# Evaluation of Feynman path integrals by Monte Carlo methods

P. K. MacKeown

Citation: American Journal of Physics **53**, 880 (1985); doi: 10.1119/1.14356
View online: https://doi.org/10.1119/1.14356
View Table of Contents: https://aapt.scitation.org/toc/ajp/53/9
Published by the American Association of Physics Teachers



forcement of the concepts of phase and phase difference; an improvement in oscillosocpe technique; and, through the audio output of the synthesizer, an appreciation that the human ear is sensitive to amplitude and frequency but not at all sensitive to phase differences between the constituent harmonics of a sound.

The students find this a valuable experiment and enjoy doing it. Musicians taking part in extension courses have derived considerable benefit and enjoyment from attempting to simulate various instrumental tonal qualities with the synthesizer.


## ACKNOWLEDGMENT

The authors gratefully acknowledge the contribution of E. R. Hodgson in the development of this experiment.



[1]R. W. Hamming, *Numerical Methods for Scientists and Engineers* (McGraw-Hill,New York, 1973), 2nd ed., pp. 505–515.
[2]T. H. Lynch, Electronics **50**, 115 (1977).
[3]R. J. Higgins, Am. J. Phys. **44**, 766 (1976).


# Evaluation of Feynman path integrals by Monte Carlo methods


P. K. MacKeown
*Department of Physics, University of Hong Kong, Hong Kong*



(Received 22 May 1984; accepted for publication 8 September 1984)



Details of a project suitable for an advanced undergraduate course in computational physics, involving the evaluation of functional integrals, are presented. The square of the ground state wavefunction for a simple system may be formulated as a Feynman path integral, and such path integrals evaluated using Monte Carlo methods on a microcomputer. Application to a system interacting through a Morse potential or through a simple harmonic potential is described, while the possible employment of over-relaxation in the latter case is explained.


## I. INTRODUCTION

One of the most noticeable aspects of the application of computers in physics is the explosion in the literature[1,2] over the past few years, of papers based on the application of Monte Carlo methods in quantum field theory calculations. Because the topic is at the forefront of research—most papers are exploring the possibility of the confinement of quarks in quantum chromodynamics—it is not easy for undergraduates to appreciate it, the more so as they generally lack experience in use of the Monte Carlo method. Such calculations, however, are evaluations essentially of Feynman path integrals; by using this technique to focus on a much simpler problem both the content of the formalism and the details of the computing method can be introduced at the undergraduate level. In this article we describe a project, used in a final year undergraduate course on computational physics, on the application of the Feynman method to a problem in elementary quantum mechanics; the students are not assumed to be familiar with functional integration beforehand. This concerns the evaluation of the square of the ground state wavefunction and its energy, of a particle in a specified potential in one dimension; the cases of simple harmonic motion and motion in a Morse potential are described explicitly.

The feasibility of this method was originally described in two rather long papers.[3] Here we aim at as simple a presentation as possible. The Monte Carlo method has often been discussed previously in the context of problems in statistical mechanics,[4] at a level similar to that in this article. Although in principle its application here is not significantly different, the relative unfamiliarity of summing over paths warrants a brief introduction. In Sec. II we briefly outline the necessary background in quantum mechanics and the extension of the formalism to imaginary time, while in Sec. III we describe the application of the Metropolis algorithm for the evaluation of the sum over histories. In Sec. IV we describe its application to the Morse potential and in Sec. V present some results for this, as well as for the simple harmonic oscillator, obtained using a Commodore CBM3032 microcomputer.

## II. THE PATH INTEGRAL FORMALISM

The path integral formalism is described in several places,[5,6] with Ref. 6 giving a useful introduction based on physical considerations. Even so, a concise presentation directed towards its immediate application in the project seems necessary for the students. This we attempt in the following.

Guided by considerations like the motion of an electron in the double-slit experiment, and an idea of Dirac, Feynman postulated an amplitude to be associated with any visualizable trajectory of a particle's motion. The amplitude for the overall resulting motion is then the sum of the trajectory amplitudes over all "permissible" trajectories. For motion in one dimension the amplitude associated with a trajectory $X(t)$ between points $X(t_0) = x_0$ and $X(t) = x$ is

assumed to equal $\exp\{iS[X(t)]/\hbar\}$, where $S[X(t)]$ is the classical action along the trajectory, i.e.,

$$S=\int_{t_0}^{t} L(X,\dot{X},t)dt\,,$$

where $L$ is the Lagrangian. The total amplitude for the motion from $(x_0, t_0)$ to $(x, t)$ is given by

$$K(x,t;x_0,t_0)=\sum_{X_i}\exp\left(\frac{i}{\hbar}S[X_i(t)]\right),\quad t>t_0; \tag{2.1}$$

a sum over all trajectories $X_i(t)$ linking the points. Among several of the formal ways of writing this quantity one frequently encounters

$$K(x,t;x_0,t_0)=\int \mathscr{D}X(t')\exp\left(\frac{i}{\hbar}S[X(t')]\right). \tag{2.2}$$

Here $\mathscr{D}X(t')$ is a measure of the number of infinitesimal segments at $t'$ of complete paths linking $(x_0, t_0)$ to $(x, t)$; in fact, the expression is no more helpful than (2.1) in telling us how to calculate the sum.

If the initial state at $t_0$ is itself a distribution characterized by a probability density $|\Psi(x_0,t_0)|^2$, the total amplitude to be at $x$ at time $t$ is just the weighted sum of trajectory amplitudes from all initial points,

$$\Psi(x,t)=\int dx_0\,\Psi(x_0,t_0)\,K(x,t;x_0,t_0)\,, \tag{2.3}$$

an expression which also explains why the sum of amplitudes in (2.1) is often called a propagator; it represents the strength with which the value of the wavefunction at any point $x_0$, $t_0$ influences its value at a specific point $x$ at a later time.

In Born's interpretation of Schrödinger's wave equation, the wavefunction $\Psi$ is related to the probability amplitude, i.e., $\Psi(x,t)$, with the appropriate initial conditions, also satisfies Schrödinger's equation:

$$H\Psi(x,t)=i\hbar\frac{\partial\Psi}{\partial t}(x,t)\,. \tag{2.4}$$

In most introductory texts on quantum mechanics[7] it is shown how a solution of (2.4) can be written formally as an expansion, with time-dependent coefficients, in the time-independent eigenstates $\psi_n(x)$ of the operator $H$, i.e.,

$$\Psi(x,t)=\sum_n c_n\exp\left[-\left(\frac{i}{\hbar}\right)E_n t\right]\psi_n(x)\,. \tag{2.5}$$

The coefficients $c_n$ here are given by

$$c_n=\int dx_0\,\Psi(x_0,0)\,\psi_n^*(x_0)\,. \tag{2.6}$$

Inserting these coefficients into the expression (2.5) and comparing the resulting expression for $\Psi(x,t)$ with (2.3) leads to the identity

$$K(x,t;x_0,0)=\sum_n \psi_n^*(x_0)\,\psi_n(x)\exp(-iE_n t/\hbar)\,.$$

We now assume that the validity of this relation extends to imaginary values of $t$; writing $t=-i\tau$, $\tau$ real, it becomes

$$K(x,-i\tau;x_0,0)=\sum_n \psi_n^*(x_0)\,\psi_n(x)\exp(-E_n\tau/\hbar)\,. \tag{2.7}$$

As some reassurance for the validity of this extension we note that such a continuation of Schrödinger's equation, (2.4), to imaginary time gives rise to the same time-independent eigenvalue problem as the original equation. The right-hand side of (2.7) poses no problem. In particular taking $x=x_0$ and assuming that the ground-state energy $E_0$ is not degenerate, then, provided the relation

$$\tau\gg\hbar/(E_1-E_0) \tag{2.8}$$

holds, where $E_1$ is the energy of the first excited state, the first term in the summation $|\psi_0(x)|^2\exp(-E_0\tau/\hbar)$ will dominate. In other words, we have

$$|\psi_0(x)|^2=\lim_{\tau\ \text{large}}\exp(E_0\tau/\hbar)\,K(x,-i\tau;x,0)\,. \tag{2.9}$$

This is the starting point for our project. It means that we can find the square of the ground-state wavefunction for a system if we can sum over the paths in (2.1) evaluated at an imaginary time $-i\tau$ (the potential of course occurring in the action $S$), with $\tau$ sufficiently large, as dictated by (2.8). Since the $E_i$ will not in general be known if the wavefunction is not, this explicit condition will not be of direct help. Sufficiently large $\tau$ can be determined only by searching for convergence[3] as a function of $\tau$.

Requiring normalization of (2.9), i.e.,

$$\int|\psi_0(x)|^2\,dx=1\,,$$

we find in conjunction with (2.1)

$$|\psi_0(x)|^2=\lim_{\tau\to\infty}K(x,-i\tau;x,0)\Big/\int_{-\infty}^{\infty}dx\,K(x,-i\tau;x,0)\,. \tag{2.10}$$

## III. EVALUATION OF THE SUM OVER PATHS

We return to the general expression (2.3), and consider the particular path shown in Fig. 1. For any $t_1<t$ we can write

$$\Psi(x,t)=\int dx_1\,\Psi(x_1,t_1)\,K(x,t;x_1,t_1)\,.$$

However, $\Psi(x_1,t_1)$ may also be expressed in terms of values at an earlier time,

$$\Psi(x_1,t_1)=\int dx_0\,\Psi(x_0,t_0)\,K(x_1,t_1;x_0,t_0)\,,$$

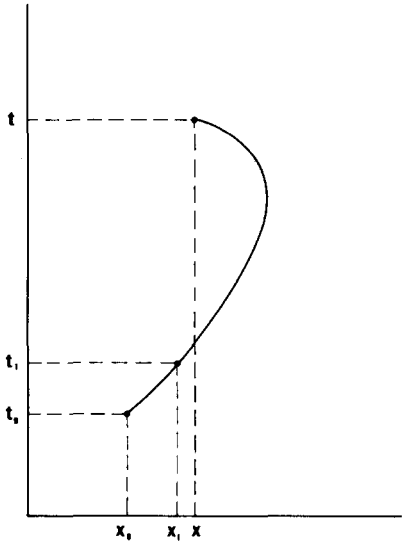


Fig. 1. An arbitrary path linking $(x_0, t_0)$ to $(x, t)$.

so we can write

$$\Psi(x,t)=\int dx_0\,\Psi(x_0,t_0)\int dx_1 \times K(x,t;x_1,t_1)\,K(x_1,t_1;x_0,t_0)\,.$$

Thus on comparison with (2.3), we have the group property

$$K(x,t;x_0,t_0)=\int dx_1\,K(x,t;x_1,t_1)\times K(x_1,t_1;x_0,t_0)\,.$$

Obviously, arbitrarily many successive times $t_i$ may be interposed in this way, at each of which time integration of the product of propagators over the space variable, denoted by $x_i$, must be carried out. With $N$ intervening times, spaced evenly by $\epsilon=(t-t_0)/N+1$, we have the following expression, with $x_{N+1}\equiv x$:

$$K(x,t;x_0,t_0)=\lim_{N\to\infty}\int dx_1,\ldots,dx_N \times\prod_{i=0}^{N}K(x_{i+1},t_{i+1};x_i,t_i)\,,$$

where the propagators in the multiple integral are to be evaluated for infinitesimal time differences. At least for systems where the potential does not depend on velocity[6] it can be shown that as far as significant contributions to this multiple integral are concerned we can write

$$K(x_{i+1},t_i+\epsilon;x_i,t_i)=A\exp\left[(i/\hbar)\,S(x_{i+1},x_i)\right],$$

where $A$ is a constant which depends on $\epsilon$ and $S$ is the stationary classical action between $x_i$ and $x_{i+1}$. In this way we can write the overall propagator as

$$K(x,t;x_0,t_0)=\lim_{N\to\infty}A^N\int dx_1,\ldots,dx_N \times\exp\left[(i/\hbar)\,S(x_0,x_1,\ldots,x_N,x)\right]. \tag{3.1}$$

The sum has been converted into a multiply infinite multiple integral, and we can use it to evaluate (2.10).

For such potentials $\Phi(x)$ which do not involve time derivatives we can write the Lagrangian for a particle as

$$L(x,\dot{x},t)=\frac{m}{2}\left(\frac{dx}{dt}\right)^2-\Phi(x)\,,$$

which in terms of $\tau$ becomes:

$$-\left[\frac{m}{2}\left(\frac{dx}{d\tau}\right)^2+\Phi(x)\right]\equiv -H(x,\tau)\,,$$

where $H$ is the Hamiltonian. Hence the action may be written as

$$S(X_i)=i\int_{X,0}^{\tau}H(x,\tau')\,d\tau'$$

and (2.10) takes the form

$$|\psi_0(x)|^2=\left[\int dx_1,\ldots,dx_N\exp\left(-\frac{1}{\hbar}\int_0^{\tau}Hd\tau\right)\right]\Big/Z\,. \tag{3.2}$$

The denominator $Z$ has the form

$$Z=\int_{-\infty}^{\infty}dx\int dx_1,\ldots,dx_N\exp\left(\frac{1}{\hbar}\int_X Hd\tau\right).$$

The label $X_i$ on the integral means that the integration

$$\int Hd\tau$$

is carried out along the trajectory $X_i$, linking the points

$$[x(0)=x,x_1(\tau_1),\ldots,x_N(\tau_N),x(\tau)=x]\,.$$

By taking these segments as straight lines, equally spaced in $\tau$ by $\epsilon\equiv\tau/N+1$, we have

$$\frac{1}{\hbar}\int Hd\tau\to\frac{\epsilon}{\hbar}\sum_0^N\left[\frac{m}{2}\left(\frac{x_{j+1}-x_j}{\epsilon}\right)^2+\Phi(x_j)\right]=\frac{\epsilon}{\hbar}\sum E_j\,, \tag{3.3}$$

and we associate an energy $E[X(\tau)]$ with a given trajectory. Equation (3.2) then assumes the form

$$|\psi_0(x)|^2=Z^{-1}\int dx_1,\ldots,dx_N \times\exp\left[-(\epsilon/\hbar)\,E(x,x_1,\ldots,x_N,x_{N+1}=x)\right].$$

It is helpful to write $x=x_0$ and integrate over $x_0$ with a delta function included, i.e.,

$$|\psi_0(x)|^2=Z^{-1}\int dx_0\,dx_1,\ldots,dx_N \times\delta(x_0-x)\exp\left[-(\epsilon/\hbar)\,E(x_0,x_1,\ldots,x_N,x_0)\right], \tag{3.4}$$

where

$$Z=\int dx_0,\ldots,dx_N\exp\left[-(\epsilon/\hbar)\,E(x_0,x_1,\ldots,x_N,x_0)\right]. \tag{3.5}$$

Expression (3.4) is of the general form:

$$\int d\mathbf{r}f(\mathbf{r})\pi(\mathbf{r}) \tag{3.6}$$

where $\pi(\mathbf{r})$ is a normalized probability distribution,

$$\pi(\mathbf{r})d\mathbf{r}=Z^{-1}\exp\left[-(\epsilon/\hbar)\,E(\mathbf{r})\right]d\mathbf{r} \tag{3.7}$$

and $f(\mathbf{r})=\delta(x_0-x)$. We now describe the evaluation of such integrals.

## IV. THE MONTE CARLO METHOD

Because of the large number of dimensions in the integral (3.6), (we will take $N=32$ below), the Monte Carlo method strongly suggests itself as a method of evaluation. An estimate of its values is just the average of the function $f(\mathbf{r})$ over a series of $M$ values $\mathbf{r}_i$ of its argument, where these values are selected at random from the distribution $\pi(\mathbf{r})$. This is the method of importance sampling. The probability distribution $\pi(\mathbf{r})$, however, contains the horrendous normalizing quantity $Z$, (3.5); in the absence of knowledge of this the only way to select variates from the distribution is by the use of Markov chains. For this the algorithm of Metropolis *et al.*[8] is most popular; we outline it in the context of a specific project below.

We investigate a pair of atoms interacting through a potential, for which the ground-state wavefunction and energy are known, namely the Morse potential[9]:

$$\Phi(r)=V_0(e^{-2a(r-r_0)}-2e^{-a(r-r_0)})\,.$$

If we write $\omega\equiv a(2V_0/\mu)^{1/2}$, $\zeta^2\equiv\hbar a(2\mu V_0)^{-1/2}$, where $\mu$ is the reduced mass of the pair, and take as our unit of length $(\hbar/\mu\omega)^{1/2}$, i.e., writing $x\equiv(r-r_0)\,(\mu\omega/\hbar)^{1/2}$, it takes the form:

$$\Phi(x)=(\hbar\omega/2\zeta^2)\,(e^{-2\zeta x}-2e^{-\zeta x})\,.$$

If, further, we take $\omega^{-1}$ as our unit of time, Eq. (3.3) takes

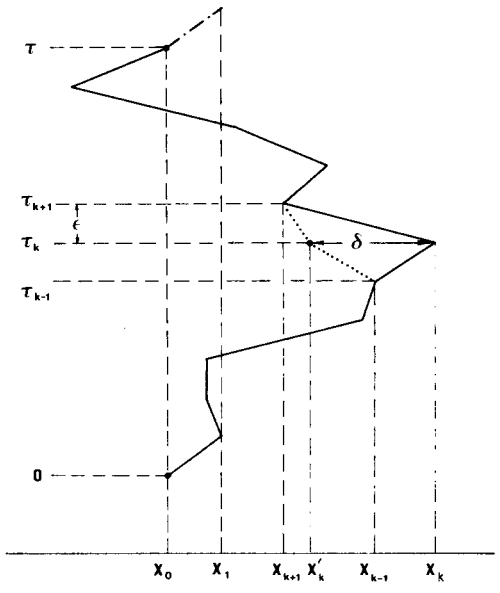


Fig. 2. A segmented path linking $(x_0, 0)$ to $(x_0, \tau)$, one of the infinity of such contributing to (3.4). A possible step $x_k \rightarrow x'_k$, on the Markov chain is shown.

the form $\epsilon E(x_0, \ldots, x_{N+1})$, where

$$E(x_0, \ldots, x_{N+1}) = \frac{1}{2}\sum_{j=0}^{N}\left[\left(\frac{x_{j+1}-x_j}{\epsilon}\right)^2 + \frac{1}{\zeta^2} \times [\exp(-2\zeta x_{j+1}) - 2\exp-(\zeta x_{j+1})]\right]. \quad (4.1)$$

The use of Markov chains to select configurations or paths is described in Ref. 10; we outline the popular version due to Metropolis *et al.*[8] Starting with an arbitrary path $(x_0, \ldots, x_{N+1} = x_0)$ successive paths are chosen a step at a time such that they differ at most in the coordinate of one node, say $x_k \rightarrow x'_k$. This step is chosen with a probability $W_{kk'} = \min(1, e^{-\epsilon\Delta E})$, where $\Delta E = E(x_0, \ldots, x'_k, \ldots, x_{N+1}) - E(x_0, \ldots, x_k, \ldots, x_{N+1})$; i.e., if $\Delta E < 0$ the coordinate is altered to $x'_k$; otherwise it is altered if $e^{-\epsilon\Delta E} > \xi$, where $\xi$ is a random variate from the uniform distribution on (0, 1). After a sufficient number of steps to erase the influence of the initial path, the trajectories so selected will be distributed as (3.7); after this the integral may be evaluated as explained above.

Any one path contributes to the wavefunction at all space points on it, e.g., the solid path in Fig. 2 contributes not only to $\psi(x_0)$, but also to $\psi(x_1)$ because $x_1$ can also be thought of as the beginning and terminating points on a path containing the same segments, with its last one, shown dashed in Fig. 2 just a repetition of the first segment. In practice a node $x_k$ is selected at random, replaced by $x'_k$ where $x'_k$ will have one of the values $x_k \pm \delta$ or $x_k$, where $\delta$ is an arbitrary amount, with the probability $W_{kk'}$, described above. This contributes unity to the integral (3.4) for $x = x'_k$. If $\delta$ is fixed, and thus the possible values of $x_i$ discrete, bins are associated with each of these possible values of $x_i$ and the one corresponding to the revised $x_k$ augmented at each step on the walk. If $\delta$ is itself allowed to vary each bin will embrace a range of values of $x$. The value of $|\psi(x_i)|^2$ is then just the number accumulated in the corresponding bin divided by the total number of steps $M$.

## V. THE PROGRAM

A program was written in BASIC[11] and run on a Commodore CBM3032 microcomputer, taking $\zeta = 1$. Paths are confined to segments linking discrete points in $-3.2 \leqslant x \leqslant 3.2$, $0 \leqslant \tau \leqslant 32\epsilon$, with mesh sizes $\delta$ and $\epsilon$ which can be assigned values, and $x(0) = x(32) = 0$. Different choices of initial path are available, and during execution the actual path is displayed continuously on the monitor. The results in Fig. 3 refer to $\epsilon = 0.55$, $\delta = 0.2$, and initial path:

$$x_i = 0.2i, \quad i = 0, \ldots, 8,$$
$$= 1.6, \quad i = 9, \ldots, 23,$$
$$= 0.2(32 - i), \quad i = 24, \ldots, 32.$$

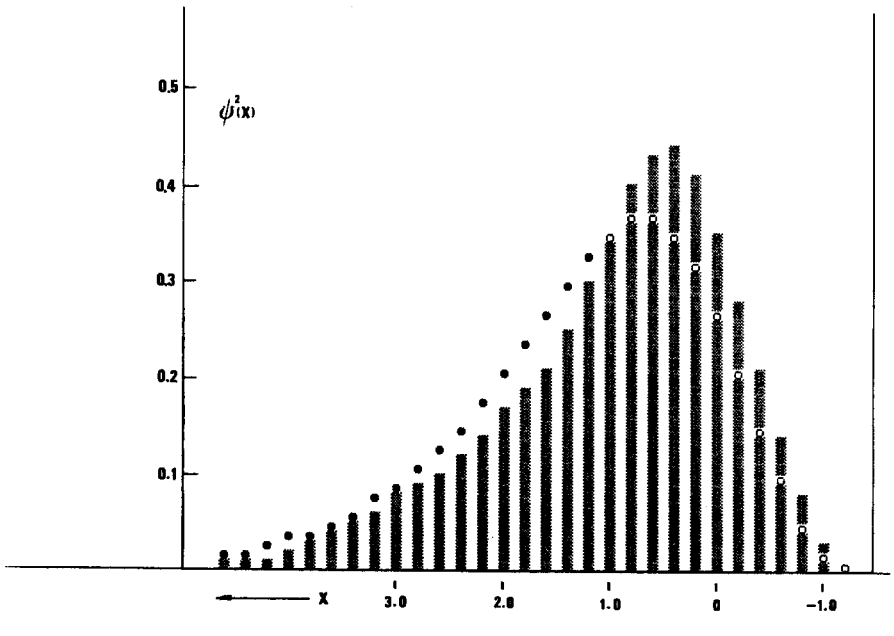


Fig. 3. The histogram shows the square of the ground-state wavefunction for the Morse potential with $\zeta = 1$, based on a chain of 100 000 steps. The known wavefunction is superimposed.

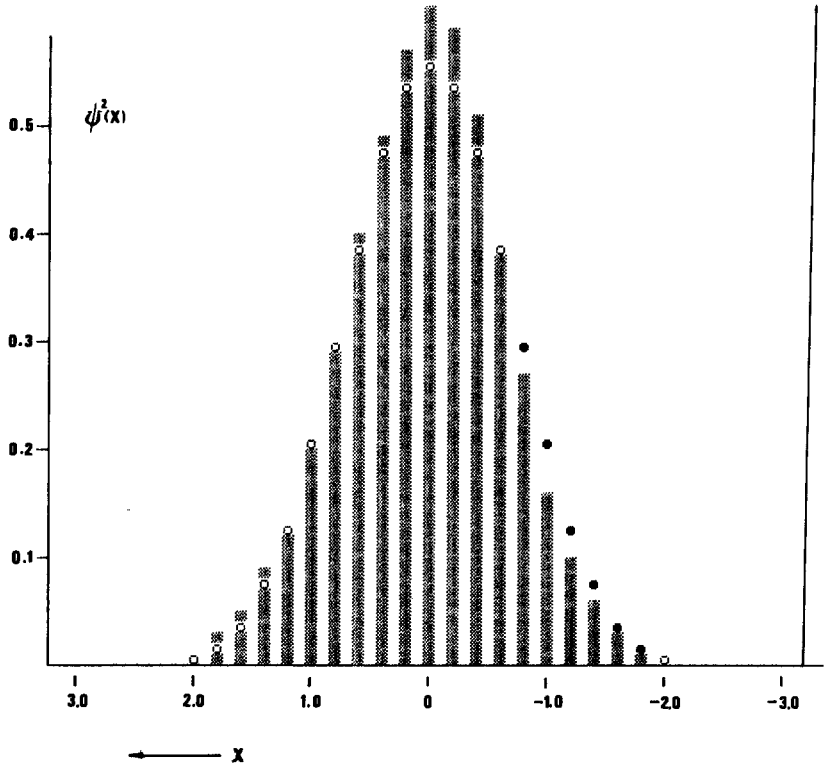


Fig. 4. The square of the ground-state wavefunction for the simple harmonic oscillator based on 50 000 steps (histogram) is compared with its known value.

Here the first 100 000 steps were ignored, it being assumed that by that time the selection process had settled down to the equilibrium one. The results in Fig. 3 are based on the subsequent $M = 100\,000$ steps. The program consists of 250 lines, much of it taken up with graphics for path monitoring and output of results, and the time required is about 1 min per 1000 steps. Because the wavefunction for the ground state has no nodes, we can take $\psi_0(x) = (|\psi_0(x)|^2)^{1/2}$ and evaluate the expectation of the Hamiltonian,

$$\int \psi_0^* H\psi_0 \, dx ,$$

using the finite difference replacement of the operator:

$$-\frac{\hbar\omega}{2}\left(\frac{d^2}{dx^2} - \frac{1}{\zeta^2}(e^{-2\zeta x} - 2e^{-\zeta x})\right).$$

The results in Fig. 3 yield $E_0/\hbar\omega = -0.110$, to be compared with the known value $(1/2) - (\zeta^2/8) - (1/2\zeta^2) = -0.125$. Also shown in Fig. 3 is the square of the known ground-state wavefunction in this case:

$$|\psi_0|^2 = 2\exp[-(x + 2e^{-x})] .$$

The determination of optimum values[3] for $\epsilon$, $\delta$, $M$, etc. is time consuming, but can be distributed among the students in the course.

The program can be adapted readily to other potentials; an interesting case is the simple harmonic potential, i.e.,

$$\Phi(x) = m\omega^2 x^2/2 .$$

With the same units as above we can write down an analogous expression to (4.1) for $E$. If we focus on the occurrences of the coordinate $x_k$ in that expression we have

$$\epsilon E = [(2 + \epsilon^2)/2\epsilon]\, x_k^2 - \tfrac{1}{\epsilon}(x_{k-1} + x_{k+1})\, x_k + \cdots .$$

When this is exponentiated in (3.7) we find that $x_k$ is distributed as a Gaussian, i.e.,

$$\pi(\ldots, x_k, \ldots) \propto \exp[-(x_k - \mu_k)^2/2\sigma^2] ,$$

where $\mu_k = (x_{k-1} + x_{k+1})/(2 + \epsilon^2)$ and $\sigma^2 = \epsilon/(2 + \epsilon^2)$. We do not now need the Metropolis algorithm to step from configuration to configuration through the Markov chain. We can select a new value for $x_k$ (independent of its previous value) $x_k' = \mu_k + \sigma\gamma$, where $\gamma$ is a random variate from the standardized Gaussian.

Results are shown in Fig. 4 for the case of $\epsilon = 0.5$, $\delta = 0.4\,(2\xi - 1)$ and the same initial path as above, taking $M = 50\,000$ after the first 10 000 steps were ignored. Also shown in Fig. 4 is the known ground-state wavefunction. The corresponding ground-state energy came out at $0.510\,\hbar\omega$, to be compared with its known value $\hbar\omega/2$.

An interesting refinement in the program in this case is the possibility of employing over-relaxation in the stepping. This is a concept with which the students are familiar from an earlier part of the course on the use of successive over-relaxation in the solution of difference equations arising from the solution of partial differential equations using finite difference methods. It is in that context also that the concept is introduced most easily; here we summarize its essential features. On average, the effect of each step is to relax that coordinate $x_k$ to a value $\mu_k$ which would minimize the contribution to the energy, or action, from the path in its neighborhood. This may not be the most effective way of minimizing the action over the whole path since $\mu_k$ depends on the values $x_{k-1}$ and $x_{k+1}$, values which in general will not already lie on the minimum, classical, path. It can be argued that a better way is to over-relax the coordinate to a value which has some "memory" of its previous value $x_k$, and on average assumes the value $\mu_k' = \omega\mu_k + (1 - \omega)\, x_k$. Here $\omega$ is a relaxation parameter $(0 < \omega < 2)$, for which an optimum value $\omega_0$ may be chosen to accelerate the relaxation to equilibrium. With such a value the new coordinate at each step is again chosen from a Gaussian with mean $\mu_k'$ and variance[12] $\omega_0(2 - \omega_0)\epsilon/(2 + \epsilon^2)$. The determination, by trial and error, of $\omega_0$ is a

straightforward extension of the project; the possibility of introducing such relaxation into cases where the energy cannot be written as a quadratic in the coordinates, i.e., where the Metropolis algorithm must be used, is a possible research level extension.

## VI. CONCLUDING REMARKS

The advent of computers has necessitated a review of the content of mathematical physics courses, with a result that students who would not be enthused greatly by some traditional topics like conformal transformations may yet, in conjunction with computers, acquire mastery of some relatively sophisticated, and at the same time very useful, techniques. We have attempted to illustrate this in the above report. Should the student continue as a physicist after graduation he may very well see the full value of these techniques as employed in statistical physics or quantum field theory calculations; should he not, the experience acquired may be valuable equally in other fields involving computing.


## ACKNOWLEDGMENT

I am very grateful to Flora Ip for assistance in writing the programs.



[1]M. Creutz, Phys. Today **36**, 35 (May 1983).
[2]C. Rebbi (Ed.), *Lattice Gauge Theories and Monte Carlo Simulations* (World Scientific, Singapore, 1983).
[3]S. V. Lewande, C. A. Jensen, and H. L. Sahlin, Comp. Phys. **3**, 416 (1969); **4**, 451 (1969).
[4]D. P. Landau and R. Alben, Am. J. Phys. **41**, 394 (1973).
[5]L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley-Interscience, New York, 1981).
[6]P. D. Mannheim, Am. J. Phys. **51**, 328 (1983).
[7]See, for example, P. T. Matthews, *Introduction to Quantum Mechanics* (McGraw-Hill, London, England, 1968), 2nd ed., Chap. 13.
[8]N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).
[9]P. M. Morse, Phys. Rev. **34**, 57 (1929).
[10]J. M. Myhre, in *Markov Chains and Monte Carlo Calculations in Polymer Science*, edited by G. G. Lowry (Marcel Dekker, New York, 1970), Chap. 2.
[11]A listing of the program is available on request.
[12]S. L. Adler, Phys. Rev. D **23**, 2901 (1981).


# On reflection and refraction of x rays by ideal mirrors and thin films


Ping Lee[a)]
*GA Technologies Inc., P.O. Box 85608, San Diego, California 92138*



(Received 10 November 1983; accepted for publication 12 September 1984)



The problem of reflection and refraction of x rays at ideal plane parallel interfaces has been examined based upon the Fresnel equations derived from the classical electromagnetic theory and it has been shown to be identical to the inhomogeneous wave model of Mahan. Furthermore, it is also shown that the reflection coefficient for a thin film in the limit of a monolayer of atoms, large angle of incidence $\theta$, and $\sin\theta/\lambda \ll 10\ \text{nm}^{-1}$ is identical to the crystal diffraction model.


## I. INTRODUCTION

Theoretical analyses of x-ray reflections by mirror surfaces are based on classical electromagnetic theory. In the x-ray region all materials are dissipative and any analysis must include a careful description of the effect of absorption on the reflected and refracted waves. For example, a parallel beam of x rays in vacuum striking a mirror surface at an oblique angle of incidence is expected to result in a beam of refracted x rays such that the planes of constant amplitude of this beam are parallel to the vacuum–mirror interface.

A plane electromagnetic wave of wavelength $\lambda$ in vacuum and of circular frequency $\omega$ propagating in a nonabsorbing medium with a real index of refraction $n$ is given by

$$e^{i(\omega t - n\mathbf{k}\cdot\mathbf{r})}. \tag{1}$$

The propagation vector $\mathbf{k}$ has a magnitude of $2\pi/\lambda$. The equation

$$n\mathbf{k}\cdot\mathbf{r} = \text{const} \tag{2}$$

represents a family of planes of constant phase and constant amplitude, all of which are perpendicular to $\mathbf{k}$. This type of wave is known as a homogeneous wave.

Many approaches and formalisms have been used for solving the boundary value problem of an electromagnetic wave at the interface between a nonabsorbing and an absorbing medium. The standard treatment[1–3] simply replaces the real index of refraction in Eqs. (1) and (2) by a complex index of refraction for the absorbing medium. This approach leads to Fresnel equations for reflection and transmission coefficients of a form identical to the case when both media are transparent. However, the nature of the refracted wave and the meaning of the complex angle in the absorbing medium must be carefully analyzed.

An alternate model presented by Mahan[4] starts from the