Simple approach to tunneling using the method of finite elements

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We use the method of finite elements to solve the operator field equations for a simple quantum-mechanical model of tunneling. For the case of just one finite element we can express the tunneling in terms of a Borel transform. We obtain excellent numerical results for short times.

I. INTRODUCTION

In a recent paper[1] it was argued that the method of finite elements may be used to obtain directly an approximate solution to the operator equations of a quantum theory. Given an approximate solution to these equations one can try to obtain such quantities as the energy levels or the Green's functions of the theory. The purpose of this paper is to investigate a very simple and natural way to use the finite-element solution to the operator equations, namely, to solve quantum-mechanical tunneling problems.

As discussed in Ref. 1, the method of finite elements gives an approximation to the operators $p(t)$ and $q(t)$ as a chain of linear approximations. We consider a sequence of time intervals of length h. On the nth interval, $(n-1)h \le t \le nh$, we introduce a local variable x defined by

$$t=(n-1)h+x \tag{1}$$

so that $0 \le x \le h$ and we approximate $p(t)$ by the linear function

$$p_{n-1}\left[1-\frac{x}{h}\right]+p_n\frac{x}{h} \quad (0 \le x \le h) \tag{2a}$$

and $q(t)$ by the linear function

$$q_{n-1}\left[1-\frac{x}{h}\right]+q_n\frac{x}{h} \quad (0 \le x \le h)\ . \tag{2b}$$

In these expressions, q_n and p_n are approximations to the exact operator functions $q(t)$ and $p(t)$ evaluated at the time $t=nh$.

The Heisenberg equations for the Hamiltonian

$$H=\frac{p^2}{2}+V(q) \tag{3}$$

are

$$\dot{q}=p \tag{4}$$

and

$$\dot{p}=-V'(q)\ . \tag{5}$$

Equations (4) and (5) together constitute a time-evolution problem: given $p(0)=p_0$ and $q(0)=q_0$, the objective is to calculate $p(t)$ and $q(t)$. We do this by computing p_n and q_n, where $n=t/h$. As the lattice spacing h becomes smaller p_n and q_n become better approximations to $p(t)$ and $q(t)$.[2]

The operators p_n and q_n satisfy the difference equations

$$\frac{q_{n+1}-q_n}{h}=\frac{p_{n+1}+p_n}{2}\ , \tag{6}$$

$$\frac{p_{n+1}-p_n}{h}=-V'\left[\frac{q_{n+1}+q_n}{2}\right]\ . \tag{7}$$

Equations (6) and (7) are obtained by substituting the linear approximations to $p(t)$ and $q(t)$ in (2a) and (2b) into the Heisenberg equations (4) and (5) and evaluating the results at the midpoint $x=h/2$.

Equations (6) and (7) are implicit equations for p_{n+1} and q_{n+1} in terms of p_n and q_n. Solving for q_{n+1} and p_{n+1} explicitly we have

$$q_{n+1}=-q_n+2g^{-1}\left[\frac{4q_n}{h^2}+\frac{2p_n}{h}\right] \tag{8}$$

and

$$p_{n+1}=-p_n-\frac{4}{h}q_n+\frac{4}{h}g^{-1}\left[\frac{4q_n}{h^2}+\frac{2p_n}{h}\right]\ , \tag{9}$$

where

$$g(x)=V'(x)+\frac{4}{h^2}x$$

is a function which contains all of the dynamics of the theory. A simple property of (8) and (9) is that the commutation relations are exactly preserved:

$$[q_{n+1},p_{n+1}]=[q_n,p_n]=\cdots=[q_0,p_0]=i\ . \tag{10}$$

In this paper we consider a Hamiltonian with a quartic potential well that exhibits tunneling:

$$H=\frac{p^2}{2}+\frac{m^2\alpha^2}{2}q^2(\sqrt{m}\,q-5)(\sqrt{m}\,q-9)\ . \tag{11}$$

Here m is a parameter having dimensions of mass (length^{-1}) and α is an adjustable constant that fixes the height of the barrier. In terms of the dimensionless variable $z=\sqrt{m}\,q$ the potential is

$$V=\frac{m\alpha^2}{2}z^2(z-5)(z-9)\ . \tag{12}$$

This potential has been chosen so that its maximum and minima occur at rational values of z: V has a minimum (position of the false vacuum state) at $z=0$ and another minimum at $z=\frac{15}{2}$ (position of the true vacuum state); V has a maximum (barrier) at $z=3$ (see Fig. 1). At $z=\frac{15}{2}$, the depth of the well is $V=-\frac{3375}{32}m\alpha^2=-105.47m\alpha^2$ and at $z=3$, the height of the barrier is $V=54m\alpha^2$. Near $z=0$ the potential is approximately harmonic:

$$H_{\text{approx}}\cong\frac{p^2}{2}+\frac{45}{2}m^2\alpha^2q^2\ . \tag{13}$$

The energy levels for H_{approx} in (13) lie at

$$E_n=(n+\tfrac{1}{2})m\alpha\sqrt{45},\quad n=0,1,2,\ldots\ . \tag{14}$$

Thus, the (false) ground state lies at $\frac{3}{2}m\alpha\sqrt{5}$. If we wish to confine exactly N false states we must choose the height of the barrier appropriately:

$$\alpha=\frac{N\sqrt{5}}{18}\ . \tag{15}$$

For the purpose of this paper we take $N=1$ and H in (12) becomes (see Fig. 1)

$$H=\frac{p^2}{2}+\frac{5m}{648}z^2(z-5)(z-9)\ . \tag{16}$$

To observe tunneling we compute the order parameter $Q(t)=\langle 0\,|\,q(t)\,|\,0\rangle$, which is the expectation value of the position operator $q(t)$ in the Gaussian *false*-vacuum state $|\,0\rangle$. The function $Q(t)$ takes a value 0 at $t=0$ and, as tunneling proceeds, tends to increase. $Q(t)$ is a measure of how much of the state has penetrated the barrier at time t. In this paper we obtain the one-finite-element approximation to $Q(t)$ and compare our results with numerical tunneling data obtained by computer.

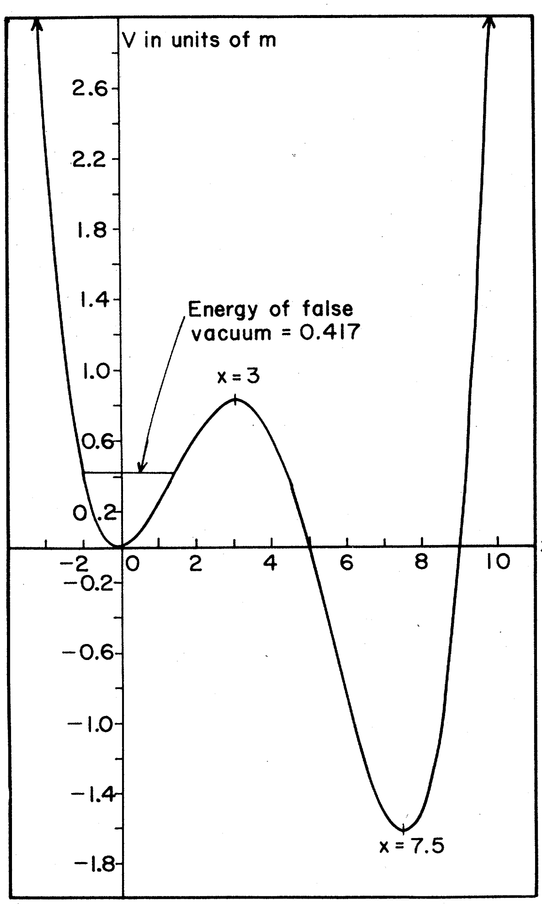

FIG. 1. The potential $V(z)$ in units of m [see (12)]. In this graph $\alpha=\sqrt{5}/18$ so that the potential confines exactly one unstable state where energy is $5m/12\simeq 0.417m$.

II. THE FALSE-VACUUM STATE

The false-vacuum state $|\,0\rangle$ is the lowest eigenstate of H_{approx} in (13). In the coordinate-space representation

$$\psi_0(x)=\langle x\,|\,0\rangle$$

is the initial ($t=0$) wave function in the false vacuum. Since H_{approx} has the form

$$H_{\text{approx}}=\frac{p^2}{2}+\frac{\omega^2}{2}q^2\ , \tag{17}$$

we see that $\psi_0(x)$ has the Gaussian form

$$\psi_0(x)=e^{-\omega x^2/2}\ . \tag{18}$$

Comparing (17) and (13) and using (15) gives the value of the frequency

$$\omega=5m/6\ . \tag{19}$$

The wave function at time t, $\psi(x,t)$, can be found by solving the Schrödinger equation in coordinate space subject to the initial condition $\psi(x,0)=\psi_0(x)$. Thus, in the Schrödinger picture the order parameter $Q(t)$ takes the form

$$Q(t)=\frac{\int \psi^*(x,t)x\psi(x,t)dx}{\int \psi^*(x,t)\psi(x,t)dx}\ . \tag{20}$$

The tunneling calculation in this paper consists of starting with the Gaussian wave function $\psi_0(x)$ in (18) which is centered around the false vacuum at $x=0$ and studying the time evolution of $Q(t)$. The frequency of "tunneling attempts" at the barrier wall is given by $\omega/(2\pi)$. As the wave function penetrates the barrier into the deeper right-hand well, $Q(t)$ grows monotonically from its initial value $Q(0)=0$. However, the wave packet in the deeper well then reflects off the right-hand wall of this well and can penetrate the barrier causing a subsequent decrease in $Q(t)$. Thus, there are two frequencies of tunneling attempts, one from the left and one from the right. As time passes $Q(t)$ will fluctuate roughly in the range between 0 and $\frac{15}{2}$ indicating that there is some probability density in both wells. [If we were to replace the right-hand wall of the deeper well by a straight horizontal line starting at the absolute minimum at $z=\frac{15}{2}$, then $Q(t)$ would just grow monotonically with time.]

Let us reexamine the problem more formally. The commutation relations for q_0 and p_0 allow us to construct in the usual way a complete set of Fock states $|n\rangle$ at time $t=0$. We introduce raising and lowering operators a and $a^\dagger$ by

$$p_0=\frac{\sqrt{m}}{\sqrt{2}\gamma}\frac{a-a^\dagger}{i} \tag{21}$$

and

$$q_0=\frac{1}{\sqrt{2m}}(a+a^\dagger)\gamma , \tag{22}$$

where a and $a^\dagger$ satisfy the standard commutation relation

$$[a,a^\dagger]=1 . \tag{23}$$

γ is an arbitrary parameter which we fix by choosing the state $|0\rangle$ to be the false-vacuum state.

To determine γ we compute the expectation value of H_{approx} in (13) with $\alpha=\sqrt{5}/18$ in the state $|0\rangle$:

$$p_0{}^2=-\frac{m}{2\gamma^2}(a^2+a^{\dagger 2}-aa^\dagger-a^\dagger a) ,$$

$$q_0{}^2=\frac{\gamma^2}{2m}(a^2+a^{\dagger 2}+aa^\dagger+a^\dagger a) ,$$

so

$$\langle 0|H_{\text{approx}}|0\rangle=\left[\frac{1}{4\gamma^2}+\frac{25\gamma^2}{144}\right]m . \tag{24}$$

Demanding that the expectation value of H_{approx} in the false vacuum be $E_0=5m/12$ gives

$$\gamma^2=\tfrac{6}{5} . \tag{25}$$

Of course, the state $|0\rangle$ is not an eigenstate of the exact Hamiltonian H in (11). However, the difference between $\langle 0|H_{\text{approx}}|0\rangle$ and $\langle 0|H|0\rangle$ is very small: $\Delta E=m/120$. Thus, $\Delta E/E_0$ is exactly 2%.

III. ONE-FINITE-ELEMENT CALCULATION OF $Q(t)=\langle 0|q(t)|0\rangle$

To observe tunneling we determine how the expectation value of $q(t)$ in the state $|0\rangle$ evolves with time. Using (8) with $n=1$ we obtain

$$\langle 0|q_1|0\rangle=2\left\langle 0\left|g^{-1}\left[\frac{4q_n}{h^2}+\frac{2p_n}{h}\right]\right|0\right\rangle . \tag{26}$$

To compute the right side of (26) we expand g^{-1} in a Taylor series:

$$g^{-1}(x)=\sum_{n=0}^{\infty}\beta_n x^n , \tag{27}$$

where

$$\begin{aligned} x&=\frac{4q_n}{h^2}+\frac{2p_n}{h}\\ &=a\left[\frac{4}{h^2}\frac{\sqrt{3}}{\sqrt{5m}}-i\frac{\sqrt{5m}}{h\sqrt{3}}\right]+a^\dagger\left[\frac{4}{h^2}\frac{\sqrt{3}}{\sqrt{5m}}+\frac{i\sqrt{5m}}{h\sqrt{3}}\right] . \end{aligned} \tag{28}$$

Using the identity

$$\langle 0|e^{t(Aa+Ba^\dagger)}|0\rangle=e^{t^2AB/2} ,$$

where A and B are c numbers, we obtain

$$\begin{aligned} &\langle 0|(Aa+Ba^\dagger)^{2n}|0\rangle=\frac{(2n)!}{n!}\left[\frac{AB}{2}\right]^n ,\\ &\langle 0|(Aa+Ba)^{2n+1}|0\rangle=0 . \end{aligned} \tag{29}$$

Hence, using (27) and (29) we have

$$\langle 0|q_1|0\rangle=2\sum_{n=0}^{\infty}\beta_{2n}\frac{(2n)!}{n!}\left[\frac{\frac{48}{h^4 5m}+\frac{5m}{3h^2}}{2}\right]^n . \tag{30}$$

This is a divergent series if (27) has a finite radius of convergence. However, we can express the sum in (30) as a Borel transform. Using

$$\frac{(2n)!}{n!}=\frac{2^{2n}\Gamma}{\sqrt{\pi}}(n+\tfrac{1}{2})=\frac{2^{2n}}{\sqrt{\pi}}\int_0^\infty e^{-t}t^{n-1/2}dt ,$$

we have

$$\begin{aligned} \langle 0|q_1|0\rangle&=\frac{2}{\sqrt{\pi}}\sum_{n=0}^{\infty}\beta_{2n}\left[\frac{96}{5mh^4}+\frac{10m}{3h^2}\right]^n\int_0^\infty dt\, e^{-t}t^{n-1/2}\\ &=\frac{2}{\sqrt{\pi}}\int_0^\infty\frac{dt\, e^{-t}}{\sqrt{t}}\sum_{n=0}^{\infty}\beta_{2n}t^n\left[\frac{96}{5mh^4}+\frac{10m}{3h^2}\right]^n\\ &=\frac{1}{\sqrt{\pi}}\int_0^\infty\frac{dt\, e^{-t}}{\sqrt{t}}\left\{g^{-1}\left[\left[t\left[\frac{96}{5mh^4}+\frac{10m}{3h^2}\right]\right]^{1/2}\right]+g^{-1}\left[-\left[t\left[\frac{96}{5mh^4}+\frac{10m}{3h^2}\right]\right]^{1/2}\right]\right\}\\ &=\frac{2}{\sqrt{\pi}}\int_{-\infty}^{\infty}dx\, e^{-s^2/2}g^{-1}\left[s\left[\frac{48}{5mh^4}+\frac{5m}{3h^2}\right]^{1/2}\right] . \end{aligned} \tag{31}$$

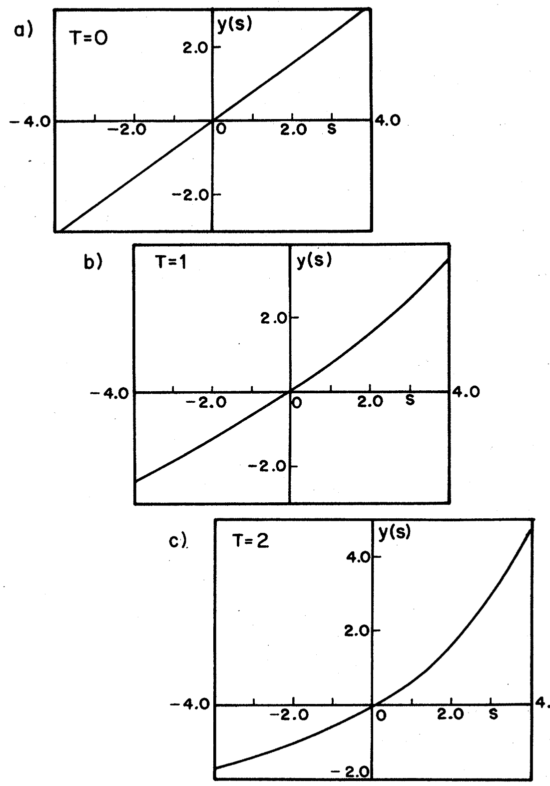

FIG. 2. Plot of the solution to the cubic equation in (34) for $y(s)$ as a function of s for (a) $T=0$, (b) $T=1$, and (c) $T=2$. At $T+0$, $y(s)$ is a straight line, but as T increases, $y(s)$ approaches $y=0$ for $s<0$ and curves away from $y=0$ for $s>0$.

For the Hamiltonian in (11)

$$g(x)=\frac{4}{h^2}x+\frac{5m^{3/2}}{324}(2m^{3/2}x^3-21mx^2+45m^{1/2}x) .$$

Thus, to compute the integrand in (31) it is necessary to solve the cubic equation

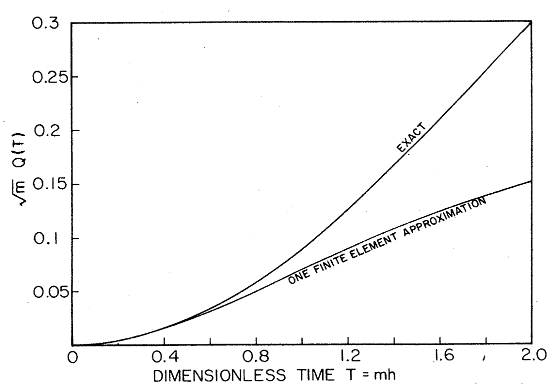

FIG. 3. $y=0$ for $s<0$ and curves away from $y=0$ for $s>0$. Comparison between the exact numerical value of $\sqrt{m}\,Q(T)$ and the one-finite-element approximation to $\sqrt{m}\,Q(T)$. Note that the one-finite-element approximation is no longer accurate when T is larger than about 1.5.

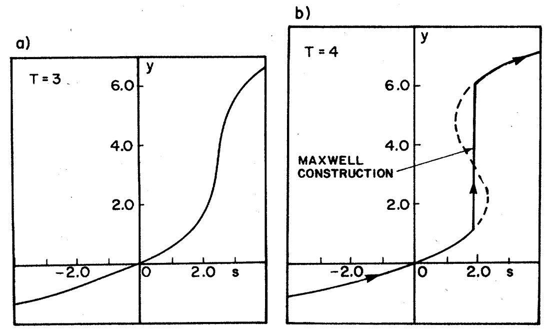

FIG. 4. Plot of the solution of (34) for $y(s)$ as a function of s for (a) $T=3$ and (b) $T=4$. When $T>T_0=\sqrt{864/95}\cong 3.02$ the curve becomes multiple valued. The ambiguity is removed by a Maxwell construction which produces a single-valued convex curve. The integration in (33) is over the solid curve and excludes the dashed curve.

$$s\left[\frac{48}{5mh^4}+\frac{5}{3}\frac{m}{h^2}\right]^{1/2}=\frac{4}{h^2}x+\frac{5m^{3/2}}{324}(2m^{3/2}x^3-21mx^2+45m^{1/2}x) \quad (32)$$

for x for each value of s in the range $-\infty<s<\infty$ and to substitute these values of x for the g^{-1} term in (31).

It is convenient to introduce dimensionless variables: we measure time in units of $1/m$

$$T=hm$$

and we let $y=x\sqrt{m}$ in (32). The final result is that

$$Q(T)=\langle 0|q_1|0\rangle=\left[\frac{2}{\pi m}\right]^{1/2}\int_{-\infty}^{\infty}ds\, e^{-s^2/2}y , \quad (33)$$

where y is the root of

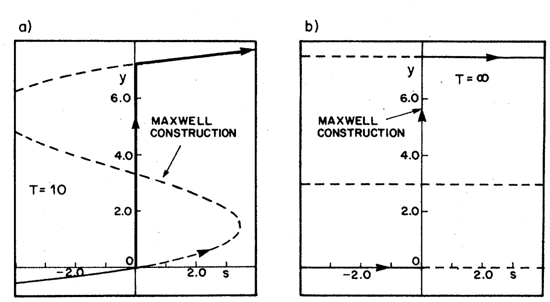

FIG. 5. Same as in Fig. 4 except that (a) $T=10$ and (b) $T=\infty$. At $T=\infty$, $y(s)=0$, 3, and 7.5. The Maxwell construction forces the integration to be done on the step function $y(s)=0$ ($s<0$, and $y(s)=7.5$ ($s\geq 0$).

$$2y^3-21y^2+\left[45+\frac{1296}{5T^2}\right]y+\frac{648s}{5T^2}\left[\frac{12}{5}+\frac{5T^2}{12}\right]^{1/2}=0\,. \qquad (34)$$

IV. NUMERICAL RESULTS

To evaluate the Borel transform integral in (33) for $Q(T)$ we must solve the cubic in (34) for y as a function of s for that value of the dimensionless time T. In Fig. 2 we plot $y(s)$ as a function of s for $T=0$, 1, and 2. Observe that as T increases from 0 the positive values of s contribute more to the Borel integral than the negative values.

The result of this calculation for $Q(T)$ $(0\leq T\leq 2)$ is shown in Fig. 3. A comparison with the exact numerical value for $Q(T)$ shows that for $T\gtrsim 1.5$ the one-finite-element approximation ceases to be accurate. [More finite elements must be used if we wish to compute $Q(T)$ accurately for larger values of T.]

What happens if we try to evaluate the integral in (33) for values of T larger than 2? In Fig. 4 we plot $y(s)$ as a function of s for (a) $T=3$ and (b) $T=4$. Observe that at $T=3$, an inflection point has developed at $s\simeq 2.5$. As T increases, it passes a critical value at $T=T_0=(864/95)\cong 3.02$ where the curve $y(s)$ becomes triple valued [see Fig. 4(b)]. At this point the integrand in (33) becomes ambiguous. One way to remove this ambiguity is to use a Maxwell (equal area) construction. This algorithm consists of following the curve $y(s)$ from $s=-\infty$ along the lower branch until it reaches that value of $s=s^*$, where $y(s)$ has a point of inflection. Then we jump to the largest value of $y(s)$ at s^* and continue on the top branch. (For the special case of a cubic curve this is the "equal area" construction.) This construction allows the integration to be performed on a single-valued and convex curve.[3]

As T continues to increase, the sigmoidal nature of the curve $y(s)$ becomes more exaggerated until, at $T=\infty$ the integration in (33) is performed over a step function: $y(s)=0$ $(s<0)$, $y(s)=7.5$ $(s\geq 0)$ (see Fig. 5). Hence, at $T=\infty$ the integral (33) can be done exactly:

$$Q(\infty)=\left[\frac{2}{\pi m}\right]^{1/2}\int_0^\infty ds\, e^{-s^2/2}(7.5)=\frac{7.5}{\sqrt{m}}\,. \qquad (35)$$

Figure 6 gives a plot of $\sqrt{m}\,Q(T)$ for $T\geq 0$. Observe that

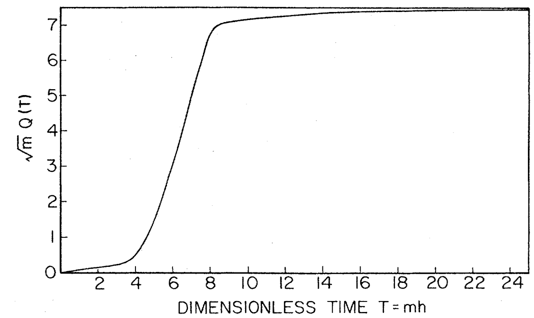

FIG. 6. The one-finite-element approximation to $\sqrt{m}\,Q(T)$ for $T>0$. Observe that as $T\rightarrow\infty$ the curve asymptotes to the value 7.5, which is exactly the position of the true vacuum of the potential (see Fig. 1).

in the one-finite-element approximation $\sqrt{m}\,Q(T)$ approaches the value 7.5 as $T\rightarrow\infty$. This is exactly the position of the absolute minimum (true vacuum) of the potential V (see Fig. 1). It is amusing that the Maxwell construction gives a result for $Q(T)$ in Fig. 6 which would be valid if the system were dissipative (after tunneling, the wave function would accumulate at the bottom of the well at $z=7.5$).

Of course, the exact value of $Q(T)$ does not rise monotonically with T. As T increases, the true $Q(T)$ has many maxima and minima that correspond to the wave function ψ in coordinate space sloshing back and forth in the potential well V in Fig. 1; as $T\rightarrow\infty$, $Q(T)$ oscillates between 0 and 7.5 and does not approach 7.5.[4] The approximate $Q(T)$ in (33) arises from a one-finite-element calculation which is too simple to have the elaborate structure of the true $Q(T)$. However, the one-finite-element approximation is remarkable in that as $T\rightarrow\infty$ it does not produce a $Q(T)$ that behaves absurdly. Indeed the $Q(T)$ in Fig. 6 appears to be in some rough sense an average over the fluctuations of the true $Q(T)$ in a model with a dissipative term. The approximate $Q(T)$ remains for a time in the false-vacuum state, rapidly tunnels to the true-vacuum state, and then remains there for all time.

ACKNOWLEDGMENTS

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[1]C. M. Bender and D. H. Sharp, Phys. Rev. Lett. **50**, 1535 (1983).

[2]The error is of order $1/n^2$. See C. M. Bender, K. Milton, and D. H. Sharp, Phys. Rev. D **31**, 383 (1985).

[3]A similar kind of problem arises in determining the convex effective potential. In that case we obtain the convex hull of the classical potential when we average over the secondary minima to obtain the Maxwell construction. See F. Cooper and B. Freedman, Nucl. Phys. **B239**, 459 (1984).

[4]The function $Q(T)$ cannot approach a constant because $\psi(x,t)$ is an infinite linear combination of eigenstates of the potential V whose eigenfrequency differences are not commensurate.