Real-Time Dynamics from Imaginary-Time Quantum Monte Carlo Simulations: Tests on Oscillator Chains

J. Bonča and J.E. Gubernatis
Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545

January 9, 2022

We used methods of Bayesian statistical inference and the principle of maximum entropy to analytically continue imaginary-time Green’s function generated in quantum Monte Carlo simulations to obtain the real-time Green’s functions. For test problems, we considered chains of harmonic and anharmonic oscillators whose properties we simulated by a hybrid path-integral quantum Monte Carlo method. From the imaginary-time displacement-displacement Green’s function, we first obtained its spectral density. For harmonic oscillators, we demonstrated the peaks of this function were in the correct position and their area satisfied a sum rule. Additionally, as a function of wavenumber, the peak positions followed the correct dispersion relation. For a double-well oscillator, we demonstrated the peak location correctly predicted the tunnel splitting. Transforming the spectral densities to real-time Green’s functions, we conclude that we can predict the real-time dynamics for length of times corresponding to 5 to 10 times the natural period of the model. The length of time was limited by an overbroadening of the peaks in the spectral density caused by the simulation algorithm.

02.70.Lq, 05.30.-d, 02.50.Wp

I. INTRODUCTION

One of the goals for doing computer simulations is the production of information useful in the interpretation and design of experiments. Notwithstanding important issues regarding Hamiltonian selection and parameterization, the interface of simulations with experiment is particularly challenging for quantum systems. The current Monte Carlo algorithms, whether they impose quantum particle statistics constraints or not, are performed either in real-time $t$ or in imaginary-time (Euclidean time) $\tau = -it$. In real-time, the propagator $\exp(itH)$ for a system, described by a Hamiltonian $H$, oscillates wildly at long-times. Analytically, these rapid oscillations self-cancel, but a Monte Carlo process, as it is typically used, has difficulty achieving this cancellation. As a consequence, modifications of the basic algorithms have been proposed to extend the simulations as long as possible in the real-time domain [1]. With these new algorithms, simulations typically produce dynamics extending to 2 to 3 times the natural periods of the systems. In imaginary-time, the propagator $\exp(-\tau H)$ is diffusive and the rapid oscillations are avoided. Correlations functions $G(\tau)$, however, are now a function of imaginary-time, and such functions do not easily convey the actual dynamics of the system. In principle, real-time correlation (Green’s) functions $\hat{G}(t)$ can be obtained from the imaginary-time ones by the process of analytic continuation. In practice, this process is difficult because it is ill-posed and because the Monte Carlo data is incomplete and noisy.

Recently, procedures were proposed to perform this analytic continuation [2]. These procedures draw heavily upon methods of Bayesian statistical inference and the principle of maximum entropy to infer from imaginary-time correlation functions their associated spectral densities $A(\omega)$. Through linear-response theory, the spectral densities represent the spectra associated with numerous real-time measurements of current-current, spin-spin, etc. correlations functions. What apparently has not yet been tried is performing the Hilbert transform of these spectral densities to obtain the frequency-dependent retarded correlation function and then Fourier transforming this quantity to obtain the real-time correlation function. In this paper, we will carry out these additional steps. By doing this, we hope to gain a greater understanding of the physical content present in the spectral density returned by the Bayesian methods. We expected that the resultant real-time information would be limited by the approximate and probabilistic nature of the analytic continuation methods. We found, however, that the distance in real-time over which our results are valid is limited primarily by the ability of the simulation algorithm to produce good data. To interface profitably with the numerical analytic continuation, the simulation algorithm has to produce high quality data consistent with the assumptions of procedures. The algorithm we used had problems doing this, and we will describe the measures taken to reduce this difficulty. Even so, in most cases we were able to extend in real-time up to factor of 10 natural periods of the physical systems. Longer extensions are possible and require longer Monte Carlo runs. For present purposes, we had no physical motivation to do so.

In Section II, we will discuss the various models studied. We simulated a particle moving in single harmonic and
double-well anharmonic potential and a collection of particles moving in chains of these potentials. For these models we know the exact solutions. By calculating their properties numerically, we can benchmark our methods. Certain properties of a single double-well potential, like the tunnel splitting, are easily obtained numerically. The phase diagram for a chain of such oscillators is also known [3]. This type of chain can exist in a symmetric or displacive state. In Section III, we summarize the numerical analytic continuation procedure we used and discuss our simulation technique. Modifying the simulation technique to be more naturally ergodic and to produce data with short statistical auto-correlation times was the most difficult and restrictive part of our study. We present our results and conclusions in Sections IV and V.

II. MODELS

We simulated five Hamiltonians. One was that for a single harmonic oscillator

$$H = \frac{p^2}{2m} + \frac{\gamma}{2} x^2$$  \hspace{1cm} (1)

which has the natural frequency $\omega_0 = \sqrt{\gamma/m}$. Another was that for a chain of $N$ such oscillators

$$H = \sum_i \frac{p_i^2}{2m} + \frac{\gamma}{2} (x_i - x_{i-1})^2$$  \hspace{1cm} (2)

Fourier transforming the displacements $x_i$ and momenta $p_i$, we can of course rewrite this second Hamiltonian as

$$H = \sum_k \frac{p_k^2}{2m} + \frac{1}{2} m \omega_k^2 x_k^2$$  \hspace{1cm} (3)

where $k = -\pi, -(N - 1)\pi/N, \ldots, \pi$ and $\omega_k^2 = 2\omega_0^2 (1 - \cos k)$. In this form, the Hamiltonian is explicitly expressed as a collection on $N$ independent simple oscillators. The natural frequency of an oscillator is $\omega_k$. The third Hamiltonian was a variant of the harmonic chain

$$H = \sum_i \frac{p_i^2}{2m} + \frac{\gamma}{2} (x_i - x_{i-1})^2 + \frac{1}{2} x_i^2$$  \hspace{1cm} (4)

which after Fourier transforming the displacements becomes

$$H = \sum_k \frac{p_k^2}{2m} + \frac{1}{2} m \omega_k^2 x_k^2$$  \hspace{1cm} (5)

where $\omega_k^2 = 1 + 2\omega_0^2 (1 - \cos k)$. In this form, the Hamiltonian is again explicitly expressed as a collection on $N$ independent simple oscillators but with a dispersion relation that has a non-zero frequency at $k = 0$. The two other Hamiltonians were a single, symmetric, double-well potential

$$H = \frac{p^2}{2m} + \frac{1}{4} (x^2 - 1)^2$$  \hspace{1cm} (6)

which has well bottoms at $x = \pm 1$ and a barrier height of unity at $x = 0$, and a chain of such potentials

$$H = \epsilon \sum_i \frac{p_i^2}{2m} + \frac{\gamma}{2} (x_i - x_{i-1})^2 + \frac{1}{4} (x_i^2 - 1)^2$$  \hspace{1cm} (7)

In the chain, $\epsilon$ sets the barrier height of every double-well. In both chains we assumed periodic boundary conditions and disallowed particle exchange.

For these Hamiltonians, our simulations obtained estimates of the imaginary-time displacement-displacement Green’s function

$$G_{ij}(\tau) = G_{i-j}(\tau) = \langle T_0 x_i(\tau)x_j(0) \rangle$$  \hspace{1cm} (8)
Here, the angular brackets denote thermal averaging. It is more convenient and illuminating to work with the spatial Fourier transform \( G_k(\tau) \) of \( g_{ij} \) and it is known \(^\square\) that

\[
G_k(\tau) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{e^{-\tau \omega} A_k(\omega)}{1 - e^{-\beta \omega}}
\]  

(9)

where \( A_k(\omega) \) is the spectral density. This function has the properties that

\[
A_k(\omega) = -A_k(-\omega)
\]

(10)

The odd symmetry of \( A_k(\omega) \) allows us to re-express \(^\square\) as

\[
G_k(\tau) = \frac{1}{2\pi} \int_{0}^{\infty} d\omega \frac{\omega[e^{-\tau \omega} + e^{-(\beta - \tau)\omega}] A_k(\omega)}{1 - e^{-\beta \omega}} 
\]

(11)

and it is straightforward to show that \( A_k(\omega) \) obeys the sum rule

\[
G_k(0) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{A_k(\omega)}{1 - e^{-\beta \omega}} = \langle x_k^2 \rangle
\]

(12)

The spectral density \( A_k(\omega) \) is also related to the frequency Fourier transform \( \hat{G}_R^R(\omega) \) of the real-time, retarded Green’s function \(^\square\)

\[
\hat{G}_R^R(t) = -i\theta(t)\langle [x_{-k}(t), x_k(0)] \rangle
\]

(13)

via

\[
\hat{G}_R^R(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega' \frac{A_k(\omega')}{\omega - \omega' + i\eta}
\]

(14)

where \( 0 < \eta \ll 1 \), from which it follows that

\[
\hat{G}_R^R(t) = -i\theta(t) \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega A_k(\omega)e^{-i\omega t}e^{-\eta t}
\]

(15)

For an individual harmonic oscillator of frequency \( \omega_k \), the eigenstates and energies are exactly known, and all the quantities in the above paragraph are known analytically:

\[
G_k(\tau) = \frac{1}{2m\omega_k} \frac{1}{\sinh(\beta \omega_k/2)} \cosh \left[ \beta \omega_k \left( \frac{1}{2} - \frac{\tau}{\beta} \right) \right]
\]

(16)

\[
A_k(\omega) = \pi [\delta(\omega - \omega_k) - \delta(\omega + \omega_k)]/m\omega_k
\]

(17)

\[
\hat{G}_R^R(\omega) = \frac{1}{2m\omega_k} \left( \frac{1}{\omega - \omega_k + i\eta} - \frac{1}{\omega + \omega_k + i\eta} \right)
\]

(18)

\[
\hat{G}_R^R(t) = \theta(t) \frac{1}{m\omega} \sin(\omega_k t)e^{-\eta t}
\]

(19)

\[
\langle x_k^2 \rangle = \frac{1}{2m\omega_k} \coth(\beta \omega_k/2)
\]

(20)

The eigenstates and energies of a single harmonic oscillator have definite, well-known characteristics: Because the potential is symmetric about \( x = 0 \), the eigenfunctions have alternating parity. The ground state has even parity and an energy \( \frac{1}{2}\omega_k \). The energies of the excited states are regularly spaced at intervals of \( \omega_k \). The double-well potential is also symmetric about \( x = 0 \), and its eigenstates also alternate in parity with the ground state again having even parity. The precise details about the energy spectrum, however, are only available numerically. When these states lie below the barrier, and particularly for deep wells, they group into widely-separated, nearly degenerate pairs. The separation in energies within and between pairs is called the tunnel splitting. The spectral density is dominated by terms with matrix elements involving states 0 and 1. Contributions from matrix elements of \( x \) involving \((0,3), (3,4), (0,5), (3,5), (5,6)\), etc. have smaller contribution to the spectral density because of smaller overlap between the eigenstates. Additionally, most can be “frozen-out” by making the temperature at least comparable to \( E_3 - E_0 \).
This temperature range is the one in which we generally worked. The nature of the energy levels and eigenstates is schematically represented in Fig. 1.

The spatial Fourier transformation of the Hamiltonian of the double-well chain does not produce as system of independent oscillators. This is the essence of its non-linearity. The model, however, has an interesting zero-temperature phase diagram as a function of the parameters $\epsilon$ and $\gamma$. Roughly, $\epsilon$ is a measure of the barrier height relative to the frequency of inter-site oscillation and the frequency of oscillation associated with the well-bottom. When the barrier height is large, the particles collectively are displaced to the left or the right of their classical equilibrium positions in a broken symmetry state characterized by a non-zero value of the mean-squared displacement. As the barrier height is lowered, a critical value is reached where because of zero-point motion and tunneling, the particles collectively make a transition to a state where the mean-squared displacement of each is zero. Accordingly, a simulation of the chain, done in one of these two thermodynamic phases, is expected to exhibit different quantum characteristics in the spectral density.

III. METHODS

A. Hybrid Path-Integral Monte Carlo Method

Our Monte Carlo simulations will be based on the Feynman path integral formulation of quantum mechanics. In imaginary-time, this formulation represents the partition function $Z$ as

$$Z = \int Dxe^{-S[x(t)]}$$

where

$$S[x(\tau)] = \int_0^\beta d\tau H[x(\tau)]$$

is the action corresponding to the path $x(\tau)$ and $H[x(\tau)]$ represents the path dependence of the Hamiltonian. The Monte Carlo method is used to perform the integration over the paths in (21). It is applied after the integral in (22) is approximated by a sum over $L$ steps in imaginary-time each of length $\Delta\tau$ and the momenta are approximated by a forward-difference approximation between successive displacements in imaginary-time:

$$p_i(\tau) = m \frac{\partial x_i(\tau)}{\partial \tau} \approx m \frac{x_i(\tau + \Delta\tau) - x_i(\tau)}{\Delta\tau}$$

For a one-dimensional system of $N$ particles, the action becomes

$$S = \Delta\tau \sum_{i,j=1}^{N,L} \frac{m}{2} \left( \frac{x_{i,j} - x_{i+1,j}}{\Delta\tau} \right)^2 + \gamma \frac{x_{i,j}^2}{2}$$

This form is similar in appearance to a classical two-body potential energy defined on a $N \times L$ lattice where at a given $\tau$ the particles interact through the potential energy function of the original problem (scaled by $\Delta\tau$), and at a given position they interact by a harmonic potential with a spring constant equal to $m/\Delta\tau$. For a single particle, the summation over the spatial coordinate $i$ is dropped and the discretized action has the interpretation of a chain where the particles at imaginary-time move in a potential $\Delta\tau V(x_j)$ while interacting with particles at neighboring times by a harmonic potential with spring constant $1/\Delta\tau$. For the models we are considering, the discretized actions are:

1. Single Harmonic Oscillator:

$$S = \Delta\tau \sum_{j=1}^{L} \frac{m}{2} \left[ \frac{x_{j+1} - x_j}{\Delta\tau} \right]^2 + \frac{\gamma}{2} x_j^2,$$

2. Harmonic Chain:

$$S = \Delta\tau \sum_{i,j=1}^{N,L} \frac{m}{2} \left[ \frac{x_{i+1,j} - x_{i,j}}{\Delta\tau} \right]^2 + \frac{\gamma}{2} (x_{i+1,j} - x_{i,j})^2,$$
3. Harmonic Chain plus on-site oscillator:

\[ S = \Delta \tau \sum_{i,j=1}^{N,L} \frac{m}{2} \left( \frac{x_{i,j+1} - x_{i,j}}{\Delta \tau} \right)^2 + \frac{\gamma}{2} (x_{i+1,j} - x_{i,j})^2 + \frac{1}{2} x_{i,j}^2, \]  

(27)

4. Single Double-Well Potential:

\[ S = \Delta \tau \sum_{j} \frac{m}{2} \left( \frac{x_{j+1} - x_{j}}{\Delta \tau} \right)^2 + \frac{1}{4} (x_{j}^2 - 1)^2. \]  

(28)

5. Double-Well Chain:

\[ S = \epsilon \Delta \tau \sum_{i,j=1}^{L,N} \frac{m}{2} \left( \frac{x_{i,j+1} - x_{i,j}}{\Delta \tau} \right)^2 + \frac{\gamma}{2} (x_{i,j} - x_{i,j+1})^2 + \frac{1}{4} (x_{i,j-1}^2 - 1)^2. \]  

(29)

The simplest way to apply the Monte Carlo method is to move repeatedly from point to point on the space-time lattice, at each point propose a change in the coordinate, \( x_{i,j} \rightarrow x'_{i,j} \), and accept the change via the Metropolis algorithm with probability \( \min[1, \exp(-\Delta S)] \) where \( \Delta S \) is the change in the value of the action proposed by the proposed change \[5\]. This method is often called path-integral Monte Carlo (PIMC).

An alternative to the Monte Carlo evaluation of the path-integral is a molecular dynamics evaluation \[6\]. Here, a fictitious momentum \( \pi_{i,j} \) is associated with each point to define a pseudo Hamiltonian

\[ H_p = \sum_{i,j=1}^{N,L} \frac{\pi_{i,j}^2}{2m_\pi} + S[x_{i,j}] \]  

(30)

and standard molecular dynamics techniques are used to sample phase space. The approach takes advantage of the classical nature of the fields in the path-integral formulation and produces the correct statistical mechanics because in classical statistical mechanics the momentum degrees of freedom can be integrated out of the partition function. The method is often called path-integral molecular dynamics.

At the core of the method we used is the hybrid Monte Carlo approach suggested by Duane et al. \[7\] which combines the molecular dynamics approach with the Monte Carlo procedure to obtain the best features of both methods. The general expectation is faster equilibration of the simulation and shorter auto-correlation times between measured quantities. With this method, the following steps are cycled: For a given set of \( x_{i,j} \) the corresponding pseudo momenta are assigned values randomly from a Maxwell-Boltzmann distribution for the velocities. The energy is computed. Next, both the momenta and displacements are evolved by molecular dynamics for some pseudo time \( t_p \). The energy is recomputed. Then the evolved displacements are accepted with probability \( \min[1, \exp(-\Delta E)] \), where \( \Delta E \) is the difference in energy between the initial and final configuration. Normally, molecular dynamics is energy conserving so the evolved displacements would always be accepted. A guiding idea behind the hybrid method is to use for the molecular dynamics with emphasis on fast integration, as opposed to accurate integration, and to adjust the size of these steps \( \Delta t \) and \( t_p \) so the Monte Carlo decision accepts 90 – 95% of the configuration. The molecular dynamics method globally updates all the displacements and is a computationally efficient procedure. The Monte Carlo procedure maintains detailed balance to ensure proper equilibrium averages and filters out the results of “bad” integrations.

We found, however, that this simple form of the hybrid method was inadequate for present purposes. The output of our simulation is to be used as input to maximum entropy procedures to execute the analytic continuation. As we will discuss below, the analytic continuation problem is an ill-posed problem and hence is very sensitive to the size of the errors associated with the input data. For a fixed amount of computer time, reducing the size of the error efficiently by a Monte Carlo method requires shortening the auto-correlation times between measurements. In our computed Green’s function, in spite of small estimates for the error bars, we would often see small (within the error bars) unphysical sawtooth-like structure in regions about \( \tau = \beta/2 \). Following a simple procedure suggested by Neal \[8\], we could generally remove this structure and also be more ergodic. His suggestion was after each Monte Carlo
decision to reverse the direction of the molecular time integration, i.e., $\Delta t \to -\Delta t$, with probability $1/2$. A smaller improvement is achieved by not using a fixed length for the time integration in the molecular dynamics simulation but rather to choose the length randomly from the interval $(t_p - \delta, t_p + \delta)$ where $t_p$ and $\delta$ are chosen so the Monte Carlo acceptance rate is in the 90 to 95 per cent range. We will refer to the combined method as the hybrid path-integral Monte Carlo method (HPIMC). Adjusting the Monte Carlo acceptance rate is not the entire story. First, it seems best to insure $t_p$ is several times larger than the natural period associated with the slowest significant modes in the systems and then choose $\delta$ to fix the acceptance ratio.

We remark that Fahy and Hamann [4] observed for the standard hybrid method the existence of a critical time $t_c$ (dependent of model parameters) demarking non-ergodic and chaotic behavior in the results of the time integration. For a harmonic system, $t_c$ is infinite which suggests the inapplicability of the method to a harmonic system. We also remark that the results of the simulations depend on the size of $\Delta t$. While necessary is insufficient. The difficulty is the inverse problem, that is, solving $A(\omega)$, is ill-posed. This condition is caused by the exponential character of the kernel at large values of $\omega$. At large $\omega$, large variations in $A(\omega)$ make little change in $G(\omega)$, and hence for a given set of $G_i$, an infinite number of $A_j$ will satisfy the least-squared estimate (36).

B. Maximum Entropy Method

The maximum entropy method [2] is used to regularize the solution of (11). Dropping the subscript $k$ for convenience, we rewrite this equations as

$$G(\tau) = \int d\omega K(\tau, \omega)[A(\omega)/\omega]$$

where the kernel

$$K(\tau) = \frac{1}{2\pi} \frac{\omega [e^{-\tau \beta} + e^{-i(\beta - \tau)}]}{1 - e^{-\beta \omega}}$$

Because both the kernel and $A(\omega)/\omega$ are regular at $\omega = 0$, we solve for $A(\omega)/\omega$ and then trivially find $A(\omega)$. For discrete values of $\tau$ and $\omega$ we approximate (31) as

$$G_i = \sum_{i,j} K_{i,j} A_j$$

where $G_i = G(\tau_i)$, $K_{i,j} = K(\tau_i, \omega_j)$, and $A_j = A(\omega_j)\Delta\omega_j/\omega_j$.

The Monte Carlo method will return estimates $G_i$ of $G_i$ and estimates of the sample variance $\sigma_j^2$ on the $G_i$. With this information, a natural solution path to $A_j$ would be to find the values of $A_j$ that minimize

$$\chi^2 = \sum_i (G_i - \bar{G}_i)^2/\sigma_i^2$$

$$= \sum_i \left( \frac{G_i - \sum_j K_{i,j} A_j}{\sigma_i} \right)^2$$

This approach, however, almost always fails. One reason is that it ignores the strong correlations that normally exist between the measured values of $G_i$, i.e., values of the Green’s function at different imaginary-times. At the very least, we must modify (35) to be

$$\chi^2 = \sum_{i,j} (\bar{G}_i - G_i)[C^{-1}]_{i,j} (\bar{G}_j - G_j)$$

where $C_{i,j}$ is the measured covariance among the values of $\bar{G}_i$. The $i$-th diagonal element of $C$ is simply $\sigma_i^2$. This modification of the definition of $\chi^2$ while necessary is insufficient. The difficulty is the inverse problem, that is, solving (11) for $A(\omega)$, is ill-posed. This condition is caused by the exponential character of the kernel at large values of $\omega$. At large $\omega$, large variations in $A(\omega)$ make little change in $G(\omega)$. The simulation, on other other hand, gives noisy and incomplete information about $G(\tau)$, and hence for a given set of $\bar{G}_i$, an infinite number of $A_j$ will satisfy the least-squared estimate (36).
The next level of solution seeks to regularize the minimization of $\chi^2$ by constraining it, i.e., minimizing

$$\chi^2 - \sum_i \alpha_i f_i(A)$$

(37)

where the $\alpha_i$ are Lagrange multipliers and the $f_i(A)$ are functions of $A_j$ representing possible constraints on the solution. Typical constraints include smoothness, non-negativity, sum rules, moments, etc. The difficulty with this approach is choosing the Lagrange multipliers. *Ad hoc* choices are commonplace. Often small changes in the values of these parameters produce massive changes in the results.

The maximum entropy approach follows from the observation that the spectral density is interpretable as a probability density function. The principle of maximum entropy states the probabilities should be assigned in such a way as to maximize

$$S = \sum_j A_j - m_j - A_j \ln(A_j/m_j)$$

(38)

Here, the $m_j$, called the *default model*, set the location of the maximum of $S$ and the value of $S$ at this point to be zero. The default model is solution for $A_j$ in the absence of other constraints on $A_j$. The method of maximum entropy maximizes

$$Q(A) = \alpha S - \frac{1}{2} \chi^2$$

(39)

To fix $\alpha$, an ad hoc procedure called *historic* maximum entropy is often used [10,11]. An more modern alternative is the Bayesian-based *classic* maximum entropy which uniquely determines $\alpha$ provided certain conditions are meet [10,11]. Under these conditions solution for $A_j$ is the most probable one. Unfortunately, these conditions seem often violated in the analytic condition problem. Accordingly, to estimate the $A_j$, we adopted a procedure suggested by Bryan.

In Bryan’s method [12], for a given value of $\alpha$, we find the $A(\alpha)$ that maximizes $Q(A)$. For the solution to (33), we take

$$\bar{A} = \int d\alpha A(\alpha) \Pr[\alpha|\bar{G}]$$

(40)

where $\Pr[\alpha|\bar{G}]$ is the probability of $\alpha$ given the data $\bar{G}$. Bayesian analysis shows that

$$\Pr[\alpha|\bar{G}] = \Pr[\alpha] \int DA \frac{e^Q}{Z_L Z_S(\alpha)}$$

(41)

where $Z_L$ is the normalization factor for $e^{-\frac{1}{2} \chi^2}$, $Z_S(\alpha)$ is the normalization factor for $e^{\alpha S}$, and $\Pr[\alpha]$ is Jeffreys’ prior. Details on the computation of this joint probability are discussed elsewhere [2]. With this function, the integral (40) is performed numerically.

The most difficult part of the problem is not evaluating the maximum entropy equations but satisfying the statistical assumptions on which they are based. The principal assumption is

$$\Pr[\bar{G}|A] = \frac{e^{-\frac{1}{2} \chi^2}}{Z_L}$$

(42)

The meaning of this assumption is the measured values of $G_j$ are statistically independent and distributed according to a multi-variable Gaussian distribution function defined by the covariance matrix $C$. Proper estimation of $C$ is paramount. Under normal circumstance the data produced by the simulations do not satisfy these assumptions. The procedures we use to have the data approximate these assumptions are discussed elsewhere [2]. When we have proper data, our solution (40) usually shows good insensitivity to the choice of the default model. Additionally, the historic and classic maximum entropy solutions usually agree well with it.

**IV. RESULTS**

To determine spectral properties of models listed in Section II, we performed HPIMC simulations with up to 800 bins of data ($N_{\text{bin}}$), each with up to 4000 measurements ($N_{\text{sweep}}$). Simulations with large bin-sizes were necessary
to avoid nonergodic behavior of the HPIMC method when used for chains with double well potentials close to the zero-temperature phase transition point. Furthermore, we set the value for the imaginary time step to $\Delta \tau = 0.25$. This choice on the one hand was small enough to avoid errors associated by the discretization of otherwise continuous imaginary time scale $\tau$, and on the other hand was large enough to avoid unphysical correlations between successive imaginary-time measurements of the Green’s function $G(\tau)$. Since our calculations were performed at the inverse temperatures $\beta$ between 1 and 10, the corresponding number of imaginary time steps $L = \beta \Delta \tau$ was between 40 and 60.

For a successful application of the HPIMC it is crucial to choose the proper value of the pseudo-time $t_p$ and the size of its step $\Delta t$ in the molecular dynamic part of the simulation. Following Faly and Hamman, we determined the value of the critical value $t_c$ for each case under consideration and then took $t_p > t_c$ to avoid running the simulation in a non-ergodic regime. Typical values for $t_p$ were between 5 and 15 for double-well cases listed below. We stress that there was not much difference in the quality of the HPIMC data if we chose $t_p > t_c$ or chose $t_p = t_c/2$. In addition, we obtained good data for the harmonic well by choosing $t_p \approx 1/\omega_0$ even though for this particular case $t_c = \infty$. If we define $\omega_0$ as the smallest nonzero frequency of the system, optimal values of the step size $\Delta t$ are between $0.05/\omega_0$ and $0.1/\omega_0$. Larger values of $\Delta t$ lead to larger errors in the pseudo-time propagation which then lead to small acceptance ratios. Smaller values of $\Delta t$ lead to longer computation times. Unless specified otherwise, we always chose $m = m_\pi = \gamma = 1$. We emphasize that the HPIMC method is insensitive of the choice of the mass $m_\pi$ associated with the fictitious momentum $\pi_{i,j}$.

In Fig. 2, we show the displacement-displacement Green’s function $G(\tau)$, for a single harmonic oscillator, obtained by evaluating (16) for various values of $\omega_0 \beta$, as a function of the imaginary-time variable $\tau$. These curves look similar to the Green’s functions that we obtained numerically for this and the other models: For some parameters and temperatures, the $G(\tau)$ varies little as a function of $\tau$; for others, it varies rapidly at the ends of the interval $[0, \beta]$ and is flat in the middle with values nearly equal to zero; and for still other parameters, it has a featureless, parabolic looking shape.

The common features of these curves have several significant implications for the analytic continuation problem. First, we remark that from the quantum Monte Carlo simulations we obtain estimates of $G(\tau)$ only at a relatively small number of discrete values $\tau_i$. The smoothness of the curves implies that the $G(\tau_i)$ at neighboring values of $\tau_i$ are correlated. The computation of the covariance matrix in (34) is thus an important part of the of the analysis of the data. While the correlations among the different $\tau$ values of $G(\tau)$ make the interpretation of the assignment of an “error-bar” to a given $\tau$ value delicate, such an assignment illustrates several difficulties inherent in the data that help to make the analytic continuation of the data often very difficult. In the case where $G(\tau)$ is nearly flat, the errors bars mean that a number of values of $G(\tau)$ are “within the error-bars” of each other. This situation, along with the correlations implied by sizable off-diagonal elements of the covariance matrix, means that only a subset, and often a small subset, of the measured values of $G(\tau)$ represent independent data useful for the analytic continuation procedure. The analytic continuation near the classical limit can be very difficult.

The situation with the rapid end-point variation and the flat nearly zero values is another difficult case. Again the flat region generates a lose of useful values of $G(\tau)$ and the smallness of $G(\tau)$ in this region can engender situations where the error bars would imply that during the simulation estimates of $G(\tau)$, which must be non-negative, were derived from ensemble values that included negative ones. The Monte Carlo algorithms in fact do not produce negative values but do produce highly skewed fluctuations about the mean. The Gaussian assumption for the likelihood function in (12) thus can only be approached in the limits of a large number of independent measurements when the central limit controls the data distribution. The ratio of the mean value to the estimated variance (signal to noise ratio) also indicates that the most effective data comes from those in the rapidly decreasing region. At low temperatures, the analytic continuation problem can become very difficult.

The details of the simulation algorithm can also impact the quality of the results and data. In Fig. 3, we show $G(\tau)/G(0)$ as a function of $\tau$ obtained by two closely related simulation techniques for a single harmonic oscillator. We remark that the scale of abscissa is $1/100$ of that of Fig. 2 and the ordinate shows $\tau$ only in a narrow region at the symmetry point $\beta/2$. The dashed curve is the analytic result obtained from (14). The data is represented by square markers were obtained by the HPIMC method without the time-reversed step; the data represented by the circles were obtained with the HPIMC method with the time-reversed step. In each case, the same number of Monte Carlo steps were made. One sees that the fluctuations with the HPIMC method without the time-reversed step are larger and that the error bars associated with the results suggest a dip into non-negative values of $G(\tau)$. More significantly, the results deviate from the exact curve by more than one standard deviation in the immediate vicinity of $\tau = \beta/2$.

The analytic continuation result for $A(\omega)$ from the data partially shown in Fig. 3 is shown in Fig. 4. From (14), the spectral density should be $0.50 (\omega - 1)$. The solid curve is obtained from the HPIMC algorithm and shows a broadened delta-function at the right location with nearly the correct weight. The fraction of a per-cent difference from the correct weight is most likely a consequence of the small error caused by discretizing the imaginary-time derivatives. On the other hand, the dashed curve, which is obtained from the data obtained from the HPIMC algorithm without
the time-reversed step, is broader, located incorrectly, and has a larger discrepancy in its weight. The increased breadth is a consequence of the larger variance in the measured data. The incorrect location and poorer weight is a consequence of the small deviation from the exact value near $\tau = \beta/2$, which in turn is a consequence of the Monte Carlo algorithm performing badly.

In Fig. 5, with the data obtained from the HPIMC algorithm, we show the full analytic continuation form $G(\tau)$ to $G^R(t)$. In Fig. 5a, the data (open circle) is compared with the exact results for $G(\tau)$ (solid line) obtained from (18). In Fig. 5b, the dashed curve is the $A(\omega)$ obtained by the analytic continuation procedure, while the solid line is a Lorentzian at the same location. The real part of $G(\omega)$ is shown in Fig. 5c, where the dashed line is the quantum Monte Carlo results and the solid line is an analytic result obtained from the Lorentzian from Fig. 5c. The width $\eta$ of the Lorentzian shown in Fig. 5b was adjusted so the $\omega = 0$ values of the two curves agreed. The single adjustment produced remarkably good agreement at high frequencies. The principal differences between the two curves are at $\omega = \pm 1$ where divergences should exist as indicated by (18). Finally, $G^R(t)$ is shown in Fig. 5d. The solid line was obtained analytically and used the Lorentzian of Fig. 5b, while the dashed line is the quantum Monte Carlo result. The agreement between the results is satisfying and comparable in quality to that possible by real-time quantum Monte Carlo methods. The width of the Lorentzian was $7/\omega_0$, i.e., about 7 times the natural period of the harmonic oscillator. This width is still controlled by the size of the variance in the measured values of $G(\tau)$.

For the case of the harmonic chain, we computed the Green’s function $G_k(\tau)$ for each independent wave number and from it found the corresponding spectral density $A_k(\omega)$. As with the single oscillator, this function should be a delta-function located at $\omega_k$ and have a weight equal to $G_k(0) = \langle x_k^2 \rangle$. As in the single oscillator case, instead of finding a delta-function, we found a Lorentzian-like peak at the correct location with the correct weight. The peaks for different values of $k$, however, had different widths. In general, the peak widths increased with increasing $k$, correlating with the increased variance associated with the $G_k(\tau)$. The spectral densities for the three lowest values of $k$ are shown in Fig. 6. The peak positions as a function of $\omega$ give the phonon dispersion relation. Our determination of this relation is compared to the exact result in Fig. 7. The agreement is excellent. There is a difficulty that must be mentioned. At $k = 0$ and $\omega_k = 0$, $G_k(\tau)$ is flat and the weight of the peak approaches infinity. For $k = 0$, not surprisingly, we were unable to do the analytic continuation. This situation is why we considered the model defined by (6). Here, $\omega_k$ at $k = 0$ is not zero and the determination of $A_k(\omega)$, and subsequently $\omega_k$, is possible for all values of $k$. The dispersion relation found from the analytic continuation agrees very well with exact result.

For a single, double-well potential, the spectral density can give direct information about tunneling processes. This situation is illustrated in Fig. 8 where the spectral densities for the Hamiltonian, described by (6), are shown for several different values of the parameter $\gamma$. It is straightforward to discretize Schroedinger’s time-independent differential equation for this potential and find the eigenvalues of the resulting eigenvalue equation. We adjusted the model parameters so only a very few (usually one) of the lowest eigenstate lied below the barrier height, similar to the situation depicted in Fig. 1a. (For deeper wells, our simulation methods would get stuck in one well or the other for large numbers of Monte Carlo steps, and hence the algorithm effectively lost ergodicity.) In the cases reported, the temperatures of the simulations were also less than the separation between the two lowest lying pairs of eigenstates. Thus, our spectral densities only exhibited the transition between these two states, and the position of the peak gives a direct measure of the lowest frequency tunnel splitting. This position agreed very well with the exact value calculated from Schroedinger’s equation. Additionally, the weight of the peak also agreed well with the sum rule (12).

For a chain of double-well potentials (5), still a different situation presents itself. At zero temperature, depending on the values of $\epsilon$ and $\gamma$, the system exists in either a broken symmetry phase, in which the mean-squared displacement is non-zero, or in a symmetric phase, in which the mean-squared displacement is zero. The model has a quantum phase transition. We found that simulation, if performed in the broken symmetry phase, stuck in one well or the other for large numbers of Monte Carlo steps, making it difficult to collect the amount of statistically independent information to do the analytic continuation. In Fig. 9, we report the $A_k(\omega)$ for two simulations done in the symmetric phase. The one in Fig. 9b is close to the zero-temperature phase boundary. As one moves closer to the $T = 0$ phase boundary by increasing $\epsilon$, the $k = 0$ peak moves towards $\omega = 0$. This movement is a consequence of the decreasing probability for tunneling between the two minima of the double-well potential as the barrier height is increased.

V. CONCLUDING REMARKS

We used methods of Bayesian statistical inference and the principle of maximum entropy to analytically continue imaginary-time Green’s function generated in quantum Monte Carlo simulations to obtain the real-time displacement-displacement Green’s functions. For test problems, we considered chains of harmonic and anharmonic oscillators whose properties we simulated by a hybrid path-integral quantum Monte Carlo method (HPIMC). From the imaginary-time, displacement-displacement Green’s function, we first obtained its spectral density. For harmonic oscillators,
we demonstrated that the peaks of this function were in the correct position and their area satisfied a sum rule. Additionally, as a function of wavenumber, the peak positions followed the correct dispersion relation. For a double-well oscillator, we demonstrated the peak location correctly predicted the tunnel splitting. Transforming the spectral densities to real-time Green’s functions, we conclude that we can predict the real-time dynamics for lengths of times corresponding to 5 to 10 times the natural period of the model. The length of time was limited by the simulation algorithm and not directly by the analytic continuation procedure.

The simulation algorithm influences the results in at least two ways. One way is the ease with which statistically independent, Gaussian-distributed data is obtained. In our experience, of the various quantum Monte Carlo methods we have used, path-integral Monte Carlo methods (PIMC) tend to produce data with long-ranged correlations, thus making statistical independence sometimes difficult to achieve. Achieving statistical independence is important for proper error estimation because of the sensitivity of ill-posed problems to errors in the data. With out statistical independence these errors are usually underestimated. That the data is Gaussian-distributed is necessary to satisfy the assumptions of the analytic continuation procedure. Currently, large amounts of data are used to force the simulation data to have proper statistical properties. The method of binned averages, with many measurements in a bin, is used to achieve statistical independence. The central limit theorem is used to obtain a Gaussian distribution of the binned averages. Because of the low computational intensity necessary for the test cases considers, producing the necessary large amounts of data was not problematic.

A second way the algorithm can influence the results is through broken ergodicity and unphysical results. Here, we are referring to the ragged structure we saw in $G(\tau)$ with the hybrid method and to the small systematic difference between the exact and computed results. We have not previously seen similar problems. Small modifications in the simulation algorithm removed the problems but it was at first difficult to determine the source of the difficulty. Because the purpose of the research was not algorithmic development, we did not do any comparisons of HPIMC and other possible methods to determine relative efficiency and other merits. Again, the computation times for these simulations is small (a few hours on a modest workstation) and so we were unmotivated to make such comparisons.

Other recently suggested approaches, e.g., \cite{13,14}, should be considered as part of further studies.

In general, we believe we have demonstrated that analytically continuing imaginary-time correlation functions, obtained from a quantum Monte Carlo simulation, to obtain real-time correlation functions is a feasible alternative to obtaining such real-time functions directly from a quantum Monte Carlo simulation done in real-time. One advantage in choosing this approach appears to be the longer length of time over which the real-time information is faithful to the correct result. Of course, this conclusion is based on one study of simple models; however, this study does strongly indicate the direction for further and more extensive work.

ACKNOWLEDGMENTS

This work was supported by the U.S. Department of Energy. We thank J. Doll and G. Berman for helpful conversations.
Present Address: Jožef Stefan Institute, University of Ljubljana, 61111 Ljubljana, Slovenia.

[1] A brief review is given by B.J. Berne and D. Thirumalai, Ann. Rev. Chem. Phys. 47, 401 (1986). More recent works include: J.D. Doll, R.D. Coalson, and D.L. Freeman, J. Chem. Phys. 87, 1641 (1987); J.D. Doll, D.L. Freeman, and T.L. Beck, Adv. Chem. Phys. 78, 61 (1990); C.H. Mak and R. Egger, Phys. Rev. A, to appear; and references therein.

[2] J.E. Gubernatis, M. Jarrell, R.N. Silver, and D.S. Sivia, Phys. Rev. B 44, 6011 (1991); M. Jarrell and J.E. Gubernatis, Phys. Rept., to appear.

[3] Xidi Wang, D.K. Campbell, and J.E. Gubernatis, Phys. Rev. B 49, 15485 (1994).

[4] G.D. Mahan, Many-Particle Physics (Plenum, New York, 1981).

[5] See for example, M. Creutz and B. Freedman, Ann. Phys. (N.Y.) 132, 427 (1981).

[6] B.J. Berne and D. Thirumalai, Ann. Rev. Phys. Chem. 37, 401 (1986).

[7] S. Duane, A.D. Kennedy, B.J. Pendleton, and D. Roweth, Phys. Lett. B 195, 216 (1987).

[8] R.N. Neal, unpublished.

[9] S. Fahy and D.R. Hamann, Phys. Rev. Lett. 69, 761 (1992).

[10] J. Skilling, in Maximum Entropy and Bayesian Methods edited by J. Skilling (Kluwer Academic, Dordrecht, 1989), p. 45.

[11] S.F. Gull, in Maximum Entropy and Bayesian Methods edited by J. Skilling (Kluwer, Dordrecht, 1989), p. 53.

[12] R.K. Bryan, Eur. Biophys. J. 18, 165 (1990).

[13] D.D. Frantz, D.L. Freeman, and J.D. Doll, J. Chem. Phys. 97, 5713 (1992).

[14] Jianshu Cao and B.J. Berne, J. Chem. Phys. 92, 1980 (1990).
FIG. 1. Schematic representation of the energy levels in a harmonic and double-well potential.

FIG. 2. Green’s function $G(\tau)$ for a particle in a harmonic-well, obtained from the analytical form (21) potential, as a function of imaginary-time $\tau$ and at different values of $\beta \omega_0$.

FIG. 3. Comparison of analytical results for the Green’s functions for a particle in an harmonic well (dashed curve) with numerical results (open circles and squares) obtained using HPIMC method (a) with and (b) without the time-reversal step in the molecular dynamic part of the algorithm.

FIG. 4. Comparison of the spectral functions obtained from the data shown in Fig. 3. As in Fig. 3, in we present spectral functions extracted from HPIMC data (a) with and (b) without the time-reversal step. We also present $G(0)$, the computed area under the curves.

FIG. 5. Comparison of the Green’s function (a) and its spectral functions for a particle in a harmonic well obtained by randomly changing the direction of the molecular dynamics time integration (open circles in (a) and full line in (b)) and by not randomly changing the integration time direction (open circles in (a) and full line in (b)). Presented is only a small portion of $G(\tau)$ around $\tau = \beta/2$ where deviations from the analytic solution (dashed line in (a)) are enhanced. Also presented are the sum rules. Analytically, $G(\tau = 0) = \langle x^2 \rangle = 0.500$.

FIG. 6. Spectral functions for the harmonic chain at different values of $k$. Arrows above spectral functions denote exact positions of peaks. We also compare the numerically calculated sum-rules $f$ with analytical values.

FIG. 7. Dispersion relation $\omega_k$ for harmonic chain with $m = 1$ and $\gamma = 1$. Open circles correspond to discrete values of $\omega_k$ for a 10-site system.

FIG. 8. Spectral functions for a single double-well potential at different values of $\gamma$ and different temperatures $1/\beta$. Arrows above spectral functions denote exact positions $\omega_0$ of peaks as obtained by numerical solution of the double-well potential. We also compare sum-rules, calculated by integrating the spectral functions $A(\omega)$ over $\omega$, with $G(\tau = 0) = \langle x^2 \rangle$, obtained directly from the QMC calculation. $\nu$ is the ratio $1/\eta t_0$ where $\eta$ was obtained by fitting $A(\omega)$ to the analytical form $G(\omega)$, see Eq. (23).

FIG. 9. Spectral functions $A(\omega)$ for a chain of 20 sites at two different values of $\epsilon$: (a) $\epsilon = 0.5$ and (b) $\epsilon = 0.75$. We present the spectral functions for different wavevectors $k$ in units of $2\pi/20$. 

12
fig. 1

V

\omega_0

X

X
\[ \frac{G(\tau)}{G(0)} = \beta \omega_0 \]
Harmonic well

G(τ)

m=γ=1
β=10
N_{sweep}=2000
N_{bin}=800

fig.3
fig. 4

Harmonic well

\[ m = \gamma = 1 \]
\[ \beta = 10 \]
\[ N_{\text{sweep}} = 2000 \]
\[ N_{\text{bin}} = 800 \]

- a) \( G(0) = 0.496 \)
- b) \( G(0) = 0.482 \)
Harmonic well

(a) $G(\tau)$

$\text{Re}(G(\omega))$

$A(\omega)$

$G(t)$

$m=\gamma=1$

$\beta=10$

$N_{\text{sweep}}=2000$

$N_{\text{bin}}=800$

$\eta=0.023$

fig. 5
\[ A(\omega) \]

\[ N = 10 \]
\[ \beta = 10 \]
\[ m = \gamma = 1 \]
\[ N_b = 800 \]
\[ N_{\text{sweep}} = 2000 \]

- \( k=1, G_k(0)=0.0806, \langle x^2_k \rangle = 0.0812 \)
- \( k=2, G_k(0)=0.0420, \langle x^2_k \rangle = 0.0425 \)
- \( k=3, G_k(0)=0.0302, \langle x^2_k \rangle = 0.0309 \)
\[
A(\omega) = \begin{cases}
\text{N}=10 \\
\beta=10 \\
m=\gamma=1 \\
N_b=800 \\
N_{\text{sweep}}=2000
\end{cases}
\]

\[
\begin{align*}
k=0, & \quad G_k(0)=0.0487, \quad \langle x_k^2 \rangle=0.0496 \\
k=1, & \quad G_k(0)=0.0423, \quad \langle x_k^2 \rangle=0.0423 \\
k=2, & \quad G_k(0)=0.0319, \quad \langle x_k^2 \rangle=0.0318 \\
k=3, & \quad G_k(0)=0.0256, \quad \langle x_k^2 \rangle=0.0257 \\
k=4, & \quad G_k(0)=0.0225, \quad \langle x_k^2 \rangle=0.0225
\end{align*}
\]
Double well, \( N_{\text{sweep}} = 4000, N_{\text{bin}} = 400-1000 \)

- \( m = 4.0, \omega_0 = 0.20, G(0) = 0.566, \langle x^2 \rangle = 0.588, \beta = 20 \)
- \( m = 2.0, \omega_0 = 0.39, G(0) = 0.602, \langle x^2 \rangle = 0.606, \beta = 15 \)
- \( m = 1.0, \omega_0 = 0.72, G(0) = 0.669, \langle x^2 \rangle = 0.670, \beta = 10 \)

\( \gamma = 1 \)

\( N_{\text{sweep}} = 4000 \)

\( N_{\text{bin}} = 400-1000 \)

fig. 8
\begin{align*}
\text{k=0, } G_k(0) &= 0.067, \quad \langle x_k^2 \rangle = 0.068 \\
\text{k=1, } G_k(0) &= 0.051, \quad \langle x_k^2 \rangle = 0.051 \\
\text{k=2, } G_k(0) &= 0.034, \quad \langle x_k^2 \rangle = 0.034 \\
\text{k=3, } G_k(0) &= 0.025, \quad \langle x_k^2 \rangle = 0.025 \\
\text{k=4, } G_k(0) &= 0.020, \quad \langle x_k^2 \rangle = 0.020
\end{align*}

\text{N=20, } \beta=15, \quad \varepsilon=0.5, \quad m=1, \quad \gamma=2, \quad N_b=600, \quad N_{\text{sweep}}=1000
fig. 9b

\[ A(\omega) \]

- \( k=0, G_k(0)=0.107, \quad \langle x_k^2 \rangle = 0.135 \)
- \( k=1, G_k(0)=0.0448, \quad \langle x_k^2 \rangle = 0.0455 \)
- \( k=2, G_k(0)=0.0247, \quad \langle x_k^2 \rangle = 0.0250 \)
- \( k=3, G_k(0)=0.0168, \quad \langle x_k^2 \rangle = 0.0175 \)

\( N=20 \)
\( \beta=15 \)
\( \epsilon=0.75, \quad m=\gamma=1 \)
\( N_b=600, \quad N_{\text{sweep}}=2000 \)