enough for the calculated quantities to have

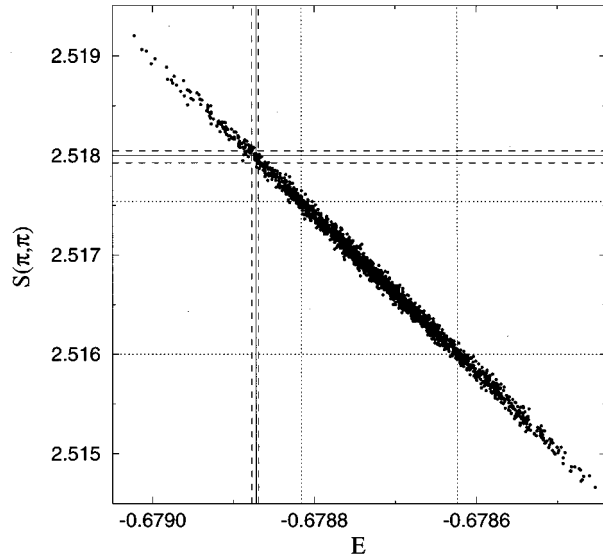


FIG. 3. Correlations between the staggered structure factor and the energy as obtained from the nearest-neighbor correlation function for a  $6 \times 6$  lattice at  $\beta=48$ . Each point represents a bootstrap sample of QMC bin averages. The solid vertical line indicates the exact energy, and the solid horizontal line is the exact structure factor [the result for  $S(\pi, \pi)$  is given “only” with 5 significant digits in Ref. 21, which actually implies a small uncertainty on the scale of this figure]. The vertical dotted and dashed lines indicate, respectively, the estimate  $\pm$  one standard deviation of the energy calculated from the nearest-neighbor correlation function and the average of  $n$ . The dotted horizontal lines indicate the conventional estimate of the structure factor, and the dashed ones the improved result obtained using the covariance method.

saturated at their ground-state values. In order to check for temperature effects, several calculations were carried out. Results at inverse temperatures  $\beta=24$  and 48 are indistinguishable within error bars, indicating that these temperatures are sufficiently low for  $L=6$ . The results presented below are for  $\beta=48$ . The simulation was divided into bins of  $5 \times 10^5$  MC step each, and a total of 600 bins were generated.

Figure 3 shows the covariance between the measured nearest-neighbor correlation function ( $E_2$ ) and  $S(\pi, \pi)$ . The plot was generated on the basis of 2000 bootstrap samples. Strong linear correlations between the two quantities are evident. Hence further knowledge of  $E$  can improve the estimate of  $S$ . The conventional average and error of  $S(\pi, \pi)$  is calculated on the basis of all the points, i.e., the distribution obtained by projecting the points onto the  $S$  axis. Having a better estimate  $E_1 \pm \sigma_1$  for  $E$ , an improved estimate of  $S$  can be calculated by weighting the points by a Gaussian centered at  $E_1$  and with a width equal to the error  $\sigma_1$ . In this case, the reduced statistical error is  $\approx 1/12$  of the conventional error. Note that the conventional estimates of both  $S$  and  $E_2$  lie outside the exact results by  $\approx 1.5$  standard deviations (not an unlikely situation statistically). The improved estimate of  $S$  is nevertheless within one standard deviation of the exact result, reflecting this being the case for the more accurate energy estimate  $E_1$  used in the procedure. In fact, this correcting property of the covariance method can even eliminate

TABLE I. Comparisons of QMC and exact results for  $4 \times 4$  and  $6 \times 6$  lattices.  $E_{\text{exact}}$  is the exact result for the ground-state energy per spin,  $E_1$  is the QMC estimate obtained from the average length of the series expansion according to Eq. (10), and  $E_2$  is the estimate obtained from the nearest-neighbor correlation function  $C(1,0)$  calculated according to Eq. (13).  $S_{\text{exact}}$  is the exact staggered structure factor,  $S_1$  is the QMC result with the accuracy increased by using the covariance with  $E_2$ , and  $S_2$  is the estimate using directly the sum of the correlation functions, Eq. (32a). The exact  $L=6$  results are from Ref. 21.

	$L=4$	$L=6$
$E_{\text{exact}}$	-0.701780	-0.678872
$E_1$	-0.701777(7)	-0.678873(4)
$E_2$	-0.70177(6)	-0.67872(9)
$S_{\text{exact}}$	1.47481	2.5180
$S_1$	1.47480(4)	2.51799(6)
$S_2$	1.4747(2)	2.5168(8)

certain systematic errors, such as those originating from finite- $T$  effects in calculations aimed at ground-state properties.<sup>37</sup>

Besides illustrating the use of the covariance method to reduce the statistical errors, Fig. 3 also clearly demonstrates to a high accuracy the absence of detectable systematic errors in the QMC data. This confirms that the SSE method indeed produces unbiased results. Table I summarizes the comparisons with the exact results for both  $4 \times 4$  and  $6 \times 6$  lattices.

As the system size increases, the fluctuations in  $S(\pi, \pi)$  as computed in the standard way increase, and accurate estimates become increasingly difficult to obtain. This is typical of algorithms utilizing local updates. The fluctuations in the energy per site as calculated from  $\langle n \rangle$  actually decrease, however (due to self-averaging). Hence, the gain in accuracy achieved with the covariance effect increases with the system size. Figure 4 shows  $L=16$  results for the staggered structure factor. For this system size the error in the energy estimate  $E_1$  is negligible on the scale of the fluctuations of  $E_2$ , and the error in the improved  $S(\pi, \pi)$  is essentially the width of the elongated shape in the vertical direction. In this case the covariance method leads to error bars  $\approx 1/100$  of those calculated in the standard way.

Unfortunately, not all quantities exhibit a strong covariance with  $C(1,0)$ . Figure 5 shows results for the staggered susceptibility (32b) of a  $6 \times 6$  system. In this case there is only a very weak covariance, and hardly any gain in accuracy can be achieved.

It is easy to understand why the covariance with  $C(1,0)$  is particularly strong for  $S(\pi, \pi)$  (or indeed any equal-time spin correlation): The system is rotationally invariant, but the simulation generates configurations in a representation where the  $z$  direction is singled out, and only this component of the correlation function is measured (the other components are not easily measurable, which is the case also with standard worldline methods). Measurements based on a particular set of configurations (a single bin or a bootstrap sample) will inevitably be affected by some deviations from perfect rotational invariance. This is manifested as amplitude fluctuations in the particular spin component measured, and cause

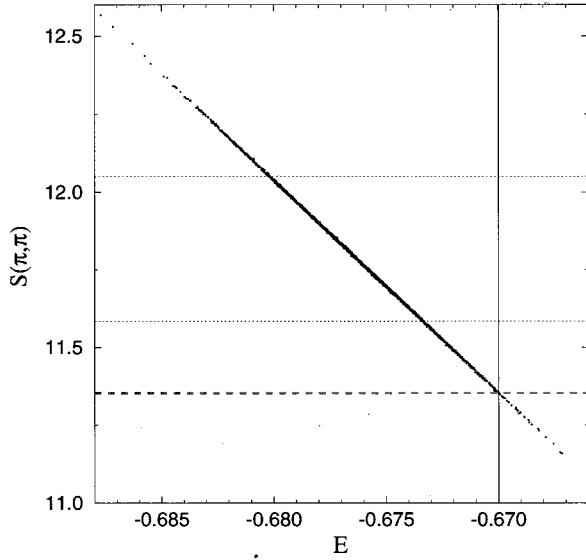


FIG. 4. Correlations between the energy as obtained from the nearest-neighbor correlation function and the staggered structure factor for a  $16 \times 16$  lattice at  $\beta = 128$ . The vertical line indicates the estimate of the energy from the average of  $n$  (the error is too small to be seen on this scale). The dotted horizontal lines indicate the value  $\pm$  one standard deviation of  $S(\pi, \pi)$  calculated using the conventional estimator. The dashed, almost indistinguishable lines indicate the improved estimate.

the covariance effects seen in the data discussed above. The ability of the local Monte Carlo updates to rotate the direction of the antiferromagnetic order in spin space diminishes with increasing size, leading to large statistical fluctuations in the conventional estimate of the correlations. The fact that the energy fluctuations do not increase with the system size can, in the same way, be traced to the rotationally invariant

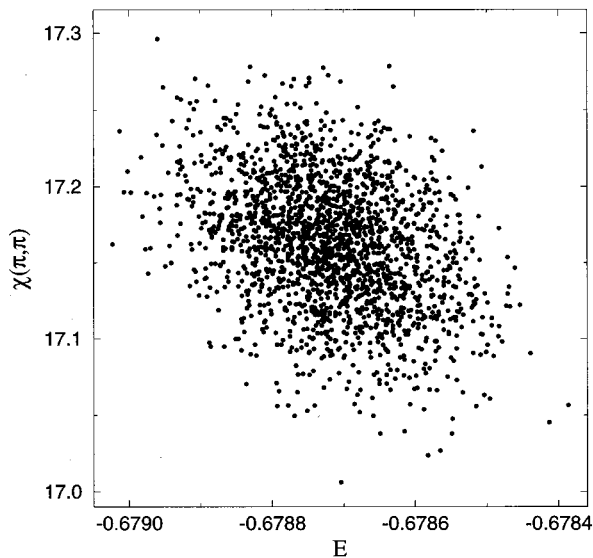


FIG. 5. Correlations between the staggered susceptibility and the energy as obtained from the nearest-neighbor correlation function for a  $6 \times 6$  lattice at  $\beta = 48$ . Due to the very weak covariance, only a modest increase in accuracy can be achieved for  $\chi(\pi, \pi)$ .

nature of the estimator (10). A somewhat more formal discussion of the covariance error reduction scheme can be found in Ref. 37.

### III. RESULTS

Simulations of  $L \times L$  systems with  $L \leq 16$  (only even  $L$ ) were carried out at inverse temperatures  $\beta = 4L$  and  $8L$ . Within statistical errors the results are indistinguishable, indicating that in both cases the ground-state completely dominates the behavior of the calculated quantities. This can also be checked using the finite-size singlet-triplet gap scaling predicted from chiral perturbation theory.<sup>27</sup> For  $L = 16$  and  $\beta = 128$ , this gives an estimate of  $\sim 10^{-7}$  for the relative error in the calculated ground-state energy due to excited states (note that since the simulations are carried out in the canonical ensemble, only  $m^z = 0$  states are mixed in). For the smaller systems the errors are even smaller (the gap scales as  $1/N$ ). All results discussed here are for  $\beta = 8L$ .<sup>52</sup>

The statistical errors of the calculated energies are as small as  $\approx 10^{-5}$  for all  $L$  studied. This accuracy exceeds by a factor 5–6 that of the most accurate results previously reported for  $L = 4$ –16, the GFMC results by Runge.<sup>16</sup> Comparing the two sets of results, they agree for  $L \leq 8$ , but for the larger sizes the GFMC data is consistently higher by 2–3 GFMC error bars. Given the agreement to a relative accuracy of less than  $10^{-5}$  between the SSE result for  $L = 6$  and the exact result, and the nonapproximate nature of the algorithm, it is hard to see why there should be any systematic errors in the SSE data for the larger lattices. Note that any remaining finite-temperature effects would lead to an overestimation of the energy, and hence could not explain the discrepancy with the GFMC data. As discussed above, care has been taken to verify that in fact the finite temperature effects are well below the statistical errors. GFMC calculations, on the other hand, are in general expected to be affected by a small systematic error originating from “population control” of the varying number of “random walkers” used in that type of simulation. In Runge’s calculation, attempts were made to remove such bias more effectively than in previous<sup>11,13</sup> GFMC calculations. However, a small remaining systematic error could not be ruled out, and the effect was expected to be an overestimation of the energy.<sup>16</sup> The discrepancy found here is therefore not completely surprising. The energies obtained with the SSE algorithm are listed in Table II. It is gratifying to note that the SSE energy is indeed nicely self-averaging—despite the considerably fewer numbers of MC steps performed for the larger systems the relative errors do not differ much from the smaller sizes.

Two definitions of the sublattice magnetization have been frequently used in previous studies,<sup>3</sup> and will be considered here as well. The first definition is in terms of the staggered structure factor,

$$M_1^2(L) = 3S(\pi, \pi)/L^2, \quad (33)$$

and the second one uses the spin-spin correlation function at the largest separation on the finite lattice,

$$M_2^2(L) = 3C(L/2, L/2). \quad (34)$$



TABLE II. QMC results for the ground-state energy, the staggered structure factor, and the spin-spin correlation function at distance  $\mathbf{r}=(L/2, L/2)$ . The accuracies of the results for  $S(\pi, \pi)$  and  $C(L/2, L/2)$  were increased by using covariance effects, as discussed in Sec. II. The simulations were carried out at inverse temperatures  $\beta=8L$ , and the total number of MC steps performed for the different systems were  $2.5 \times 10^8$  ( $L=4$ ),  $3 \times 10^8$  ( $L=6$ ),  $10^8$  ( $L=8$ ),  $10^8$  ( $L=10$ ),  $3 \times 10^7$  ( $L=12$ ),  $1.5 \times 10^7$  ( $L=14$ ), and  $10^7$  ( $L=16$ ).

$L$	$-E$	$S(\pi, \pi)$	$C(L/2, L/2)$
4	0.701777(7)	1.47480(4)	0.059872(5)
6	0.678873(4)	2.51799(6)	0.050856(3)
8	0.673487(4)	3.7939(2)	0.045867(5)
10	0.671549(4)	5.3124(3)	0.042851(6)
12	0.670685(5)	7.0780(7)	0.040873(9)
14	0.670222(7)	9.090(1)	0.03945(1)
16	0.669976(7)	11.352(2)	0.03839(2)

The factors 3 are included to account for rotational averaging of the  $z$  component of the correlations.  $M_1(L)$  and  $M_2(L)$  should, of course, scale to the same sublattice magnetization in the thermodynamic limit. Using covariance error reduction, both were determined to within relative statistical errors of  $\approx 10^{-4}$  (slightly larger for the largest systems). This accuracy also exceeds that of previous studies. The results for both  $S(\pi, \pi)$  and  $C(L/2, L/2)$  are listed in Table II.

As discussed in Sec. II, the spin stiffness can be obtained directly by measuring the square of the fluctuating winding number. However, as pointed out recently by Einarsson and Schulz,<sup>22</sup> the two terms in Eq. (26) have different leading size corrections;  $\sim 1/L^3$  for  $E$  and  $\sim 1/L$  for  $\Lambda_s$ . Therefore,  $\Lambda_s$  is also calculated separately. There is a small discrepancy between the QMC results for  $L=4$  and  $L=6$ , and the Lanczos results reported in Ref. 22. Adjusting for different factors in the definitions, the Lanczos results are  $\Lambda_s(4)=0.04832$  and  $\Lambda_s(6)=0.06723$ , whereas the QMC results obtained here are  $\Lambda_s(4)=0.04841(2)$  and  $\Lambda_s(6)=0.06791(3)$ . The reason for the discrepancy is not clear, but carrying out  $4 \times 4$  exact diagonalizations with weak twist fields included in the Hamiltonian, and subsequently calculating the derivative in Eq. (20) numerically, gives  $\Lambda_s(4)=0.04840$ , in good agreement with the QMC result. Hence, there is reason to believe that the QMC results are correct.

The uniform susceptibility has typically been obtained in numerical studies via a definition in terms of the singlet-triplet excitation gap.<sup>12,16,21</sup> Here a different approach is taken, not requiring simulations in the  $S=1$  sector. The  $\mathbf{q}$ -dependent susceptibility,

$$\chi(q_x, q_y) = \frac{1}{N} \sum_{j,k} e^{i[q_x(x_j - x_u) + q_y(y_j - y_u)]} \chi(j, k), \quad (35)$$

is calculated using Eq. (15), and its value at the longest wavelength,  $q_1 = 2\pi/L$ , is taken as the definition of the finite-size uniform susceptibility [due to the finite-size gap and the conserved magnetization,  $\chi(q=0)$  of course vanishes identically]. In order to give the correct transverse sus-

ceptibility of a system with broken symmetry in the thermodynamic limit, the result has to be adjusted by a factor  $3/2$ . Hence, the definition is

$$\chi_\perp(L) = \frac{3}{2} \chi(2\pi/L, 0). \quad (36)$$

The spin-wave velocity can be obtained from the infinite-size values of  $\rho_s$  and  $\chi_\perp$  according to the general hydrodynamic relation

$$c = \sqrt{\rho_s / \chi_\perp}. \quad (37)$$

The above quantities will now be scaled to the thermodynamic limit using  $\chi^2$  fits to appropriate scaling forms. Chiral perturbation theory gives the following scaling behavior for the ground-state energy and the sublattice magnetization defined according to Eq. (33) [parameters without the argument  $L$  will henceforth denote the infinite-size values]:

$$E(L) = E + \beta c \frac{1}{L^3} + \frac{c^2}{4\rho_s} \frac{1}{L^4} + \dots, \quad (38a)$$

$$M_1^2(L) = M^2 + \alpha \frac{M^2}{c\chi_\perp} \frac{1}{L} + \dots, \quad (38b)$$

where  $\alpha = 0.62075$  and  $\beta = -1.4377$ .<sup>27</sup> The leading corrections have been obtained also from renormalization-group calculations for the nonlinear  $\sigma$  model,<sup>25,26</sup> and their orders also agree with spin-wave theory.<sup>53</sup> Spin-wave theory also predicts that the leading corrections to  $\Lambda_s$  and  $M_2$  are  $\sim 1/L$ ,<sup>22,53</sup> and this should be the case also for  $\chi_\perp(L)$  due to the linear spin-wave spectrum for small  $q$ .

Individually fitting all the parameters, it is found that the high accuracy of  $E(L)$  necessitates the inclusion also of a term  $\sim 1/L^5$  in Eq. (38a). Both  $M_1^2(L)$  and  $M_2^2(L)$  require corrections up to order  $1/L^3$ . The QMC results for  $\Lambda_s(L)$  and  $\chi_\perp(L)$  are less accurate, and only linear and quadratic terms are needed. Hence, the following size dependences are assumed:

$$E(L) = E + \frac{e_3}{L^3} + \frac{e_4}{L^4} + \frac{e_5}{L^5}, \quad (39a)$$

$$M_1^2(L) = M^2 + \frac{m_1}{L} + \frac{m_2}{L^2} + \frac{m_3}{L^3}, \quad (39b)$$

$$M_2^2(L) = M^2 + \frac{n_1}{L} + \frac{n_2}{L^2} + \frac{n_3}{L^3}, \quad (39c)$$

$$\Lambda_s(L) = \Lambda_s + \frac{l_1}{L} + \frac{l_2}{L^2}, \quad (39d)$$

$$\chi_\perp(L) = \chi_\perp + \frac{x_1}{L} + \frac{x_2}{L^2}. \quad (39e)$$

The predicted scaling forms (38), together with the hydrodynamic relation (37) and the expression (26) for the spin stiffness  $\rho_s$ , imply the following constraints among the parameters and size corrections:

$$\Lambda_s = -(1/3)[E + 2\alpha M^2 e_3 / (\beta m_1)], \quad (40a)$$

$$\chi_{\perp} = \alpha \beta M^2 / (m_1 e_3), \quad (40b)$$

$$e_4 = m_1 e_3 / (4 \alpha \beta M^2). \quad (40c)$$

All the scaling forms (39) are hence coupled to a high degree, and a good simultaneous fit of all parameters will strongly support the field theoretical predictions (38).

Data for all sizes  $L=4-16$  can be included in fits with good values of  $\chi^2$  per degree of freedom ( $\chi^2/\text{DOF}$ ), except in the case of  $\chi_{\perp}(L)$  for which  $L=4$  has to be excluded (not surprising, since the smallest wave-vector  $q_1$  used in the definition is as large as  $\pi/2$  for  $L=4$ ). Both  $\Lambda_s(16)$  and  $\chi_{\perp}(16)$  have error bars too large to be useful, and are therefore also excluded.

Extrapolating the infinite-size parameters from fits to a relatively small number of points, one has to take into account the fact that there are higher-order corrections present, which by necessity have been neglected in the scaling forms used. The statistical errors of the extrapolated parameters may be smaller than the systematic errors introduced due to this neglect (even though the fit may be good). In order to minimize this type of subtle errors, the  $L=4$  data were excluded from all the fits discussed in the following. This leads to larger statistical fluctuations but should significantly reduce the risk of underestimating the errors (the largest neglected correction to  $E$  is 11 times larger for  $L=4$  than for  $L=6$ , and for the other quantities 3–5 times larger).

Before considering the full fit (39) with all the constraints (40), it is instructive to consider first the results of individual, unconstrained fits to all the different quantities. The effects of including the constraints can then be judged in light of these results.

Completely independent fits give  $E = -0.66943(2)$ ,  $M = 0.3062(6)$  [from  $M_1(L)$ ],  $M = 0.3068(9)$  [from  $M_2(L)$ ],  $\rho_s = 0.179(4)$ , and  $\chi_{\perp} = 0.063(1)$ . Note that  $M_1(L)$  and  $M_2(L)$  give the same sublattice magnetization  $M$  within statistical errors, as they should. Using Eq. (37) the spin-wave velocity is  $c = 1.69(2)$ . These parameters are in good general agreement with previous calculations, except that the energy is slightly lower than the best GFMC estimate,<sup>16</sup> due to the discrepancies in the finite-size data discussed above. The sublattice magnetization is a bit lower than the recent result by Beard and Wiese<sup>19</sup> [ $M = 0.3085(2)$ ].

The consistency with the scaling forms (38) can of course also be tested with these independent fits. The leading energy correction is found to be  $e_3 = -2.43(11)$ , whereas Eq. (38a) in combination with the above estimate for  $c$  gives  $e_3 = \beta c = 2.43(3)$ . The constant of the linear term in  $M_1(L)$  is  $m_1 = 0.574(9)$ , whereas the right-hand side of the scaling form (38b) gives  $m_1 = \alpha M^2 / (c \chi_{\perp}) = 0.550(10)$ . The subleading energy correction of the fit is  $e_4 = 4(1)$ , and Eq. (38a) gives  $e_4 = c^2 / (4 \rho_s) = 4.0(1)$ . Hence, there is good consistency with the predicted scaling forms, within a few percent for the leading terms, but with a statistical uncertainty as large as  $\approx 25\%$  for the subleading energy correction.

The leading corrections have been derived in several different ways.<sup>25–27</sup> Given then the good numerical agreement found above, it is now reasonable to enforce the constraints (40a) and (40b) which involve these terms. From such a fit, with the constraint on the subleading energy correction (40c) left unenforced, one can get a better estimate of the size of

the subleading term. The constraint that  $M_1(L)$  and  $M_2(L)$  extrapolate to the same  $M$  is also enforced.

First, a remark on the scaling of the ground state energy: One of the early nonlinear  $\sigma$  model calculations of the finite-size behavior indicated that the subleading correction to  $E$  was  $\sim 1/L^5$ , not  $\sim 1/L^4$ .<sup>26</sup> Previous numerical calculations were not accurate enough to distinguish between these forms. However, Runge noted that the value of  $c$  extracted from the leading correction was in rather poor agreement with other estimates if a  $1/L^5$  subleading correction was used, and that a slightly better value was obtained using  $1/L^4$ . Even with the accuracy of the QMC results for  $E(L)$  obtained here, individual fits using the two different subleading corrections (and including also the next higher-order correction in both cases) cannot by themselves definitely rule out the absence of the  $1/L^4$  term, although the fit including it is better. However, it is not at all possible to obtain a good fit constrained by Eq. (40a) and (40b) without the  $1/L^4$  term (including  $1/L^5$  and  $1/L^6$  terms),  $\chi^2/\text{DOF}$  being as high as  $\approx 50$  in this case. With the  $1/L^4$  (and  $1/L^5$ ) term  $\chi^2/\text{DOF} \approx 0.9$ . Hence, knowing the constraints on the leading corrections, the present data unambiguously require that the subleading energy term is  $\sim 1/L^4$ .

The parameters obtained in the partially constrained fit are  $E = -0.669436(5)$ ,  $M = 0.3071(3)$ ,  $\rho_s = 0.176(2)$ ,  $\chi_{\perp} = 0.0623(10)$ , and  $c = 1.681(14)$ . The statistical errors are here significantly reduced relative to the previous unconstrained fits, and the two sets of parameters are consistent with each other. The leading corrections to  $E$  and  $M$  are now, of course, in complete agreement with the theoretical prediction. The subleading energy correction of the fit is  $e_4 = 4.17(23)$ , whereas Eq. (38a) with the above parameters gives  $e_4 = c^2 / (4 \rho_s) = 4.01(7)$ . Hence, it is now also confirmed, at the 5% accuracy level, that the size of the subleading energy correction agrees with the chiral perturbation theory prediction by Hasenfratz and Niedermayer.<sup>27</sup> It is remarkable that the derivation of this very detailed theoretical result is based purely on symmetry and dimensionality considerations.<sup>27</sup>

With the subleading energy correction now firmly established, the last constraint (40c) can also be enforced, and the parameters of this fit are taken as the final results. This fully coupled fit still has  $\chi^2/\text{DOF} \approx 0.9$  (the total number of parameters is 14, and a total of 28 data points were used). Looking at  $\chi^2$  for the five individual curves, they all represent good fits to their respective data sets. Hence, the constrained fit is in all respects a good one. All the ground-state parameters obtained from the fit are listed in Table III, along with the leading and subleading corrections to the energy and the sublattice magnetization. There are only minor changes relative to the previous partially constrained fit, the main improvement in accuracy being for the spin-wave velocity. The errors of the parameters were calculated using the bootstrap method,<sup>51</sup> i.e., fits were carried out for a large number of bootstrap samples of the QMC data, and the error is defined as one standard deviation of the parameters of those fits. As explained in Sec. II B, this should be a very accurate method for calculating statistical errors even in highly nonlinear situations such as the constrained  $\chi^2$  fit. The QMC data used, along with the fitted curves, are shown in Figs. 6–9.

In the figures, it can be observed that even though the  $L=4$  data are not included in the fit, the fitted curves ex-

TABLE III. The ground-state parameters and the leading and subleading corrections to  $E$  and  $M$ , as obtained from a fit fully constrained by the predictions of chiral perturbation theory.

Parameters	
$E$	$-0.669437(5)$
$M$	$0.3070(3)$
$\rho_s$	$0.175(2)$
$\chi_\perp$	$0.0625(9)$
$c$	$1.673(7)$
Size corrections	
$e_3$	$-2.405(10)$
$e_4$	$4.00(6)$
$m_1$	$0.560(6)$
$m_2$	$1.08(5)$

trapolated to  $L=4$  are quite close to these QMC points, except in the case of  $\chi_\perp(4)$  (for which this point cannot even be included in an individual fit). In fact, calculating also the statistical errors of the extrapolations to  $L=4$  gives strong further support to the reliability of the procedures used. For all quantities except the energy, the statistical errors are found to be comparable at  $L=4$  and  $L=\infty$ . For the energy the fluctuations are more than 20 times larger at  $L=4$ , due to the high order of the leading correction. The exact results for

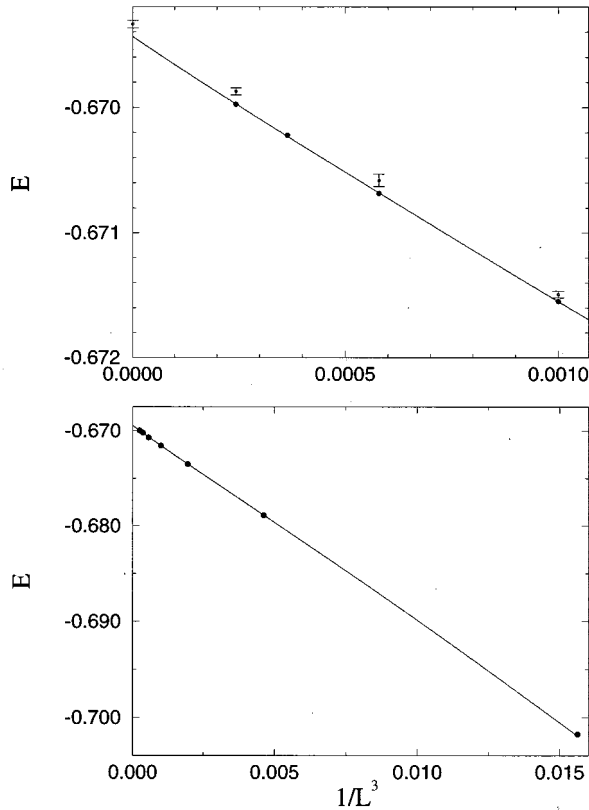


FIG. 6. The ground-state energy vs  $1/L^3$  on two different scales. The solid circles are the QMC data. On the scale of the top graph, the error bars are smaller than half the radius of the circles. The smaller circles with error bars in the top graph are the GFMC and extrapolated results by Runge (Ref. 16). The result of the constrained fit including the  $L>4$  data is indicated by the curves.

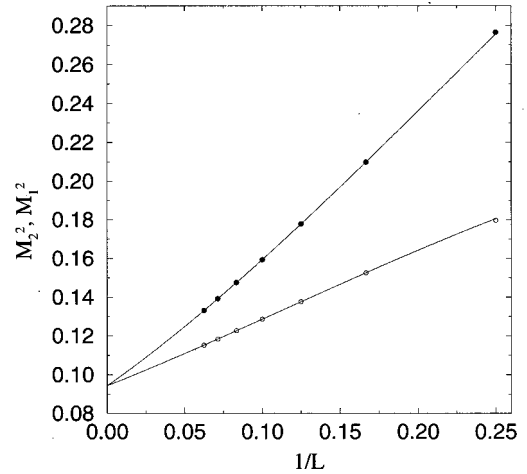


FIG. 7. The sublattice magnetization squared, as defined by Eqs. (33) and (34), vs inverse system size. The solid and open circles are the QMC data for  $M_1(L)$  and  $M_2(L)$ , respectively, and the curves are the results of the constrained fit including the  $L>4$  data. The QMC error bars are much smaller than the circles.

both  $E(4)$  and  $\Lambda_s(4)$  are within one standard deviation of the extrapolated results. The sublattice magnetizations  $M_1(4)$  and  $M_2(4)$  both deviate by 2.5 standard deviations, and  $\chi_\perp$  deviates by 3 standard deviations. These rather small deviations clearly indicate that there are only minor effects of neglected higher-order corrections. The extrapolations to  $L=\infty$  should of course be significantly less sensitive to systematic errors, since the neglected corrections rapidly vanish for the larger sizes. As already discussed above, the neglected corrections are several times larger at  $L=4$  than at  $L=6$  (the smallest size considered in the fits). Hence, any remaining systematic errors in the infinite-size extrapolations listed in Table III should be well below the indicated statistical errors.

#### IV. SUMMARY AND DISCUSSION

An extensive study of the ground-state parameters of the 2D Heisenberg model has been presented. Using the stochas-

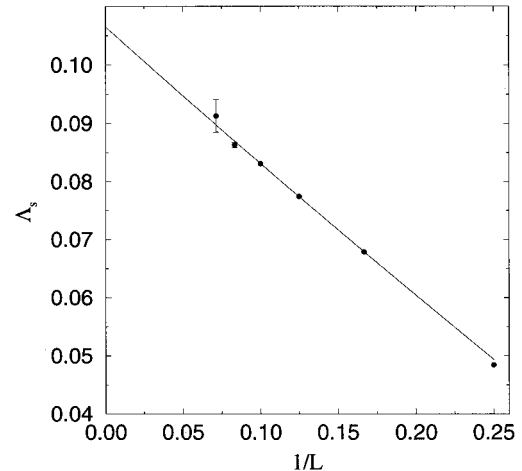


FIG. 8. The spin current-current correlator, Eq. (25), vs the inverse system size, along with the result of the coupled fit to the  $L>4$  data.

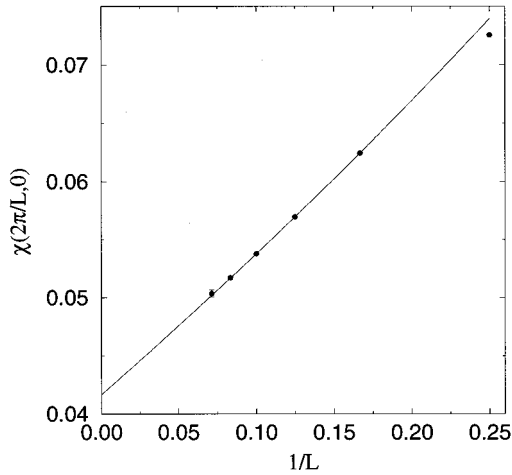


FIG. 9. The long-wavelength spin susceptibility [ $2/3$  of  $\chi_{\perp}(L)$ ] vs inverse system size, along with the result of the constrained fit to the  $L > 4$  data.

tic series expansion QMC method<sup>35,36</sup> in combination with a data analysis scheme utilizing covariance effects,<sup>37</sup> results of unprecedented accuracy were obtained for the ground-state energy and the sublattice magnetization for systems of linear dimensions up to  $L = 16$ . The long-wavelength susceptibility and the spin stiffness were also directly calculated in the simulations.

The QMC data was extrapolated to the thermodynamic limit using scaling forms predicted from chiral perturbation theory,<sup>27</sup> supplemented by higher-order terms necessary to obtain good fits. Both the leading and subleading corrections were found to agree in magnitude with the theoretical predictions to within a few percent. To the author's knowledge, this is the first numerical verification of the predictions of chiral perturbation theory<sup>27</sup> to subleading order.

The ground-state energy extracted from the fit is the most accurate estimate obtained to date, and is slightly higher than the best Green's function Monte Carlo result.<sup>16</sup> This discrepancy is most likely due to a "population control" bias in the GFMC calculation.<sup>16</sup> The spin stiffness and the sublattice magnetization are both lower than the results of a recent low-temperature loop algorithm QMC study.<sup>19</sup> The discrepancy appears to be marginally larger than what could be explained by statistical fluctuations alone. For the spin-wave velocity the results are consistent with each other.

In the QMC study by Beard and Wiese<sup>19</sup> the size and temperature dependence of the uniform and staggered susceptibilities were fit to scaling forms from chiral perturbation theory. Hence, the underlying theory for analyzing the data is the same as used in the present study, but the physical quantities used are different, as is the temperature regime (low but finite  $T$  versus  $T=0$  in this study). Since both QMC algorithms are "exact," the discrepancies must originate from the scaling procedures. In this paper the effects of neglected higher-order corrections were discussed, and attempts were made to minimize these as much as possible. Furthermore, as a quantitative check of remaining effects of this nature, the calculated scaling functions were extrapolated to lattices smaller ( $L=4$ ) than the smallest size used in the fit ( $L=6$ ).

The close agreement with the actual calculated results, along with the high orders of the largest neglected corrections, show that any effects of the higher-order terms on the extrapolations to infinite size should be well below the carefully computed statistical errors. It can be noted that Beard and Wiese also included subleading corrections,<sup>19</sup> but not to the same high orders as was necessary in the present study (due to the high accuracy of the SSE results for the energy and the sublattice magnetization). Another reason to believe that the present study is more reliable is that the fit involves in a direct manner the  $T=0$  finite-size definitions of the same infinite-size parameters sought, not functions of those parameters.

In combination with the covariance error reduction scheme,<sup>37</sup> the SSE method is a very efficient method for calculating correlation functions of isotropic spin models, as exemplified by the results presented here. The covariance scheme is most efficient in cases where there are strong long-ranged correlations (where the "bare" estimator for the correlation function does not behave well). It is currently being applied in a study of the temperature dependence of the correlation length of the weakly coupled Heisenberg bilayer, for larger lattices and lower temperatures than previously<sup>39</sup> possible. This is motivated by recent results obtained from a mapping to a nonlinear  $\sigma$  model for this system,<sup>54</sup> predicting a much faster divergence of the correlation length as  $T \rightarrow 0$  than for the single layer. The SSE algorithm has also proven useful in the case of critical, or near-critical systems, such as the bilayer Heisenberg model close to its quantum critical point. More accurate finite-size scalings than previously reported for this,<sup>40</sup> as well as other models exhibiting quantum critical behavior,<sup>41</sup> are possible with the data enhanced using the covariance method.

QMC methods based on the loop-cluster algorithm,<sup>31</sup> have proven to be very efficient in several studies of  $S=1/2$  Heisenberg models,<sup>18,19,55</sup> and are clearly more efficient than the SSE method in many cases. For example, it was shown here that the covariance method cannot significantly improve the accuracy of calculated static susceptibilities, which appear to be very accurately given in loop algorithm simulations.<sup>19</sup> The method used here for calculating the spin stiffness directly from the winding number fluctuations would probably also be more accurate with loop algorithms. However, it is not clear whether loop algorithms can easily produce more accurate results for equal-time correlation functions or energies than those presented in this paper.

The methods discussed here can also be easily extended to higher-spin models. In fact, the covariance scheme has an additional advantage for  $S > 1/2$ , in that the on-site correlation  $(S_i^z)^2$  is known exactly (in the isotropic case), but fluctuates in the simulation and exhibits strong covariance with other correlation functions.<sup>37</sup> Detailed studies of various higher-spin models should therefore now be feasible also in 2D.

## ACKNOWLEDGMENTS

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