

## Loop Algorithms for Monte Carlo Simulations of Quantum Spin Systems

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We present a new algorithm for world line Monte Carlo simulations of quantum spin systems. The algorithm consists of a stochastic pairing and a stochastic flipping procedure, and the formula for the pairing probability is explicitly given for Heisenberg models. As an illustration of the algorithm, we calculated autocorrelation times for simulations of the  $S = 1$  antiferromagnetic Heisenberg chain. The rapid increase in autocorrelation times which is seen in the conventional world line method as the imaginary-time spacing decreases is eliminated by the present algorithm.

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Since the pioneering work of Heisenberg, quantum spin models have provided useful descriptions of the magnetic properties of materials. For example, quantum spin models have been attracting the interest of a number of researchers because in quasi-one-dimensional systems, a novel property which strongly depends on the length of the spin was conjectured by Haldane [1] and was confirmed numerically [2] for the  $S = 1$  Heisenberg model. In recent years, important information about the finite-temperature properties of these models has been learned using the world line quantum Monte Carlo simulation [3]. For example, with this method, and numerical methods of analytic continuation [4], experimentally accessible quantities, such as the dynamic structure factor, can be obtained from the simulations [5]. This and related information are hard to obtain by other means. However, as recently realized [6], the world line Monte Carlo technique has another difficulty—long autocorrelation times making error estimation difficult and in some cases impossible. The long autocorrelation time is due either to a physical phase transition, a zero-temperature singularity, or a small value of the imaginary-time spacing in the Suzuki-Trotter approximation.

Several attempts to reduce the autocorrelation times in quantum Monte Carlo simulations have been made by using new types of cluster algorithms [7,8]. The attempts were most successful for the  $S = \frac{1}{2}$  XXZ model. When transformed by the Suzuki-Trotter formula into a problem with classical degrees of freedom, this model maps onto a special case of the six-vertex model so one can use the loop algorithm of Evertz and Marcu [9]. With this algorithm, Wiese and Ying [8] reported high precision results for the properties of the two-dimensional,  $S = \frac{1}{2}$  antiferromagnetic Heisenberg model. In this paper, we present a generalization of the loop algorithm for spin systems with an arbitrary length of spins in arbitrary dimensions. The generalization is not a straightforward extension of the  $S = \frac{1}{2}$  case. In the  $S = \frac{1}{2}$  case, the existence of the loop algorithm followed directly from the solution of a linear system of equations of order 3. As we discuss below, for larger spins the

analogous system of equations has a much larger order so even proving the existence of a meaningful solution is nontrivial. We will not only show that a nontrivial solution exists, but we will also present a compact analytic expression for the solution of ferromagnetic and antiferromagnetic Heisenberg models. We will illustrate the efficiency of the algorithm for the specific case of the  $S = 1$  antiferromagnetic Heisenberg chain. The method presented contains the loop algorithm for the  $S = \frac{1}{2}$  XXZ model and the Swendsen-Wang (SW) cluster algorithm [10] for classical Potts model as special cases.

The following analogy might be helpful for understanding the new algorithm. In SW algorithm, two labels, frozen and deleted, are assigned probabilistically to each bond in the lattice depending on whether the pair of lattice sites have the same Potts state or not. When the frozen bonds are connected, clusters are formed, and each cluster can be flipped independently. For the loop algorithm, a plaquette plays a role analogous to a bond. Similarly, circles seen below correspond to the lattice sites, and various kinds of pairing will correspond to freezing and deleting. When paired circles are connected, loops form. These loops can be flipped independently. Our Hamiltonian is

$$\mathcal{H} = \sum_{(i,j)} \mathcal{H}_{i,j} = - \sum_{(i,j)} J_{i,j} (S_i^x S_j^x + S_i^y S_j^y + \lambda S_i^z S_j^z), \quad (1)$$

where  $S_i^\alpha$  is the spin operator which satisfies  $S_i^2 = (S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2 = S(S+1)$ , and  $[S_i^\alpha, S_i^\beta] = (i/2)S_i^\gamma$  with  $(\alpha, \beta, \gamma) = (x, y, z), (y, z, x),$  or  $(z, x, y)$ . The symbol  $(i, j)$  represents an arbitrary nearest neighbor pair. We assume  $J_{i,j} \geq 0$ . When  $\lambda = 1$ , we have the ferromagnetic Heisenberg model; when  $\lambda = -1$ , the antiferromagnetic Heisenberg model. In the case of antiferromagnets, if the lattice is bipartite, we have no sign problem. For simplicity, we will assume such lattices.

The first important step is to express a spin operator in terms of sum of  $2S$  Pauli operators,  $\sigma_{i,\mu}^\alpha$  ( $\alpha = x, y, z$ ):

$$S_i^\alpha = \frac{1}{2} \sum_{\mu=1}^{2S} \sigma_{i,\mu}^\alpha. \quad (2)$$

Then, using the Suzuki-Trotter formula and (2), we can express the partition function for our Hamiltonian as

$$Z = \sum_{\{n\}} \prod_{k=1}^M \prod_{(i,j) \in \mathcal{B}_k} w_{i,j}(\mathbf{n}_i^{(k+1)}, \mathbf{n}_j^{(k+1)}, \mathbf{n}_i^{(k)}, \mathbf{n}_j^{(k)}). \quad (3)$$

Here,  $\mathbf{n}_i^{(k)}$  is a set of  $2S$  one-bit variables,  $(n_{i,1}^{(k)}, n_{i,2}^{(k)}, \dots, n_{i,2S}^{(k)})$ , where  $n_{i,\mu} = 0$  or  $1$ .  $\mathcal{B}_k$  is a subset of the nearest neighbor pairs and depends on the decomposition of the lattice we use. The product over  $k$  corresponds to a step in imaginary time of length  $\Delta\tau$  where  $\Delta\tau = \beta/M$ . We decompose the lattice by the usual checkerboard scheme in the  $x\tau, y\tau$ , etc. planes for whatever number of dimensions we wish to consider.

We work with complete sets of states that satisfy

$$\sigma_{i,\mu}^z |\mathbf{n}_i^{(k)}\rangle = (2n_{i,\mu}^{(k)} - 1) |\mathbf{n}_i^{(k)}\rangle. \quad (4)$$

The function  $w_{i,j}$  is simply the matrix element of  $\exp(-\Delta\tau \mathcal{H}_{i,j})$  in this basis, i.e.,

$$w_{i,j}(\mathbf{n}'_i, \mathbf{n}'_j, \mathbf{n}_i, \mathbf{n}_j) \equiv \langle \mathbf{n}'_i, \mathbf{n}'_j | \times P_i P_j \exp(-\Delta\tau \mathcal{H}_{i,j}) P_i P_j | \mathbf{n}_i, \mathbf{n}_j \rangle. \quad (5)$$

The operator  $P_i$  is a projector onto the space where  $S_i^2 = S(S+1)$ . Thus, as characteristic of the world line method, we have transformed the original quantum problem into a problem with classical degrees of freedom. The classical problem has  $8S$ -body interactions described by (3). In what follows, we call a *plaquette* the group of  $8S$  variables on which the  $8S$ -body interaction  $w_{i,j}$  is defined.

To construct a cluster algorithm, we will follow the general scheme proposed recently by several authors [11,12]. We start with

$$P_{i,j}(b|a) = v_{i,j}(b)/w_{i,j}(a), \quad (6)$$

$$\sum_b \delta(a,b) v_{i,j}(b) = w_{i,j}(a), \quad (7)$$

where  $a$  is a state of a plaquette, i.e.,  $a = (\mathbf{n}'_i, \mathbf{n}'_j, \mathbf{n}_i, \mathbf{n}_j)$ , and  $b$  is a label, and  $P_{i,j}(b|a)$  is the probability with which the label  $b$  is assigned to a plaquette in the state  $a$ . This probability is what we need to find. Because we know  $w_{i,j}$ , to find it we need  $v_{i,j}$  which we determine from the linear equations (7). The function  $\delta(a,b)$  has the value of 1 if the state  $a$  is allowed when the label is  $b$  and has the value of 0 otherwise. Because in what follows we focus on a given plaquette, we will omit the subscript  $i, j$ .

In general, the linear equations (7) are either overdetermined or underdetermined. The central claims of the present paper are that at least one nontrivial solution exists for isotropic models, i.e., for the ferromagnetic and antiferromagnetic Heisenberg models, and that this solution leads to an ergodic loop algorithm. We will present the mathematical proof of the claim elsewhere.

In the present case, a state  $a$  can be depicted by a plaquette with  $2S$  circles at each corner [Fig. 1(a)].

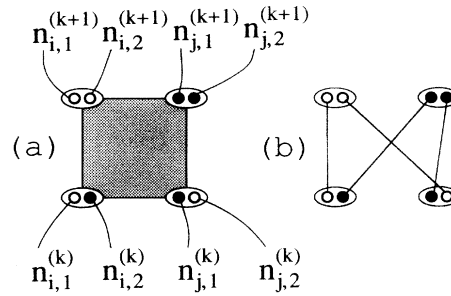


FIG. 1. (a) A pictorial representation of a plaquette and its state for  $S = 1$ . (b) One possible label (pairing) for the plaquette.

Because of the conservation rule, the total number of possible states for  $a$  is  $N_{st} \equiv \sum_{k=0}^{4S} \binom{4S}{k}^2$ . Each circle represents one of  $2S$  variables defined on a corner. In Fig. 1, a solid circle means  $n_{i,\mu} = 1$ , and an open circle,  $n_{i,\mu} = 0$ . In the loop algorithm, which is a special case of a cluster algorithm, a label  $b$  is identified with a pairing of the  $8S$  circles as described below.

There are  $(4S)!$  possible ways to connect pairwise the  $8S$  circles on a given plaquette in such a way that changing the color of two circles of any pair does not violate the local conservation rule. Each connected pair will be flipped simultaneously, in analogy to flipping pairs of neighboring spins connected by the freezing-deletion procedure in the SW algorithm. The label  $b$  in the present case is one of several ways of pairing. An example is shown in Fig. 1(b). The allowed states from this label are those reachable by changing colors of some set of pairs. Obviously, there are  $2^{4S}$  possible states for any label because a label consists of  $4S$  pairs. In other words, given a label  $b$ , the function  $\delta(a,b)$  takes the value of 1 if and only if  $a$  is one of these  $2^{4S}$  states. Thus, the meaning of (7) is clarified in the present specific case. For later use, we need to define what we mean by the *class* of a label: two labels belong to the same class if and only if they are identical ways to connect four corners if the distinction between circles at the same corner is neglected. A class is identified with a diagram in which each corner is the end point of  $2S$  line segments (for an example, see Fig. 2).

The solution we present in this Letter has the following special properties:  $v(b)$  depends only on the class to which  $b$  belongs, and  $v(b)$  is nonvanishing if and only if the class of  $b$  can be decomposed into a combination of two kinds of elemental diagrams. For the ferromagnetic Heisenberg model, one of these elemental diagrams is a pair of vertical lines, and the other is a pair of diagonal lines [Fig. 2(a)]. For the antiferromagnetic Heisenberg model, one is a pair of vertical lines, and the other is a pair of horizontal lines [Fig. 2(b)]. Therefore, we have  $2S + 1$  distinct classes of labels in either case. Accordingly, there are  $2S + 1$  independent variables in Eq. (7).

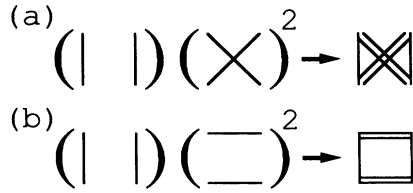


FIG. 2. A label class which can be constructed from the two elemental diagrams for the  $S = \frac{3}{2}$  (a) ferromagnetic and (b) antiferromagnetic Heisenberg chain.

We will let  $(2S - l, l)$  denote the class which is characterized by the combination of  $2S - l$  elemental diagrams of the first kind and  $l$  diagrams of the second kind. Accordingly, we define  $v(2S - l, l)$  as the value of  $v(b)$  when  $b$  belongs to the class  $(2S - l, l)$ .

To see that only one solution exists having the properties just mentioned, it is sufficient to note the following: If we first define classes of states similar to the classes of labels, then we say that two states belong to the same class if and only if they are identical if we neglect the distinction of circles at the same corner. Consequently, a state  $(n_1, n_2, n_3, n_4)$  belongs to the class which is characterized by four numbers  $(m_1, m_2, m_3, m_4)$  where  $m_i \equiv \sum_{\mu=1}^{2S} n_{i,\mu}$ . For the ferromagnetic case, if we pick from the  $N_{st}$  equations (7) an equation for which  $a$  belongs to a class characterized by  $(l, 2S - l, 0, 2S)$  ( $l = 0, 1, \dots, 2S$ ), then it is easy to see that this equation is  $[(2S)!]^2 v(2S - l, l) = w(l, 2S - l, 0, 2S)$ , where  $w(m_1, m_2, m_3, m_4)$  equals  $w(a)$  with  $a$  belonging to the class  $(m_1, m_2, m_3, m_4)$ . Thus, we arrive at the solution for the ferromagnetic Heisenberg model,

$$v(2S - l, l) = \frac{1}{(2S)!} \binom{2S}{l}^{-1} \times \langle\langle l, 2S - l | \exp(-\Delta\tau \mathcal{H}_{i,j}) | 0, 2S \rangle\rangle. \tag{8}$$

For antiferromagnetic case, the equation for the class of states characterized by  $(l, 0, 0, l)$  is

$$v(2S - l, l) = \frac{1}{(2S)!} \binom{2S}{l}^{-1} \langle\langle l, 0 | \exp(-\Delta\tau \mathcal{H}_{i,j}) | 0, l \rangle\rangle. \tag{9}$$

The state  $|m_i, m_j\rangle\rangle$  stands for the eigenfunction of  $S_i^2, S_j^2, S_i^z,$  and  $S_j^z$  with  $S_i^2 = S_j^2 = S(S + 1), S_i^z = m_i,$  and  $S_j^z = m_j$ . The formulas (8) and (9) completely determine our loop algorithm.

We remark that a loop algorithm is advantageous from the computational point of view because the loop identification takes a computational time proportional to the number of variables  $N_v$ , whereas cluster identification takes at least  $N_v \log(N_v)$ . As pointed out in [12], the  $S = \frac{1}{2}$  XXZ model with Ising-like anisotropy does not have loop algorithm solution of (7); that is, no solution to (7) exists if the label is restricted to the pairing.

However, we have a cluster solution in that case if we introduce another type of label [12]. In the limit of strong anisotropy, this solution reduces to the SW algorithm for the Ising models [12]. In general, the computation time for one Monte Carlo step of the loop algorithm is only a small multiple of the standard method.

To illustrate the efficiency of the present algorithm, we simulated the  $S = 1$  Heisenberg chain. We just want to show how drastically autocorrelation times are reduced. Others [13] have already intensively studied various important properties such as the magnitude of the gap and the correlation length at zero temperature. Figure 3 shows the integrated autocorrelation time for the magnetization and the magnetic susceptibility for a chain of length 32 at the inverse temperature  $\beta = 10$ . To calculate the autocorrelation time, we have divided sequences of up to  $3 \times 10^7$  Monte Carlo data points for a quantity  $X$  into bins of length  $l$ . If  $X_b(l)$  is the average of the data in the  $b$ th bin, then the integrated autocorrelation is estimated by the asymptotic value of  $\tau_X(l) \equiv l\sigma_X^2(l)/2\sigma_X^2(1)$ , at large  $l$  [14]. Here,  $\sigma_X^2(l)$  is the variance of the bin averages  $\bar{X}_b(l)$ .

Because antiferromagnetic Heisenberg models with integer spins are believed to be disordered and have a finite correlation length ( $\xi = 6.2$  in the case of  $S = 1$ ) [13], we expect that our measured autocorrelation time for either the conventional or the new algorithm does not depend strongly on the system size if the system is sufficiently long. We also expect that with fixed imaginary-time spacing this autocorrelation time is also independent of the inverse temperature if the temperature is sufficiently low because once we map the original problem onto the classical system, the imaginary-time

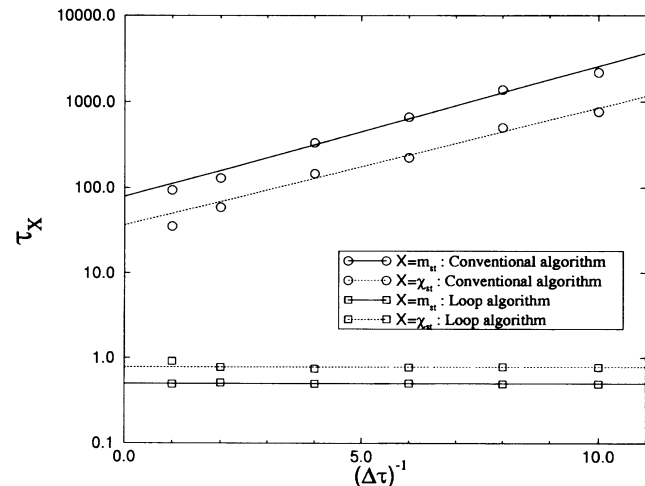


FIG. 3. The integrated autocorrelation time versus inverse imaginary-time spacing for the staggered magnetization ( $m_{st}$ ) and the staggered susceptibility ( $\chi_{st}$ ) for an antiferromagnetic Heisenberg chain with  $S = 1$  and length  $L = 32$  at  $T = 0.1$ . The lines are guidelines to eye.

spacing is the only relevant coupling constant and the inverse temperature only plays the role of the system size in the imaginary-time direction. We actually observe both of these features by doing the simulations for shorter chains ( $L = 16$ ) and at higher temperatures.

In the case of integer spins, the long autocorrelation times arise only from small imaginary-time spacings. Because the ordinary checkerboard decomposition has a systematic error proportional to  $(\Delta\tau)^{-2}$ , we must take small spacings to get accurate results (and to maintain the quantum character of the results). However, as this spacing decreases, the acceptance ratio of a local movement of a world line in the conventional method becomes small because each diagonal segment of a world line contributes to the total weight  $w$  by the factor proportional to  $\Delta\tau$ . To improve the accuracy of the results in the conventional method, we thus have to expect longer autocorrelation times as well as the expense of the larger system sizes in the imaginary-time direction.

We calculated the autocorrelation times  $\tau_X$  for  $X =$  energy, staggered magnetization, and staggered susceptibility. Although the correlation time of the energy for the conventional algorithm is longer than that for the loop algorithm, the difference is not as significant as for the other two quantities. As we can see in Fig. 3, the autocorrelation time for the magnetization is enormously long for the conventional world line method. On the other hand, for the present algorithm it is identically  $\frac{1}{2}$  because in the loop algorithm any loop is flipped with probability  $\frac{1}{2}$  and therefore two subsequent configurations are completely decorrelated as far as the magnetization is concerned. As for the susceptibility, although the difference is slightly less significant than that for the magnetization, we see the same qualitative property: a rapid increase in  $\tau_X$  as the imaginary-time spacing decreases for the conventional algorithm, whereas for the loop algorithm it does not depend on the spacing. We conclude that the present algorithm is particularly useful for the integer spins. For half integer spins, we expect that the efficiency of the present algorithm is even more crucial because the autocorrelation time for the conventional algorithm will increase as a function of the inverse temperature and the system size as well as the function of the inverse of the imaginary-time

spacing whereas the performance of the new algorithms is quite insensitive to changes in these parameters [6].

Finally, we remark that we have found some simple analytic solutions for anisotropic models. Of course, the previous work where the  $S = \frac{1}{2}$  anisotropic XXZ models is mapped to the six-vertex model is the simplest example of an anisotropic model. Specifically, we actually found solutions for anisotropic models with larger spins, such as the  $S = 1$  XY model. These results will be presented elsewhere. Further study of constructing general formula of the anisotropic XXZ models and applying the present algorithm to half integer spin cases is under way.

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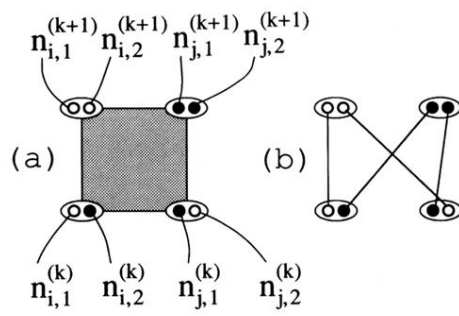


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