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Solving the sign problem in quantum Monte Carlo dynamics

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A method of solving the sign problem in the Monte Carlo path-integral simulations of quantum dynamics is presented. Our method is based on the distortion of integration contours in conjunction with a stationary-phase filtering method. Using this importance sampling, correlation functions for the spin-boson model have been computed for real times much longer than $\beta\hbar$.

The equilibrium properties of many quantum systems in condensed phase have been studied using Monte Carlo (MC) methods.[1,2] Calculations of quantum dynamics by this approach, however, have seemed intractable. The major difficulties in dynamical simulations arise from the appearance of complex exponentials in real-time path integrals. This difficulty inherent in quantum dynamical MC simulations is often referred to as the "alternating-weight" or "sign" problem. An analogous difficulty arises in treating fermionic systems.[3] Earlier attempts to avoid the alternating-weight problem in quantum dynamics (or for fermionic systems) have relied on the self-consistent-field approximation (the analog of Hartree-Fock[4]) or else these attempts were limited to short times[5,6] (which would be analogous to infrequent fermionic exchange[7]).

In this Rapid Communication, we report a method we have discovered for solving the alternating-weight problem as it appears in quantum dynamics. Primary elements of our method are found in earlier works on quantum MC.[5,8-12] To illustrate our method, we consider the spin-boson model: A two-level system (TLS) coupled to an infinite set of harmonic oscillators. The Hamiltonian is

$$H=-K\sigma_x+\sum_j\left(\frac{p_j^2}{2m_j}+\frac{m_j\omega_j^2x_j^2}{2}\right)+\phi\sigma_z\,, \tag{1}$$

where $2K$ is the tunnel splitting of the TLS, σ_z and σ_x are the Pauli spin matrices, and m_j,ω_j are the mass and frequency of the jth oscillator. The local field is $\phi=\sum_j c_jx_j$, where c_j is the strength of the coupling to the jth oscillator. The spectral density of the bath is

$$J(\omega)\equiv(\pi/2)\sum_j(c_j^2/m_j\omega_j)\delta(\omega-\omega_j)=\eta\omega/(1+\tau^2\omega^2)\,.$$

This somewhat arbitrary choice of $J(\omega)$ ensures a well-defined classical friction η, and bath correlation decays exponentially with a time τ.[13] The spin-boson model is often used to describe self-trapping of molecular polaron,[14] spin-phonon relaxation,[15] macroscopic tunneling, and quantum coherence,[16] and nonadiabatic effects in chemical dynamics.[17]

Although in the case $\phi=0$ the two subsystems can each be solved, the coupled system is a nonlinear many-body system which evolves through tunneling processes. The system exhibits a broken symmetry for sufficiently large coupling.[16] In the adiabatic limit, this localization transition occurs when the localization parameter $L\equiv\eta/2\tau K$ reaches a critical value of unity.[18] Exact solutions of the spin-boson model are not known, except for some special cases such as the adiabatic limit. Further, the model is intractable by basis set techniques except for the nondissipative case of a few oscillators. Although dynamical quantum MC simulations have been attempted in the past, they have been limited to short time.[5] In the future, we will use our MC procedure to carry out an extensive examination of the spin-boson model and the approximate theories used to treat it. In the present context, however, this model serves as a nontrivial illustration of the dynamical algorithm we will discuss.

The relevant correlation function is

$$\langle h_A(0)h_A(t)\rangle=\mathrm{Tr}e^{-\beta H}h_Ae^{itH/\hbar}h_Ae^{-itH/\hbar}/Z\,,$$

where $h_A=(1+\sigma_z)/2$ and $Z=\mathrm{Tr}e^{-\beta H}$. For the uncoupled TLS, $\langle h_A(0)h_A(t)\rangle$ oscillates in a sinusoidal fashion reflecting perfect quantum coherence. In the presence of dissipation, however, the rate of tunneling diminishes, accompanied by a loss of coherence.[16] By the fluctuation-dissipation theorem, the rate of change of the population is[19]

$$k(t)=\frac{-1}{\beta\hbar\langle h_A\rangle}\,\mathrm{Im}[\langle h_A(0)h_A(t)\rangle]\,, \tag{2}$$

which exhibits a plateau at long times if the relaxation is exponential. In that case, the tunneling rate constant is the plateau value[20] of $k(t)$.

Correlation functions such as $\langle h_A(0)h_A(t)\rangle$ may be represented by a discretized path integral[5,21]

$$\langle h_A(0)h_A(t)\rangle=\frac{\int dr_1\cdots dr_{P+2Q}\mathcal{O}(r_1,r_2,\ldots,r_{P+2Q})h_A(r)h_A(r')}{\int dr_1\cdots dr_{P+2Q}\mathcal{O}(r_1,r_2,\ldots,r_{P+2Q})}\,, \tag{3}$$

in the coordinate representation $|r\rangle\equiv|\sigma,\{x_i\}\rangle$ where σ is the position of the TLS. $\mathcal{O}$, the statistical object that governs the dynamics in real time, is depicted in Fig. 1. The forward (reverse) real-time path has a total length of $iT(-iT)$ with Q subsegments, and $t\le T$; the imaginary-time path has a length of $\beta\hbar$ and P subsegments. Due to the real-time paths,

$\mathcal{O}$ is an oscillatory function of $\{r_i\}$.

The statistical object was considered before us by Wolynes and co-workers.[5(a)] Its advantages are twofold: (1) From a single Monte Carlo trajectory, one obtains the correlation function for all real-time points t, less than T. Separate calculations for each different t are not required. (2) Simultaneously, one accounts for all possible constructive and destructive interferences, and quantum coherence is exposed, rather than hidden by complex time. Alternative formulations[5(b),6,8(b)] focusing on separate probability amplitudes and/or different forms of correlation functions do not have these advantages.

Since the bath is harmonic and its coupling to the TLS is linear, an integration over the bath degrees of freedom reduces Eq. (3) to sum over spin paths

$$\langle h_A(0)h_A(t)\rangle = \sum_{\{\sigma\}} \exp\left[\sum_{i,j}\sigma_i M_{ij}\sigma_j/2\right] h_A(\sigma)h_A(\sigma') \Big/ \sum_{\{\sigma\}} \exp\left[\sum_{i,j}\sigma_i M_{ij}\sigma_j/2\right], \tag{4}$$

where $\sum_{i,j}\sigma_i M_{ij}\sigma_j/2 = S_{\mathrm{TLS}}[\sigma] + I[\sigma]$.[5] Here, S_{TLS} is the action for the free TLS and $I[\sigma] = \sum_{i,j}\sigma_i I_{ij}\sigma_j$ is the influence functional containing nonlocal complex-valued couplings

$$I_{ij} \equiv \frac{\hbar}{\pi}\Delta_i\Delta_j \int_0^\infty d\omega\, J(\omega) \frac{\cosh[\hbar\omega(\Delta t_{ij} - \Delta t_{ji})/2]}{\sinh(\beta\hbar\omega/2)}, \tag{5}$$

where

$$\Delta_i = \begin{cases} \beta\hbar/P, & 1 \le i \le P \\ iT/Q, & P+1 \le i \le P+Q \\ -iT/Q, & P+Q+1 \le i \le P+2Q, \end{cases} \tag{6}$$

and $\Delta t_{ij} \equiv \sum_{k=i}^{j-1}\Delta_k$. For technical reasons that will be apparent shortly, we rewrite Eq. (4) in continuum form by making use of the Hubbard-Stratonovich transformation[22]

$$\langle h_A(0)h_A(t)\rangle = \int \prod_{k=1}^{P+2Q} ds_k\, W[s] h_A(s)h_A(s') \Big/ \int \prod_{k=1}^{P+2Q} ds_k\, W[s], \tag{7}$$

where

$$W[s] = \exp\left[-\sum_{i,j} s_i (M+A)^{-1}_{ij} s_j/2 + \sum_i \ln(2\cosh s_i)\right],$$

$h_A(s) = e^{-s}/2\cosh s$, and A is an arbitrary diagonal matrix with elements $a_1, \ldots, a_{P+2Q}$. This transformation is valid as long as $\mathrm{Re}(M+A)$ is positive definite. This can be ensured by letting $a_1 = a_2 = , \ldots , = a_0$ and choosing a_0 such that $a_0 + \min_j \mathrm{Re}(\lambda_j) > 0$, where λ_j are the eigenvalues of M. So the basic task appears in Eq. (7).

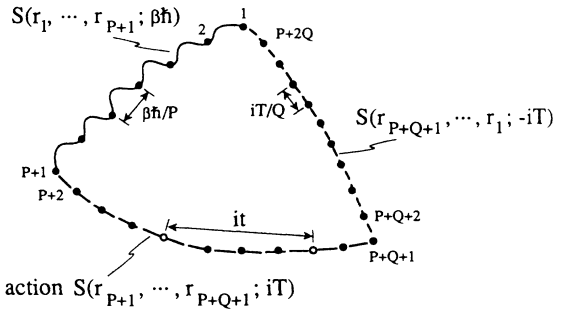

FIG. 1. $\mathcal{O}$, the statistical object that governs the dynamics in real time. $S(r_1, \ldots, r_{P+1}; \beta\hbar)$ is the discretized action for the imaginary-time path with a total length of $\beta\hbar$ and P subsegments. $S(r_{P+1}, \ldots, r_{P+Q+1}; iT)$ and $S(r_{P+Q+1}, \ldots, r_1; -iT)$ are the actions for the forward and reverse real-time paths, each with total length iT and Q subsegments. The correlation function $\langle h_A(0)h_A(t)\rangle$ is computed by sampling $h_A(r)h_A(r')$ for every pair of points r and r' (denoted by the open circles) separated by it.

Integration over oscillatory functions such as those in Eq. (7) are encountered in all quantum dynamics simulations. The complex-valued exponent of W renders classical MC methods useless. A primitive way to deal with the non-positive-definite nature of W is to rewrite $W[s]$ as $\rho[s]\exp(if[s])$, where $\rho[s]$ is positive definite and $f[s]$ is real. Then $\rho[s]$ can be used as a weight function. But a straightforward implementation of this idea fails because it is inefficient. Indeed, for long enough real time, due to rapid phase cancellations, the accuracy is lost in the roundoff errors on the computer. We refer to this as the primitive approach.

A better idea is based on the observation that the most significant contributions to the integral come from regions of configuration space where the phase $f[s]$ is nearly stationary. A successful scheme to perform the integration in Eq. (7) must concentrate sampling near these stationary-phase regions. This is the idea behind the stationary-phase Monte Carlo (SPMC) method.[8] In particular, to focus sampling near stationary-phase regions, one may incorporate a filtering function D into the integrand,

$$D[s] \equiv \int \prod_{k=1}^{P+2Q} dy_k P[y] \left[\frac{\rho[s-y]}{\rho[s]}\right] e^{if[s-y]-if[s]}, \tag{8}$$

where $P[y] = N\exp(-\sum_j y_j^2/2\epsilon_j^2)$ and N is a normalization constant. In general, the exact analytical form of $D[s]$ is unknown, so it is approximated by its first-order approximant $D_0[s] = \exp[-\sum_j \epsilon_j^2(\partial f/\partial s_j)^2/2]$. The

widths $\{\epsilon_j\}$ are chosen according to $\epsilon_j = \epsilon_0 \Delta_j$, where Δ_j is the characteristic width[23] of $\rho[s]$ in the variable s_j. ϵ_0 is chosen to maximize damping while at the same time minimize the error introduced by the approximation D_0.[24] A correction to D_0 can be estimated by computing $\Delta D = D - D_0$ by the Monte Carlo as proposed by Doll. A small value of ϵ_0 results in a small correction ΔD, but it also produces little filtering of the integrand so the sign problem overwhelms the calculation. On the other hand, a large ϵ_0 produces heavy filtering, so the integrand appears highly smoothed, but the correction ΔD becomes large and the Monte Carlo estimation of ΔD now suffers from the same alternating weight. We have merely shifted the sign problem to another part of the calculation. Therefore we must aim for a compromise between these two extremes. The correction ΔD may be used as a guide for searching for this compromise. In a successful application of SPMC, the difference between the uncorrected results and the corrected ones must be small.

We have tried to apply the SPMC method to evaluate Eq. (7), and we find no acceptable compromise for ϵ_0. The reason is that the dynamics of the spin-boson model is dominated by tunneling. For such nonclassical processes, there are no real-time stationary paths in real-configuration space. Indeed, we can easily observe from Eq. (7) that the true stationary point where $\rho[s]$ is maximum and $f[s]$ is stationary does not lie on the real axis. Hence, we have been led to modify the SPMC to allow for distortion of integration contours. If the distorted integration contour goes into the complex plane and passes near the stationary point, the efficiency of the MC sampling can be enhanced. In principle, the best distorted contour is the steepest-descent trajectory emanating from the stationary point. However, such a contour seems difficult to parametrize. Instead, we perform a simple rotation of the integration contour. Rotations like this were considered before,[12] but the reasoning and applications are significantly different. In the cases that we have studied, such a simple distortion already produces significant improvement over the unrotated contour. The exact location of the stationary point is unimportant, as long as the rotated contour passes through the *vicinity* of it. The *approximate* location of the stationary point can be found by simulated annealing[25] with minimal work. In general, there may be more than one such point; therefore, ideally one might wish to sample near each of them. But in our studies of the spin-boson model with large L, we find that the stationary point that has the largest weight dominates the results. Through the calculations with ΔD, the accuracy of the procedure is checked *a priori*. The uncorrected results differ from the corrected ones by only a small factor, typically 5%.

Thus the method we have discovered is a two-step procedure: approximate annealing followed by filtering. Figure 2(a) illustrates the quality of the results we obtain. The function $k(t)$ plotted there is a particularly demanding quantity as it is the time derivative of the population correlation function. We have performed the calculations

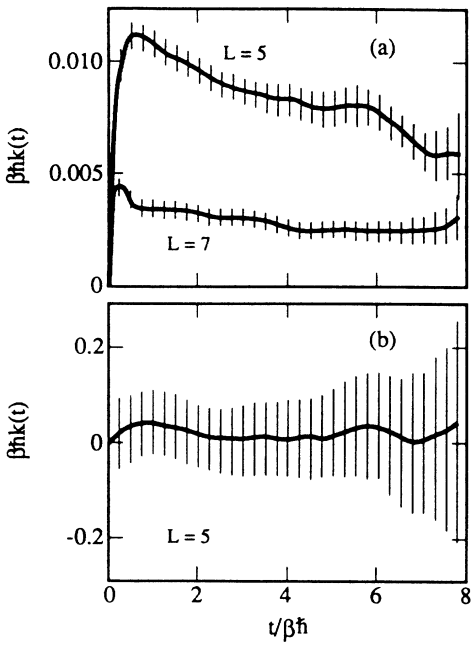

FIG. 2. (a) $k(t)$ for $L=5$ and 7, both with $\tau=\beta\hbar/2$, computed using a combination of integration contour distortion and SPMC filtering. (b) Corresponding results for $L=5$ without contour distortion—note the change in the vertical scale. In both (a) and (b), vertical bars indicate one standard deviation.

out to times much larger than $\beta\hbar$, times so long that we can observe the plateau behavior in $k(t)$. No other techniques are available to obtain results of this quality for this length of time. Figure 2(a) shows that for $L=5$ and $\tau=\beta\hbar/2$, the relaxation is nonexponential, indicated by the absence of a plateau. For $L=7$ and $\tau=\beta\hbar/2$, $k(t)$ begins to exhibit a well-defined plateau giving the tunneling rate constant. The statistical uncertainties are largest at the end point $t \to T$, since the number of equivalent pairs is reduced to one (see Fig. 1).

As a basis for comparison, the corresponding results for $L=5$ *without* contour distortion using the same number of passes are shown in Fig. 2(b). We see that if only SPMC filtering but no contour distortion is used, the statistical uncertainty arising from the oscillating signs makes the results obtained in this way meaningless. The primitive approach lacking any form of importance sampling for the alternating signs is necessarily worse, indeed useless even for times comparable to $\beta\hbar$.

For some systems, the complex action may possess an enormous multitude of comparably important stationary paths. These cases can be troublesome in much the same way as glassy behavior is difficult to treat in classical simulations.[26] Nevertheless, our results demonstrate the exact numerical solution of the spin-boson model and the wide class of natural systems for which the spin-boson model is a caricature. These systems are unapproachable by any other technique.

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