Flat-histogram methods in quantum Monte Carlo simulations: Application to the t-J model

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Abstract. We discuss that flat-histogram techniques can be appropriately applied in the sampling of quantum Monte Carlo simulation in order to improve the statistical quality of the results at long imaginary time or low excitation energy. Typical imaginary-time correlation functions calculated in quantum Monte Carlo are subject to exponentially growing errors as the range of imaginary time grows and this smears the information on the low energy excitations. We show that we can extract the low energy physics by modifying the Monte Carlo sampling technique to one in which configurations which contribute to making the histogram of certain quantities flat are promoted. We apply the diagrammatic Monte Carlo (diag-MC) method to the motion of a single hole in the t-J model and we show that the implementation of flat-histogram techniques allows us to calculate the Green’s function in a wide range of imaginary-time. In addition, we show that applying the flat-histogram technique alleviates the “sign”-problem associated with the simulation of the single-hole Green’s function at long imaginary time.

1. Introduction
The quantum Monte Carlo simulation technique has been very successful when dealing with equilibrium properties of system of particles which do not obey Fermi statistics[1]. This technique cannot be applied directly to real-time dynamics and one resorts in the calculation of correlation functions in imaginary-time. From the behavior of these correlation functions in imaginary-time, ground-state properties can be accurately calculated. In principle, an accurately known correlation function at long imaginary-time scales can yield useful information about the low-lying energy excitations. However, typical imaginary-time correlation functions calculated in quantum Monte Carlo are subject to exponentially growing errors as the range of imaginary-time grows. Here, we show that this problem can be significantly alleviated by applying flat-histogram ideas[2, 3, 4] in the Monte Carlo sampling of configurations which contribute to making the histogram of such correlation functions in imaginary-time flat.

Flat-histogram ideas have been successfully applied to classical simulations of systems undergoing first order phase transitions, systems with rough energy landscapes, etc. The Wang-Landau algorithm[4] (WLA), a particularly useful flat-histogram algorithm, has been applied to the simulation of equilibrium statistical mechanical properties of quantum systems[5]. Following this work, Gull et al.[6] have applied the idea to the continuous-time quantum Monte Carlo...
Carlo approach to the quantum impurity solver needed for all dynamical mean-field theory applications.

The main idea used in the present paper has been demonstrated\cite{7} in the past using the Fröhlich polaron problem\cite{8} by combining the so-called multicanonical\cite{2} (MUCA) or the Wang-Landau algorithm\cite{4} with the diagrammatic Monte Carlo (diag-MC) method\cite{9, 10}. In the present paper, we illustrate the benefit of applying flat-histogram techniques to the diag-MC sampling\cite{9, 10} in order to reveal the imaginary-time dependence of the single-hole Green’s function moving in an antiferromagnetic background as described by the two-dimensional (2D) t-J model\cite{11, 12, 13, 14, 15}. The t-J model is probably the simplest non-trivial quantum many-body model to capture the interplay between charge-carrier motion and antiferromagnetic fluctuations and it is as basic as the Ising model for classical systems. Therefore, we feel that we should not proceed any further with quantum simulation of electronic systems without having a technique which can accurately simulate such a model.

First, we use the diag-MC method in conjunction with the flat-histogram technique to the problem of a single-hole in a modified soluble version of t-J model, where, the diag-MC sampling space is restricted to the diagrams which are summed up by the non-crossing approximation (NCA). This allows us to assess the correct implementation and accuracy of the method and to have an “exact” solution to compare with the results obtained with and without application of the flat-histogram method.

Next, we sample all the diagrams without any restriction which corresponds to the fully linearized version of the t-J model without any further approximation. In this case, the sampling technique should sum up amplitudes which are not positive definite and, thus, they cannot be simply interpreted as probability in the Monte Carlo sampling technique. Namely, we encounter the so-called “sign-problem” in the application of the Monte Carlo method. We show that even in this case, where there is the “sign-problem”, we can still extract more accurate results for the imaginary-time dependence of the single-hole spectral function and, thus, more accurate results for the low-lying spectrum of the problem.

We will use two different implementations of the diag-MC method. One in which the imaginary-time dimension is not sampled by the Markov process and it is treated as a fixed parameter in a particular simulation. This requires repetition of the simulation for each one of the different values of imaginary-time needed. In the second implementation the imaginary-time is one additional dimension of the sampling space. While the latter approach may be more efficient, we will also use the former approach to demonstrate a different way to apply the flat-histogram idea in which the distribution of the order $n$ contribution to the perturbation expansion is made flat.

2. The Hamiltonian

We use a simplified version of the 2D t-J model in which the Hamiltonian and the hole-hopping terms are linearized within the spin-wave approximation to obtain a polaron-like Hamiltonian (\cite{11, 13, 14}), i.e.,

\[
\hat{H} = - \sum_{\vec{k}, \vec{q}} g(\vec{k}, \vec{q}) a_{\vec{k} + \vec{q}}^\dagger a_{\vec{k}} b_{\vec{q}}^\dagger + H.c. + \sum_{\vec{k}} \hbar \omega(\vec{k}) b_{\vec{k}}^\dagger b_{\vec{k}},
\]

\[
g(\vec{k}, \vec{q}) = \frac{4t}{\sqrt{N}} (u_{\vec{q}} \gamma_{\vec{k} - \vec{q}} + v_{\vec{q}} \gamma_{\vec{k}}), \quad \gamma_{\vec{k}} = -2t (\cos(k_x a) + \cos(k_y a)),
\]

where $b_{\vec{q}}^\dagger$ is the Bogoliubov spin-wave creation operator, $\omega(\vec{k})$ is the spin-wave dispersion of the square lattice quantum antiferromagnet and $a_{\vec{k}}^\dagger$ is the hole creation operator. Also the $g(\vec{k}, \vec{q})$ is the coupling of the hole to spin waves and $u_{\vec{q}}$ and $v_{\vec{q}}$ are the coefficients of the Bogoliubov transformation. For details of the derivation of this simplified version of the t-J model, which
remains a non-trivial quantum many-body problem, as well as for the definitions of the operators and the expression for $\omega_k$, $u_\eta$, $v_\eta$ and $g(k, \eta)$, the reader is referred to Refs. [11, 13, 14].

In order to demonstrate the importance of applying flat-histogram techniques, we will consider two cases. First, no guidance function is used in the diag-DMC simulation, which we will refer to as “bare” diag-MC, which is the straightforward way to apply the diag-MC. This is not the same as the standard implementation of diag-MC[9, 10] where some different “tricks” are applied to assist the simulation at long imaginary time. The second approach which will discuss is when a flat-histogram technique is implemented in the diag-MC simulation. When we apply any of the flat-histogram techniques in conjunction with diag-MC, we will refer to it as flat-histogram diag-MC.

3. Fixed-time diagrammatic Monte Carlo

The diagrammatic Monte Carlo technique[9, 10] is a Markov process in a space defined by all the terms (or diagrams) which appear in perturbation theory. For example, it samples the terms of the perturbation expansion of the imaginary-time single-particle Green’s function, which can be schematically written as follows:

$$G(\tau) = \sum_{\lambda} O_\lambda(\tau), \quad O_n(\tau) = \sum_{\lambda} D_n^{(\lambda)}(\tau)$$

$$D_n^{(\lambda)}(\tau) = \int d\vec{x}_1 d\vec{x}_2 ... d\vec{x}_n S_n^{(\lambda)}(\vec{x}_1, \vec{x}_2, ..., \vec{x}_n, \tau),$$

where $O_n$ represents the sum of all the diagrams of order $n$, $O_0(\tau) = G^0(\tau)$ is the Green’s function in zeroth order, and $\lambda$ is a variable which labels the contribution $D_n^{(\lambda)}$ of a particular diagram of order $n$. As the order $n$ of the expansion increases, the number of integration variables increases in a similar manner. Notice that when we refer to the $n^{th}$ order in the case of the t-J model we mean that the number of spin-wave-propagators contained in the diagrams is $n$; therefore, the order in perturbation expansion is $2n$. 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 which represents the number of times $N_n(\tau)$ the order $n$ appeared in the Markov process. Since we can compute a low order diagram analytically, say for example the zeroth order $O_0(\tau)$, the absolute value of all other orders is computed as follows:

$$O_n(\tau) = \frac{N_n(\tau)}{N_0(\tau)} O_0(\tau).$$

3.1. The problem with “bare” application of diag-MC

First, we restrict our QMC computation of $G(\tau)$ to sample the subspace spanned only by the diagrams included in the non-crossing approximation (NCA). We do that because in this case, the NCA diagrams can be summed up “exactly” ([13, 14]) and we can use this “exact” solution to judge the accuracy of our results.

In Fig. 1(a) $O_n(\tau)$ as a function of $n$ is shown for a fixed value of $\tau$ as calculated for this soluble model. Notice that the distribution of the order $n$ is Gaussian-like which peaks at a value of $n = n_{\text{max}}(\tau)$. Fig. 1(b) shows $O_n(\tau)$ 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 $O_n(\tau)$ 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 $n = 0$
Figure 1. (a) $O_n(\tau)$ as a function of $n$ for fixed $\tau$. (b) $O_n(\tau)$ as a function of $n$ for three different values of $\tau$ plotted on a logarithmic scale.

Figure 2. (a) $O_n(\tau)$ as a function of $n$ for $\tau = 5$ as calculated by repeating the diag-MC for 3 different starting configurations. (b) Same as part (a) for $\tau = 7$.

is zero or very small, it leads to a fatal situation in our attempt to calculate the absolute value of $O_n(\tau)$, because this is obtained using the formula (7) and a very small $N_0(\tau)$ implies a large uncertainty in the absolute value of all $O_n(\tau)$.

This is illustrated in Fig. 2 where the calculated $O_n(\tau)$ is shown as a function of $n$ for $\tau = 5$ and $\tau = 7$ as calculated by repeating a diag-MC simulation of $3 \times 10^8$ MC steps for 3 different starting configurations. Notice that the statistical fluctuations from one simulation to another affect the values of $O_n$ uniformly for all $n$ by the same fluctuating scale factor, i.e., $1/N_0(\tau)$. If we are to calculate the error from these fluctuations for each value of $n$, the size of the error bars would be much larger than the size of the fluctuations of the points for successive values of $n$. Namely, the points which represent $O_n(\tau)$ 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. 7. Note that using the same number of MC steps becomes impossible to calculate $O_n(\tau)$ beyond this value of $\tau = 12$ because the ratio $O_{n_{\text{max}}} / O_0$ becomes much larger than the number of MC steps.

3.2. Application of the flat-histogram technique

Here, we will solve the problem discussed in the previous subsection by adopting flat-histogram techniques which have been applied in simulations of classical statistical mechanics[2, 4]. 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 $O_n(\tau)$ to the density of states which corresponds to the corresponding configurations. The flat-histogram method renormalizes the density of states $O_n(\tau)$ for each $n$ by known factors (which can be easily estimated) and, then, samples a more-or-less flat-histogram of such populations.

![Figure 3](image.png)

**Figure 3.** (a) The evolution of the re-weighted distribution as a function of the multicanonical steps. Notice that the range where the distribution has a significant value expands as we repeat the multicanonical steps and after 6 such iterations (green curve labeled MUCA(6)) it becomes more or less flat in the entire domain. (b) $O_n(\tau)$ as a function of $n$ for $\tau = 7$ as calculated by using multicanonical diag-MC for 3 different starting configurations and by applying the multicanonical method.

Next, we use the idea of the MUCA algorithm[2] as follows: First, for a given fixed value of $\tau$ we carry out an initial exploratory run, where we find that the distribution $O_n$ of the values of $n$ peaks at some value of $n = n_{\text{max}}$, which depends on the chosen value of $\tau$. The black solid curve in Fig. 3(a) 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 $O_m$ is practically zero. Then, we modify the probabilities associated with a particular configuration of the $n^{th}$ order by dividing the original probabilities by a factor $f_n = \max (1, N_n)$. Using these modified probabilities we carry out another set of $M_0$ diag-MC steps which yields a new histogram with populations $N'_n$ shown by the red curve in Fig. 3(a). In the next step, we divide the probabilities associated with a particular configuration of the $n^{th}$ order by the factor $f'_n = f_n \times \max (1, N'_n)$. Using these modified probabilities we carry out a new set of $M_0$ diag-MC
steps which yields a new histogram with populations $N''$, etc. The blue and green curves in Fig. 3(a) are obtained in the third and sixth iteration of this process. Notice that already at the $6^{th}$ step the histogram is reasonably flat. When the histogram becomes more-or-less “flat” at some $k^{th}$ 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 $O_n(\tau)$ and $G(\tau)$.

Fig. 3(b) shows the results of applying the MUCA 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 curves in Fig. 2(b). Notice the significant reduction of the statistical fluctuations between the three different simulations. Furthermore, the flat-histogram approach allows us to calculate $O_n(\tau)$ for almost any $\tau$, something which is not possible using bare diag-MC.

4. Sampling the imaginary time $\tau$ in the diag-MC

Here we discuss the usual implementation of the diag-MC where the imaginary time variable is also a dimension of the sampling space. In this case the random walk makes a series of transitions between states $\{n, \lambda, \vec{R}, i\} \rightarrow \{n', \lambda', \vec{R}', i'\}$, where $\vec{R} = (\vec{x}_1, \ldots, \vec{x}_n)$, $n$ is the perturbation order, $\lambda$ is a particular diagram, and $i$ (or $i'$) is the label of a particular imaginary time interval $(\tau_i - \delta\tau/2, \tau_i + \delta\tau/2)$ (where $\delta\tau = \tau_{i+1} - \tau_i$). Namely, in this case we sample the histogram of $G(\tau)$ by including the imaginary time as an extra dimension of the sampling space. In this case, the value $G_i$ of the histogram $G(\tau_i)$ in the $i^{th}$ $\tau$-interval is found by using the known value of $G_0$ in the first interval, namely,

$$G_i = \frac{N_i}{N_0} G_0, \quad (6)$$

where $N_i$ is the number of occurrences of the MC random walk in the $i^{th}$ interval.

In Fig. 4 we illustrate what the problem is with the bare diag-MC. We first notice that the error in $G(\tau)$ for a given number of MC steps grow exponentially with the maximum value of $\tau_{\text{max}}$ used in this simulation. The reason is that because the exponential dependence of $G(\tau)$ on $\tau$ itself (See Fig. 4(a)), given a fixed number of MC steps, when $\tau$ is sampled, during the Markov process, the number of occurrences $N_0$ in the $\tau = 0$ interval is exponential small with the value of $\tau_{\text{max}}$ used. Since the value of $N_0$ enters in the Eq. 6 for $G_i$, the fluctuations in $G_i$ increase exponentially with increasing $\tau_{\text{max}}$ in this case. This is illustrated in Fig. 4(b) where the relative errors in $G_i$ are given for various values of $\tau_{\text{max}}$. For comparison, the relative errors obtained by using the Wang-Landau technique to make the histogram of $G_i$ flat and for approximately the same amount of CPU time to that used in the bare diag-MC simulation, is also shown in Fig. 4(b). Notice that by increasing $\tau_{\text{max}}$ the error in the bare diag-MC increases more or less uniformly for all values of $\tau$ and it is much larger than the error obtained after the application of the WLA.

5. Results for the full t-J model

Here, we present the results for the full t-J model, where we sample all the diagrams using diag-MC. First, we will keep the imaginary time fixed and in the second part we will present the case when $\tau$ is also sampled.

5.1. Fixed-time diagrammatic Monte Carlo

First, we note that some terms in a given order $O_n$ have a positive contribution, while some other terms have a negative contribution. We separate these contributions to $O_n^+$ and $-O_n^-$ such that $O_n = O_n^+ - O_n^-$ where both $O_n^\pm$ are positive.
The diag-MC process for fixed $\tau$ discussed in Sec. 3 generates a histogram which represents the number of times $N^+_{n}(\tau)$ and $N^-_{n}(\tau)$ a given order $n$ appeared in the Markov process with positive or negative sign. Then, we can compute $O^\pm_{n}$ using the ratio of these occurrences, i.e.,

$$O^\pm_{n}(\tau) = \frac{N^\pm_{n}(\tau)}{N^0_{n}(\tau)}O^0_{0}(\tau). \quad (7)$$

Notice that we have used $O^+_{0}$ as a reference in both cases because $O^-_{0} = 0$.

In Fig. 5 we illustrate both contributions $O^\pm_{n}$ obtained by applying the diag-MC+MUCA sampling for $3 \times 10^8$ MC steps for $\tau = 4$ and $\tau = 5$. Notice that the two contributions $O^+_{n}$ and $O^-_{n}$ are close and their relative difference decreases exponentially with $\tau$, thus, the statistical error increases exponentially with $\tau$. This is a manifestation of the so-called “sign-problem” in quantum Monte Carlo simulation. In this case the problem with the bare application of the diag-MC discussed in Sec. 3.1, is significantly enhanced due to the increased fluctuations in each of the $N^\pm_{n}$ distributions themselves with increasing $\tau$.

We can apply the flat-histogram technique as discussed in Sec.3.2 to each of the distributions $O^\pm_{n}$ simultaneously as illustrated in Fig. 6(a). This approach by reducing the statistical fluctuations in $O^\pm_{n}(\tau)$, for large $\tau$, allows us to obtain a more accurate $G(\tau)$ as illustrated in Fig. 6(b). In Fig. 6(b) we present $G(\tau)$ for the full t-J model using $J/t = 0.3$ and for $\vec{k} = (\pi/2, \pi/2)$ calculated for 20 different diag-MC runs using diag-MC with (red crosses) and without (open blue circles) the application of the multicanonical approach and for the same number of MC steps in each one of these MC simulations. Notice that as $\tau$ increases the statistical fluctuations of $G(\tau)$ obtained with bare diag-MC are larger than those obtained with the application of the flat-histogram technique.

### 5.2. Sampling the histogram of $G(\tau)$.

We can also apply the flat-histogram approach when we include $\tau$ as a dimension of the sampling space for the full t-J model. In this case, as in Sec. 4, we make the histogram of $G(\tau)$ flat.

Once again we wish to demonstrate the need for the application of flat-histogram techniques. In Fig. 7(a) we present the positive and negative contributions $G^\pm(\tau)$ to $G(\tau)$ calculated with
**Figure 5.** The calculated $O_n^\pm(\tau)$ for the full t-J model using $J/t = 0.3$ and for $\vec{k} = (\pi/2, \pi/2)$ for (a) $\tau = 4$ and (b) $\tau = 5$.

**Figure 6.** (a) Demonstration of the application of the flat-histogram approach to make both histograms $N_n^\pm(\tau)$ flat as a function of $n$. This is illustrated for $\tau = 5$ after one application of multicanonical step (MUCA(1)) and after a second multicanonical step (MUCA(2)). (b) $G(\tau)$ calculated for 20 diag-MC runs using diag-MC without (open blue circles) and with (red crosses) the application of flat-histogram technique.

The bare diag-MC and in Fig. 7(b) we present the results of the calculation of $G(\tau)$ and the $G^2(\tau)$ contributions using diag-MC with the application of the WLA. We note that while both calculations were carried out for approximately the same amount of CPU time (200 repetitions of $10^8$ MC steps each), for the bare diag-MC case we used $\tau_{max} = 3.8$, while for diag-MC+WLA we used $\tau_{max} = 4.8$. If we were to extend the value of $\tau_{max}$ for the former calculation to the value used in the latter calculation, most like there would be no occurrences of the Markov...
process in the crucial interval of $\tau = 0$. The reason is that the exponential growth of $G(\tau)$ “pushes” all the occurrences of the Markov process at high value of $\tau$. This is evident for this smaller value of $\tau_{\text{max}}$ by the large fluctuations which are more clearly noticeable at low values of $\tau$. In Fig. 8(a) we show the relative errors for various values of $\tau_{\text{max}}$ when calculated with the bare diag-MC method. Notice that the error in $G^{\pm}(\tau)$ for a given number of MC steps grows exponentially with the maximum value of $\tau_{\text{max}}$ used in this simulation because of the exponential dependence of $G^{\pm}(\tau)$ on $\tau$ itself. In Fig. 8(a) we also present the error obtained when the WLA is applied in conjunction with the diag-MC for approximately the same amount of CPU time. This comparison suggests that the gain of the application of the WLA is significant.

In Fig. 8(b) the relative errors of $G^{\pm}(\tau)$ and $G(\tau)$ are shown. We can understand the reduction of error when applying the flat-histogram technique in a very simple way as follows. For a given value of $\tau$ the error on both $G^{+}(\tau)$ and $G^{-}(\tau)$ is significantly reduced when combining the diag-MC technique with the flat-histogram technique. The reason for this is essentially the same as in the case of the NCA (Sec. 4) where every diagrammatic contribution is positive definite. As a result the error in the difference $G(\tau) = G^{+}(\tau) - G^{-}(\tau)$ is also significantly reduced. Thus, the flat-histogram technique is reducing the error in $G(\tau)$ itself.

6. Discussion
We demonstrated that the combination of the flat-histogram techniques with the diag-MC method yields a significant improvement over the bare diag-MC method. This combination has been applied to extract the imaginary-time single-hole Green’s function $G(\tau)$ in the t-J model.

First, we restricted our sampling space to only those non-crossing diagrams whose contribution is positive-definite and, thus, can be regarded as a probability distribution. We found that the combination of flat-histogram techniques with the diag-MC method yields much more accurate results for $G(\tau)$ over a wide range of the imaginary-time $\tau$.

Second, when we sampled the entire diagrammatic space, without the NCA restriction, there are both positive and negative contributions from non NCA diagrams. The positive and
negative contributions approach each other exponentially as we increase $\tau$, thus, the error in the difference, i.e., $G(\tau)$, grows exponentially with increasing $\tau$. This is very similar to the “sign” problem in other quantum Monte Carlo simulations of fermions where the statistical error increases exponentially as a function of the particle number. The application of the flat-histogram technique with the diag-MC allows us to obtain more accurate results on both the positive and the negative contributions to $G(\tau)$. This enables us to compute $G(\tau)$ in a wider range of $\tau$.

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