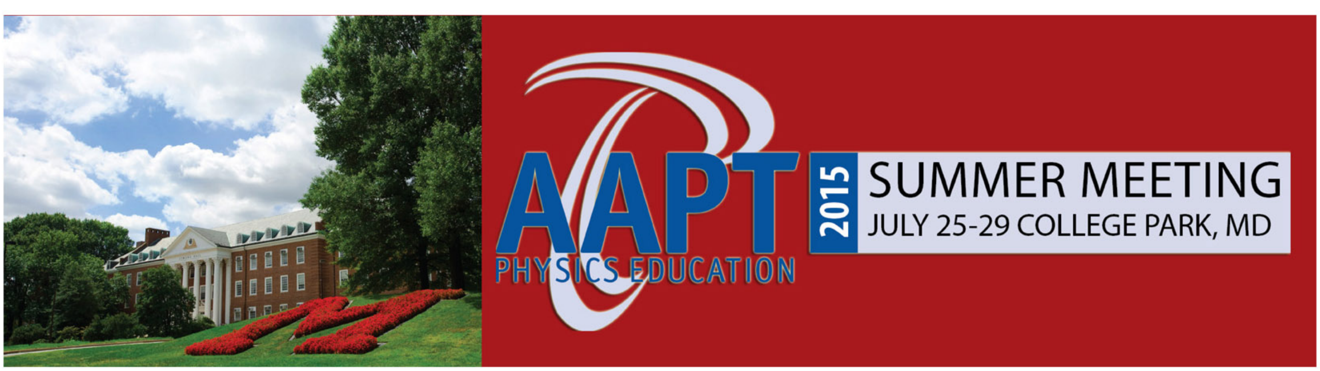
AMERICAN JOURNAL of PHYSICS

Path integral for the quantum harmonic oscillator using elementary methods

S. M. Cohen

Citation: American Journal of Physics **66**, 537 (1998); doi: 10.1119/1.18896
View online: http://dx.doi.org/10.1119/1.18896
View Table of Contents: http://scitation.aip.org/content/aapt/journal/ajp/66/6?ver=pdfcov
Published by the American Association of Physics Teachers



Path integral for the quantum harmonic oscillator using elementary methods

S. M. Cohen
Department of Physics, Portland State University, Portland, Oregon 97207

(Received 12 September 1997; accepted 12 November 1997)

We present a purely analytical method to calculate the propagator for the quantum harmonic oscillator using Feynman's path integral. Though the details of the calculation are involved, the general approach uses only matrix diagonalization and well-known integrals, techniques which an advanced undergraduate should understand. The full propagator, including both the prefactor and the classical action, is obtained from a single calculation which involves the exact diagonalization of the discretized action for the system. © *1998 American Association of Physics Teachers.*

I. INTRODUCTION

Since their introduction,[1] Feynman path integrals have become a powerful method of calculation for quantum mechanical problems.[2,3] Though until recently exact solutions were available for only the simplest cases, great advances in developing methods of solving these integrals have been made in the last 15 years.[4] Yet even before these advances, the approach bore fruit in many ways. For example, the derivation[5] of the ''Feynman rules'' was an extremely important contribution which greatly simplified calculations in perturbation theory.

In a recent article, English and Winters[6] have presented a method of calculating the Feynman path integral for the prefactor of the propagator of the quantum harmonic oscillator. The motivation for their work was ''to introduce a formulation of quantum mechanics which is usually considered beyond the scope of most undergraduate courses.'' We agree with these authors that it is of interest to make alternative approaches to quantum mechanics accessible to the undergraduate. We believe that path integrals have great beauty in the simplicity of their basic formulation. They also clarify various aspects of quantum mechanics, such as the uncertainty principle. The clarification in this particular case follows immediately from the central idea upon which the path integral formulation is based: that all paths in configuration space contribute to the evolution of the wave function. Thus there is an intrinsic uncertainty as to the evolution of any system (we cannot know the trajectory the system follows), and this uncertainty is explicitly illustrated in this approach.

In this note, we give an alternative presentation which we believe is somewhat more direct than that of English and Winters. The method used by these authors required the use of a symbolic computational program, and an intermediate result written in terms of continued fractions. (But see our Appendix for a discussion of how the approach of these authors may be completed analytically.) Our method does not require the use of a computer and is straightforward, formally, so it should be accessible to students. An understanding of Gaussian integrals, and of matrices and their eigenvectors and eigenvalues, are the only prerequisites to following this approach.

Although this problem has been addressed in numerous other works,[2,3,6,7] our presentation is new in some important ways. First, we discretize the action from the very beginning, allowing us to obtain a final result which is exact for arbitrary N (the number of intervals chosen for the discretization—see below). These results are thus directly transferable to the case of a polymer chain with nonvanishing bond lengths confined in a harmonic potential. Additionally, we show how the classical action arises naturally, along with the prefactor, from a single calculation. This differs from previous approaches in which only the prefactor was calculated, the appearance of the classical action being assumed due to a theorem given by Feynman.[2]

II. FORMAL EVALUATION OF THE PATH INTEGRAL

The quantum propagator, $K(b,a)$ for a particle beginning at position $x(t_a)=a$ and ending at $x(t_b)=b$, is given as[2]

$$K(b,a)=\int D[x(t)]\exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b}\mathscr{L}[x(t),\dot{x}(t)]\right), \tag{1}$$

where

$$\mathscr{L}[x(t),\dot{x}(t)]=\tfrac{1}{2}m\dot{x}^2-\tfrac{1}{2}m\omega^2x^2 \tag{2}$$

is the classical Lagrangian, and the symbol $\int D[x(t)]$ represents integration over all paths in configuration space beginning at a and ending at b. As is common practice, these integrals may be done by first partitioning the time interval into N pieces of width ϵ each, so that $T=t_b-t_a=N\epsilon$. At the end of the calculation the limits $N\rightarrow\infty$, $\epsilon\rightarrow 0$, are taken, such that $T=N\epsilon$ is held constant. Then, with $x_j=x(j\epsilon)$, we may write

$$K(b,a)=\lim_{\substack{N\rightarrow\infty\\ \epsilon\rightarrow 0}}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2}\times\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}dx_1dx_2\cdots dx_{N-1}\times e^{im/2\hbar\epsilon\Sigma_{j=1}^{N}\{(x_j-x_{j-1})^2-\epsilon^2\omega^2x_j^2\}}. \tag{3}$$

The argument of the exponential contains the quadratic form

$$Q=\sum_{j=1}^{N}[(x_j-x_{j-1})^2-\epsilon^2\omega^2x_j^2]=x_0^2+x_N^2-\epsilon^2\omega^2x_N^2-2x_1x_0-2x_Nx_{N-1}+Q', \tag{4}$$

where we may write, $Q'=\vec{x}^T\mathbf{A}\vec{x}$. Here,

$$\vec{x}^T=(x_1x_2\cdots x_{N-1}) \tag{5}$$

is the transpose of $\vec{x}$, and

$$\mathbf{A}=\begin{pmatrix} 2-\epsilon^2\omega^2 & -1 & 0 & 0 & \cdots \\ -1 & 2-\epsilon^2\omega^2 & -1 & 0 & \cdots \\ 0 & -1 & 2-\epsilon^2\omega^2 & -1 & \cdots \\ 0 & 0 & -1 & 2-\epsilon^2\omega^2 & \\ \vdots & \vdots & \vdots & & \ddots \end{pmatrix}. \tag{6}$$

If, using a change of variables from the x_j to new variables z_j, we can rewrite Q' into the form

$$Q'=\text{constant}+\sum_{j=1}^{N-1}\lambda_j z_j^2, \tag{7}$$

where the constant does not depend on the z_j, then the (coupled) integrals in Eq. (3) will have been reduced to $N-1$ separate Gaussian integrals. First, we will find a transformation of variables,

$$\vec{x}=\mathbf{O}\vec{y}, \tag{8}$$

such that

$$\mathbf{O}^T\mathbf{A}\mathbf{O}=\Lambda, \tag{9}$$

with Λ a diagonal matrix, $\Lambda_{ij}=\lambda_j\delta_{ij}$, and $\mathbf{O}$ will be orthogonal since A is symmetric and real. Then we may write

$$Q=x_0^2+x_N^2-\omega^2\epsilon^2x_N^2-2x_N\sum_{j=1}^{N-1}\mathbf{O}_{N-1,j}y_j -2x_0\sum_{j=1}^{N-1}\mathbf{O}_{1,j}y_j+\sum_{j=1}^{N-1}\lambda_j y_j^2. \tag{10}$$

Completing the squares, we change variables once again to

$$z_j=y_j-\frac{x_N\mathbf{O}_{N-1,j}+x_0\mathbf{O}_{1,j}}{\lambda_j}, \tag{11}$$

yielding

$$Q=\sum_{j=1}^{N-1}\lambda_j z_j^2+x_0^2+x_N^2-\omega^2\epsilon^2x_N^2 -\sum_{j=1}^{N-1}\frac{(\mathbf{O}_{N-1,j}x_N+\mathbf{O}_{1,j}x_0)^2}{\lambda_j}. \tag{12}$$

Since $\mathbf{O}$ is orthogonal, det $\mathbf{O}=1$, and the Jacobian of both transformations, Eqs. (8) and (11), is unity. Hence we have the replacement

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}dx_1dx_2\cdots dx_{N-1}\Rightarrow\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}dz_1dz_2\cdots dz_{N-1} \tag{13}$$

in Eq. (3) along with the transformation of variables. We obtain

$$K(b,a)=\lim_{\substack{N\to\infty\\ \epsilon\to 0}}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{N/2}\exp\left\{\frac{im}{2\hbar\epsilon}\left[x_0^2+x_N^2-\omega^2\epsilon^2x_N^2 -\sum_{j=1}^{N-1}\frac{(\mathbf{O}_{N-1,j}x_N+\mathbf{O}_{1,j}x_0)^2}{\lambda_j}\right]\right\} \times\prod_{j=1}^{N-1}\left[\int_{-\infty}^{\infty}\exp\left(\frac{im}{2\hbar\epsilon}\lambda_j z_j^2\right)dz_j\right]. \tag{14}$$

The integrals are now simple Gaussians, as advertised above, yielding

$$K(b,a)=\lim_{\substack{N\to\infty\\ \epsilon\to 0}}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2}\exp\left\{\frac{im}{2\hbar\epsilon}\left[x_0^2+x_N^2-\omega^2\epsilon^2x_N^2 -\sum_{j=1}^{N-1}\frac{(\mathbf{O}_{N-1,j}x_N+\mathbf{O}_{1,j}x_0)^2}{\lambda_j}\right]\right\}\left(\prod_{j=1}^{N-1}\lambda_j\right)^{-1/2} =e^{i/\hbar\, S_{\text{cl}}}\lim_{\substack{N\to\infty\\ \epsilon\to 0}}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{1/2}(\det\mathbf{A})^{-1/2}\equiv F(T)e^{i/\hbar\, S_{\text{cl}}}. \tag{15}$$

We will show below that

$$S_{\text{cl}}=\lim_{\substack{N\to\infty\\ \epsilon\to 0}}\frac{m}{2\epsilon}\left[x_0^2+x_N^2-\omega^2\epsilon^2x_N^2 -\sum_{j=1}^{N-1}\frac{(\mathbf{O}_{N-1,j}x_N+\mathbf{O}_{1,j}x_0)^2}{\lambda_j}\right] \tag{16}$$

is indeed the classical action, as it must be; and we will find det $\mathbf{A}$ and thus the prefactor $F(T)$, as well.

III. DIAGONALIZATION OF THE MATRIX, A

To implement the transformation of variables, Eq. (8), we must find the matrix $\mathbf{O}$ which diagonalizes $\mathbf{A}$. As is well known, $\mathbf{O}$ is the matrix of the eigenvectors of $\mathbf{A}$. It is not difficult to show that a complete set of eigenvectors, which we shall denote as $\vec{e}_j$, is given in terms of their components by

$$(\vec{e}_j)_i=\sqrt{\frac{2}{N}}\sin\left(\frac{\pi ij}{N}\right), \tag{17}$$

with $1\leqslant i,\ j\leqslant N-1$. The corresponding eigenvalues are

$$\lambda_j=2-\omega^2\epsilon^2-2\cos\left(\frac{\pi j}{N}\right)=4\sin^2\left(\frac{\pi j}{2N}\right)-\omega^2\epsilon^2, \tag{18}$$

leading directly to the result

$$\det\mathbf{A}=\prod_{j=1}^{N-1}\lambda_j=\prod_{j=1}^{N-1}\left[\left(4\sin^2\left(\frac{\pi j}{2N}\right)-\omega^2\epsilon^2\right)\right] =\frac{(-4)^{N-1}}{\sin^2\theta-1}\prod_{j=1}^{M/2}\left[\sin^2\theta-\sin^2\left(\frac{\pi j}{M}\right)\right], \tag{19}$$

where we have written $\sin\theta$ for $\omega\epsilon/2=\omega T/2N$, and $M=2N$. The product appearing in the final form of this equation is given in Hansen,[8]

$$\prod_{j=1}^{M/2}\left[\sin^2\theta-\sin^2\left(\frac{\pi j}{M}\right)\right]=(-1)^{M/2}2^{1-M}\sin(M\theta)\cot\theta, \tag{20}$$

and we find[9]

$$\det \mathbf{A}=\frac{\sin(2N\theta)}{\sin(2\theta)}, \tag{21}$$

correct for all $N\geqslant \omega T/2$. Furthermore, taking

$$\mathbf{O}_{ij}=(\vec{e}_j)_i, \tag{22}$$

we may calculate

$$\begin{aligned} S_{\mathrm{cl}}(N)&=\frac{mN}{2T}\left[x_0^2+x_N^2-\frac{\omega^2T^2}{N^2}x_N^2\right.\\ &\left.\quad-\sum_{j=1}^{N-1}\frac{(\mathbf{O}_{N-1,j}x_N+\mathbf{O}_{1,j}x_0)^2}{\lambda_j}\right]\\ &=a_Nx_N^2+a_0x_0^2+a_{0N}x_0x_N. \end{aligned} \tag{23}$$

Now,

$$a_N=\frac{mN}{2T}\left(1-\frac{\omega^2T^2}{N^2}-\sum_{j=1}^{N-1}\frac{\mathbf{O}_{N-1,j}^2}{\lambda_j}\right). \tag{24}$$

But,

$$\begin{aligned} \sum_{j=1}^{N-1}\frac{\mathbf{O}_{N-1,j}^2}{\lambda_j}&=\frac{2}{N}\sum_{j=1}^{N-1}\frac{\sin^2\left(\frac{\pi j(N-1)}{N}\right)}{4\sin^2\left(\frac{\pi j}{2N}\right)-\sin^2\theta}\\ &=\frac{2}{N}\sum_{j=1}^{N-1}\frac{\sin^2\left(\frac{\pi j}{N}\right)}{4\sin^2\left(\frac{\pi j}{2N}\right)-\sin^2\theta}\\ &=\frac{1}{2N}\sum_{j=1}^{M/2-1}\frac{1-\cos\left(\frac{4\pi j}{M}\right)}{\cos\phi-\cos\left(\frac{2\pi j}{M}\right)}, \end{aligned} \tag{25}$$

with, as before, $M=2N$, $\sin\theta=\omega T/2N$, and also $\cos\phi=1-\omega^2T^2/2N^2$. This sum may also be found in Hansen,[10]

$$\begin{aligned} \sum_{j=1}^{M/2-1}&\frac{\cos\left(\frac{2\pi jk}{M}\right)}{\cos\phi-\cos\left(\frac{2\pi j}{M}\right)}\\ &=-\frac{M}{2}\csc\phi\csc\frac{M\phi}{2}\cos\left\{\left(\frac{M}{2}-k\right)\phi\right\}\\ &\quad+\frac{1}{4}\csc^2\left(\frac{\phi}{2}\right)-\frac{1}{4}(-1)^k\sec^2\left(\frac{\phi}{2}\right), \end{aligned} \tag{26}$$

where in our case we need $k=0,2$. Then we have

$$a_N=\frac{mN}{2T}\left(1-\frac{\omega^2T^2}{N^2}-\frac{\cos((N-2)\phi)-\cos(N\phi)}{2\sin\phi\sin(N\phi)}\right). \tag{27}$$

The evaluation of a_0 is identical to that of a_N, apart from the term proportional to $1/N$; that is,

$$a_0=\frac{mN}{2T}\left(1-\frac{\cos((N-2)\phi)-\cos(N\phi)}{2\sin\phi\sin(N\phi)}\right). \tag{28}$$

In the same way, we find

$$\begin{aligned} a_{0N}&=-\frac{mN}{T}\sum_{j=1}^{N-1}\frac{\mathbf{O}_{N-1,j}\mathbf{O}_{1,j}}{\lambda_j}\\ &=\frac{m}{T}\sum_{j=1}^{N-1}\frac{(-1)^j\sin^2\left(\frac{\pi j}{N}\right)}{\cos\phi-\cos\left(\frac{\pi j}{N}\right)}=-\frac{mN}{T}\frac{\sin\phi}{\sin(N\phi)}. \end{aligned} \tag{29}$$

In writing the last equality, we have again referred to Hansen,[11]

$$\sum_{j=1}^{N-1}\frac{(-1)^j\sin^2\left(\frac{\pi j}{N}\right)}{\cos\phi-\cos\left(\frac{\pi j}{N}\right)}=-N\sin\phi\csc N\phi. \tag{30}$$

IV. EXACT PROPAGATOR FOR N DISCRETE TIME INTERVALS

Using the above results, we can determine the propagator for an arbitrary number, N, of divisions of the time interval T. This expression may be useful for students and others doing numerical work with path integrals, as a check of their discrete-time algorithms. The result is

$$K_N(b,a)=\left(\frac{mN\sin(2\theta)}{2\pi i\hbar T\sin(2N\theta)}\right)^{1/2}e^{i/\hbar\, S_{\mathrm{cl}}(N)}, \tag{31}$$

with

$$\begin{aligned} S_{\mathrm{cl}}(N)&=\frac{mN}{2T}\left\{\left(1-\frac{\cos((N-2)\phi)-\cos(N\phi)}{2\sin\phi\sin(N\phi)}\right)a^2\right.\\ &\quad+\left(1-\frac{\omega^2T^2}{N^2}-\frac{\cos((N-2)\phi)-\cos(N\phi)}{2\sin\phi\sin(N\phi)}\right)b^2\\ &\quad\left.-\frac{2\sin\phi}{\sin(N\phi)}ab\right\}, \end{aligned} \tag{32}$$

$$\theta=\arcsin\left(\frac{\omega T}{2N}\right), \tag{33}$$

and

$$\phi=\arccos\left(1-\frac{\omega^2T^2}{2N^2}\right). \tag{34}$$

Note that we have used $x_0=a$, $x_N=b$.

Finally, the true propagator is obtained as

$$K(b,a)=\lim_{N\to\infty} K_N(b,a)$$
$$=\left(\frac{m\omega}{2\pi i\hbar \sin \omega T}\right)^{1/2} \times\exp\left\{\frac{im\omega}{2\hbar \sin \omega T}[(a^2+b^2)\cos \omega T-2ab]\right\}, \tag{35}$$

having used the fact that for large N,

$$\theta\cong\frac{\omega T}{2N},$$

and

$$\phi\cong\frac{\omega T}{N}.$$

In conclusion, we have presented a strictly analytical method by which the full propagator for the quantum harmonic oscillator may be obtained using Feynman's path integral approach. Though the details are involved, the general approach should be accessible to advanced students. In particular, our presentation may be of interest to those instructors of graduate-level quantum mechanics who would like to introduce path integrals into their courses.

ACKNOWLEDGMENTS

We would like to thank Pui-Tak Leung for helpful comments and for bringing Ref. 6 to our attention.

APPENDIX

In Ref. 6, it is shown that the prefactor, $F(T)$, may be written as a product of factors,

$$F(T)=\left(\frac{m}{2\pi i\hbar T}\right)^{1/2}\lim_{N\to\infty}\left[N\prod_{j=1}^{N-1}\frac{A_j}{B_j}\right]^{1/2}, \tag{A1}$$

where the A_j and B_j satisfy the same recursion relations,

$$A_j=\gamma A_{j-1}-A_{j-2}, \tag{A2}$$

$$B_j=\gamma B_{j-1}-B_{j-2}, \tag{A3}$$

with $\gamma=2-\omega^2T^2/N^2$, and starting conditions, $A_{-1}=-1$, $A_0=0$, $B_{-1}=0$, and $B_0=1$. As these authors observe, $A_{j+1}=B_j$. What we would like to point out is that these relations brand these objects as Chebyshev polynomials of the second kind.[12] Specifically,

$$B_j=U_j\left(\frac{\gamma}{2}\right)=\frac{\sin[(j+1)\arccos(\gamma/2)]}{\sin[\arccos(\gamma/2)]}. \tag{A4}$$

Therefore, the product appearing in the formula for $F(T)$ is just

$$\prod_{j=1}^{N-1}\frac{A_j}{B_j}=\prod_{j=1}^{N-1}\left\{\frac{\dfrac{\sin[j \arccos(\gamma/2)]}{\sin[\arccos(\gamma/2)]}}{\dfrac{\sin[(j+1)\arccos(\gamma/2)]}{\sin[\arccos(\gamma/2)]}}\right\}$$
$$=\frac{\sin[\arccos(\gamma/2)]}{\sin[N \arccos(\gamma/2)]}. \tag{A5}$$

Thus we have

$$F(T)$$
$$=\left(\frac{m}{2\pi i\hbar T}\right)^{1/2}\lim_{N\to\infty}\left\{N\frac{\sin\left[\arccos\left(1-\dfrac{\omega^2T^2}{2N^2}\right)\right]}{\sin\left[N \arccos\left(1-\dfrac{\omega^2T^2}{2N^2}\right)\right]}\right\}^{1/2}$$
$$=\left(\frac{m}{2\pi i\hbar T}\right)^{1/2}\lim_{N\to\infty}\left\{N\frac{\sin\left[\dfrac{\omega T}{N}\right]}{\sin\left[N\left(\dfrac{\omega T}{N}\right)\right]}\right\}^{1/2}$$
$$=\left(\frac{m}{2\pi i\hbar T}\right)^{1/2}\left\{\frac{\omega T}{\sin(\omega T)}\right\}^{1/2}. \tag{A6}$$

Finally, then

$$F(T)=\left(\frac{m\omega}{2\pi i\hbar \sin(\omega T)}\right)^{1/2}. \tag{A7}$$

This is the desired result, once again obtained by purely analytical means.

[1] R. P. Feynman, ''Space-time approach to nonrelativistic quantum mechanics,'' Rev. Mod. Phys. **20**, 367–387 (1948).
[2] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw–Hill, New York, 1965).
[3] L. S. Schulman, *Techniques and Applications of Path Integration* (Wiley-International, New York, 1981).
[4] C. Grosche and F. Steiner, ''How to solve path integrals in quantum mechanics,'' J. Math. Phys. **36**, 2354–2385 (1995), and references therein.
[5] R. P. Feynman, ''An operator calculus having applications in quantum electrodynamics,'' Phys. Rev. **84**, 108–128 (1951).
[6] L. Q. English and R. R. Winters, ''Continued fractions and the harmonic oscillator using Feynman's path integrals,'' Am. J. Phys. **65**, 390–393 (1997).
[7] J. T. Marshall and J. L. Pell, ''Path-integral evaluation of the space-time propagator for quadratic Hamiltonian systems,'' J. Math. Phys. **20**, 1297–1302 (1979).
[8] Eldon R. Hansen, *A Table of Series and Products* (Prentice-Hall, Englewood Cliffs, NJ, 1975), p. 497, Eq. #91.1.18.
[9] This result has been obtained previously in H. Kleinert, *Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics* (World Scientific, Singapore, 1990), p. 85, Eq. #2.140.
[10] Reference 8, p. 272, Eq. #41.2.19.
[11] Reference 8, p. 272, Eq. #41.2.25.
[12] I. S. Gradshteyn and I. M. Rhyzik, *Table of Integrals, Series, and Products* (Academic, Orlando, FL, 1980), pp. 1032–1033.