Universal SSE algorithm for Heisenberg model and Bose Hubbard model with interaction

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I. INTRODUCTION

Recently, significant progress in quantum Monte Carlo methods has been observed. During the last two decades, advanced quantum Monte Carlo algorithms have been developed. First quantum Monte Carlo methods, so-called world line algorithms, were based on Suzuki-Trotter approximation and used local updates \[1, 2\]. It has been replaced by the loop algorithms, which use non-local updates. Using of non-local loop updates allows to decrease autocorrelation times by orders of magnitude \[3\]. Later the loop algorithms in continuous imaginary time have been developed \[4\]. The continuous-time implementation of the loop algorithm has eliminated errors resulting from the Trotter discretization and, hence, loop algorithms have become numerically exact methods.

Unfortunately, loop algorithms are inefficient in the presence of external field \[5\]. The origin of this slowdown results from the method of including external field into the simulations. External field is taken into account through the global weight, which increases with field increase. To construct efficient algorithm one should take into account external field locally, in the loop construction. For the first time this idea was implemented in the framework of the worm algorithm \[6\].

Both worm and loop algorithms work directly in continuous imaginary time. At the same time there is a numerically exact quantum Monte Carlo method, which works in the discrete basis. It is Stochastic Series Expansion (SSE) method. SSE algorithm is based on power series expansion of an partition function. Initially SSE method was developed with local updates \[7\]. Later the algorithm with loop updates was proposed \[8\]. Applying loop updates for SSE method has same favorable consequence as for world line algorithms and SSE method has become powerful tool for exploring quantum many-body systems. Recently Sandvik and Syljuåsen introduce the concept of directed loops in stochastic series expansion, which allows to perform simulation in wide range of external fields \[9\].

Last years loop algorithms and SSE algorithm have been used for exploring of different quantum systems. Investigations of quantum spins \[10, 11, 12, 13\], bosons \[11\] and one-dimensional fermion systems \[12\] have been performed. However, at the present moment investigations of hard-core bosons and spin \(S = 1/2\) systems are predominant in literature.

The authors of the papers \[12\] investigate spin systems with spin \(S > 1/2\) by loop algorithms. But they do not take into account external field. And they use the spin-split representation, i.e. replace the original spin operators by the sum of \(2S\) Pauli operators. Such representation is uncomfortably because it requires extra memory resources and it cannot be applied directly for soft-core bosons.

P. Henelius et al. have studied ferromagnetic Heisenberg model with spin up to \(S = 2\) in the wide range of external field by using of the SSE algorithm \[14\]. Our calculations indicate that the standard SSE algorithm is quite effective in the case of ferromagnetic Heisenberg model but for simulation Heisenberg antiferromagnet it is necessary to increase efficiency of the algorithm.

Until now we do not know about simulations of soft-core bosons by the loop or SSE algorithms. Very recently Kawashima et al. develop method for free soft-core bosons based on the mapping of bosonic models to the spin models \[15\]. For simulation of spin system they use coarse-grained loop algorithm with the spin-split representation. Unfortunately, the authors do not give any quantitative characteristics of their algorithm efficiency.

In the present work we propose universal algorithm based on SSE method, which allows to investigate both spin systems with arbitrary spin in the presence of external field and systems of interacting soft-core bosons in the presence of chemical potential. Also we develop simple procedure, which allows to increase efficiency of the SSE algorithm in the general case.
II. THE ALGORITHM

During the construction of the algorithm we follow the ideas of the work [2], therefore we do not describe SSE method in details but briefly outline it.

Let us to consider Heisenberg model in the case of arbitrary spin $S$, in the presence of external longitudinal field $h$

$$\hat{H} = \pm J \sum_{<i,j>} S_i S_j - h \sum_i S_i^z, \quad (1)$$

and Bose Hubbard model with interaction

$$\hat{H} = -t \sum_{<i,j>} (b_i^+ b_j + b_i b_j^+) + V \sum_{<i,j>} n_i n_j + U \sum_i n_i^2 - \mu \sum_i n_i, \quad (2)$$

where $\langle i, j \rangle$ denotes summation over the pairs of nearest-neighbor sites. Following to the ideas of the SSE method, we rewrite the Hamiltonians (1,2) as a sum over diagonal and off-diagonal bond operators

$$\hat{H} = -J \sum_{<i,j>} (\hat{H}_{ij}^{(d)} \mp \hat{H}_{ij}^{(n)}), \quad (3)$$

where minus corresponds to antiferromagnet, plus corresponds to ferromagnet and Hubbard model (for Hubbard model $J$ corresponds to $t$). In the case of the Heisenberg model the operators are

$$\hat{H}_{ij}^{(d)} = C \mp S_i^z S_j^z \mp \frac{h}{2J} (S_i^z + S_j^z)$$

and, correspondingly, in the case of the Bose Hubbard model the operators are

$$\hat{H}_{ij}^{(d)} = C \mp \frac{V}{t} n_i n_j \mp \frac{U}{2t} (n_i^2 + n_j^2) + \frac{\mu}{2t} (n_i + n_j)$$

$$\hat{H}_{ij}^{(n)} = b_i^+ b_j + b_i b_j^+.$$ (4)

One should guarantee non-negativity of all matrix elements of the operators (4) by appropriate choosing of constants $C$.

The SSE algorithm is based on the series expansion of the partition function $Z$ with respect to inverse temperatures $\beta$ powers. To simplify Monte Carlo simulation, Sandvik et al. [8, 9] propose to introduce unit operators $I$ and cut off the expansion at $n = L$ power. It should be point out, that unit operators can be distributed in different ways. So we obtain the formula for the partition function

$$Z = \sum_{\alpha} \sum_{\langle S_L \rangle} \frac{(J\beta)^n (L-n)!}{L!} (\alpha) \prod_{k=1}^{L} \hat{H}_k(\gamma)(\alpha), \quad (6)$$

where $\gamma$ denotes the operator type - unit, diagonal, non-diagonal, $S_L$ is a sequence of operator indices and $n$ is the number of non-unit operators in $S_L$.

The Monte Carlo simulation is carried out with diagonal and loop updates. The simulation starts with an arbitrary state $\langle \alpha \rangle$ and operator string $S_L$ containing only unit operators. During the diagonal update one attempts to interchange diagonal and unit operators with the probabilities

$$P(\hat{I} \to \hat{H}_{ij}^{(d)}) = \frac{J N \beta(\alpha(p)) \hat{H}_{ij}^{(d)} |\alpha(p)\rangle}{L - n}$$

$$P(\hat{H}_{ij}^{(d)} \to \hat{I}) = \frac{L - n + 1}{J N \beta(\alpha(p)) \hat{H}_{ij}^{(d)} |\alpha(p)\rangle},$$

where $|\alpha(\rho)\rangle$ is the system state after $p$ operators been applied to it, $N$ is a number of bonds. Note that diagonal update changes the expansion power $n$ by $\pm 1$.

In the stage of loop update interchanging of diagonal and non-diagonal operators is carried out with the fixed expansion power $n$. At the same time state $\langle \alpha \rangle$ can be changed.

In the case of spin $S = 1/2$ loop update is executed in the following way. Non-unit operators can be represented as vertices with four legs (Fig. 1(a)). One of the $n$ vertices is selected and one of its four legs is selected at random. After that exit leg of the vertex is selected according with appropriate probabilities and the spins at both the entrance and exit legs are flipped. Note that the exit leg uniquely points to the entrance leg of the next vertex. The loop is constructed such way until it closed.

At $S > 1/2$ split-spin representation of spin operators is widely used (Fig. 1(b)). In this case vertex contains $4(2S + 1)$ variables, which can take the value $\pm 1$. During the construction of the loop spins at the entrance and the exit legs are flipped. But now loop propagates through the vertices with $4(2S + 1)$ legs. And therefore a number of possible loop paths increases rapidly with spin increase.
SSE algorithm allows to refuse spin-split representation and to apply filling number representation which is applicable both for Heisenberg and Bose Hubbard model. In order to do it we use well known expressions for the matrix elements of corresponding operators

\[ \langle s|S^+|s-1\rangle = \langle s-1|S^-|s\rangle = \sqrt{(S+s)(S-s+1)} \]
\[ \langle n|b^+|n-1\rangle = \langle n-1|b|n\rangle = \sqrt{n}. \]  

Now vertex has only four legs at arbitrary spin or at arbitrary maximum filling number for bosons (Fig. 1). However, variables connected with legs take values \(-S,...,S\) for spins or \(0,...,n_{\text{max}}\) for bosons. Therefore during the construction of the loop we cannot use only flip of states at entrance and exit legs. So we introduce increasing and decreasing processes. To avoid discontinuous loop pathes during the construction of loops we use a simple rule: if state at the exit leg is decreased (increased) then at the entrance leg of the next vertex decreasing (increasing) process will be chosen.

III. OPTIMIZATION OF THE ALGORITHM

Recently Sandvik and Syljuåsen showed that in order to fulfill detailed balance for loop update one should to solve the set of equations

\[ W_i = \sum_j a_{ij}, \]  

where \(W_i\) are matrix elements of the operators \((4,5)\), and \(a_{ij}\) are all allowed processes. For example \(a_{ii}\) denotes bounce process, which does not change matrix element \(W_i\), and \(a_{ij}\) denotes process which transforms \(W_i\) to \(W_j\). It should be point out that all \(a_{ij}\) must be nonnegative and because of detailed balance principle \(a_{ij} = a_{ji}\). From \(a_{ij}\) one can obtain probabilities of all processes \(P(W_i \rightarrow W_j) = a_{ij}/W_i\) and correspondingly \(P(W_j \rightarrow W_i) = a_{ij}/W_j\).

We found that in the case of arbitrary spin, set of all processes \(\{a_{ij}\}\) is decomposed into closed groups containing one, three and six non-bounce processes. The group with one non-bounce process is described by equations set with two equations, and groups with three and six non-bounce processes are described by equations sets with three and four equations correspondingly. So the equations set is decomposed into sets consisting of two, three and four equations. Relations between number of various groups is different at different values of spin. For example in the case of \(S = 1/2\) there are only groups containing three non-bounce processes. However at \(S = 1\) groups containing three and six non-bounce processes appear. And number of such groups grows with increase of spin until spin value becomes \(S = 5/2\). At \(S = 5/2\) part of groups with non-bounce process is \(4/15\), with three non-bounce processes is \(3/15\) and with six non-bounce processes is \(8/15\). At \(S > 5/2\) the relations between number of groups are the same as for \(S = 5/2\).

It is obvious that there is particular non-negative solution of the equations set. It is so-called heat-bath solution.

\[ a_{ij} = \frac{W_i W_j}{\sum_k W_k}. \]  

In the denominator sum is over all matrix elements belonging to the group. Unfortunately heat-bath solution gives rise to the inefficient algorithm since all bounce processes \(a_{ii}\) are nonzero. In order to increase efficiency of algorithm, one should to exclude bounce processes. Let us to do it for different types of groups.

In the case of the group with one non-bounce process corresponding set of equations is

\[ W_1 = a_{11} + a_{12} \]
\[ W_2 = a_{22} + a_{21}. \]  

So we can always exclude one of bounce processes by choosing \(a_{12} = W_2, a_{11} = W_1 - W_2, a_{22} = 0\) if \(W_1 > W_2\) and \(a_{12} = W_1, a_{22} = W_2 - W_1, a_{11} = 0\) otherwise. It is obvious that if \(W_1 = W_2\) bounce processes are absent at all.

Sandvik and Syljuåsen for \(S = 1/2\) Heisenberg model have analysed analytically groups with three non-bounce processes, which are described by the equations set

\[ W_1 = a_{11} + a_{12} + a_{13} \]
\[ W_2 = a_{22} + a_{21} + a_{23} \]
\[ W_3 = a_{33} + a_{31} + a_{32}. \]
Then solution of Eq. (12) takes the form

\[ a = \frac{1}{J} \]

They proposed different solutions of the equations set \( \{12\} \) for various parameters of the model. It should be point out, that some solutions contain two bounce processes. At the same time for the case of arbitrary spin one cannot analytically analyse all allowed processes and obtain corresponding probabilities because number of processes grows rapidly as spin increase.

We considered the equations set \( \{12\} \) in general and concluded that only one bounce process is needed at any \( W_i \). And there is no need to solve equations set \( \{12\} \) analytically, but it is possible to use simple procedure for obtaining non-negative solution of Eq. \( \{12\} \).

First we demand all bounce processes \( a_{ii} \) to be zero. Then solution of Eq. \( \{12\} \) takes the form

\[
\begin{align*}
a_{12} &= \frac{W_1 + W_2 - W_3}{2} \\
a_{13} &= \frac{W_1 + W_3 - W_2}{2} \\
a_{23} &= \frac{W_2 + W_3 - W_1}{2}.
\end{align*}
\]

(We take into account that \( a_{ij} = a_{ji} \).) If one of \( a_{ij} \) is negative then two others are certainly positive. So we need only one bounce process. Let \( a_{12} < 0 \) to be negative, then we should introduce bounce \( a_{33} \) in a such way that \( a_{12} \) becomes positive and \( a_{13}, a_{23} \) do not change the sign. Let \( W_1 > W_2 \), then by choosing \( a_{33} = W_3 - W_1 - W_2/\delta \) we get new solution of Eq. \( \{12\} \)

\[
\begin{align*}
a_{12} &= \frac{W_2}{2} (1 - \frac{1}{\delta}) \\
a_{13} &= W_1 + \frac{W_2}{2} (\frac{1}{\delta} - 1) \\
a_{23} &= W_2 (1 + \frac{1}{\delta}).
\end{align*}
\]

It is obvious that at any \( \delta > 1 \) solution \( \{14\} \) is positive. If \( W_2 > W_1 \), then we should interchange \( W_1 \) by \( W_2 \) in \( \{14\} \). It should be point out that at \( \delta = 1 \) solution \( \{12\} \) coincides with some solutions proposed in Ref. 9. We do not assert that our solution is most effective, but given procedure is universal and it can be applied at arbitrary spin.

The groups with six non-bounce processes are described by the equations set

\[
W_1 = a_{11} + a_{12} + a_{13} + a_{14} \\
W_2 = a_{22} + a_{21} + a_{23} + a_{24} \\
W_3 = a_{33} + a_{31} + a_{32} + a_{34} \\
W_4 = a_{44} + a_{41} + a_{42} + a_{43}.
\]

As well in the case of group with three non-bounce processes, we demand \( a_{ii} = 0 \) and take into account \( a_{ij} = a_{ji} \). Then we obtain the equations set with four equations and six variables, i.e. we have two free parameters. Let us assume \( a_{23} = a_{34} = a_{13} \), then we obtain solution of Eq. \( \{16\} \)

\[
\begin{align*}
a_{12} &= \frac{W_1 + W_2 - W_4}{2} - \frac{W_3}{6} \\
a_{13} &= \frac{W_3}{3} \\
a_{14} &= \frac{W_1 + W_4 - W_2}{2} - \frac{W_3}{6} \\
a_{24} &= \frac{W_2 + W_4 - W_1}{2} - \frac{W_3}{6}.
\end{align*}
\]

We can guarantee positivity of terms like \( (W_1 + W_2 - W_4)/2 \), by using procedure which we apply for the equations set with three equations. Thus we introduce one bounce process. After that we obtain expressions like \( a = W_3/6 \) with positive \( a \). If latter expression is negative

FIG. 3: Integrated autocorrelation times for the magnetization and energy vs external field in ferromagnetic (upper plot) and antiferromagnetic (lower plot) Heisenberg model with different spin \( S \) at \( N_s = 16 \) and \( \beta = 10 \). Coupling constant is \( J = 1.0 \).

FIG. 4: Integrated autocorrelation times for the mean number of bosons and energy vs chemical potential in the Bose Hubbard model with different maximum site filling at \( N_s = 16 \) and \( \beta = 10 \). Hopping constant is \( t = 1.0, U = 0.5, V = 0.5 \).
IV. TEST CALCULATIONS

SSE algorithm is universal in any dimension. With increase of dimension extra bonds arise, but ideas of loop construction remain the same. Therefore we test the proposed scheme on 1D systems.

We calculate magnetization $M$ for Heisenberg model, a mean number of bosons $N_b$ for Bose Hubbard model, and energy for both models. We use well-known estimators

$$E = -\frac{\langle n \rangle}{\beta}$$

$$M = \frac{1}{N_s} \sum_{i=1}^{N_s} \langle S_i^z \rangle$$

$$N_b = \frac{1}{N_s} \sum_{i=1}^{N_s} \langle n_i \rangle,$$

where $n$ is a number of non-unit operators in operator string and $N_s$ is a number of sites. We have checked our results with exact diagonalization and have found that relative deviation our results from exact is less than $10^{-3} - 10^{-4}$.

It is well-known that integrated autocorrelation times is a quantitative measure of efficiency of a Monte Carlo sampling. We calculate autocorrelation times using binning method, which described in Ref. 3

First of all it is interesting to analyse influence of bounce processes on efficiency of the algorithm. To this end we calculate for Heisenberg antiferromagnet integrated autocorrelation times for magnetization by using heat-bath solution and optimized algorithm described in the previous section. We consider spin $S = 5/2$ because at this value all types of groups are present and relations between number of groups do not change with further spin increase. As shown in Fig. 2, in the case of the optimized algorithm bounce probabilities are less then in the case of heat-bath solution. Accordingly autocorrelation times are less for the optimized algorithm. For other calculations reported here the optimized algorithm has been used.

Fig. 3 shows autocorrelation times for magnetization versus external field for ferromagnetic (upper plot) and antiferromagnetic (lower plot) Heisenberg model with different spin $S$. Calculations have been done for the chain with $N_s = 16$ sites at $\beta = 10$.

One can see some increase of autocorrelation times with spin increase for the antiferromagnet chain. However it is difficult to compare efficiency of the algorithm at fixed temperature and different spin. Mean number of non-unit operators can be roughly estimated as $N_s J/\beta S^2$.

It is clear that this value grows rapidly with the spin $S$ increase. We observe that the mean number of non-unit operators $\langle n \rangle \sim 100$ at $\beta = 10$ and $N_s = 16$ in the case of spin $S = 1/2$ whereas in the case of spin $S = 5/2$ at the same conditions $\langle n \rangle \sim 2000$. Thus simulation of $S = 5/2$ Heisenberg antiferromagnet at $\beta = 10$ is as hard as simulation of $S = 1/2$ Heisenberg antiferromagnet at $\beta \sim 100$. Hence the origin of autocorrelation time increase is clear and, with the other hand, it is obvious that the algorithm is very efficient. It should be point out that the algorithm works efficiently in wide range of external fields.

For the ferromagnet chain we obtain good autocorrelation times for magnetization in wide range of external fields with the exception of zero field. At zero field autocorrelation times for magnetization become very large (we do not show corresponding points at Fig. 3). It is a known sequence of degeneracy states with spins up and spins down.

Also we done calculations for Bose Hubbard model with interaction. As seen from Fig. 4 autocorrelation

![FIG. 5: Lower plot - integrated autocorrelation times for the mean number of bosons in the Bose Hubbard model at $N_s = 16$ and $\beta = 10$, $N_{max} = 5$. Hopping constant is $t = 1.0$, $V = 0.0$, $\mu = U$. Dark circles correspond to the optimized algorithm, open circles correspond to the heat-bath algorithm, squares correspond to chain with $N_s = 50$. Middle plot - bounce probabilities for optimized and heat-bath algorithms. Upper plot - mean length of loops in units of $\langle n \rangle$ for optimized and heat-bath algorithms accordingly. The arrow points to the critical point "Mott insulator-superfluid"

one can add process $a_{33} = W_3(1 - 1/\delta_3)$. And we can provide positivity of solution by choosing $\delta_2$ sufficiently large.
times for energy is order of unity. Autocorrelation times for mean number of bosons grow with maximum filling number $N_{\text{max}}$ increase. Note that we can use any maximum filling number $N_{\text{max}}$, and for large class of problems the value $N_{\text{max}} \sim 5...10$ is quite enough.

Investigation of many-body quantum system behavior near the critical points is one of interesting problem in condensed matter physics. Kawashima et al. have tested SSE directed loop algorithm for 3D system and failed to obtain estimates for the observables near the critical point [16]. It is well known that 1D Bose Hubbard model experiences superfluid-insulator transition at $(t/U)_c = 0.608$, $V = 0$, $\mu = U$ [17]. We calculate autocorrelation times near the critical point for $N_s = 16$, $N_s = 50$ chains at $\beta = 10$, $N_{\text{max}} = 5$. As seen from Fig. (5) autocorrelation times for both optimized and heat-bath algorithms are quite reasonable. But bounce probabilities in the case of heat-bath algorithm are very large and exceed bounce probabilities in the case of optimized algorithm by order of magnitude. Large bounce probabilities give rise to enormous loops, which walk around system many times until closed. Construction of such big loops takes a lot of time and simulation becomes inefficient. So we can conclude that SSE algorithm allows to perform simulations near the critical point (at least near superfluid-insulator transition in 1D), however it is desirable to exclude bounce processes.

V. SUMMARY

In conclusion it should be emphasized that the algorithm introduced here allows to explore Heisenberg model with arbitrary spin and Bose Hubbard model with interaction. With the help of filling number representation we create the unified code for both models. Note that from algorithmic point of view differences between the models arise only at stage of matrix elements calculation.

We propose universal procedure for excluding bounce processes. It has been obtained that for groups with one and three processes only one bounce is needed and in the case of group with six processes maximum two bounces are needed. We found that relations between number of various groups are different up to spin $S = 5/2$ (maximum filling number $N_{\text{max}} = 5$). After spin $S = 5/2$ the relations do not change.

Calculations of integrated autocorrelation times demonstrate increase efficiency of the algorithm under bounce processes excluding. We show that the proposed algorithm works in wide range of external fields both for Heisenberg model with arbitrary spin $S$ and for Bose Hubbard model with interaction. Also we found that the algorithm is efficient near the superfluid-insulator transition.

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