A quantum Monte Carlo algorithm realizing an intrinsic relaxation

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We propose a new quantum Monte Carlo algorithm which realizes a relaxation intrinsic to the original quantum system. The Monte Carlo dynamics satisfies the dynamic scaling relation $\tau \sim \xi^z$ and is independent of the Trotter number. Finiteness of the Trotter number just appears as the finite-size effect. An infinite Trotter number version of the algorithm is also formulated, which enables us to observe a true relaxation of the original system. The strategy of the algorithm is a compromise between the conventional worldline local flip and the modern cluster loop flip. It is a local flip in the real-space direction and is a cluster flip in the Trotter direction. The new algorithm is tested by the transverse-field Ising model in two dimensions. An accurate phase diagram is obtained.

KEYWORDS: quantum Monte Carlo method, nonequilibrium relaxation method, quantum dynamics, transverse-field Ising model

The Monte Carlo method is a powerful tool to investigate the condensed matter physics. The method directly benefits from a progress of microprocessors. It is also suitable for the parallel computing. Developments of various Monte Carlo algorithms consist of an important part of the statistical physics in these decades.\(^1\)

The quantum version is called a quantum Monte Carlo (QMC) method.\(^2\) A $d$-dimensional quantum system is decomposed into a $(d+1)$-dimensional classical system, where the actual simulations are performed. The additional dimension is called the Trotter direction and its length is denoted by the Trotter number $m$. The original quantum system is recovered in the limit of the infinite Trotter number.

The first update algorithm in QMC is the worldline local flip. A worldline, which is an outcome of the local spin conservation, is moved locally in the $(d+1)$-dimensional lattice. An acceptance ratio of this flip becomes worse and the Monte Carlo dynamics freezes as the Trotter number increases to approach the original quantum system. This is purely a technical problem not from a physical origin as the critical slowing down. Recently, the loop flip algorithm in QMC\(^3\)\(^-\)\(^6\) is developed in order to solve this problem. It is also possible to take the infinite Trotter number limit beforehand.\(^6\) A nonlocal loop is defined in the $(d+1)$-dimensional lattice for the update. All spins on the loop
are simultaneously flipped. This loop corresponds to the correlated spins in this \((d+1)\)-dimensional lattice. Therefore, the algorithm drastically reduces the correlation time.

The loop algorithms, or generally cluster algorithms, are a trend of recent developments in Monte Carlo methods. It accelerates the Monte Carlo simulations suffering from the slow dynamics. Another trend is the nonequilibrium relaxation (NER) method\(^7\). The NER method positively makes use of the critical slowing down to detect the phase transition. One observes a relaxation function of a physical quantity at each temperature. If it exhibits an algebraically slow relaxation, the temperature is judged to be a critical point. The method works very well in the slow-dynamic systems\(^10\). A Monte Carlo investigation on the relaxation process is a good approach to the critical phenomena.

An updating algorithm in the NER simulation must realize an intrinsic relaxation of the system. For example, an algebraic relaxation should be observed at the critical point. A relaxation in the paramagnetic phase should be exponential with a finite correlation time corresponding to a finite correlation length. The requirement is guaranteed by updating degrees of freedom with the same length at each time step. One realization is a single spin flip algorithm in the classical spin systems.

In regard to the QMC method, however, an algorithm which realizes a relaxation intrinsic to the original quantum system has not been invented yet. A relaxation function by the loop algorithm has nothing to do with the physics. The NER analysis is possible by using the worldline local flip.\(^13\) A ratio between the inverse temperature \(J/T\) and the Trotter number \(m\) is fixed finite. The simulation exhibits a relaxation of the \((d+1)\)-dimensional classical system. It suffers from the freezing as the Trotter number increases.

Aim of this Letter is to propose a new QMC algorithm realizing the relaxation intrinsic to the original quantum system. A shortcoming of the worldline local flip algorithm is a mixture of a physical relaxation and an unphysical relaxation causing the freezing. The new algorithm extracts only a physical relaxation part. The unphysical one is eliminated by using an idea of the loop algorithm. The infinite Trotter number version is also formulated.

A basic idea of the present algorithm is to make an update local in the real-space direction and global in the Trotter direction. The former one is to ensure the Monte Carlo dynamics reflecting the physics of the original quantum system. We typically choose one real-space interaction bond or one real-space spin as a local unit of the updating. One Monte Carlo step corresponds to a time unit in which a change of this real-space length occurs. The latter idea is realized by a cluster flip extending only in the Trotter direction. Each updating unit is connected along the Trotter direction in a same manner as the Swendsen-Wang algorithm\(^14\) in one dimension. A cluster of the connected updating units is flipped simultaneously. A length of the cluster corresponds to the correlation in the Trotter direction. Therefore, the freezing due to the Suzuki-Trotter decomposition is solely eliminated. The present update algorithm can be considered as a single quantum-spin flip.
We consider an $S = 1/2$ Heisenberg chain for a simple explanation of the algorithm.

$$\mathcal{H} = \sum_i J S_i \cdot S_{i+1}$$  \hspace{1cm} (1)$$

The system is decomposed into a checkerboard plane as shown in Fig. 1(a). An updating unit is four spins consisting of a blank plaquette as depicted in Fig. 1(b). If a worldline runs vertically in the left (right) side of the plaquette, a pseudo-spin pointing to the right (left) is assigned. If there is no vertical worldline or there are two worldlines in both sides, no pseudo-spin is assigned. A pseudo-spin represents a possible worldline move. It changes the direction, if the spin flip is accepted. The worldline local flip is regarded as a single spin flip of this pseudo-spin.

An actual procedure of the updating is as follows. We choose one real-space bond to try an update (the double-line bond connecting two solid spins in Fig. 1(a)). Pseudo-spins in regard with these two real-space spins are updated. (Bold arrows in the figure.) A Boltzmann weight $W$
participating in this update is written as a product of two parts.

\[ W = W_p \times A. \] (2)

One consists of weights of plaquettes on the updating bond (\( \boxtimes \)) as denoted by \( W_p \). These plaquettes can be considered as effective bonds connecting pseudo-spins on the updating bond. They are used to define a cluster of pseudo-spins. The other part consists of weights of plaquettes on the neighboring bonds (\( \boxcirc \)) as denoted by \( A \). The weights determine a probability to accept the cluster flip.

If two pseudo-spins neighboring along the Trotter direction point to the same direction, they are connected to form a cluster with a probability \( 1 - p \) of

\[ p \equiv \frac{\boxtimes}{\boxcirc} = \tanh(\frac{J}{mT}) \sim \frac{J}{mT}. \] (3)

Pseudo-spins in a cluster are flipped simultaneously with a probability calculated from the weights of plaquettes on the neighboring bonds \( A \). A product of the weights of plaquettes adjacent to each pseudo-spin in the cluster is calculated before (\( A_{\text{initial}} \)) and after (\( A_{\text{final}} \)) the flip. We accept the flip with a probability

\[ \frac{A_{\text{final}}}{A_{\text{initial}} + A_{\text{final}}} \] (4)

We try this flip for each cluster independently. A new worldline configuration is obtained by new pseudo-spin configurations.

The ergodicity of this update algorithm is same as the worldline local flip. The worldline global flip is necessary to change the magnetization. The present algorithm is an adoption of the Swendsen-Wang algorithm under the external field. Here, a molecular field from the neighboring real-space spins is regarded as the external field. Therefore, the detailed balance is also satisfied as is guaranteed in the Swendsen-Wang algorithm. An important notice is that the acceptance of a flip does not depend on the Trotter number nor the temperature. An average size of the cluster is about \( 1/p \sim \frac{mT}{J} \). Then, the contribution from the neighboring interaction bonds \( A \) is an order of \( \exp \left[ \frac{\frac{4}{mT} \times \frac{1}{p}}{} \right] \sim O(1) \). The freezing due to the decomposition is solely eliminated by this relation. A cluster analysis is easy because it is performed only in one dimension. It enables us to write a fast program without difficulties for various systems. An actual computational time of one Monte Carlo step is almost same as that of the conventional local flip one.

It is possible to take the infinite Trotter number limit beforehand. In this scheme we introduce a 'breakup', which is a domain wall of the pseudo-spins, i.e., where a worldline hops.\(^3\)\(^-\)\(^5\) A location of a breakup is stored in memory to define a state. A probability of a breakup to exist is \( p \sim \frac{J}{mT} \). An average number of the breakups is \( \frac{J}{T} \) in the infinite \( m \) limit. Therefore, among the pseudo-spins on a selected updating bond we put breakups by Poisson random numbers with the expectation number \( \frac{J}{T} \). The pseudo-spins between the neighboring breakups are flipped by using the probability of
Eq. (4). Here, we do not discriminate between the newly-assigned breakups and the already-existing breakups.

An updating procedure for the transverse-field Ising model is almost same as for the Heisenberg model. Only a difference is that there is no local spin conservation in this model. An updating unit, which is a plaquette in the Heisenberg model, shrinks to a single spin. Therefore, the single-spin flip is possible in the \((d + 1)\)-dimensional lattice. The Hamiltonian is

\[
\mathcal{H} = \sum_{\langle i,j \rangle} J S_i^z S_j^z - \sum_i \Gamma S_i^x.
\]

(5)

The Suzuki-Trotter decomposition is shown in Fig. 1(c). A Boltzmann weight is assigned to each interaction bond. First, we choose one real-space spin to try an update. Spins along a line in the Trotter direction will be updated. (Solid circles in Fig. 1(c).) A cluster is defined by connecting two spins neighboring in the Trotter direction with a probability \(1 - p\) of

\[
p = \tanh(\Gamma/mT) \sim \Gamma/mT,
\]

(6)

if they take same spin value. The clusters are shown by rectangles in Fig. 1(c). They are flipped with a probability of Eq. (4). The weights \(A_{\text{initial}}\) and \(A_{\text{final}}\) are calculated by molecular fields from the spins neighboring in the real-space direction to the cluster. The infinite Trotter number version in this model is also trivial. We put breakups with the expectation number \(\Gamma/T\) along a line in the Trotter direction of the updated spin. A cluster between two breakups is flipped by Eq. (4).

As a demonstration of the new algorithm we consider the transverse-field Ising model in two dimensions. The classical phase transition occurs at a temperature which varies with \(\Gamma/J\). The quantum phase transition occurs at \(T = 0\) for a finite \(\Gamma/J\) value.

Figure 2 shows NER plots of the magnetization \(M\) at \(T/J = 0.1\) and \(\Gamma/J = 3.05\). This point is in the vicinity of the transition point. The relaxation functions depend on the Trotter number in the conventional algorithm as shown in Fig. 2(a). As the Trotter number increases, it becomes later for the algebraic relaxation to begin. On the other hand, the relaxation functions by the new algorithm essentially do not depend on the Trotter numbers as shown in Fig. 2(b). The relaxation function of the infinite Trotter number is depicted by a line. The figure clearly shows that the Trotter number dependence only appears as the finite-size effect. Before it appears, the relaxation coincides with that of the infinite Trotter number. The relaxation of the original quantum system is considered to be realized. The equilibrium data of small Trotter numbers are consistent between two algorithms. The logarithmic slope of the relaxation \(-\beta/z\nu\) also coincides with each other. Therefore, we can conclude that two algorithms are observing the same critical phenomenon. A computational time for one Monte Carlo step is almost same between two algorithms. The total necessary computation time to achieve the same resolution is reduced to 1/10.
Fig. 2. NER plots of the magnetization of 2D transverse-field Ising model near the critical point. $\Gamma/J = 3.05, T/J = 0.1$. The real-space system size is $400 \times 400$. (a) By the conventional local flip algorithm. (b) By the new flip algorithm proposed in this Letter. Data of the infinite Trotter number version ($m = \infty$) is depicted by a line.

Figure 3 shows a phase diagram obtained by the NER analysis of the magnetization using the infinite Trotter number version of the present algorithm. The smallest value of $\Gamma$ at which the relaxation exhibits the exponential decay is the lower bound of the paramagnetic phase. The largest value of $\Gamma$ at which the relaxation converges to a finite value is the upper bound of the ferromagnetic phase. The phase boundary line is in between. The lowest temperature we have carried out the simulation is $T/J = 0.01$. Within the system size ($149 \times 150$) and the time range (1000 steps) of the simulation at this temperature there is no temperature effect and the data can be considered as those of the ground state. Our estimate of the quantum transition point is $\Gamma_c = 3.044(2)$. In the classical limit ($\Gamma/J = 0$) the phase transition of the 2D classical Ising
model occurs at $T/J = 2.269$. We have also verified this temperature and the critical exponents by using the same program. The phase diagram is obtained very accurately compared with previous investigations.\textsuperscript{15} The shape of the phase diagram qualitatively agrees with the experimental result of LiHoF$_4$,\textsuperscript{16} which is considered to realize the transverse-field Ising model in three dimensions.

![Phase Diagram](image)

Fig. 3. A phase diagram of 2D transverse-field Ising model obtained by the NER using the infinite Trotter number algorithm. The real-space system size is $199 \times 200$ ($T/J \geq 0.1$) and $149 \times 150$ ($T/J = 0.01$). The time range is 1000 steps.

Figure 4 shows an NER plot on the phase boundary line when changing the temperature. The logarithmic slopes $-\beta/z\nu$ converge to the same value in the long time limit at high temperatures. It indicates that they belong to the same universality class. The slope is consistent with a choice of $\beta = 1/8$, $\nu = 1$, and $z = 2.16$, which is the exponents of the 2D classical Ising model. As the temperature decreases, it takes a longer time to observe the 2D classical Ising behavior. In the low temperature limit ($T/J = 0.01$) the relaxation exhibits the universality of the 3D classical Ising model, which is equivalent to the quantum phase transition of the present model. The slope is consistent with the exponents $\beta = 0.325$, $\nu = 0.635$, and $z = 2.05$.\textsuperscript{17} We observe in this figure a systematic crossover from the 2D Ising to the 3D Ising universality. A relaxation function traces the trail of the ground-state ($T/J = 0.01$) until the temperature effect appears. Then, it changes the behavior to the 2D classical Ising universality.

In summary, a quantum Monte Carlo algorithm realizing the relaxation intrinsic to the original quantum system is formulated. Analyses on the relaxation of a quantum system are done without an ambiguity of the Suzuki-Trotter decomposition. This is made possible by updating single-
quantum-spin degrees of freedom as the updating unit. Since a length scale updated in one Monte Carlo step is definite, the algebraic relaxation is expected to be realized in the critical phase. It is an open question whether or not the dynamics of this algorithm explains a time evolution of a quantum system which strongly couples with the heat reservoir. It is expected that the use of the present algorithm helps a progress of the field. We remark here that the negative-sign problem is not solved by this algorithm. Therefore, applications to the various transverse-field Ising models and to the non-frustrated Heisenberg/XY models are fruitful.

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1) The Monte Carlo Method in Condensed Matter Physics, edited by K. Binder (Springer-Verlag, Berlin, 1995).
2) Quantum Monte Carlo methods in Condensed Matter Physics, edited by M. Suzuki (World Scientific, Singapore, 1994).
3) H. G. Evertz, G. Lana and M. Marcu: Phys. Rev. Lett. 70 (1993) 875.
4) U. -J. Wiese and H. -P. Ying: Z. Phys. B 93 (1994) 147.
5) H. G. Evertz: cond-mat/9707221.
6) B. B. Beard and U. -J. Wiese: Phys. Rev. Lett. 77 (1996) 5130.
7) D. Stauffer: Physica A 186 (1992) 197.
8) N. Ito: Physica A 196 (1993) 591.
9) N. Ito and Y. Ozeki: Int. J. Mod. Phys. 10 (1999) 1495.
10) T. Shirahata and T. Nakamura: Phys. Rev. B 65 (2002) 024402.
11) T. Nakamura and S. Endoh: J. Phys. Soc. Jpn. 71 (2002) 2113.
12) T. Nakamura: J. Phys. Soc. Jpn. 72 (2003) 789.
13) Y. Nonomura: J. Phys. Soc. Jpn. 67 (1998) 5.
14) R. H. Swendsen and J.-S. Wang: Phys. Rev. Lett. 58 (1987) 86.
15) For example, T. Ikegami, S. Miyashita and H. Rieger: J. Phys. Soc. Jpn. 67 (1998) 2671.
16) D. Bitko, T. F. Rosenbaum and G. Aeppli: Phys. Rev. Lett. 77 (1996) 940.
17) N. Ito, S. Fukushima, H. Watanabe and Y. Ozeki: in Computer Simulation Studies in Condensed-Matter Physics XIV, edited by D. P. Landau, S. P. Lewis and H. B. Schuettler, Springer Proceedings in Physics Vol.89 (Springer-Verlag, 2002) p.27.