The Single Histogram Method and the Quantum Harmonic Oscillator: Accuracy Limits

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In a recent work, M. Troyer, F. Alet and S. Wessel proposed a way to extend histogram methods to quantum systems in the World Line Quantum Monte Carlo (WLQMC) formulation. The strategy, also proposed in [2], allows to compute quantum averages on a narrow temperature range from a single Monte Carlo run at a fixed temperature. This is achieved by fixing $N$, the number of temporal divisions in the Trotter-Suzuki expansion of WLQMC, and by changing $\epsilon=1/(Nk_B T)$. In this work we apply this strategy to construct a single histogram Monte Carlo method for a canonical ensemble of one-dimensional quantum harmonic oscillators and we explore its accuracy limits. We obtain that fixing $N$ imposes a limit of minimal temperature to the properly performance of the method, which is $T_{\text{min}}=1.9(2)N^{-0.80(6)}$ in our example. This limit is a consequence of the fact that the Trotter-Suzuki expansion fails for large $\epsilon$ values, and, therefore, should be taken into account in all applications of this histogram method for quantum systems.

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INTRODUCTION

Histogram Monte Carlo methods are powerful and robust techniques to investigate classical systems, both with discrete or continuous degrees of freedom. Such methods have many advantages over traditional Monte Carlo ones. For example, one can obtain mean values of thermodynamical quantities over a broad range of temperatures by using data from a single run. Also it is possible to compute thermodynamic potentials, like the free energy, that are not accessible by other methods. All these methods bases on defining a density of states, let say $g(E)$, i.e. the number or states with the same energy. Once obtained, $g(E)$ allows to compute averages like the mean energy and the specific heat at any desired temperature. Therefore, the problem of averaging over all states is transformed into a problem of counting and, therefore, should be taken into account in all applications of this histogram method for quantum systems.

There are histogram methods for analysis and histograms methods for sampling. Some examples of the first ones are the Single Histogram Method (SHM), first proposed by Z. W. Salsburg in 1959 and popularized by A. M. Ferrenberg and R. H. Swendsen in 1988; the Broad Histogram Method (BHM) formulated in 1996 by P. C. M. de Oliveira, T. J. P. Penna and H. J. Herrmann, and the Transition Matrix Monte Carlo method (TMMC) proposed by J. S. Wang, T. K. Tay and R. H. Swendsen in 1998 which reduces to BHM when a single energy jump is chosen. In the second class we find, for example, the Multicanonical Method, proposed by B. A. Berg (also formulated by J. Lee as the Entropic Sampling method), the Flat-Histogram method of Wang and Lee and the Wang-Landau method. These methods take samples uniformly distributed on the energy axis.

Recently, M. Troyer, F. Alet and S. Wessel proposed a way to extend histogram Monte Carlo methods to canonical ensembles of quantum systems, in the world line quantum Monte Carlo (WLQMC) formulation. In contrast with previous proposals, this idea, also proposed in [2], resembles the full power of the classical histogram methods, since it is able, for instance, to calculate mean values on a narrow temperature range from a single Monte Carlo run at a fixed temperature (SHM). The idea bases on the observation that interactions in time and space in the equivalent classical system of WLQMC are weighted by the temperature in different ways, as we will illustrate below. Thus, it is useful to define two new quantities, $k_1$ and $k_2$, which summarize spatial and temporal interactions, and also a density of states $g(k_1, k_2)$ on them. Such density can be computed by using any histogram method and allows to obtain averages at different temperatures from a single run. This strategy has been used by Troyer, Alet and Wessel to investigate the three-dimensional quantum Heisenberg model with excellent results.

In this work we illustrate this strategy by studying a much more simple system: a canonical ensemble of non-coupled one-dimensional quantum harmonic oscillators. By doing so, interesting aspects of the method like its range of accuracy and its dependence on the simulation parameters will be explored. The article is organized as follows. First, the World Line Quantum Monte Carlo method is revised. Next, the quantities $k_1$, $k_2$ and $g(k_1, k_2)$ for a quantum single-particle system are defined, and it is shown how this density of states allows to compute expectation values for the kinetic, potential and total energy operators at any desired temperature. Then, we implement the SHM for the one-dimensional quantum har-
monic oscillator, and we investigate how the temperature range of accuracy is affected by the number of divisions on the axis of imaginary time. Finally, we summarize our main results and conclusions.

THE WORLD LINE QUANTUM MONTE CARLO METHOD

The World Line Quantum Monte Carlo method (WLQMC) was formulated in 1982 by J. E. Hirsch, R. L. Sugar, D. J. Scalapino and R. Blankenbecler [13]. It has been used to study one particle systems as well as many particle systems, like interacting bosons and system of strong correlated fermions. The WLQMC employs path integrals to change the partition function of a quantum system to the partition function of an equivalent classical system in one higher dimension [14]. To illustrate the method, let us consider a quantum system with a separable Hamiltonian

\[ \hat{H} = \hat{T} + \hat{V}(\hat{X}) = \frac{\hat{p}^2}{2m} + \hat{V}(\hat{X}), \]

where \( \hat{V}(\hat{X}) \) and \( \hat{T} = \frac{\hat{p}^2}{2m} \) are the potential and kinetic energy operators respectively. In the canonical ensemble, the partition function is

\[ Z = \text{Tr}[e^{-\beta \hat{H}}], \]

where \( \beta = \frac{1}{k_B T} \) is the imaginary time, \( \hat{H} \) is given by [11] and \( k_B \) is the Boltzmann constant.

Since \( \hat{X} \) and \( \hat{P} \) do not commute, the exponential in [2] cannot be separated into a product of exponentials. Therefore, the imaginary time \( \beta \) is written as \( \beta = N \epsilon \), and a Trotter–Suzuki approximation is used [21, 22, 23] to write the partition function [2] as

\[ Z = \lim_{N \to \infty} \lim_{\epsilon \to 0} Z_{tr} = \lim_{N \to \infty} \lim_{\epsilon \to 0} \text{Tr}[e^{-\epsilon \hat{T}} e^{-\epsilon \hat{V}(\hat{X})}]^N. \]

To compute [3], the trace is expressed as a sum over a complete set of position eigenstates, and a new completeness relation is introduced between each of the \( N \) factors in that expression, obtaining

\[ Z_{tr} = \left( \frac{m}{2 \pi \epsilon} \right)^{N/2} \int Dx \exp[-\epsilon H(x)], \]

\[ H(x) = \sum_{i=0}^{N-1} V(x_i) + \frac{1}{2} m \sum_{i=0}^{N-1} \left( \frac{x_i - x_{i+1}}{\epsilon} \right)^2, \]

where \( Dx = dx_0 dx_1 \cdots dx_{N-1} \). The partition function for the quantum system is now expressed as a multidimensional integral over classical variables. The expression [4] can be interpreted as the energy of a chain of \( N \) classical oscillators with potential energy \( V(x) \) coupled through springs of constant \( k = m/\epsilon^2 \). In this case, \( x = \{x_0, x_1, \ldots, x_{N-1}\} \) will denote a specific configuration of this classical system.

By following the same procedure described above, one obtains

\[ \langle \hat{V} \rangle_{tr} = \left( \frac{Dx}{N} \int Dx \frac{V(x_0) \exp[-\epsilon H(x)]}{\int Dx \exp[-\epsilon H(x)]} \right) \]

\[ \langle \hat{T} \rangle_{tr} = \frac{1}{2} \int Dx \frac{(x_0 - x_1)^2 \exp[-\epsilon H(x)]}{\int Dx \exp[-\epsilon H(x)]}, \]

for the expectation values of the potential and kinetic energy operators respectively, where \( x_0 \) and \( x_1 \) can be replaced by any pair \( (x_i, x_{i+1}) \) of neighboring classical oscillators. For the total energy we have \( \langle \hat{H} \rangle_{tr} = \langle \hat{T} \rangle_{tr} + \langle \hat{V}(\hat{X}) \rangle_{tr} \).

Expressions [5] and [6] show that the expectation values for quantum operators are now expressed as multidimensional integrals over the configuration space of the classical system. This integral can be computed by using standard Monte Carlo methods. For example, we can use the Metropolis algorithm to compute the total energy average \( \langle \hat{H} \rangle_{tr} \) as follows. First, an oscillator \( i \) in configuration \( x \) is chosen at random and its position \( x_i \) is changed to a new value \( x_i + r \), where \( r \) is a uniformly distributed random number in \([-1, 1]\). Next, this new configuration \( x' \) is accepted with rate \( A(x' \mid x) = \min\{1, e^{-\epsilon (\hat{H}(x') - \hat{H}(x))}\} \). Finally, energy averages are computed as arithmetic means over the sample set.

The temperature can be fixed by varying either \( N \) or \( \epsilon \), since \( \beta = 1/k_B T = N \epsilon \). When \( N \) is fixed and \( \epsilon \) varies to fix the temperature, errors in the Trotter–Suzuki approximation are greater at low temperatures.

HISTOGRAM METHODS FOR QUANTUM SYSTEMS IN THE WLQMC FORMULATION

For a classical system in the canonical ensemble, the average energy at temperature \( T \) is given by

\[ \langle E \rangle_T = \frac{\sum_x E_x e^{-\frac{E_x}{k_B T}}}{\sum_x e^{-\frac{E_x}{k_B T}}}, \]

where \( g(E) \) is the number of configurations with the same energy \( E \). If \( g(E) \) is known, one can use [7] to obtain \( \langle E \rangle_T \) as a continuous function of temperature. So, the problem of summing over all states has been transformed into a problem of counting to find \( g(E) \).

In the classical SHM, samples are taken with probability proportional to \( e^{-E_x/k_B T} \) (canonical distribution) at fixed temperature \( T \), and a histogram of visits \( \mathcal{V}(E) \) is accumulated as the number of samples with energy \( E \). From such histogram, the density of states \( g(E) \) is
approximated as
\[ g(E) \simeq \frac{\mathcal{V}(E)}{\mathcal{N}} \exp[E/k_B T], \]  
where \( \mathcal{N} \) is the total number of samples. By replacing \( \mathcal{N} \) in \( \mathcal{N}_k \), we can obtain averages at temperatures \( T' \neq T \).

To extend histogram methods to quantum systems, one has to define a density of states. As proposed in [1, 2], this is achieved by defining two quantities in the WLQMC classical system, which resummes the interactions in space and time directions:
\[ k_1 = \sum_{l=0}^{N-1} V(x_l), \quad k_2 = \sum_{l=0}^{N-1} (x_l - x_{l+1})^2, \]
with periodic boundary conditions. The partition function \( Z' \) and the averages \( \langle \hat{V} \rangle \) and \( \langle \hat{T} \rangle \) can be written in terms of \( k_1 \) and \( k_2 \) as
\[ Z'_{tr} = \left( \frac{m}{2\pi \epsilon} \right)^{N/2} \int dk_1 dk_2 \, g(k_1, k_2) e^{-\epsilon H(k_1, k_2)}, \]
\[ \langle \hat{V} \rangle_{tr} = \frac{1}{N} \int \frac{dk_1 dk_2}{dk_1 dk_2} \frac{g(k_1, k_2)}{k_1} e^{-\epsilon H(k_1, k_2)}, \]
\[ \langle \hat{T} \rangle_{tr} = \frac{1}{2\epsilon} - \frac{m}{2N \epsilon^2} \int \frac{dk_1 dk_2}{dk_1 dk_2} \frac{g(k_1, k_2)}{k_2} e^{-\epsilon H(k_1, k_2)}, \]
where \( H(k_1, k_2) = k_1 + mk_2/2\epsilon^2 \), and \( g(k_1, k_2) \) is the number of configurations \( x = \{x_0, x_1, \ldots, x_{N-1}\} \) of the classical system with same values of \( k_1 \) and \( k_2 \) for fixed \( N \).

Expressions (11)–(13) are continuous equivalent to those of classical systems \( \mathcal{N}_k \). We can use any histogram method to compute \( g(k_1, k_2) \). Let us use the SHM to illustrate this point. First, we fix the simulation temperature \( T_{sim} = 1/N \epsilon_{sim} \) by choosing \( N \) and the initial \( \epsilon_{sim} \). Then, samples are taken with probabilities proportional to \( e^{-\epsilon H(x)} \) by using the Metropolis algorithm described above, and an histogram of visits \( \mathcal{V}(k_1, k_2) \) is cumulated as the number of samples with values \( k_1 \) and \( k_2 \). Next, the density of states \( g(k_1, k_2) \) is estimated as
\[ g(k_1, k_2) \simeq \frac{\mathcal{V}(k_1, k_2)}{\mathcal{N}} \exp[\epsilon H(k_1, k_2)]. \]
Once \( g(k_1, k_2) \) is computed, averages at different temperatures are obtained by changing \( \epsilon \) in equations (12)–(13).

**THE SHM FOR THE ONE-DIMENSIONAL QUANTUM HARMONIC OSCILLATOR**

The system we chose is a canonical ensemble of non-coupled one-dimensional quantum harmonic oscillators.

![Figure 1: Average potential energy for the one–dimensional quantum harmonic oscillator at various simulation temperatures.](image1)

![Figure 2: Average kinetic energy for the one–dimensional quantum harmonic oscillator at various simulation temperatures.](image2)

![Table I: Simulation Parameters](table)

| \( N \) | \( \epsilon_{sim} \) | \( T_{sim} \) | CPU time(s) |
|-------|-----------------|-------------|-------------|
| 40    | 0.25            | 0.10        | 412.294     |
| 30    | 0.09            | 0.37        | 312.607     |
| 10    | 0.10            | 1.00        | 117.532     |

For this system, \( k_1 \) takes the form \( k_1 = \frac{1}{2} m \omega^2 \sum_{l=0}^{N-1} x_l^2 \), with \( m \) the mass and \( \omega \) the frequency. The exact expressions for the expectation values are [21, 24]
\[ \langle \hat{H} \rangle = 2\langle \hat{T} \rangle = 2\langle \hat{V} \rangle = \hbar \omega \left( \frac{1}{2} + \frac{1}{e^{\hbar \omega} - 1} \right). \]

Figures 1, 2, and 3 shows the expectation values of the potential, kinetic and total energy, at three different simulation temperatures, \( T_{sim} \). The parameters for each simulation are shown in table I. In all cases, the total number of samples was 60000, \( k_B = 1 \), 30000 mcss were discarded before sampling, and 10 mcss were performed between successive samples. To make statistic, the whole procedure was run ten times with different seeds of the random number generator.

Errors in the Trotter–Suzuki aproximation are proportional to \( \epsilon^2 \) [19]. Since the SHM fixes \( N \) and changes the
temperature by varying $\epsilon$, the errors will be greater for lower temperatures. There is a minimum temperature, $T_{\text{min}}$, where the simulation results includes the theoretical ones between the error bars. Such a $T_{\text{min}}$ is a function of $N$. By looking at the total energy, we found for the SHM

$$T_{\text{min}} = 1.9(2)N^{-0.80(6)}.$$  \hspace{1cm} (16)

Following the same procedure for the WLQMC we found

$$T_{\text{min}} = 2.0(6)N^{-0.81(6)}.$$  \hspace{1cm} (17)

This two results are very similar and are plotted in Figure 4. They actually show that the minimum temperature in SHM is a consequence of the errors in the Trotter–Suzuki approximation. This limit is important for the correct performance of the method and should be taken into account for all applications of histogram methods for quantum systems in the WLQMC formulation.

Increasing $N$ or decreasing $\epsilon$ gives exacter results at low temperatures, but at price of longer CPU times, just because correlation times increases with decreasing $\epsilon$. Nevertheless, the use of SHM spares large amounts of CPU times. For example, it takes 118 sec on a Pentium 4 at 1.6 GHz to compute $\langle \hat{H} \rangle_T$ over the whole temperature range $0.7 \leq T \leq 1.7$, at simulation temperature $T_{\text{sim}} = 1.0$, in contrast with the 35 sec of a single point by WLQMC.

**CONCLUSIONS**

In this work we have employed the extension of histogram methods for quantum systems in the WLQMC formulation proposed in \cite{1,2} to the case of a canonical ensemble of one-dimensional quantum harmonic oscillators. By doing so, we have explored the ranges of accuracy of the method as a function of the number of divisions $N$ in time direction. Actually, since the method fixes $N$ and varies $\epsilon$ to change $T$, the corrections in the Trotter-Suzuki expansion fixes a minimum temperature for the correct performance of the SHM. We obtained that the method is accurate for temperatures above $T_{\text{min}}=1.9(2)N^{-0.80(6)}$. That is corroborated by direct WLQMC simulations, equation \cite{17} This $T_{\text{min}}$ can be lowered by increasing $N$, but at cost of larger CPU times, because correlation times grow with decreasing $\epsilon$. Perhaps SHM needs smaller CPU times than WLQMC.

The definitions of $k_1$ and $k_2$ and the density of states $g(k_1,k_2)$, expressions \cite{10} and \cite{14}, allow to apply any histogram Monte Carlo method to quantum systems in the WLQMC formulation, with all the power and advantages that histogram methods have deserve for classical ones. However, the restrictions founded here applies to all of them, because they relies on the fail of the Trotter-Suzuki expansion for lower $\epsilon$ values, and should be always taken into account. Further analysis, like the theoretical study of the errors in this method, are interesting areas of future work.

The strategy of extending histogram methods to quantum systems in the WLQMC formulation is completely general, and is able to give accurate results for many kinds of systems. We expect that our work will be useful to the right use of the method for many systems in the future.

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