Diffusion in the Continuous-Imaginary-Time Quantum World-Line Monte Carlo Simulations with Extended Ensembles

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The dynamics of samples in the continuous-imaginary-time quantum world-line Monte Carlo simulations with extended ensembles are investigated. In the case of a conventional flat ensemble on the one-dimensional quantum $S = 1$ bi-quadratic model, the asymmetric behavior of Monte Carlo samples appears in the diffusion process in the space of the number of vertices. We prove that a local diffusivity is asymptotically proportional to the number of vertices, and we demonstrate the asymmetric behavior in the flat ensemble case. On the basis of the asymptotic form, we propose the weight of an optimal ensemble as $1/\sqrt{n}$, where $n$ denotes the number of vertices in a sample. It is shown that the asymmetric behavior completely vanishes in the case of the proposed ensemble on the one-dimensional quantum $S = 1$ bi-quadratic model.

KEYWORDS: diffusion, extended ensemble, quantum Monte Carlo, first-passage time, bi-quadratic model

Properties of various quantum exotic states and phase transitions between them have been extensively investigated. For example, quantum paramagnetic and valence-bond-solid states related to a possible mechanism to support a novel superconductivity in cuprates,\(^1\) and the existence of non-Landau-Ginzburg-Wilson type phase transitions between different broken symmetries.\(^2\) In order to numerically investigate such quantum states and phenomena, unbiased quantum world-line Monte Carlo (QMC) methods based on a Markov chain are powerful tools, because they can be applied to large scale systems at low temperatures and are not limited to the one-dimensional case, if no negative-sign problem exists. However, even for no negative-sign cases, it is sometimes difficult to get accurate data from the conventional QMC simulations, because Monte Carlo samples are trapped near a metastable state in configuration space. In general, the quality of QMC simulations deteriorates at low temperatures, because metastable states are related to degenerate ground states. In fact, the autocorrelation time of samples in QMC simulations becomes exponentially large to overcome barriers between metastable states. In order to eliminate the rapid increase in autocorrelation times in Monte Carlo simulations, two approaches were proposed over the last two decades. One is to change the update method of samples in a Markov process to a global one that connects metastable states directly. In fact, the loop algorithm\(^3\) has been successful in studies of quantum magnetic phases due to the global update whose shape is like a loop and which corresponds to a magnetic correlated domain. However, in some cases using the loop algorithm, we encountered rapid increases in autocorrelation time: For example, valence-bond-solid states that break spatial symmetries on the two and quasi-one dimensional lattice.\(^4,5\) For such cases, the second approach is probably effective, in which a canonical ensemble is replaced by an artificial extended ensemble such that Monte Carlo samples would not be trapped near metastable states. For classical systems, the extended weight is adjusted such that the appearance ratio of energy $E$ samples would be flat. They are not trapped near a metastable state because Monte Carlo samples diffuse in a wide energy range. Therefore, these methods have been extensively used for studies of spin glasses and frustrated classical models. However, for quantum models, they have been tested only in a few cases.\(^6,7\) In order to get conclusive numerical results for quantum strong correlated phenomena as mentioned above, we need to understand the property of QMC methods with extended ensembles, and it is important to improve their efficiencies. In this letter, we will concentrate the diffusive behavior of samples in the continuous-imaginary-time QMC simulations with an extended ensemble. We will report the asymmetric behavior in the diffusion process for the one-dimensional quantum $S = 1$ bi-quadratic (BQ) model case. On the basis of our proven asymptotic form of the local diffusivity of samples, we will propose an optimal ensemble. The performance of the proposed ensemble will be shown for the case of the one-dimensional BQ model.

Although the first formulation of QMC methods with extended ensembles (EEQMC) was based on high-temperature series expansion,\(^6\) it can be also done on the path-integral representation with a continuous-imaginary-time limit (see §2.15 in ref. 8). In order to provide a brief description of the EEQMC algorithms on the path-integral representation, we first consider the definition of the exponential operator:

$$\exp\left(-\beta \sum_b \mathcal{H}_b\right) = \lim_{M \to \infty} \left[ \prod_b \left(1 - \frac{\beta \mathcal{H}_b}{M}\right) \right]^M. \quad (1)$$

Inserting the identity operator $1 = \sum_\alpha |\alpha\rangle\langle\alpha|$ with a complete orthonormal basis $\{|\alpha\rangle\}$ between two adjacent factors in the right-hand side of eq. (1), we obtain the discrete-imaginary-time path-integral representation of a partition function as

$$Z \approx \sum_{\{S_b(t)\}} \prod_{t=1}^M \prod_{b=1}^K (S_{b+1}(t) | 1 - \beta \mathcal{H}_b \Delta | S_b(t)), \quad (2)$$
where \( H_b \) is the \( b \)-th interaction Hamiltonian, \( \beta \) is an inverse temperature, \( \Delta = 1/M \), \( S_{K+i}(t) \equiv S_i(t+1) \), and \( S_1(M+1) \equiv S_1(1) \). Next, we introduce new auxiliary variables \( G_u(t) \) called graph variables as \( (1 - \beta H_b \Delta) = \sum G_u(t) = 0 (-\beta H_b \Delta G_u(t) \). Then, eq. (2) is rewritten as
\[
Z \approx \sum_S G^n(S,G) W_0(S,G) = \sum_n \beta^n \Omega(n),
\]
\[
W_0(S,G) = \prod_u \langle S_u | - (\beta H_u \Delta) G_u | S_u \rangle,
\]
\[
\Omega(n) = \sum_S \sum_{\{G|n(G)=n\}} W_0(S,G),
\]
where \( u, u', S, \) and \( G \) denote \( b, t \), \( b+1, t \), \( \{S_u\} \), and \( \{G_u\} \), respectively, and \( n(G) = \sum_u G_u \). In the following, a graph variable \( G_u \) that takes a value 1 is called a vertex and the number of vertices \( n(G) \) is called a vertex number. This representation is the mathematical background required to describe the remarkable QMC algorithms that have been developed during the last two decades. In particular, we can take a limit of a continuous-imaginary time, \( \Delta \to 0 \), in the level of QMC algorithms (see §2.5 in ref. 8 for details). In the remainder of this paper, we consider the EEQMC algorithm on the continuous-imaginary time, because it has no systematic error from the discretization of an imaginary time.

The vertex number \( n(G) \) in a canonical ensemble statistically corresponds to an inverse temperature \( \beta \) because \( \langle n(G) \rangle_\beta = \beta \langle -H \rangle_\beta \), where \( \langle \cdot \rangle_\beta \) is a canonical ensemble average. Therefore, if we adjust the weight of a configuration \( (S,G) \) so that the frequency of obtaining the vertex number \( n \) would be independent of \( n \), i.e., flat, we can sample various configurations in a wide inverse temperature range. From eq. (3), \( \Omega(n) \) is regarded as the density of states with a fixed vertex number \( n \). Hence, if the factor \( \beta^{n(G)} \) in eq. (3) is replaced by \( 1/\Omega(n(G)) \), it can be done. In general, in order that the appearance ratio of configurations with a vertex number \( n \) is \( P_n(n) \), the extended ensemble weight of a configuration \( (S,G) \) has to be \( P_n(n(G)) W_0(S,G) / \Omega(n(G)) \). However, we need to guess \( \Omega(n) \) from the QMC samples themselves, because \( \Omega(n) \) is not known a priori. Fortunately, some sophisticated methods have been proposed. In our simulations, we have used the broad-histogram relation for the vertex number as
\[
\frac{\Omega(n+1)}{\Omega(n)} = \frac{\langle \text{diag}(-H) \rangle_n}{n + 1 - (n_K + 1)},
\]
where \( \langle Q \rangle_n \) denotes the micro-canonical ensemble average of an operator \( Q \) at a fixed vertex number \( n \), \( \text{diag}(Q) \) refers to the diagonal part of an operator \( Q \), and \( n_K \) is the number of kinks at which a state changes, i.e., \( \langle S_u | S_u \rangle = 0 \). Because the right-hand side in eq. (6) can be directly estimated in the EEQMC simulations, \( \Omega(n) \) can be calculated from this recursion formula. We should note that this estimation method is independent of the dynamics of the EEQMC samples; it is not based on the histogram of the appearance of a vertex number in the EEQMC simulations.

However, after \( \Omega(n) \) is sufficiently estimated, the dynamics of the EEQMC samples do not seem to be a regular random walk in the vertex number space. In particular, in order to investigate this behavior, we focus on the first-passage time (FPT) of EEQMC samples regarded as random walkers in a vertex number space. The FPT is defined as the time at which a random walker first reaches a threshold value. Because the movement of an EEQMC sample is usually restricted to the interval \( [N_a, N_b] \) in the vertex number space, two types of FPTs are defined as a QMC sample moves from \( N_b \) to \( N_a \), and vice versa. In the following, the former is called forward and the latter is called backward.

![Figure 1](image-url)  
**Figure 1.** First-passage times (FPT) of EEQMC samples for the one-dimensional quantum S = 1 bi-quadratic model. Filled triangle and square symbols are forward and backward FPTs for a flat ensemble, respectively. Triangle and square symbols are forward and backward FPTs for the ensemble defined by eq. (15), respectively. In the inset, the ratios of backward and forward FPTs are shown.
EEQMC algorithm consists of three steps: (i) deciding a new vertex number \( n' \) under a given \( S \)-configuration, (ii) assigning new graphs \( G' \) with the vertex number \( n' \) to a given \( S \)-configuration, and (iii) choosing a new \( S' \)-configuration under the given graphs \( G' \). It is possible to measure observables only at the time that these three steps are completed. In Fig. 1, forward and backward FPTs for a flat ensemble increase almost linearly, but the backward FPT is always larger than the forward one: For example, the ratio of two FPTs is 7.0(5) for \( L = 256 \) (see the inset of Fig. 1). Thus, the EEQMC samples for a flat ensemble move quickly from high temperatures to low ones, but slowly in the reverse direction. In order to improve the efficiency of the EEQMC algorithms, it is necessary to correct this asymmetric behavior.

When we make a new \( G' \) configuration under a fixed \( S \)-configuration, the vertex \( (G_a = 1) \) at a kink cannot be removed, because the local weights in \( W_0(S, G) \) at a kink becomes zero: \( \langle S_u' | S_u \rangle = 0 \). Therefore, if the number of kinks is \( n_K \), the probability \( p(n'|n_K) \) to choose the next vertex number \( n' \) in step (i) is proportional to the sum of weights of the configurations that have unchanged \( n_K \) vertices at kinks and new inserted \( (n' - n_K) \) ones into a given \( S \)-configuration:

\[
p(n'|n_K) \propto \frac{P_v(n') \left[ \sum_{(u|G_u=0)} \langle S_u' | (-H_u\Delta) | S_u \rangle \right]^{(n'-n_K)}}{\Omega(n')(n' - n_K)!}.
\]

For finite-size systems, if the vertex number is sufficiently large, the right-hand side in eq. (6) is converged. Using limiting values as \( w_0 = \lim_{n \to \infty} (\text{diag}(-H))_n \) and \( r_K = \lim_{n \to \infty} (n_K)_n / n \), the asymptotic form of \( \Omega(n) \) is as

\[
\Omega(n) \approx \frac{\Omega(n-1)}{n} \left( \frac{w_0}{1-r_K} \right) \propto \frac{1}{n!} \left( \frac{w_0}{1-r_K} \right)^n.
\]

Substituting eq. (8) into eq. (7), we find that the main factor of \( p(n'|n_K) \) is the negative binomial distribution. Using the limit theorem for the negative binomial distribution, we obtain the asymptotic form of \( p(n'|n_K) \propto P_v(n') \exp \left[ -(n' - m_0)^2 / 2(m_0/r_K) \right] \), where \( m_0 \equiv (r_K^{-1} - 1)n_K \). Here, we assume that \( P_v(n') \) is a slowly varying function. And if we assume that the probability \( p(n_K|n) \) that the number of kinks in a configuration with a vertex number \( n \) is \( n_K \) is equivalent to the probability \( p(n|n_K) \), the probability to choose the next vertex number \( n' \) from configurations with a vertex number \( n \) is

\[
p(n \to n') = \int_0^t d n_K \ p(n'|n_K)p(n_K|n),
\]

\[
= \frac{1}{n} \left[ \frac{1-r_K}{r_K} \right] n, \quad (10)
\]

where \( N_G(m, \sigma^2) \) denotes the Gaussian distribution with mean \( m \) and variance \( \sigma^2 \). Thus, the EEQMC samples almost seem to be random walkers in the vertex number space, but the local diffusivity \( D(n) \) increases linearly as

\[
D(n) \approx \left[ \frac{1-r_K}{r_K} \right] n, \quad (11)
\]

where \( n \) is the number of vertices in a configuration. Figure 2 shows the local diffusivity \( D(n) \) for a flat ensemble \( (P_v(n) = 1) \) in the EEQMC simulations of the one-dimensional quantum \( S = 1 \) bi-quadratic model. The chain length \( L \) is 128 and the total number of MCSs is \( 1.05 \times 10^8 \). The local diffusivity in Fig. 2 is approximately linear in the region above the vertex number 100 (see also the left-top inset of Fig. 2). The solid line in Fig. 2 is a linear function predicted in eq. (11) with \( r_K = 0.6108(1) \), which is evaluated from the QMC simulations. The predicted line is consistent with the local diffusivity in the region above the vertex number 1000. And the discrepancy between them is never more than 6% at all vertex numbers below 1000 but zero. Next, we checked the dependence of the local diffusivity on extended ensembles. In the right-bottom inset of Fig. 2, the ratios between local diffusivities in two different ensembles are shown. Because these values are approximately equal to one, the local diffusivity is almost unaffected by the choice of extended ensembles. For other system-size cases, the same results were obtained. Therefore, the local diffusivity of the EEQMC samples is described well by eq. (11).

From eq. (10), the behavior of the samples in the EEQMC simulations may be described well by a Fokker-Planck equation (FPE) on a vertex number range \([N_a, N_b] \). Using the theory of first-passage processes,\(^{14}\) we can explicitly obtain the first-passage times for a one-dimensional FPE as

\[
T_{FP}(N_a \to n) = \int_{N_a}^n dx^0 P_v(x) \int_x^n \frac{dx'}{D(x')} P_v(x'),
\]

\[
T_{FP}(N_b \to n) = \int_n^{N_b} dx^0 P_v(x) \int_n^{x} \frac{dx'}{D(x')} P_v(x').
\]

If we assume the linear increase of the local diffusivity
While it typically cannot be uniquely determined, a side in eq. (12) would be equivalent to that in eq. (13). Asemble with eq. (11).

The behavior of the EEQMC samples is described well by one and their ratio varies slowly. Thus, the qualitative and the backward one is always larger than the forward at an inverse temperature \( \beta \). Here, although eq. (11) is the asymptotic form, we use calculate a canonical ensemble average of an observable at inverse temperatures. But that for the ensemble \( P_{v}^{OPT} \) decreases at low temperatures.

In summary, we considered the diffusion of samples in the continuous-imaginary-time EEQMC simulations. In particular, the asymmetric behavior of FPTs of EEQMC samples was reported in detail. We proved that the local diffusivity of the EEQMC samples is asymptotically proportional to the vertex number. And it was shown that the asymptotic form is consistent with the local diffusivity in the EEQMC simulations of the one-dimensional BQ model in the wide region of the vertex numbers. Using this result and the theory of first-passage processes, we demonstrated the asymmetric behavior of FPTs for a flat ensemble case and proposed an optimal ensemble for the continuous-imaginary-time EEQMC simulations in order to correct the asymmetric behavior. It was shown that the asymmetric behavior on the one-dimensional BQ model completely vanishes in the case of the proposed ensemble.

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