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Stochastic Method for Real-Time Path Integrations

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A new stochastic method for the direct computation of real-time Green's functions is proposed. The inherent sign problem is circumvented by partitioning the path integration into two parts, one of which involves conventional stochastic sampling, and the other explicit or analytical summation. Using this method, the dynamics of the spin-boson model may be computed up to several tunneling periods. The results reveal surprisingly complex relaxation behaviors near the coherent-incoherent boundary at low temperatures.

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In his space-time formulation of quantum mechanics, Feynman demonstrated that Green's functions of quantum systems may be represented by functional integrals over space-time paths [1,2]. Since its conception, Feynman's elegant approach has led to advances in many branches of modern physics. But attempts to implement Feynman's path integration ideas in direct numerical simulations of real-time quantum dynamics have been far less illustrious and much fewer [3–11] compared to formal theories. The numerical difficulties associated with real-time path integrations are collectively called the "sign problem," and they are the result of the oscillatory nature of the integrand appearing in Feynman integrals. Interestingly, Feynman himself was the first to recognize the fundamental difficulties associated with the sign problem [2] long before the first numerical path integration [3] was undertaken.

In this Letter, we propose a novel stochastic method to directly sample the Feynman integral in real time. Numerical evidence will show that this method partially circumvents the sign problem and is stable up to large values of real time. We apply this new method to compute real-time correlation functions of condensed phase tunneling systems, in particular, the spin-boson model [12], and observe surprisingly complex behaviors near the coherent-incoherent boundary at low temperatures.

Consider the Green's function for a system whose generalized coordinate is x (x may be a continuous or discrete variable),

$$G(x_a,t_a;x_b,t_b)=\int_a^b \mathcal{D}x(t)e^{iS[x(t)]/\hbar}, \tag{1}$$

where $S[x(t)]$ is the action. Let $\bar{x}(t)$ be any path satisfying the boundary conditions $\bar{x}(t_a)=x_a$ and $\bar{x}(t_b)=x_b$. In terms of $\bar{x}$ and fluctuations y,

$$G(x_a,t_a;x_b,t_b)=e^{iS[\bar{x}(t)]/\hbar}\int_0^0 \mathcal{D}y(t)e^{i\delta S[\bar{x}(t),y(t)]/\hbar}, \tag{2}$$

where $\delta S[\bar{x}(t),y(t)]=S[x(t)]-S[\bar{x}(t)]$. Notice that Eq. (2) is true for *any* $\bar{x}(t)$; therefore, summing over all possible $\bar{x}(t)$ yields a quantity that is equal to a multiple of $G(x_a,t_a;x_b,t_b)$, and when expressed in terms of this sum, the Green's function becomes

$$G(x_a,t_a;x_b,t_b)=A^{-1}\sum_{\text{all }\bar{x}(t)} e^{iS[\bar{x}(t)]/\hbar} \times\int_0^0 \mathcal{D}y(t)e^{i\delta S[\bar{x}(t),y(t)]/\hbar} \tag{3a}$$

$$=\int_a^b \mathcal{D}\bar{x}(t)e^{iS[\bar{x}(t)]/\hbar}D[\bar{x}(t)], \tag{3b}$$

where $D[\bar{x}(t)]\equiv A^{-1}\sum_{\text{all }y(t)}\exp\{i\delta S[\bar{x}(t),y(t)]/\hbar\}$, A is a normalization constant, and we have interchanged the summation and the integration to avoid mathematical ambiguities concerning the measure. Now Eq. (3b) may serve as the basis for a Monte Carlo (MC) sampling after the functional integral is broken up using the conventional Trotter formula. There is a key difference between Eq. (3b) and the direct application of Eq. (1)—Eq. (3b) *is free of any sign problem.* This crucial observation is true because Eq. (2) is true for all $\bar{x}(t)$, and therefore the integrand in Eq. (3b) is a *constant* of $\bar{x}(t)$, and so no sign problem exists.

First, $D[\bar{x}(t)]$ is itself a path sum, and its exact form is in general unknown. A nested Monte Carlo scheme for Eq. (3b), in which $D[\bar{x}(t)]$ is first evaluated by an inner Monte Carlo sampling, would offer no advantage because this would merely shift the sign problem to a different part of the calculation. In order for Eq. (3b) to be useful, a reasonable analytical approximation for $D[\bar{x}(t)]$ has to be formulated. Next, we explore some possibilities for approximants to $D[\bar{x}(t)]$. In this Letter, we focus specially on systems with a discrete Hilbert space [13], where $\bar{x}(t)$ and $y(t)$ are paths in *state space*. Let each $\bar{x}(t)$ be parametrized on a discrete time line from 0 to t at $P+1$ grid points separated by t/P, where eventually $P\rightarrow\infty$. For any $\bar{x}(t)$, a fluctuation is generated by displacing the states at any number of internal grid points to new states, and all fluctuations contribute to $D[\bar{x}(t)]$. The contributions to $D[\bar{x}(t)]$ can be grouped by order, where fluctuations differing from $\bar{x}(t)$ at one grid point are called first order, those differing from $\bar{x}(t)$ at two grid points are called second order, etc. Except for a few trivially solvable cases, summing over all fluctuations is clearly impossible. The nth-order approximant $D^{(n)}[\bar{x}(t)]$ neglects fluctuations of order $n+1$ or higher: $D^{(n)}[\bar{x}(t)]=A^{-1}(1+\sum_{j=1}^{n}C^{(j)})$, where $C^{(j)}$ is the contribution due to jth-order fluctuations, and $A=1+\sum_{j=1}^{n}A^{(j)}$, where $A^{(j)}$ is the number of elements in the set of jth-order fluctuations. In practice, it is feasible to employ only a small number of low-order terms. This suggests a resummation to approximately account for the missing terms,

$$D^{(n)}[\bar{x}(t)]=A^{-1}\exp\sum_{j=1}^{n}\xi^{(j)}+O(C^{(n+1)}), \tag{4}$$

where $\xi^{(1)}=C^{(1)}$, $\xi^{(2)}=C^{(2)}-C^{(1)2}/2$, etc., and according to the linked cluster theorem, the exponent only contains terms associated with connected diagrams [14]. The computational effort required for the evaluation of $D^{(n)}$ should therefore grow only linearly with system size for models with short-ranged interactions. As it stands, Eq. (4) is not a very good approximant to D for small n, because the $O(C^{(n+1)})$ term is not small in general. Instead, we use the geometrically damped series $D_{\epsilon}^{(n)}=A_{\epsilon}^{-1}(1+\sum_{j=1}^{n}\epsilon^{j}C^{(j)})$, where $0\leq\epsilon\leq 1$ and $A_{\epsilon}=1+\sum_{j=1}^{n}\epsilon^{j}A^{(j)}$, which gives upon resummation

$$D_{\epsilon}^{(n)}[\bar{x}(t)]\approx A_{\epsilon}^{-1}\exp\sum_{j=1}^{n}\epsilon^{j}\xi^{(j)}, \tag{5}$$

where the neglected terms are $O(\epsilon^{n+1}C^{(n+1)})$. In the limit $\epsilon\rightarrow 0$, $D_{\epsilon}^{(n)}\rightarrow 1$ and reduces Eq. (3b) back to Eq. (1), the exact expression for the path integral. But in this limit, the sign problem renders the Monte Carlo sampling unstable. In the other limit $\epsilon\rightarrow 1$, $D_{\epsilon}^{(n)}\rightarrow D^{(n)}$ and the resulting inaccuracy is large. In practice, one aims for a small but finite ϵ between these two limits to achieve the largest level of filtering while retaining reasonable accuracy.

Several features distinguish the current method from other recent approaches to real-time path integrations [4,7–9,11]. All other approaches treat extended systems only [4,7–9], which immediately excludes a large and important class of discrete quantum systems. Furthermore, these methods are most useful when the system possesses one or more "classical" stationary paths. This reliance precludes treatment of many quantum processes which have no classical analogs, such as tunneling. These limitations may be partially circumvented [11] by first using a continuum transformation to turn discrete systems into extended ones, and then extending the space of integration to include complex-valued space-time paths in order to capture nonclassical stationary trajectories. The present method, however, does not succumb to any of these limitations of the former methods because its formulation [cf. Eqs. (3)] applies equally well to *both extended and discrete systems* and therefore provides a unified framework for treating both classes of quantum processes on the same footing.

The proposed method will first be illustrated for a two-state tunneling system with the Hamiltonian $H_0=-\hbar\Delta\sigma_x/2$, where σ_x is the Pauli spin matrix and Δ is the tunnel splitting. Notice that this system evolves purely by tunneling and its dynamics exhibits perfect quantum coherence. Its Hilbert space has dimension 2 and the basis vectors $\{\sigma\}$ are the eigenvectors of σ_z. The Green's function $G(\sigma,0;\sigma',t)=\langle\sigma|e^{-itH_0/\hbar}|\sigma'\rangle$ is given by a path integral which is isomorphic to a 1D Ising model with complex-valued exchange interaction after the conventional Trotter breakup [6]. First, we examine the results of direct Monte Carlo sampling *without* filtering. The diagonal element of the Green's function is

$$G(\sigma,0;\sigma,t)=i^{N/2}\cosh(\Delta t/2)\left\langle\exp iJ''\sum_{j=1}^{N}\sigma_j\sigma_{j+1}\right\rangle_{W[\sigma]}, \tag{6}$$

where the brackets denote an average over $W[\sigma]=\exp J'\sum_{j=1}^{N}\sigma_j\sigma_{j+1}$, N is the number of discretization points, and periodic boundary condition applies; $J'=-\frac{1}{2}\ln\tanh(Kt/N)$, and $J''=-\pi/4$. Notice that with these definitions for J' and J'', Eq. (6) is *exact* to all orders of N. Comparing Eq. (6) to the trivial analytical solution $G(\sigma,0;\sigma,t)=\cos(\Delta t/2)$, one observes that $\langle\exp iJ''\sum\sigma_j\sigma_{j+1}\rangle_W$ would vanish *exponentially* with t (or with N if t/N is kept fixed), and the average would be lost in the noise if a direct Monte Carlo evaluation of G was performed via Eq. (6). Numerical results in Fig. 1(a), which shows $P(t)\equiv|G(\sigma,0;\sigma,t)|^2$, reveal this instability of the direct method, where the statistical errors at long times diverge according to our expectation. Interestingly, Fig. 1(a) shows that the sign problem is *not* the only pathology of the direct method. Even for short-time data points with small statistical errors, the direct method yields erroneous results. The origin of this error can be traced back to the Monte Carlo evaluation of Eq. (6),

which is valid only if the quantity to be averaged is smooth on the length scale of the weight function. For all real-time path integrations, this quantity is nonpositive definite and highly oscillatory, in violation of the smoothness requirement.

Now we demonstrate how the proposed method may be used to circumvent the sign problem. Inserting the approximate $D_\epsilon^{(n)}[\bar{x}(t)]$ into both the numerator and denominator in Eq. (6),

$$G(\sigma,0;\sigma,t)\approx i^{N/2}\cosh(\Delta t/2)\left\langle \exp iJ''\sum_{i=1}^{N}\sigma_i\sigma_{i+1}D_\epsilon^{(n)}\right\rangle_W \Big/ \langle \tilde{D}_\epsilon^{(n)}\rangle_W . \tag{7}$$

Notice in Eq. (7) that the filtering functions for the numerator $D_\epsilon^{(n)}$ and the denominator $\tilde{D}_\epsilon^{(n)}$ are not identical [15]. Numerical results using Eq. (7) with the same number of MC passes as those in Fig. 1(a) are shown in 1(b). For these calculations, a first-order ($n=1$) approximant to D was used, with $\epsilon=0.015$, computed by explicitly summing over all first-order fluctuations. Figure 1(b) shows that the results do not suffer from the sign problem and they are in excellent agreement with the exact results up to more than two tunneling periods. In addition to eliminating the large statistical errors, the systematic errors are also eliminated, because the filtering function D significantly damps the oscillations.

Now we apply the proposed method to a highly nontrivial problem—the computation of real-time correlation functions of condensed phase tunneling systems—for which we embed the two-state tunneling system described above in a bosonic bath [16], with the total Hamiltonian $H=H_0+\sum_j(p_j^2/2m_j+m_j\omega_j^2x_j^2/2+c_jx_j\sigma_z)$, where c_j is the strength of the coupling to the jth oscillator. This so-called spin-boson model has been the subject of extensive studies and is a model for macroscopic quantum

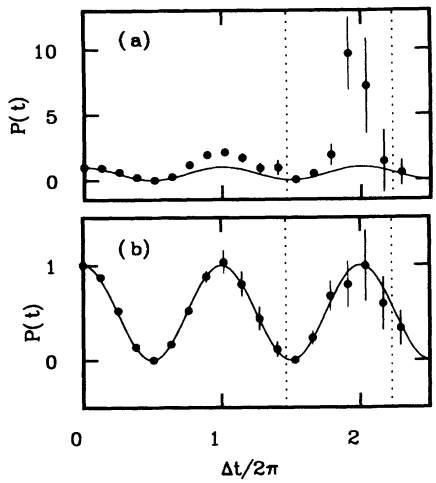

FIG. 1. The probability of return $P(t)$ for a bare two-state tunneling system from Monte Carlo sampling. The number of discretization N for each t is given by $\Delta t/2N=0.1333$. 2×10^4 MC samples were used to obtain results in the leftmost region indicated by the dotted line, 2×10^5 in the middle, and 1×10^6 in the rightmost region. Solid curves are exact solutions. Vertical bars indicate errors of 1 standard deviation. (a) Results from the direct method, Eq. (6); (b) results using the proposed method, Eq. (7). [Note the change in scale from (a) to (b).]

coherence [17], Josephson junctions [12], and light particle transport in crystals [18]. Previous functional-integral theories employing the noninteracting blip approximation have predicted extremely rich behaviors for the spin-boson model with an Ohmic bath [12], including a transition from coherent to incoherent relaxation at finite temperatures [19], power-law tails in the relaxation at intermediate coupling strength α [20,21], and nonexponential temperature dependence of the incoherent relaxation rate [22]. The noninteracting blip approximation has yielded reliable results for all but a tiny region in the parameter space. Interestingly, this small region, $\frac{1}{2}<\alpha<1$ at low temperatures, for which the noninteracting blip approximation breaks down, is also one of the most intriguing because it is in this region that the spin-boson model is "equivalent" to the Kondo problem [23–25] (spin-$\frac{1}{2}$ system interacting with a fermionic bath). We present here results of the first numerical simulations for this region, up to two tunneling periods [26].

Figure 2(a) shows Monte Carlo results for the spin-correlation function $C(t)=\mathrm{Re}[\mathrm{Tr}e^{-\beta H}\sigma_z\sigma_z(t)]/\mathrm{Tr}e^{-\beta H}$ for $\alpha=0.64$ with an Ohmic bath cutoff frequency $\omega_c=1.25\Delta$ [27] at several temperatures. The results were obtained by first expanding the Green's functions using the Trotter formula similar to that in Eq. (6) [6,28]. The harmonic bath was then integrated out, dressing the spin path with nonlocal influence functionals, and the Monte Carlo averages were performed using $D_\epsilon^{(2)}$ with $\epsilon=0.030$. The same data are replotted in Fig. 2(b) on a semilog scale. The results show that at high temperature, the system relaxes purely exponentially, in agreement with the "golden rule" [12]. At a lower temperature $kT\lesssim\hbar\Delta(\Delta/\omega_c)^{\alpha/(1-\alpha)}$, the relaxation proceeds via a fast initial (underdeveloped) exponential decay, followed by a much slower *second exponential decay*. This is in disagreement with the prediction of the noninteracting blip approximation that the long-time incoherent relaxation in this region follows a power law $\sim t^{-2(1-\alpha)}$ [20]. In addition, at even lower temperatures, the relaxation becomes oscillatory, with the correlation function approaching zero seemingly from below in the long-time limit. Again, this observation is in contrast with the prediction of the noninteracting blip approximation that the relaxation for $\alpha>\frac{1}{2}$ is purely incoherent [19]. On the other hand, our result lends support to recent evidence which suggests that initial system preparation with Boltzmann weighting

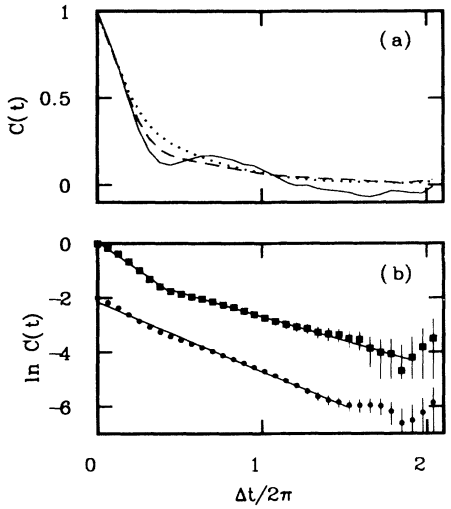

FIG. 2. (a) Real-time spin-correlation functions for $\alpha=0.64$ from Monte Carlo sampling: $T/\Delta=1.25$ (dotted line), using 4×10^5 samples; $T/\Delta=0.625$ (dashed line), using 1.2×10^6 samples; $T/\Delta=0.3125$ (solid line), using 1.2×10^6 samples. (b) Data from (a) on a semilog scale: $T/\Delta=1.25$ (circles, offset vertically by -2), relaxation is purely exponential characterized by one time constant indicated by the straight line; $T/\Delta=0.625$ (squares), an initial exponential decay is followed by a second, much slower exponential, indicated by the two straight lines. Vertical bars indicate statistical errors of 1 standard deviation.

may significantly alter the conclusions of the noninteracting blip approximation at low temperatures [18].

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[1] R. P. Feynman, Rev. Mod. Phys. **20**, 367 (1948).
[2] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
[3] A. P. Vinogradov and V. S. Filinov, Dokl. Acad. Nauk SSSR [Sov. Phys. Dokl. **26**, 1044 (1981)].
[4] V. S. Filinov, Nucl. Phys. **B271**, 717 (1986).
[5] D. Thirumalai and B. J. Berne, J. Chem. Phys. **79**, 5029 (1984); **81**, 2512 (1984).
[6] E. C. Behrman, G. A. Jongeward, and P. G. Wolynes, J. Chem. Phys. **79**, 6277 (1983).
[7] J. D. Doll, D. L. Freeman, and M. J. Gillan, Chem. Phys. Lett. **143**, 277 (1988); J. D. Doll, T. L. Beck, and D. L. Freeman, J. Chem. Phys. **89**, 5753 (1988).
[8] N. Makri and W. H. Miller, Chem. Phys. Lett. **139**, 10 (1987); J. Chem. Phys. **89**, 2170 (1988).
[9] R. E. Cline, Jr., and P. G. Wolynes, J. Chem. Phys. **88**, 4334 (1987).
[10] B. A. Mason and K. Hess, Phys. Rev. B **39**, 5051 (1989).
[11] C. H. Mak and D. Chandler, Phys. Rev. A **41**, 5709 (1990).
[12] A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fischer, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).
[13] The present method applies equally well to extended systems and yields results similar to those previously derived by other authors based on different arguments (see Refs. [4,7,8]).
[14] R. Kubo, J. Phys. Soc. Jpn. **17**, 1100 (1962).
[15] The numerator involves a complex action but the denominator involves a real action.
[16] A. O. Caldeira and A. J. Leggett, Phys. Rev. Lett. **46**, 211 (1981); Ann. Phys. (N.Y.) **149**, 374 (1984); A. J. Leggett, Phys. Rev. B **30**, 1208 (1984).
[17] A. J. Bray and M. A. Moore, Phys. Rev. Lett. **49**, 1546 (1982).
[18] M. Sassetti and U. Weiss, Phys. Rev. A **41**, 5383 (1990).
[19] A. Garg, Phys. Rev. B **32**, 4746 (1985).
[20] A. J. Leggett and A. Garg, Phys. Rev. Lett. **54**, 857 (1985).
[21] H. Grabert and U. Weiss, Phys. Rev. Lett. **54**, 1605 (1985).
[22] U. Weiss, H. Grabert, P. Hanggi, and P. Riseborough, Phys. Rev. B **35**, 9535 (1987).
[23] J. Kondo, Physica (Amsterdam) **125B**, 279 (1984); J. Kondo, in *Fermi Surface Effects*, edited by J. Kondo and A. Yoshimori, Springer Series in Solid-State Sciences Vol. 77 (Springer-Verlag, Berlin, 1988).
[24] K. Yamada, Prog. Theor. Phys. **72**, 195 (1984); K. Yamada, A. Sakurai, and S. Miyazima, *ibid.* **73**, 1342 (1985).
[25] L.-D. Chang and S. Chakravarty, Phys. Rev. B **31**, 154 (1985).
[26] High-quality numerical data for long real times are necessary to determine the nature of the slow incoherent relaxations (see Ref. [28]).
[27] Previous short-time calculations have shown that even for $\omega_c \gtrsim \Delta$, the rich dynamical behaviors of the spin-boson model are already well described by the noninteracting blip approximation, except in the Kondo region (see Ref. [28]).
[28] C. H. Mak and D. Chandler, Phys. Rev. A **44**, 2352 (1991).