

Universal stochastic series expansion algorithm for Heisenberg model and Bose-Hubbard model with interaction

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We propose a universal stochastic series expansion (SSE) method for the simulation of the Heisenberg model with arbitrary spin and the Bose-Hubbard model with interaction. We report the calculations involving soft-core bosons with interaction by the SSE method. Moreover, we develop a simple procedure for increased efficiency of the algorithm. From calculation of integrated autocorrelation times we conclude that the method is efficient for both models and essentially eliminates the critical slowing down problem.

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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 It has been replaced by the loop algorithms that use nonlocal updates. Using nonlocal 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 slow-down results from the method of including external field into the simulations. External field is taken into account through the global weight, which increases as the field increases. 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 that works in the discrete basis. It is a stochastic series expansion (SSE) method. SSE algorithm is based on power series expansion of a partition function. Initially SSE method was developed with local updates [7]. Later the algorithm with loop updates (worm updates) was proposed [8]. Applying loop updates for SSE method has the 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 have introduced the concept of directed loops in stochastic series expansion, which allows to perform the simulation in a wide range of external fields [9].

In the last few years, loop algorithms and SSE algorithm have been used for exploring different quantum systems. In-

vestigations of quantum spins [10,13–15], bosons [11], and one-dimensional fermion systems [12] have been performed. However, at present, investigations of hard-core bosons and spin $S = 1/2$ systems are predominant in literature.

The authors of Ref. [13] have investigated spin systems with spin $S > 1/2$ by loop algorithms. But they have not taken into account the external field. Rather they have used the spin-split representation, i.e., they have replaced the original spin operators by the sum of $2S$ Pauli operators. Such representation is not suitable because it requires extra memory resources and it cannot be applied directly for soft-core bosons.

Henelius *et al.* have studied ferromagnetic Heisenberg model with spin up to $S = 2$ in a wide range of external field by using the SSE algorithm [15]. Our calculations indicate that the standard SSE algorithm is quite effective in the case of ferromagnetic Heisenberg model, but for the simulation of Heisenberg antiferromagnet it is necessary to increase efficiency of the algorithm.

Till now we do not know about simulations of soft-core bosons by the loop or SSE algorithms. Very recently Kawashima *et al.* have developed a method for *free* soft-core bosons based on the mapping of bosonic models to the spin models [16]. For the simulation of spin system they have used coarse-grained loop algorithm with the spin-split representation. Unfortunately, the authors have given any quantitative characteristics of their algorithm efficiency.

In the present work we propose universal algorithm based on the SSE method that 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 a simple procedure that allows us 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 of Ref. [9]; therefore, we do not describe the SSE method in details but outline it briefly.

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

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$$\hat{H} = \pm J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - h \sum_i S_i^z, \quad (1)$$

and the Bose Hubbard model with interaction

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

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

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

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

$$\hat{H}_{ij}^{(d)} = C \mp S_i^z S_j^z + \frac{h}{2J} (S_i^z + S_j^z), \quad (4)$$

$$\hat{H}_{ij}^{(n)} = \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+),$$

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

$$\hat{H}_{ij}^{(d)} = C - \frac{V}{t} n_i n_j - \frac{U}{2t} (n_i^2 + n_j^2) + \frac{\mu}{2t} (n_i + n_j), \quad (5)$$

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

One should guarantee non-negativity of all matrix elements of operators (4) and (5) by appropriate choosing of constants C .

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

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

where γ denotes the operator type—unit, diagonal, nondiagonal; S_L is a sequence of operator indices; and n is the number of nonunit operators in S_L .

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

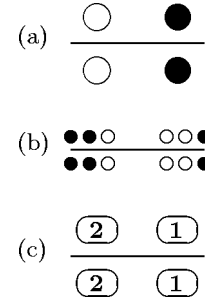


FIG. 1. An example of different vertices. (a) In the case of hard-core bosons or $S=1/2$ Heisenberg model. (b) In the case of the spin-split representation for the $S=3/2$ Heisenberg model. (c) Vertex (b), in the filling number representation. “1” is identified with the spin projection $S^z = -1/2$, “2” is identified with the spin projection $S^z = 1/2$. For the Bose Hubbard model one can identify “1” with one boson per site, “2” with two bosons per site.

$$P(\hat{I} \rightarrow \hat{H}_{ij}^{(d)}) = \frac{JN\beta \langle \alpha(p) | \hat{H}_{ij}^{(d)} | \alpha(p) \rangle}{L-n}, \quad (7)$$

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

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

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

In the case of spin $S=1/2$ loop update is executed in the following way. Nonunit 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 to 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 in such a way that it closes.

At $S > 1/2$, spin-split representation of spin operators is widely used [Fig. 1(b)]. In this case vertex contains $4(2S+1)$ variables, which can take the value ± 1 . During the construction of the loop, spins at the entrance and the exit legs are flipped. But now the loop propagates through the vertices with $4(2S+1)$ legs, and therefore a number of possible loop paths increase rapidly as spin increases.

The SSE algorithm allows us to refuse spin-split representation and to apply filling number representation, which is applicable both for the Heisenberg and for the Bose Hubbard models. In order to do it, we use well-known expressions for the matrix elements of corresponding operators

$$\langle s | S^{\dagger} | s-1 \rangle = \langle s-1 | S^{-} | s \rangle = \sqrt{(S+s)(S-s+1)}, \quad (8)$$

$$\langle n | b^{\dagger} | n-1 \rangle = \langle n-1 | b | n \rangle = \sqrt{n}.$$

Now vertex has only four legs at arbitrary spin or at arbitrary maximum filling number for bosons [Fig. 1(a)]. However,

variables connected with legs take values $-S, \dots, S$ for spins or $0, \dots, n_{max}$ 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 paths during the construction of the 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 [9] have shown that in order to fulfil detailed balance for loop update one should solve the set of equations

$$W_i = \sum_j a_{ij}, \quad (9)$$

where W_i are the matrix elements of operators (4) and (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 the process that transforms W_i to W_j . It should be pointed out that all a_{ij} must be non-negative 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 have found that in the case of arbitrary spin, set of all processes $\{a_{ij}\}$ is decomposed into closed groups containing one, three, and six nonbounce processes. The group with one nonbounce process is described by the set of equations with two equations, and groups with three and six nonbounce processes are described by the sets of equations with three and four equations, respectively. So the set of Eqs. (9) is decomposed into sets consisting of two, three, and four equations. Relations between number of various groups are different at different values of spin. For example, in the case of $S = 1/2$, there are only groups containing three nonbounce processes. However, at $S = 1$, groups containing three and six non-bounce processes appear. Number of such groups grows with increase in spin until spin value becomes $S = 5/2$. At $S = 5/2$ part of groups with one nonbounce process is $4/15$, with three nonbounce 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 a particular non-negative solution of the set of Eqs. (9). It is so-called heat-bath solution:

$$a_{ij} = \frac{W_i W_j}{\sum_k W_k}. \quad (10)$$

In the denominator, the 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 exclude bounce processes. Let us do it for different types of groups.

In the case of the group with one nonbounce process, corresponding set of equations is

$$W_1 = a_{11} + a_{12}, \quad (11)$$

$$W_2 = a_{22} + a_{21}.$$

So we can always exclude one of the 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.

Sandvik and Syljuåsen for $S = 1/2$ Heisenberg model have analyzed analytically groups with three nonbounce processes [9], which are described by the set of equations

$$W_1 = a_{11} + a_{12} + a_{13}, \quad (12)$$

$$W_2 = a_{22} + a_{21} + a_{23},$$

$$W_3 = a_{33} + a_{31} + a_{32}.$$

They proposed different solutions of the set of Eqs. (12) for various parameters of the model. It should be pointed out that some solutions contain two bounce processes. At the same time for the case of arbitrary spin one cannot analytically analyze all allowed processes and obtain corresponding probabilities because the number of processes grows rapidly as spin increases.

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

First we demand all bounce processes a_{ii} to be 0. Then solution of Eqs. (12) takes the form

$$a_{12} = \frac{W_1 + W_2 - W_3}{2}, \quad (13)$$

$$a_{13} = \frac{W_1 + W_3 - W_2}{2},$$

$$a_{23} = \frac{W_2 + W_3 - W_1}{2}.$$

(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 Eqs. (12):

$$a_{12} = \frac{W_2}{2} \left(1 - \frac{1}{\delta} \right), \quad (14)$$

$$a_{13} = W_1 + \frac{W_2}{2} \left(\frac{1}{\delta} - 1 \right),$$

$$a_{23} = \frac{W_2}{2} \left(1 + \frac{1}{\delta} \right).$$

It is obvious that at any $\delta > 1$ solution (14) is positive. If $W_2 > W_1$, one should interchange W_1 by W_2 in Eqs. (14). It should be pointed out that at $\delta = 1$ solution (14) coincides with some solutions proposed in Ref. [9]. We do not assert that our solution is most effective, but the given procedure is universal and can be applied to arbitrary spin.

The groups with six nonbounce processes are described by the set of equations

$$W_1 = a_{11} + a_{12} + a_{13} + a_{14}, \quad (15)$$

$$W_2 = a_{22} + a_{21} + a_{23} + a_{24},$$

$$W_3 = a_{33} + a_{31} + a_{32} + a_{34},$$

$$W_4 = a_{44} + a_{41} + a_{42} + a_{43}.$$

As well in the case of group with three nonbounce processes, we demand $a_{ii} = 0$ and take into account $a_{ij} = a_{ji}$. Then we obtain the set of equations 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 Eqs. (15):

$$a_{12} = \frac{W_1 + W_2 - W_4}{2} - \frac{W_3}{6}, \quad (16)$$

$$a_{13} = \frac{W_3}{3},$$

$$a_{14} = \frac{W_1 + W_4 - W_2}{2} - \frac{W_3}{6},$$

$$a_{24} = \frac{W_2 + W_4 - W_1}{2} - \frac{W_3}{6}.$$

We can guarantee positivity of terms, such as $(W_1 + W_2 - W_4)/2$, by using a procedure that we apply for the set of equations with three equations. Thus, we introduce one bounce process. After that we obtain expressions such as $a - W_3/6$ with positive a . If latter expression is negative, one can add process $a_{33} = W_3(1 - 1/\delta_2)$, and we can provide positivity of solution (16) by choosing δ_2 sufficiently large.

IV. TEST CALCULATIONS

The SSE algorithm is universal in any dimension. With increase in 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 the Heisenberg model, a mean number of bosons N_b for the Bose Hubbard model, and energy for both models. We use well-known estimators [9]

$$E = -\frac{\langle n \rangle}{\beta}, \quad (17)$$

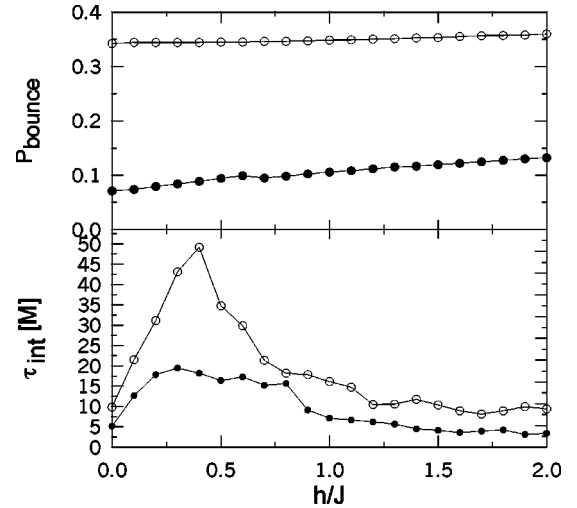


FIG. 2. Upper plot: bounce probabilities vs external field in the $S = 5/2$ antiferromagnetic Heisenberg model at $N_s = 16$ and $\beta = 10$. Coupling constant is $J = 1.0$. Dark circles correspond to the optimized algorithm and open circles correspond to the heat-bath algorithm. Lower plot: integrated autocorrelation times for the magnetization vs external field in the cases of optimized and heat-bath algorithms.

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

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

where n is the number of nonunit operators in operator string and N_s is the number of sites. We have checked our results with exact diagonalization and have found that the relative deviation of our results from the 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 is described in Ref. [3]

First of all it is interesting to analyze influence of bounce processes on efficiency of the algorithm. To this end we calculate for the Heisenberg antiferromagnet integrated autocorrelation times for magnetization by using heat-bath solution and optimized algorithm described in the preceding 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 than 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.

Figure 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 $\beta = 10$.

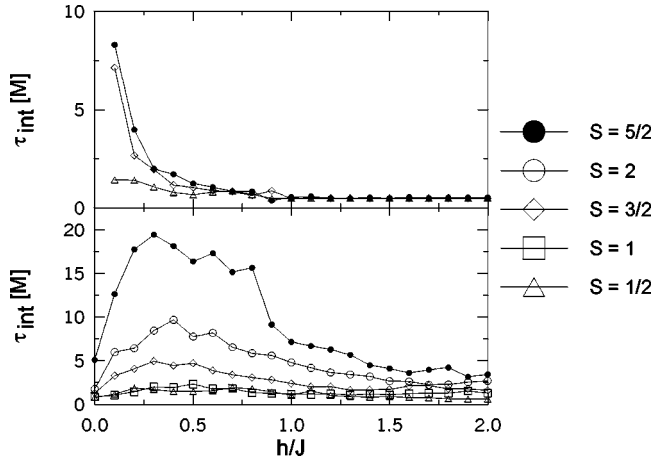


FIG. 3. Integrated autocorrelation times for the magnetization and energy vs external field in ferromagnetic (upper plot) and anti-ferromagnetic (lower plot) Heisenberg model with different spin S at $N_s = 16$ and $\beta = 10$. Coupling constant is $J = 1.0$.

One can see some increase of autocorrelation times with spin increase for the anti-ferromagnet chain. However, it is difficult to compare efficiency of the algorithm at fixed temperature and different spin. Mean number of nonunit 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 nonunit 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, the simulation of $S = 5/2$ Heisenberg anti-ferromagnet at $\beta = 10$ is as hard as the simulation of $S = 1/2$ Heisenberg anti-ferromagnet at $\beta \sim 100$. Hence, the origin of autocorrelation time increase is clear and, on the other hand, it is obvious that the algorithm is very efficient. It should be pointed out that the algorithm works efficiently in a wide range of external fields.

For the ferromagnet chain we obtain good autocorrelation times for magnetization in a 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 have done calculations for the Bose Hubbard model with interaction. As seen from Fig. 4 autocorrelation times for energy is of the order of unity. Autocorrelation times for mean number of bosons grow with increase maximum filling number N_{max} . Note that we can use any maximum filling number N_{max} , and for large class of problems the value $N_{\text{max}} \sim 5, \dots, 10$ is quite enough.

Investigation of many-body quantum system behavior near the critical points is one of the interesting problems 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

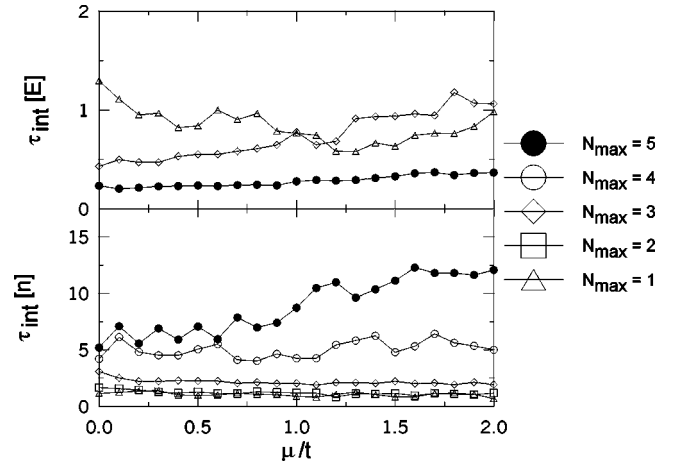


FIG. 4. Integrated autocorrelation times for the mean number of bosons and energy vs chemical potential in the Bose Hubbard model with different maximum site filling at $N_s = 16$ and $\beta = 10$. The hopping constant is $t = 1.0$, $U = 0.5$, $V = 0.5$.

bounce probabilities in the case of heat-bath algorithm are very large and exceed bounce probabilities in the case of optimized algorithm by the order of magnitude. Large bounce probabilities give rise to enormous loops, which walk around the system many times until closed. Construction of

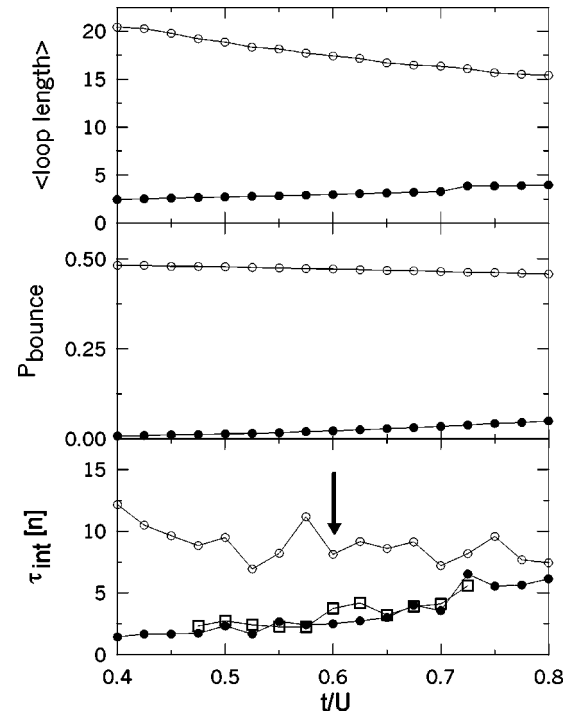


FIG. 5. Lower plot: integrated autocorrelation times for the mean number of bosons in the Bose Hubbard model at $N_s = 16$ and $\beta = 10$, $N_{\text{max}} = 5$. Hopping constant $t = 1.0$, $V = 0.0$, $\mu = U$. Dark circles correspond to the optimized algorithm, open circles correspond to the heat-bath algorithm, and 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.”

such big loops takes a lot of time and the simulation becomes inefficient. So we can conclude that the SSE algorithm allows us 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 us to explore the Heisenberg model with arbitrary spin and the 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 the stage of matrix elements calculation.

We propose a 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

groups with six processes maximum two bounces are needed. We have found that relations between number of various groups are different up to spin $S=5/2$ (maximum filling number $N_{max}=5$). After spin $S=5/2$ the relations do not change.

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

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