Stochastic series expansion method with operator-loop update

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A cluster update (the ''operator loop'') is developed within the framework of a numerically exact quantum Monte Carlo method based on the power series expansion of $\exp(-\beta H)$ (stochastic series expansion). The method is generally applicable to a wide class of lattice Hamiltonians for which the expansion is positive definite. For some important models the operator-loop algorithm is more efficient than loop updates previously developed for ''worldline'' simulations. The method is here tested on a two-dimensional anisotropic Heisenberg antiferromagnet in a magnetic field. [S0163-1829(99)50722-4]

The path-integral formulation of quantum statistical mechanics is a useful starting point for numerical studies of interacting many-body systems in cases where positive definiteness can be assured. Monte Carlo algorithms based on the ''Trotter decomposition''[1,2] in discrete imaginary time, commonly referred to as ''worldline'' methods, have been used extensively for studies of quantum spins and bosons, as well as fermions in one dimension (in higher dimensions the fermion path integral is not positive definite).[3] Recently, two important technical developments have lead to significantly more efficient simulation algorithms. A generalization[4] of cluster updates used in classical Monte Carlo simulations[5] can reduce the autocorrelation times of some simulations by orders of magnitude,[6,7] thereby enabling studies of models in parameter regimes where standard local updating schemes do not efficiently explore the configuration space. Algorithms have also been constructed that work directly in the imaginary time continuum,[8–11] thus producing results free of systematic errors without extrapolations.

There are, however, still unresolved issues for these improved algorithms. For some important models the loop schemes do not take into account all interactions in the system, and hence an *a posteriori* acceptance probability has to be assigned after the loop clusters have been constructed.[7,12] This degrades the simulation efficiency. Some loop algorithms also break down due to ''freezing,''[4,13] when the probability is high for a single cluster to encompass the whole system. It is also often a nontrivial task to construct an algorithm for a new Hamiltonian — it would clearly be desirable to have a more general method.

Here a general loop-type updating scheme is constructed within the ''stochastic series expansion'' (SSE) (Refs. 8 and 14) framework. This approach to quantum simulations is based on sampling the diagonal matrix elements of the power series expansion of $\exp(-\beta H)$ and is related to a less general method proposed by Handscomb.[15] The SSE scheme is as general in applicability as the worldline method, and like the continuous time variant, it is numerically exact (there is also a strong relationship between the two methods).[11] SSE algorithms have been applied to numerous problems over the past several years, but so far only local updating schemes have been used. The ''operator-loop'' algorithm introduced here has the same favorable effects on autocorrelation times

as the loop updates developed within the worldline scheme. In addition, the method overcomes the problems discussed above; all interactions are taken into account in the loop construction, there does not appear to be any problems related to freezing, and the algorithm is very easily implemented for a wide range of models.

For definiteness and sake of simplicity, the operator-loop algorithm will here be described for simulations of the anisotropic $S=1/2$ Heisenberg model in a magnetic field, defined in standard notation by the Hamiltonian

$$H=J\sum_{\langle i,j\rangle}\left[\Delta S_i^z S_j^z+\frac{1}{2}(S_i^+ S_j^- + S_i^- S_j^+)\right]-h\sum_i S_i^z, \quad (1)$$

where $\langle i,j\rangle$ denotes a pair of interacting spins on a lattice in any number of dimensions. In addition to serving as an illustration for a general SSE operator-loop algorithm, simulation results for this model will show explicitly that problems present with other loop algorithms are avoided. With the standard worldline loop algorithms, freezing occurs for $\Delta > 1$.[4,13] The loop construction also does not take into account a nonzero magnetic field h,[12] hence making simulations of large $h>0$ systems problematic. In the present algorithm, h is explicitly taken into account in the loop construction and simulation results show that $\Delta > 1$ poses no problems.

For the construction of the SSE configuration space the Hamiltonian is first written as

$$H=-J\sum_{b=1}^{M}[H_{1,b}-H_{2,b}], \quad (2)$$

where $H_{1,b}$ and $H_{2,b}$ are symmetric bond operators corresponding to an interacting spin pair $\langle i(b),j(b)\rangle$;

$$H_{1,b}=C-\Delta S_{i(b)}^z S_{j(b)}^z+\frac{h}{2J}(S_{i(b)}^z+S_{j(b)}^z),$$

$$H_{2,b}=\frac{1}{2}(S_{i(b)}^+ S_{j(b)}^- + S_{i(b)}^- S_{j(b)}^+). \quad (3)$$

The constant C only shifts the energy and can be chosen to assure a positive definite expansion for any nonfrustrated lat-

tice. The number of spins in the system is denoted by N; the number of bonds $M=Nd$ for a cubic lattice in d dimensions.

The partition function $Z=\mathrm{Tr}\{e^{-\beta H}\}$ is expanded as

$$Z=\sum_{\alpha}\sum_{n=0}^{\infty}\frac{(-\beta)^n}{n!}\langle\alpha|H^n|\alpha\rangle, \qquad (4)$$

in the basis $\{|\alpha\rangle\}=\{|S_1^z,S_2^z,\ldots,S_N^z\rangle\}$. This expansion converges exponentially for $n\sim N\beta$. A truncation at $n=L$ of this order is imposed, and a unit operator $H_{0,0}=1$ is introduced to rewrite Eq. (4) as[8,14]

$$Z=\sum_{\alpha}\sum_{S_L}\frac{\beta^n(L-n)!}{L!}\left\langle\alpha\left|\prod_{i=1}^{L}H_{a_i,b_i}\right|\alpha\right\rangle, \qquad (5)$$

where S_L denotes a sequence of operator indices;

$$S_L=[a_1,b_1]_1,[a_2,b_2]_2,\ldots,[a_L,b_L]_L, \qquad (6)$$

with $a_i\in\{1,2\}$ and $b_i\in\{1,\ldots,M\}$, or $[a_i,b_i]=[0,0]$, and n denotes the number of non-$[0,0]$ elements in S_L. In principle, each term in Eq. (5) should be multiplied by a factor $(-1)^{n_2}$, where n_2 is the total number of $[2,b]$ elements in S_L. However, for a nonfrustrated lattice this number must always be even for the matrix element to be nonzero. Therefore, choosing C in Eq. (3) such that all matrix elements of $H_{1,b}$ are positive, the expansion is positive definite. A Monte Carlo procedure can therefore be used to sample the terms (α,S_L) according to their relative weights. Previously,[14] sampling schemes were devised based on (i) local substitutions of single diagonal operators, $[0,0]_p\leftrightarrow[1,b]_p$, and (ii) pairs of diagonal and off-diagonal operators $[1,b]_{p_1}[1,b]_{p_2}\leftrightarrow[2,b]_{p_1}[2,b]_{p_2}$. The diagonal update (i) will also be used here. The new operator-loop update involves any number of diagonal and off-diagonal operators and is much more efficient than the simple pair update (ii).

It is convenient to introduce the notation $|\alpha(p)\rangle$ for states obtained by acting on $|\alpha\rangle$ in Eq. (5) with the first p elements of the operator string,

$$|\alpha(p)\rangle\sim\prod_{i=1}^{p}H_{a_i,b_i}|\alpha\rangle, \qquad (7)$$

and to define states $|\alpha_b(p)\rangle=|S_{i(b)}^z(p),S_{j(b)}^z(p)\rangle$ on the bonds. For a contributing term, $|\alpha(L)\rangle=|\alpha(0)\rangle=|\alpha\rangle$.

The simulation starts with some random state $|\alpha\rangle$ and an "empty" operator string $[0,0]_1,\ldots,[0,0]_L$. L is chosen arbitrarily and adjusted during the equilibration phase of the simulation so that it will always be larger than the highest n reached (hence leading to no detectable truncation error). The diagonal update $[0,0]_p\leftrightarrow[1,b]_p$ is carried out sequentially at each position $p=1,\ldots,L$ for which $[a_p,b_p]=[0,0]$ or $[1,b]$. Such an update changes the expansion power n by ±1. Acceptance probabilities that satisfy detailed balance are obtained using Eq. (5) and the fact that there are M random choices for b in the $\rightarrow$ direction;[14]

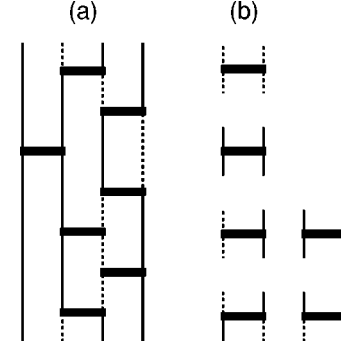$$P([0,0]_p\rightarrow[1,b]_p)=\frac{M\beta\langle\alpha_b(p)|H_{1,b}|\alpha_b(p)\rangle}{L-n},$$

FIG. 1. (a) Representation of an $M(\alpha,S_n)$, with $n=7$, for a four-spin system. The vertical solid and dashed lines indicate the spin states acted on by the operators H_b, which are represented by the horizontal bars. (b) shows the allowed vertices, corresponding to the nonzero matrix elements (10).

$$P([1,b]_p\rightarrow[0,0]_p)=\frac{L-n+1}{M\beta\langle\alpha_b(p)|H_{1,b}|\alpha_b(p)\rangle}, \qquad (8)$$

where $P>1$ should be interpreted as probability one. The state $|\alpha(0)\rangle$ is stored at the beginning of an updating cycle. Each time an off-diagonal operator $[2,b]_p$ is encountered the corresponding spins are flipped so that the states in Eq. (8) will be available when needed.

The second, new type of update is carried out with n fixed. It is then convenient to disregard the $[0,0]$ unit operator elements in S_L and instead work with sequences S_n containing only the Hamiltonian operators $[1,b]$ and $[2,b]$. The propagation index p will in the following refer to this reduced sequence. Further, full bond operators including both the diagonal and off-diagonal terms are defined; $H_b=H_{1,b}+H_{2,b}$. The matrix element in Eq. (5) can then be written as

$$M(\alpha,S_n)=\prod_{p=1}^{n}\langle\alpha_{b_p}(p)|H_{b_p}|\alpha_{b_p}(p-1)\rangle. \qquad (9)$$

The nonzero matrix elements are

$$\langle\downarrow,\downarrow|H_b|\downarrow,\downarrow\rangle=C-\Delta/4-h/(2J),$$

$$\langle\uparrow,\uparrow|H_b|\uparrow,\uparrow\rangle=C-\Delta/4+h/(2J),$$

$$\langle\downarrow,\uparrow|H_b|\downarrow,\uparrow\rangle=\langle\uparrow,\downarrow|H_b|\uparrow,\downarrow\rangle=C+\Delta/4, \qquad (10)$$

$$\langle\uparrow,\downarrow|H_b|\downarrow,\uparrow\rangle=\langle\downarrow,\uparrow|H_b|\uparrow,\downarrow\rangle=1/2.$$

C should be chosen such that all diagonal matrix elements are larger than (or equal to) zero. $M(\alpha,S_n)$ can be graphically represented as a set of n vertices connected to the propagated spins, as shown in Fig. 1(a) for a system with four spins. Two spin states "enter" each vertex, and "exit" in either the same states or flipped (the direction of the propagation is clearly irrelevant). The allowed types of vertices, corresponding to the nonzero matrix elements (10), are shown in Fig. 1(b). Figure 1(a) displays all the full spin states at each "event," but clearly there is much redundant information in this picture. The spin states at the four "legs" of the n vertices completely specify the full spin configuration (except for spins that happen not to be connected to any vertex). In order to carry out the operator-loop update, a
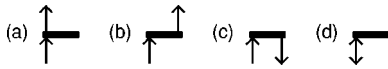
FIG. 2. The four paths on a vertex in the case of the entrance point being the low-left leg. The entrance and exit legs are indicated by the arrows. The spins at these legs are flipped in the process; the states at the other legs remain unchanged.

linked list of the vertices with their four spin states is constructed using the current state $|\alpha\rangle$ and the index sequence S_L. The list is doubly linked, so that it is possible to move in either direction from any leg of a given vertex to the leg of the next or previous vertex connected to the same spin.

The principles of the operator-loop update are now quite simple to state: One of the n vertices is first chosen at random, and one of its four legs is randomly selected as the entrance point. One of its legs is then chosen as the exit point from the vertex, according to probabilities to be specified below. The four possible vertex paths, in the case of the entrance being the low-left leg, are illustrated in Fig. 2. The spins at both the entrance and exit legs are flipped. [Note that the entrance and the exit can be the same leg, Fig. 2(d), in which case the net effect is no spin flip; only a reversal of direction of movement in the list.] The chosen exit leg points to a leg of another vertex in the linked list, the spin at which is also flipped. From this vertex, an exit leg is again chosen, which points to another vertex, etc. After some varying number of steps, the exit of the last visited vertex will point to the original entrance point of the update. The loop then closes and the result has been to flip all the spins along the random path followed in the process. Since the operator list is a periodic structure [because $|\alpha(n)\rangle = |\alpha(0)\rangle$], any state $|\alpha(p)\rangle$ can be affected in the update, and the sum over states $|\alpha\rangle$ in Eq. (5) is therefore, implicitly, also sampled in the process.

The probabilities for the four different choices of exits from a given visited vertex are proportional to the matrix elements (10) for the resulting vertices, i.e., when the entrance and exit spins have been flipped. It is intuitively clear that this operator-loop procedure satisfies detailed balance and, in combination with the diagonal single-operator update, is ergodic in the grand canonical ensemble (fluctuating total z component of the magnetization), including all winding number sectors. A rigorous proof will not be presented here.

Note that one of the paths (a)–(c) in Fig. 2 will always have zero probability, since the Hamiltonian (1) does not contain operators $S_i^+ S_j^+$ or $S_i^- S_j^-$. The probability of the ''bounce'' process (d) is always in principle nonzero. However, in some cases it is possible to exclude this path. Consider the XY model in zero field, i.e., $\Delta = h = 0$. If $C = 1/2$ is chosen, all the nonzero matrix elements in Eqs. (10) equal 1/2. Detailed balance is then satisfied also by only choosing, with equal probabilities, among the two allowed paths (a)–(c). For the isotropic Heisenberg model, i.e., $\Delta = 1$, $h = 0$, and with $C = 1/4$, the bounce can also be neglected. The only allowed path is then always the ''switch and reverse'' (c) (which corresponds to a substitution $[1,b] \leftrightarrow [2,b]$ in terms of the operators in S_L), and hence the loop construction is completely deterministic in this important case.

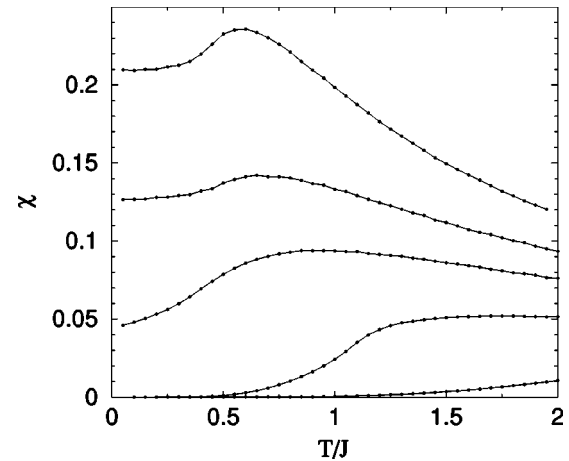A full updating cycle consists of the following steps: First

FIG. 3. Magnetic susceptibility vs temperature for the zero-field Heisenberg model with anisotropy parameter $\Delta = 0$, 0.5, 1, 2, and 4 (top to bottom).

the diagonal single-operator update is carried out at all positions in S_L with diagonal operators. The linked list of vertices is then constructed and a number of loop updates are performed. The typical size of a loop depends strongly on the model parameters. The number of loops to be constructed in each cycle is therefore chosen such that on average a total of $\sim \langle n \rangle$ vertices are visited. The updated vertices are finally mapped onto the corresponding operator indices $[a,b]$ and written into S_L.

To demonstrate the efficiency of the new algorithm, results are next presented for two different cases where previous loop algorithms have encountered difficulties:[12,13] the anisotropic model in zero field and the isotropic case with a field. The estimators for various observables of interest have been discussed in detail in Ref. 14. The correctness of the simulation code was verified by comparing results for a 4 $\times$ 4 lattice with exact results obtained by diagonalizing the Hamiltonian. The results to be presented next were obtained using lattices sufficiently large to eliminate finite-size effects. For the lowest temperatures considered, 64×64 spins were typically used, and on the order of 10^6 updating cycles were carried out.

The susceptibility, $\chi = \beta \langle (\Sigma_i S_i^z)^2 \rangle / N$, for $h = 0$ is shown in Fig. 3 for several Δ values. Unlike with the standard worldline loop algorithm,[4,13] there are no problems with ''freezing'' for $\Delta > 1$. The exponential decay of χ to 0 as $T \to 0$ for $\Delta > 1$ reflects the presence of a spin gap. For the isotropic case ($\Delta = 1$), the results are in perfect agreement with previous calculations.[16] For the XY model ($\Delta = 0$), a temperature-independent behavior is seen at low temperature ($T/J \lesssim 0.2$), in agreement with a prediction of chiral perturbation theory.[17] Quantitatively, the T-independent value should be $\chi = \rho_s / c^2$, where ρ_s is the spin stiffness and c the spin-wave velocity.[17] The result $\chi = 0.2095(3)$ obtained here at $T/J = 0.05$ is consistent with this prediction and recent ground-state calculations of ρ_s and c.[18]

The magnetization, $m = \langle \Sigma_i S_i^z \rangle / N$, is shown for an isotropic interaction and several strengths of the magnetic field in Fig. 4. In all cases, there is a maximum in m between $T/J = 0.5$ and 1, reflecting the crossover between high-temperature independent spin behavior and antiferromag-
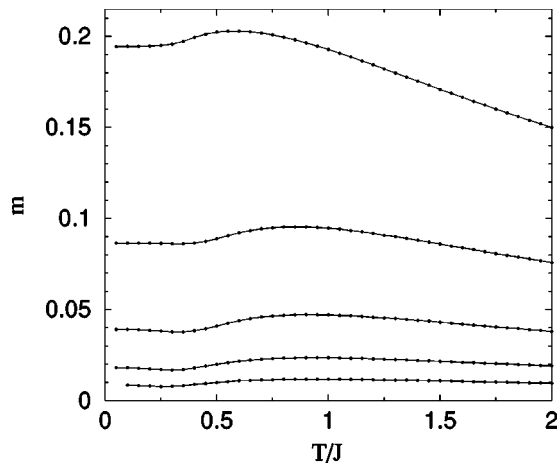
FIG. 4. Magnetization vs temperature for the isotropic Heisenberg model ($\Delta = 1$) in magnetic fields $h/J = 2$, 1, 1/2, 1/4, and 1/8 (top to bottom).

netic correlations developing at lower T (also seen in the zero-field susceptibility in Fig. 3). Note the shallow minimum at lower temperatures for $h/J \lesssim 1$, reflecting the temperature scale at which the short-range antiferromagnetic correlations are the strongest.

The simulations are very efficient for any strength of the field, since a $h > 0$ is taken into account in the loop construction. With other loop algorithms,[4,10] an *a posteriori* acceptance probability has to be assigned for updates in which the total magnetization changes. This probability decreases rapidly with increasing field strength, leading to an autocorrelation time which increases exponentially with h/T.[12] Previous simulations[12] were therefore restricted to $h/T \lesssim 4$. Figure 4 shows results up to $h/T = 40$, and there are no signs of increasing autocorrelation times even for much higher values.

To conclude, the operator-loop algorithm introduced here has several advantages over other loop methods suggested recently.[4,10] The most important is that all interactions, in-

cluding external fields, are taken into account in the loop construction, thus eliminating the need for *a posteriori* acceptance probabilities that restrict the applicability of the previous methods.[12] Like the continuous-time version of the worldline algorithm,[9–11] the SSE method is completely approximation free. The configuration space is, however, discrete, and the only floating point operation required in the simulation is the generation of uniformly distributed random numbers. In the continuous-time worldline algorithms,[9–11] on the other hand, high-precision values of imaginary times have to be manipulated. One can therefore expect that the operator-loop algorithm is faster in many cases, in particular for the uniform Heisenberg model, where the loop construction is deterministic. It is also interesting to note that certain expectation values have simpler estimators in the SSE framework than for worldline methods.[11]

The method has here been demonstrated for the anisotropic Heisenberg in a magnetic field. Generalizations to other models with two-body interactions are straightforward. The vertices depicted in Fig. 1 only involve other degrees of freedom at the ''legs.'' For example, for Hubbard-type models the legs can have charge $c = 1$ and spin $s = \pm \frac{1}{2}$, or $s = 0$ and $c = 0,2$. The paths in Fig. 2 involve changing these quantum numbers by some values $(\delta c, \delta s)$ at the entrance leg, and by $(\delta c, \delta s)$ at an exit leg in the same direction [paths (a) and (b) in Fig. 2] or $(-\delta c, -\delta s)$ at an exit in the reverse direction [paths (c) and (d)]. Implementation for a new model thus essentially involves specifying all allowed vertices, i.e., all nonzero matrix elements of type (10).

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