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Monte Carlo Integration of the Feynman Propagator in Imaginary Time[1]

S. V. LAWANDE[2]

Department of Applied Science, University of California, Davis, California 95616

AND

C. A. JENSEN AND H. L. SAHLIN

Department of Applied Science, University of California, Davis–Livermore, California 95616

and

Lawrence Radiation Laboratory, University of California, Livermore, California 94550

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ABSTRACT

The Feynman propagator or "integral over paths" is written with time t replaced by $-i\tau$. The result is a propagator, corresponding to a diffusion equation with the classical Lagrangian replaced by the classical Hamiltonian in the kernel. An evaluation of this propagator, over a sufficiently long time, yields the absolute square of the ground-state wavefunction, viz., $|U_0(x)|^2$ of the quantum system. A biased Monte Carlo integration scheme, where the biasing is exponential in the energy of the system, is used to evaluate functional integrals in the case of the quantum mechanical particle in a box, oscillator, and Morse potential. This scheme and the results of the integrations are described.

I. INTRODUCTION

The formalism of functional or path integrals first suggested by Feynman [1], [2], offers an alternative approach towards solving many problems of quantum mechanics. The close similarity between the Feynman integrals and the ones used by Wiener [3–5] in his studies of Brownian motion has been discussed in several recent papers [6–9]. This latter fact makes the functional integral method a useful

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tool for studying certain problems of statistical mechanics [10–13]. An excellent summary of earlier work on path integrals is found in an article by Brush [14].

In the present paper we propose to discuss the application of functional integrals to the numerical calculation of quantum mechanical wavefunctions. We shall attempt to show that, at least in principle, Feynman path integrals provide a rather direct and intuitively appealing method for computing the ground states of quantum systems, based on a simple approach with a minimum number of assumptions. As examples of this, we shall present computer results for three simple quantum systems, viz. harmonic oscillator, particle in a box, and a particle acted on by a Morse Potential. Particular problems associated with multicenter potentials, singular potentials, and the appropriate use of statistics are pointed out, as is the promise of the method in terms of the reduction of machine time required for evaluation of wavefunctions for many-particle systems.

II. Formulation of the Appropriate Path Integral

We outline below the path integral formulation of the nonrelativistic Schrödinger equation. Our treatment is not the most rigorous one, but it is included here for completeness and general understanding of the method.

Consider the time-dependent Schrödinger equation for a single particle of mass m, in a potential field $V(\mathbf{X})$:

$$\hat{H}\psi(\mathbf{X}, t) = i\hbar \frac{\partial \psi}{\partial t}(\mathbf{X}, t), \tag{1}$$

where the Hamiltonian $\hat{H}$ is given by

$$\hat{H} \equiv -\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{X}). \tag{2}$$

Introduce the orthonormal set of the eigenfunctions of the time-independent equation

$$\hat{H}U_n(X) = E_n U_n(X), \tag{3}$$

where

$$\int U_n^*(\mathbf{X})\, U_m(\mathbf{X})\, d^3\mathbf{X} = \delta_{nm} \tag{4}$$

and

$$\sum_n U_n^*(\mathbf{X}_1)\, U_n(\mathbf{X}_2) = \delta(\mathbf{X}_2 - \mathbf{X}_1). \tag{5}$$

Consider the expansion

$$\psi(\mathbf{X}, t) = \sum_n C_n(t)\, U_n(\mathbf{X}), \tag{6}$$

where

$$C_n(t) = \int U_n^*(\mathbf{X})\, \psi(\mathbf{X}, t)\, d^3\mathbf{X}. \tag{7}$$

Substitute it for $\psi(\mathbf{X}, t)$ in Eq. (1), multiply both sides of the resulting equation by $U_m^*(\mathbf{X})$ and integrate over the entire space of $\mathbf{X}$ to obtain

$$E_m C_m(t) = i\hbar \frac{dC_m}{dt}(t), \tag{8}$$

which may be readily solved to yield

$$C_m(t_2) = C_m(t_1) \exp\left\{-\frac{iE_m}{\hbar}(t_2 - t_1)\right\} \qquad (t_2 > t_1). \tag{9}$$

Hence we may write for $t_2 > t_1$

$$\begin{aligned}
\psi(\mathbf{X}_2, t_2) &= \sum_n C_n(t_2)\, U_n(\mathbf{X}_2) \\
&= \sum_n C_n(t_1) \exp\left\{-\frac{i}{\hbar} E_n(t_2 - t_1)\right\} U_n(\mathbf{X}_2) \\
&= \sum_n \left\{\int \psi(\mathbf{X}_1, t_1)\, U_n^*(\mathbf{X}_1)\, d^3\mathbf{X}_1\right\} U_n(\mathbf{X}_2) \exp\left\{-\frac{i}{\hbar} E_n(t_2 - t_1)\right\} \\
&= \int \psi(\mathbf{X}_1, t_1)\left[\sum_n U_n^*(\mathbf{X}_1)\, U_n(\mathbf{X}_2) \exp\left\{-\frac{iE_n}{\hbar}(t_2 - t_1)\right\}\right] d^3\mathbf{X}_1 \\
&= \int K(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1)\, \psi(\mathbf{X}_1, t_1)\, d^3\mathbf{X}_1,
\end{aligned} \tag{10}$$

where we have introduced the Feynman propagator or Green's function

$$K(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1) = \sum_n U_n^*(\mathbf{X}_1)\, U_n(\mathbf{X}_2) \exp\left\{-\frac{iE_n}{\hbar}(t_2 - t_1)\right\} d^3\mathbf{X}_1. \tag{11}$$

Equation (10) expresses the time development of the wavefunction in terms of the propagator K, and the initial form of the wavefunction. Several properties of K are now evident. First, from Eq. (11) we note that

$$K(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1) = \sum_n \psi_n^*(\mathbf{X}_1, t_1)\, \psi_n(\mathbf{X}_2, t_2), \tag{12}$$

where the $\psi_n(\mathbf{X}, t)$ are time-dependent solutions of Eq. (1), and also

$$\begin{aligned}
K(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1) &= \exp\left\{-\frac{i\hat{H}_2}{\hbar}(t_2 - t_1)\right\} \sum_n U_n^*(\mathbf{X}_1)\, U_n(\mathbf{X}_2) \\
&= \exp\left\{-\frac{i\hat{H}_2}{\hbar}(t_2 - t_1)\right\} \delta(\mathbf{X}_2 - \mathbf{X}_1),
\end{aligned} \tag{13}$$

where $\hat{H}_2$ stands for the Hamiltonian involving only the coordinates $\mathbf{X}_2$. The exponential operator in Eq. (13) is to be regarded as the power series expansion of the exponent. It is easy to see from

$$\psi(\mathbf{X}_3, t_3) = \int K(\mathbf{X}_1, \mathbf{X}_3, t_3 - t_1)\, \psi(\mathbf{X}_1, t_1)\, d^3\mathbf{X}_1, \tag{14}$$

and

$$\begin{aligned}\psi(\mathbf{X}_3, t_3) &= \int K(\mathbf{X}_2, \mathbf{X}_3, t_3 - t_2)\, \psi(\mathbf{X}_2, t_2)\, d^3\mathbf{X}_2 \\ &= \iint K(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1)\, K(\mathbf{X}_2, \mathbf{X}_3, t_3 - t_2)\, \psi(\mathbf{X}_1, t_1)\, d^3\mathbf{X}_2\, d^3\mathbf{X}_1\end{aligned} \tag{15}$$

that the semigroup composition law

$$K(\mathbf{X}_1, \mathbf{X}_3, t_3 - t_1) = \int K(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1)\, K(\mathbf{X}_2, \mathbf{X}_3, t_3 - t_2)\, d^3\mathbf{X}_2 \tag{16}$$

holds. This convolution property of the propagator is characteristic of stochastic processes.

Since we are concerned with the forward propagation in time ($t_2 > t_1$), it is convenient to redefine a new propagator $\overline{K}$ as

$$\overline{K}(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1) = K(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1)\, \theta(t_2 - t_1), \tag{17}$$

where $\theta(t_2 - t_1)$ is a step function defined by

$$\theta(t_2 - t_1) = \begin{cases} 1 & t_2 \geqslant t_1, \\ 0 & t_2 < t_1. \end{cases} \tag{18}$$

The temporal development of the wavefunction may then be written as

$$\psi(\mathbf{X}_2, t_2)\, \theta(t_2 - t_1) = \int \overline{K}(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1)\, \psi(\mathbf{X}_1, t_1)\, d^3\mathbf{X}_1, \tag{19}$$

which is the quantum mechanical form of the "Huygens' Principle" in classical optics. Mathematically, the propagator or kernel $\overline{K}/i\hbar$ is the Green's function of the Schrödinger equation (1). For,

$$\begin{aligned}&\left(i\hbar \frac{\partial}{\partial t_2} - \hat{H}_2\right) \frac{\overline{K}}{i\hbar}(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1) \\ &\quad = \frac{\partial \theta}{\partial t_2}(t_2 - t_1)\, K(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1) \\ &\qquad + \frac{\theta}{i\hbar}(t_2 - t_1) \sum_n \psi_n^*(\mathbf{X}_1, t_1)\left[i\hbar \frac{\partial \psi_2}{\partial t}(\mathbf{X}_2, t_2) - \hat{H}_2 \psi(\mathbf{X}_2, t_2)\right] \\ &\quad = \delta(t_2 - t_1)\, \delta(\mathbf{X}_2 - \mathbf{X}_1),\end{aligned} \tag{20}$$

where we have used the fact that

$$\frac{\partial \theta}{\partial t_2}(t_2 - t_1) = \delta(t_2 - t_1), \tag{21}$$

and that

$$\lim_{t_2 \to t_1} K(\mathbf{X}_1, \mathbf{X}_2, t_2 - t_1) = \delta(\mathbf{X}_2 - \mathbf{X}_1), \tag{22}$$

as can be seen from the relation (12).

In order to obtain the path integral form of the propagator, we use Eq. (13) and consider a small interval of time $\epsilon = t_2 - t_1$. Thus

$$K(\mathbf{X}_1, \mathbf{X}_2, \epsilon) = e^{-i\epsilon H_2/\hbar}\delta(\mathbf{X}_2 - \mathbf{X}_1). \tag{23}$$

Equation (23) expresses the fact that the propagator for an infinitesimally small time could be generated from its initial δ-function value [cf. Eq. (22)] through a unitary transformation in time.

We now use the operator relation

$$\exp\{\epsilon(\hat{A} + \hat{B})\} \simeq e^{\epsilon\hat{B}}e^{\epsilon\hat{A}} \exp\left\{\frac{\epsilon^2}{2}[\hat{A}, \hat{B}]\right\}, \tag{24}$$

which is exact if $\hat{A}$ and $\hat{B}$ commute with their commutator $[\hat{A}, \hat{B}]$ and correct up to second order in ϵ, otherwise. This reduces Eq. (23) to the following form

$$K(\mathbf{X}_1, \mathbf{X}_2, \epsilon) \simeq \exp\left\{-\frac{i\epsilon V_2}{\hbar}\right\} \exp\left\{\frac{\epsilon^2}{4m}(\nabla_2^2 V_2 - V_2\nabla_2^2)\right\}$$
$$\times \exp\left\{\frac{i\epsilon\hbar}{2m}\nabla_2^2\right\} \delta(\mathbf{X}_2 - \mathbf{X}_1) \qquad (V_2 = V(\mathbf{X}_2)). \tag{25}$$

Now if we use the Fourier representation of the δ-function

$$\delta(\mathbf{X}_2 - \mathbf{X}_1) = \int_{-\infty}^{\infty} \exp\{i\mathbf{k} \cdot (\mathbf{X}_2 - \mathbf{X}_1)\} \frac{d^3\mathbf{k}}{(2\pi)^3} \tag{26}$$

in Eq. (25) and carry out the operation, we arrive at the result

$$K(\mathbf{X}_1, \mathbf{X}_2, \epsilon) = \exp\left\{-\frac{i\epsilon V_2}{\hbar}\right\} \exp\left\{\frac{\epsilon^2}{4m}\nabla_2^2 V_2\right\}$$
$$\times \int_{-\infty}^{+\infty} \exp\left\{i\left\{\frac{\epsilon^2}{2m}\mathbf{k} \cdot \nabla_2 V_2 - \frac{\epsilon\hbar\mathbf{k}^2}{2m} + \mathbf{k} \cdot (\mathbf{X}_2 - \mathbf{X}_1)\right\}\right\} \frac{d^3\mathbf{k}}{(2\pi)^3}. \tag{27}$$

The integral is evaluated in the usual manner, and we obtain

$$K(\mathbf{X}_1, \mathbf{X}_2, \epsilon) = K_0(\mathbf{X}_1, \mathbf{X}_2, \epsilon) \cdot C(\mathbf{X}_1, \mathbf{X}_2, \epsilon), \tag{28}$$

where

$$K_0(\mathbf{X}_1, \mathbf{X}_2, \epsilon) = \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{3/2} \exp\left\{\frac{i\epsilon}{\hbar}\left[\frac{m}{2}\left(\frac{\mathbf{X}_2 - \mathbf{X}_1}{\epsilon}\right)^2 - V(\mathbf{X}_2)\right]\right\} \tag{29}$$

and

$$C(\mathbf{X}_1, \mathbf{X}_2, \epsilon) = \exp\left\{\frac{i\epsilon}{\hbar}\left[\frac{(\mathbf{X}_2 - \mathbf{X}_1)}{2} \cdot \nabla V_2 - \frac{i\hbar\epsilon}{4m}\nabla_2^2 V_2\right]\right\}. \tag{30}$$

The expression (28) for the propagator is correct to second order in ϵ. As long as ϵ is small, the correction term $C(\mathbf{X}_1, \mathbf{X}_2, \epsilon)$ is unimportant, and in the subsequent discussion we shall use only K_0.

We wish to point out here that our method of derivation holds only for Cartesian coordinates. Some care has to be taken to obtain the appropriate form of the propagator for coordinate systems other than Cartesian [15].

The expression for the propagator for a finite time interval $t_2 - t_1$ can be obtained from Eq. (29) by dividing the time interval into N equal parts each of length ϵ and applying successively the composition law of Eq. (16). This gives

$$K(\mathbf{X}_1, \mathbf{X}_{N+1}, t_2 - t_1 = N\epsilon)$$
$$= \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{3N/2} \int \cdots \int \exp\left\{\frac{i\epsilon}{\hbar}\left[\sum_{j=1}^{N} \frac{m}{2}\left(\frac{\mathbf{X}_{j+1} - \mathbf{X}_j}{\epsilon}\right)^2 - V(\mathbf{X}_{j+1})\right]\right\} \prod_{k=2}^{N} d^3\mathbf{X}_k. \tag{31}$$

In the limit of $\epsilon \to 0$, $N \to \infty$ and $N\epsilon$ finite, we obtain the Feynman form [2],

$$\lim_{\substack{\epsilon\to 0 \\ N\to\infty}} K(\mathbf{X}_1, \mathbf{X}_{N+1}, t_2 - t_1 = N\epsilon) = \int \exp\left\{\frac{i}{\hbar}\int_{t_1}^{t_2} L(\mathbf{X}, \dot{\mathbf{X}}, t)\, dt\right\} D\mathbf{X}(t), \tag{32}$$

where $L(\mathbf{X}, \dot{\mathbf{X}}, \epsilon)$ is the classical Lagrangian of the particle, and the symbol $D\mathbf{X}(t)$ denotes integration over all possible, yet unspecified, paths of the particle. Equation (31) is thus a Riemann multiple integral approximation to the Feynman propagator of Eq. (32) with the paths specified by "broken-line" curves. Other parametrizations of the paths are possible and have been discussed in the literature [16-20].

An interesting aspect of the Feynman path integral form of Eq. (31) is that it allows us to consider the classical limit $\hbar \to 0$. As $\hbar$ approaches zero, the integrand of Eq. (31) becomes a very rapidly oscillating function. Very small changes in the action would therefore result in large changes in the phase, which in turn would

imply a strong tendency towards mutual cancellation of the contributions from neighboring paths. If however, the path is classical, for which the action $\int_{t_2}^{t_1} L\,dt$ is stationary, the nearby paths will contribute equally to the integral. In other words, the contributions in the immediate neighborhood of the classical path tend to interfere constructively. Thus in the limit $\hbar \to 0$, the greatest contribution comes from the paths close to the classical path.

III. The Propagator in Imaginary Time

The expression (31) for the propagator involves oscillatory integrals and hence is not suitable for obtaining the ground state wavefunction. For this purpose, it is convenient to use the imaginary time coordinate which renders the integrals real Thus, if we replace "it" by τ, the Schrödinger equation (1) changes over to

$$\hat{H}\psi(\mathbf{X}, \tau) = -\hbar \frac{\delta \psi}{\delta \tau}(\mathbf{X}, \tau) \tag{33}$$

which has the form of a diffusion equation. This does not introduce any changes in the time independent eigenvalue equation (3). It is thus permissible to replace "it" in Eq. (11) and "$i\epsilon$" in Eq. (31) by τ. We then obtain the equation

$$K(\mathbf{X}_1, \mathbf{X}_2, \tau_2 - \tau_1) = \sum_n \exp\left\{-\frac{E_n}{\hbar}(\tau_2 - \tau_1)\right\} U_n^*(\mathbf{X}_1)\, U_n(\mathbf{X}_2), \tag{34}$$

corresponding to Eq. (11) and the result

$$\begin{aligned} &K(\mathbf{X}_1, \mathbf{X}_{N+1}, \tau_2 - \tau_1 = N\tau) \\ &\quad = \left(\frac{m}{2\pi\hbar\tau}\right)^{3N/2} \int \cdots \int \exp\left\{-\frac{\tau}{\hbar}\left[\sum_{j=1}^{N}\left\{\frac{m}{2}\left(\frac{\mathbf{X}_{j+1} - \mathbf{X}_j}{\tau}\right)^2 + V(\mathbf{X}_{j+1})\right\}\right]\right\} \\ &\qquad \times \prod_{k=2}^{N} d\mathbf{X}_k{}^3 \end{aligned} \tag{35}$$

corresponding to Eq. (31). The limiting form when $\tau \to 0$, $N \to \infty$, $N\tau$ finite is then given by

$$\lim_{\substack{\tau \to 0 \\ N \to \infty}} K(\mathbf{X}_1, \mathbf{X}_{N+1}, N\tau = \tau_2 - \tau_1) = \int \exp\left\{-\frac{1}{\hbar}\int_{\tau_1}^{\tau_2} H dt\right\} D\mathbf{X}(\tau), \tag{36}$$

where H is the classical Hamiltonian. Equations (35) and (36) are in fact related to Wiener integrals, which have been extensively studied in the literature [3], [4],

[21–25]. It is interesting to note here that on account of the real nature of the integrand and finiteness of $\hbar$, the greatest contribution to the propagator comes from the path which makes the total action $\int_{t_1}^{t_2} H\, d\tau$ a minimum. This is analogous to the "classical path" of the preceding section. However, since the exponent is real, contributions from all paths add together with some being large and others being small.

Consider now the propagator $K(\mathbf{X}, \mathbf{X}, \tau)$ for a sufficiently long time interval τ. We have from Eq. (34)

$$K(\mathbf{X}, \mathbf{X}, \tau) = \sum_n \exp\left\{-\frac{E_n \tau}{h}\right\} \mid U_n(\mathbf{X})\mid^2$$

$$\cong \exp\left\{-\frac{E_0 \tau}{h}\right\} \mid U_0(\mathbf{X})\mid^2 \tag{37}$$

for large enough τ, provided that the ground state and the first-excited states are well separated from each other in energy. The behavior of the propagator for various times is illustrated in Fig. 1 for the harmonic oscillator, for which an exact analytical form of $K(\mathbf{X}, \mathbf{X}, \tau)$ is available [2].

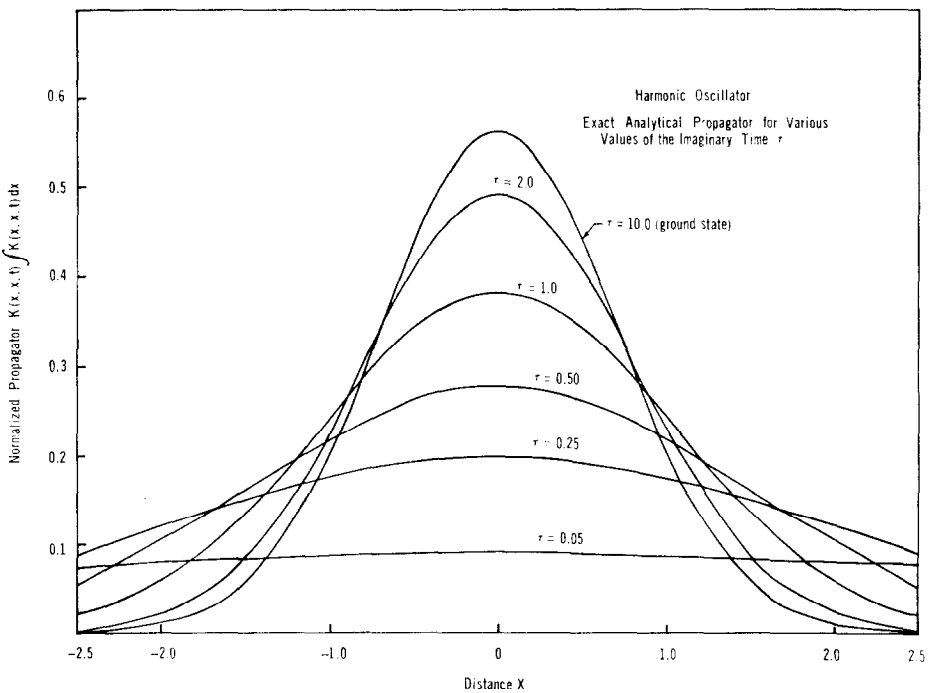

FIG. 1. An exact analytic evaluation of the one-dimensional harmonic-oscillator propagator for various imaginary times.

Equation (37) implies that if we let $\mathbf{X}_{N+1} = \mathbf{X}_1$ in Eq. (35), then, for large time differences, we obtain the absolute square of the ground-state wavefunction-of the system times a multiplying factor, which is a simple function of the energy of the ground state. In fact, if we evaluate the normalized path integral,

$$K(\mathbf{X}_1, \mathbf{X}_1, \tau) = \frac{\int K(\mathbf{X}_1, \mathbf{X}_{N+1}, \tau)\, \delta(\mathbf{X}_1 - \mathbf{X}_{N+1})\, d^3\mathbf{X}_{N+1}}{\int K(\mathbf{X}_1, \mathbf{X}_1, \tau)\, d^3\mathbf{X}_1} \tag{38}$$

for a sufficiently large value of τ, we obtain the absolute square of the ground state wave function. The problem is thus reduced to the numerical estimation of the R.H.S. of Eq. (38). This may be carried out in a convenient manner, by means of a Monte Carlo procedure described in Section V. Once the ground state wave function is determined, the corresponding energy may be determined in two ways. One way is to compute the average potential energy using the generated wavefunction and apply the Virial Theorem. An alternative method is to obtain the average of the Hamiltonian operator itself.

While the quantum mechanical use of path integrals for the numerical evaluation of ground states is a relatively new[3] application, functional integrals have been used for some time in statistical mechanics [12], [26–29]. This is because the partition function is equal to the integral of the diagonal elements of the propagator, if we make the substitution $\tau/\hbar = \beta = 1/kT$, in Eq. (34). We obtain thereby

$$\begin{aligned} \int K(\mathbf{X}, \mathbf{X}, \tau)\, d^3\mathbf{X} &= \sum_n \left(\int |\, U_n(\mathbf{X})|^2\, d^3\mathbf{X} \right) e^{-\beta E_n} \\ &= \sum_n e^{-\beta E_n} \\ &= Z(\beta), \end{aligned} \tag{39}$$

where $Z(\beta)$ is the partition function. An important difference exists between statistical mechanical calculations and the present problem. This difference lies in the values of β or τ which need to be used in these two cases. If one is interested in the quantum mechanical ground state, it is necessary to use a sufficiently large value of τ so that the ground state is the only important contributor to the final result. This corresponds to a value of β equivalent to a very low temperature. Most statistical mechanical calculations performed up to now have not approached these low temperatures, where the effects of quantum mechanical statistics represent more than a small perturbation.

[3] However, a method for finding the smallest eigenvalue and eigenfunction of the Schrödinger equation, based on functional integrals, has been proposed by Donsker and Kac [30]. Since then the idea has been reverberating in the literature [8], [21], [25], [31], [33].

We shall indicate below that, while this is relatively easy to do in principle, in practice very serious problems concerning accuracy arise using the standard form of the propagator. This forces us to consider the question of statistics very carefully and also to pay considerable attention to those parameters and procedures which make a given evaluation as accurate as possible.

IV. Use of a Monte Carlo Method

The evaluation of the multiple integrals of Eq. (38) by the standard quadrature methods is impractical, since N is usually a large number. In fact, the time required to compute a one-dimensional integral using a simple quadrature formula involving p number of points would be proportional to p. A straightforward generalization of this would imply that the time required for evaluating an N-dimensional integral would be p^N. On the other hand, a simple Monte Carlo method based on a uniform sampling of points from the integration space would involve a time which is only linear in N. A Monte Carlo method may not be as efficient as an ordinary quadrature technique when integrals of very few dimensions are involved; but as the dimensionality N of the integrals is increased, Monte Carlo soon gains efficiency, and when N is very large it probably becomes the only feasible method to use.

A numerical technique for directly integrating the time-dependent Schrödinger equation in imaginary time has been discussed in recent literature [33]. When only one spatial dimension is present, this technique may be more efficient than the method using the path integrals. This is because in the latter method one is dealing with an integral with a large multiplicity. However, when more than one spatial dimension is involved, the present Monte Carlo path integral approach is expected to be a better method.

In general, the Monte Carlo procedure will require a minimum of around 100,000 configurations to evaluate the path integral to approximately 1 % accuracy. An offhand guess of the number of configurations n could be obtained from the amount of statistical fluctuation ($\sim n^{-1/2}$) one is willing to tolerate in the results. The exact value of n will probably depend on the particular potential being studied and on the magnitude of the time step τ. Actual numerical evaluations of the path integrals for some elementary quantum mechanical problems have indicated that the above estimate for n yields results of reasonable accuracy.

We discuss the details of the calculations below. However, by way of illustration, Figs. 2 and 3 give results of some of these calculations for the harmonic oscillator for various times. In Fig. 2 the Monte Carlo computer evaluation is plotted as well as an analytic evaluation of the ground state of the one-dimensional harmonic oscillator. Here, the integration time is chosen to be sufficiently large so that the

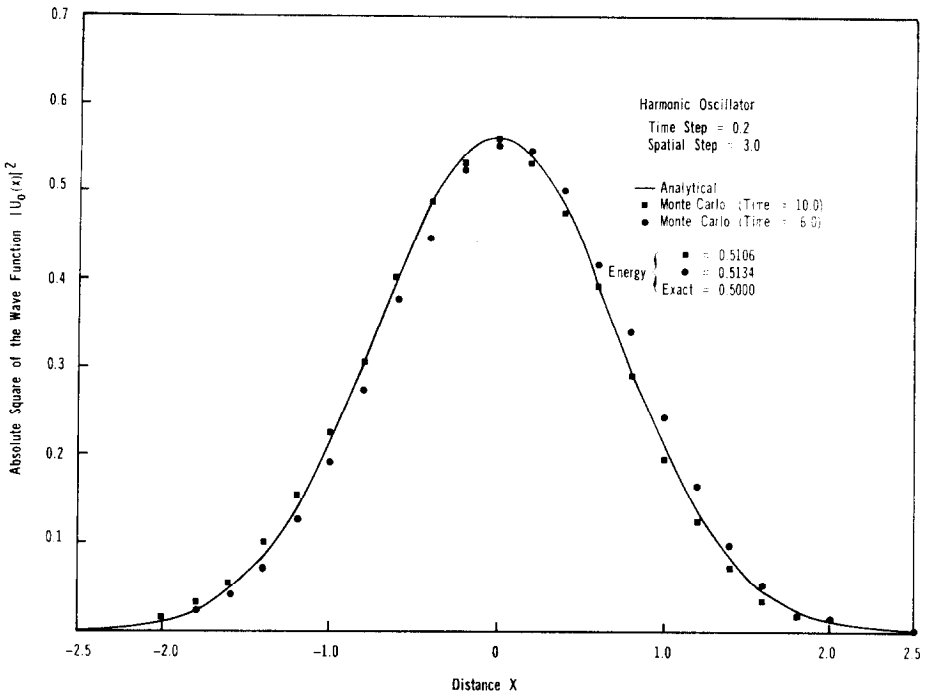

FIG. 2. Comparison of an analytic evaluation of the harmonic-oscillator propagator and two Monte Carlo evaluations.

ratio of the contribution of the first-excited state to that of the ground state is approximately 10^{-4}. Also shown in the same figure are results of a similar calculation for a shorter time. Figure 3 shows the Monte Carlo results compared with analytic evaluations of the propagator for three different times. The results for the largest time gives almost pure ground state. The results for two smaller times show the mixture of the ground and the excited states.

V. DESCRIPTION OF THE NUMERICAL PROCEDURE[4]

In order to evaluate the functional integrals involved in Eq. (38), we use a method which is basically the same as the one proposed by Metropolis *et al.* [29], and employed in many statistical mechanical calculations. It is thus necessary to

[4] This discussion is for a one-dimensional problem, generalization to more than one dimension being quite straightforward.

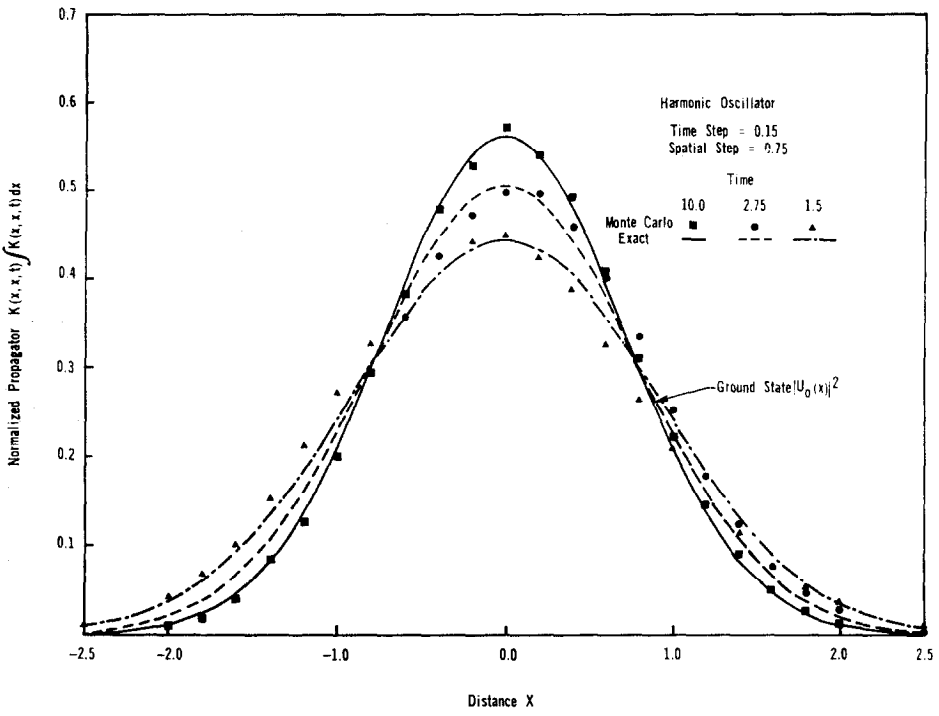

FIG. 3. Comparison of analytic and Monte Carlo evaluations of the harmonic oscillator propagator for three different imaginary times.

give only an outline of the procedure here, in terms of the following steps taken on a computer.

1. First, an initial configuration is chosen. This consists in generating an initial path by choosing the N points $x_1, \ldots, x_N$, randomly, within the interval $[a, b]$. If the interval $[a, b]$ is assumed to be equally divided in M subintervals, each of these points would fall in at least one of these subintervals. We call these subintervals X-boxes.

2. Next, an integer $j(1 \leqslant j \leqslant N)$ is chosen at random. This integer specifies the point x_j for which a trial move is constructed. The trial move is made by choosing a random displacement which lies anywhere from to $-\alpha$ to $+\alpha$. Thus for a random j, a trial move for x_j would be

$$x_j \to x_j + \alpha(2\eta_1 - 1),$$

where η_1 is a random number between 0 and 1.

3. A decision whether to accept or reject the trial move is then made on the basis of the following criteria:

> The old and new path quantities $\bar{E}(x_1 \cdots x_N)$ and the difference $\Delta\bar{E}$ is calculated, where

$$\bar{E}(x_1, \ldots, x_N) = \Big[\sum_{j=1}^{N} \Big\{ \frac{m}{2} \Big(\frac{x_{j+1} - x_j}{\tau} \Big)^2 + V(x_{j+1}) \Big\} \Big]_{x_{N+1}=x_1}$$

if $\Delta\bar{E} < 0$, that is, if the new "energy" is less than the old "energy", the trial move is accepted, and we obtain a new path. If $\Delta\bar{E} > 0$, the trial move is accepted with probability $\exp(-\tau\Delta\bar{E}/\hbar)$. This is done by picking a random number η_2 between zero and one, and comparing it with $\exp(-\tau\Delta\bar{E}/\hbar)$. If $\eta_2 < \exp(-\tau\Delta\bar{E}/\hbar)$, the move is accepted; if otherwise, the move is rejected.

If the move is rejected, the old path is counted as a new configuration for averaging purposes.

4. The contribution of the new path to the integral is calculated and added to that of the previous paths. A new cycle is then generated starting from step 2.

Using a sufficiently long Markov chain of configurations constructed in the above manner one can obtain the value of the integral (38), or of any similar integral defining the average of a function of configurations, simply by averaging over all members of the chain. In fact, as the length of the Markov chain goes to infinity, the limiting frequency of each configuration would be proportional to the exponential factor $\exp(-\tau\bar{E}/\hbar)$ for that configuration.

It may be remarked here that one could also do a straightforward Monte Carlo calculation by choosing configurations at random rather than as members of a Markov chain and then assign weights. Such a method, in the present context, would have the tendency to pick with high-frequency paths for which $\exp(-\tau\bar{E}/\hbar)$ is small and hence are relatively improbable. (This has the consequence of making the wavefunction unnecessarily accurate for small values of $|\psi|^2$.) This method is therefore inefficient as compared to the "importance sampling" procedure of the Markov-chain method [32] outlined here.

The procedure as outlined above only calculates the propagator at one value of the coordinate, viz. $X_1 = X_{N+1}$. In order to calculate the entire wavefunction it would thus seem that this procedure is to be repeated for all possible values of the coordinate or for some appropriate coordinate grid. It is possible to avoid this duplication of effort in the following manner. A typical path is shown as a space–time plot in Fig. 4(top). The closing path shown in Fig. 4(bottom) from X_N to $X_{N+1} = X_1$ implies that no one point in the path is unique. Therefore, the same path which contributes to the wavefunction at X_1 contributes an equal amount to

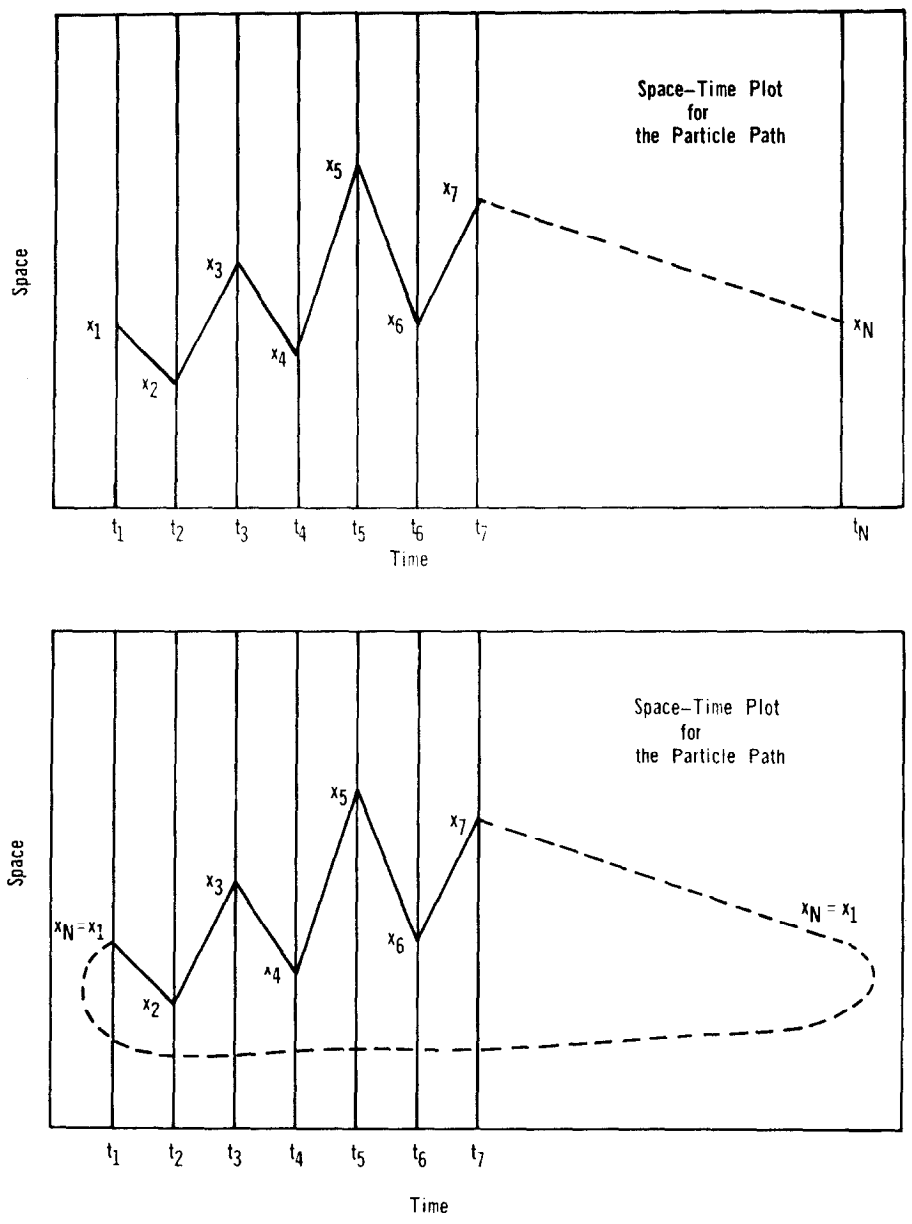

FIG. 4. (top) Open space–time plot for a single path; (bottom) closed space–time plot for a single path.

the wavefunction at X_2, at X_3, etc. In fact, any one of the points $X_2, \ldots, X_N$ could have been considered, in place of X_1, as playing the role of the beginning and end point of the path. An efficient numerical method should take advantage of this fact that one path contains information about the wavefunction at many points. Since the particular X coordinate which is subjected to the trial move is the only coordinate contributing new information during the execution of the logical cycle, there is no need of repeated application of the information contained in the other X coordinates. We may therefore, concentrate all of our attention on the X coordinate we attempt to move, by regarding this particular coordinate as the joint origin and terminal point for the path.

The statistics are taken as follows: since the paths are selected with an exponential bias, and since the contribution of any one path to the propagator is the very same exponential, whenever we have obtained a new X coordinate we put a count of unity in a box corresponding to that particular X coordinate. By placing unity in a box instead of the actual value of the exponential, we remove the biasing factor contributed by our sampling scheme. After we have gone through a sufficient number of cycles to obtain the required degree of accuracy, all of these counts in the various X boxes are divided by a normalization factor which is equal to the product of the size of the X box times the total number of cycles.

To summarize, we have a situation in which an arbitrarily chosen path, if carried through a sufficient number of cycles of movements, relaxes to an equilibrium position, within fluctuations, in such a way that further continuation of the cycling procedure will give only configurations with the "exponential" bias. The entire integration procedure then consists of arbitrarily picking an initial path, allowing this path to relax without taking any statistics, and, then, after sufficient cycles of relaxation, continuing the procedure while taking statistics until the desired accuracy is achieved. It is clear that this procedure remains virtually the same in every case regardless of the physical system under consideration or the time for which the integration is carried out. It is, therefore, at least in principle, possible to think of writing one computer code which could handle any physical system, assuming that a computer of sufficient speed and storage capacity is made available In actuality, however, this is hardly the case, and much of the rest of this paper is concerned with a discussion of the problems encountered in evaluating path integrals even in one-dimensional systems with well-behaved potentials.

VI. Effects of the Potential

For preliminary investigations, it was found convenient to treat the one-dimensional harmonic-oscillator potential. The Coulomb potential would have been more interesting, but because it goes to infinity at $R = 0$, the origin, it imposes more

severe requirements on the method, and it was felt that problems associated with a particular potential should be avoided in a preliminary investigation. One would offhand guess from the nature of the method described above that if one tried to use it in a straightforward manner on the Coulomb potential, the system would fall to the center ($R = 0$), in the case of zero angular momentum. Such an occurrence is indeed the case. There is, of course, some interest both from computer-experimental and theoretical points of view in determining precisely those conditions on the coefficient of the positive $1/R^2$ centrifugal energy term, which keep the configuration from falling to the center.

Some results were obtained for the Morse potential and the particle in the box to further verify the method, and, in the latter case, to determine if the singularity in the first derivative of the potential energy at the edges of the box introduced any additional problems.

One cautionary note has to be sounded when one is dealing with the harmonic oscillator. It has been shown that the form of the propagator for the harmonic oscillator in real time is such that only the classical path contributes to the result. All other paths cancel each other exactly and leave no net contribution. When one goes to imaginary time, paths do not cancel, and, in fact, all possible paths contribute to some extent to the propagator. It is important to note this fact concerning the harmonic oscillator, since one might expect it to give rise to unexpected results in the integrations. Such an effect might arise because it is quite possible that one could throw away terms in the harmonic oscillator without effecting the final result if one took care to throw away terms in such a manner that whenever one eliminated one path from the integral, one also eliminated the twin which would have the opposite sign when the integration is performed in real time. One of the effects of picking a finite value of time step, ϵ, for the numerical integration is to throw away paths which cannot be approximated to sufficient accuracy by broken line segments with this time-step size. Thus, one might expect to obtain, in the case of the harmonic-oscillator potential, anomalously good results for time steps too large to be justified on a theoretical basis.

It is conceivable that similar considerations apply for the case of the Coulomb potential. It may be the finiteness of the time step, ϵ, which amounts to the imposition of a sharper singularity on the system than the $1/R$ potential can itself impose, which causes the "fall" to the center not observed in the usual treatment, using the Schrödinger equation. For the relatively large values of epsilon that one is likely to choose in a numerical evaluation of the path integral it is unlikely that the problems associated with the kinetic-energy term for very small epsilon will be important [1].

VII. Uniqueness of the Markov Chain

The final point which should be noted before discussing the experimental results is that there is a question about whether or not one Markov chain, as we have described it, is sufficient to adequately cover the space of the functional integral. This is not necessarily equivalent to asking whether or not the system as we have described it is ergodic. It is quite possible for one Markov chain to have the ability to eventually cover all of the appropriate space, but to do so sufficiently slowly so that this characteristic is of no practical value. Thus, the question of how many Markov chains are needed breaks up into two questions. The first question is, does one Markov chain have the ability to cover all of the appropriate phase space? And the second question is, if it has the ability to do so, will it do so sufficiently quickly to be of practical value?

In the case of the second question, it is quite likely that a full answer will depend on the particular potential and the particular value of time step, ϵ, chosen in a given case. A third parameter of considerable significance in this respect is the maximum size α for an attempted move of a given coordinate, and a fourth parameter is the total number of time steps N, since the rate at which one can remove a "memory" of a previous configuration should go roughly as the inverse square of this quantity.

VIII. Experimental

Before beginning an actual computer run it is necessary to select parameters such as the time step, total time, maximum spatial displacement, and the various grid sizes. The first parameter which must be determined is the total time. If the energy-level structure of the system is understood at least approximately, a reliable estimate of a proper integration time can easily be determined by making the exponential in the difference in energies between the first-excited state and the ground state divided by $\hbar$ smaller than the error which one is willing to tolerate in the total Monte Carlo integration. If, however, the energy-level structure is not understood, then it will be necessary to regard the integration time as a parameter to be determined, and one will have to make at least two integrations for two different times to determine whether or not one has picked a time sufficiently large so that one is obtaining essentially the ground state. It may be worth mentioning here that some caution is necessary when one is dealing with potentials which exhibit classically metastable configurations (e.g., a potential with a double or triple minima). In such cases, one may end up with metastable paths rather than paths corresponding to the true ground state. An effective way to remedy this defect would then depend upon the potential being studied. Similarly, if the first-excited state is reasonably well

separated in energy from the second-excited state, then integrations for at least two times, one of which is of such a length that the first-excited state contributes significantly to the wavefunction while with the other time the first-excited state does not so contribute, will presumably yield a value for the wavefunction and energy of the first-excited state.

A precise estimate of the time step ϵ is generally difficult to obtain, and is perhaps unnecessary. In practice, it suffices to choose ϵ much smaller than the characteristic times of quantum motion involved in a given problem. One usually has some idea of the latter, if not entirely from theory, then from computer experiments in the worst circumstances, when one is dealing with a relatively unknown system. For example, for the harmonic-oscillator a range of values from 0.1 to 0.5 (in units of $\hbar = m = w = 1$) have been found to yield reasonable results.

The correct procedure for determining the maximum spatial step size α is not so obvious. Previous experience might be helpful. However, a variational-type approach might be employed. Provided that ϵ and the total time are chosen appropriately, a trial value of α would yield a wavefunction which in turn yields an upper bound to the ground-state energy. By changing α, one could obtain several estimates for the ground state and the corresponding energy. The minimum of all these values for the energy would then be the best estimate for the energy, and the corresponding parameter α may then be used to generate the best possible estimate of the ground-state wavefunction. This is partly illustrated in Fig. 5, where Monte Carlo results for the wavefunction for various values of the parameter α are shown.

In order to achieve a faster relaxation, one may temporarily increase the time step during the early period of the cycle. This has the effect, as can be seem from expression (11), of filtering out the excited states more rapidly. Increasing the total time while retaining the same number of time steps is equivalent to increasing the value of ϵ. For small values of ϵ the kinetic energy term, which is proportional to $((X - X')/\epsilon)^2$, is large compared to the potential energy terms which does not contain ϵ. Thus increasing the value of epsilon allows the configuration to see the potential more quickly during any given attempted move and forces it towards the minimum of the potential. However, such a procedure should not be used for the entire relaxation period, but instead toward the end of the relaxation period one should return to the value of time step which one intends to use in the actual integration. Actual experiments on the machine indicate that this is a reasonably good way to achieve quick relaxation.

One can think of several ways of estimating how well a system has relaxed. The simplest one is the condition for the equilibrium of a statistical mechanical system, viz., that the total number of upward transitions equal the total number of downward transitions. If one keeps statisties on these numbers and assumes that relaxation has occurred when these conditions have been achieved, one has one possible measure of the time required for relaxation. Unfortunately, our results indicate

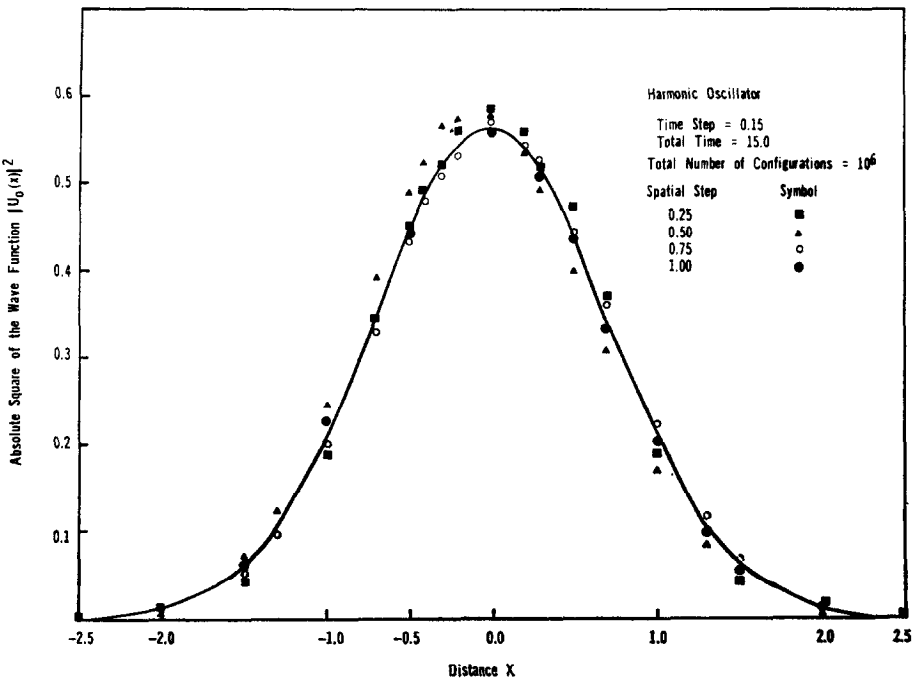

FIG. 5. Comparison of the analytic propagator and several Monte Carlo evaluations with different maximum spatial steps, α.

that equilibrium in this sense is attained long before the system is sufficiently relaxed so that good statistics could be obtained for all parts of the wavefunction. Similar results are obtained for the root-mean-square distance moved per configuration. That is, this number becomes constant before really good statistics can be taken. Normally, we have been forced to compare statistics taken on sets of consecutive configurations to determine when relaxation is reasonably complete.

We have found that one Markov chain is not in general completely reliable or with it in a reasonable length of time. In the case of the harmonic oscillator and other potentials for which one already knows the answer, it is generally possible to pick a particular set of values of ϵ and the maximum step size α such that one Markov chain gives very good results. However, when one is seeking the characteristics of an unknown system, a more reliable procedure would be to generate many Markov chains, allow each one to go through a relaxation period, collect statistics after these relaxation periods for a certain length of time, and add the statistics for all of the different chains together to obtain the total wavefunction. Figure 6

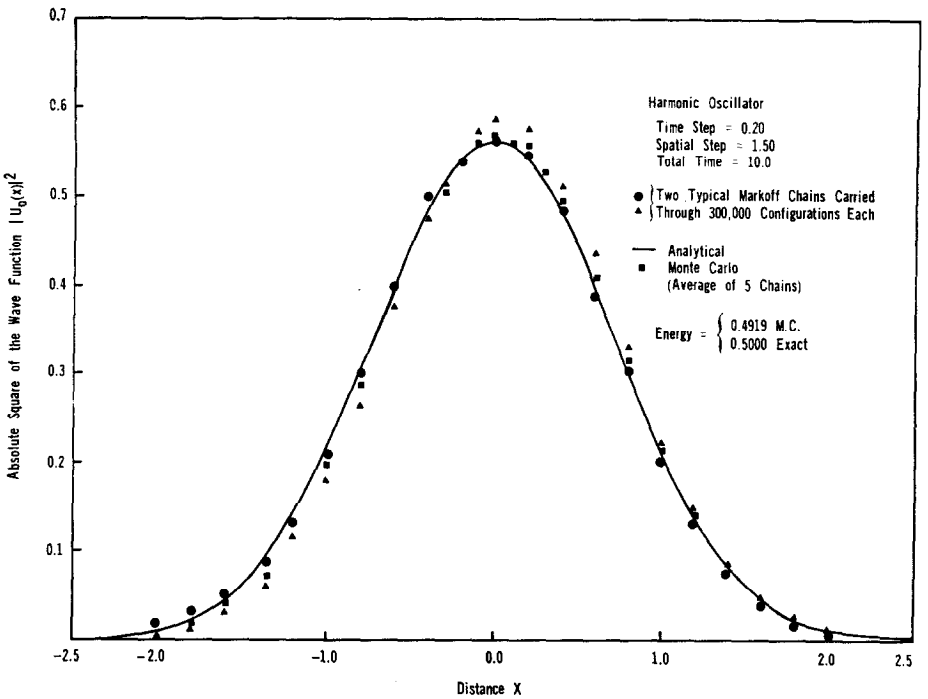

FIG. 6. Plots of the harmonic-oscillator propagator for calculations using the summed results of several individual Markov chains.

gives plots of wavefunctions in which the same number of configurations has been used for the statistics but several different Markov chains have been generated. For these plots values of ϵ and α were chosen which did not give good results for a single Markov chain, although the choices of these parameters seemed to be as reasonable as the choices which did give good results for a single Markov chain.

Several questions arise, naturally, concerning the details of the relaxation process. When one is dealing with many time steps it is very unlikely that during the random choice of the initial path one finds a path whose relaxation will require an inordinately long time. We have examined several paths chosen at random and found that each of these transforms into a reasonably broad spectrum of components with no one component represented to an inordinately large extent. One question of concern during the relaxation process is whether or not a configuration is pure in the sense that it is made up of only one component, because if this happens, it would represent a kind of metastable situation. Another question is, are there components which relax more slowly than others? And if so, are they related in any important fashion to the entire wavefunction or to special regions of the wavefunction? Figure 7 shows the kind of wavefunction produced as a result

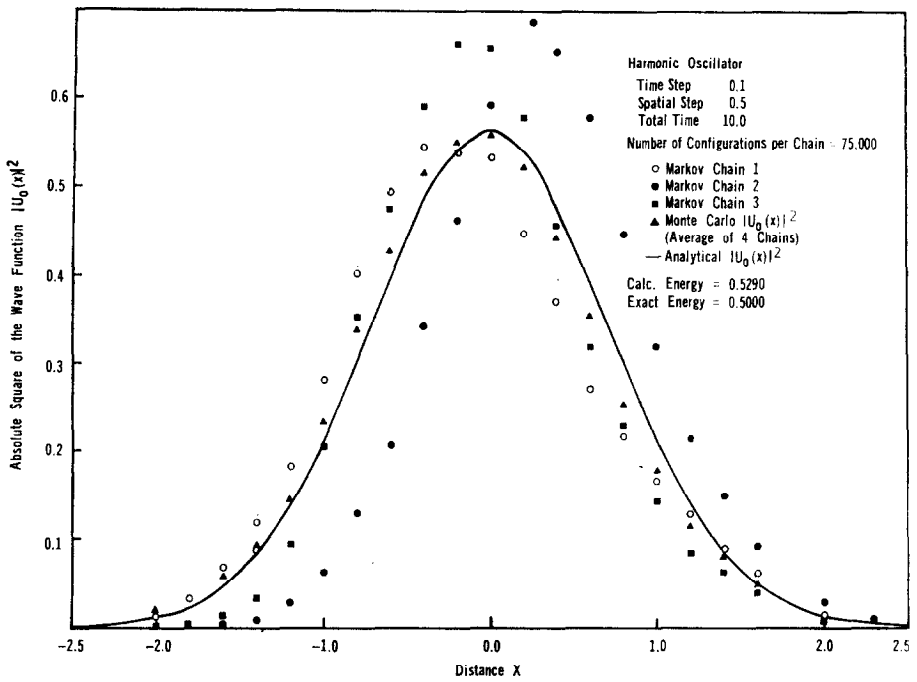

FIG. 7. Plots of three individual Markov chains and their sum under conditions in which statistics were taken before each chain had fully relaxed.

of adding up the statistics of many independent Markov chains but in which the relaxation period in a given Markov chain was too short to allow complete relaxation. It is clear that some components in the path relax more slowly than others and that these components are associated with the peak of the absolute square of the wavefunction. Figure 8 shows the intermediate stages of a relaxation process during a single Markov chain of 200,000 configurations. It is possible to allow the system to relax for a longer time so that those slowly relaxing components associated with an incorrect peak can be eliminated.

There is another set of unwanted components associated with a given configuration which relax very slowly. These components appear when one is dealing with a rather small time step. If one has a very small time step, then the peak of the absolute square of the wavefunction is both too narrow and too high. These components are apparently associated with the fact that with small time steps one is to a certain extent emphasizing the contribution from the higher-energy components. Experimentally, the effect of these high-energy components is not evident until a given path has gone through a great many configurations. Thus, these components relax extremely slowly, practically not at all in fact, and while they are small in

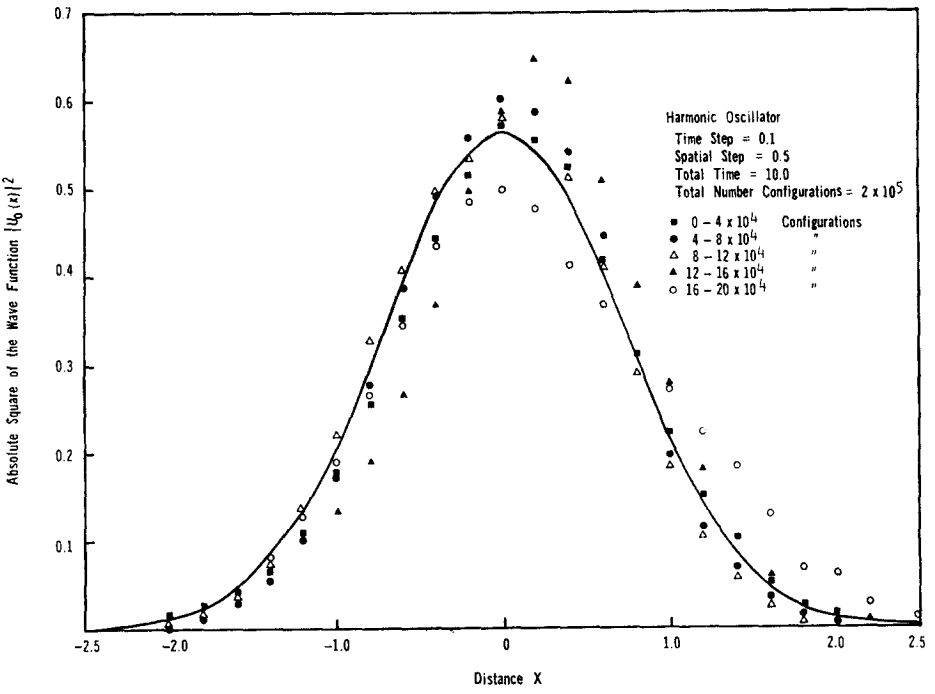

FIG. 8. Plots of statistics for the same Markov chain during different intervals of its history.

an initially unrelaxed and even in a quasi-relaxed path, they seem to represent the principal undesirable contribution remaining in a configuration resulting after a great many steps. Averaging over many independent runs tends to de-emphasize these components, since their effect does not become important during the number of configurations one is likely to use in any one of a set of relatively short independent runs.

A summary then of the empirically determined rules for selecting the best parameters is the following:

1. Pick as large a time step size ϵ, as is consistent with the accuracy desired. This will ensure that those path components which cause too highly peaked paths will be minimized.

2. Pick as short a total integration time as is consistent with the attainability and the accuracy of the ground state. This will allow one to select all of the different time steps relatively rapidly in the sampling procedure so that the memory of a previous configuration disappears as soon as possible.

3. Pick a maximum spatial step size such that one is successful in moving a point only 10 to 30 % of the time. While this means that one does not move a coor-

dinate so often, it means that when a coordinate is moved, it is likely to be a relatively large step so that the configuration moves through phase space more rapidly.

4. Use several (for example, five or ten) independent Markov chains, and without spending too large a fraction of the computer run in initial relaxation, take the statistics, using a total number of configurations about two or three times as large as the number of configurations required for initial relaxation.

Finally, Figs. 9 and 10 show the optimum results obtained for a particle in a box and a particle acted on by the Morse potential. The Monte Carlo results are shown along with the analytical results, and the values of the ground state energies are indicated. These results further confirm the discussion of the present section.

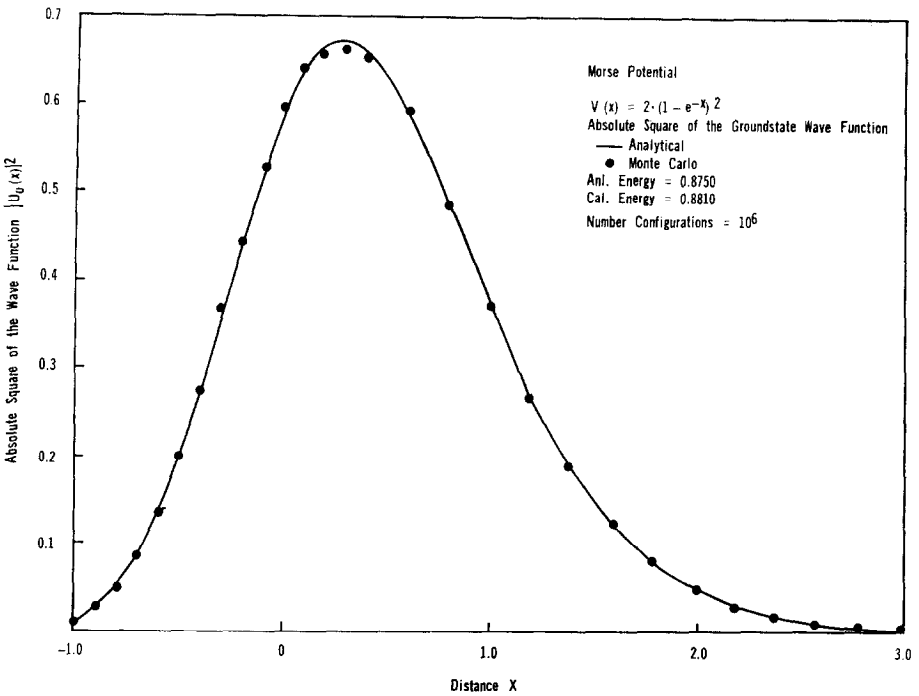

FIG. 9. Comparison of analytic and Monte Carlo evaluations of the one-dimensional Morse-potential propagator. Space and time steps were experimentally optimized.

IX. EXCITED STATES AND STATISTICS

We mentioned above how one might be able to calculate the first-excited state if the second-excited state is relatively well separated from it in energy. Under the

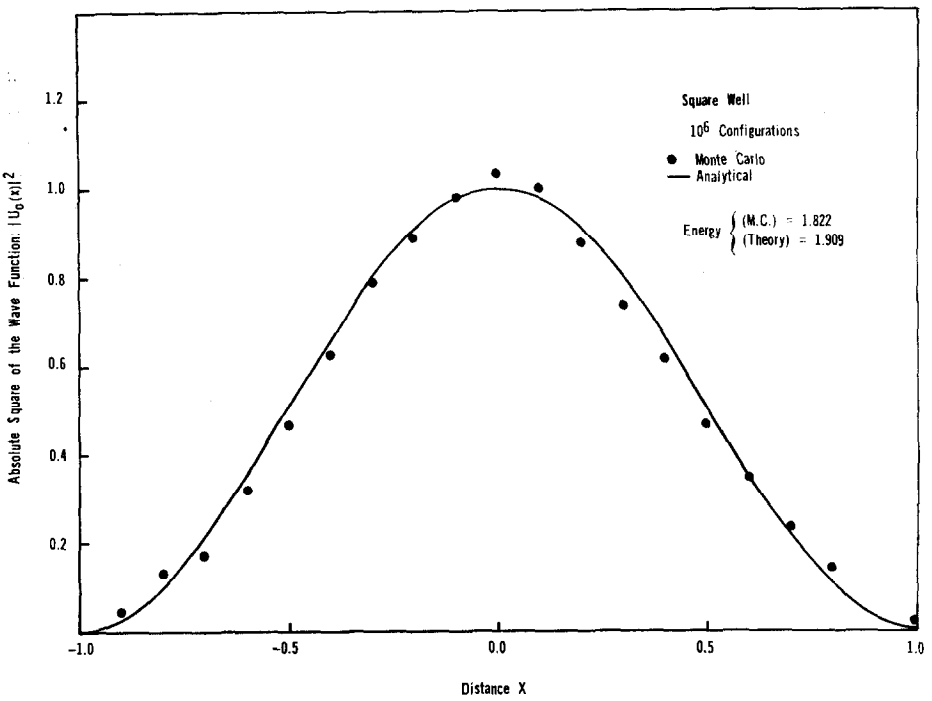

FIG. 10. Comparison of analytic and Monte Carlo evaluations of the one-dimensional particle-in-a-box propagator.

same condition, one could obtain the absolute square of the wavefunction of the first-excited state by making one run which gave one pure ground state and a second run with a shorter integration time which gave the mixture primarily of the first-excited state and the ground state. The contribution of the ground state to this result can then be subtracted out leaving the first-excited state. Unfortunately, since this will involve taking the difference between two large numbers which are not known too accurately, the resulting wavefunction will not be too accurate.

Taking exchange statistics into account is somewhat similar to the problem of determining excited states. We know that

$$\begin{aligned}\Psi(1, 2, t) &= \frac{1}{\sqrt{2}}[\psi(1, 2, t) \pm \psi(2, 1, t)] \\ &= \frac{1}{\sqrt{2}}\int [K(1, 2; 1', 2', t) \pm K(2, 1; 1', 2', t)]\, \Psi(1', 2', 0)\, dX_1\, dX_2\end{aligned} \tag{40}$$

gives the wavefunction of a two-particle, one-dimensional system at time t as a function of the wavefunction of the same system at time zero. The plus sign corresponds to Bose statistics and the minus sign to Fermi statistics. The two propagators are very nearly the same, except that in the second one the labels on the particles at time t have been interchanged. In order to determine the absolute square of the total wavefunction for two Fermi particles, one would subtract the second [redacted] particles at time t equal to the coordinates of the particles at time zero. Figure 11(top) is a stylized drawing of the two paths associated with the integration of the propagator in which no exchange has taken place. Figure 11(bottom) is the equi-

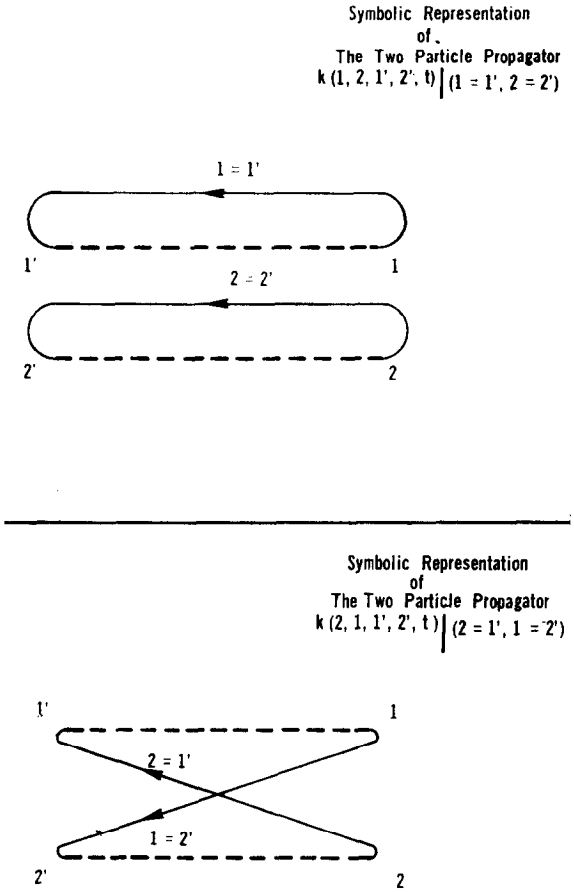

FIG. 11. (top) A symbolic representation of the unpermuted half of the one-dimensional two-particle propagator; (bottom) a symbolic representation of the permuted half of the one-dimension two-particle propagator.

valent stylized drawing for the paths of the second particle in which the final positions have been interchanged and then the coordinates at time t have been set equal to the coordinates at time zero.

For the case of the two Fermi particles we are considering it is clear that the propagator for the exchanged system is equivalent to the propagator for a single particle in which the time is twice as long. We know that when we are dealing with two Fermi particles, which are in the same potential well but which do not interact with each other, the ground state of the total system will be that for which one of the particles is in the one-particle ground state and the other is in the first excited one-particle state. In

$$\Psi^2 \simeq K(1, 2; 1', 2', t)|_{1=1',2=2'} - K(2, 1; 1', 2', t)|_{2=1',1=2'}$$

$$\cong e^{-E_1 t/\hbar} U_1^2 + e^{-E_2 t/\hbar} U_0^2 - c e^{-2E_2 t/\hbar} U_0^2 \tag{41}$$

we have used these facts, that is, the first two terms on the right hand side of the equation come from the first propagator and give a contribution from the ground state and from the first excited state. The second propagator being only a one-particle propagator, in essence, contains only a contribution from the one-particle ground state. This contribution gives rise to the third term in expression (41) in which c is a constant to be evaluated. Equation (41) rewritten as

$$\Psi^2 \cong e^{-E_0 t/\hbar}[e^{-(E_1-E_0)t/\hbar} U_1^2 + (1 - c e^{-E_0 t/\hbar})\, U_0^2] \tag{42}$$

implies that the constant c is given by

$$e^{-(E_1-E_0)t/\hbar} = 1 - c e^{-E_0 t/\hbar}. \tag{43}$$

As a consequence of this, one is essentially left with the same problem in the case of exchange statistics that one had while dealing with the excited states. As the number of particles in the system increases, the problem becomes more severe, because one will be adding and subtracting several propagators corresponding to all the various exchange classes to obtain the total wavefunction. This then would require more detailed investigation and is beyond the scope of the present paper.

X. Conclusions and Summary

We have discussed a method for determining the ground states of quantum mechanical systems on the computer in which essentially no approximations are required. We have shown that, in the case of the harmonic-oscillator, particle-in-

the-box, and Morse potentials, the procedure works reasonably well. We have also discussed some of the practical experimental difficulties in obtaining accuracy on the computer. However, the problems associated with exchange statistics, singular potentials, and non-cartesian coordinates need to be overcome before the method could be profitably used to handle complex unknown systems.

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