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” 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). Recently, two important technical developments have lead to significantly more efficient simulation algorithms. A generalization of cluster updates used in classical Monte Carlo simulations can reduce the autocorrelation times of some simulations by orders of magnitude, 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 thus producing results free of systematic errors without the extrapolations to zero discretization which are required in order to obtain numerically exact results using the Trotter decomposition.

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. This can seriously affect the efficiency of simulations. Some loop algorithms also break down due to “freezing” when the probability is high for a single cluster to encompass the whole system. It is also often a highly non-trivial task to construct an algorithm for a new Hamiltonian — it would clearly be desirable to have a simple recipe for an arbitrary model.

In this Communication, a general loop-type updating scheme is constructed within the “stochastic series expansion” (SSE) framework. This approach to quantum simulations is based on sampling the diagonal matrix elements of the power series expansion of \( \exp(-\beta H) \) [where \( H \) is the Hamiltonian and \( \beta \) the inverse temperature] and is related to a less general method proposed by Handscomb. 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). 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

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

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 \( \Delta > 1 \). The loop construction also does not take into account a non-zero magnetic field \( h \), 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

\[
H = -J \sum_{b=1}^{M} [H_{1,b} - H_{2,b}], \tag{2}
\]

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

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

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

The constant \( C \) only shifts the energy and can be chosen to assure a positive definite expansion for any non-frustrated lattice. The number of spins in the system is
denoted by $N$; the number of bonds $M = N d$ for a cubic lattice in $d$ dimensions.

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

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

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 (for a more thorough discussion, see Ref. [4])

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

where $S_L$ denotes a sequence of operator-indices;

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

with $a_i \in \{1, 2\}$ and $b_i \in \{0, \ldots, M\}$, 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 (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 non-frustrated lattice this number must always be even for the matrix element to be non-zero. Choosing $C$ in (3) such that all matrix elements of $H_{1, b}$ are positive, the expansion is then positive definite. A Monte Carlo procedure can therefore be used to sample the terms $\{\alpha, S_L\}$ according to their relative weights. Previous sampling schemes were devised based on (i) local substitutions of single diagonal operators, $|0, 0\rangle_p \leftrightarrow |1, b\rangle_p$, and (ii) pairs of diagonal and off-diagonal operators $|1, b\rangle_p |1, b\rangle_p \leftrightarrow |2, b\rangle_p |2, b\rangle_p$. 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. (3) with the first $p$ elements of the operator string,

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

and to define states $|\alpha_b(p)\rangle = |S_{a_0}^{(2)}(p), S_{a_2}^{(2)}(p)\rangle$ 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 operator string $[0, 0]_1, \ldots, [0, 0]_L$ containing only unit operators. The cut-off $L$ 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 $[0, 0]\leftrightarrow [1, b]$ is carried out sequentially at each position $p = 1, \ldots, L$ for which $|a_p, b_p| = |0, 0|$ or $|1, b|$. When accepted, such an update changes the expansion power $n$ by $\pm 1$. Acceptance probabilities that satisfy detailed balance are obtained using Eq. (3) and the fact that there are $M$ random choices for $b$ in the $\rightarrow$ direction.

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

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

where a number larger than 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 Eqs. (3) 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 (2) can then be written as

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

The non-zero matrix elements are

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

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

$$\langle \downarrow, \uparrow | H_b | \downarrow, \uparrow \rangle = \langle \uparrow, \downarrow | H_b | \uparrow, \downarrow \rangle = C + \Delta A/4,$$

$$\langle \uparrow, \downarrow | H_b | \uparrow, \downarrow \rangle = \langle \downarrow, \uparrow | H_b | \uparrow, \downarrow \rangle = 1/2.$$
Note that one of the paths (a)-(c) in Fig. 2 will always have zero probability, since the Hamiltonian does not contain operators $S_i^+ S_j^+$ or $S_i^- S_j^-$. These operators could be included in a more general model and then all four paths would be allowed. The probability of the “bounce” process (d) is always in principle non-zero. 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 non-zero matrix elements in Eq. (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 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 $\sim (n)$ 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. 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, $64 \times 64$ spins were typically used, and on the order of $2 \times 10^5$ updating cycles were carried out.

The susceptibility, $\chi = \beta (\sum_i S_i^z)^2 / N$, for the case $h = 0$ is shown in Fig. 3 for several values of the anisotropy $\Delta$. Unlike with the standard worldline loop algorithm, there are no problems with “freezing” in simulations for $\Delta > 1$. The exponential decay of $\chi$ to zero as $T \to 0$ for $\Delta > 1$ reflects the opening of a gap in the spectrum for these systems. For the isotropic case ($\Delta = 1$), the results are in perfect agreement with previous calculations. 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. Quantitatively, the T-independent value should be $\chi = \rho_s c^2$ where $\rho_s$ is the spin stiffness and $c$ the spin-wave velocity. The result $\chi = 0.2095(3)$ obtained here at $T/J = 0.05$ is consistent with this prediction and recent ground state calculations of $\rho_s$ and $c$.14

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**FIG. 1.** (a) Representation of a matrix element product $M(\alpha, S_n)$, Eq. (11), with $n = 7$, for a 4-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, which are associated with the non-zero matrix elements $L$. (a) (b) (c) (d)

**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. 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, e.t.c.. 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. (3) is therefore, implicitly, also sampled in the process.

The probabilities for the four different choices of exits from a given visited vertex are simply proportional to the matrix elements $L$ corresponding to the resulting vertices, i.e., those where the spins at the entrance and exit legs 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. For lack of space, a rigorous proof will not be presented here.
The magnetization per spin, $m = \langle \sum_i S_i^z \rangle / N$, is shown for an isotropic interaction and several strengths of the magnetic field in Figure 4. For all field-strengths, there is a maximum in $m$ between $T/J = 0.5$ and 1, reflecting the cross-over between high-temperature independent spin behavior and antiferromagnetic correlations developing at lower $T$ (also seen in the zero-field susceptibility in Fig. 3). Note the shallow minimum at lower temperatures for $h/J \leq 1$. This reflects the temperature scale at which the local, short-range antiferromagnetic correlations are the strongest.

The operator-loop simulations are very efficient for any strength of the field, since an $a$ posteriori acceptance probability has to be assigned for updates in which the total magnetization changes. This acceptance probability decreases rapidly with increasing field strength, leading to an autocorrelation time which increases exponentially with $h/T$. Previous simulations were therefore restricted to $h/T \lesssim 4$. Fig. 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. The most important is that all interactions, including external fields, are taken into account in the loop construction, thus eliminating the need for an $a$ posteriori acceptance probabilities that restrict the applicability of the previous methods. Like the continuous-time version of the worldline algorithm, 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, 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.

The method has here only been demonstrated for the anisotropic Heisenberg in a magnetic field. Generalizations to other models with two-body interactions are almost trivial, however. 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 $c = 0$. The vertex paths in Fig. 2 then involve changing these quantum numbers by some values ($\delta c, \delta s$) at the entrance leg, and changing them 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 non-zero matrix elements of type (10).

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