Flat histogram diagrammatic Monte Carlo method

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The diagrammatic Monte Carlo (Diag-MC) method is a numerical technique which samples the entire diagrammatic series of the Green’s function in quantum many-body systems. In this Letter, we incorporate the flat histogram principle in the diagrammatic Monte method and we term the improved version “Flat Histogram Diagrammatic Monte Carlo” method. We demonstrate the superiority of the method over the standard Diag-MC in extracting the long-imaginary-time behavior of the Green’s function, without incorporating any a priori knowledge about this function, by applying the technique to the polaron problem.

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Quantum Monte Carlo methods for bosonic systems continue to provide very useful insight into the nature of such systems and can be carried out on very large size systems which allows extrapolation to the thermodynamic limit. Interacting fermion systems and frustrated spin systems in more than one dimension, however, are plagued with the infamous so-called minus-sign problem, which leads to exponential growth of the statistical error with the system size. Since most real systems are “deep down” fermionic, including the electronic structure of solids, and the nuclear, neutron and quark matter, computational physics faces a bottleneck of paramount importance.

The diagrammatic Monte Carlo (diag-MC) method¹,², which has been successfully applied to a wide variety of problems in a range of fields, including ultra-cold atoms trapped in optical lattices³, superconductivity³, the Fermi-polaron problem⁴, systems of correlated fermions⁵,⁶,⁷, in systems of excitons⁸, and frustrated quantum spin systems⁹, is based on the interpretation of the entire sum of all Feynman diagrams as an ensemble averaging process over their corresponding configuration space. Thus, a Markov sequence \(d_0, d_1, \ldots, d_n, \ldots\), can be defined by means of transitions \(d \rightarrow d'\) based on the weights of the particular series of Feynman diagrams, which samples these diagrammatic terms with the exact relative weights as in the diagrammatic expansion. One of the great advantages of the method is that it sums only the linked diagrams and, thus, in the case of fermion systems, the infamous minus-sign problem could become a minus-sign “blessing”¹¹.

In addition to the large cancellation due to the interference terms due to the fermion statistics, which severely limits the “signal-to-noise” ratio in MC simulation of fermionic systems, we also face the problem of extracting the low-energy physics in most many-body problems. In calculating the Green’s function in imaginary time \(\tau\), this problem shows up in our attempt to estimate the long-time behavior of these functions as a function of \(\tau\). In this limit the Green’s function decays rapidly (because of the other high energy excitations) and, it quickly becomes very small and the information about the low-lying excitations gets lost in the noise of numerical data.

The so-called “flat histogram methods”¹² ¹⁴ have been used to improve the Monte-Carlo simulation of classical systems, for example for systems undergoing first order phase transitions, systems with rough energy landscapes, etc. In addition, the Wang-Landau algorithm¹⁴ has been applied to the simulation of equilibrium statistical mechanical properties of quantum systems¹³. More precisely, Troyer et al.¹⁵ have used the fact that quantum Monte Carlo simulation uses the mapping of a quantum many-body system to a classical system which allows them to generalize the use of the flat histogram method to this case. Using this generalization, they show that the algorithm becomes efficient by greatly reducing the tunneling problem in first order phase transitions and, in addition, the algorithm allows them to calculate directly the free-energy and entropy.

In this Letter, we introduce a new version of the diag-MC which is superior to standard diag-MC because it allows us to extract the long imaginary-time (low energy) behavior of the Green’s function \(G(\tau)\) accurately without using any a priori knowledge about the behavior of \(G(\tau)\). The idea of this new method is based on combining the principle of flat histograms¹² ¹⁴ and the diag-MC method. This “flat histogram diagrammatic Monte Carlo” (FHDMC) method allows us to calculate accurately and directly, without introducing any “tricks”² and with no a priori knowledge, the imaginary-time dependence of the Green’s function which varies over many orders of magnitude. In this Letter, we first introduce the general method of the FHDMC and, then, the efficiency of the method is demonstrated in the example of the Fröhlich polaron problem¹⁶ ¹⁷ where the standard diag-MC method has been extensively shown to be inaccurate¹ ².

First, let us consider a simple case of the diagrammatic
Monte Carlo method in order to illustrate the new idea. The Diag-MC method is a Markov process which samples an infinite series of the form:

\[ G(\tau) = \sum_{n}^\infty I_n(\tau), \quad I_0(\tau) = G^0(\tau), \quad (1) \]

\[ I_n(\tau) = \int d\vec{x}_1 d\vec{x}_2 ... d\vec{x}_n F_n(\vec{x}_1, \vec{x}_2, ..., \vec{x}_n, \tau), \quad (2) \]

where as the order \( n \) of the expansion increases, the number of integration variables increases in a similar manner.

The Diag-MC method is a Markov process \( n \to n' \) which generates the distribution \( I_0(\tau), I_1(\tau), I_2(\tau), ..., I_n(\tau), ... \). The entire sum \( G(\tau) \) can be calculated stochastically if we know the exact value of one of the terms, say, \( I_0(\tau) \). Then,

\[ I_n(\tau) = \frac{N_n}{N_0} I_0(\tau), \quad (3) \]

where \( N_k \) is the number of times the \( n^{th} \) term appears in the Markov sequence. As a result the fluctuations (and the error) in estimating \( I_n(\tau) \) depends crucially on the fluctuations of \( N_0 \). As a result if the value of \( I_0(\tau) \) relative to other terms of the series is small, then, the population \( N_0 \) could be a small fraction of the total population \( N_T = \sum_{n=0}^\infty N_n \), which is the total number of MC steps, and, thus, the error in the estimate of \( I_n(\tau) \) by using the above expression will be large. To be more concrete, as the value of \( \tau \) increases the values of \( n \) giving the most significant contribution to \( G(\tau) \) increases exponentially with \( \tau \). Namely, \( I_n \), as a function of \( n \), peaks at a value \( n = n_{\text{max}} \) which increases exponentially with increasing \( \tau \). Therefore, for large enough values of \( \tau \) the ratio \( I_{n_{\text{max}}}/I_0 \) becomes many orders of magnitude larger than unity. This corresponds to the problem of critical slowing down in classical MC simulation, a problem which can be addressed by the flat histogram methods\(^{[12–14]}\).

The flat histogram method renormalizes these populations by known factors (which can be easily estimated) and, then, samples a more-or-less flat histogram of such populations.

We will apply flat histogram methods\(^{[12–14]}\) on two different versions of applying the diag-MC.

**Sampling of \( G(\tau) \) for a fixed value of \( \tau \):** In order to apply any flat histogram technique to our problem we map the particular value of \( n \) to the “energy” level in standard flat histogram methods for classical statistical mechanics and the integrals \( I_n(\tau) \) to the density of states which corresponds to the corresponding configurations.

**Sampling of the histogram of \( G(\tau) \):** We divide the range of \( \tau \), i.e., \([0, \tau_{\text{max}}]\) into \( L \) equal intervals \( \delta_\tau = [\tau_i, \tau_{i+1}] \), where \( \tau_{i+1} = \tau_i + \Delta \tau \). In this case the variable \( \tau \) is also sampled by the same Markov process.

The histogram \( g_l \) of \( G(\tau) \) defined as

\[ g_l = \frac{1}{\Delta \tau} \int_{\tau_{l-1}}^{\tau_l} d\tau G(\tau), \quad (4) \]

requires the histograms \( I_k^{(l)} \) of \( I_k(\tau) \) defined by

\[ I_k^{(l)} = \frac{1}{\Delta \tau} \int_{\tau_{l-1}}^{\tau_l} d\tau I_k(\tau), \quad (5) \]

such that

\[ g_l = \sum_{k=0}^{\infty} I_k^{(l)} \quad (6) \]

The FHDMC can be applied in a similar way to the one discussed in the case for fixed \( \tau \). Here, we apply the flat histogram methods to find the histogram \( g_l \) by mapping the value of the interval \( l \) to the “energy” level and \( g_l \) to the “density-of-states” in the classical case.

For each one of these two cases we have chosen to apply both multicanonical\(^{[12]}\) and the Wang-Landau (W-L) algorithm\(^{[14]}\).

The standard Diag-MC has been extensively applied to the Fröhlich polaron Hamiltonian which describes a single electron in a phonon field:

\[ H = \sum_k e(k) a_k^\dagger a_k + \omega_0 \sum_k b_k^\dagger b_k + \frac{1}{2} \]

\[ + \sum_{k,q} V(q)(b_k^\dagger b_{-q}^\dagger a_k a_{-q}) \]

\[ V(q) = \frac{i}{\sqrt{\Lambda}} \sqrt{2 \pi} \frac{1}{q} e(k) = \frac{k^2}{2} \quad (8) \]

where the summation extends over the first Brillouin zone and \( \Lambda \) is the volume of the system. This Hamiltonian takes into account a single optical phonon with fixed frequency \( \omega_0 \) and \( a_k^\dagger \) and \( b_k^\dagger \) are electron and phonon creation operators. Here, we will work in imaginary time at \( T = 0 \). The free electron and phonon propagators are respectively given by

\[ G^0(k, \tau_2 - \tau_1) = e^{-e(k)(\tau_2 - \tau_1)} \Theta(\tau_2 - \tau_1), \quad (9) \]

\[ D(q, \tau_2 - \tau_1) = e^{-\omega_0(\tau_2 - \tau_1)}. \quad (10) \]

While the Diag-MC algorithm and our computer program are quite general and can solve exactly (within statistical errors) the single polaron problem, we choose to restrict ourselves to sampling only the diagrams of the infinite series shown in Fig. 1. The reason is that we can sum up this infinite series of selected diagrams exactly and this allows us to compare the results of the standard Diag-MC and the FHDMC with the exact solution. This series is summed by solving Dyson’s equation which for the case of \( k = 0 \) is given as:

\[ G(\tau) = G^0(\tau) + \int d\tau_2 \int d\tau_1 G^0(\tau_1) \Sigma(\tau_2 - \tau_1) \]

\[ \times G(\tau - \tau_2), \quad (11) \]

\[ \Sigma(\tau') = 2\alpha \sqrt{2\pi} \int \frac{d^3 q}{(2\pi)^3} \frac{1}{q^2} e^{-(q^2/2+1)\tau'}. \quad (12) \]
where we have taken $\omega_0 = 1$. This equation can be transformed in Laplace’s space, using the properties of convolution integrals, as follows:

$$G(s) = \tilde{G}^0(s) + \tilde{G}^0(s)\tilde{\Sigma}(s)G(s), \tag{13}$$

$$\tilde{G}^0(s) = \frac{1}{s}, \quad \tilde{\Sigma}(s) = \frac{\alpha}{\sqrt{s+1}} \quad \Re(s) > -1 \tag{14}$$

which yields

$$\tilde{G}(s) = \frac{\sqrt{s+1}}{s\sqrt{s+1} - \alpha}. \tag{15}$$

The inverse Laplace transform is given by

$$G(\tau) = \frac{1}{2\pi i} \lim_{T \to \infty} \int_{\sigma-iT}^{\sigma+iT} \tilde{G}(s)e^{\tau s} ds, \quad \sigma > 0. \tag{16}$$

Using the corresponding Bromwich contour we obtain:

$$G(\tau) = A_0 e^{s_1\tau} + \frac{e^{-\tau}}{2\pi i} \int_0^\infty \frac{2\alpha \sqrt{t} e^{-\tau t}}{t^2 + \alpha^2} dr, \tag{17}$$

$$A_0 = \frac{s_1^2 + s_1 + \alpha \sqrt{s_1 + 1}}{(s_1 - s_2)(s_1 - s_3)}, \tag{18}$$

where $s_1, s_2, s_3$ are the three roots of the equation $s^3 + s^2 - \alpha^2 = 0$, $s_1$ is the real root and $s_2$ and $s_3$ are complex conjugate to each other. For $\alpha = 2$ we find that $s_1 = 1.314596$ and $A_0 = 0.7788386$. Asymptotically for $\tau \to \infty$ we have

$$G(\tau) = A_0 e^{s_1\tau}. \tag{19}$$

Therefore, the polaron ground state energy in the approximation given by the series in Fig. 1 is $E_0 = -s_1$. For a finite chemical potential $\mu$, $G(\tau)$ should be modified to $A_0 \exp((s_1 + \mu)\tau)$.

**Fixed \( \tau \) diag-MC**: As discussed earlier we have applied the diag-MC for fixed $\tau$. The fixed-$\tau$ diag-MC is very similar to the approach outlined by Prokof’ev et al. [1]. It includes only transitions from order $n$ to $n + 1$ where we select the beginning $\tau_1$, the end $\tau_2$ and the momentum $q$ of the phonon propagator. In addition, it includes transitions from $n$ to $n - 1$ (except when $n = 0$; this exception modifies the acceptance rate from 0 to 1 compared to all other transitions originating from $n \neq 0$) where the phonon propagator is removed. We modify this part of the general simulation algorithm in order to simulate only the series in Fig. 1 as follows: when we attempt the MC move $n \to n + 1$, i.e., we attempt to add a new phonon propagator at time instants $\tau_1^{(n+1)}$ and $\tau_2^{(n+1)}$, the free fermion line where the instant $\tau_1^{(n+1)}$ is to be inserted is selected to be one of those existing free-fermion lines which do not have the same ends with one and the same phonon propagator, and $\tau_2^{(n+1)}$ is selected to be between $\tau_1^{(n+1)}$ and the end of the selected free-fermion line.

**Sampling of the histogram of \( G(\tau) \)**: As discussed earlier in this case we consider the histogram in the intervals $\delta_i$. Using the behavior of $G(\tau)$ for large $\tau$ we calculate the ground state energy. The updating procedure between different orders $n$ is the same as in the case of fixed $\tau$ discussed in the previous paragraph. In addition, here, we allow transitions to a different time $\tau'$ which may belong to a different interval. The value of $\tau'$ is selected as in Ref. [1], with the only difference that $\tau'$ is selected in the interval $[\tau_{\text{end}}, \tau_{\text{max}}]$, instead of the interval $[\tau_{\text{end}}, \infty]$ (where $\tau_{\text{end}}$ is the end of the last phonon propagator in the particular diagram).

**Fig. 2** presents the results of our calculation of $G(\tau)$ for fixed values of $\tau$. The results of FHDMC were obtained with the application of multicanonical [12] and Wang-Landau [14] (W-L) algorithm for the reduced polaron problem. We calculated $G(\tau)$ for $\tau = 25.0, 26.0, ..., 49.0$ and for approximately the same number of diag-MC steps which corresponds to approximately the same amount of CPU time for comparison.

In our multicanonical simulation for a given value of $\tau$, our tolerance for the value of histogram of $I_n(\tau)$ for any $n$ was lower than twice and higher than half the value of the histogram for $I_0(\tau)$. Renormalization of the “density of states” was performed every $10^9$ iterations for a total number of $2 \times 10^8$ iterations. We also carried out calculations were histogram updates were made every $10^4$ and $10^5$ iterations keeping the same total number of iterations, however, the error was larger.

In our simulation using the W-L algorithm, we gave

![FIG. 1: (Color online) Top: An infinite series of selected diagrams contributing to the single electron Green’s function. Bottom: The Dyson equation which sums the selected series. The wiggly line denotes a phonon propagator, while a thin (thick) solid line denotes the bare (renormalized) fermion propagator.](image-url)
the modification factor \( f \) the initial value \( f = 1 \) and we reduce it according to \( f_{i+1} = \sqrt{f_i} \) every time the histogram became “flat” within our tolerance. Our tolerance for “flatness” was such that the absolute value of the difference of the histogram \( H_n \) for each value of \( n \) from the average value of the histogram \( \bar{H} \) to be less than \( \frac{\bar{H}}{10} \). The “flatness” of the histogram was assessed every \( 10^5 \) iterations. Choosing the final value for \( f \) to be \( 1.000007629 \), the total number of iterations required was \( 8 \times 10^8 \).

Notice that, while the W-L algorithm works better, both flat histogram algorithms yield \( G(\tau) \) for any \( \tau \) including very long-\( \tau \) where \( G(\tau) \) varies over many orders of magnitude. By fitting the long imaginary-time part of the Green’s function to a single exponential \( G(\tau) = Ze^{-E_0\tau} \), we find that in the case of multicanonical the ground state energy is \( E_0 = -1.31 \pm 0.01 \) and \( Z = 0.77 \pm 0.33 \), while in the case of the W-L algorithm \( E_0 = -1.311 \pm 0.004 \) and \( Z = 0.88 \pm 0.12 \). The exact values are \( E_0 = -1.3146 \) and \( Z = 0.77883 \).

Fig. 3 compares the results of our FHDMC for \( g_1 \) obtained with the W-L algorithm with the results of the standard implementation of the diag-MC where a finite chemical potential \( \mu \) is used as a “tunable” parameter. Our simulation using the W-L algorithm was done as described earlier when discussing the results of Fig. 2 for the calculation of \( G(\tau) \) for constant \( \tau \). The total number of iterations were \( 3.07 \times 10^8 \) and this required a final value of the factor \( f = 1.000006100 \). For comparison the diag-MC method was also applied for the same number of iterations. This, however, does not include the time to determine the “optimum” value of \( \mu \). We notice that the results of the FHDMC and the standard diag-MC shown in Fig. 3 are similar. If \( \mu = 0 \) or a different \( \mu \) than its optimum value is used, the results of the diag-MC for this range of \( \tau \) are very bad.

The diag-DMC, as has been applied in the polaron problem \cite{2}, uses the chemical potential as a “tunable parameter” to reduce the statistical variance at long-\( \tau \). In this particular problem, the exact asymptotic solution for \( G(\tau) \) is a single exponential, \( G(\tau) = Z \exp(-E_0\tau) \), where \( E_0 \) is the ground state. Therefore, using the chemical potential \( \mu \), which corresponds to multiplying \( G(\tau) \) by an exponential factor \( \exp(\mu \tau) \), with \( \mu \) as a tunable parameter, is effectively a simple way to make the histogram flat at long-\( \tau \), which occurs when \( \mu \sim E_0 \). This works when there is a gap in the problem, i.e., where there is a single exponential governing the asymptotic behavior of \( G(\tau) \). However, this is not a general enough method to be applied to a different problem where the long-\( \tau \) behavior is not governed by a single exponential, or we are interested, in addition to the ground state, to other low lying excitations. The method presented here, however, constructs the exact “density of states”, with no a priori knowledge about it.

In conclusion, we have presented the FHDMC method to improve the standard diag-MC based on the idea of
flat histogram methods. This idea was demonstrated on an exactly soluble problem, however, our method is very general and can be implemented for any problem where the diagrammatic MC method can be applied. We have shown with this method that the statistical fluctuations can be controlled even for very large values of the imaginary time without the need for any a priori knowledge about the behavior of $G(\tau)$.

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