I. INTRODUCTION

Quantum Monte Carlo simulation, an undeniable useful tool in addressing a number of issues in quantum many-body physics, cannot be used to simulate real-time dynamics. By means of analytic continuation to Euclidean time \( t \to -i\tau \), however, the Schrödinger equation turns into a diffusion equation, which can be simulated using random walks which explore the potential landscape by spending proportionately more “time” near the valleys of the potential and less “time” near the potential heights. The transformation into imaginary time turns the path integral representation of the evolution operator from an integral over paths of computationally “nasty” phase factors, a problem almost impossible to treat stochastically, into an integral over paths in imaginary time weighted by a real and positive “Boltzmann-like” weight; this weight is interpreted as a well-behaved probability for a particular path to contribute to the sum and this interpretation allows a straightforward stochastic treatment\(^6\).

This transformation, by itself, is useful because it yields the interacting ground state and physical quantities related to the equilibrium statistical mechanical description of a quantum many-body system. However, if we are interested in obtaining information about the real-time dynamics and information about the excitations of the system, an “inversion” of this ill-defined transformation for the results of correlation functions \( C(\tau) \) of an operator \( \hat{O} \) representing a physical observable, namely,

\[
C(\tau) = \langle \hat{T}_\tau \hat{O}(\tau) \hat{O}^\dagger(0) \rangle,
\]

(1)

(where \( \hat{T}_\tau \) is the imaginary-time ordering operator) from the imaginary time \( \tau \) back to real time \( t \) is required.

The analytic continuation to real-time proceeds by means of a “numerical inversion” of the QMC data on \( C(\tau) \) to find the spectral function \( A(\omega) \). These inversion techniques, such as the so-called maximum entropy method\(^2\) or its generalization, the so-called stochastic analytical inference (SAI) method\(^3,4\), require very accurate QMC data on \( C(\tau) \). Since collective phenomena emerge at energy scales significantly smaller than the typical short-range interaction energy scale, we are mainly interested in sampling the long imaginary part of such response or correlation functions. Such response functions obtained by QMC are noisy data and in a limited \( \tau \) range. If we are interested in extracting the low energy excitations, this information hides more clearly in the long-imaginary-time evolution of the correlation functions which is typically obscured by statistical errors.

Flat histogram methods have been very useful in classical systems\(^5,8\) where they have been used to overcome problems in simulations of first order phase transitions, systems with rough energy landscapes, etc. The flat histogram idea has been extended in quantum many-body systems and, in particular, in stochastic series expansion\(^9\) to overcome the tunneling problem in first order phase transitions, in the continuous-time quantum Monte Carlo approach to the impurity solver problem used in dynamical mean-field-theory DMFT\(^10\) and the diagrammatic Monte Carlo method\(^11\).

The main idea presented in this paper, in simple terms, is the following. We show that the flat-histogram method can be applied to the QMC method itself to make the histogram of \( C(\tau) \) flat for all \( \tau \) by sampling the variable \( \tau \), and keeping track of the factors in each imaginary-time interval needed to achieve this result. In this way, the stochastic error on \( C(\tau) \) becomes the same for the entire range of \( \tau \) of our interest. This approach allows us to achieve much greater degree of accuracy when inverting the information contained in \( C(\tau) \) to find its corresponding spectral function \( A(\omega) \) in the entire range of values of \( \omega \) of our interest.

In order to demonstrate the idea in the present paper, we need to make specific choices of i) a non-trivial quantum many-body problem, ii) a specific QMC method, iii) a specific correlation function \( C(\tau) \), and iv) a method
to carry out the analytic continuation. Using the same methods and techniques we will calculate the spectral function \(A(\omega)\) using QMC with and without the application of the flat histogram method during the QMC runs which produce the data on \(C(\tau)\). We will show that the flat histogram QMC method is superior to the standard QMC for such important observables. Using our past specific experience with models and QMC techniques, we choose the problem of the Green’s function \(G_{\vec{k}}(\tau)\) of a single hole in the \(t-J\) model[12, 13] with the diagrammatic Monte Carlo (DMC) method[11] using the method of the stochastic analytical inference[3] for the analytic continuation to obtain the spectral function \(A_{\vec{k}}(\omega)\) from the QMC data obtained for \(G_{\vec{k}}(\tau)\).

The paper is organized as follows. In Sec. II we describe the problem, the model, and the general approach we will follow. Sec. III describes the computational details and our implementation of the analytic continuation technique which we adopted. In Sec. IV we present the results of the spectral function obtained with our method, which are compared to what we believe to be the “exact” results of a soluble but restricted version of the \(t-J\) model. In addition, our results are compared to those obtained without the application of the flat histogram idea during the DMC simulation. Lastly, in Sec. V we present the main conclusions of the paper.

II. THE METHOD

In order to be precise we take the example where the operator \(\hat{O}^\dagger\) is the single particle creation operator \(a_{\vec{k}}^\dagger\) in which case \(C(\tau)\) becomes the single particle Green’s function \(G_{\vec{k}}(\tau)\) in imaginary time. In this case the spectral function \(A_{\vec{k}}(\omega)\) is related to \(G\) as follows

\[
G_{\vec{k}}(\tau) = \int d\omega K(\tau, \omega) A_{\vec{k}}(\omega),
\]

where the so-called kernel \(K(\tau, \omega)\) is simply \(e^{-\omega \tau}\). The spectral function is a non-negative quantity normalized to unity.

We consider a finite imaginary time range, \(0 < \tau < \tau_{\text{max}}\) and we divide it into \(L\) equal intervals. By integrating Eq. 2 in each time interval \(i\) we obtain

\[
G_{\vec{k}}^i = \int d\omega \bar{K}(i, \omega) A_{\vec{k}}^i(\omega),
\]

\[
G_{\vec{k}}^i = \frac{1}{\Delta \tau} \int_{\tau_{i-1}}^{\tau_i} G_{\vec{k}}(\tau) d\tau,
\]

and \(\bar{K}(i, \omega)\) is the average value of the kernel \(K(\tau, \omega) = e^{-\omega \tau}\) in the \(i\) interval, i.e., \(\bar{K}(i, \omega) = \frac{e^{-\omega \tau_i} - e^{-\omega \tau_{i-1}}}{\Delta \tau}\).

In Ref. 11, we have shown that we can apply the flat histogram technique on the so-called diagrammatic Monte Carlo method[14, 15] to make the histogram \(G_{\vec{k}}^i(\tau)\) of \(G_{\vec{k}}(\tau)\) flat. The idea was demonstrated on the Fröhlich polaron problem. The results of the flat histogram DMC (FHDMC) on the estimate for the polaron ground state were significantly better than the result of the standard-DMC. However, as argued in the paper[11] the polaron problem spectrum was characterized by a gap, and the full advantage of the flat histogram method over standard-DMC could not fully demonstrated.

In the present paper we use a simplified version of the \(t-J\) model, in which the Heisenberg and the hole-hopping terms are linearized within the spin-wave approximation to obtain a polaron-like Hamiltonian[20], i.e.,

\[
\hat{H} = \frac{t_2}{\sqrt{N}} \sum_{\vec{k}, \vec{q}} g(\vec{k}, \vec{q}) h^\dagger_{\vec{k}+\vec{q}} h_{\vec{k}} h_{\vec{q}} + H.c.
\]

\[
+ \sum_{\vec{k}} \hbar \omega(k) b^\dagger_{\vec{k}} b_{\vec{k}},
\]

where the operator \(b_{\vec{k}}\) is the Bogoliubov spin-wave creation operator, \(\omega(k)\) is the spin-wave dispersion of the square lattice quantum antiferromagnet[21] and \(h_{\vec{k}}\) is the hole creation operator. Here \(g(\vec{k}, \vec{q})\) is the coupling of the hole to spin waves and its expression in terms of the coefficients of the Bogoliubov transformation is given in Refs.[13, 20].

It is well-known that the single-hole spectral function of the above Hamiltonian can be obtained within the non-crossing approximation (NCA)[12, 13, 20]. The diagrammatic Monte Carlo (DMC) method with or without[10–10] the incorporation of the flat histogram technique can be applied to the problem of a single-hole. In this paper in order to demonstrate the method, we wish to restrict our DMC to the sampling of only the diagrams contributing to the NCA. This restriction is actually a more difficult approach to numerically implement than the one in which the Markov process samples all the connected diagrams contributing to \(G_{\vec{k}}(\tau)\). The reason for restricting ourselves within the NCA diagrammatic space, is because in this case there is an “exact” solution to the problem which we can use to measure the success of the approach discussed here.

Our QMC data analyzed in this paper are obtained by the application of the FHDMC and the standard DMC to calculate \(G_{\vec{k}}(\tau)\) for \(\vec{k} = (\pi/2, \pi/2)\) and \(J/t = 0.2\). In order to obtain the “exact” solution, we have recalculated the single-hole Green’s function within the NCA approach described in Ref. 13 for \(\vec{k} = (\pi/2, \pi/2)\) for a \(32 \times 32\) size square lattice and a finite imaginary part was used in the free-hole propagator with \(\epsilon = 0.002\) (in units of the hopping parameter \(t\) which smears the lowest energy quasiparticle peak. Note that as discussed in Ref. 13 on this size lattice the finite-size effects were found to be small. The results of these calculations will be used as default models and we will refer to them as “exact” solutions. We have carried out QMC simulations for a range of \(J/t\) to compare with the exact results in order to make sure that our computer programs are correct.
Now imagine that we obtain a set of data \( G_k^{(d)}(i, j) \) for \( i = 1, \ldots, L \) and \( j = 1, \ldots, N_d \) on \( G_k(i) \) obtained by QMC, where the \( j \) denotes the data bin. For the analytic continuation we will use a generalization of the maximum entropy method, the so-called stochastic analytical inference (SAI) technique. In the later approach, \( A_k(\omega) \) is obtained as the average over all its possible forms in a Monte Carlo integration where the particular form of \( A_k(\omega) \) is selected from a distribution determined by the so-called default model \( D_k(\omega) \) and the probability of any proposed form of \( A_k(\omega) \) to be the true form given the input data \( G_k^{(d)}(i, j) \) is given by

\[
P[A_k/G_k^{(d)}] \sim e^{-\chi^2[A/\bar{k}]/2}, \tag{6}
\]

where \( \chi^2[A] \) is the \( \chi^2 \) determined from the data \( G_k^{(d)}(i, j) \) on \( G_k(i) \) and the result which is obtained from Eq.\( \ref{2} \) using the proposed form of \( A_k(\omega) \). In the evaluation of \( \chi^2[A] \) the covariance matrix of the data is used. The technical details of how one selects the particular proposed \( A_k(\omega) \) according to a given default model \( D(\omega) \) as well as how to make the optimum choice of the “temperature” \( \alpha \) and other important details of this calculation are discussed in Sec.\( \ref{III} \). In Sec.\( \ref{III} \) we show that for a given fixed \( D(\omega) \) the “optimum” temperature \( \alpha \) and quality of the QMC data (i.e., the size of the relative error in \( G^{(d)} \)) are strongly interdependent. We show that, using a given \( D(\omega) \) to select the proposed “configurations” of \( A_k(\omega) \), the acceptance rate, rather than \( \alpha \), is a better criterion to use for optimizing the results of the analytic continuation to real time. We find that when we tune \( \alpha \) to achieve an acceptance rate of 0.1, the results of the SAI are still influenced by the \( D(\omega) \), while for an acceptance rate of 0.01, the results are independent of the \( D(\omega) \). The results presented in this paper are for the latter value of the acceptance rate.

In the process of the analytic continuation we will work with two very different default models. We will analyze the same QMC data, obtained with either FHDMC or standard-DMC, using two different default models. In one series of results presented in this paper, we will as default model the “exact” solution to the problem and a different default model which differs significantly from the “exact” solution and call it the “wrong” default model. These two choices are discussed in Sec.\( \ref{III} \) in detail.

### III. COMPUTATIONAL DETAILS

As discussed in the previous Section, we are going to apply the FHDMC to obtain QMC data on the imaginary time single particle Green’s function \( G_k(\tau) \). Details of this method as applied to the Fröhlich Hamiltonian have been discussed in Ref.\( \ref{11} \). The only difference in this problem is in the forms of the hole and spin-wave propagators (which are the analogues of the electron and phonon propagators in the polaron problem) which are given in Ref.\( \ref{13} \).

Furthermore, we will restrict our DMC approach to sample the diagrammatic subspace spanned only by the diagrams included in the non-crossing approximation\( \ref{12} \). The only reason for this restriction is that the problem of the single-hole spectral function can be solved exactly and, this can be used to test the accuracy of the results of QMC method.

#### A. Application of the Stochastic Analytical Inference method

Since our data on \( G_k(\tau) \) obtained by either standard DMC or FHDMC are for a specific fixed value of \( \bar{k} \), they will be simply denoted as \( G_k^{(d)}(i, j) \) and the histogram of \( G_k(\tau) \) will be denoted as \( \bar{G}(i) \), and \( A(\omega) \) is an abbreviation for \( A_k(\omega) \) for fixed \( k \). There are \( N_d \) data bins \( G_k^{(d)}(i, j) \), \( j = 1, 2, \ldots, N_d \) obtained for \( G(i) \) in each imaginary time slice \( i \) and \( i = 1, 2, \ldots, L \).

Because as we produce the data table \( G_k^{(d)}(i, j) \) the imaginary time \( \tau \) is sampled during the FHDMC or the standard DMC updates, there is strong correlation between the data for the different imaginary time intervals. Therefore, in order to compute \( \chi^2 \) we need the data covariance matrix \( \mathbf{C} \) defined from its matrix elements as follows:

\[
C(k, l) = \frac{1}{N_d(N_d - 1)} \sum_{j=1}^{N_d} \left[ \bar{G}^{(d)}(k) - G^{(d)}(k, j) \right] \times \left[ \bar{G}^{(d)}(l) - G^{(d)}(l, j) \right], \quad k, l = 1, 2, \ldots, L, \tag{7}
\]

where \( \bar{G}^{(d)}(k) \) is the average of the data for the \( k \)-time slice, i.e.,

\[
\bar{G}^{(d)}(k) = \frac{1}{N_d} \sum_{j=1}^{N_d} G^{(d)}(k, j). \tag{8}
\]

In terms of \( \mathbf{C} \), \( \bar{G}^{(d)} \) and the proposed \( A(\omega) \) which gives a \( \bar{G}(i) \) via Eq.\( \ref{2} \) the \( \chi^2 \) is given as

\[
\chi^2 = (\bar{G}(d) - \bar{G})^T \mathbf{C}^{-1} (\bar{G}(d) - \bar{G}), \tag{9}
\]

where \( (\bar{G}(d))_T \equiv (\bar{G}^{(d)}(1), \bar{G}^{(d)}(2), \ldots, \bar{G}^{(d)}(L)) \) and \( \mathbf{G}^T \equiv (\bar{G}(1), \bar{G}(2), \ldots, \bar{G}(L)) \).

We determine the orthogonal matrix \( \mathbf{O} \) and the diagonal matrix \( \mathbf{d} \) such that:

\[
\mathbf{C} = \mathbf{dO} \mathbf{O}^T. \tag{10}
\]

Then, we can simply write \( \chi^2 \) as follows:

\[
\chi^2 = (\bar{G}_f^{(d)} - G_f)^T (\bar{G}_f^{(d)} - G_f), \tag{11}
\]

\[
\bar{G}_f^{(d)} = \mathbf{d}^{-1/2} \mathbf{O}^T \bar{G}(d), \tag{12}
\]

\[
G_f = \mathbf{d}^{-1/2} \mathbf{O}^T \bar{G}. \tag{13}
\]
In the SAI method, $A(\omega)$ is obtained as the average over all its possible forms in a Monte Carlo integration where the particular form of $A(\omega)$ is selected from a distribution determined by the so-called default model $A(\omega)$ and the probability of any proposed form of $A(\omega)$ to be the true form given the input data $G^{(d)}(i, j)$ is given by Eq. [9] where $\chi^2 [A]$ is obtained using Eq. [11] determined from the data $G^{(d)}(i, j)$ on $G(i)$ and $G(i)$ determined from the assumed values of $A(\omega)$. The optimum choice of the “temperature” $\alpha$ will be discussed in the next Subsection.

We apply the Metropolis algorithm using the expression given by Eq. [8] as the acceptance probability and we calculate the average spectral function $A(\omega)$. In the application of the Metropolis algorithm we use as selection probability of a particular $A(\omega)$ a distribution which is related to the so-called default model $D(\omega)$, which contains our prior knowledge about the actual $A(\omega)$. We consider the frequency interval $[\omega_{\text{min}}, \omega_{\text{max}}]$ and we assume that $A(\omega)$ is zero outside this interval. First, we slice this frequency interval into $N_\omega$ intervals $\Delta\omega(i)$ around a middle-frequency $\omega(i)$, $i = 1, 2, ..., N_\omega$. We define a normalized histogram based on the default model $D(\omega)$ as

$$
D(i) = \frac{D(\omega(i))}{\sum_{j=1}^{N_\omega} D(\omega(j)) \Delta\omega(j)},
$$

and based on it we define a new variable $x(i)$ which takes values in the interval $[0, 1]$, which is sliced in intervals $[x(i-1), x(i)]$ of width

$$
\Delta x(i) = D(i) \Delta\omega(i), \quad i = 1, 2, ..., N_\omega,
$$

such that we can define the following

$$
x(0) = 0, \quad x(i) = \sum_{j=1}^{i} \Delta x(j), \quad x(N_\omega) = 1.
$$

We select normalized “configurations” of $n(x)$ ($n(x) \geq 0$, $\int_{0}^{1} n(x) dx = 1$) from the uniform distribution $\mathbb{E}$. The height $A(i)$ of the histogram of $A(\omega)$ in the interval $\Delta\omega(i)$ of $\omega$ is obtained as

$$
A(i) = \frac{1}{\Delta\omega(i)} \int_{x(i-1)}^{x(i)} n(x) dx.
$$

### B. Choice of the default models

In all of our simulations presented in this paper, we will compute, using either FHDMC or standard DMC, the histogram of the imaginary-time Green’s function $G^{(d)}_\omega(\tau)$ for $\vec{k} = (\pi/2, \pi/2)$ and for $J/t = 0.2$. Using the FHDMC method [11] or the standard DMC method we produce for the imaginary-time histogram of the Green’s function $G(\tau)$ a table of data $G^{(d)}(i, j)$, where $i = 1, 2, ..., N_d$ is the index for the different bins and $j = 1, 2, ..., L$ is the index for the imaginary-time interval.

In order to invert these data using the SAI method discussed in the previous subsection, we need a default model. Since we have the “exact” solution to this modified problem, i.e., where we have restricted the DMC sampling to the NCA diagrams, we can use as default model, (a) the “exact” solution or (b) another default model which differs from the “exact” solution and examine the extent to which the analytic continuation method is capable of finding.

In the present paper, when we refer to the “exact” default model, we imply the solution obtained within NCA by solving the Dyson’s equation self-consistently as was done in Ref. [12, 13]. For this purpose we have re-calculated the spectral function for $A_\omega(\omega)$ for the same value of $J/t = 0.2$ within NCA but for $k = (0.0)$. This spectral function will be used as an option for a default model in the SAI method. In the following, we refer to this choice for default model as the “wrong” default model, because this is not the correct solution that corresponds to the QMC data for $\vec{k} = (\pi/2, \pi/2)$.

### C. Acceptance rate and “temperature” $\alpha$

Here, we discuss that the optimum value for the “temperature” $\alpha$, which enters in the statistical analytical inference (SAI) $\mathbb{E}$ and the statistical error in the QMC input data are interdependent. We also discuss that the parameter which needs to be tuned in order to achieve results which are not influenced by the default model is the acceptance rate in the Monte Carlo sampling used in the SAI technique.

First, we wish to compare the results for the distribution of $A(\omega)$ obtained for two different sets of data characterized by different degree of precision. In both sets of data, $G_1^{(d)}(i, j)$ and $G_2^{(d)}(i, j)$, we take $\tau_{\max} = 12$ (in units of the inverse hopping matrix element $t$) $L = 600$ and $N_d = 1200$. The data $G_1^{(d)}(i, j)$ are characterized by a relative statistical variance $\sigma_{\tau 1} \simeq 1.3 \times 10^{-2}$, while the data $G_2^{(d)}(i, j)$ is characterized by a relative statistical variance of $\sigma_{\tau 2} \simeq 3 \times 10^{-3}$.

We ask ourselves the following question: If we apply the SAI method on the first set of data to find the probability distribution $P_1(\omega)$ of $A(\omega)$, using the same default model, and we use a “temperature” $\alpha_1$, is it possible to find a different temperature $\alpha_2$, such that the probability distribution $P_2(\omega)$ of $A(\omega)$ for the second set of data to be the same with $P_1(\omega)$. If the answer to this question is affirmative, it would mean that our freedom on how to choose the value of $\alpha$ is severely restricted.

The variance and the relative statistical variance for a
particular time interval $j$ are defined as
\[ \sigma^2_\nu(j) = \langle (G^\nu_v(j))^2 \rangle - \langle G^\nu_v(j) \rangle^2, \] (18)
\[ \omega^2_\nu(j) = \frac{\sigma^2_\nu(j)}{\langle G^\nu_v(j) \rangle^2}, \quad \nu = 1, 2, \] (19)

a) First we note that, assuming that the set of data in both cases is large enough, using the central limit theorem, we have that
\[ \bar{G}^\nu_{1}(j) = \bar{G}^\nu_{2}(j), \quad \text{for all } j = 1, ..., L. \] (20)

b) In order to accept or reject a “configuration” during the process of sampling $A(\omega)$ to invert the two sets of data $G^\nu_1$ or $G^\nu_2$, we need $\chi^2$. Let us assume that the covariance matrix is roughly diagonal and that the diagonal elements are roughly the same. We note that in our FHDMC method the relative statistical variance is approximately the same for all time intervals. The values of $\chi^2$ for the two different sets of data can be approximated as
\[ \chi^2_\nu = \sum_{j=1}^{L} \frac{(\bar{G}^\nu_v(j) - G(j))^2}{\sigma_\nu(j)^2}, \]
\[ \simeq \frac{1}{\sigma^2_{r\nu}} \sum_{j=1}^{L} \frac{(\bar{G}^\nu_v(j) - G(j))^2}{\bar{G}^\nu_v(j)^2}, \] (21)
where $\nu = 1, 2$ for the two different sets of data, and $\sigma_{r\nu}$ is the relative variance which is taken to be roughly the same for all time intervals. $G(j)$ is the value of the exact histogram of $G(\tau)$ in the $j$ time-interval which is given in terms of $A(\omega)$ by Eq. 2.

c) In the process of sampling $A(\omega)$ to invert the two sets of data $G^\nu_1$ or $G^\nu_2$, the proposed “configurations” of $A(\omega)$ are drawn from the same distribution because we use the same default model. Therefore, the values of $G(j)$ used to calculate $\chi^2$ are “drawn” from the same distribution. The acceptance probability is determined from the “Boltzmann factor” given by Eq. 6. Therefore, in order to obtain the same distribution of accepted configurations $A(\omega)$ in both cases of the data-to-be-inverted, the two different temperature values $\alpha_1$ and $\alpha_2$ used to invert the two sets of data should be related by the following
\[ \alpha_1 \sigma^2_{r1} = \alpha_2 \sigma^2_{r2}. \] (22)

The acceptance rates for these two simulations to find $A(\omega)$ are shown in Fig. 1(a). Fig. 1(a) illustrates that if the temperature $\alpha$ is scaled according to Eq. 22 the acceptance rates obtained for the two data set collapse and they become the same.

Therefore, the above analysis leads to the conclusion that the optimum “temperature” $\alpha$ and the relative statistical variance of the data are two interdependent variables. In addition, we will see in the next sections that the acceptance rate is a better quantity to tune in order to find the correct value of $\alpha$ for a given set of data such that during the SAI procedure the default model is not weighing more it should in this process.

In Fig. 1(b) we present the dependence of the average $\chi^2/L$ and acceptance rate characterizing the SAI proce-
FIG. 2: (Color on-line) In subfigures (a) and (b) the $\alpha$-dependence of the $\chi^2/L$ is shown for the cases where the “exact” and the “wrong” default are used in the SAI approach for the FHDMC (a) and standard DMC data (b). In subfigures (c) and (d) the $\alpha$-dependence of the acceptance rate is shown for the cases where the “exact” and the “wrong” default model is used for the FHDMC (c) and standard DMC data (d).

These dependencies could be used to judge the extent to which a given default model is close to the exact solution of a given problem when using the SAI method.

IV. RESULTS

As already discussed we will restrict our DMC approach to sample the diagrammatic subspace spanned only by the diagrams included in the NCA. The reason is that we can solve the problem of the single-hole spectral function exactly and, this, can be used to test the accuracy of the results of QMC method. Furthermore, we will work with two sets of QMC data obtained for the histogram of $G_{\vec{k}}(\tau)$ for $\vec{k} = (\pi/2, \pi/2)$
FIG. 3: (Color on-line) Analytic continuation of FHDMC and standard DMC data of the $t-J$ model for $J/t = 0.2$ for $\mathbf{k} = (\pi/2, \pi/2)$ obtained from the SAI technique using (a) FHDMC data and $\alpha = 0.5$ (which yields an acceptance rate of 0.013), (b) FHDMC data and $\alpha = 8$ (which yields an acceptance rate of 0.13) using as default model the “exact” solution. (c) Standard DMC and $\alpha = 500$ (which yields an acceptance rate of 0.013) and (d) standard DMC $\alpha = 4000$ (which yields an acceptance rate of 0.105) using as default model the “exact” solution.

and $J/t = 0.2$. One set is obtained with FHDMC and the other with standard DMC, both for approximately the same amount of CPU time in order to compare. These results for the histogram of $G_{\mathbf{k}}(\tau)$ are obtained for $0 < \tau < 12$ (in units of the inverse hopping matrix element $t$) and for 600 $\tau$-intervals ($L=600$) and the number of data bins $N_d = 1200$ for each time-interval. The relative statistical error on FHDMC results is more or less independent of $\tau$ (see also Fig. 6(a)) and it was approximately $\sigma_{\tau} = 3 \times 10^{-3}$ while for the results obtained using standard-DMC $\sigma_{\tau}$ ranges from $2 \times 10^{-3}$ for small $\tau$ up to $2 \times 10^{-2}$ for large $\tau$. These relative errors were obtained by using approximately the same amount of CPU time such that the comparison between FHDMC and standard-DMC to be meaningful.

To each set of these data we apply the SAI method for different values of $\alpha$. Here, we will present the results for just two representative values of $\alpha$. In addition, we will apply two different default models one which is the “exact” solution and a second which we will call the “wrong” default model because it is the “exact” solution for $\mathbf{k} = 0$ instead of the “exact” solution for $\mathbf{k} = (\pi/2, \pi/2)$.

In Fig. 3(a) and Fig. 3(b) we present the results of the analytic continuation of the FHDMC data obtained from the SAI technique using as default model the “exact” solution (discussed in Sec. III B) and (a) $\alpha = 0.5$, which yields an acceptance rate of 0.013 and an average $\chi^2/L$ of 2.0, and (b) $\alpha = 8$, which yields an acceptance rate of
0.13 and an average $\chi^2/L$ of 2.2. Notice that at the high temperature the SAI result follows the default model. At the lower temperature, the result is somewhat different and it can, in fact, find some difference between what we call “exact”. This difference is due to the fact that the “exact” calculation uses a finite value of $\epsilon$ which broadens the peaks (which is necessary because the calculation was done on a finite $32 \times 32$ square lattice), while the FHDMC corresponds to an infinite square lattice and does not require any broadening parameter. Furthermore, notice that for a value of $\alpha$ which leads to an acceptance rate of $\sim 0.1$ the SAI procedure follows the default model, while when the acceptance rate is of the order of 0.01 (lower temperature) it does not. We will reach the same conclusion, next, when we use a default model which is not close to the exact.

In Fig. 3(c) and Fig. 3(d) we present the results of applying the SAI method to data obtained with the standard DMC. In Fig. 3(c) we have used $\alpha = 500$ which yields an acceptance rate of 0.013. In Fig. 3(d) we have used $\alpha = 4000$ which yields an acceptance rate of 0.0105. In both cases we used as default model the “exact” solution. As can be seen from these figures when we use the standard-DMC technique the agreement of the ana-
FIG. 5: (Color on-line) The results of the SAI approach using as input data QMC results with higher degree of precision. (a) and (b) respectively present the results with FHDMC data and with the standard DMC at high enough values of $\alpha$ where the acceptance rate is of the order of 0.1. (c) and (d) respectively present the results with FHDMC data and with the standard DMC at low enough values of $\alpha$ where the acceptance rate is of the order of 0.01.

Analytic continuation is dramatically worse than the present method. Nevertheless notice that for a value of $\alpha$ which leads to an acceptance rate of $\sim 0.1$ the SAI procedure follows the default model.

The true test of the method comes when we use a default model that is different from the exact answer. Towards this goal, we have used the “exact” spectral function $A_{(0,0)}(\omega)$ obtained for $\mathbf{k} = 0$ as the default model $D(\omega)$ in the SAI approach to invert the FHDMC and standard-DMC data on $\Omega(\pi,2\pi)$. As discussed in Sec. III B we call this $D(\omega)$, the “wrong” default model. Using this “wrong” default model in the SAI technique we obtained the results illustrated in Fig. 4. The default model is shown by the red open circles. The “exact” result is shown by the black dashed line in all subfigures. Notice that in Fig. 4(a), which is obtained using the FHDMC data and “temperature” $\alpha = 6$ yielding an acceptance rate of 0.13, the results are influenced by the default model. On the other hand, in Fig. 4(b), which is obtained using the FHDMC data and “temperature” $\alpha = 8 \times 10^7$ yielding an acceptance rate of 0.046, the results are not influenced by the default model.
\(\alpha = 0.1\) yielding an acceptance rate of 0.04, the results are not influenced by the default model and they agree reasonably well with the “exact” results.

When we use the results of the standard DMC to carry out the SAI analysis, the results at the high temperature yielding an acceptance rate of 0.06 are influenced by the default model (Fig. 4(c)). When we lower the temperature further to obtain an acceptance rate of 0.003 the results still in significant disagreement with the exact results (Fig. 4(d)). If we lower the temperature further, the result do not change in any significantly way. Therefore, we conclude that using a value of \(\alpha\) such that the acceptance rate to be around 0.01 the results of the SAI method are not influenced by the default model.

In order to see if the results of the analytic continuation of the standard DMC data will improve by increasing the accuracy of the input DMC data, we run longer and collected data with relative error ranging from \(2 \times 10^{-4}\) for small values of \(\tau\) to \(2 \times 10^{-3}\) for large \(\tau\). These data and, for comparison we obtained data using the FHDMC running for the same amount of CPU time with average relative error of \(8 \times 10^{-4}\) are shown in Fig. 5. In both cases we provide the results of the application of the SAI using the “wrong” default model for two different values of \(\alpha\) which yield acceptance rates of the order of 0.1 (Fig. 5(a) and Fig. 5(b)) and 0.01 (Fig. 5(c) and Fig. 5(d)). For the former the results of the inversion are influenced by the default model and in the latter they are not. Notice that the results obtained using the FHDMC data are significantly better than those obtained using the standard DMC data.

Is there a simple way to understand the reason for the superiority of the application of the flat histogram technique during the QMC simulation? Fig. 6(a) illustrates the relative error for \(G_{\vec{k}}(\tau)\) as a function of the imaginary-time interval obtained using standard-DMC and FHDMC for the same amount of CPU time. Notice that the error in \(G_{\vec{k}}(\tau)\) as obtained by standard-DMC as a function of \(\tau\) increases. When using FHDMC the relative error is more-or-less constant for all values of \(\tau\) sampled. An exponential “guidance function” was used to approximately capture the long \(\tau\) behavior of \(G\) in the standard-DMC[14, 15].

As can be seen from Fig. 6(a) this is not enough, because of the fact that in this case (and most non-trivial cases) the dependence of \(G(\tau)\) with \(\tau\) involves many (a continuum) set of exponentials. Why this behavior of the relative error, which is expected in any QMC method, is not good for obtaining an accurate analytic continuation? The values of \(\chi^2\) can be approximated as

\[
\chi^2[A] = \sum_{i=1}^{L}[(\tilde{G}^{(d)}(i) - G(i))\sigma_i^{-2}(\tilde{G}^{(d)}(i) - G(i))],
\]

where \(\tilde{G}^{(d)}(i)\) and \(\sigma_i^2\) are the averages and the variances of the data \(G^{(d)}(i, j)\) in the \(i^{th}\) time interval. Notice that in the integration over all possible configurations of \(A(\omega)\), the time intervals with relatively small relative error \(G_{\vec{k}}(i)\) obtained by the QMC method, will make the most substantial contribution to the probability in Eq. 6. As a result, in the Monte Carlo sampling of \(A(\omega)\) involved in the SAI inversion process, the “configurations” of \(A(\omega)\) which would be likely accepted, would be those that yield a \(G_{\vec{k}}(i)\) in close agreement with the data \(G_{\vec{k}}^{(d)}(i, j)\) at small values of \(\tau\) and the data at large values of \(\tau\) would be mostly irrelevant. If, however, the flat histogram technique is applied within the QMC method to make the
histogram of $G_F(\tau)$ flat, this problem is no longer there.

Another problem associated with standard-DMC is the strong correlations in the statistical correlations of the standard-DMC data as can be inferred from Fig. 6(b). In Fig. 6(b) we present standard-DMC data (using a value of $\mu = -2.58$ in units of the hopping matrix element $t$) starting from different configurations. The solid red line gives the average obtained from various DMC runs. Notice that the results for any particular standard-DMC run stay mostly on the same side of the average. These correlations were also discussed and their origin was explained in Ref. 11 and they are largely absent in the FHDMC data. They give rise to very large off-diagonal elements in the covariance matrix and severely hinder the analytic continuation technique which is based on the value of the $\chi^2$.

V. CONCLUSIONS

We have shown that by combining flat histogram techniques\cite{6,7,8} and the QMC method in such a way to make the histogram of an imaginary-time correlation function $C(\tau)$ flat\cite{11}, we are able to carry out an accurate analytic continuation to real time. The reason for this dramatic improvement of the results of the analytic continuation is that the flat histogram application in the QMC sampling improves the quality of information contained in $C(\tau)$ across all time scales. This has been demonstrated using the DMC method which can be modified to simulate an exactly soluble problem. This is within the flexibility of the DMC method, because we can select the set of Feynman diagrams to sample. Thus, by selecting the diagrammatic series to be the one which takes into account all the diagrams which contribute to the single-hole spectral function of the 2D $t - J$ model within the NCA approximation, we can compare the results of the analytic continuation directly to the “exact” solution\cite{12,13,14}.

We have used the SAI\cite{3} approach, a generalization of the maximum entropy method, to carry out the analytic continuation to real time. We find that the QMC data obtained using the FHDMC method\cite{11}, which incorporates flat histogram ideas to make the histogram of the $C(\tau)$ flat in imaginary time, when “inverted” with the SAI method, yield a spectral function in excellent agreement with the “exact” spectral function. On the other hand, using simply standard DMC data, without incorporating flat histogram techniques during the QMC sampling, yield spectral functions of far inferior quality.

We have also attempted to reason that, in general, if we incorporate the flat histogram idea with any QMC technique, in such a way to make the histogram of $C(\tau)$ flat, the results of the analytic continuation to real time should be of significantly better statistical quality. The arguments given are based on the fact that the quality of the QMC data on $C(\tau)$ obtained when such flat histogram techniques are incorporated into the QMC algorithm, is the same across all imaginary-time scales. This allows the analytic continuation techniques, which use the $\chi^2$ as the measure to judge various “proposals” for the spectral function, to take equally seriously the values of $C(\tau)$ at all time-scales. Furthermore, we find that the quality of the QMC data is significantly better when flat histogram techniques are incorporated in the QMC sampling, because in such case, the QMC data for different time-intervals are significantly less correlated.

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