Continued Fractions and the Harmonic Oscillator Using Feynman's Path Integrals

L.Q. English and R.R. Winters[a)]

Department of Physics

Denison University

Granville OH 43023

Abstract

The Simple Harmonic Oscillator plays a prominent role in most undergraduate Quantum Mechanics courses. The study of this system using path integrals can serve to introduce a formulation of Quantum Mechanics which is usually considered beyond the scope of most undergraduate courses. However given the current interest in the interpretation and foundations of Quantum Mechanics, non-standard approaches such as Feynman's path integral formalism can be helpful in developing insights into the structure of Quantum Mechanics. In this paper we evaluate the path integration appearing in Feynman's treatment in a natural and direct manner utilizing a symbolic computational program. This approach makes the use of the path integral formulation of Quantum Mechanics accessible to most undergraduate physics majors.

As a byproduct of our approach, we find a representation of the reciprocal of the sinc function, $sinc(x) \equiv \frac{\sin(x)}{x}$, in terms of an infinite product of partial approximates of a continued fraction. We have not found this representation in the literature.

I. Introduction

Given the interest[1,2,3] in the conceptual foundations of the Quantum Mechanics, it is important to introduce undergraduate physics majors to non-standard developments of Quantum Mechanics. One very interesting approach is the use of path integrals by Feynman and Hibbs[4] in their book **Quantum Mechanics and Path Integrals**. This approach speaks to the superposition of alternative processes in a way different from the more standard approach[5] using states in a Hilbert Space. While remarkable progress in the development of path integration techniques has been realized lately [6], such general methods are beyond the scope of most undergraduate Quantum Mechanics courses. Even such a simple system as the one-dimensional simple harmonic oscillator (SHO) is formidable. In fact, Feynman and Hibbs[4] chose to solve this problem with a less than straight-forward approach using Fourier transforms. Marshall and Pell[7] report a general solution for quadratic Hamiltonians such as for the SHO, however, their solution seems too complicated to be accessible to most undergraduate students. We have calculated the propagator for the SHO by directly evaluating the infinitely recursive integrations appearing in the integration over all paths. The motivation for re-examining this problem is to provide an alternative development which we believe is accessible to undergraduate physics majors. Our treatment utilizes a computer-based symbolic manipulator to evaluate a recursive relationship and a limit required in our approach to computing the path integrations. It is the use of the symbolic computational program which places our treatment of the SHO well within the abilities of most undergraduate physics majors.

II. The Propagator for the SHO

The quantum mechanical propagator, K(b,a), describes the probability amplitude for the transition of a system from point x_a in configuration space at time t_a to point x_b at time t_b. The action S[x(t)] of a particular path connecting $x_a=x(t_a)$ and $x_b=x(t_b)$ determines the phase of the amplitude associated with that (particular) path. To compute K(b,a), the amplitudes corresponding to all paths are added. The phase factors corresponding to individual paths can all be written in the form[4], $e^{\frac{i}{\hbar}S[x(t)]}$, where $S[x(t)]=\int_{t_a}^{t_b} L(x,\dot{x},t)dt$ and $L(x,\dot{x},t)$ is the Lagrangian for the system. Thus the propagator is given[4] by

$$K(b,a) = \int e^{\frac{i}{\hbar}S[x(t)]}\, \hat{D}[x(t)] , \tag{1}$$

where the symbol $\int \hat{D}[x(t)]$ is used to represent the integration over all paths connecting the initial and final points.

One approach[4,8] to carrying out the path integration for a one-dimensional system, such as the SHO, is to first partition the time interval into N pieces each of "width" ϵ, such that $t_b-t_a = N\epsilon$. Defining[4] x_ℓ as the positions of the particle at times $t_a+\ell\epsilon$, $\ell=0,1,2,...N$, one possible path between $x_0=x_a$ and $x_N=x_b$ can be formed by joining a given set of x_ℓ's by line segments. All such paths can be generated by varying each x_ℓ for $\ell=1,2,...N-1$ over the real numbers. Thus the propagator generated by all paths joining initial and final states is,

$$K(b,a) = \lim_{\substack{\epsilon\to 0\\ N\to\infty}} \int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}S[x(t)]} dx_1 dx_2 \ldots dx_{N-1} \left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N}{2}} , \qquad \textbf{(2)}$$

where in the $\lim_{\substack{\epsilon\to 0\\ N\to\infty}} N\epsilon \equiv T \equiv t_b - t_a$. The endpoints, $x_0 = x_a$ and $x_N = x_b$, are fixed, while the intermediate positions x_ℓ assume all real values. The factor $\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N}{2}}$ in Eq.(2) properly normalizes[4] the propagator so that $\lim_{\epsilon\to 0} K(x(t+\epsilon),x(t)) = \delta(x),$ where $\delta(x)$ is the Dirac delta function.

III. The One-Dimensional Oscillator

Consider a particle of mass m in a one-dimensional harmonic oscillator potential $U=\frac{1}{2} m\omega^2 x^2$. The action can be expressed[4,8] as the limit of a Riemann sum in terms of the integration variables $x_1, x_2, \ldots, x_{N-1}$,

$$S[x(t)] = \int_{t_a}^{t_b} L[x(t)]\ dt = \sum_{\ell=1}^{N} \left[\frac{1}{2}m \left(\frac{x_\ell - x_{\ell-1}}{\epsilon}\right)^2 \epsilon - U_\ell\ \epsilon\right] . \qquad \textbf{(3)}$$

Note that the kinetic energy at $t_a+\ell\epsilon$ has been written in terms of the change in the position over the time interval ϵ, i.e. in terms of the mean velocity. The potential energy U_ℓ must correspond to the position of the particle within that same time-interval, i.e. between x_ℓ and $x_{\ell+1}$. The exact position is a matter of choice since eventually we will let ϵ go to zero. Departing from the Fourier Transform approach of Feynman and Hibbs[4] , we choose to write U_ℓ in a natural way, $U_\ell = U(x_\ell) = \frac{1}{2}\omega^2 x_\ell^2$, and compute the integration directly. At this point we could insert Eq.(3)

into Eq.(2) and start the integration process. However, we make use of a very helpful transformation[4] of variables,

$$y(t) = x(t) - \chi(t), \tag{4}$$

where χ(t) represents the path taken by the classical particle and y(t) represents the deviation of the path x(t) from χ(t). For the SHO the classical path can be expressed as

$$\chi(t) = \frac{x_b \sin[\omega(t - t_a)] + x_a \sin[\omega(t_b - t)]}{\sin[\omega(t_b - t_a)]}, \tag{5}$$

which makes clear that $y(t_a) = y(t_b) = 0$, i.e., x(t) must pass through x_a at t_a and x_b at t_b. As Feynman and Hibbs[4] demonstrate for the case of any Hamiltonian quadratic in x and $\dot{x}$ this transformation allows separation of the propagator into two factors,

$$K(b,a) = e^{\frac{i}{\hbar} S_{cl}} \int_0^0 e^{\frac{i}{\hbar} S[y(t)]} \hat{D}[y(t)] . \tag{6}$$

The limits of integration should not be taken literally; they are supposed to remind the reader that for all paths, y(t) is zero at the endpoints. The classical action S_{cl} can be expressed[4] as

$$S_{cl} = \frac{\omega}{2\sin(\omega T)} [(x_a{}^2 + x_b{}^2)\cos(\omega T) - 2x_a x_b]. \tag{7}$$

It is the second factor, the path integral in Eq.(6), that presents computational difficulties.

IV. Computation of $\int_0^0 e^{\frac{i}{\hbar} S[y(t)]} \hat{D}[y(t)]$

The path integral in Eq.(6) can now be written[4] in terms of the coordinate y(t) as

$$\lim_{\substack{\epsilon \to 0 \\ N \to \infty}} \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{\frac{N}{2}} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{\frac{im}{2\hbar\epsilon} \sum_{i=1}^{N} [(y_i - y_{i-1})^2 - \omega^2 \epsilon^2 y_i^2]} dy_1 dy_2 \ldots dy_{N-1}, \qquad \textbf{(8)}$$

where $y_o = y(t_a) = 0$ *and* $y_N = y(t_b) = 0$. The innermost integration in Eq.(8), i.e. over the variable $y_{1,}$ involves only those terms in the sum which contain y_1; all others are treated as constants and can be factored out of the integration. Thus the innermost integral in Eq.(8) is

$$\int_{-\infty}^{\infty} e^{\frac{im}{2\hbar\epsilon} [(y_2 - y_1)^2 + (y_1 - y_0)^2 - \omega^2 \epsilon^2 y_1^2]} dy_1 . \qquad \textbf{(9)}$$

This integral is readily solved by completing the square in the exponent and by choosing a suitable substitution of variables yielding

$$C_1 \left(\frac{m}{2\pi i \hbar \epsilon} \right)^{-\frac{1}{2}} e^{\frac{im}{2\hbar\epsilon} [(y_2^2 + y_0^2) - \frac{1}{\gamma}(y_2 + y_0)^2]} , \qquad \textbf{(10)}$$

where $C_1 \equiv \sqrt{\frac{1}{\gamma}}$ and where

$$\gamma \equiv 2 - \frac{(\omega T)^2}{N^2} \ . \qquad \textbf{(11)}$$

The second innermost integration in Eq.(8), involving y_2, can now be written,

$$C_1 \left(\frac{m}{2\pi i\hbar\epsilon} \right)^{-\frac{1}{2}} \int_{-\infty}^{\infty} e^{\frac{im}{2\hbar\epsilon}[(y_3 - y_2)^2 - \omega^2\epsilon^2 y_2^2]} \ e^{\frac{im}{2\hbar\epsilon}\ [(y_2{}^2 + y_0{}^2) \ - \ \frac{1}{\gamma}(y_2 + y_0)^2]} \ dy_2 \ . \qquad \textbf{(12)}$$

This integration yields

$$C_2 \left(\frac{m}{2\pi i\hbar\epsilon} \right)^{-\frac{1}{2}} C_1 \left(\frac{m}{2\pi i\hbar\epsilon} \right)^{-\frac{1}{2}} e^{\frac{im}{2\hbar\epsilon}\left[\left(y_3{}^2 + (1 - \frac{1}{\gamma})\ y_0{}^2 \right) - \frac{1}{\gamma - \frac{1}{\gamma}}(y_3 + \frac{1}{\gamma} y_0)^2 \right]} \ , \qquad \textbf{(13)}$$

where $C_2 \equiv \sqrt{\frac{1}{\gamma - \frac{1}{\gamma}}}$. This procedure is repeated for every y_ℓ up to y_{N-1}. After a few integrations a pattern emerges. The pth constant, C_p, can be written as

$$C_p \ = \ \sqrt{\frac{1}{\gamma - \frac{1}{\gamma - \frac{1}{\gamma - \frac{1}{\ddots_p}}}}} \ , \qquad \textbf{(14)}$$

where the symbol $\ddots_p$ indicates that the pattern continues to the pth denominator.

The radicand is recognized as the pth partial approximate of the continued fraction,

$$C_\infty^2 = \cfrac{1}{\gamma - \cfrac{1}{\gamma - \cfrac{1}{\gamma - \cfrac{1}{\ddots}}}} \quad , \tag{15}$$

where the fraction extends to an infinite number of denominators. After the N-1 integrations, the result multiplied by the normalization factor, $\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N}{2}}$, in Eq.(2) is,

$$C_{N-1}C_{N-2}...C_1\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{-\frac{N-1}{2}} e^{\frac{im}{2\hbar\epsilon}\left[\left(y_N{}^2+F_{N-1}\,y_0{}^2\right)-C_{N-1}^2\left(y_N+\prod_{k=1}^{N-1}C_k^2\,y_0\right)^2\right]}\left(\frac{m}{2\pi i\hbar\epsilon}\right)^{\frac{N}{2}} \quad , \tag{16}$$

where F_{N-1} is a finite function of a finite number of the partial approximates of the continued fraction $C_\infty{}^2$. Both y_0 and y_N are zero, so that $e^{\frac{im}{2\hbar\epsilon}\left[\left(y_N{}^2+F_{N-1}\,y_0{}^2\right)-C_{N-1}^2\left(y_N+\prod_{k=1}^{N-1}C_k^2\,y_0\right)\right]}$ reduces to unity prior to taking the limit in Eq.(8). Substitution of the limit of Eq.(16) into Eq.(6), yields for the propagator,

$$K(b,a) = \left(\frac{m}{2\pi i\hbar T}\right)^{1/2} e^{\frac{i}{\hbar}S_{cl}} \lim_{N\to\infty}\left[\,N\prod_{p=1}^{N-1}C_p^2\,\right]^{1/2}, \tag{17}$$

where we have used ϵ=T/N to replace the ϵ appearing in the two radicals appearing in Eq.(16). Writing the partial approximates $C_p{}^2$ in terms of γ makes clear the continued fraction structure of the SHO propagator,

$$K(b,a) = \left(\frac{m}{2\pi i\hbar T}\right)^{½} e^{\frac{i}{\hbar}S_{cl}} \lim_{N\to\infty} \left[N \; \frac{1}{\gamma} \; \frac{1}{\gamma - \frac{1}{\gamma}} \; \frac{1}{\gamma - \frac{1}{\gamma - \frac{1}{\gamma}}} \; \cdots \; \frac{1}{\gamma - \frac{1}{\gamma - \frac{1}{\gamma - \frac{1}{\ddots_{N-1}}}}} \right]^{½} . \qquad \textbf{(18)}$$

Evaluation of the limit in Eq.(18) is not trivial because γ is a function of N (See Eq.(11)). In the following section of this paper we show that this limit is $\frac{\omega T}{\sin(\omega T)}$.

V. The Limit of the Product of Partial Approximates

We can convert the p[th] partial approximate of any continued fraction to a rational function of the form $\frac{A_p}{B_p}$, the numerator and denominator of which are given by well known recursion relations[9]. For the continued fraction C_∞^2, the recursive relations yield,

$$C_p^2 \;=\; \frac{A_p}{B_p} \;=\; \frac{\gamma A_{p-1} - A_{p-2}}{\gamma B_{p-1} - B_{p-2}} . \qquad \textbf{(19)}$$

The starting conditions for the recursions are $A_{-1} = -1$, $A_0 = 0$ and $B_{-1} = 0$, $B_0 = 1$. Examination of Eq.(19) with the starting conditions reveals that B_p is equal to A_{p+1} for all p. Thus in the calculation of the finite product of partial approximates of C_∞^2 from p=1 to p=N, each successive numerator A_p is canceled by the previous denominator B_{p-1}, so that the finite product is simply

$\frac{A_1}{B_N} = \frac{1}{B_N}$. Now Eq.(17 or 18) can be rewritten as,

$$K(b,a) = \left(\frac{m}{2\pi i\hbar T}\right)^{½} e^{\frac{i}{\hbar}S_{cl}} \lim_{N\to\infty}\left[\frac{N}{B_N}\right]^{½} . \tag{20}$$

We used the symbolic manipulator MAPLE[10] to solve the recursion relation satisfied by the B_p, i.e., $B_p = \gamma B_{p-1} - B_{p-2}$ yielding,

$$B_p = 2\frac{i\left(\frac{2}{\gamma + i\sqrt{4-\gamma^2}}\right)^p}{\sqrt{4-\gamma^2}(\gamma + i\sqrt{4-\gamma^2})} + 2\frac{i\left(-\frac{2}{-\gamma + i\sqrt{4-\gamma^2}}\right)^p}{\sqrt{4-\gamma^2}(-\gamma + i\sqrt{4-\gamma^2})} . \tag{21}$$

The right-hand side of this relationship reduces to the real numbers for $N^2 > (\omega T)^2$, i.e., N sufficiently large that γ is real. Again using MAPLE[10], the limit of $\frac{B_N}{N}$ has the intriguingly simple form of the sinc function,

$$\lim_{N\to\infty}\frac{B_N}{N} = \frac{\sin(\omega T)}{\omega T} \equiv sinc(\omega T). \tag{22}$$

We note that the infinite product in our development plays a role similar to that of the function G in Eq.(52) of the paper by Marshall and Pell[7]. The partial approximates C_p^2 play a role analogous to that of the determinants D_p^α of the matrices G_p^α appearing in Eq.(3.10) in the work by Junker and Leschke[11]. In fact, Junker and Leschke[11] show that the D_p^α satisfy the same recursion relationship as satisfied by the B_p and that the D_p^α are related to the sine, cosh, and sinh functions in ways similar to, but different from, our Eq.(22).

Using the limit from Eq.(22) in Eq.(20), we arrive at the final form for the propagator for the SHO,

$$K(b,a) = \left(\frac{m\omega}{2\pi i\hbar\sin(\omega T)}\right)^{\frac{1}{2}} e^{\frac{im\omega}{2\hbar\sin(\omega T)}\left[(x_a^2+x_b^2)\cos(\omega T) - 2x_a x_b\right]} . \qquad \textbf{(23)}$$

This expression agrees with the result of Feynman and Hibbs[4] and others[7,11,12,13,14] obtained by different methods. Given the propagator, reclaiming wave functions and energy spectrum for the SHO can be accomplished without recourse to the Schrödinger's equation[12,13]. Of course, developing the Schrödinger's equation from the propagator is a worthwhile exercise[4].

V. Conclusion

We believe that the use of MAPLE[10] (or any other symbolic manipulator program) has greatly simplified our development of the SHO propagator and that most undergraduates can follow our approach. We emphasize that the crucial step in our approach is the evaluation of the limit of the product of partial approximates of the continued fraction C_∞^2, viz.,

$$\lim_{N\to\infty}\left[N\prod_{p=1}^{N}C_p^2\right]^{\frac{1}{2}} = \frac{\omega T}{\sin(\omega T)} \equiv \frac{1}{sinc(\omega T)}. \qquad \textbf{(24)}$$

As far as we know, this representation of the reciprocal of the sinc function has not been reported in the literature on continued fractions[9,15,16].

Acknowledgments

The authors are very grateful for the careful readings of this manuscript by the Referees and by M.D. Westmoreland, who also provided the demonstration that the form for the B_p in Eq.(21) reduces to a real quantity for real γ.

References

[a)]This work supported in part by Grant #P116B30079 from the Department of Education (FIPSE Program) and a Grant from the W.M. Keck Foundation.

[1]N.D. Mermin, "Quantum mysteries refined", Am. J. Phys. **62**, 880-886 (1994).

[2]T.F. Jordan, "Quantum mysteries explored", Am. J. Phys. **62**, 874-880 (1994).

[3]R. Jones, "Resource Letter CD-1: Causality and determinism in physics", Am. J. Phys. **64**, 208-215 (1996) and references therein.

[4]R.P. Feynman and A.R. Hibbs, **Quantum Mechanics and Path Integrals**, (McGraw-Hill, New York, NY, 1965).

[5]P.A.M. Dirac, **Quantum Mechanics**, (Oxford University Press, Amen House, London, 1958).

[6] A. Inomata, H. Kuratsuji and C.C. Gerry, "Path Integrals and Coherent States of SU(2) and SU(1,1)", (World Scientific, Singapore, 1992).

[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]R.P. Feynman, "Space-Time Approach to Non-Relativistic Quantum Mechanics", Rev. Mod. Phys. **20**, 367-387 (1948).

[9]H.S. Wall, **Analytic Theory of Continued Fractions**, (Chelsea Publishing Co., New York, NY, 1973).

[10]**MAPLE**, Version V, Release 4, (Waterloo Maple Software, Waterloo, ON, 1996).

[11]G. Junker and H. Leschke, "Remarks on the quasi-classical propagator of area-preserving maps", Physica D, **56**, 135-150 (1992).

[12]L.S. Schulman, **Techniques and Applications of Path Integration**, (Wiley-International, New York, 1981).

[13]H. Kleinert, **Path Integrals in Quantum Mechanics, Statistics, and Polymer Physics**, (World Scientific, Singapore, 1990).

[14]P.K. MacKeown, "Evaluation of Feynman path integrals by Monte Carlo methods", Am. J. Phys. **53**, 880-885 (1985).

[15]Oskar Perron, **Die Lehre von den Kettenbruechen**, (Chelsea Publishing Co., New York, NY, 1950).

[16]A.Y. Khinchin, **Continued Fractions**, (University of Chicago Press, Chicago, IL, 1964).