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Matrix methods in discrete-time quantum mechanics

Carl M. Bender
Department of Physics, Washington University, St. Louis, Missouri 63130

L. M. Simmons, Jr.
Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

Richard Stong
Department of Physics, Washington University, St. Louis, Missouri 63130

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The operator difference equations that arise in the finite-element treatment of a quantum theory are implicit and therefore difficult to solve. By introducing a matrix formulation it is possible to circumvent the implicit character of these equations and obtain explicit closed-form solutions for arbitrary matrix elements of any operator.

I. INTRODUCTION

In a previous paper[1] we showed how to approximate the Heisenberg equations of motion for a quantum-mechanical system having one degree of freedom by a system of operator difference equations. For the Hamiltonian

$$H=\tfrac{1}{2}p^2+V(q) \tag{1.1}$$

the Heisenberg equations in the continuum are

$$\dot{q}=p,\quad \dot{p}=-V'(q)\ . \tag{1.2}$$

This system of evolution equations exactly preserves the values of the equal-time commutator

$$[q(t),p(t)]=i\ . \tag{1.3}$$

In Ref. 1 we discretize the differential equations (1.2) by introducing a time lattice with lattice spacing h. On this lattice the equations of motion become

$$\frac{q_{n+1}-q_n}{h}=\frac{p_{n+1}+p_n}{2}\ , \tag{1.4a}$$

$$\frac{p_{n+1}-p_n}{h}=-V'\left[\frac{q_{n+1}+q_n}{2}\right], \tag{1.4b}$$

where q_n is the approximation to $q(nh)$. The error in this approximation[1] is of order h^2 for small h.

There are, of course, many discretizations of (1.2). The virtue of the operator difference equations (1.4) is that they exactly preserve the equal-time commutation relations at each lattice point:

$$[q_{n+1},p_{n+1}]=[q_n,p_n]=i\ . \tag{1.5}$$

On the other hand, the system of operator equations (1.4) is difficult to solve because it is implicit.

The implicit character of these equations is illustrated by the algebraic equation $y=g(x)$. In all quantum systems studied in the finite-element method it is necessary to obtain the solution $x=g^{-1}(y)$ in order to solve exactly the operator difference equations. For nontrivial (nonharmonic) potentials, the function g^{-1} may be complicated, unwieldy, and difficult to obtain in closed form. It is remarkable that, in the matrix formulation discussed in this paper, one can obtain exact closed-form expressions for arbitrary matrix elements of any operator in terms of the function g. The function g^{-1} never appears. The main purpose of this paper is to demonstrate the matrix formalism necessary to solve this implicit set of operator equations.

We introduce a one-parameter set of Fock states, $|\,n\,\rangle$, which can be constructed because q_0 and p_0 satisfy canonical commutation relations. We take

$$p_0=\frac{a-a^\dagger}{i\gamma\sqrt{2}},\quad q_0=\frac{\gamma}{\sqrt{2}}(a+a^\dagger)\ , \tag{1.6}$$

where $[a,a^\dagger]=1$. The Fock states satisfy

$$a\,|\,n\,\rangle=\sqrt{n}\,|\,n-1\,\rangle\ ,$$
$$a^\dagger\,|\,n\,\rangle=\sqrt{n+1}\,|\,n+1\,\rangle\ . \tag{1.7}$$

The parameter γ is a measure of the width of these states:

$$\langle\, n\,|\,q_0{}^2\,|\,n\,\rangle=\gamma^2(n+\tfrac{1}{2})\ . \tag{1.8}$$

In terms of these Fock states we construct our matrix mechanics and obtain explicit closed-form expressions for $\langle n\,|\,q_1\,|\,m\rangle$, $\langle n\,|\,p_1\,|\,m\rangle$, $\langle n\,|\,q_1{}^2\,|\,m\rangle$, $\langle n\,|\,p_1{}^2\,|\,m\rangle$. These results, which are derived in Sec. II, are valid for a broad class of potentials $V(q)$. Our matrix formulas are solutions to the one-time-step problem. That is, given the initial operators q_0 and p_0 and the set of Fock states $|\,n\,\rangle$ defined in terms of q_0 and p_0 we can calculate the matrix elements of the operators q_1 and p_1 at the next point on the time lattices. By iterating the solution to the one-time-step problem one can find the matrix elements of the operators p_n and q_n at later points $t=nh$. We also examine in Sec. II the asymptotic limits and other behavior of these matrix elements, relate the results to the tunneling problem, and calculate some specific examples.

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In a continuum theory the most important operator is the Hamiltonian, which is the generator of infinitesimal time translations. On a lattice no such operator exists because there are no infinitesimal translations. There is, however, a unitary operator U that advances the field operators q_n, p_n by one time step:

$$q_{n+1}=Uq_nU^{-1},\quad p_{n+1}=Up_nU^{-1}\ . \tag{1.9}$$

In Sec. III we calculate the matrix elements of the operator U and show how to use these matrix elements to calculate explicitly the matrix element of any operator at the time step n.

II. DETERMINATION OF MATRIX ELEMENTS

In this section we calculate the general matrix elements of monomials of the operators q_1 and p_1.

A. Calculation of $\langle m \mid q_1 \mid n \rangle$

We begin with the difference equations (1.4) with $n=0$:

$$\frac{q_1-q_0}{h}=\frac{p_1+p_0}{2}\ , \tag{2.1a}$$

$$\frac{p_1-p_0}{h}=-V'\left[\frac{q_1+q_0}{2}\right]\ . \tag{2.1b}$$

We solve (2.1a) for p_1,

$$p_1=-p_0+\frac{2}{h}(q_1-q_0)\ , \tag{2.2}$$

and substitute this result into (2.1b) to obtain

$$\frac{2p_0}{h}+\frac{4}{h^2}q_0=V'\left[\frac{q_1+q_0}{2}\right]+\frac{4}{h^2}\frac{q_1+q_0}{2}\ . \tag{2.3}$$

We let

$$x=\tfrac{1}{2}(q_1+q_0)\ , \tag{2.4a}$$

$$y=\frac{2p_0}{h}+\frac{4}{h^2}q_0\ , \tag{2.4b}$$

and[2]

$$g(x)=V'(x)+\frac{4}{h^2}x\ . \tag{2.4c}$$

Then (2.3) has the form

$$g(x)=y\ , \tag{2.5}$$

which is the crucial implicit equation that must be solved, as discussed in Sec. I. Under the assumption that the potential $V(x)$ is such that $g(x)$ has a unique inverse, the solution of (2.5) is $x=g^{-1}(y)$. It is sufficient that $V'(x)$ be monotonically increasing or that $V(x)$ be a single-well potential. Then

$$q_1=-q_0+2g^{-1}\left[\frac{2p_0}{h}+\frac{4q_0}{h}\right]\ , \tag{2.6a}$$

$$p_1=-p_0-\frac{4}{h}q_0+\frac{4}{h}g^{-1}\left[\frac{2p_0}{h}+\frac{4q_0}{h}\right]\ . \tag{2.6b}$$

We now take the m,n matrix element of (2.6a) in the complete set of Fock states introduced in Sec. I:

$$\langle m \mid q_1 \mid n\rangle=-\langle m \mid q_0 \mid n\rangle+2\langle m \mid g^{-1}(y) \mid n\rangle\ . \tag{2.7}$$

From (1.6) and (1.7) we get

$$\langle m \mid q_0 \mid n\rangle=\frac{\gamma}{\sqrt{2}}(\sqrt{n}\,\delta_{m,n-1}+\sqrt{n+1}\,\delta_{m,n+1})\ . \tag{2.8}$$

To compute the second term in (2.7) we make one more assumption about the potential $V(x)$, namely, that $g^{-1}(y)$ has a Taylor expansion:

$$g^{-1}(y)=\sum_{n=0}^{\infty}a_n y^n\ . \tag{2.9}$$

Thus, the problem is to calculate

$$M_{mn}=\langle m \mid g^{-1}(y) \mid n\rangle=\sum_{k=0}^{\infty}a_k\langle m \mid y^k \mid n\rangle\ . \tag{2.10}$$

We obtain $\langle m \mid y^k \mid n\rangle$ by introducing the generating function $G(t)=\langle m \mid e^{ty} \mid n\rangle$ and using the identity $e^{A+B}=e^Ae^Be^{-[A,B]/2}$, which holds if $[A,B]$ is a c number. We substitute the result in (2.10) and use the identity

$$\frac{(2p+2l+m-n)!}{p!}=\frac{2^{2p+1}}{\sqrt{\pi}}\int_0^{\infty}dx\,e^{-x^2}\times\left[\frac{d}{dx}\right]^{m-n+2l}x^{2p+2l+m-n}\ . \tag{2.11}$$

A straightforward calculation produces

$$M_{mn}=\left[\frac{m!n!}{\pi}\right]^{1/2}\left[\frac{e^{-i\theta}}{\sqrt{2}}\right]^{m-n}\sum_{l=0}^{\infty}\frac{2^{-l}}{l!(n-l)!(m-n+l)!}\int_{-\infty}^{\infty}dx\,e^{-x^2}\left[\frac{d}{dx}\right]^{m-n+2l}g^{-1}(2xR)\ , \tag{2.12}$$

where we have introduced

$$Re^{i\theta}=\frac{2\gamma}{h^2}+\frac{1}{ih\gamma}\ . \tag{2.13a}$$

With this definition

$$R^2=\frac{4\gamma^2}{h^4}+\frac{1}{h^2\gamma^2}\ , \tag{2.13b}$$

$$e^{2i\theta}=\frac{2i\gamma^2+h}{2i\gamma^2-h}\ , \tag{2.13c}$$

$$\cos\theta=\frac{2\gamma}{Rh^2}\ . \tag{2.13d}$$

We integrate (2.12) by parts[3] repeatedly and use the definition of the Hermite polynomial

$$H_n(x)=(-1)^n e^{x^2}\frac{d^n}{dx^n}e^{-x^2}\ .$$

[With this definition the first few Hermite polynomials are $H_0(x)=1$, $H_1(x)=2x$, $H_2(x)=4x^2-2$.] Then

$$M_{mn}=\left[\frac{m!n!}{\pi}\right]^{1/2}\left[\frac{e^{-i\theta}}{\sqrt{2}}\right]^{m-n}\times\sum_{l=0}^{\infty}\frac{2^{-l}}{l!(n-l)!(m-n+l)!}\times\int_{-\infty}^{\infty}dx\,g^{-1}(2xR)e^{-x^2}H_{m-n+2l}(x)\ . \qquad (2.14)$$

We perform the sum using the identity[4]

$$\sum_{k=0}^{\min(m,n)}2^k k!\binom{m}{k}\binom{n}{k}H_{m+n-2k}(x)=H_m(x)H_n(x)\ , \qquad (2.15)$$

and obtain

$$M_{mn}=\frac{e^{i\theta(n-m)}}{(m!n!\pi 2^{n+m})^{1/2}}\times\int_{-\infty}^{\infty}dx\,e^{-x^2}g^{-1}(2xR)H_n(x)H_m(x)\ . \qquad (2.16)$$

The integral in (2.16) contains a clumsy and difficult to calculate function $g^{-1}(2xR)$. Fortunately the simple change of variables $z=g^{-1}(2xR)$ allows us to express the matrix element M_{mn} entirely in terms of the function g. Using (2.7) and (2.8), our final result is

$$\langle m\,|q_1|\,n\rangle=\frac{-\gamma}{\sqrt{2}}(\sqrt{n}\,\delta_{m,n-1}+\sqrt{m}\,\delta_{n,m-1})+\frac{e^{i\theta(n-m)}}{R(\pi 2^{n+m}n!m!)^{1/2}}\int_{-\infty}^{\infty}dz\,z\,e^{-g^2(z)/4R^2}g'(z)H_n\left[\frac{g(z)}{2R}\right]H_m\left[\frac{g(z)}{2R}\right]\ . \qquad (2.17)$$

A similar result can be obtained for $\langle m\,|p_1|\,n\rangle$ by taking the m,n matrix element of (2.2) and using (2.17).

B. Calculation of $\langle m\,|q_1{}^2|\,n\rangle$

From the expression (2.17) for $\langle m\,|q_1|\,n\rangle$ and the completeness of the Fock states we can express $\langle m\,|q_1{}^2|\,n\rangle$ as a sum:

$$\langle m\,|q_1{}^2|\,n\rangle=\sum_{k=0}^{\infty}\langle m\,|q_1|\,k\rangle\langle k\,|q_1|\,n\rangle\ . \qquad (2.18)$$

To perform the summation we use the identity[5]

$$\sum_{k=0}^{\infty}\frac{(\frac{1}{2})^k}{k!}H_k(x)H_k(y)=e^{x^2}\sqrt{\pi}\,\delta(x-y)\ . \qquad (2.19)$$

The result is

$$\langle m\,|q_1{}^2|\,n\rangle=\frac{\gamma^2}{2}\{[n(n-1)]^{1/2}\delta_{m,n-2}+(2m+1)\delta_{m,n}+[m(m-1)]^{1/2}\delta_{n,m-2}\}+\frac{e^{i\theta(n-m)}}{R(\pi n!m!2^{n+m})^{1/2}}\times\int_{-\infty}^{\infty}dz\,z\,e^{-g^2(z)/(4R^2)}g'(z)\left[2zH_n(z)H_m(z)-\frac{\gamma g(z)}{R}\cos\theta H_n(z)H_m(z)-i\gamma\sin\theta[H_n(z)H_m'(z)-H_n'(z)H_m(z)]\right]\ . \qquad (2.20)$$

Matrix elements of higher powers of q_1 and p_1 can be determined in the same way by the insertion of a complete set of Fock states.

C. Asymptotic behavior of matrix elements

The large-h asymptotic behavior of these matrix elements is particularly simple. This limit may seem inappropriate because the usual rationale for a lattice theory is as an approximation to an underlying continuum theory; thus the usual concern is with the limit $h\to 0$. The lattice theory we are investigating here, in addition to being a useful approximation to the continuum theory as $h\to 0$, is also a completely consistent quantum theory in its own right. In the limit $h\to\infty$ we can see the connection between an initial quantum state and a final quantum state in the far future.

One might expect that the matrix elements of powers of the position and momentum operators would become infinite as $h\to\infty$. This is what would happen in a typical finite difference or "shooting method" discretization of a classical differential equation. It is surprising that as $h\to\infty$ the matrix elements calculated in this section approach finite limiting values that can be obtained easily using Laplace's method for the asymptotic expansion of integrals.

In the limit $h\to\infty$ we know from (2.13b) that $R\sim 1/\gamma h$ and from (2.4c) that $g(z)\sim V'(z)$. In the integral in (2.17) the saddle point z_0 occurs where the derivative of the exponent $[V'(z)]^2$ vanishes. Because $V''(z)>0$ for all z, the saddle point satisfies

$$V'(z_0)=0\ . \qquad (2.21)$$

Expanding the entire integral in Taylor series about $z=z_0$ and evaluating the resulting Gaussian integral gives an extremely simple expression for the asymptotic form of the matrix element of q_1:

$$\lim_{h\to\infty}\langle m\,|q_1|\,n\rangle=\frac{-\gamma}{\sqrt{2}}(\sqrt{n}\,\delta_{m,n-1}+\sqrt{m}\,\delta_{n,m-1})+2z_0\delta_{n,m}\ . \qquad (2.22)$$

Similarly, we can use Laplace's method on the integral in (2.20) to find the asymptotic behavior of the matrix element of $q_1{}^2$:

$$\lim_{h\to\infty}\langle m\,|q_1{}^2|\,n\rangle=\delta_{n,m}[\gamma^2(m+\tfrac{1}{2})+4z_0{}^2]-2z_0\gamma\sqrt{2}(\delta_{m,n-1}\sqrt{n}+\delta_{n,m-1}\sqrt{m}\,)+\frac{\gamma^2}{2}\{\delta_{m,n-2}[n(n-1)]^{1/2}+\delta_{n,m-2}[m(m-1)]^{1/2}\}\ . \qquad (2.23)$$

Of course, (2.23) also follows directly from (2.22) and the completeness of the Fock states. This procedure can be extended to obtain the asymptotic behavior of the matrix element of any power of q_1 or p_1.

D. A simple example: The displaced harmonic oscillator

We illustrate the general results obtained so far with a simple example. Consider the continuum Hamiltonian for the displaced harmonic oscillator,

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}m^2(q-a)^2\ . \qquad (2.24)$$

The continuum Heisenberg equations of motion are $\dot{q}=p$ and $\dot{p}=-m^2(q-a)$. On the lattice these give the difference equations

$$\frac{q_1-q_0}{h}=\frac{p_1+p_0}{2}\ , \qquad (2.25a)$$

$$\frac{p_1-p_0}{h}=-m^2\left[\frac{q_1+q_0}{2}-a\right]\ . \qquad (2.25b)$$

The solutions to these equations are

$$q_1=\frac{q_0(4-m^2h^2)+4hp_0+2am^2h^2}{4+m^2h^2}\ , \qquad (2.26a)$$

$$p_1=\frac{p_0(4-m^2h^2)-4m^2hq_0+4m^2ha}{4+m^2h^2}\ . \qquad (2.26b)$$

Observe that

$$\lim_{h\to\infty}q_1=-q_0+2a\ , \qquad (2.27a)$$

$$\lim_{h\to\infty}p_1=-p_0\ . \qquad (2.27b)$$

The m,n matrix element of (2.27a) is consistent with the asymptotic behavior of $\langle m\,|q_1|\,n\rangle$ calculated in (2.22).

As a special case consider the behavior of $\langle 0|q_1|0\rangle$ and $\langle 0|p_1|0\rangle$ as functions of h. As $h\to\infty$ this first matrix element approaches $2a$ and, in general,

$$\langle 0|q_1|0\rangle=\frac{2am^2h^2}{4+m^2h^2}\ , \qquad (2.28a)$$

$$\langle 0|p_1|0\rangle=\frac{4m^2ah}{4+m^2h^2}\ . \qquad (2.28b)$$

Notice that as h ranges from zero to infinity $\langle 0|q_1|0\rangle$ increases monotonically from zero to $2a$ following a curve that has an inflection point at $h=2/(m\sqrt{3})$. Moreover this matrix element reaches half of its maximum value when $h=2/m$. The matrix element $\langle 0|p_1|0\rangle$ increases monotonically from zero to its maximum value ma as h ranges from zero to $2/m$ and then decreases to zero as $h\to\infty$.

These lattice results are very different from the oscillating behavior of $\langle 0|q(t)|0\rangle$ and $\langle 0|p(t)|0\rangle$ in the continuum theory. In particular,

$$\langle 0|q(t)|0\rangle=a[1-\cos(mt)]\ , \qquad (2.29a)$$

$$\langle 0|p(t)|0\rangle=am\sin(mt)\ , \qquad (2.29b)$$

in the continuum theory. These continuum theory results show that the wave packet begins at $\langle q\rangle=0$ with $E=m/2+m^2a^2/2$ and oscillates between the classical turning points at $a\pm(a^2+1/m)^{1/2}$. In contrast, the lattice results in (2.28) show that the wave packet moves to the right and reaches a maximum momentum ma at $\langle 0|q_1|0\rangle=a$, when $h=2/m$. Past this point the wave packet gradually decelerates and comes to rest on the right side of the well at $\langle 0|q_1|0\rangle=2a$, without ever reaching the classical turning point. Thus, the discrete-time quantum theory results are very different from the continuum theory and violate continuum theory intuition.

A numerical comparison of (2.28) and (2.29) shows that the one-time-step finite-element approximation is useful for times up to about one-fourth the classical period of oscillation $T=2\pi/m$. To be specific, at $h=t=T/16$ the relative error between (2.29a) and (2.28a) is -2.5% and the relative error between (2.29b) and (2.28b) is -1.2%. At $T/8$ and $T/4$ the corresponding results are $(-9\%, -4\%)$ and $(-25\%,-3\%)$.

On the basis of these results we feel that it is reasonable, in general, to use the one-time-step finite-element approximation for times of order $h\leq\frac{1}{4}T$, where T is the classical period of oscillation for the potential at hand.[6]

III. MATRIX ELEMENTS OF THE TIME-EVOLUTION OPERATOR

In Ref. 1 we derived the unitary operator U that produces time translations on the lattice [see (1.9)]. For the Hamiltonian (1.1) the explicit form of U is

$$U=e^{ip_n{}^2h/4}e^{iA(q_n)h}e^{-ip_n{}^2h/4}\ , \qquad (3.1)$$

where[2]

$$A(a)=\frac{2}{h^2}\left[q-\frac{4}{h^2}g^{-1}(q)\right]^2+V\left[\frac{4}{h^2}g^{-1}(q)\right]\ . \qquad (3.2)$$

In (3.1) U is given at the nth lattice site, that is, it is expressed in terms of the operators q_n and p_n. It is easy to see,[1] however, that U is independent of the choice of lattice site, n.

To calculate $\langle m\,|U|\,n\rangle$ one inserts complete sets of position and momentum eigenstates between the factors in (3.1) and computes the integrals that arise. The result is

$$\langle m \mid U \mid n \rangle = \frac{e^{-i\theta(m+n+1)}}{\pi^{1/2}(m!n!2^{m+n})^{1/2}h^2R} \int_{-\infty}^{\infty} dz\, g'(z) H_m\left[\frac{g(z)}{2R}\right] H_n\left[\frac{g(z)}{2R}\right] \exp\left[ihV(z)+i\frac{h^3}{8}[V'(z)]^2-\frac{e^{-i\theta}}{\gamma h^2 R}g^2(z)\right]. \tag{3.3}$$

This is equivalent to the operator expression

$$U = e^{-i\theta a^\dagger a}\exp\left[ihA(h^2Rq/\gamma)-\frac{ih}{2}q^2\right]e^{-i\theta a a^\dagger}. \tag{3.4}$$

Also notice that (3.3) has the same general form as (2.17). In the expression (2.17) for $\langle m \mid q_1 \mid n \rangle$, a factor of $z\exp[-g^2(z)R^{-2}/4]$ appears in the integral. In the expression (3.3) for $\langle m \mid U \mid n \rangle$, this factor is replaced by an exponential.

The matrix element in (3.3) can be used to calculate the m,n matrix element of any operator (consisting of any combination of p and q operators) at any time step N. We need only premultiply and postmultiply by N powers of the matrix elements of U and U^{-1} summing over the intermediate states. This operation can be performed on a computer by truncating the matrix (3.3) to a dimension appropriate to the numerical accuracy required. The results of such numerical calculations will be discussed elsewhere.

[1]C. M. Bender, K. A. Milton, D. H. Sharp, L. M. Simmons, Jr., and R. Stong, Phys. Rev. D 32, 1476 (1985).

[2]We caution the reader that the definition of $g(x)$ used in this paper differs from that in Ref. 1 by a factor of $h^2/4$, which produces a change in the corresponding definitions of g^{-1} and A.

[3]One can integrate by parts in (2.12) unless $g^{-1}(z)$ diverges at least as strongly as e^{z^2} as $z\to\infty$. Such behavior implies that $g(z)$ grows very slowly as $z\to\infty$. For example, $g^{-1}(z)\sim e^{z^2}$ implies that $g(z)\sim\sqrt{\ln z}$ $(z\to\infty)$. This contradicts the definition of $g(z)$, (2.4c), which implies that $g(z)$ grows at least linearly for large z.

[4]*Higher Transcendental Functions,* edited by A. Erdélyi (McGraw-Hill, New York, 1953), Vol. 2, p. 195, Eq. 10.13(37).

[5]The identity (2.19) is simply the statement of the completeness of the harmonic-oscillator wave functions. Alternately, it can be derived as a special case, in the limit $z\to 1$, of Mehler's formula [see Ref. 4, p. 194, Eq. 10.13(22)]

$$\sum_{k=0}^{\infty}\frac{(z/2)^k}{k!}H_k(x)H_k(y) = (1-z^2)^{-1/2}\exp\left[\frac{2xyz-z^2(x^2+y^2)}{1-z^2}\right].$$

[6]Roughly the same accuracy is obtained for potentials more complicated than single-well potentials. In a recent study of tunneling in the finite-element approximation using a quartic double-well potential [C. M. Bender, F. Cooper, V. P. Gutschick, and M. M. Nieto, Phys. Rev. D 32, 1486 (1985)] it was found that the one-time-step approximation to $\langle 0 \mid q(t) \mid 0\rangle$ is almost exact at $t=T/16$, has a relative error of 19% at $t=T/8$, and a relative error of 45% at $t=T/4$. Here T is the period of oscillation of the metastable (false vacuum) state.