MONTE CARLO INTEGRATION WITH OSCILLATORY INTEGRANDS: IMPLICATIONS FOR FEYNMAN PATH INTEGRATION IN REAL TIME ☆

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A new method is described for the Monte Carlo evaluation of integrals of the form $\int_{-\infty}^{\infty} dx \exp[iS(x)]$ that occur in the Feynman path integral representation of the time evolution operator, $\exp(-iHt/\hbar)$. The method is general, strictly Monte Carlo based (and thus applicable to high dimensionality), and has the desirable feature that the stationary phase (i.e. semiclassical) approximation to the integral is obtained in its *worst* limit. Application to a non-trivial test case (the Airy integral) illustrates these features.

1. Introduction

There is considerable interest in developing Monte Carlo methods for the evaluation of the Feynman path integral representation [1] of the time evolution operator $\exp(-iHt/\hbar)$, or propagator. A path integral representation of the propagator is desirable since it often allows one to integrate out "bath" degrees of freedom without approximation [1, pp. 68–71, 343–354], and Monte Carlo methods appear to be necessary if one is to deal with systems of more than two or three degrees of freedom. Such methods exist, and have been used with considerable success, for evaluating the Boltzmann operator (i.e. the imaginary time propagator), $\exp(-\beta H)$, and thus equilibrium statistical mechanical properties of complex systems [2–7]. One needs the real time propagator, however, in order to describe quantum dynamics. We have in mind, in particular, evaluation of the reactive flux correlation function [8] for chemical reactions.

The obvious difficulty in evaluating the path integral expression for $\exp(-iHt/\hbar)$, compared to $\exp(-\beta H)$, is that the exponent of the integrand is imaginary rather than real, so that the integrand is not positive definite, thus invalidating normal Monte Carlo methods. Though some progress [8–13] has been made in circumventing this problem, there is as yet no generally satisfactory solution.

The purpose of this paper is to present a new approach to the Monte Carlo evaluation of integrals of the type occurring in the path integral expression for the time evolution operator. The method is quite general, and has the highly desirable feature that it incorporates the stationary phase approximation, i.e. the semiclassical limit of the path integral, as its *worst* limit. Section 2 develops the method, and section 3 illustrates the method by application to a simple but non-trivial example.

2. The method

For simplicity of presentation, we consider the generic one-dimensional integral

$$K=\int_{-\infty}^{\infty} dx \exp[iS(x)] \; ; \qquad (1)$$

the multidimensional generalization, which is the form of real time path integrals, will be noted below. Following Filinov [14], one inserts unity in the form

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$$1=\int_{-\infty}^{\infty} dx_0\,\sqrt{B/2\pi}\,\exp[-\tfrac{1}{2}B(x-x_0)^2] \quad (2)$$

into the integrand of eq. (1) and interchanges the order of integration:

$$K=\int_{-\infty}^{\infty} dx_0\,\sqrt{B/2\pi}$$

$$\times\int_{-\infty}^{\infty} dx\,\exp[iS(x)-\tfrac{1}{2}B(x-x_0)^2]\,. \quad (3)$$

Since the Gaussian factor ensures that values of x near x_0 dominate the integral over x, $S(x)$ is expanded about x_0 through quadratic terms

$$S(x)\approx S(x_0)+S'(x_0)(x-x_0)$$
$$+\tfrac{1}{2}S''(x_0)(x-x_0)^2\,, \quad (4)$$

and the integral over x then evaluated:

$$K\approx K(B)$$

$$\equiv\int_{-\infty}^{\infty} dx_0\,\exp[iS(x_0)]\,[1-iS''(x_0)/B]^{-1/2}$$

$$\times\exp[-\tfrac{1}{2}S'(x_0)^2/[B-iS''(x_0)]\,. \quad (5)$$

At this point we depart from Filinov's procedure and note that eq. (2) is true if B is complex, and is approximately true even if B is a function of x_0, i.e. we allow $B\to B(x_0)$, and then make the specific choice

$$B(x_0)=iS''(x_0)+c^{-1}\,, \quad (6)$$

where c is a constant. Eq. (5) then becomes

$$K\approx K(c)$$

$$\equiv\int_{-\infty}^{\infty} dx\,\exp[iS(x)]\,[1+icS''(x)]^{1/2}$$

$$\times\exp[-\tfrac{1}{2}cS'(x)^2]\,, \quad (7)$$

where we have re-labeled the integration variable x_0 as simply x.

The Monte Carlo prescription for evaluating $K(c)$ of eq. (7) is to choose the (unnormalized) sampling function $P(x)$ as

$$P(x)=\exp[-\tfrac{1}{2}cS'(x)^2]\,, \quad (8)$$

so that the Monte Carlo approximation to the integral is then

$$K(c)=\left(\int_{-\infty}^{\infty} dx\,P(x)\right)$$

$$\times\frac{1}{N}\sum_{k=1}^{N}\exp[iS(x_k)]\,[1+icS''(x_k)]^{1/2}\,, \quad (9)$$

where the N values x_k are chosen at random from the distribution $P(x)$. The Metropolis algorithm [15], the stochastic dynamics algorithm [16], etc., are standard ways of doing this. The error in eq. (9) decreases with increasing N as $N^{-1/2}$.

Eqs. (7)–(9) essentially define the method we are proposing, and we now discuss some of its characteristics. Quite generally, one sees that $P(x)$ of eq. (8) weights the stationary phase regions of the integrand, i.e. regions where $S'(x)=0$, if these exist, or in any event, regions where $|S'(x)|$ is smallest. These are clearly the correct regions to be sampled in any integration procedure, and this important feature was first incorporated in Doll's "stationary phase Monte Carlo" method [17].

Eqs. (7)and (8) are, in fact, quite similar to certain versions of Doll's expressions, though they differ in some significant (and advantageous) aspects. More explicitly, note the limits of large and small c. For large c, $P(x)$ becomes a narrow Gaussian about stationary phase points x_{SP}, so that the Monte Carlo statistics are excellent. Furthermore, it is simple arithmetic to show that in this limit eq. (7) gives

$$\lim_{c\to\infty}K(c)=\sum_{x_{SP}}\exp[iS(x_{SP})]\,[2\pi i/S''(x_{SP})]^{1/2}\,, \quad (10)$$

which one recognizes as the standard stationary phase approximation [18] to the integral K.

Conversely, in the limit $c\to 0$ one sees that $K(c)$ of eq. (7) reverts to the original integral K, eq. (1), but in this limit the Monte Carlo statistics are poor because $P(x)$, eq. (8), becomes infinitely broad. For the case that $S(x)$ is a *quadratic* function of x, it is easy to show that $K(c)=K$ identically for *all* values of c.

In summary, as $c\to\infty$ the Monte Carlo statistics of eq. (9) are excellent but $K(c)$ approaches the stationary phase approximation to K rather than the correct value; as $c\to 0$, $K(c)$ approaches the correct value of the integral K but the Monte Carlo statistics become poor. If $S(x)$ happens to be a quadratic function of x, then $K(c)=K$ identically for all values of c. In practical situations, therefore, one should vary the value of c, taking it as small as Monte Carlo statistics allow, knowing always that the *worst* limit, $c\to\infty$, gives the stationary phase approximation.

Finally, we note the multidimensional generalization of eqs. (1) and (7):

$$K=\int_{-\infty}^{\infty} d\boldsymbol{x}\, \exp[iS(\boldsymbol{x})]\,, \tag{11}$$

$$K(\mathbf{c})=\int_{-\infty}^{\infty} d\boldsymbol{x}\, \exp[iS(\boldsymbol{x})][\det(\mathbf{1}+i\mathbf{c}\cdot\boldsymbol{S}_2(\boldsymbol{x}))]^{1/2} \times\exp[-\tfrac{1}{2}\boldsymbol{S}_1(\boldsymbol{x})\cdot\mathbf{c}\cdot\boldsymbol{S}_1(\boldsymbol{x})]\,, \tag{12}$$

where $\boldsymbol{S}_1(\boldsymbol{x})=\partial S/\partial\boldsymbol{x}$, $\boldsymbol{S}_2(\boldsymbol{x})=\partial^2S/\partial\boldsymbol{x}\,\partial\boldsymbol{x}$, and $\mathbf{c}$ is a constant matrix. One may choose $\mathbf{c}=c\,\mathbf{1}$, or in any way desired.

3. Example: the Airy function

Since the method of section 2 is exact for quadratic functions $S(x)$, a non-trivial test requires a more complicated phase function. The integral representation of the Airy function [19]

$$\mathrm{Ai}(-z)=\frac{1}{2\pi}\int_{-\infty}^{\infty} dx\, \exp[i(xz-\tfrac{1}{3}x^3)] \tag{13}$$

is of the form of eq. (1) with $S(x)=xz-\frac{1}{3}x^3$, and this integral has the generic behavior of coalescing stationary phase points in the limit $z\to 0$.

For $z\gg 1$ the stationary phase (i.e. semiclassical, WKB) approximation to $\mathrm{Ai}(-z)$

$$\mathrm{Ai}(-z)\approx\frac{\sin(\frac{1}{4}\pi+\frac{2}{3}z^{3/2})}{\pi^{1/2}z^{1/4}} \tag{14}$$

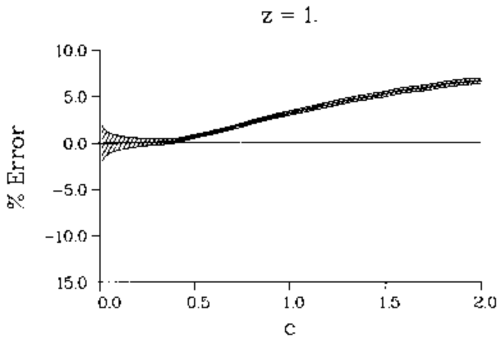

Fig. 1. The percentage error (cf. eq. (15)) given by eqs. (7)–(9) for the Airy integral, eq. (13), for $z=1$, as a function of the constant c. The width of the shaded curve shows the Monte Carlo statistical error for $N=5000$. The stationary phase limit, $c\to\infty$, is 4.6% for this case.

is extremely accurate [19], so that here the method of section 2 will be accurate and efficient for a wide range of values of the constant c. To provide a challenge to the method, therefore, we consider small values of z.

Figs. 1–4 show the percentage error,

$$100\times\frac{(\text{approximate})-(\text{exact})}{(\text{exact})}\,, \tag{15}$$

given by eq. (9) for the Airy integral, eq. (13), for $z=1$, 0.5, 0, and -0.5, respectively, as a function of the parameter c. In each case the shaded region of the curve denotes the Monte Carlo statistical error for $N=5000$; the reader can obtain results for different values of N simply by scaling the width of the curves by $(5000/N)^{1/2}$; e.g., the results correspond-

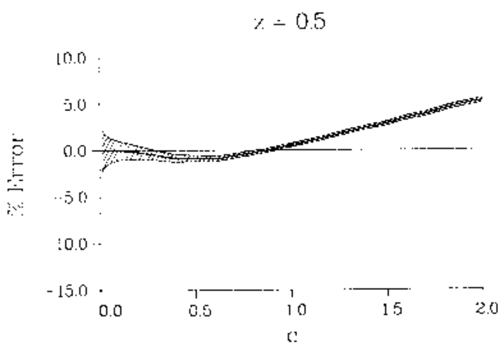

Fig. 2. Same as fig. 1 except for $z=0.5$. The stationary phase limit, $c\to\infty$, is 20%.

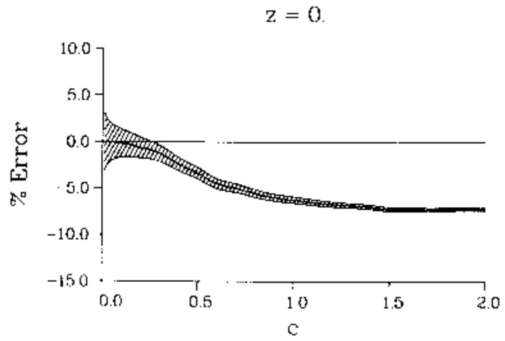

Fig. 3. Same as fig. 1 except for $z=0$. Here the stationary phase limit is divergent.

ing to $N=1000$ are obtained by expanding the width of the shaded curves by $\sqrt{5}\approx 2.2$.

For $z=1$ (fig. 1) the stationary phase approximation is still quite good (better than 5%), so there is a wide range of c for which the Monte Carlo result, eq. (9), is accurate and efficient (i.e. a small statistical error). Smaller z is more of a challenge, but even for $z=0$ – where the stationary phase result, eq. (14), diverges – there is a significant range of c for which eq. (9) is both accurate and efficient. For $z<0$ there are no (real) points of stationary phase, yet eq. (9) still provides usefully accurate results ($\approx 10\%$) when c is large enough to have acceptable statistical error. If one distorted the integration path from the real x axis – a trick that has already been shown to be very useful in Monte Carlo path integration [12,13] – then much more accurate results could be obtained for $z<0$.

Finally, fig. 5 shows similar results for $z=1$ using Filinov's original expression, eq. (5), as a function

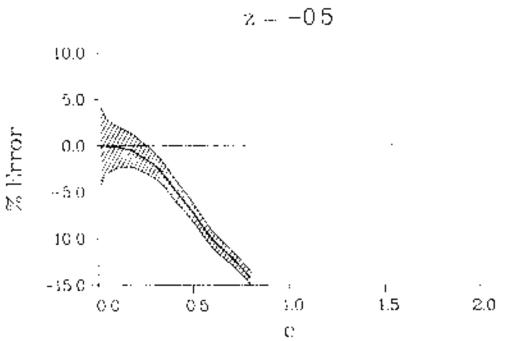

Fig. 4. Same as fig. 1 except for $z=-0.5$. There are no (real) stationary phase points in this case.

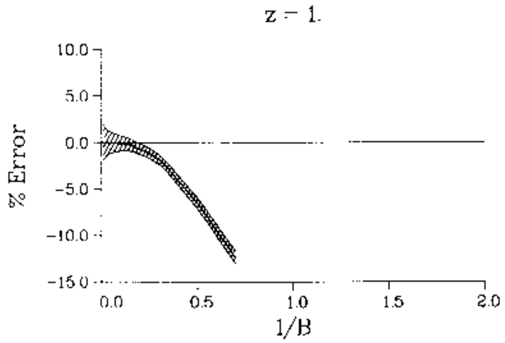

Fig. 5. Same as fig. 1 (also $z=1$), for the original Filinov method, eq. (5), using the real part of the exponent to define the sampling function $P(x)$ rather than eq. (8).

of the constant B^{-1}. (Here one divides the complex exponent $-\frac{1}{2}S'(x_0)^2/[B-iS''(x_0)]$ into real and imaginary parts and uses the real part to define the Monte Carlo sampling function.) The results are essentially the same as shown in fig. 5 for all values of z tested and behave not nearly so well as those discussed above. One can show analytically that the stationary phase approximation is *not* obtained in the limit $B^{-1}\to\infty$ (or any other limit); in fact, $K(B)\to 0$ as $B^{-1}\to\infty$, i.e. -100% error. The *modified* Filinov expression, eq. (7), is thus clearly superior.

4. Concluding remarks

We believe that the method described in section 2 has essentially all the desirable properties one is looking for in a Monte Carlo algorithm for such integrals. The example treated in section 3 illustrates these features in a most encouraging fashion. Application to real time path integrals is straightforward, and this work is in progress.

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