Quantum roll: A study of the long-time behavior of the finite-element method

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Using the method of finite elements we investigate the quantum behavior of a particle starting in an unstable equilibrium at the top of a potential hill and rolling down. In order to study the numerical accuracy of the method for large times we consider the exactly solvable model with $V(q)=-\frac{1}{2}q^2$ and an initial Gaussian wave function at $t=0$, $\psi(q)\propto\exp(-\frac{1}{2}q^2)$ so that the initial state $|0\rangle$ has $\langle 0|q^2|0\rangle=\langle 0|p^2|0\rangle=\frac{1}{2}$. We study the accuracy of the large-time approximations to $\langle 0|q^2(t)|0\rangle$ based upon single finite elements of degree n. The Taylor series is exact up to t^{2n} and even the coefficient of t^{2n+2} is a very accurate representation of the exact coefficient. We then consider the convergence properties of the (N,n) approximations consisting of N iterations of the finite element of degree n. For these approximations the corrections to the Taylor-series coefficients in higher orders vanish as N^{-2n}.

I. INTRODUCTION

One of the outstanding problems in field theory is that there are no nonperturbative methods for studying processes in real time. Monte Carlo techniques, which have come to be an important tool in understanding field theory, require calculation in Euclidean space or at finite temperatures so that a probabilistic interpretation can be provided to the path integral. As yet no one has found a practical way for evaluating Minkowski-space path integrals. An interesting alternative to the path integral is provided by the Heisenberg operator equations of motion, which describe the time evolution of quantum-mechanical operators. Many questions can be answered by studying the time evolution of the Heinsenberg operators. For example, in the early universe one would like to understand how a field rolls down a relatively flat potential or tunnels from a false vacuum into a true vacuum. If the initial state is Gaussian all the matrix elements of $\phi(t=0),\pi(t=0)$ are easy to calculate. If one can solve for $\phi(t),\pi(t)$ in terms of $\phi(0),\pi(0)$ by a time iteration scheme that preserves the canonical commutation relation, then one can calculate $\langle 0|\phi^n(t)|0\rangle$ and watch in real time the average motion of the field in a dynamical situation. The other alternative is to consider functional Schrödinger equations and try to watch the time development of the initial wave functional. We feel that the Heisenberg approach is more feasible if we are interested in knowing only a few selected matrix elements.

Recently two methods have been proposed for iterating the Heisenberg equations in a canonical fashion: the implicit finite-element method of Bender *et al.*[1–5] and the explicit method of Moncrief.[6] In both methods one is dealing with operators so the iteration methods are symbolic. One obtains at the Nth-time iteration $\pi_N=f_N(\pi_0,\phi_0)$, $\phi_N=g_N(\pi_0,\phi_0)$, and the calculations must be done exactly algebraically. Numerical evaluations enter only at the stage where matrix elements of π_N and ϕ_N must be obtained in terms of the matrix elements of ϕ_0,π_0 in the initial state. Since we want to study the long-time behavior of quantum processes it is important to understand whether one needs a low-order scheme with many iterates or a high-order scheme with a few iterates, or whether a moderate-order scheme with a moderate number of iterations is optimum to ensure that the algebra be tractable and the accuracy reasonable. To illuminate such questions we study a solvable model, a Gaussian wave packet "rolling" down a quantum-mechanical hill, where $V(q)=-q^2/2$.

II. THE FINITE-ELEMENT APPROXIMATION

As a laboratory for studying the long-time behavior of the finite-element approximation in quantum mechanics, we consider the inverted, one-dimensional harmonic oscillator,

$$H=\frac{p^2}{2}-\frac{q^2}{2}\,. \tag{1}$$

This model has the virtue of being exactly solvable, but the operator $q(t)$ is not periodic, so we can study its evolution for large times. Previous work[1–5] on the finite-element approach to quantum mechanics has concentrated on the short-time behavior, as, for example, in the extraction of the level spacings for the anharmonic oscillator,[5] by identifying the first few terms in the Taylor expansion

of $e^{i\omega t}$. In exploring the large-t behavior of the finite-element approximation we have several goals in mind: (1) to examine the limits of validity of a single nth-degree finite element, (2) to study the convergence of repeated iterates of the nth-degree finite element, and (3) to compare the accuracy of high-order iterates of low-degree finite elements with low-order iterates of high-degree finite elements.

The general finite-element approach was discussed in detail in Ref. 5. We solve Hamilton's equations of motion, here

$$\dot{q}=p,\ \dot{p}=q\ , \tag{2}$$

by dividing the time interval from 0 to t into N steps of length $h=t/N$. On each interval we represent the operators p and q by polynomials in the time with operator coefficients:

$$p(t)=\sum_{k=0}^{n} a_k(x/h)^k\ ,$$
$$q(t)=\sum_{k=0}^{n} b_k(x/h)^k\ , \tag{3}$$

where x is a local variable, $0\leq x\leq h$. We determine the $2n+2$ operators a_k and b_k by imposing continuity at the boundaries of the intervals and by applying the two equations of motion n times on each interval, at the Gauss points given by the zeros of the nth Legendre polynomial $P_n(-1+2x/h)$. At the initial time we impose the canonical commutation relation

$$[q(0),p(0)]=i\ . \tag{4}$$

As demonstrated in Ref. 5, this procedure guarantees that the canonical commutation relations are preserved exactly at each lattice site. Moreover, for the specific examples discussed in Refs. 3 and 5, the relative error is of order N^{-2n}, just as in classical applications.[5,7]

For illustration we carry out this procedure for a single linear finite element. We rewrite Eqs. (3) as

$$q(t)=q_0\left[1-\frac{t}{h}\right]+\frac{t}{h}q_1\ ,$$
$$p(t)=p_0\left[1-\frac{t}{h}\right]+\frac{t}{h}p_1\ . \tag{5}$$

We impose the equations of motion (2) at the Gauss point $t/h=\frac{1}{2}$:

$$\frac{q_1-q_0}{h}=\frac{p_1+p_0}{2}\ ,$$
$$\frac{p_1-p_0}{h}=\frac{q_1+q_0}{2}\ . \tag{6}$$

Regarding p_0 and q_0 as known operators, we solve for p_1 and q_1, the finite-element approximations to the momentum and position operators at time $t=h$:

$$p_1=\frac{(h^2+4)p_0+4hq_0}{4-h^2}\ ,$$
$$q_1=\frac{(h^2+4)q_0+4hp_0}{4-h^2}\ . \tag{7}$$

Note that Eqs. (7) possess singularities at $h=\pm 2$, which limit the domain of applicability of these solutions. The existence of such singularities is a general feature that will occur in the higher-degree finite-element approximations. The occurrence of these singularities is a result of the implicit nature of the differencing scheme embodied in (6), which is a system of equations that must be simultaneously solved for the operators p_1 and q_1 and is not specific to the inverted oscillator potential

We have explicitly solved for p_1 and q_1 using finite elements of degree $n=1$, 2, 3, 4, and 5. The denominators are of the form $D_n(h)D_n(-h)$ where $D_n(h)$ is the polynomial of degree n, given in Table I. The distance d_n to the nearest singularity (also shown in Table I) controls the range in h over which the single-finite-element approximation is valid.

We observe that for odd n the nearest zero of $D_n(h)$ lies on the negative real axis, while for even n there are no real zeros. We also note that all of the singularities lie in a rather narrow annulus of outer radius comparable to d_n.

These observations can be extended and made rigorous as follows. Note that $D_n(h)$ can be written as

$$D_n(h)=\sum_{k=0}^{n}\frac{h^k(2n-k)!}{k!(n-k)!}=\sum_{l=0}^{n}\frac{h^{n-l}(n+l)!}{l!(n-l)!}$$
$$=\frac{h^{n+1/2}e^{h/2}}{\sqrt{\pi}}K_{n+1/2}(\tfrac{1}{2}h)\ ,$$

where $K_\nu(z)$ is the modified Bessel function of the third kind.[8] One can, therefore, write $D_n(h)$ in many different closed forms, for example,

$$D_n(h)=\frac{h^n}{n!}\int_0^\infty dt\, e^{-t}t^n(1+t/h)^n\ .$$

They satisfy the recurrence relation

TABLE I. For the single-finite-element approximation of degree n, the solutions q_1 and p_1 have denominators of the form $D_n(h)D_n(-h)$. The range over which the finite-element approximation can be used is controlled by the magnitude d_n of the zero of $D_n(h)$ nearest to the origin.

n	$D_n(h)$	d_n
1	$h+2$	2.0
2	$h^2+6h+12$	3.464
3	$h^3+12h^2+60h+120$	4.644
4	$h^4+20h^3+180h^2+840h+1680$	6.047
5	$h^5+30h^4+420h^3+3360h^2+15\,120h+30\,240$	7.293

$$D_{n+1}(h)=(4n+2)D_n(h)+h^2D_{n-1}(h)\ .$$

Using known results[8,9] on the zeros of $K_\nu(z)$ one can discuss the zeros of $D_n(h)$. In general, it follows that $D_n(h)$ has only simple zeros and has no zeros in the right-half plane, $|\arg h|\le\frac{1}{2}\pi$, and that $D_n(h)$ and $D_{n+m}(h)$, $m=1,2,\ldots$, have no common zero. For large odd n the zero of $D_n(h)$ nearest the origin occurs[9] at $d_n\sim 0.662\,74(2n+1)$. This asymptotic estimate has a relative error of only -0.6% at $n=1$. For even n this estimate is roughly correct. The rms distance to the zeros of $D_n(h)$, $[D_n(0)]^{1/n}\sim 4n/e$, is asymptotically larger than d_n by only 11%.

To make numerical comparisons among the different finite-element approximations, we consider an initial state consisting of a Gaussian centered at the origin,

$$\begin{aligned}&\langle q_0\rangle=\langle p_0\rangle=0\ ,\\ &\langle q_0^2\rangle=\langle p_0^2\rangle=\tfrac{1}{2}\ .\end{aligned}\tag{8}$$

The exact continuum solution of the equations of motion gives

$$\langle q^2(t)\rangle=\tfrac{1}{2}+\sinh^2 t=\tfrac{1}{2}+t^2+\frac{t^4}{3}+\frac{2t^6}{45}+\frac{t^8}{315}+\frac{2t^{10}}{14\,175}+\frac{2t^{12}}{467\,775}+\cdots\ .\tag{9}$$

We find for a single nth-degree finite element agreement with this exact result through order t^{2n}:

$$\begin{aligned}
n=1:&\ \langle q_1^2\rangle=\tfrac{1}{2}+t^2+(\tfrac{1}{3}+\tfrac{1}{6})t^4+\cdots\ ;\\
n=2:&\ \langle q_1^2\rangle=\tfrac{1}{2}+t^2+\tfrac{1}{3}t^4+(\tfrac{2}{45}-\tfrac{1}{360})t^6+\cdots\ ;\\
n=3:&\ \langle q_1^2\rangle=\tfrac{1}{2}+t^2+\tfrac{1}{3}t^4+\tfrac{2}{45}t^6\\
&\qquad+(\tfrac{1}{315}+\tfrac{1}{50\,400})t^8+\cdots\ ;\\
n=4:&\ \langle q_1^2\rangle=\tfrac{1}{2}+t^2+\tfrac{1}{3}t^4+\tfrac{2}{45}t^6+\tfrac{1}{315}t^8\\
&\qquad+(\tfrac{2}{14\,175}-\tfrac{1}{12\,700\,800})t^{10}+\cdots\ ;\\
n=5:&\ \langle q_1^2\rangle=\tfrac{1}{2}+t^2+\tfrac{1}{3}t^4+\tfrac{2}{45}t^6+\tfrac{1}{315}t^8+\tfrac{2}{14\,175}t^{10}\\
&\qquad+(\tfrac{2}{467\,775}+\tfrac{1}{5\,029\,516\,800})t^{12}+\cdots\ .
\end{aligned}\tag{10}$$

Note that the nth-degree finite-element approximation not only agrees with the exact result (9) through order t^{2n}, but the error in the coefficient of $t^{2(n+1)}$ gets rapidly smaller as n increases. A similar phenomenon occurs for the higher coefficients. This is the reason the finite-element method works much better than might be expected. This is indicated in Table II.

TABLE II. The single-finite-element approximation of degree n for $\langle q_1^2\rangle$ agrees with the exact result through the term t^{2n} in the Taylor series. The next term, t^{2n+2}, in the Taylor series for the approximation has a coefficient that closely approximates the correct coefficient. As shown in this table the relative error in the coefficient of t^{2n+2} decreases dramatically with increasing n.

n	Relative error in coefficient of $t^{2(n+1)}$
1	$+5\times10^{-1}$
2	-6.25×10^{-2}
3	$+6.25\times10^{-3}$
4	-5.58×10^{-4}
5	$+4.65\times10^{-5}$

III. THE ITERATED FINITE-ELEMENT APPROXIMATION

We now turn to iterated finite elements to pursue the long-time development of $\langle q^2(t)\rangle$. We note that the equations of motion can be diagonalized by introducing α and β defined by

$$q=\frac{1}{\sqrt{2}}(\alpha+\beta),\quad p=\frac{1}{\sqrt{2}}(\alpha-\beta)\ ,\tag{11}$$

which give

$$\dot\alpha=\alpha,\quad \dot\beta=-\beta\ .\tag{12}$$

We represent α and β by nth-degree polynomials in x on each interval and impose (12) at the Gauss points. For one finite element we find

$$\alpha_1=\alpha_0F_n(h),\quad \beta_1=\beta_0/F_n(h)\ ,\tag{13}$$

where

$$F_n(h)=\frac{D_n(h)}{D_n(-h)}\ ,\tag{14}$$

and $D_n(h)$ is the polynomial in h of order n given above and in Table I.

If we express α_0 and β_0 in terms of p_0 and q_0, the operators q_N and p_N at the Nth lattice sites are

$$\begin{aligned}&q_N=\tfrac{1}{2}q_0(F_n^{\,N}+F_n^{\,-N})+\tfrac{1}{2}p_0(F_n^{\,N}-F_n^{\,-N})\ ,\\ &p_N=\tfrac{1}{2}p_0(F_n^{\,N}+F_n^{\,-N})+\tfrac{1}{2}q_0(F_n^{\,N}-F_n^{\,-N})\ ,\end{aligned}\tag{15}$$

which we can compare to the continuum answer

$$\begin{aligned}&q(t)=q_0\cosh t+p_0\sinh t\ ,\\ &p(t)=p_0\cosh t+q_0\sinh t\end{aligned}\tag{16}$$

by making the replacement $Nh=t$.

Once again we will examine $\langle q_N^2\rangle$ with the initial condition (8) and compare with the continuum result (9). The (N,n) approximant is given by

$$\langle q_N^2\rangle=\frac{1}{4}\left\{\left[F_n\left[\frac{t}{N}\right]\right]^{2N}+\left[F_n\left[\frac{-t}{N}\right]\right]^{2N}\right\}.\tag{17}$$

It is interesting to write out the first few terms in the Taylor expansion of this function:

$$n=1:\ \langle q_N{}^2\rangle=\tfrac{1}{2}+t^2+\frac{1}{3}\left[1+\frac{1}{2N^2}\right]t^4+\cdots\ ;$$

$$n=2:\ \langle q_N{}^2\rangle=\tfrac{1}{2}+t^2+\tfrac{1}{3}t^4+\frac{2}{45}\left[1-\frac{1}{16N^4}\right]t^6+\cdots\ ;$$

$$n=3:\ \langle q_N{}^2\rangle=\tfrac{1}{2}+t^2+\tfrac{1}{3}t^4+\tfrac{2}{45}t^6+\frac{1}{315}\left[1+\frac{1}{160N^6}\right]t^8+\cdots\ ; \tag{18}$$

$$n=4:\ \langle q_N{}^2\rangle=\tfrac{1}{2}+t^2+\tfrac{1}{3}t^4+\tfrac{2}{45}t^6+\tfrac{1}{315}t^8+\frac{2}{14\,175}\left[1-\frac{1}{1792N^8}\right]t^{10}+\cdots\ ;$$

$$n=5:\ \langle q_N{}^2\rangle=\tfrac{1}{2}+t^2+\tfrac{1}{3}t^4+\tfrac{2}{45}t^6+\tfrac{1}{315}t^8+\tfrac{2}{14\,175}t^{10}+\frac{2}{467\,775}\left[1+\frac{1}{21\,504N^{10}}\right]t^{12}+\cdots\ .$$

We note that the first term that disagrees with the continuum result (9), $O(t^{2n+2})$, has a relative error of order N^{-2n}, with an exponentially decreasing coefficient (compare Table II).

In Table III we compare the various (N,n) approximations for a large value of t, $t=10$, for which the continuum result $\langle q^2(10)\rangle=1.212\,912\,988\,524\,474\times10^8$. We note that for n odd, the pole in q_N is crossed for low N, and $\langle q_N{}^2\rangle$ converges to the continuum result from above. For even n, the poles lie off the real axis, and $\langle q_N{}^2\rangle$ converges to the continuum result from below.

Recently, Moncrief[6] has proposed an explicit differencing scheme

$$q_{k+1}=q_k+hp_k-\tfrac{1}{2}h^2\frac{dV}{dq_k}(q_k)\ ,$$
$$p_{k+1}=p_k-\tfrac{1}{2}h\frac{dV(q_k)}{dq_k}-\tfrac{1}{2}h\frac{dV(q_{k+1})}{dq_{k+1}}\ . \tag{19}$$

These equations are canonical in that they preserve the equal-time commutation relations. Because they are explicit rather than implicit, they do not have the large-time singularities of the finite-element method displayed in Table I. On the other hand, it is not clear how to generalize this scheme to higher degree. With Moncreif's scheme, for the Hamiltonian (1), we obtain at time step N

$$q_N=\tfrac{1}{2}q_0\{[f(h)]^N+[f(-h)]^N\}+\tfrac{1}{2}p_0\left[1+\frac{h^2}{4}\right]^{-1/2}\{[f(h)]^N-[f(-h)]^N\}\ , \tag{20}$$

where

$$f(h)=1+h\left[1+\frac{h^2}{4}\right]^{1/2}+\tfrac{1}{2}h^2\ . \tag{21}$$

TABLE III. At $t=10$ the exact result is $\langle q^2(10)\rangle=1.212\,912\,988\,524\,474\times10^8$. We display the results of applying the nth-degree finite-element approximation iterated N times. For convenience in comparison we underline those digits that agree with the exact result. Entries marked * must be disregarded because the magnitude of the pole of the finite-element approximation (see Table I) falls within the range $[0,10/N]$ for that iteration order. The last six entries, marked $n=M$, are the results of iterating the explicit differencing scheme of Moncrief (see text and Ref. 6). Note that this scheme, which does not have singular points, here works somewhat slightly better than the linear ($n=1$) finite element.

n	N	$\langle q_N{}^2\rangle$
1	1	*
1	2	*
1	3	*
1	5	*
1	10	8.72×10^8
1	100	$\underline{1.2}33\times10^8$
2	1	*
2	2	*
2	3	*
2	5	7.06×10^7
2	10	$\underline{1.}18\times10^8$
2	100	$\underline{1.212\,910}\times10^8$
3	1	*
3	2	*
3	3	$\underline{1.}86\times10^8$
3	5	$\underline{1.2}31\times10^8$
3	10	$\underline{1.213}2\times10^8$
3	100	$\underline{1.212\,912\,988}\,76\times10^8$
4	1	*
4	2	6.84×10^7
4	3	$\underline{1.}19\times10^8$
4	5	$\underline{1.212}\,64\times10^8$
4	10	$\underline{1.212\,912}\,01\times10^8$
4	100	$\underline{1.212\,912\,988\,524\,464}\times10^8$
5	1	*
5	2	$\underline{1.2}55\times10^8$
5	3	$\underline{1.213}\,4\times10^8$
5	5	$\underline{1.212\,915}\,7\times10^8$
5	10	$\underline{1.212\,912\,99}0\,9\times10^8$
5	100	$\underline{1.212\,912\,988\,524\,476}\times10^8$
M	1	1.35×10^3
M	2	7.52×10^4
M	3	7.75×10^5
M	5	8.48×10^6
M	10	5.15×10^7
M	100	$\underline{1.201}\,4\times10^8$

This implies, for our initial conditions (8),

$$\langle q_N{}^2\rangle=\left[\tfrac{1}{4}\{[f(h)]^{2N}+[f(-h)]^{2N}\}+\frac{h^2}{32}\{[f(h)]^N+f(-h)^N\}^2\right]\left[1+\frac{h^2}{4}\right]^{-1}\ . \tag{22}$$

The first few terms in the Taylor expansion of (22) are ($t=Nh$)

$$\langle q_N{}^2\rangle = \tfrac{1}{2}+t^2+\frac{1}{3}\left[1-\frac{5}{8N^2}\right]t^4+\cdots . \tag{23}$$

For small t, Moncrief's scheme is less accurate than the linear finite element [see (18)].

In Table III we also display numerical results for $\langle q_N{}^2\rangle$ at $t=10$ as predicted by the Moncrief scheme; for large t this scheme is somewhat more accurate than linear finite elements.

IV. CONCLUSIONS

We have studied the large-time behavior of the finite-element approximation to quantum mechanics for a simple explicitly solvable model of an inverted harmonic potential. We believe that the general qualitative features will persist in nonlinear problems, which are currently under investigation.

The nth-degree finite-element solution has $2n$ complex singularities in mirror pairs in the t plane, all occurring in a narrow annulus about the origin. For odd n two of these singularities occur on the real axis. The presence of these singularities implies that there is a value of t (the magnitude of the distance to the nearest singularity) beyond which one cannot sensibly extend a single-finite-element approximation. As the degree of the finite element increases, the pole nearest the origin moves out, so that finite-element approximations of higher degree have a larger range of t over which they can be applied.

The single-finite-element approximation of degree n agrees exactly with the Taylor series of the continuum solution through the term t^{2n} and the coefficient of the t^{2n+2} term rapidly converges to the continuum result as n increases.

Each of the degree-n finite-element solutions can be iterated N times to carry the solution to large time. In the N-fold iterated nth-degree finite-element solution the error in the t^{2n+2} coefficient decreases as N^{-2n}. Moreover, the coefficient of this error term decreases exponentially with n. As a result we were able to extend solutions to very large times with extremely high accuracy by straightforward iteration of the basic one-step solution.

Finally we studied the explicit differencing scheme of Moncreif and found that it is of slightly lower accuracy than the linear finite element at short times and of slightly greater accuracy at long times.

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