Application of flat histogram methods to extract the long imaginary-time behavior in diagrammatic Monte Carlo

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\textbf{Abstract}

We demonstrate that using flat histogram methods we can extract the imaginary-time behavior of the Green’s function $G$ from diagrammatic Monte Carlo simulations very accurately even when $G$ changes by many orders of magnitude.

\begin{keyword}
Computational techniques, computer modelling and simulation, Monte Carlo method
\end{keyword}

\section{1. Introduction}

Flat histogram techniques (Berg and Neuhaus (1991); Oliviera et al. (1996); Wand and Landau (2001)) have been shown to be very important methods in order to allow efficient sampling of the entire phase space and transitions between configurations in classical systems undergoing a first order phase transition.

Troyer et al. (Troyer, Wessel and Alet (2003)) have applied flat histogram methods to simulation of equilibrium quantum statistical mechanics and showed that it also makes the quantum Monte Carlo algorithm efficient in handling the tunneling problem in first order phase transitions. Furthermore, following this idea, Gull et al. (Gull et al. (2011)) have applied the flat histogram method to the continuous-time quantum Monte Carlo approach to the quantum impurity solver needed for all dynamical mean-field theory applications.

The goal of the present paper is to show that one can use flat histogram techniques in order to accurately extract the long imaginary-time behavior of the Green’s function in quantum many-body systems. More precisely, here we apply the flat histogram method to the diagrammatic-Monte Carlo (diag-MC) method in order to extract $G(\tau)$ for large $\tau$.

To illustrate the idea we choose the Fröhlich polaron problem (Fröhlich, Pelzer and Zieau (1950)) where the diag-MC has been previously fruitfully applied (Prokof’ev and Svistinov (1998); Michencko et al. (2000)). Some results of the idea presented in this paper have been published (Diamantis and Manousakis (2013)) and the reader is referred to that work because it contains complementary information.

\section{2. The problem}

The diagrammatic Monte Carlo technique (Prokof’ev and Svistinov (1998); Michencko et al. (2000)) is a Markov process in a space defined by all the terms (or diagrams) which appear in perturbation theory. Take for example the...
perturbation expansion of the imaginary-time single-particle Green’s function, which can be schematically written as follows:

\[
G(\tau) = \sum_{n}^\infty I_n(\tau), \quad I_n(\tau) = \sum_{\lambda} I^{(\lambda)}_n(\tau), \quad I_0(\tau) = G^0(\tau),
\]

(1)

\[
I^{(\lambda)}_n(\tau) = \int d\vec{x}_1 d\vec{x}_2 ... d\vec{x}_n F^{(\lambda)}_n(\vec{x}_1, \vec{x}_2, ..., \vec{x}_n, \tau),
\]

(2)

where \( n \) can be the order of the diagram and \( \lambda \) is a variable which labels the diagrams within the same order. As the order \( n \) of the expansion increases, the number of integration variables increases in a similar manner. In diag-MC the random walk makes a series of transitions between states \( \{n, \lambda, \vec{R}\} \rightarrow \{n', \lambda', \vec{R}'\} \), where \( \vec{R} = (\vec{x}_1, ..., \vec{x}_n) \). Through such a Markov process the entire series of terms is sampled.

This process generates a histogram of the number of times \( N_n \) the order \( n \) appears in the Markov process. Since we can compute a low order diagram analytically, say for example the zeroth order \( I_0(\tau) \), the absolute value of all other orders is computed as follows:

\[
I_n(\tau) = \frac{N_n}{N_0} I_0(\tau).
\]

(3)

For illustration of the method we will use a simplified version (Diamantis and Manousakis (2013)) of the Fröhlich polaron problem (Fröhlich, Pelzer and Zieau (1950)) which has an exact solution and, this allows us to compare the Monte-Carlo results with exact results. When we refer to the \( n^{th} \) order in this case we mean that the number of phonon-propagators contained in the diagrams is \( n \); therefore, the order in perturbation expansion is \( 2^n \), because there are \( 2n \) vertices when there are \( n \) phonon propagators. In Fig. 1(a) the calculated \( I_n(\tau) \) as a function of \( n \) is shown for a fixed value of \( \tau \) as calculated for this model. Notice that the function \( I_n \) is a Gaussian-like distribution which peaks at a value of \( n = n_{\text{max}}(\tau) \). Fig. 1(b) shows \( I_n(\tau) \) on a logarithmic scale for \( \tau = 8, 12 \) and 16. Notice that as a function of \( \tau \), \( n_{\text{max}}(\tau) \) grows almost linearly with \( \tau \), the value of \( I_n(\tau) \) at the maximum grows dramatically with increasing \( \tau \). Namely, as \( \tau \) increases higher and higher order diagrams give the most significant contribution. As a result, for large enough \( \tau \), for any given limited number of Monte Carlo steps, the number of walks landing in small values of \( n \) becomes very small or non-existent. However, when the number of MC steps which land in the state \( n = 0 \) is zero or very small, it leads to a fatal situation in our attempt to calculate the absolute value of \( I_n(\tau) \), because this is obtained using the formula (3) and a very small \( N_0 \) implies a large uncertainty in the absolute value of all \( I_n(\tau) \). This is illustrated in Fig. 2(a) where the red points with error bars are obtained with the diag-MC process. Notice that the
size of the error bars is much larger than the size of the fluctuations of the points for successive values of \( n \). Namely, the points which represent \( I_n(\tau) \) form a rather smooth curve. This seems unusual given the size of the error bars. This can be explained by the fact that the error is due to the poor estimation of \( N_0 \) which propagates through the formula given by Eq. 3. Note that using the same number of MC steps becomes impossible to calculate \( I_n(\tau) \) beyond this value of \( \tau = 12 \) because the ratio \( I_{n_{\text{max}}}(\tau)/I_0 \) becomes much larger than the number of MC steps.

3. How to solve the problem

Here, we will solve the problem discussed in the previous section by adopting the flat histogram techniques which have been applied to simulation of classical statistical mechanics (Berg and Neuhaus (1991); Wand and Landau (2001)). We map the particular value of \( n \) to the “energy” level in standard flat histogram methods for classical statistical mechanics and the sum of the terms giving \( I_n(\tau) \) to the density of states which corresponds to the corresponding configurations. The flat histogram method renormalizes the density of states \( I_n(\tau) \) for each \( n \) by known factors (which can be easily estimated) and, then, samples a more-or-less flat histogram of such populations.

Next, we use the idea of the multicanonical algorithm (Berg and Neuhaus (1991)) as follows: First, for a given fixed value of \( \tau \) we carry out an initial exploratory run, where we find that the distribution \( I_n \) of the values of \( n \) peaks at some value of \( n = n_{\text{max}} \), which depends on the chosen value of \( \tau \). The curve labeled 0 in Fig. 2(b) shows the result obtained for the histogram using \( M_0 = 10^6 \) diag-MC steps. This distribution falls off rapidly for \( n > n_{\text{max}} \), and, thus, we can determine the maximum value \( n_c \) of \( n \) visited by the Markov process. We choose a value of \( m \) safely greater than \( n_c \), such that the value of \( I_m \) is practically zero. Then, we modify the probabilities associated with a particular configuration of the \( n^{\text{th}} \) order by dividing the original probabilities by a factor \( f_n^{(0)} = \max(1, N_n) \). Using these modified probabilities we carry out another set of \( M_0 \) diag-MC steps which yields a new histogram with populations \( N_n^{(1)} \) shown by curve labeled by 1 in Fig. 2(b). In the next step, we divide the probabilities associated with a particular configuration of the \( n^{\text{th}} \) order by the factor \( f_n^{(1)} = f_n^{(0)} \cdot \max(1, N_n^{(1)}) \). Using these modified probabilities we carry out a new set of \( M_0 \) diag-MC steps which yields a new histogram with populations \( N_n^{(2)} \) shown by curve labeled by 2 in Fig. 2(b). We continue this process several times where the probabilities at the \( i^{\text{th}} \) step are divided by a factor \( f_n^{(i)} = f_n^{(i-1)} \cdot \max(1, N^{(i)}) \) where \( N^{(i)} \) is the population of the \( n^{\text{th}} \) order at the \( i^{\text{th}} \) step. The curves labeled 3, 4, 5 and 6 in Fig. 2(b) are obtained by repeating this process four more times. Notice that already at the 6th step the histogram is reasonably flat including for small \( n \). When, the histogram becomes more-or-less “flat” at some \( k^{\text{th}} \) step, we begin a Markov process for a relatively large number of MC steps, by dividing the original probabilities by the factor \( f_n^{(k)} \), and, by re-weighting the observables by the biasing factor \( f_n^{(k)} \) we determine \( I_n(\tau) \) and \( G(\tau) \).
Fig. 3. The results obtained using the fixed-\(\tau\) diag-MC (a) with application of the multicanonical algorithm to make the histogram of \(I_n(\tau)\) as a function of \(n\) flat. (b) with application of the WL algorithm to make the histogram of \(I_n(\tau)\) as a function of \(n\) flat. The results in both cases are compared with the exact results.

Fig. 2(a) shows the results of applying the multicanonical algorithm as discussed in the previous paragraph for the same number of MC steps and approximately the same amount of CPU time as in the calculation with the straightforward application of the diag-MC to obtain the red curve in Fig. 2(a). Notice the significant reduction of the error bars. Furthermore, the flat histogram approach allows us to calculate \(I_n(\tau)\) for almost any \(\tau\), something which is not possible using simple diag-MC.

In Fig. 3 we compare with the exact results the results for \(G(\tau)\) obtained for various values of \(\tau\) using the multicanonical method to make the histogram flat (Fig. 3(a)) or the W-L algorithm (Fig. 3(b)). Notice that the agreement holds over a range where \(G(\tau)\) changes by 14 orders of magnitude.

4. Sampling the histogram of \(G(\tau)\)

Instead of fixing \(\tau\), we can divide the interval of \(\tau\) in small intervals of fixed duration \(\delta \tau\) and we define \(g_l\) as the time average of \(G(\tau)\) inside the particular interval \(l\). In this case, what we regard as the “state” in the Markov process acquires an additional label \(l\) and becomes \(\{l, n, \lambda, \vec{R}\}\) (where \(n\) is the order, \(\lambda\) a particular diagram of order \(n\), and \(\vec{R} = (\vec{x}_1, \ldots, \vec{x}_n)\), the integration variables. Thus, we can also have transitions between different \(l\) values. In this case in order to calculate \(g_l\) we create a list \(N_l\) of the number of times the Markov random walker lands in the interval \(l\) and we can calculate the absolute value of \(g_l\) as

\[
g_l = \frac{N_l}{N_0} g_0,
\]

where \(g_0 = 1\). Notice that \(g_l/g_0\) can be a very large number, and if \(\tau\) is large enough it can be much larger than the total number of MC steps. In this case because \(N_l\) is expected to be either 0 or a very small number (and, thus, with large error), it makes sense in order to apply the flat histogram method, to map the “energy level” in the classical MC and the density of states to the particular interval \(l\) and \(g_l\) respectively. This way, the histogram of \(g_l\) becomes flat.

Fig. 3(a) compares the results obtained without application of the flat histogram method (red circles with error bars) with those obtained using the W-L method (blue squares, the size of the error in this case is smaller than the symbol-size and it omitted for clarity) to make the histogram of \(g_l\) flat. We have limited the maximum value of \(\tau\) in order to make it possible to obtain results with the simple diag-MC method, i.e., to obtain a non-zero value of \(N_0\). Again the reason for the errors in the standard diag-MC without applying the flat histogram method, is the fact that
\( N_0 \) is very small and, by using the expression (4) its error propagates to all other values of \( l \). This is shown in Fig. 3(b) where the results of different runs, each with the same number of MC steps are compared. Notice that the various lines are almost parallel to each other starting with different value at \( l = 0 \).

5. Conclusions

We have combined the idea of flat histogram methods with diagrammatic MC quantum simulation technique in order to extract the single Green function at long imaginary time. We have shown that

a) Simple application of the standard diag-MC, without some a priori knowledge about the behavior of \( G(\tau) \) at long \( \tau \), leads to either very large errors or it becomes impossible to estimate \( G(\tau) \) if \( \tau \) is large enough. We consider \( \tau \) to be large when the range of values of \( \ln(\tau) \) for various values of \( n \) or the range of values of \( G(\tau) \) in the interval \((0,\tau)\) involves many orders of magnitude.

b) To cure this problem, we used the idea of flat histogram methods: In the case where we need to apply the diag-MC by keeping \( \tau \) fixed, we made the histogram of \( \ln(\tau) \) flat for various values of \( n \). In the case where we allowed \( \tau \) to vary, which enables us to sample \( \tau \) also, we made flat the histogram of \( G(\tau) \) as function of \( \tau \).

c) We find that this is a crucial improvement over the standard diag-MC in order to extract the imaginary time behavior of the Green’s function. This allows us to extract the low-energy physics of many-body systems.

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