Monte Carlo approach to phase transitions in quantum systems

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Abstract. We propose algorithms of the path-integral-based quantum Monte Carlo simulation, which is otherwise prohibitively slow. While the basic idea is the loop-cluster update, there are some important “tricks” that are vital to make the simulation practical. In the present paper, we show two such techniques and their successful applications to the two-dimensional SU(N) Heisenberg model and the three-dimensional Bose Hubbard model. In the former, we obtain a new type of the valence-bond-solid state for the two-boson representation, while in the latter we equilibrate a system of which the size is comparable to a typical experiment of optical lattices.

1. Introduction
Quantum Monte Carlo simulation [1] is a robust tool for investigating novel phenomena in strongly correlated quantum systems, potential candidates for a quantum computer. Various quantum systems on lattices are investigated recently as candidates of quantum computers, such as squid arrays [2], trapped ions [3], optical lattices [4], and quantum dots [5]. In most of such systems, the basic degrees of freedom (q-bits) are some discrete quantum degrees of freedom defined on a discrete space (i.e., lattice). Therefore, in theoretical studies of the quantum computers, quantum lattice models, such as the transverse Ising model or the XXZ model, often appear as convenient play-grounds. Boson models are also of a considerable interest from the same view-point since the model system can be the Bose-Hubbard model in some cases such as bosonic atoms trapped in an optical lattice. In addition, these lattice quantum models are worth studying in their own right, since these models exhibits strange quantum phases and critical phenomena which may lead to discovery of novel and fundamental quantum phenomena.

In the present paper, we first review one of the most powerful numerical methods developed recently for quantum lattice models, namely, the world-line Monte Carlo method with directed-loop algorithm (DLA) [6]. This is a simple framework suitable for general use, ranging from quantum spin systems to soft-core boson systems. It is also the basis of the new methods discussed in the present paper. Then, we discuss two typical examples, the SU(N) Heisenberg model and the Bose-Hubbard model, and show that a straight-forward application of the DLA to these models does not necessarily yield a practical algorithm but the problem can be solved with some additional improvements.

The SU(N) Heisenberg model is the simplest generalization of the conventional SU(2) Heisenberg model to higher symmetry. For the ground state of this model, there is an interesting theoretical predictions [7] that the ground state is characterised by broken lattice-translational
and lattice-rotational symmetry and that the symmetry of the ground state depends periodically
on the number of bosons in the representation of the model. The broken-symmetry state are
generally called “valence-bond-solid (VBS)” states. In some quantum systems, including the
SU($N$) Heisenberg model, there is a phase transition between the VBS state and the Néel state
as some parameter ($N$ in the case of SU($N$) model) is changed. The nature of this phase
transition is one of the subjects of the most intense arguments in recent year, because if the
phase transition is of the second order, it does not fit in the conventional Landau-Fisher-Wilson
framework of critical phenomena. However, this is not the main subject of the present paper.

The Bose-Hubbard model is considered to be the model of the ultra-cold atom systems [8]
trapped in an optical lattice. [9] Many researchers in condensed-matter physics expect that this
system will eventually provide us with a variety of “real” strongly-correlated quantum systems
which otherwise are mere toys of theoreticians. The Bose-Hubbard model is the first example
system that is materialized in the optical lattice. Here, the central issue is to check various
theoretical predictions in a real system, such as the relationship between the superfluidity and
the condensation, the development of interference pattern in the static structure factor and its
temperature dependence, etc. [10] A Monte Carlo simulation for a uniform system has been done
to reveal that the periodic structure in the interference pattern does not precisely characterize
the onset of the superfluidity [11], while the larger scale simulation with non-uniform chemical
potential, which may be directly comparable with experiments, are still missing.

For both systems, the SU($N$) model and the BH model, a straight-forward application of the
directed-loop update algorithm becomes unpractical in several crucial conditions. In the case of
the SU($N$) Heisenberg model, as we go to larger $N$ and higher representations the number of
local states becomes too large to handle in the form of a simple array in the computer memory.
[12] In the case of the BH model, as we go to larger on-site repulsion $U$, the number of vertices,
which is proportional to $U$ and the squared upper-bound for the particle numbers, increases.
This slows the simulation significantly. [13, 14] In the present paper, we show methods
for solving these problems. A part of the application results has been published in [12] for the
SU($N$) model, and more details of the method together with some application results will be
published in [14].

2. Directed-Loop Update in Quantum Monte Carlo

The directed-loop update was proposed [6] as a method of updating the configuration in the
stochastic series expansion [15, 16]. Since the SSE formulation and the world-line Monte Carlo
simulation based on the path-integral are identical in some limit [1], the directed-loop update
can be regarded as a method of updating the world-line pattern in the path-integral Monte
Carlo simulation. Since the present algorithm is based on the world-line quantum Monte Carlo
simulation with the directed-loop update, we first give a brief review on this framework. For
more details, see [1].

Suppose we want to study static properties of a $d$-dimensional quantum system characterized
by the Hamiltonian $H$. The problem is reduced to computing expectation values of various
quantities $Q(\Sigma)$ with the weight $W(\Sigma)$. Here, $\Sigma(r, \tau)$ is the scalar field defined on a ($d + 1$)-
dimensional space-time, and $Q$ and $W$ are some functionals of $\Sigma$. In the present case, $\Sigma(r, \tau)$
is an integer field called world-line configuration with $r$ specifying a point on a discrete lattice
$\Lambda$ and $\tau \in [0, \beta)$ a continuous imaginary time. The weight $W$ is given by the Feynman path
integral

$$W(\Sigma) \equiv \exp \left( - \int_0^\beta d\tau L(\Sigma(\tau), \partial_\tau \Sigma(\tau)) \right). \quad (1)$$

A simulation with the world-line Monte Carlo method is a Markov process in the space of the
world-line configurations. The updating procedure defines the transition matrix of the Markov
process and is arranged so that the resulting transition matrix satisfies the detailed-balance condition. In the directed-loop algorithm, a Monte Carlo step (often referred to as a sweep) consists of two phases. In the first phase we place vertices that represents various terms in the Hamiltonian. Vertices are often depicted as equal-time (horizontal) lines connecting several spatial positions. For instance, a two-body interaction corresponds to a vertex connecting two spatial positions. In the second phase we modify the world-line configurations. These two phases corresponds to the graph-updating process and the configuration-updating process in a more general framework of loop-cluster algorithm [17]. The procedure of the second phase is achieved by repeating a worm-updating cycles a number of times. In the directed-loop algorithm, this is done by extending a phase space. We extend the phase space by introducing two special points, which we call the head and the tail of the worm at which the continuity condition of the world-line configuration is violated. A worm-updating cycle consists of three procedures: creating a worm, moving the head, and annihilating a worm. The head moves along the temporal axis and changes its direction when it hits a vertex. When a worm head hits a vertex it can also change its spatial position (to which the current position is connected by the vertex).

As a result, the Monte Carlo simulation is characterized by the following ingredients: (1) the vertex assignment density for the first phase, (2) the worm creation/annihilation probability for the second phase, and (3) the scattering probability of the head at vertices for the second phase. In general, one can study any lattice model with this prescription provided that it does not have the notorious negative sign problem. However, in practice, one often encounter problems in various specific applications. In what follows, we see what kind of problems may exist and how we can solve those.

3. SU($N$) Model and VBS States

We first consider the simple generalization of the conventional Heisenberg model, i.e., the SU($N$) Heisenberg model. The model Hamiltonian we discuss is defined as

$$H = \frac{J}{N} \sum_{(r,r')} \sum_{\alpha,\beta=1}^N S^{\alpha\beta}(r) \bar{S}^{\beta\alpha}(r')$$  (2)

where the operators $S^{\alpha\beta}$ and $\bar{S}^{\alpha\beta}$ are the generators of the SU($N$) algebra. Here we consider the simple square lattice with the periodic boundary condition. Similar to the case of the conventional SU(2) Heisenberg model, we need to specify the representation of the algebra we work with. Unlike the SU(2) case, however, since the conjugate representation is not identical to the original representation, we have two options in generalizing the SU(2) antiferromagnetic Heisenberg model to the SU($N$) symmetry. Namely, we can use two representations, conjugate to each other, for two sub-lattices, while we can also use the same representation for all spins. While both options are equally natural extension of the conventional antiferromagnetic Heisenberg model, we use the first option, i.e., the alternating representation. In Eq.(2), we have used the symbol, $\bar{S}$, for spins on one sub-lattice to remind ourselves of the fact that they belong to a different representation.

In this paper, we further specify the model by considering only the symmetric representations (for the sub-lattice A). This corresponds to the Young tableaux with a single row. Still we have a tunable parameter, i.e., the number of columns, which we refer to as $n$ in what follows. This number corresponds to $2S$ in the SU(2) case. Accordingly, the representation on the sub-lattice B is characterized by the $N - 1$ rows and $n$ columns.

Based on the $1/N$ expansion treatment, Read and Sachdev [7] predicted that the model with sufficiently large $N$ has a valence-bond-solid (VBS) ground state with spontaneously-broken lattice symmetry. The nature of the ground states may depend on the representation, somewhat analogous to what is known as Haldane’s conjecture in the SU(2) models in one dimension. More
specifically, it was suggested [18, 7] that, for the model with the Young tableaux with m rows and n columns, the $N$-$n$ phase diagram does not strongly depend on $m$, and has a line of phase transition separating the small-$N$ Neél region from the large-$N$ VBS region. It was also argued that the nature of the VBS ground state can be classified according to the quotient of the division of $n$ by 4. If $n \equiv 1$ or 3 (mod 4), the ground state has a columnar ordering with both the translational symmetry and the 90-degree rotational symmetry both broken, whereas if $n \equiv 2$ (mod 4) it has a “nematic” VBS ordering with only the lattice-rotational symmetry broken. Finally, if $n$ is a multiple of 4, there is no spontaneous breaking of the lattice symmetry.

A direct check of the spontaneous breaking-down of the translational symmetry for $m \equiv n \equiv 1$ was carried out in the previous paper [19], which yielded the transition value of $N$, namely $4 < N^*(m = n = 1) < 5$.

When we try to apply the above-mentioned framework of the directed-loop algorithm to this system, we immediately encounter the difficulty arising from very large number of local states of a vertex. In order to study systematically the $N$ and $n$ dependence of the ground state we need to generate tables of the scattering probabilities with which the head of the worm scatters at each vertex. The size of this table is proportional to $N^4$, where $N_s$ is the number of local state on a site. It is related to $N$ and $n$ by $N_s \propto N^m$, which makes the table size proportional to $N^{4n}$. Since the VBS state appears in the region $N > 5n$, in order to study, for example, the first uniform VBS state, which is expected around $n = 4$ and $N \sim 20$, the table size will be $20^{16}$, which is well beyond the capacity of the computer memory. We could reduce this number by making use of the fact that for a given initial state the number of possible final states is much smaller than $N^{2n}$. This may reduce the table size down to $\propto N^{2n}$, which is $20^{8}$ in the previous example. However, this may be still too large. Of course, instead of storing the whole table in the memory, we could compute the probability every time the head hits the vertex. However, if this is done in an arbitrary way, it slows down the simulation considerably.

Now we consider how we can handle this problem in a systematic and economical way. The solution is based on splitting an original SU($N$) spin into $n$ “smaller” spins each corresponding to the fundamental representation. Once the splitting is done, the remaining task is simply applying the algorithm (for the fundamental representation) to each pair of smaller spins in which no large table of scattering probability is involved. In the familiar SU(2) case, we split a large spin of the magnitude $S$ into $2S$ Pauli spins, which was originally proposed in [20]. In the present case, formally we replace the original SU($N$) spin operator with the $n$-boson representation by the sum of operators corresponding to the fundamental (i.e., the single-boson) representation.

$$S^{\alpha\beta}(r) \Rightarrow \tilde{S}^{\alpha\beta}(r) \equiv \sum_{\mu=1}^{n} \sigma^{\alpha\beta}_{\mu}(r).$$

(3)

with $\sigma^{\alpha\beta}_{\mu}(r)$ being an SU($N$) spin in the fundamental representation. Accordingly, the phase space summation should be replace by

$$\text{Tr}_{n}(f\{S^{\alpha\beta}(r)\}) = \text{Tr}_{\sigma}(Pf\{\tilde{S}^{\alpha\beta}(r)\}).$$

(4)

Here $P \equiv \prod_{r}P(r)$ where $P(r)$ is the symmetrizer of $n$ particles on the site $r$.

Let us assume that a site $r'$ belongs to the sub-lattice B for which the conjugate representation is used. Note that there is a one-to-one correspondence between states in one representation and those in the conjugate representation. In the case of the conjugate to the fundamental representation, for example, if we define

$$|\tilde{\alpha}\rangle_{r'} \equiv |1, 2, \ldots, \alpha - 1, \alpha + 1, \ldots, N\rangle_{r'},$$

(5)
the singlet state can be formed between two sites \( r \) and \( r' \) by

\[
|\text{singlet}\rangle = \sum_{\alpha=1}^{N} |\alpha\rangle_r \otimes |\bar{\alpha}\rangle_{r'}
\]  

(6)

provided that the states \(|\bar{\alpha}\rangle_{r'}\) are defined with appropriate signs. By using \(|\bar{\alpha}\rangle_{r'}\) as the basis vector for the sub-lattice B, the operator \( \sigma^{\alpha\beta}_{\mu}(r') \) can be expressed as the same matrix that represents \(-\sigma^{\beta\alpha}_{\mu}(r)\) on sub-lattice A. Therefore, we can rewrite the pair Hamiltonian in the following way.

\[
\mathcal{H}_{rr'} = -\frac{J}{N} \sum_{\mu,\nu=1}^{n} \sum_{\alpha,\beta=1}^{N} \sigma^{\beta\alpha}_{\mu}(r) \sigma^{\alpha\beta}_{\nu}(r').
\]  

(7)

This form of the Hamiltonian immediately suggests a loop algorithm to be used. Namely, we should assign a graph (i.e., a vertex) which may be represented by two horizontal lines (figure 1(a)). In the directed loop framework, this vertex means that when a worm head arrives at one of the four legs of a vertex, it should hop, with probability 1, to the neighboring site and change the direction of the motion. (Because of this deterministic nature of the vertex, the resulting directed-loop algorithm is almost identical with the loop algorithm.) The density of the vertices is \( J/N \) for a given pair of \( \sigma \)-spins if the local states on both ends are identical. Otherwise, the density is 0. With this density, we assign the vertices to all the \( n^2 \) pairs of \( \sigma \)-spins. As in the SU(2) case, the symmetrization operator can be taken into account by random reconnection of the ends of the \( n \) lines at \( \tau = \beta \) to those at \( \tau = 0 \). [20]

In figure 1(b), loops of a system with only 4 spins are illustrated as an example. Along a loop, the local state is the same on any point, and it is one of the \( N \) values. Different loops can have different values.

Figure 1. The split-spin algorithm for the SU(N) Heisenberg model in the case of two-boson representation. The elementary graph (a) and an example loop pattern in a 4-spin system (b).

In an actual simulation, we do not directly work with each individual \( \sigma \) spins. The actual computer program is written based on the “occupation number”, i.e., the number of bosons that has a specified color,

\[
n_{\alpha}(r) \equiv \sum_{\mu=1}^{n} \sigma_{\mu}(r)
\]  

(8)

where \( \sigma_{\mu}(r) = 1, 2, \cdots, N \) is the local state (color) of the \( \mu \)-th boson. Shifting to this “second-quantized” picture can be done by the “coarse-graining” introduced in [21].
As a demonstration of the new algorithm, we here present results of simulation of the SU(15) Heisenberg model with the two-boson representation up to \( L = 32 \). According to the theoretical predictions [7], the ground state of the two-boson representation model should be the nematic VBS state at sufficiently large value of \( N \). This is the state where the translational symmetry is preserved while the 90-rotational symmetry is broken. In other words, the correlation between two nearest-neighbor spins is uniform but direction dependent. In our previous paper [19], we presented some results on the higher representations as well as the results on the fundamental representation. However, no clear evidence was found for the spontaneous rotational symmetry breaking in the case of two- and three-boson representations even if \( N \) is larger than the critical value, in contrast to the theoretical prediction.

In the present paper, we carry out further parameter search and obtain an evidence of the rotational symmetry breaking. We define the following local quantity.

\[
A(r) \equiv B_x(r) - B_y(r) \tag{9}
\]

where

\[
B_\mu(r) \equiv \frac{1}{n^2} \sum_{\alpha=1}^{N} n_\alpha(r) n_\alpha(r + e_\mu). \tag{10}
\]

When integrated over all the lattice points, \( A(r) \) clearly yields the order parameter characterizing the spontaneous rotational symmetry breaking. Instead of measuring the integrated quantity, however, we here compute the two-point correlation with respect to this local quantity at the distance \( L/2 \) where \( L \) is the system size, \( \langle A(0,0)A(L/2,0) \rangle \). If there is a finite long-range ordering, the correlation must converge to a finite value as \( L \) increases, whereas it should decrease exponentially when there is no long-range ordering.

In figure 2, we plot the correlation as a function of the system size in log-log scale. The horizontal axis is slightly shifted according to the simulation length, so that the convergence as a function of the simulation length becomes more evident. (The rightmost one in each cluster of symbols represents the longest simulation.) In the initial equilibration stage of the simulation, we intentionally make the coupling constant asymmetric, so that the system is forced to have a finite asymmetry. The effect of the initial stage decays quickly when the system size is small, resulting in a flat shape of the symbol cluster. (See the top-left clusters for example.) On the other hand, for larger systems, the effect is visible resulting in clear trend of decreasing. (See the right-most clusters.) At the highest temperature \( \beta J/N = 1 \), the simulation has reached the equilibrium for all system sizes, and the correlation decays exponentially as a function of \( L \). At the lowest temperature \( \beta J/N = 4 \), on the other hand, it is not clear whether the system has reached the equilibrium for \( L = 16 \) and 32 (the two symbol clusters on the right). However, even in these cases, we see a clear trend of upward curving, showing that the simulation is close to the convergence (i.e., equilibrium). When we focus on the \( L \) dependence of the right-most symbol in each cluster, the trend is very clear that at sufficiently low-temperature, the two-point correlation function does not exponentially decay (as a function of \( L \)). Rather, it is likely to converge to a finite value.

4. Bose Hubbard Model

The second example of recent progress in the quantum Monte Carlo method we see in the present paper is the Bose Hubbard model. The Bose-Hubbard model is considered to be the model of the ultra-cold atom systems [8] trapped in an optical lattice. Recently the Mott-superfluidity phase transition was observed in an optical lattice system [9]. Since the real system is “small” unlike most conventional solid-state-physics experiments, direct comparison between experiments and numerical simulation is possible. The system size in a well-known experiment by Greiner et al.
Figure 2. The two-point correlation function of A, the rotation-symmetry-breaking order-parameter, of the SU(15) Heisenberg model as a function of the system size. In order to show the dependence on the length of the simulation, we plot 6 sets of results corresponding to 6 different lengths of the Monte Carlo sequence. For the sake of clarity, symbols are slightly shifted horizontally according to the simulation length. (Each symbol corresponds to a simulation 4 times longer than the one represented by its next left neighbor.)

[22] was $L = 64$. In the present paper we present some result of a simulation of the same systems size together with the technique that makes the simulation of such large systems possible.

In the present paper, we consider the following Bose Hubbard model in a non-uniform chemical potential.

$$\mathcal{H} = -\frac{t}{2} \sum_{(RR')} (b_R^\dagger b_{R'} + \text{h.c.}) + \frac{U}{2} \sum_R n_R (n_R - 1) - \sum_R \mu_R n_R$$

(11)

The non-uniform chemical potential $\mu_R$ represents the trapping potential which is usually approximated by a parabolic form $\mu_R = \mu_0 - \Omega r^2$.

In the directed loop algorithm, the number of local states must be finite. Therefore, when we apply the algorithm to the BH model, we have to truncate the number of the particles on a single lattice point. If this artificial upper bound is not touched (so frequently) in the actual simulation, the error due to the truncation can be neglected. Therefore, in order to reduce the systematic error due to this truncation, we might want to make the maximum number as large as possible. However, this may make the number of vertices very large because the vertex density increases as a function of the artificial upper bound [13, 14]. To be more specific, the number of vertices is proportional to $U$ and the squared upper-bound. Existence of too many vertices slows down the simulation significantly. In the previous paper [13], we presented a method for solving this problem. However, the increase of the computational time is not the only problem that arises in the Boson simulation. Another problem may arise from the memory requirement when the worm passes straight through most of the two-site vertices. In the present paper, we discuss a method for solving this problem and demonstrate the efficiency of the resulting algorithm by
performing a large scale simulation whose size is the same as the above-mentioned experiment [22].

The essential idea is to skip all the stochastic events that actually do not change the direction or the spatial position of the worm head. In the first modification [13], we only skipped the straight-passings at one-site vertices. In the present paper, we propose a procedure in which straight-passings of all types of vertices are skipped. As a result, we no longer carry out the first phase, i.e., the phase of placing the vertices, separately. The vertices are created only when the worm head changes the direction and/or the position and, as a result, a kink is generated there. In this regard, the resulting algorithm is very close to the worm algorithm [23], in which there is no notion of vertices. However, the present algorithm may be simpler in that we consider only scattering processes of the worm head whereas in the worm algorithm several different types of procedures, such as jumps/anti-jumps and reconnections must be executed in addition to somewhat complicated processes of choosing the next position of the worm head according to the “mean-field” that the head feels [23].

Figure 3. The head’s motion in the improved directed-loop algorithm for the Bose-Hubbard model. The open triangle indicates the position and the direction of the worm head just after the previous step, whereas the filled triangle represents the worm head at the end of the current step. The short right-pointing arrow indicates the position of the stochastically generated first scattering time $\tau_{\text{first}}$. The local states are indicated by the thickness of the vertical lines. The dashed vertical line represents the part that will be changed by the current step. The dashed horizontal ones are vertices. Three cases are illustrated: (a) the first scattering time $\tau_{\text{first}}$ is outside of the current constant-environment interval, $I$, and there is no change in the state on the current site at the end of $I$, (b) $\tau_{\text{first}}$ is beyond the boundary of $I$, and there is a change in the state at the end of $I$, (c) $\tau_{\text{first}}$ is within $I$.

The actual prescription of avoiding all the straight-passing processes is simple. It is analogous to the decay of a radio active atom. When the decay rate is $\lambda$, the probability of having a decay event in an infinitesimal time interval $\Delta \tau$ is $\lambda \Delta \tau$ provided that the event has not taken place at any earlier time. We can simulate this decaying process by discretizing the time. Namely, starting from the first time window, we stochastically decide whether the atom decays or not for each time window, and when the decay event finally takes place at some time window we stop there. An alternative procedure which is statistically equivalent to the former is that we first stochastically generate the first decay time, wait until this time, let the atom decay, and stop there. Although statistically equivalent, in the first procedure, the number of operation is proportional to the skipped time-windows whereas the number of operations is $O(1)$ in the latter procedure.
If we apply this analogy to the process of a worm head passing a number of two-site vertices, we obtain the following prescription. Consider a head traveling along a vertical line and an “constant-environment” interval $I$ is ahead of the worm. In this imaginary-time interval, there is no change in the environment, namely, there is no change in the local state at any of the site that interacts with the current site. In other words, the constant-environment interval is an interval in which the molecular field felt by the worm’s head is constant. Because of this definition of the interval, the vertex density is uniform in this interval. Here we have to consider all types of vertices, i.e., all the interaction terms in the Hamiltonian that involves the current site. We here use the index $i$ to specify the type of the vertex. For example, if the Hamiltonian consists of two-body interaction terms only, $i$ specifies the nearest neighbor site to which the head is to be scattered. We let $\rho_i$ denote the vertex density of the type $i$ in the current interval $I$. The probability of having a scattering event in the imaginary time interval $\Delta\tau$ is

$$\Delta\tau\lambda = \Delta\tau \times \sum_i \rho_i p_i^{(\text{scatter})}$$

where $p_i^{(\text{scatter})}$ is the probability of the head being scattered provided that it encounters a vertex of type $i$. Then we can generate the first scattering time $\tau_{\text{first}}$ according to the distribution

$$P(\tau_{\text{first}}) \propto e^{-\lambda \tau}.$$  

(13)

This can be achieved by generating a uniform random number $r \in [0,1)$ and define

$$\tau_{\text{first}} = \lambda^{-1} \log \frac{1}{r}.$$  

(14)

If this turns out to fall out of the constant-environment interval $I$ we simply let the head proceed to the end of the interval. In case the head hits a kink as a result, let it be scattered at the kink in the same way as the conventional directed-loop update (figure 3(b)). If there is no kink there, we do nothing other than moving the head to the end of $I$ (figure 3(a)).

On the other hand, if $\tau_{\text{first}}$ falls within $I$, we let the head advance by $\tau_{\text{first}}$ and is scattered there. We now need to choose the type $i$ of the vertex that actually scatters the head. This should be done with the probability,

$$P_i \propto \rho_i p_i^{(\text{scatter})}.$$  

(15)

Once the type of the vertex $i$ is chosen, we place a vertex of this type at the head’s position and let the head be scattered by this vertex. The scattering procedure at the vertex is the same as that of the conventional directed-loop update, except that “passing through” event is not allowed.

Then, in all cases, we start again from the beginning with the new constant-environment interval $I'$ ahead of the head’s new position.

In order to demonstrate that the present method makes it possible to simulate a system of which the size is comparable to the real experiment, we perform a Monte Carlo simulation with the parameters which are close to the ones used in the experiment [22]. Figure 4 presents (a) the phase diagram of the BH model in three dimensions, and (b) the density profile at $U = 20t$, $\mu_0 = 60t$, $\Omega = 0.08t$, $\beta t = 5.0$ and $n_{\text{max}} = 15$. The system size is $L = 64$. With these parameters, the average number of bosons is $1.8 \times 10^5$. Both the system size and the number of particles are close to the experimental values [22].

The phase diagram clearly exhibits so-called “Mott-lobe” structure, and is consistent with theoretical prediction by Fisher et al.[24]. No clear system-size dependence can be seen in the
scale of the figure. The phase boundary is obtained through the calculation of the particle and hole gaps inside the Mott region. In the density profile, the characteristic shape, which is often referred to as "big wedding cake" structure, is clearly observed. Terraces correspond to Mott phases with different occupation number, while slopes superfluid regions inbetween. The equilibration has been confirmed by performing the simulation with various simulation lengths and checking the absence of systematic dependence on the length of the simulation.

Figure 4. (a) The phase diagram of the uniform Bose-Hubbard model, and (b) the 'big-wedding-cake' structure in the particle density profile. The parameters used here are $U = 20t$, $\mu_0 = 66t$, $\Omega = 0.08t$, $\beta t = 5.0$, $n_{\text{max}} = 15$. The phase boundary is estimated based on the Mott gap [25].

5. Summary
In the present paper, we have reviewed the directed loop algorithm, one of the standard method that provides a robust and general framework for the quantum Monte Carlo simulation of a very broad variety of quantum systems. Based upon this framework, we develop two algorithms for quantum spin and boson models. While in both cases a straight-forward application of the conventional directed loop algorithm is not practical, we have demonstrated that there are solutions to the problems that greatly enhances the efficiency of the method. We have also presented some new physical results in order to illustrate the efficiency of the resulting algorithms. In the case of the SU(N) model, in particular, we have presented the result that suggests the spontaneous breaking of the lattice rotational symmetry at $N = 15$ for the two-boson representation model.

Acknowledgments
The computation in the present work is executed on computers at the Supercomputer Center, Institute for Solid State Physics, University of Tokyo. The present work is financially supported by MEXT Grant-in-Aid for Scientific Research (B) (19340109), MEXT Grant-in-Aid for Scientific Research on Priority Areas “Novel States of Matter Induced by Frustration” (19052004), and by Next Generation Supercomputing Project, Nanoscience Program, MEXT, Japan.
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