

Integration of the Heisenberg equation of motion for quantum tunneling

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A method of integration of the Heisenberg equation of motion is proposed in which the time evolution of the basis set $\{T_{m,n}(t)\}$ of the Weyl-ordered operators introduced by Bender and Dunne [Phys. Rev. D **40**, 3504 (1989)] is obtained from the Taylor expansion and is expressible in terms of the initial $\{T_{m,n}(0)\}$'s. In the absence of damping forces, the constant values of the energy and the position-momentum commutation relation are used to check the accuracy of the integration. This method is applied to obtain the mean position and velocity of the particle as a function of time as well as the dwell time of the particle inside the barrier. In the example that is considered here, the potential is assumed to be the sum of a harmonic and a cubic term, and the calculation is done with and without dissipative coupling.

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I. INTRODUCTION

Bender and collaborators, in a series of papers, have outlined a number of different schemes for the integration of operator differential equations using a discrete time version of the equation of motion [1-3]. Among other applications, Bender *et al.* have used one finite-element calculation to study quantum tunneling in a double-well potential [2]. However, this method for a general tunneling problem, like the one considered in this paper, is not adequate. For an acceptable and accurate result, it is shown that one can start with the basis set of Weyl-ordered operators of Bender and Dunne [4,5], study their time evolution, and use the result to determine the solution of the operator equation of motion. The most interesting feature of the solution of the operator equation is a demonstration of the nonlocal character of the solution, e.g., the wave packet feels the effect of the deep well that lies on the other side of the barrier.

In Sec. II the time dependence of the basis set is studied, and it is shown that by combining the Taylor expansion and analytical continuation one can find the basis set $\{T_{m,n}(t)\}$ at a later time in terms of its initial value, i.e., $\{T_{m,n}(0)\}$. In Sec. III an expression for the position operator is obtained that explicitly depends on $\{T_{m,n}(0)\}$. This is used to study the motion of a wave packet for normal quantum tunneling. Section IV deals with dissipative quantum tunneling using Heisenberg's equation of motion. In the present formulation there is no need to construct a Lagrangian or a Hamiltonian for the dissipative system. Here it is shown that the equal time commutation relation is not only time dependent but is also a q number [6]. A specific example of tunneling through an anharmonic potential is studied in Sec. V, and in Sec. VI numerical results for this problem are given.

II. TAYLOR EXPANSION AND THE TIME EVOLUTION OF THE BASIS SET

Consider the operator equations of motion for a particle of unit mass

$$\frac{dp}{dt} = f(q), \quad \frac{dq}{dt} = p, \quad (2.1)$$

where $f(q)$ is a polynomial in q . The operators $q(t)$ and $p(t)$ satisfy the commutation relation

$$[q(t), p(t)] = i. \quad (2.2)$$

We want to integrate (2.1) subject to the initial conditions

$$q(t=0) = q(0) \quad \text{and} \quad p(t=0) = p(0), \quad (2.3)$$

assuming that the force $f(q)$ is such that the only singularities in the solution of (2.1) are fixed poles. Following the classical example of Taylor and Laurant series, Bender and Dunne propose a Weyl-ordered operator basis $\{T_{m,n}\}$ in powers of $p(t)$ and $q(t)$ defined as

$$T_{m,n} = \left(\frac{1}{2}\right)^n \sum_{k=0}^n \{n! / [(n-k)!k!]\} q^k p^m q^{n-k}. \quad (2.4)$$

Using the commutation relation (2.2) we can write (2.4) in an equivalent form

$$T_{m,n} = \left(\frac{1}{2}\right)^m \sum_{j=0}^m [m! / (m-j)!j!] p^j q^n p^{m-j}. \quad (2.5)$$

It is also possible to write $T_{m,n}$ as a totally symmetrized form containing m factors of p and n factors of q , divided by the number of terms in the expression. We can also extend this basis to include negative powers of p and q . Bender and Dunne [4,5] show that $T_{m,n}$'s form an algebra closed under multiplication and that the properties of this algebra can be deduced from the product formula [5]

$$T_{m,n} T_{r,s} = \sum_{j=0}^{\infty} [(i/2)^j / j!] \sum_{k=0}^j (-1)^{j-k} [j! / (j-k)!k!] [\Gamma(n+1)\Gamma(m+1)\Gamma(r+1) \times \Gamma(s+1)] T_{m+r-j, n+s-j} [\Gamma(m-l+1)\Gamma(n+l-2j)\Gamma(r+l-2j)\Gamma(s-l+1)]^{-1}, \quad (2.6)$$

where $m, n, r,$ and s can be positive or negative integers. One of the important results of this algebra, which will be used in the present work, is the commutator of $T_{m,n}$ and $T_{r,s}$,

$$\begin{aligned}
 [T_{m,n}, T_{r,s}] = & 2 \sum_{j=0}^{\infty} [(i/2)^{2j+1}/(2j+1)!] \\
 & \times \sum_{k=0}^j (-1)^k [(2j+1)!/(2j+1-k)!k!] \\
 & \times [\Gamma(n+1)\Gamma(m+1)\Gamma(r+1)\Gamma(s+1)] T_{m+r-2j+1, n+s-2j+1} \\
 & \times [\Gamma(m-k+1)\Gamma(n+k-2j)\Gamma(r+k-2j)\Gamma(s-k+1)]^{-1}.
 \end{aligned}
 \tag{2.7}$$

From the definition of $T_{m,n}$'s we have

$$q(t) = T_{0,1}(t) \tag{2.8}$$

and

$$p(t) = T_{1,0}(t). \tag{2.9}$$

To solve the operator differential equation (2.1) using this basis set we start with the Taylor expansion of $q(\Delta t)$,

$$\begin{aligned}
 q(\Delta t) = & q(0) + (-i\Delta t)[q(0), H] + (-i\Delta t)^2[[q(0), H], H] + \dots \\
 = & q(0) + [(\Delta t)/1!](dq/dt)_0 + [(\Delta t)^2/2!](d^2q/dt^2)_0 + [(\Delta t)^3/3!](d^3q/dt^3)_0 + \dots,
 \end{aligned}
 \tag{2.10}$$

where H is the Hamiltonian $H = \frac{1}{2}p^2 + V(q)$.

The right-hand side of (2.10) is expressible in terms of $T_{m,n}(0)$'s

$$q(\Delta t) = T_{0,1} + [(\Delta t)/1!]T_{1,0} + [(\Delta t)^2/2!]f(T_{0,1}) + \frac{1}{2}[(\Delta t)^3/3!][T_{1,0}f'(T_{0,1}) + f'(T_{0,1})T_{1,0}] + \dots, \tag{2.11}$$

where f' is the derivative of $f(q)$ with respect to q , and $f(q) = -(\partial V/\partial q)$. Note that when f is a polynomial in q , then $f(T_{0,1})$ and $f'(T_{0,1})$ are expressible as sums involving $T_{0,j}$. A similar relation can be obtained for $p(\Delta t)$. In general if t_j denotes the time $j\Delta t$ with j an integer, then $q(t_{j+1})$ and $p(t_{j+1})$ are expressible in terms of $T_{m,n}(t_j)$:

$$\begin{aligned}
 q(t_{j+1}) = & T_{0,1}(t_j) + \Delta t T_{1,0}(t_j) + (1/2!)(\Delta t)^2 f(T_{0,1}(t_j)) \\
 & + \frac{1}{2}(1/3!)(\Delta t)^3 [T_{1,0}(t_j)f'(T_{0,1}(t_j)) + f'(T_{0,1}(t_j))T_{1,0}(t_j)] + \dots
 \end{aligned}
 \tag{2.12}$$

and

$$p(t_{j+1}) = T_{1,0}(t_j) + (\Delta t)f(T_{0,1}(t_j)) + \frac{1}{2}(1/2!)(\Delta t)^2 [T_{1,0}(t_j)f'(T_{0,1}(t_j)) + f'(T_{0,1}(t_j))T_{1,0}(t_j)] + \dots. \tag{2.13}$$

Thus if $\{T_{m,n}\}$'s are known at t_j , then $q(t_{j+1})$ and $p(t_{j+1})$ can be calculated from Eqs. (2.12) and (2.13). Using $q(t_{j+1})$ and $p(t_{j+1})$, we can calculate $T_{m,n}$ at a later time using Eqs. (2.4) or (2.5):

$$T_{m,n}[q(t_{j+1}), p(t_{j+1})] = T_{m,n}(t_{j+1}). \tag{2.14}$$

We note that $T_{m,n}(t_{j+1})$ depends on the products of the elements of the set $\{T_{m,n}(t_j)\}$, which can be simplified using the product formula (2.6). But the elements $T_{m,n}(t_j)$ in turn are given in terms of $\{T_{m,n}(t_{j-1})\}$ and so on. Therefore the result of integration will be given as a series in $\{T_{m,n}(0)\}$. For the position operator, we can write

$$q(t) = \sum_{m,n} c_{m,n}(t) T_{m,n}(0), \tag{2.15}$$

where $c_{m,n}(t)$ is the time-dependent real coefficient of $T_{m,n}(0)$.

Similarly for $p(t)$ we have

$$p(t) = \sum_{m,n} (dc_{m,n}/dt) T_{m,n}(0). \tag{2.16}$$

Either from Eqs. (2.15) and (2.16) or from (2.12) and (2.13) we can calculate the equal time commutator. For instance, from the latter equation we find

$$\begin{aligned}
 [q(t_{j+1}), p(t_{j+1})] = & [T_{0,1}(t_j), T_{1,0}(t_j)] \\
 = & [T_{0,1}(0), T_{1,0}(0)] \\
 = & i.
 \end{aligned}
 \tag{2.17}$$

The energy of the particle, in the absence of dissipative forces, remains constant, and its ground-state expectation value is equal to the sum of expectation values of the kinetic and potential energies,

$$\langle 0|E|0\rangle = \frac{1}{2}\langle 0|p^2|0\rangle + \langle 0|V(q)|0\rangle, \tag{2.18}$$

where $V(q)$ is defined by

$$f(q) = - \left[\frac{\partial V}{\partial q} \right]. \tag{2.19}$$

III. MOTION OF THE WAVE PACKET

Consider a normalized Gaussian wave packet

$$\psi(q) = (\nu/\pi)^{(1/4)} \exp(-\frac{1}{2}\nu q^2), \quad (3.1)$$

where ν is a parameter with the dimension of frequency. Using this wave function we find the ground-state expectation value of $T_{m,n}(0)$ to be

$$\begin{aligned} \langle 0|T_{m,n}|0\rangle &= \int_{-\infty}^{+\infty} \psi^*(q) T_{m,n}(0) \psi(q) dq \\ &= \nu^{(1/2)(m-n)} (m-1)!! (n-1)!! (\frac{1}{2})^{(m+n)/2}, \\ &\quad \text{when } m \text{ and } n \text{ are even} \\ &= 0 \text{ otherwise.} \end{aligned} \quad (3.2)$$

For a displaced Gaussian wave packet

$$\psi(q - q_0) = (\nu/\pi)^{(1/4)} \exp[-(\nu/2)(q - q_0)^2], \quad (3.3)$$

this expectation value becomes

$$\begin{aligned} \langle 0|T_{m,n}(0)|0\rangle_{q_0} &= \int_{-\infty}^{+\infty} \psi^*(q - q_0) T_{m,n}(0) \psi(q - q_0) dq \\ &= \sum_{j=0}^n \{n! / [(n-j)! j!]\} \\ &\quad \times q_0^j \langle 0|T_{m,n}(0)|0\rangle. \end{aligned} \quad (3.4)$$

From Eqs. (2.15) and (2.16) we calculate the expectation values of $q(t)$ and $p(t)$ with the displaced Gaussian wave packet $\psi(q - q_0)$,

$$\langle 0|q(t)|0\rangle_{q_0} = \sum_{m,n} c_{m,n}(t) \langle 0|T_{m,n}|0\rangle_{q_0}, \quad (3.5)$$

$$\langle 0|p(t)|0\rangle_{q_0} = \sum_{m,n} (dc_{m,n}/dt) \langle 0|T_{m,n}|0\rangle_{q_0}, \quad (3.6)$$

in addition we find the expectation value of the commutator, i.e.,

$$\langle 0|[q(t), p(t)]|0\rangle = i. \quad (3.7)$$

IV. DISSIPATIVE TUNNELING

The Heisenberg equation of motion for dissipative tunneling can be derived from a conservative many-body Hamiltonian, and the resulting operator equation is a nonlinear integrodifferential equation with a kernel that is dependent on the form of coupling to the heat bath [6,7]. For the present work we consider a phenomenological damping term proportional to the momentum of the particle, i.e., $-\lambda p$, and add it to the original equation of motion:

$$\frac{dp}{dt} = -\lambda p + f(q), \quad \frac{dq}{dt} = p. \quad (4.1)$$

This operator equation is subject to the same initial condition Eq. (2.3), where $p(0)$ and $q(0)$ satisfy the commutation relation

$$[q(0), p(0)] = i. \quad (4.2)$$

At any other time Eq. (2.2) is not satisfied, and in fact the commutator $[q(t), p(t)]$, in our approximation, is not a

c -number, because of the finite number of terms $\{T_{m,n}\}$. To show this, consider the Taylor expansion of (4.1) similar to (2.11),

$$\begin{aligned} q(\Delta t) &= T_{01} + (\Delta t/1!) T_{10} \\ &\quad + (1/2!)(\Delta t)^2 [-\lambda T_{10} + f(T_{01})] + \dots, \end{aligned} \quad (4.3)$$

$$p(\Delta t) = T_{10} + (\Delta t/1!) [-\lambda T_{10} + f(T_{01})] + \dots. \quad (4.4)$$

From these we calculate $[q(\Delta t), p(\Delta t)]$,

$$\begin{aligned} [q(\Delta t), p(\Delta t)] &= [T_{01}, T_{10}] \\ &\quad + (\Delta t)[T_{01}, -\lambda T_{10} + f(T_{01})] \\ &\quad + (\Delta t)[T_{10}, f(T_{01})] + \dots \\ &= i\{1 - (\Delta t)[1 - f'(q(0))]\} + \dots, \end{aligned} \quad (4.5)$$

which shows the q -number nature of the commutator at the time Δt . Only when f is constant or is a linear function of q (i.e., harmonic potential), the commutator will be a c -number.

V. A SPECIFIC CASE OF QUANTUM TUNNELING

The simplest model of quantum tunneling that has been discussed frequently in the literature is the case of the anharmonic potential

$$V(q) = \frac{1}{2}\nu^2 q^2 - \frac{1}{3}\mu^3 q^3, \quad (5.1)$$

where ν and μ are constants. For this potential we can simplify our calculation by introducing a set of dimensionless operators

$$Q(\theta) = (\mu^3/\nu^2)q(t), \quad P(\theta) = (\mu^3/\nu^3)p(t), \quad \theta = \nu t. \quad (5.2)$$

In terms of these variables the equations of motion (4.1) become

$$\frac{dP}{d\theta} = -\lambda' P - Q + Q^2, \quad \frac{dQ}{d\theta} = P, \quad (5.3)$$

where

$$\lambda' = \lambda/\nu \quad (5.4)$$

is a dimensionless damping constant. The basis set $\{T_{m,n}(p, q)\}$ is also replaced by the dimensionless set $\tau_{m,n}(P, Q, \theta)$, where

$$\tau_{m,n}(P, Q, \theta) = (\mu^3/\nu^2)^n (\mu^3/\nu^3)^m T_{m,n}(t). \quad (5.5)$$

The commutator $[Q(\theta), P(\theta)]$, in the absence of damping, can be found from $[q(t), p(t)] = i$, i.e.,

$$[Q(\theta), P(\theta)] = \gamma [q(t), p(t)] = i\gamma, \quad (5.6)$$

where γ is a dimensionless constant

$$\gamma = \mu^6/\nu^5, \quad (5.7)$$

remembering that we have set $\hbar = 1$.

After changing to these dimensionless variables, the only parameter that is left in the calculation is γ . In

terms of Q the potential has a minimum at $Q=0$ and a maximum at $Q=1$, and the height of the potential barrier at this point is $V_0 = \frac{1}{6}$. Using Eqs. (2.18) and (3.2), we find the expectation value of the energy in the absence of damping to be

$$\langle 0|H(t)|0\rangle_{Q_0} = \frac{1}{2}\langle 0|P^2(t)|0\rangle_{Q_0} + \frac{1}{2}\langle 0|V[Q(t)]|0\rangle_{Q_0} \tag{5.8}$$

or

$$\langle 0|H(f)|0\rangle_{Q_0} = \frac{1}{2}[\gamma(1-Q_0)+Q_0^2] - \frac{1}{3}Q_0^3, \tag{5.9}$$

where

$$Q_0 = (\mu^3/\nu^2)q_0, \tag{5.10}$$

$$\langle 0|E|0\rangle_{Q_0} = (\nu/\mu)^6\langle 0|H|0\rangle_{Q_0}.$$

In what follows for the sake of simplicity we omit the

$$\langle 0|\tau_{m,n}(\theta)|0\rangle = \begin{cases} \sum_{k=0}^n \{n!/ [k!(n-k)!]\} Q_0^k (m-1)!!(k-1)!!(\gamma/2)^{(k+m)/2} & (m \text{ even}) \\ 0 & (m \text{ odd}). \end{cases} \tag{5.13}$$

The initial wave packet in terms of the dimensionless quantities is given by

$$\psi(Q-Q_0) = (1/\pi\gamma)^{(1/4)} \exp[-(Q-Q_0)^2/\gamma], \tag{5.14}$$

the position of this wave packet at any later time is given by (5.11). The results of the numerical integration of Eq. (5.3) will be given in the next section.

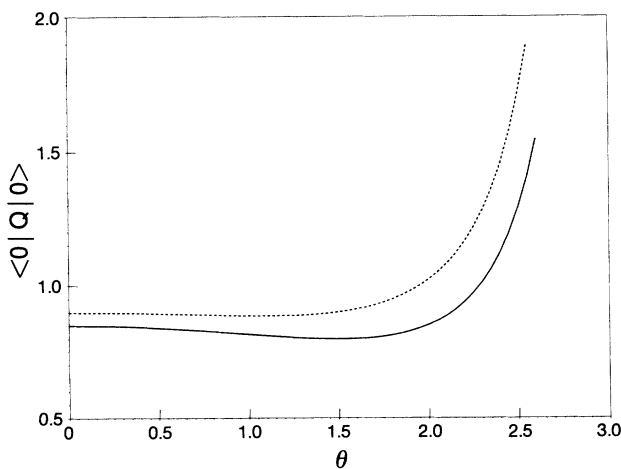


FIG. 1. The expectation value of the position operator $\langle 0|Q(\theta)|0\rangle_{Q_0}$ as a function of $\theta = \nu t$ (both $\langle 0|Q(\theta)|0\rangle_{Q_0}$ and θ are dimensionless numbers). The solid line is for the initial position of the wave packet $Q_0=0.85$ and corresponds to the energy lower than the height of the barrier V_0 . The dashed line is for $Q_0=0.9$, i.e., for an energy slightly lower than V_0 . Both of these are obtained for $\gamma=0.1$.

subscript Q_0 from the expectation values.

If the energy $\langle 0|H|0\rangle$ is less than the maximum height of the barrier, i.e., for $\langle 0|H|0\rangle < V_0$, then tunneling occurs. Thus by changing the values of Q_0 or γ , we can adjust the energy of the packet and satisfy this inequality.

By writing Eq. (2.15) in terms of Q and τ we can calculate the expectation value of the position operator Q as a function of the dimensionless time $\theta = \nu t$,

$$\langle 0|Q(\theta)|0\rangle = \sum_{m,n} d_{m,n} \langle 0|\tau_{m,n}|0\rangle, \tag{5.11}$$

where

$$d_{m,n} = (\nu^2/\mu^3)^{(n-1)}(\nu/\mu)^3 c_{m,n}. \tag{5.12}$$

A similar expectation can also be found for $\langle 0|P(\theta)|0\rangle_{Q_0}$. Now from Eqs. (3.2), (3.4), and (5.5) we have

VI. RESULTS

Before we discuss the results of the present formulation of the problem, it is important to consider the criteria for quantum tunneling when we use a localized wave packet like (3.3). Since such a wave packet is a superposition of different energy eigenstates, it may be argued that due to the possibility of a large contribution from the eigenstates of the Hamiltonian above the potential barrier, one may be looking at the passage of the particle over the barrier, rather than quantum tunneling. Here we impose two physically reasonable conditions that differentiate between the passage over the barrier and quantum tunneling.

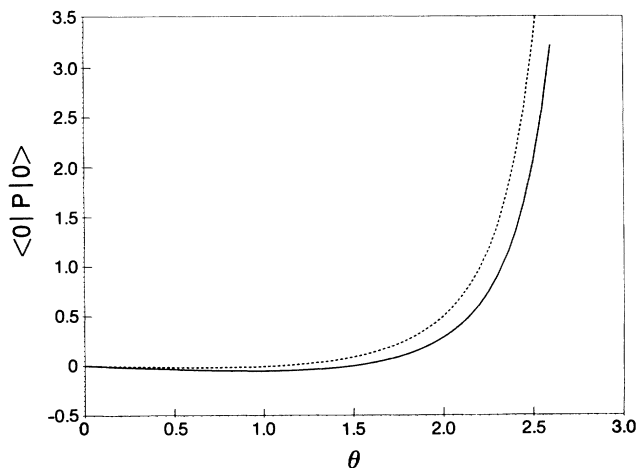


FIG. 2. The expectation value of the momentum operator $\langle 0|P|\theta\rangle$ as a function of θ for the two cases $Q_0=0.9$ (dashed line) and $Q_0=0.85$ (solid line) with $\gamma=0.1$.

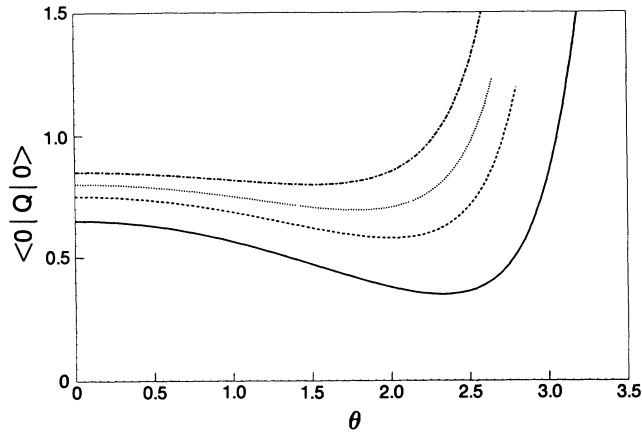


FIG. 3. The expectation value of $\langle 0|Q|0\rangle$ for dissipative tunneling ($\lambda'=0.1$). Different lines corresponds to different values of Q ; $Q_0=0.65$ (solid line), $Q_0=0.75$ (dashed line), $Q_0=0.8$ (dotted line), and $Q_0=0.85$ (dot-dashed line). All these curves are obtained for the dimensionless parameter $\gamma=0.1$.

(1) The expectation value of the energy of the wave packet $\langle 0|H|0\rangle$ should be less than the height of the barrier.

(2) If we calculate the expectation values of the initial position and momentum $\langle 0|q(0)|0\rangle$, $\langle 0|p(0)|0\rangle$ using the wave packet (3.3) and then choose these as initial values for the classical $q(0)$ and $p(0)$ and solve the classical equation of motion, we should obtain two turning points. That is, the classical limit of quantum tunneling results in bounded oscillations about the equilibrium $q=0$. In our formulation both of these conditions are satisfied.

The method of integration that we have used to obtain $\langle 0|Q(\theta)|0\rangle$ is outlined in Sec. II. We start with the Taylor expansion (2.12) and (2.13) and keep terms proportional to $(\Delta t)^8$ in the expansion and a basis set of 253 terms of $\tau_{m,n}$'s, i.e., all terms with $(m+n)\leq 22$. The procedure of substitution and reduction of the products of $\tau_{m,n}(t_j)$ generates a $\tau_{0,1}$ (or $\tau_{1,0}$) also containing 253

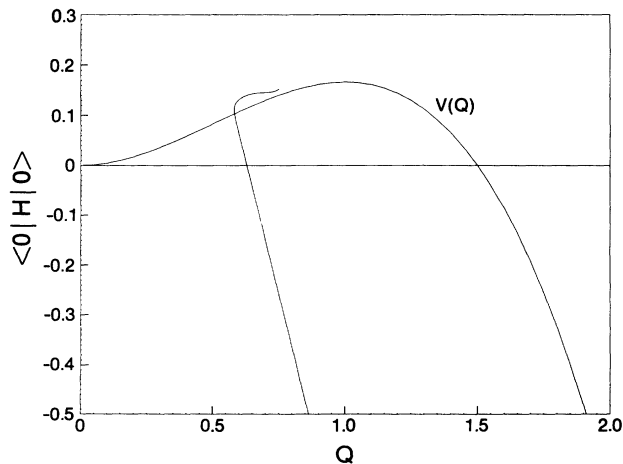


FIG. 4. Dissipation of energy in the initial phase of tunneling. Note that initially the motion of the wave packet is in the direction of the center of the potential $Q=0$. The parameters used are $Q_0=0.75$, $\gamma=0.1$, and $\lambda'=0.1$.

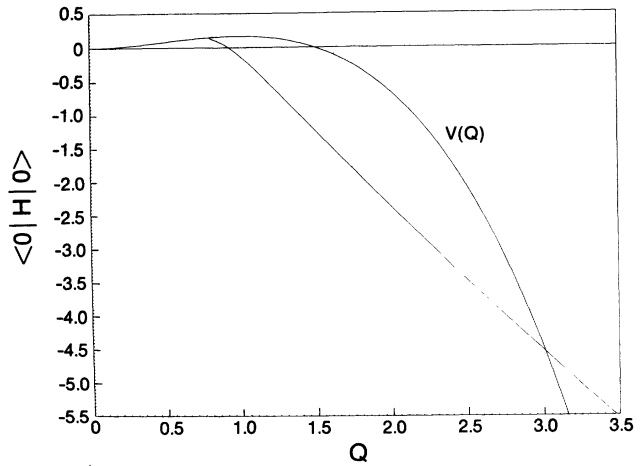


FIG. 5. Details of the energy loss of a wave packet tunneling through the barrier $V(Q)$. The two points of intersection of $\langle 0|H|0\rangle$ and $V(Q)$ correspond to the classical turning points. The constants used are $Q_0=0.85$, $\gamma=0.1$, and $\lambda'=0.1$.

terms in $\{\tau_{m,n}(0)\}$. In the absence of dissipative force, i.e., when $\lambda'=0$, the wave packet, which is initially located at Q_0 , starts moving in the direction of the minimum of the potential at $Q=0$, similar to the motion of a classical particle in this potential well. However this inward motion is of short duration (see Figs. 1 and 2), and the wave packet moves back and approaches the classical turning point with increasing momentum. With this momentum it enters the classically inaccessible region (under the barrier), and even here it gains momentum, i.e., it feels the presence of a very deep well on the other side of the barrier. Finally the packet escapes the barrier after spending a very short time $\Delta\theta$ traversing it. During the course of the motion, the total energy as calculated from (5.9) and the commutation relation obtained from (5.6) remain constant. Comparing the expectation values of $Q(\theta)$ and $P(\theta)$ for energies slightly below the barrier $\langle 0|H_1|0\rangle=0.16404$ ($Q_0=0.85$) and just above the bar-

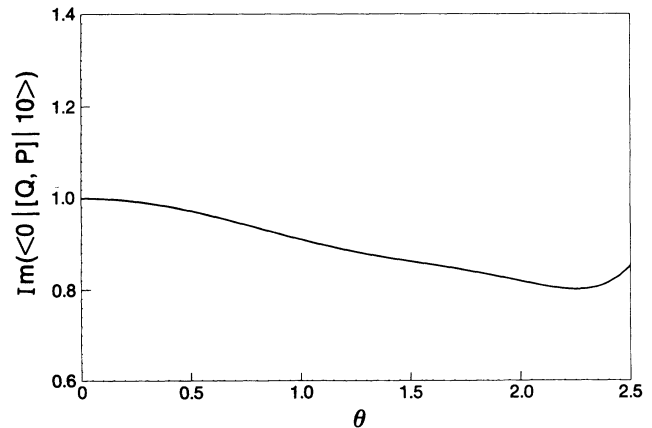


FIG. 6. In the presence of dissipative forces the commutator $[Q,P]$ changes with time. Here the expectation value of the commutator in units of γ is shown as a function of θ for $\lambda'=0.1$ and $\gamma=0.1$. This shows that our approximation of $[Q,P]$ by finite series in $\{T_{m,n}\}$ is valid for short times.

rier $\langle 0|H_2|0\rangle=0.167$ ($Q_0=0.9$) with $\gamma=0.1$ shows that unlike the classical situation there is no qualitative change in motion. In fact when $\langle 0|H_2|0\rangle > V_0$, the wave packet first moves to the left, before turning back and passing over the barrier. Figures 1 and 2 also show the motion of the wave packet in the classically forbidden region and the dwell time, i.e., the time that the wave packet spends under the barrier. For $\gamma=0.1$ and $\langle 0|H|0\rangle=0.153$ ($Q_0=0.75$), the dwell time $\Delta\theta$ is 0.175, whereas for the same γ but for $\langle 0|H|0\rangle=0.164$ ($Q_0=0.85$), $\Delta\theta$ changes to 0.178. When the dissipative force $\lambda'(dQ/dt)$ is present, the barrier $V(Q)=\frac{1}{2}Q^2-\frac{1}{3}Q^3$ allows for tunneling no matter how strong the damping constant λ' is. Unlike the cases where the depth of the potential is finite, here there is no critical damping and therefore no localization of the wave packet in the shallower well, i.e., around $Q=0$ (Figs. 3–5) [8]. The wave packet loses energy during the course of its motion, therefore its total energy can be positive zero or negative.

For a dissipative system it is more difficult to determine the classical turning points and hence the dwell time, since the energy is not conserved. If one plots the energy $\langle 0|H|0\rangle$ as a function of the mean position operator $\langle 0|Q|0\rangle$, one finds that this curve intersects the barrier at two points, Fig. 5, the difference $\Delta\theta_D=\theta_2-\theta_1$ corresponding to the coordinates of the two turning points is the dwell time. This $\Delta\theta_D$ can be very different from the dwell time in the absence of damping, but approaches $\Delta\theta$ for a conservative case as $\lambda'\rightarrow 0$. For instance for $\lambda'=0.1$, $\gamma=0.1$, and $Q_0=0.8$, one finds $\Delta\theta_D$ to be 1.62, and for the same λ' and γ but with $Q_0=0.75$ the corresponding dwell time is $\Delta\theta_D=1.04$. The expectation value of the commutator in the presence of damping is

$$\langle 0|[Q(\theta),P(\theta)]|0\rangle=i\gamma\langle 0|C(\theta)|0\rangle, \quad (6.1)$$

where $C(\theta)$ is a dimensionless operator depending on θ and approaches one as λ' goes to zero, Fig. 6. For a most general quadratic potential the commutator is a c -number [6], i.e.,

$$[Q(\theta),P(\theta)]=i\gamma C(\theta). \quad (6.2)$$

For this class of potentials one can calculate $C(\theta)$ by differentiating (6.2), and then substituting for $dP/d\theta$ from (5.3), with the result that

$$C(\theta)=C(0)\exp(-\lambda'\theta). \quad (6.3)$$

But the expectation value obtained from (6.1) shows a different result because of our approximation.

In the present formulation we have studied the example of a barrier given by the anharmonic potential, a simple case that has been considered by a number of authors [9–11]. However the present formulation can also be applied to other forms, e.g., a combination of the form

$$V(r)=(a/r)-(b/r^2)+(c/r^3), \quad (6.4)$$

with $b^2 > 4ac$ and $c > 0$. For such a case the basis set consists of the elements $\{T_{m,n}\}$, where n now is a negative integer or zero.

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