Stochastic Cluster Series expansion for quantum spin systems

Kim Louis and C. Gros

Fakultät 7, Theoretische Physik, University of the Saarland, 66041 Saarbrücken, Germany.

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In this paper we develop a cluster-variant of the Stochastic Series expansion method (SCSE). For certain systems with longer-range interactions the SCSE is considerably more efficient than the standard implementation of the Stochastic Series Expansion (SSE), at low temperatures. As an application of this method we calculated the \(T = 0\)-conductance for a linear chain with a (diagonal) next nearest neighbor interaction.

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Introduction— The development of efficient Quantum Monte Carlo (QMC) methods with loop-updates, like the original loop-algorithm and the SSE\(^{2,3,4,5}\), has been a major advancement. They are very efficient for the anistropic Heisenberg models, like the \(xxz\)-chain and can be generalized to more complicated Hamiltonians, but in some cases only with reduced performance.

Here we study the \(xxz\)-chain with a diagonal next nearest neighbor interaction. This model is better suited to find a way to reduce the bounce weight.

Here we report, that a new implementation of the SSE-algorithm, the cluster-SSE, yields a considerably smaller bounce weight than the standard SSE, improving thus the efficiency considerably at low temperatures.

Conventional SSE— We will now briefly discuss the conventional SSE-implementation and point out its difficulties. Our model of interest is a frustrated chain with a diagonal next-nearest neighbor interaction: (see Fig.1)

\[
H = \sum_n \left( \frac{J_x}{2}(S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+)ight) + J_z S_n^z S_{n+1}^z + J_{zz} S_n^z S_{n+2}^z \right). \tag{1}
\]

Note that only the interaction part is frustrated such that a Monte Carlo simulation will not suffer from the sign problem. Following Ref.\(^2\) we start by splitting the Hamiltonian into a set of local operators, i.e., \(H = \sum_{h \in \mathcal{H}} h\) with \(\mathcal{H} = \{h_{n,n+1}, h_{n,n+2} : t = 1, 2, 3; n \in \mathbb{N}\}\) and where the constants \(C\) and \(C_2\) are needed to ensure that all matrix elements between \(S^z\)-eigenbasis-states are positive. Using the Taylor expansion, the partition function may be written as

\[
Z = \sum_{M,\phi,\alpha} \frac{(-\beta)^M}{M!} \prod_{m=1}^M \langle \alpha_m, \phi(m) \alpha_{m+1} \rangle \tag{3}
\]

where \(M \in \mathbb{N}\), \(\phi : \{1, \ldots, M\} \to \mathfrak{h}\), and the \(\alpha_m\) run over all \(S^z\)-eigenbasis states with periodic boundary-conditions \(\langle \alpha_1 \rangle = \langle \alpha_{M+1} \rangle\) along the imaginary-time axis. The factors \(\langle \alpha_m, \phi(m) \alpha_{m+1} \rangle\) in Eq. \(\mathbb{E}\) are called plaquettes and are non-negative due to \(\phi\). Hence, we can obtain the partition function by sampling the terms in Eq. \(\mathbb{E}\) with their relative weight factors over all spin-configurations \(|\alpha_m\rangle\) and local operators \(\phi(m) \in \mathfrak{h}\).

Since each operator \(\phi(m)\) acts only on two sites we may write

\[
W_{n_1,n_2}(s_{n_1}^m, s_{n_2}^m, s_{n_1}^{m+1}, s_{n_2}^{m+1}) := \langle \alpha_m, \phi(m) \alpha_{m+1} \rangle
\]

where \(s_n^m = S_n^z|\alpha_m\rangle\) are spin variables and \(W_{n_1,n_2}\) is given by the prefactors of \(\mathbb{E}\). Note that because of translation invariance \(W_{n_1,n_2}\) depends actually only on \(n_2 - n_1\). For brevity we will in the sequel denote the four arguments, which we call plaquette legs, by one super-argument, which we call the plaquette state. The SSE knows two updates:

- In the diagonal update an insertion/removal of one plaquette is considered.
- The loop update (constructs and) flips a sub-set of the spin variables such that the new configuration is allowed—that means has non-zero weight.

The loop update may be achieved step by step. In each step we consider only one plaquette, whose state will be
changed from $i$ to $j$ by flipping two legs $l_i$ and $l_j$. The “in-going” leg $l_i$ is given and we have to choose the “out-going” leg $l_j$ with a certain probability $p(i \rightarrow j, l_i, l_j)$. Of course, the probability for a transition $i \rightarrow j$ must be zero, if one of the states $i$ or $j$ has zero weight.

These probabilities—yet to be determined—will play a central rôle in what follows. Therefore, we will explain in detail how they are obtained.

They may equivalently be represented by $(2^4 \cdot 4) \times (2^4 \cdot 4)$-matrices $a^{n_1,n_2}$ with entries

$$a^{n_1,n_2}_{(i,l_i)(j,l_j)} := p(i \rightarrow j, l_i, l_j) W_{n_1,n_2}(i).$$

The fact that the $p(i \rightarrow j, l_i, l_j)$ are probabilities imposes for each $l_i$ and $i$ the following conditions:

$$W_{n_1,n_2}(i) = \sum_{j,l_j} a^{n_1,n_2}_{(i,l_i)(j,l_j)}. \quad (4)$$

The detailed balance condition is satisfied if the matrices $a^{n_1,n_2}$ are symmetric.

Closer inspection shows that the matrices $a^{n_1,n_2}$ are block diagonal where the dimension of the blocks $d$ equals half the number of allowed plaquette states. Hence, if $n_2 - n_1 = 1$, we have $d = 3$ (as for the $xzx$-chain); it would be four if pair creation and pair annihilation were not forbidden, whereas $d = 2$ for $n_2 - n_1 = 2$.

All the elements in one single block of $a^{n_1,n_2}$ differ in at least one state index. Hence, we may drop the leg indices $l_i$ and $l_j$ without causing ambiguities. Moreover, we will also omit the explicit indication of the site indices $n_1$ and $n_2$ in $a$ and $W$.

For the blocks of length 3 a formal solution for the non-diagonal entries $a_{ij}$ which meets detailed balance and Eqs. (4) can easily be stated:

$$a_{ij} = \frac{W(i) + W(j) - W(k)}{2} + [a_{kk} - a_{ii} - a_{jj}] / 2 \quad (5)$$

where $k$ is the third plaquette state in the same block of $a$ as $i$ and $j$. One sees that the diagonal entries of the matrices $a$ remain free—apart from the final restriction that all probabilities (entries of $a$) need be positive.

Ref. 5 tells us how to dispose of the remaining degrees of freedom: The diagonal entries of a (baptized bounces) since they correspond to the choice $l_j = l_i$ are always allowed, but turn out to be inefficient as they impede the update scheme. As a general rule, one can say that the most favorable among all possible solutions to Eqs. (4) is the one with minimal diagonal entries.

In the blocks of length three all bounce weights may be put to zero for a wide parameter range but in the blocks of dimension two Eqs. (4) dictate one of the two bounces $a_{ii}$ and $a_{jj}$ to be equal to $[W(i) - W(j)] = J_{zz}/2$. A situation which is far from optimal.

**Cluster variant (SCSE)—** The problem with the SSE method is that some plaquettes—associated with operators $h^{(4)}$—have only four allowed (diagonal) states. This can be avoided by splitting the Hamiltonian into small clusters instead of mere two-sites operators. We now introduce the Stochastic Cluster Series expansion (SCSE).

![FIG. 1: The model Hamiltonian that will be discussed in this paper. Solid lines indicate a full Heisenberg-like interaction between the sites; dashed lines stand for sites coupled only by a $zz$-term (Ising-like interaction). Two clusters—as defined in the text—are indicated by thicker lines.](image1.png)

![FIG. 2: Pictorial representation of the plaquettes similar to the one used in Ref. 6. The operator itself is indicated by the horizontal central bar. The symbols stand for the six legs of the plaquettes. Equal symbols mean equal spins, and filled and empty symbols mean opposite spins. In this way the left diagram represents the eight diagonal plaquettes, and the right diagram, four non-diagonal plaquettes. The remaining non-diagonal plaquettes may be obtained by reflection with respect to the vertical central plaquette-axis and are not shown here.](image2.png)

In the case of the frustrated chain we split the Hamiltonian $H$ not into two-sites but three-sites operators (see Fig. 1):

$$h_{n,n+1,n+2}^{(1)} = J_x S_n^x S_{n+1}^x S_{n+2}^x / 4$$

$$h_{n,n+1,n+2}^{(2)} = J_y S_n^y S_{n+1}^y S_{n+2}^y / 4$$

$$h_{n,n+1,n+2}^{(3)} = J_z S_n^z S_{n+1}^z S_{n+2}^z / 4$$

$$h_{n,n+1,n+2}^{(4)} = J_x S_n^x S_{n+1}^x S_{n+2}^x + J_{zz} S_n^z S_{n+1}^z S_{n+2}^z + C. \quad (6)$$

Note the factor $1/4$ instead of $1/2$ for $h^{(t)}$ with $t = 1, 2, 3, 4$. It stems from the fact that each non-diagonal operator is “distributed” between two clusters. The possible plaquette states are shown in Fig. 2.

The diagonal update and loop construction remain unchanged with respect to the SSE. In the loop update the only difference is that $W$ is now a function of 6 variables. Let us now turn to the matrix $a$. The transitions of the form $h^{(l)} \rightarrow h^{(r)}$, when $t \in \{1, 2\}$ and $r \in \{3, 4\}$ will be ruled out from the beginning (for simplicity and because we do not expect that they will give assistance in minimizing the bounce.) All other transitions may have positive probability.

For a given plaquette — associated with an operator $h^{(l)}$— and a given in-going leg, whose site index is $n_i \in \{n, n+1, n+2\}$, we can directly tell the dimension of the corresponding block of $a$ and give a solution for its entries. There are three cases to be considered:

1) For $t = 1, 2$ and $n_i = n + 2$ (or $t = 3, 4$ and $n_i = n$) we get only two equations from Eqs. (4). Since both pla-
diagonal operators; we call them blocks of the same dimension may be obtained by reflection or vertical axis. (Note that in-going legs may always be out-going legs.) Upon flipping the two connected legs and interchanging in-and out-going leg one diagram becomes another. The other blocks of the same dimension may be obtained by reflection operations of the plaquettes.

FIG. 3: Example of a block of dimension 2 (top) and 3 (bottom) of Eqs. (1). (Notation see Fig. 2) In- and possible out-going legs are indicated by arrows and connected by a line. (Note that in-going legs may always be out-going legs.)

FIG. 4: Two examples of a block of dimension 4 of Eqs. (4) similar to Fig. 3. The other blocks of the same dimension may be obtained by reflection with respect to the horizontal or vertical axis.

plaque states (corresponding to non-diagonal \( h^{(t)} \) have equal weights, we can put the bounce weight to zero. The proceeding of the loop is then deterministic. (see top of Fig. 3)

II) Otherwise if \((t = 5, \ n_i \neq n + 1)\) or \((t \neq 5, \ n_i = n + 1)\) we have to consider three equations which may be treated as in the SSE. (see Eqs. (5) and bottom of Fig. 3)

III) In the remaining cases we need to solve a sub-system of Eqs. (4) of not less than four equations. (see Fig. 4). Among the four plaquette states involved in this block we find two states corresponding to non-diagonal \( h^{(t)} \) — which we call \( i_n \) and \( j_n \). From Fig. 4 we infer that if \( i_n \) corresponds to \( t \in \{1, 2\} \), \( j_n \) corresponds to \( t \in \{3, 4\} \), et vice versa. The remaining two states correspond to diagonal operators; we call them \( i_d \) and \( j_d \). The entries of \( a \) are given by

\[
a_{i_n,i_d} = \max\{W(i_d)/2 + W(i_n) - W(j_d)/2, 0\}
a_{i_n,j_d} = \min\{W(j_d)/2 + W(i_n) - W(i_d)/2, 0\}
a_{i_d,j_d} = \min\{W(i_d) + W(j_d) - 2W(i_n)/2, W(i_d)\}
a_{j_d,j_d} = \max\{0, W(j_d) - W(i_d) - 2W(i_n)\}
a_{j_n,k} = a_{i_n,k}, \quad k = i_d, j_d.
\]

Note that we assumed \( W(i_d) \leq W(j_d) \) and exploited \( W(i_n) = W(j_n) \). With this choice only one diagonal entry (namely, \( a_{i_d,j_d} \)) may be non-negative. To be concrete: only the situation depicted in the upper part of Fig. 4 admits \( a_{i_d,j_d} = (J_x - J_z)/2 > 0 \) if \( J_x > J_z \).

The SCSE is more intricate (one has to consider several cases separately) and the bounce cannot always be avoided, but there is a considerable improvement (at low temperatures) with respect to the SSE.

Numerical results—In this paper we use the method proposed in Ref. 3 to calculate the conductance for the Hamiltonian 1. We evaluate the expression

\[
g(\omega_M) = -\omega_M/h \int_0^{\hbar/\beta} \cos(\omega_M \tau) \langle P_x P_y (i\tau) \rangle d\tau \quad (6)
\]

at the Matsubara frequencies \( \omega_M = 2\pi M/(\beta h) \), \( M \in \mathbb{N} \). The conductance is obtained by extrapolating \( g(\omega) \) from the Matsubara frequencies to \( \omega = 0 \). The operators in Eq. (6) are given by \((e \text{ is the charge unit})\)

\[P_x = e \sum_{n \geq 2} S_n^x.\]

The \( \omega = 0 \)-value of \( g \) does not depend on \( x \) or \( y \),

To illustrate the improvement gained by introducing SCSE we performed for a special choice of parameters \((J_x = 2J_z)\) simulations of \( g(\omega_M) \). In Fig. 5 we plotted the ratios of the time consume along with the ratio of the statistical error in \( g(\omega_M) \) (for \( M = 1, \ldots, 10) \). The SSE is slightly faster (about 80 percent) but while the statistical error grows linearly with \( J_x \) for SSE, it grows more modestly for the SCSE.

Frustrated system—Using the Lanczos-method Zhu-ravlev, Katsnelson and coworkers \( \ddagger \) obtained a very complete picture of the frustrated system given by the Hamiltonian 1. They set up a low-temperature phase
diagram with two gapped and a gap-less phase. In the gap-less phase the system is—for a large range of parameters—very well-described by the Luttinger liquid picture. In Fig. 6 $g(\omega = 0)$—extrapolated by a quadratic fit—is plotted versus $J_{z2}$ for various $J_z < J_x$. For this region in parameter space Ref. 8 finds a phase boundary between the gap-less and the gapped phase at $J_{z2} = J_x$.

In a Luttinger liquid the conductance equals the Luttinger parameter $\Delta$ and may hence be viewed as an effective interaction. Since $J_{z2}$ mediates a nearest neighbor attraction and thereby reduces the effective interaction, the conductance first grows with $J_{z2}$ and then assumes its maximum approximately when $2J_{z2} = J_z$ is satisfied. We see that within error bars the conductance does not vary on the phase boundary.

As we work at a finite temperature of $k_B T = 0.01J_x$, the conductance goes smoothly to zero in the gapped phase such that a determination of the phase boundary from Fig. 6 becomes difficult.

A remarkable fact of the phase diagram in Ref. 8 is the fact that the gap-less phase is not bounded in parameter space; it contains, e.g., the line with $2J_{z2} = J_z$. It is therefore interesting to study the behavior of the conductance on this line. However, if we increase $J_z$ and $J_{z2}$ simulating the conductance becomes more difficult. (The statistical error grows.)

Only the SCSE allows us to compute the conductance for as large interaction values as $J_z = 5$, $J_{z2} = 2.5$. The conductance is plotted in Fig. 7. Beside the statistical error we have an extrapolation error depending on our extrapolation scheme. In Fig. 7 we compared two schemes: a quadratic fit to the first three Matsubara frequencies and a linear fit from the first six Matsubara frequencies. The former should give a smaller extrapolation error, but it enhances the statistical error of $g(\omega)$. The latter has a larger extrapolation error, but it suppresses the statistical error of $g(\omega)$. For small parameters the two fits almost coincide. But for larger parameter values—when the statistical error increases—the quadratic fit starts to fluctuate.

For this system the DC-Drude weight $D$ and the susceptibility $\chi$ at $T = 0$ may be obtained by exact diagonalization. The same is true for the conductance via the relation $g = \pi \sqrt{D/\chi}$ valid for a Luttinger liquid. Fig. 7 provides also the exact diagonalization data showing good agreement with the SCSE data within error bars.

**Conclusion**—In this letter we showed that the performance of the SSE can be substantially improved by selecting a different splitting of the Hamiltonian. We used this strategy for an $xxz$-chain with next-nearest-neighbor-interaction, but it should also apply to systems which have additional plaquettes with a reduced number of plaquette states. These systems include fermionic chains with arbitrary interaction part, which may also be coupled by an interaction term as well as (not necessarily one-dimensional) spin systems that have at the same time Heisenberg-like and Ising-like interaction bonds.

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