cal point. I am deeply grateful to I. R. Krichevskii who many years ago introduced me to the "critical wonderland."

[1]L. D. Landau and E. M. Lifshitz, *Statistical Physics* (Pergamon, New York, 1977).
[2]M. Gitterman, Rev. Mod. Phys. **50**, 85 (1978).
[3]I. Prigogine and R. Defay, *Chemical Thermodynamics* (Longmans, Green, London, 1954).
[4]I. R. Krichevskii, Russ. J. Phys. Chem. **41**, 1332 (1967).
[5]M. A. Anisimov, Russ. J. Phys. Chem. **45**, 439 (1973).
[6]L. G. Randall, Sep. Sci. Technol. **17**, 1 (1982).
[7]M. Gitterman and I. Procaccia, J. Chem. Phys. **78**, 2648 (1983).
[8]I. Procaccia and M. Gitterman, J. Chem. Phys. **78**, 5275 (1983).
[9]A. C. Moweny and D. T. Jacobs, Am. J. Phys. **51**, 542 (1983); S. B Ngubane and D. T. Jacobs, Am. J. Phys. **83**, 5888 (1985).

Numerical path integration without Monte Carlo

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A numerical procedure for evaluating Feynman's path integral in imaginary time without using the Monte Carlo "heat bath" method is discussed. The method is essentially iterative matrix multiplication and bears a close resemblance to the Feynman procedure of summing all paths by time slicing and then integrating. The procedure is used to determine ground-state energy eigenvalues for the harmonic oscillator, double-well anharmonic oscillator, and the Morse oscillator.

I. INTRODUCTION

In the past few years there has been a proliferation of articles dealing with the machine calculation of Feynman's path integral.[1,2] The motivation behind this activity in large part stems from the attempt to obtain nonperturbative results from the currently accepted theory of strong interactions—quantum chromodynamics.[3] It may also be of some interest, however, to obtain numerical results in ordinary quantum mechanics when the exact Feynman propagator is not available. It is well known that the process of path integration can be carried out exactly only when the integrals in the time-sliced propagator are Gaussian or are reducible to Gaussian form by employing some kind of canonical transformation. Since most interesting potentials do not fit into this category, the motivation for numerical path integration is obvious.

The method of numerical path integration most often employed is the importance sampling Monte Carlo (MC) method. In particular, one uses the Metropolis[4] algorithm in which the propagator is evaluated in imaginary time, giving the quantum mechanical system the appearance of a statistical ensemble interacting with a heat bath. The first application of this method to quantum mechanics appears to be that by Lawande *et al.*,[5] who applied it to obtain the ground-state wavefunctions and energy eigenvalues for a few common potentials, namely, the particle in a box, the harmonic oscillator, and the Morse oscillator. More recently, Creutz and Freedman[6] have discussed a modified Metropolis algorithm and have obtained results for the harmonic oscillator as well as for the double-well potential where one expects instanton (tunneling state) contributions to the propagator. They also obtained correlation functions by the MC method. Recently, in this Journal, there appeared a paper by MacKeown[7] in which an MC method (essentially that of Ref. 5) was described that may be suitable for use in advanced undergraduate courses in computational physics or quantum mechanics. The potentials used for the purpose of illustration in that article were the Morse oscillator and the harmonic oscillator.

It might be argued that the MC method of numerical path integration is somewhat removed from the idea of Feynman, where all paths are supposed to contribute to the propagator. The introduction of the imaginary time actually has two effects. First, it can be shown on general grounds (see below) that in the region of large imaginary time the propagator is dominated by the ground state. Thus, if one is interested solely in the ground-state wavefunction and energy eigenvalue, only this asymptotic limit of the propagator need be known. On the other hand, in the actual calculation of the path integral most of the conceivable paths make no contribution, the most important paths being those along the steepest descent. In the MC algorithm, paths are accepted or rejected according to a Markov process until one obtains "thermal equilibrium." It would appear that this is conceptually quite far from the original idea of calculating the path integral by time slicing and integrating over all space at each intermediate time.

In this article we wish to apply a numerical method that is more along the original lines of Feynman. This method (to be described below), which is basically matrix multiplication, was first described by Thirumalai *et al.*[8] and still uses imaginary time, so we are going to obtain ground-state information only. In Ref. 8, the authors applied this tech-

nique to proton tunneling in a bistable potential. We also wish to examine some of the potentials previously considered from the MC point of view in Refs. 5–7.

The article is organized as follows. In Sec. II, we briefly discuss the path integral formulation of the propagator and its analytic continuation to imaginary time. (This is similar to Sec. II of Ref. 7.) In Sec. III, the matrix method of evaluating the propagator and correlation functions is described. Applications to the harmonic oscillator, the double-well potential, and the Morse oscillator are made in Sec. IV. Section V contains our concluding remarks.

II. PATH INTEGRALS

The path integral formulation of quantum mechanics is well presented in a number of textbooks[1,2,9] so here we shall give only a brief review of the salient features relevant to the calculations to be presented.

Feynman's path integral formulation of quantum mechanics is a global formulation rather than a local one, such as the differential equation of Schrödinger. The object of interest is not the wavefunction but rather the propagator $K(x'',t'';x',t')$, which is the transition amplitude associated with the motion of a particle from x' at t' to x'' at t'',

$$K(x'',t'';x',t') = \langle x''t''|x't'\rangle = \langle x''|\exp[-iH(t''-t')/\hbar]|x'\rangle, \quad (1)$$

if the Hamiltonian H is independent of time. Now, according to Feynman, this amplitude can be given as the sum

$$K(x'',t'';x',t') = \mathcal{N}\sum_{\text{paths}} \exp\frac{iS(\text{path})}{\hbar}, \quad (2)$$

where S is the classical action

$$S = \int_{t_1}^{t_2} L(x,\dot{x})dt, \quad (3)$$

L is the Lagrangian, $L = \frac{1}{2}m\dot{x}^2/2 - V(x)$, and $\mathcal{N}$ is the normalization factor. In a more formal notation, the propagator may be written as

$$K(x'',t'';x',t') = \int_{x'}^{x''} \mathcal{D}x(t)\exp\left(\frac{i}{\hbar}\int_{t'}^{t''} L(x,\dot{x})dt\right), \quad (4)$$

where $\mathcal{D}x(t)$ is a "measure" of the infinitesimal path segments at time t. As this expression is no more helpful than Eq. (2) an operational procedure must be given to actually perform the sum over all paths. To this end, Feynman proposed that time be sliced into N intervals of length ϵ such that $t''-t' = N\epsilon$. Then, at intermediate times, $t_j = j\epsilon + t'$, one sets $x(t_j) = x_j$ for $j = 0,1,\ldots,N$, where $x_0 = x'$, $x_N = x''$, $t_0 = t'$, and $t_N = t''$. A particular path is the limit, as $N\to\infty$, of the polygonal path linking the nodes at x_j for $0<j<N$. The propagator then becomes

$$K(x'',t'';x',t') = \lim_{N\to\infty} A^N \int_{-\infty}^{\infty}\prod_{j=1}^{N-1} dx_j \times\exp\left(\frac{i}{\hbar}\sum_{j=0}^{N-1} S(x_{j+1},x_j)\right), \quad (5)$$

where $S(x_{j+1},x_j)$ is the short time action given by

$$S(x_{j+1},x_j) = \tfrac{1}{2}m(x_{j+1}-x_j)^2/\epsilon - (\epsilon/2)[V(x_{j+1}) + V(x_j)] \quad (6)$$

and the normalization factor A is given by

$$A = (m/2\pi i\hbar\epsilon)^{1/2}.$$

Thus we may write

$$K(x'',t'';x',t') = \lim_{N\to\infty}\int_{-\infty}^{\infty}\prod_{j=1}^{N-1} dx_j \prod_{j=1}^{N-1} K(x_{j+1},x_j;\epsilon), \quad (7)$$

where $K(x_{j+1},x_j;\epsilon)$ is the short time propagator

$$K(x_{j+1},x_j;\epsilon) = (m/2\pi i\hbar\epsilon)^{1/2}\times\exp[(i/\hbar)S(x_{j+1},x_j)]. \quad (8)$$

On the other hand, the propagator can be represented in terms of the eigenfunctions and energy eigenvalues as[9]

$$K(x'',t'';x',t') = \sum_{n=0}^{\infty} e^{-iE_n(t''-t')/\hbar}\psi_n(x'')\psi_n^*(x'). \quad (9)$$

If we now set $t' = 0$ and $t'' = -i\hbar\tau$, we obtain

$$K(x'',x';-i\hbar\tau) = \sum_{n=0}^{\infty} e^{-E_n\tau}\psi_n(x'')\psi_n^*(x'). \quad (10)$$

This is, in fact, the density matrix

$$\rho(x'',x',\tau) = K(x'',x';-i\hbar\tau) \quad (11)$$

for a canonical ensemble in thermal equilibrium if τ is interpreted as the Boltzmann factor. In the limit $\tau\to\infty$, the right side of Eq. (10) is dominated by the ground state $n = 0$. Since the wavefunctions $\psi_n(x)$ are normalized the partition function is

$$Z = \operatorname{tr}\rho = \int_{-\infty}^{\infty} dx\,\rho(x,x;\tau) = \sum_{n=0}^{\infty} e^{-E_n\tau}. \quad (12)$$

Thus the ground-state wavefunction is determined from

$$|\psi_0(x)|^2 = \lim_{\tau\to\infty}[\rho(x,x;\tau)/Z]. \quad (13)$$

The ground-state energy is determined from

$$E_0 = -\lim_{\tau\to\infty}(1/\tau)\log Z. \quad (14)$$

Now from Eqs. (7) and (8) the path integral expression for the density matrix may be obtained by making the replacement $\epsilon\to -i\hbar\epsilon$. This yields

$$\rho(x'',x';\tau) = \lim_{N\to\infty}\int_{-\infty}^{\infty}\prod_{j=1}^{N-1} dx_j \prod_{j=D}^{N-1}\rho(x_{j+1},x_j;\epsilon), \quad (15)$$

where

$$\rho(x_{j+1},x_j;\epsilon) = (m/2\pi\hbar^2\epsilon)^{1/2}\times\exp\{-(m/2\hbar^2\epsilon)(x_{j+1}-x_j)^2 - (\epsilon/2)[V(x_{j+1}) + V(x_j)]\} \quad (16)$$

is the short "time" density matrix. It is this form of the path integral that will be the starting point for our numerical calculation.

III. NUMERICAL METHOD

In order to evaluate the propagator of Eq. (15) we set up a grid of equally spaced points between $-L/2$ and $+L/2$ on the x axis. Let Δ be the spacing between the grid points and let $2M+1$ be the total number of points in the interval $(-L/2, L/2)$. Thus $L = M\Delta$. Any set of points x_i, x_j can be specified as $i\Delta, j\Delta$ on the grid.

Now, using a trapezoidal rule, the first integral in Eq. (15) becomes essentially the matrix multiplication

$$\rho(i\Delta,j\Delta;2\epsilon)=\Delta\sum_{k=-M}^{M}\rho(i\Delta,k\Delta;\epsilon)\rho(k\Delta,j\Delta;\epsilon), \quad (17)$$

where

$$\rho(i\Delta,j\Delta;\epsilon)=(m/2\pi\hbar^2\epsilon)^{1/2}\exp\{-(m\Delta^2/2\hbar^2\epsilon)(i-j)^2 - (\epsilon/2)[V(i\Delta)+V(j\Delta)]\} \quad (18)$$

is the short time propagator on the right side of Eq. (17). The second integral can then be performed to obtain

$$\rho(i\Delta,j\Delta;3\epsilon)=\Delta\sum_{k=-m}^{m}\rho(i\Delta,k\Delta;\epsilon)\rho(k\Delta,j\Delta;2\epsilon). \quad (19)$$

Following this procedure, one obtains the Nth integral as

$$\rho(i\Delta,j\Delta,N\epsilon)=\Delta\sum_{k=-M}^{M}\rho(i\Delta,k\Delta;\epsilon)\rho(k\Delta,j\Delta,(N-1)\epsilon). \quad (20)$$

In practice, this procedure is rather time consuming. As is shown in Ref. 8, a more efficient procedure is to do the calculation iteratively. From Eq. (17) we obtain $\rho(i\Delta,j\Delta,2\epsilon)$. Substituting back into (17) we obtain $\rho(i\Delta,j\Delta;\psi\epsilon)$. After n iterations we have $\rho(i\Delta,j\Delta,2^n\epsilon)$.

The probability density for the ground-state wave function, $P(x)=|\psi_0(x)|^2$ is obtained according to Eq. (13), where the partition function is evaluated according to

$$Z=\mathrm{tr}\,\rho=\frac{\Delta}{2}\sum_{k=-M}^{M}\{\rho[(k+1)\Delta,(k+1)\Delta;2^n\epsilon] + \rho(k\Delta,k\Delta;2^n\epsilon)\}. \quad (21)$$

Now, in evaluating the integral of Eq. (15) using the iterative procedure, the number of iterations n should be high enough so that the high-temperature approximation of Eq. (16) is valid. Also, for a given grid spacing, it should be large enough so that the exponential term does not decrease too rapidly for large $i-k$. As pointed out in Ref. 8, this implies that one should choose the quantity $\delta=m\Delta^2 2^n/2\hbar\tau^2$ as small as possible. A value of $\delta<0.3$ seems to ensure good convergence. In our calculation, we generally set $m=\hbar=1$ and typically choose $\epsilon=0.1$ and with Δ in the range 0.1 to 0.15 and with $n=6$. This gives a δ well within the range suggested in Ref. 8. Typically we take M in the range 50–60. We shall say more on how the accuracy depends on ϵ,Δ in Sec. V.

IV. APPLICATIONS

A. Harmonic oscillator

We consider the harmonic oscillator with the potential energy

$$V(x)=\tfrac{1}{2}x^2. \quad (22)$$

The square of the ground-state wavefunction we obtain is shown in Fig. 1 along with the analytic result

$$|\psi_0(x)|^2=(1/\sqrt{\pi})e^{-x^2}=0.564e^{-x^2}. \quad (23)$$

Our numerical $|\psi_0(x)|^2$ peaks at a value of 0.568 whereas the MC results of Creutz and Freedman[6] peak at about 0.59. The energy determined from Eq. (14) is $E_0=0.499$ in excellent agreement with the exact result of 0.50.

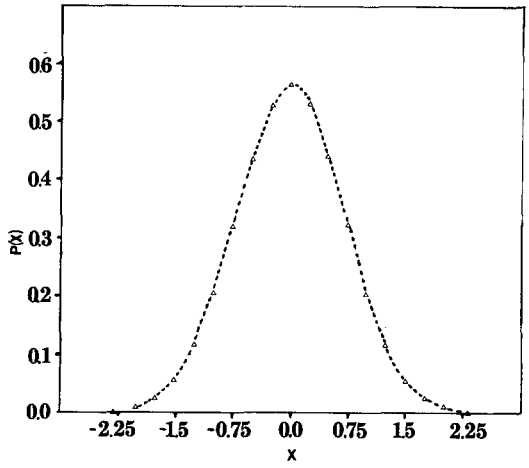

Fig. 1. The probability density $P(x)=|\psi_0(x)|^2$ for the harmonic oscillator ground state. The dashed line is the exact result and the triangles are from our numerical calculations.

B. Double-well anharmonic oscillator

We next consider the anharmonic oscillator treated in Ref. 6 by MC methods. The potential is written in the form

$$V(x)=\lambda(x^2-f^2)^2, \quad (24)$$

where the zeros of the potential occur at the classical minima $x=\pm\sqrt{f^2}$. For $f^2=2.0$ and $m=0.5$ we obtain the ground-state probability density $\rho(x)=|\psi_0(x)|^2$ shown in Fig. 2 along with the exact result. As in the case of the MC results, one clearly sees the effects of the tunneling or "instanton" solutions. The energy eigenvalue of the ground state is determined to be $E_0=2.257$ while the exact result from the continuum theory[10] is $E_0=2.290$. On the other hand, the MC result for E_0 also appears to be a little lower than the exact result as can be seen in Fig. 10 of Ref. 6. Unfortunately, it is not possible to determine the precise value from the graph.

C. Morse oscillator

Finally we consider the Morse oscillator, in the form as discussed by Lawande *et al.* in Ref. 5. They write the poten-

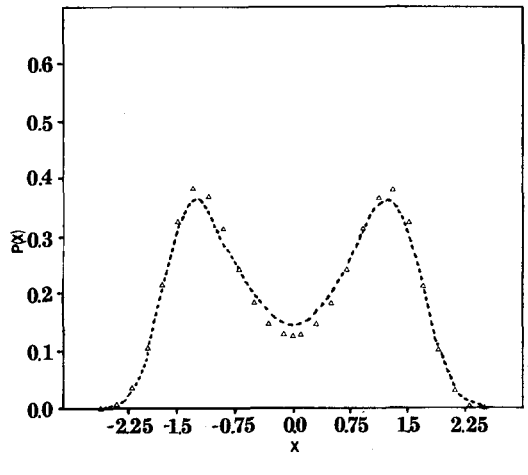

Fig. 2. The probability density for the ground state of a double well with $f^2=2.0$.

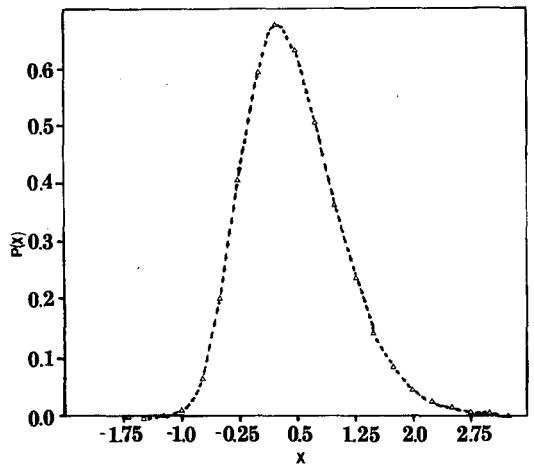

Fig. 3. The probability density for the ground state of the Morse oscillator.

tial (for the s states) as

$$V(x) = 2(1 - e^{-x})^2. \tag{25}$$

The probability density for the ground state is shown in Fig. 3 along with the exact results. The energy determined as $E_0 = 0.887$ while the exact result is 0.881. The MC result of Ref. 5 is $E_0 = 0.875$.

V. CONCLUSION

The iterative matrix multiplication method of evaluating path integrals appears to be of at least comparable accuracy to the Monte Carlo method and in some cases (such as the harmonic oscillator) somewhat more accurate. A question arises, then, as to the effect of a given set of parameters (ϵ,Δ,M,n) on the accuracy of the result. To indicate how these parameters affect the calculated energy, we consider again the double-well potential for various ϵ and Δ. We take $M = 60$ and set the number of iterations $n = 6$. These choices allow us to perform the calculations in a reasonable amount of time. The results are in Table I. We note that with $\epsilon = 0.1$ the energy obtained does not seem to depend on Δ, at least to the accuracy displayed. For large values of ϵ, such as $\epsilon = 0.15$, decreasing Δ improves the result. On the other hand, ϵ can be made too small for which the results get worse (e.g., $\epsilon = 0.05$, $\Delta = 0.05$). This result could probably be improved by taking more iterations, thus slowing down the calculation. We should also say that the matrix method used here is more than two orders of magnitude faster than an MC routine which gives comparable accuracy.[8]

Table I. The dependence of the ground-state energy of the double well on the choice of ϵ and Δ.

ϵ	Δ	Energy
0.1	0.15	2.257
0.1	0.1	2.257
0.1	0.05	2.257
0.15	0.15	2.215
0.15	0.10	2.236
0.15	0.05	2.237
0.05	0.05	2.218

Finally, we mention that this method can be generalized for two dimensions, at least, though with increased memory requirements and decreasing speed. Nevertheless, we are currently implementing the method for a nonseparable potential in two dimensions. It is apparent, however, that for higher dimensions some form of the Monte Carlo method is the only realistic approach. Nevertheless, for low-dimensional systems, or for systems that are separable, the method discussed here is an attractive alternative to the Monte Carlo method.

[1]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).
[2]L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley–Interscience, New York, 1981).
[3]M. Creutz, *Quarks, Gluons, and Lattices* (Cambridge U.P., Cambridge, 1983).
[4]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).
[5]S. V. Lawande, C. A. Jensen, and H. L. Sahlin, Comp. Phys. **3**, 416 (1969).
[6]M. Creutz and B. Freedman, Ann. Phys. (N.Y.) **132**, 427 (1981).
[7]P. K. MacKeown, Am. J. Phys. **53**, 880 (1985).
[8]D. Thirumalai, E. J. Bruskin, and B. J. Berne, J. Chem. Phys. **79**, 5063 (1983).
[9]Two recent quantum mechanics textbooks that discuss path integral quantization are R. Shankar, *Principles of Quantum Mechanics* (Plenum, New York, 1980) and J. J. Sakurai, *Modern Quantum Mechanics* (Benjamin, New York, 1985).
[10]R. Blankenbecher, T. Degrande, and R. L. Sugar, Phys. Rev. D **21**, 1055 (1980).