Quantum Tunneling Using Discrete-Time Operator Difference Equations

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Canonical discrete-time operator difference equations are introduced as an alternative approach to the numerical solution of a quantum field theory. We apply these techniques to the solution of the operator Heisenberg equations of motion describing the problem of quantum-mechanical tunneling. Our numerical solutions accurately depict the time evolution of $\langle q^n \rangle$ and of a local probability measure.

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As an alternative approach to the numerical solution of a quantum field theory it has recently been proposed[1] that the operator field equations be solved directly by time stepping of the operator on a Minkowski lattice. The canonical operator difference equations can be either implicit, as derived from a finite-element approach,[1] or explicit, as derived from a finite-difference approach.[2] These techniques are canonical in the sense that the iteration scheme exactly preserves the equal-time commutation relations at every lattice point. Furthermore, they lead to a consistent formulation of fermions[3] and of gauge invariance.[4]

Quantum mechanics provides a convenient laboratory for the study of these techniques[5,6] and for the development of them into practical computational tools. In one-dimensional quantum mechanics one obtains operator difference equations on a time lattice as an approximation to the operator Heisenberg equations of motion and these equations provide a nonperturbative method for the study of quantum processes in real time. It seems natural to apply these new computational ideas to quantum tunneling.

Certain aspects of this problem have recently been studied.[7,8] Using the finite-element method Bender *et al.*[7] investigated tunneling in a quartic potential in a one-finite-element approximation and obtained good results for short times. In a second paper Cooper, Milton, and Simmons[8] studied the long-time behavior of the motion of a wave packet in the classically allowed region of an inverted parabolic potential. That study compared the numerical accuracy of various implicit and explicit quantum differencing schemes.

The purpose of this paper is to extend the development of operator-difference techniques to a practical computational scheme for quantum problems. We use an explicit differencing scheme[2] to study the motion of an initial Gaussian wave packet in a degenerate double-well potential.

The continuum Hamiltonian is $H=\frac{1}{2}p^2+V(q)$, where

$$V(q)=4q^2(q-\beta)^2/\beta^2. \tag{1}$$

This potential is symmetric about $q=\frac{1}{2}\beta$ and has approximately harmonic wells centered at $q=0$ and $q=\beta$. Near $q=0$ the approximate potential is $V_{\text{approx}}(q)=4q^2$ whose eigenvalues are $E_n=\sqrt{8}\times(n+\frac{1}{2})$. The normalized ground-state wave function of V_{approx} is

$$\phi_0(q)=(\omega/\pi)^{1/4}\exp(-q^2\omega/2), \tag{2}$$

where $\omega=\sqrt{8}$. We choose ϕ_0 as the initial coordinate-space wave packet, centered at $q=0$ in the left well when $t=0$. If $\omega/2<\beta^2/4$, the barrier height, the particle represented by the wave packet ϕ_0 is classically confined and the wave function tunnels with a frequency determined by the energy splitting of the almost degenerate ground state and first excited state.

We study this tunneling process in the Heisenberg picture by directly solving the Heisenberg equations of motion,

$$\dot{q}(t)=p(t), \quad \dot{p}(t)=-\frac{dV(q)}{dq}, \tag{3}$$

on a discrete time lattice and by measuring matrix elements of appropriate operators in the false vacuum state represented by (2).

The recurrence relations that we use to express the quantum operators at time step $n+1$ in terms of those at time step n are[2]

$$q_{n+1}=q_n+hp_n-\tfrac{1}{2}h^2V'(q_n), \tag{4a}$$

$$p_{n+1}=p_n-\tfrac{1}{2}h[V'(q_n)+V'(q_{n+1})], \tag{4b}$$

where h is the time-lattice spacing Δt and q_n and p_n are the Heisenberg operators on the discrete time lattice. q_n and p_n are accurate approximations to the position

and momentum operators $q(t)$ and $p(t)$ at time $t=nh$, with error of order h^3. This differencing scheme shares with the finite-element method the property that it is canonical; that is, it exactly preserves the equal-time commutation relation $[q_n,p_n]=i$ at every time step (it is a unitary scheme).[2]

The equal-time commutation relation for $n=0$ (that is, $t=0$) allows us to define a Fock space of states $|k\rangle$ such that $a_0|0\rangle=0$, where

$$q_0=(2\omega)^{-1/2}(a_0+a_0^\dagger) \tag{5a}$$

and

$$p_0=i(\tfrac{1}{2}\omega)^{1/2}(a_0^\dagger-a_0). \tag{5b}$$

The coordinate-space representation of $|0\rangle$ is ϕ_0 given in (2). To study tunneling in the Heisenberg picture we calculate

$$F_l(t)=\langle 0|q^l(t)|0\rangle \tag{6a}$$

$$=\int \psi_0^*(x,t)x^l\psi_0(x,t)dx, \tag{6b}$$

where $\psi_0(x,t)$ is the wave packet that evolves from $\psi_0(x,0)=\phi_0(x)$ under the action of the Hamiltonian.

Another quantity of interest is the fractional probability, as a function of time, for the wave packet to remain in the left well; this directly measures the tunneling time. In the Schrödinger picture such a probability measure is

$$P_L(t)=\int_{-\infty}^{\beta/2}\psi_0^*(x,t)\psi_0(x,t)dx. \tag{7}$$

In the Heisenberg picture it is more convenient to measure an operator that has most of its support in the left well. We choose

$$\tilde{P}_L(t)=\langle 0|\beta/(\beta+q^4)|0\rangle, \tag{8}$$

which has behavior quite similar to $P_L(t)$. We find that $\tilde{P}_L(0)=0.97$.

The recurrence relations (4) are attractive because they allow, in principle, an exact symbolic iteration by means of an algebraic-manipulation program such as MACSYMA. One organizes the iterates q_n and p_n, for $n=1,2,\ldots,N$, expressed in terms of the Fock-space operators a and $a^\dagger$, in normal-ordered form. It is then trivial to calculate any matrix element of any polynomial in q_0 and p_0. The replacement $t=h/N$ then produces an approximate Taylor series in t for the matrix elements, exact to order t^2, and converging to the exact Taylor series as N^{-2}, where N is the number of iterations. Because of the nonlinear nature of the equations (4) the algebraic complexity of the iterates grows very rapidly. With our present MACSYMA techniques it is impractical to calculate more than four or five iterates.

Alternatively, one can recognize that finite-dimensional numerical matrices can be used to circumvent the algebraic complexity. Because

$$\langle j|q_0|k\rangle=(2\omega)^{-1/2}(\sqrt{j}\,\delta_{j,k+1}+\sqrt{k}\,\delta_{k,j+1}), \tag{9}$$

where $j,k=0,1,2,\ldots,$ it is not difficult to see that $\langle 0|q_0^{2N}|0\rangle$ can be calculated exactly by matrix multiplication with a matrix representation of q_0 of dimensionality $d=1+N$; of course, $\langle 0|q_0^{2N+1}|0\rangle=0$. From the form of the potential $V(q)$ in (1) and the recurrence relations (4) it then follows that we can calculate $\langle 0|q_N|0\rangle$ exactly using the finite-dimensional matrix representations

$$(q_0)_{jk}=(2\omega)^{-1/2}(\sqrt{j}\,\delta_{j,k+1}+\sqrt{k}\,\delta_{k,j+1}), \tag{10a}$$

$$(p_0)_{jk}=i(\tfrac{1}{2}\omega)^{1/2}(\sqrt{j}\,\delta_{j,k+1}-\sqrt{k}\,\delta_{k,j+1}), \tag{10b}$$

for $1\leq j,k\leq D$, where $D=\frac{1}{2}(3^N+1)$. The matrix size for this exact calculation grows very rapidly with the number of iterations and the limit imposed by computer memory and computational time is likely to be $N\leq 7$.

Because of the difficulties described above in the exact iteration scheme, we found for practical purposes that a numerical approach was needed. The numerical approach is to approximate the infinite matrices p_0 and q_0 by sequences of larger and larger $D\times D$ matrices given by (10) and to iterate (4) with fixed values of D and h. We have implemented the scheme in FORTRAN and studied the numerical stability and convergence as a function of D and h.

At fixed D we studied convergence of our results as a function of h. We found at all D that for $h\leq 0.07$ the results were stable to at least two significant figures; for $h\leq 0.008$ we found a four-significant-figure stability. Of course, at small D the answers at large t are far from the correct infinite-D limit.

We next kept $h=0.008$ and studied convergence to the infinite-D limit as a function of t (at small t finite matrices are exact.) We note that the dimension D controls the number of harmonic-oscillator basis states in the $t=0$ Fock space. We compared larger and larger $D\times D$ matrices and found for the potential (1) with $\beta=2.5$ the following times of validity with four-place accuracy: For $D=4$, $t\leq 1.6$; $D=8$, $t\leq 3$; $D=16$, $t\leq 10$; $D=32$, all t examined ($t\leq 30$). These internally consistent results were then confirmed by comparison with a numerical integration of the Schrödinger equation[9] which gave also a four-significant-figure agreement with the $D=32$ results at all times $t\leq 30$. Running up to $t=30$ sufficed to display two complete oscillations in the tunneling.

In Figs. 1 and 2 we display our numerical results for iteration of the system (4) using 32×32 matrices and $h=0.008$, extending out to $t=30$. This calculation is enough to display two complete oscillations in the tunneling. This $D=32$ calculation agrees to four significant figures with a numerical integration of the

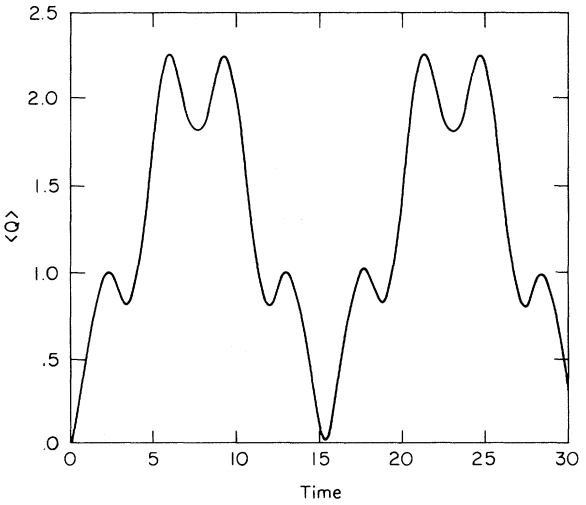

FIG. 1. Time dependence of $\langle 0|q(t)|0\rangle$ in the potential (1), with $\beta=2.5$, where $|0\rangle$ is the initial Gaussian wave packet (2). This calculation used 32×32 matrix representations for q_0 and p_0 as given in (10) and a value of $h=0.008$.

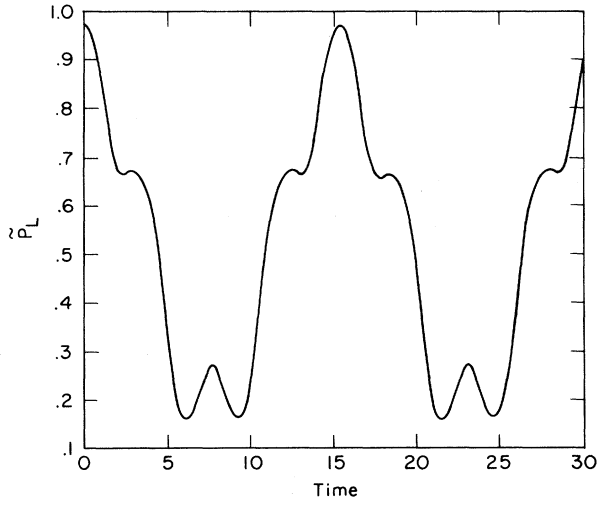

FIG. 2. Time dependence of $\tilde{P}_L(t)=\langle 0|\beta/(\beta+q^4)|0\rangle$, a measure of the probability for the wave packet $|0\rangle$ to remain in the left well. This calculation used the same parameters as in Fig. 1.

Schrödinger equation.[9]

We also calculated $\langle 0|q^2|0\rangle$ and $\langle 0|q^4|0\rangle$, which display the same oscillatory behavior as shown in Figs. 1 and 2. It is trivial to calculate other moments of q (and p); the accuracy of these results will be governed by the matrix-dimensionality considerations above.

We believe that the accuracy of our results establishes that direct iteration of the Heisenberg equations (3) with an operator-difference approximation such as (4) and finite-dimensional approximations for q_0 and p_0 offers a practical alternative to the conventional Schrödinger-equation approach. (The calculation described here with $h=0.008$ required 5 min of CPU time on a Cray-1 computer; for two-significant-figure accuracy one needs only 40 sec.)

As remarked earlier, our motivation for studying operator-difference techniques is to develop alternative methods for the numerical solution of a quantum field theory. For example, in a $(1+1)$-dimensional field theory the field operators $\phi(x,t)$ and $\pi(x,t)$ must first be discretized on a space lattice of volume Na by $x\rightarrow ja$. For example,

$$\dot{\phi}_j(t)=\pi_j(t), \tag{11a}$$

$$\dot{\pi}_j(t)=\frac{\phi_{j+1}(t)+\phi_{j-1}(t)-2\phi_j(t)}{a^2}-\frac{\partial V(\phi)}{\partial\phi_j}, \tag{11b}$$

$j=1,2,\ldots,N$. These operator equations are the analogs of (3) and can be discretized in time by use of a technique such as (4). For a spatial lattice of volume Na there are $2N$ equations (11) to be differenced and iterated, in place of the pair of equations (3). This calculation is under study.

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