Discrete-time quantum mechanics

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The finite-element (collocation) method enables us to construct discrete time-lattice quantum systems that accurately approximate continuum quantum systems. The discrete quantum systems so generated are fully consistent quantum-mechanical systems in their own right. This paper gives a comprehensive treatment of such quantum systems. We examine various finite-element schemes, construct the effective lattice Hamiltonian, and calculate eigenvalues. Numerical results are extremely easy to obtain and are very accurate.

I. INTRODUCTION

A recent series of papers[1–3] proposed a new approach to quantum field theory on a lattice. This approach consists of formulating a completely consistent quantum theory in which the field operators are defined on discrete lattice sites in space-time instead of on the space-time continuum. The field operators in this theory satisfy difference equations (instead of differential equations) whose solution exactly satisfies canonical equal-time commutation relations at the lattice sites. In the limit as the lattice spacing h approaches zero, the solution to the discrete theory approaches that of the continuum theory. We emphasize that the lattice is not just an artifice for the approximate evaluation of functional integrals; rather, for every value of h we have a fully consistent quantum theory in which time is a discrete parameter.

Given a continuum quantum theory it is not easy to construct the analogous discrete theory; the equal-time commutation relations are not ordinarily satisfied. (The differencing schemes usually used in the Monte Carlo evaluation of functional integrals lead to inconsistent quantum field theories.) To find a consistent discretization procedure, we use the finite-element (collocation) method.[4] In Refs. 1–3 we used the simplest finite-element procedure, in which the finite elements are linear. The results we have obtained so far are very satisfying. We have applied the method in both quantum mechanics and quantum field theory and we have applied it to both boson and fermion theories. For the case of fermion theories we have shown that the differencing scheme is local and unitary, and chiral invariance is preserved in the massless limit, yet there is no fermion doubling.[2] We have succeeded in formulating an Abelian gauge-invariant set of difference equations, and we have used this approach to solve the massless Schwinger model.[3] We have successfully computed the chiral anomaly in this model; the value of the chiral anomaly in discrete space-time differs from the value of the chiral anomaly in the continuum by a relative error of order N^{-2}, where N is the number of spatial lattice sites.[3]

The purpose of this paper is to present an organized and systematic discussion of discrete time quantum-mechanical systems. (In a second paper we intend to extend this discussion to quantum field theories.) In Sec. II we discuss the use of an rth-degree polynomial finite element and show how to discretize on a time lattice the Hamilton's equations of quantum mechanics. We prove that a consistent discrete quantum mechanics requires that the continuum equations of motion be imposed at the Gauss points (zeros of the rth-degree Legendre polynomial).

The relative error between the exact continuum result and the solution obtained by using N rth-degree finite elements is N^{-2r} when the Gauss points are used. In Sec. III we illustrate the phenomenal accuracy of rth-degree finite elements by examining some simple nonlinear differential equations.

In Sec. IV we show that linear finite elements have a number of advantages: First, the discrete operator equations can be easily converted from implicit to explicit form; second, from the explicit form of the operator difference equations we derive a closed expression for the transfer operator U (the unitary time evolution operator that advances operators forward in time by one lattice step). The effective Hamiltonian for this discrete lattice system is $\mathscr{H}=(\ln U)/(ih)$. The Hamiltonian $\mathscr{H}$ has a Taylor expansion in powers of h^2, $\mathscr{H}=\sum_{n=0}^{\infty}\mathscr{H}_{2n}h^{2n}$, where $\mathscr{H}_0$ is the Hamiltonian for the analogous continuum theory. It is interesting to note that as $h\to\infty$,

$U \to \mathcal{P}$, where $\mathcal{P}$ is the parity operator.

Finally, in Sec. V we address the difficult question of how to use the solution to the discrete lattice theory to determine the spectrum of the Hamiltonian for the underlying continuum theory. Promising approaches are discussed which give excellent numerical results.

II. CONSISTENT DISCRETIZATION OF QUANTUM MECHANICS

Throughout this paper we will consider quantum-mechanical systems defined by a continuum Hamiltonian of the form

$$H=\frac{p^2}{2}+V(q)\ . \tag{2.1}$$

Hamilton's equations for the operators p and q are

$$\dot{q}=p \tag{2.2}$$

and

$$\dot{p}=f(q)\ , \tag{2.3}$$

where

$$f(q)=-V'(q) \tag{2.4}$$

is the force. Equations (2.2) and (2.3) define a time-evolution problem, where, in quantum mechanics, the initial condition takes the form of an equal-time commutation relation

$$[q(0),p(0)]=i\ . \tag{2.5}$$

By virtue of Hamilton's equations, the operators q and p satisfy the canonical equal-time commutation relation for all times:

$$[q(t),p(t)]=i\ . \tag{2.6}$$

The finite-element method provides a simple means of converting a differential equation into a difference equation. Let $y(t)$ satisfy a first-order ordinary differential equation in t:

$$\dot{y}=F(y)\ . \tag{2.7a}$$

An initial condition,

$$y(0)=y_0\ , \tag{2.7b}$$

is given and the goal is to find $y(T)$. We divide the interval $(0,T)$ into N intervals of length h where $Nh=T$. On the nth interval, $(n-1)h \le t \le nh$, we introduce a local variable x defined by

$$x=t-(n-1)h\ , \tag{2.8}$$

so that $0 \le x \le h$. We then approximate $y(t)$ on the nth interval by an rth-degree polynomial of the form $\sum_{k=0}^{r} a_k (x/h)^k$. If we can determine the coefficients a_k on the first interval, we then have a good approximation to $y(t)$ on that interval. In particular, we have an approximation y_1 to $y(h)$:

$$y_1=\sum_{k=0}^{r} a_k \cong y(h)\ . \tag{2.9}$$

We continue this procedure, obtaining subsequent approximations $y_2, y_3, \ldots$ to $y(2h), y(3h), \ldots$. After N steps, we obtain y_N, the N-finite-element approximation to $y(T)$.

To find the sequence of approximations $y_1, y_2, y_3, \ldots, y_N$ it is necessary to determine the $r+1$ coefficients a_k on each interval. However, the procedure is quite ambiguous. If we impose the differential equation d times on the nth interval, then it is necessary to impose $r+1-d$ joining conditions (continuity, continuity of the first derivative, continuity of the second derivative, ...) at $t=(n-1)h$. On the first interval, there are no joining conditions at $t=0$; rather we must impose $r+1-d$ initial conditions, in which the values of $y(0), \dot{y}(0), \ddot{y}(0), \ldots$, are specified. These values are obtained by successively differentiating the differential equation (2.7a) and substituting the initial value (2.7b). We say that as the number of joining conditions increases the approximation becomes *stiffer.*

In one extreme, the stiffest approximation, the differential equation is imposed once on the interval, and in the other extreme, the floppy approximation, the method we will use in this paper, the differential equation is imposed r times, and we require that the approximation only be continuous.

A. Failure of the stiff approximation

We do not use a stiff approximation in this paper because it is forbidden by quantum mechanics. For a quantum-mechanical system with operators p and q the rth-degree finite-element approximation is given in terms of the expansions

$$p(t)=\sum_{k=0}^{r} a_k (x/h)^k\ ,$$

$$q(t)=\sum_{k=0}^{r} b_k (x/h)^k\ ,$$

where $0 \le x \le h$. While we could determine the coefficients a_k on the nth interval from those on the $(n-1)$st interval, attempting to determine the coefficients on the first interval, even in principal, leads to an inconsistency. This is because the coefficients a_k are operators.

We illustrate this problem by a simple example for which $r=2$. On the first interval we represent

$$p(x)=p_0+a_1\frac{x}{h}+a_2\frac{x^2}{h^2} \tag{2.10}$$

and

$$q(x)=q_0+b_1\frac{x}{h}+b_2\frac{x^2}{h^2}\ . \tag{2.11}$$

For the sake of complete generality we impose the differential equations (2.2) and (2.3) at αh and βh, respectively, where $0 \le \alpha, \beta \le 1$ are as yet undetermined:

$$\frac{b_1}{h}+\frac{2b_2}{h}\alpha=p_0+a_1\alpha+a_2\alpha^2\ , \tag{2.12}$$

$$\frac{a_1}{h}+\frac{2a_2}{h}\beta=f(q_0+b_1\beta+b_2\beta^2)\ . \tag{2.13}$$

Next, we impose the initial conditions. The condition (2.5) reads

$$[q_0,p_0]=i\ . \tag{2.14}$$

We also impose two more commutator conditions which we obtain from the continuum equations at $t=0$:

$$[q(0),\dot{p}(0)]=[q_0,a_1]=0\ , \tag{2.15}$$

$$[\dot{q}(0),p(0)]=[b_1,p_0]=0\ . \tag{2.16}$$

There are two more commutator conditions that follow from the equations of motion (2.12) and (2.13):

$$[b_1+2\alpha b_2,p_0+\alpha a_1+\alpha^2 a_2]=0\ , \tag{2.17}$$

$$[a_1+2\beta a_2,q_0+\beta b_1+\beta^2 b_2]=0\ . \tag{2.18}$$

The five commutators, (2.14)–(2.18), are kinematical in nature; they make no reference to the dynamical content of the theory, which is embodied in the function f.

For this quantum system to be internally consistent, (2.14)–(2.16), the analogs of the three equal-time commutators, must hold again at $t=h$; that is

$$[q_0+b_1+b_2,p_0+a_1+a_2]=i\ , \tag{2.19}$$

$$[q_0+b_1+b_2,a_1+2a_2]=0\ , \tag{2.20a}$$

$$[p_0+a_1+a_2,b_1+2b_2]=0\ . \tag{2.20b}$$

We can show that if (2.20) is assumed to hold, then (2.19) holds so long as $\alpha+\beta=1$. However, (2.20) does not hold in general unless $\alpha=1$ and $\beta=1$, which implies the failure of (2.19).

This kind of demonstration can be given for any stiff approximation to a quantum system. Thus, on the basis of quantum-mechanical consistency we reject any kind of stiff finite-element scheme in which more than a single initial commutator is imposed.

Furthermore, even if a consistent stiff approximation could be found, we would prefer not to use it, because it is not as accurate as the floppy approximation; a maximally stiff approximation yields a relative error of N^{-r} between $y(t)$ and y_N. On the other hand, for a floppy approximation, the relative error between these two quantities is N^{-2r}.

B. Consistency of floppy approximation

The failure of the stiff approximation discussed in the previous section is not very surprising and it is all the more remarkable that the floppy approximation *is* successful. We begin by examining the case $r=1$, using the notation of the preceding section.

1. Case $r=1$

Imposing Eqs. (2.2) and (2.3) at $t=\alpha h$ and $t=\beta h$, respectively, yields [here $q_1=q(1h)$, $p_1=p(1h)$]

$$\frac{q_1-q_0}{h}=p_0(1-\alpha)+p_1\alpha\ , \tag{2.21}$$

$$\frac{p_1-p_0}{h}=f(q_0(1-\beta)+q_1\beta)\ , \tag{2.22}$$

in the first finite element. Since $p(0)=p_0$ and $q(0)=q_0$ we have

$$a_0=p_0,\quad b_0=q_0$$

and the continuity conditions at $t=h$ are

$$a_1=p_1-p_0,\quad b_1=q_1-q_0\ .$$

Is there a choice for α and β such that (2.21) and (2.22) together with the equal-time commutator at $t=0$, (2.5), imply that $[q_1,p_1]=i$? Equations (2.21) and (2.22) yield the following commutators:

$$[q_1-q_0,p_0(1-\alpha)+p_1\alpha]=0\ , \tag{2.23}$$

$$[q_0(1-\beta)+q_1\beta,p_1-p_0]=0\ . \tag{2.24}$$

Combining the three commutation relations (2.5), (2.23), and (2.24) does indeed yield $[q_1,p_1]=i$ provided that α and β satisfy the constraint

$$\alpha+\beta=1\ . \tag{2.25}$$

Having shown consistency with quantum mechanics on the first finite element, it follows on all finite elements by virtue of the continuity condition on $p(t)$ and $q(t)$ at the boundaries of adjacent finite elements, $t=nh$.

In this paper we are primarily interested in the symmetric choice $\alpha=\beta=\frac{1}{2}$, where the equations of motion are imposed at the midpoints of the finite elements. Any other choice for α and β breaks time-reversal symmetry and leads to numerical approximations which are not as accurate as in the symmetric case. We will return to this point in Secs. IV and V.

2. Case $r=2$

Here we impose the equations of motion (2.2) and (2.3) twice on each finite element. In view of our above remarks with regard to symmetry and numerical accuracy, we will restrict our attention to the symmetric case where both of the equations of motion are imposed at the *same* points $x=\alpha_1 h$ and $x=\alpha_2 h$.

On the $n=1$ finite element we have

$$p(x)=p_0+a_1\frac{x}{h}+a_2\frac{x^2}{h^2}\ ,$$

$$q(x)=q_0+b_1\frac{x}{h}+b_2\frac{x^2}{h^2}\ .$$

Imposing (2.2) and (2.3) at $x=\alpha_1 h$ and $\alpha_2 h$ gives

$$\begin{aligned}
&\frac{b_1}{h}+\frac{2b_2}{h}\alpha_1=p_0+a_1\alpha_1+a_2\alpha_1^2\ ,\\
&\frac{a_1}{h}+\frac{2a_2}{h}\alpha_1=f(q_0+b_1\alpha_1+b_2\alpha_1^2)\ ,\\
&\frac{b_1}{h}+\frac{2b_2}{h}\alpha_2=p_0+a_1\alpha_2+a_2\alpha_2^2\ ,\\
&\frac{a_1}{h}+\frac{2a_2}{h}\alpha_2=f(q_0+b_1\alpha_2+b_2\alpha_2^2)\ .
\end{aligned} \tag{2.26}$$

From these equations we obtain the kinematical commutators:

$$[p_0+a_1\alpha_1+a_2\alpha_1^2, b_1+2b_2\alpha_1]=0\ ,$$
$$[a_1+2a_2\alpha_1, q_0+b_1\alpha_1+b_2\alpha_1^2]=0\ ,$$
$$[p_0+a_1\alpha_2+a_2\alpha_2^2, b_1+2b_2\alpha_2]=0\ , \tag{2.27}$$
$$[a_1+2a_2\alpha_2, q_0+b_1\alpha_2+b_2\alpha_2^2]=0\ .$$

By adding these commutators we can prove that

$$[q_1,p_1]=[q_0,p_0]=i$$

if and only if α_1 and α_2 are given by

$$\alpha_1=\frac{1}{2}-\frac{1}{\sqrt{12}},\quad \alpha_2=\frac{1}{2}+\frac{1}{\sqrt{12}}\ . \tag{2.28}$$

This is the condition for quantum consistency.

3. Case $r=3$

Now we impose the equations of motion three times on each finite element at $x=\alpha_1 h$, $\alpha_2 h$, and $\alpha_3 h$. Taking

$$p(x)=p_0+a_1x/h+a_2x^2/h^2+a_3x^3/h^3$$

and

$$q(x)=q_0+b_1x/h+b_2x^2/h^2+b_3x^3/h^3$$

we obtain six equations analogous to (2.26) from which we derive six commutator conditions analogous to (2.27). Once again we add the six commutator conditions together. However, now the two commutators at $x=\alpha_2 h$ are weighted by the factor $\frac{8}{5}$. The condition for quantum consistency is now

$$\alpha_1=\tfrac{1}{2}-\sqrt{3/20},\quad \alpha_2=\tfrac{1}{2},\quad \alpha_3=\tfrac{1}{2}+\sqrt{3/20}\ . \tag{2.29}$$

4. The general case

The sequence of points α at which the operator equations of motion must be imposed, $\frac{1}{2}$ for $r=1$; $\frac{1}{2}\pm 1/\sqrt{12}$ for $r=2$; $\frac{1}{2}, \frac{1}{2}\pm\sqrt{3/20}$ for $r=3$, fits a well-known pattern. These numbers are the zeros of the rth Legendre polynomial $P_r(2\alpha-1)$. The first three such polynomials are

$$P_1=2\alpha-1\ ,$$
$$P_2=6\alpha^2-6\alpha+1\ ,$$
$$P_3=(2\alpha-1)(10\alpha^2-10\alpha+1)\ .$$

These zeros are the so-called Gaussian knots or nodes which are used to perform a quadrature integration. The weighting of the commutators necessary to derive the consistency condition (the factor of $\frac{8}{5}$ mentioned above, for example) is exactly the weighting used in Gaussian quadrature.[4]

We conclude this section by reemphasizing that the only way to preserve the equal-time commutation relations is to impose the operator equations of motion at the Gaussian quadrature nodes. If the commutator relations are preserved at successive intervals of time, then the theory is unitary; that is, the transfer operator is unitary and probability is conserved. This same point has been observed in a totally different context by Durand,[5] who showed that a lattice discretization of the Schrödinger equation preserves orthonormality of the wave functions only if the lattice points lie at the Gaussian knots.

III. FINITE-ELEMENT METHOD FOR CLASSICAL EQUATIONS

Using quantum mechanics we have determined in Sec. II the type of finite-element method to be used, namely, that we work at the Gaussian knots. The purpose of this brief section is to illustrate the astounding accuracy of the finite-element methods.

We begin by considering the linear differential-equation initial-value problem

$$y'=y,\quad y(0)=1,\ \text{to find}\ y(1)=e\ . \tag{3.1}$$

Using a simple linear finite element and imposing the differential equation at the Gaussian point $\frac{1}{2}$, we predict $y_1=3$, which has a relative error of 10%. N linear finite elements gives

$$y_N=\left[\frac{2N+1}{2N-1}\right]^N\sim e\left[1+\frac{1}{12N^2}\right]\quad (N\to\infty)\ . \tag{3.2}$$

Next we solve problem (3.1) using quadratic ($r=2$) finite elements. A single quadratic finite element with the differential equation imposed at the Gaussian points $\frac{1}{2}\pm 1/\sqrt{12}$ yields $y_1=\frac{19}{7}$ which differs from e by -0.14%. N quadratic finite elements gives

$$y_N\sim e\left[1-\frac{1}{720N^4}\right]\quad (N\to\infty)\ . \tag{3.3}$$

The corresponding results for the cubic finite elements are, for one finite element, $y_1=\frac{193}{71}$, which has a relative error of 0.0010%. N cubic finite elements gives

$$y_N=e\left[1+\frac{1}{100\,800N^6}\right]\quad (N\to\infty)\ . \tag{3.4}$$

We now examine some nonlinear examples. First, consider

$$y'=\frac{1}{y},\quad y(0)=1,\ \text{to find}\ y(1)=\sqrt{3}\ . \tag{3.5}$$

A single linear finite element gives the exact answer. The single quadratic finite element also gives the exact answer.

Second, consider

$$y'=\sqrt{y},\quad y(0)=1,\ \text{to find}\ y(1)=\tfrac{9}{4}\ . \tag{3.6}$$

A single linear finite element gives $y_1=(5+\sqrt{17})/4\simeq 2.2808$, which corresponds to a relative error of 1.3%. However, a single quadratic finite element gives the exact answer.

Finally, we consider

$$y'=\tfrac{1}{2}y^2,\quad y(0)=1,\ \text{to find}\ y(1)=2\ . \tag{3.7}$$

A single linear finite element gives the exact answer. However, this is a fortuitous event. This is a good problem to illustrate the convergence rate of the quadratic finite-element method which does not give the exact

answer. For one finite element we find $y_1=1.999\,831$ which has a relative error of -0.0085%. For two finite elements the prediction for $y(1)$ is $y_2=2.000\,012$, which has a relative error of $0.000\,60\%$, which is consistent with the expectation that the relative error decreases like N^{-4} (the relative error is smaller by roughly a factor of 16).

In general,[4] the rth-degree finite-element method using Gaussian knots gives results with relative errors which go like N^{-2r}. It is not easy to make *a priori* estimates of relative errors when the finite-element method is applied to quantum differential equations. However, our experience so far is that in quantum systems, numerical predictions are equivalently accurate.[3,6] Indeed the dependence of the relative error on the number of finite elements is the same as for classical differential equations (see Secs. IV and V).

IV. THE TRANSFER OPERATOR FOR LINEAR FINITE ELEMENTS

For the Hamiltonian $H=p^2/2+V(q)$ the case of linear ($r=1$) finite elements is special. This is because it is possible to recast the equations (2.21) and (2.22), which give an implicit relation between p_1,q_1 and p_0,q_0, into an explicit relation, which expresses p_1 and q_1 as functions of p_0 and q_0. On the nth finite element

$$p(x)=p_{n-1}\left[1-\frac{x}{h}\right]+p_n\frac{x}{h}\ ,$$
$$q(x)=q_{n-1}\left[1-\frac{x}{h}\right]+q_n\frac{x}{h}\ . \tag{4.1}$$

[Recall that q_n and p_n are our approximations to the exact operator functions $q(t)$ and $p(t)$ evaluated at the time $t=nh$ and that x is the local variable defined on the nth interval by (2.8).] Treating this problem with full generality, we impose the equations of motion (2.2) and (2.3) at the points $x=\alpha h$ and $x=\beta h$, respectively. As we showed in Sec. II, quantum-mechanical consistency requires

$$\alpha+\beta=1\ . \tag{4.2}$$

The resulting implicit operator recurrence relations are

$$\frac{q_n-q_{n-1}}{h}=p_{n-1}(1-\alpha)+p_n\alpha\ , \tag{4.3}$$

$$\frac{p_n-p_{n-1}}{h}=f(q_{n-1}(1-\beta)+q_n\beta)\ . \tag{4.4}$$

To rewrite these equations in explicit form, we define the function $g(x)$ by

$$g(x)=x-\alpha\beta h^2 f(x)\ . \tag{4.5}$$

Then, in terms of the inverse function $g^{-1}(x)$, we have

$$q_n=-\frac{\alpha}{\beta}q_{n-1}+\frac{1}{\beta}g^{-1}(q_{n-1}+h\beta p_{n-1})\ , \tag{4.6}$$

$$p_n=-\frac{\beta}{\alpha}p_{n-1}-\frac{q_{n-1}}{h\alpha\beta}+\frac{1}{h\alpha\beta}g^{-1}(q_{n-1}+h\beta p_{n-1})\ . \tag{4.7}$$

The derivation of these equations depended crucially on the form of the Hamiltonian. If we generalize the form of the Hamiltonian even slightly to $H=K(p)+V(q)$, the implicit relations

$$\frac{q_n-q_{n-1}}{h}=K'(p_{n-1}(1-\alpha)+p_n\alpha)\ ,$$
$$\frac{p_n-p_{n-1}}{h}=f(q_{n-1}(1-\beta)+q_n\beta)\ , \tag{4.8}$$

do preserve the canonical commutation relation,

$$[q_n,p_n]=[q_{n-1},p_{n-1}]=i\ , \tag{4.9}$$

provided that (4.2) holds, but they can no longer be solved for p_n and q_n.

The same features hold for finite elements with $r>1$. Namely, the canonical commutation relations are preserved if the equations of motion are imposed at the Gaussian knots, but again the implicit equations cannot be recast into explicit form.

A. Derivation of transfer operator

Once we have found the explicit form for the recursion relation in (4.6) and (4.7) it is possible to find a closed-form expression for the transfer operator U, which advances the operators p_n and q_n one time step. The construction proceeds as follows: First, we rewrite (4.3) in the form

$$q_n-h\alpha p_n=q_{n-1}+h\beta p_{n-1}\ . \tag{4.10}$$

Next, we use the identity

$$e^{ip^2s}qe^{-ip^2s}=q+2sp\ , \tag{4.11}$$

where s is a c number, to rewrite (4.10) as

$$e^{-ip_n^2\alpha h/2}q_n e^{ip_n^2\alpha h/2}=e^{ip_{n-1}^2\beta h/2}q_{n-1}e^{-ip_{n-1}^2\beta h/2}$$

or

$$q_n=e^{ip_n^2\alpha h/2}e^{ip_{n-1}^2\beta h/2}q_{n-1}e^{-ip_{n-1}^2\beta h/2}e^{-ip_n^2\alpha h/2}\ . \tag{4.12}$$

The unitary transfer operator U can be written in the form

$$U=e^{i\mathscr{H}h}\ . \tag{4.13}$$

This operator has the property that

$$q_n=Uq_{n-1}U^{-1},\quad p_n=Up_{n-1}U^{-1}\ . \tag{4.14}$$

A comparison with (4.12), suggests the ansatz

$$U=e^{ip_n^2\alpha h/2}e^{ip_{n-1}^2\beta h/2}e^{iAh}\ . \tag{4.15}$$

Substituting this form in (4.14) gives

$$e^{iAh}q_{n-1}e^{-iAh}=q_{n-1}\ .$$

Therefore, we observe that A is a function of q_{n-1} only:

$$A=A(q_{n-1})\ . \tag{4.16}$$

Next we use (4.14) and (4.15) to write

$$p_n = e^{ip_n^2\alpha h/2} e^{ip_{n-1}^2\beta h/2} e^{iA(q_{n-1})h} p_{n-1} e^{-iA(q_{n-1})h} e^{-ip_{n-1}^2\beta h/2} e^{-ip_n^2\alpha h/2} . \tag{4.17}$$

To simplify this equation we premultiply by $e^{-ip_n^2\alpha h/2}$ and postmultiply by $e^{ip_n^2\alpha h/2}$. Then, we replace p_n by the right-hand side of (4.7),

$$-\frac{\beta}{\alpha}p_{n-1} - \frac{1}{h\alpha\beta}q_{n-1} + \frac{1}{h\alpha\beta}g^{-1}(q_{n-1}+h\beta p_{n-1}) = e^{ip_{n-1}^2\beta h/2} e^{iA(q_{n-1})h} p_{n-1} e^{-iA(q_{n-1})h} e^{-ip_{n-1}^2\beta h/2} .$$

This equation simplifies if we premultiply by $e^{-ip_{n-1}^2\beta h/2}$ and postmultiply by $e^{ip_{n-1}^2\beta h/2}$. The result is

$$-\frac{\beta}{\alpha}p_{n-1} - \frac{1}{h\alpha\beta}(q_{n-1}-\beta h p_{n-1}) + \frac{1}{h\alpha\beta}g^{-1}(q_{n-1}) = e^{iA(q_{n-1})h} p_{n-1} e^{-iA(q_{n-1})h}$$

$$= p_{n-1} - A'(q_{n-1})h ,$$

where we have used the identity (4.11). This gives a differential equation for A:

$$A'(q_{n-1}) = \frac{1}{h^2\alpha\beta}[q_{n-1} - g^{-1}(q_{n-1})] . \tag{4.18}$$

It is even possible to find a closed-form solution to (4.18). Integrating both sides of (4.18) gives

$$A(x) = \frac{1}{h^2\alpha\beta}\left[\tfrac{1}{2}x^2 - \int^x ds\, g^{-1}(s)\right] . \tag{4.19}$$

To evaluate the integral we make the change of variable $u = g^{-1}(s)$,

$$A(x) = \frac{1}{h^2\alpha\beta}\left[\tfrac{1}{2}x^2 - \int^{g^{-1}(x)} du\, g'(u)u\right] .$$

We evaluate this integral by parts:

$$A(x) = \frac{1}{h^2\alpha\beta}\left[\tfrac{1}{2}x^2 - xg^{-1}(x) + \int^{g^{-1}(x)} du\, g(u)\right] .$$

Finally, we refer to (4.5) and recall that $f(x) = -V'(x)$:

$$A(x) = \frac{1}{h^2\alpha\beta}\{\tfrac{1}{2}x^2 - xg^{-1}(x) + \tfrac{1}{2}[g^{-1}(x)]^2\} + V[g^{-1}(x)]$$

$$= \frac{1}{2h^2\alpha\beta}[x - g^{-1}(x)]^2 + V[g^{-1}(x)] . \tag{4.20}$$

Having found the exact expression for A we return to (4.15) and rewrite it as

$$U = Ue^{ip_{n-1}^2\alpha h/2} U^{-1} e^{ip_{n-1}^2\beta h/2} e^{iA(q_{n-1})h} .$$

Solving for U we find

$$U = e^{ip_{n-1}^2\beta h/2} e^{iA(q_{n-1})h} e^{ip_{n-1}^2\alpha h/2} . \tag{4.21}$$

This is our final closed-form expression for the transfer operator.

It is important to note that while U in (4.21) depends on p_{n-1} and q_{n-1}, U is independent of n [just as the Hamiltonian $H = p^2/2 + V(q)$ is independent of time t even though p and q are functions of t]. To prove that U is independent of n, we simply multiply (4.21) by U on the left-hand side and U^{-1} on the right-hand side. This transformation does not change U, of course, but has the effect of replacing p_{n-1} and q_{n-1} in (4.21) by p_n and q_n, respectively.

B. Continuum limit

It is easy to compute the continuum limit of the transfer operator. If h is small, $g(x) = x + O(h^2)$. Thus $g^{-1}(x) = x + O(h^2)$ and $A(x)$ in (4.20) is approximately $V(x)$ with corrections of order h^2. Therefore, from (4.21) we have

$$U \simeq e^{ip_{n-1}^2\beta h/2} e^{iV(q_{n-1})h} e^{ip_{n-1}^2\alpha h/2} .$$

If we take the logarithm of this and divide by ih we obtain

$$\frac{\ln U}{ih} = \mathscr{H} \simeq \frac{\alpha+\beta}{2}p_{n+1}^2 + V(q_{n+1}) + O(h) . \tag{4.22}$$

Since $\alpha+\beta = 1$, we have obtained the continuum Hamiltonian in the limit as $h \to 0$.

C. Transfer operator for the harmonic oscillator

For the harmonic oscillator, whose Hamiltonian is given by $H = p^2/2 + m^2q^2/2$, $A(x)$ in (4.21) is

$$A(x) = \frac{m^2x^2}{2(1+\alpha\beta h^2m^2)} . \tag{4.23}$$

Thus, the transfer operator is exactly

$$U = \exp(ip^2\beta h/2) \exp\frac{ihm^2q^2}{2(1+\alpha\beta h^2m^2)} \exp(ip^2\alpha h/2) . \tag{4.24}$$

The three exponentials in (4.24) can be combined exactly into a single exponential:

$$U = e^{i\mathscr{H}h} , \tag{4.25}$$

where

$$\mathscr{H} = \frac{1}{hm} \frac{\arctan\left[\dfrac{mh[1-\frac{1}{4}m^2h^2(1-4\alpha\beta)]^{1/2}}{1-\frac{1}{2}m^2h^2(1-2\alpha\beta)}\right]}{\left[1-\dfrac{m^2h^2}{4}(1-4\alpha\beta)\right]} \times \left[\tfrac{1}{2}p^2 + \tfrac{1}{2}m^2q^2 + \tfrac{1}{2}m^2h(\beta-\alpha)\left[\frac{pq+qp}{2}\right]\right] . \tag{4.26}$$

For small h,

$$\mathscr{H}=\tfrac{1}{2}p^2+\tfrac{1}{2}m^2q^2+\tfrac{1}{4}m^2h(\beta-\alpha)(pq+qp)+O(h^2)\ . \tag{4.27}$$

Observe that $\mathscr{H}$ differs from the continuum Hamiltonian by terms of order h, unless $\alpha=\beta$. The case $\alpha=\beta$ is clearly very special. If $\alpha=\beta=\frac{1}{2}$, only even powers of h occur in the expansion of $\mathscr{H}$ because the equations of motion have been imposed in a time-reversal symmetric manner. If we set $\alpha=\beta=\frac{1}{2}$ in (4.26) we obtain

$$\mathscr{H}=\frac{2}{hm}\arctan\left[\frac{mh}{2}\right](\tfrac{1}{2}p^2+\tfrac{1}{2}m^2q^2)\ . \tag{4.28}$$

D. Cubic anharmonic oscillator

For the quantum-mechanical model whose Hamiltonian is

$$H=\frac{p^2}{2}+\frac{\lambda}{3}q^3\ , \tag{4.29}$$

$$f(x)=-\lambda x^2\ , \tag{4.30}$$

and

$$g^{-1}(x)=\frac{-1+(1+4\alpha\beta h^2\lambda x)^{1/2}}{2\alpha\beta h^2\lambda}\ , \tag{4.31}$$

where the sign of the square root is determined by requiring that g^{-1} be smooth in the limit $h\to 0$. The transfer operator is given by (4.21) where

$$A(x)=\frac{x^2}{2\alpha\beta h^2}+\frac{x}{2\alpha^2\beta^2h^4\lambda}-\frac{(1+4\alpha\beta h^2\lambda x)^{3/2}-1}{12\alpha^3\beta^3h^6\lambda^2}\ . \tag{4.32}$$

If we expand U as a series in powers of h and compute $\mathscr{H}=(1/ih)\ln U$ we obtain

$$\mathscr{H}=\frac{p^2}{2}+\frac{\lambda}{3}q^3-(\beta-\tfrac{1}{2})\lambda hqpq+O(h^2)\ \ (h\to 0)\ . \tag{4.33}$$

Once again, observe that in the special case $\alpha=\beta=\frac{1}{2}$, the corrections are of order h^2. Since first-order corrections to $\mathscr{H}$ vanish in the symmetric case, evidently numerical accuracy will be optimized in this case. We will see this point explicitly in Sec. V. Therefore, for the rest of this section we will assume $\alpha=\beta=\frac{1}{2}$. In the symmetric case the first few terms in the expansion of $\mathscr{H}$ are

$$\mathscr{H}=\tfrac{1}{2}p^2+\tfrac{1}{3}\lambda q^3+h^2\left[\frac{\lambda}{12}pqp+p^3\right]+\cdots\ . \tag{4.34}$$

E. Quartic anharmonic oscillator

For the continuum system described by the Hamiltonian

$$H=\frac{p^2}{2}+\frac{\lambda}{4}q^4\ , \tag{4.35}$$

the effective lattice Hamiltonian is

$$\mathscr{H}=\tfrac{1}{2}p^2+\tfrac{1}{4}\lambda q^4-\frac{h^2}{8}\left[\frac{\lambda^2q^6}{3}+\lambda qp^2q\right]+\frac{h^4}{160}(3\lambda^3q^8-3\lambda^2q^2+7\lambda^2q^2p^2q^2+\tfrac{7}{6}\lambda p^4)+O(h^6)\ \ (h\to 0)\ . \tag{4.36}$$

If we use quadratic finite elements, $\mathscr{H}$ (which we cannot obtain in closed form) will differ from H by terms of order h^4, cubic finite elements will give a difference of order h^6, and so on.

F. Large-lattice-spacing limit

Although the large-lattice-spacing limit is not a physically relevant region, it is mathematically interesting. In the symmetric case, $\alpha=\beta=\frac{1}{2}$, the recursion relations (4.6) and (4.7) become extremely simple in the limit $h\to\infty$. Specifically, they read

$$\begin{aligned} p_n&=-p_{n-1}+O(1/h)\ ,\\ q_n&=-q_{n-1}+O(1/h)\ . \end{aligned} \tag{4.37}$$

Apparently, then, in this limit, the transfer operator in the case of linear finite elements becomes the parity operator.

To see this limit explicitly, we set $h=\infty$ in the expression for $h\mathscr{H}$ for the harmonic oscillator in (4.28):

$$\lim_{h\to\infty}\mathscr{H}h=\frac{\pi}{2}\left[\frac{p^2}{m}+mq^2\right]\ . \tag{4.38}$$

This gives

$$U=e^{i\pi(p^2/m+mq^2)/2}\ , \tag{4.39}$$

which is a representation of the parity operator $\mathscr{P}$ (there are many unitarily equivalent representations).

In general for any Hamiltonian H when $\alpha=\beta=\frac{1}{2}$, we have

$$\lim_{h\to\infty}U=\mathscr{P}\ . \tag{4.40}$$

V. COMPUTING THE ENERGY SPECTRUM

The finite-element method yields a fully consistent and regulated (completely finite) quantum theory which approximates the underlying continuum theory. The immediate result of solving the discrete theory is to give discrete approximations, q_n and p_n to $q(t)$ and $p(t)$. The problem is now to extract physical information from these results. One can immediately extract information on tunneling; this will be discussed elsewhere.[6] Of much greater importance is the determination of the energy spectrum.

There are a number of ways to obtain energy eigenvalues. The simplest procedure consists of determining the time dependence of the operators $q(t)$ and $p(t)$ for short times. The energy spectrum can be deduced in an extremely quick and simple fashion from the oscillation frequencies of these operators.

A. Symmetric linear finite-element calculation

We illustrate the method for the quartic anharmonic oscillator

$$H=\tfrac{1}{2}p^2=\tfrac{1}{4}\lambda q^4 \tag{5.1}$$

for the case of symmetric linear finite elements ($r=1$, $\alpha=\beta=\frac{1}{2}$). We begin by solving the recursion relations for a single finite element

$$\frac{q_1-q_0}{h}=\tfrac{1}{2}(p_1+p_0)\,, \tag{5.2}$$

$$\frac{p_1-p_0}{h}=-\lambda\left[\frac{q_1+q_0}{2}\right]^3, \tag{5.3}$$

as a series in powers of the lattice spacing h. The result is

$$q_1=q_0+p_0h-\frac{\lambda}{2}q_0{}^3h^2+\cdots\,, \tag{5.4}$$

$$p_1=p_0-\lambda q_0{}^3h-\frac{3\lambda}{2}q_0p_0q_0h^2+\cdots\,. \tag{5.5}$$

We stop at order h^2 because we know that the symmetric linear finite-element prescription is accurate to this order.

Next we introduce a set of Fock states by constructing a pair of creation and annihilation operators a and $a^\dagger$ in terms of p_0 and q_0:

$$q_0=\frac{\gamma(a+a^\dagger)}{\sqrt{2}},\quad p_0=\frac{(a-a^\dagger)}{i\sqrt{2}\gamma}\,, \tag{5.6}$$

where

$$[a,a^\dagger]=1\,. \tag{5.7}$$

It is possible to define these creation and annihilation operators because p_0 and q_0 satisfy canonical commutation relations. The parameter γ is completely arbitrary, and is the coordinate-space width of the Fock states $|\,n\,\rangle$ generated by $a^\dagger$. In our calculation γ will be determined by a simple self-consistency requirement. Note that the states $|\,n\,\rangle=[(a^\dagger)^n/\sqrt{n!}]\,|\,0\,\rangle$ are *not* the energy eigenstates of the anharmonic oscillator.

To obtain oscillation frequencies we take matrix elements of (5.4) and (5.5) between adjacent Fock states:

$$\langle 1\,|\,p_1\,|\,0\rangle=\langle 1\,|\,p_0\,|\,0\rangle(1+i\tfrac{3}{2}h\lambda\gamma^4-\tfrac{3}{4}h^2\lambda\gamma^2+\cdots)\,, \tag{5.8}$$

$$\langle 1\,|\,q_1\,|\,0\rangle=\langle 1\,|\,q_0\,|\,0\rangle\left[1+\frac{ih}{\gamma^2}-\tfrac{3}{4}h^2\lambda\gamma^2+\cdots\right]. \tag{5.9}$$

Any matrix element of any time-dependent operator, such as $p(t)$ or $q(t)$, has the general form $\sum_k c_k e^{i\omega_k t}$, where c_k are complete amplitudes and ω_k are all possible energy differences. Here, we choose γ so that to order h^2 only a single frequency ω appears. That is,

$$\frac{\langle 1\,|\,p_1\,|\,0\rangle}{\langle 1\,|\,p_0\,|\,0\rangle}\simeq e^{i\omega h}\simeq 1+i\omega h-\frac{\omega^2}{2}h^2\,, \tag{5.10}$$

$$\frac{\langle 1\,|\,q_1\,|\,0\rangle}{\langle 1\,|\,q_0\,|\,0\rangle}\simeq e^{i\omega h}\simeq 1+i\omega h-\frac{\omega^2}{2}h^2\,. \tag{5.11}$$

Comparing powers of h in (5.10) and (5.11) with (5.8) and (5.9) gives a simple system of algebraic equations

$$\omega=\tfrac{3}{2}\lambda\gamma^4,\quad \omega=\frac{1}{\gamma^2},\quad \omega^2=\tfrac{3}{2}\lambda\gamma^2\,. \tag{5.12}$$

Note that this procedure produces four equations (three different ones) for only two unknowns, ω and γ. However, all but two equations are redundant. The solutions are

$$\gamma=\left[\frac{2}{3}\frac{1}{\lambda}\right]^{1/6} \tag{5.13}$$

and

$$\omega=(\tfrac{3}{2}\lambda)^{1/3}=1.144\,71\lambda^{1/3}\,. \tag{5.14}$$

We regard the determination of γ as a kind of variational fit which gives the optimal width that suppresses all other frequencies to this order. The value of ω is a remarkably good approximation to the exact numerical value of E_1-E_0 which is $1.088\,45\lambda^{1/3}$. The relative error of our approximation is 5.2%.

This same procedure can be used to find other adjacent energy differences. If we take n, $n+1$ matrix elements of (5.4) and (5.5) we find

$$\omega_{n+1,n}=\left[\frac{3(n+1)}{2}\lambda\right]^{1/3}=1.144\,71(n+1)^{1/3}\lambda^{1/3}\,. \tag{5.15}$$

This approximation becomes more accurate as n increases. For example, when $n=1$, $\omega_{2,1}=1.4423\lambda^{1/3}$, which corresponds to a relative error of -0.5%. When n is large we can compare (5.15) with the WKB approximation to $E_{n+1}-E_n$, which becomes exact as $n\to\infty$:

$$(E_{n+1}-E_n)_{\rm WKB}=\lambda^{1/3}\left[\tfrac{3}{2}\sqrt{\pi}\frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}\right]^{4/3}\tfrac{4}{3}(n+1)^{1/3}$$

$$=1.156\,19(n+1)^{1/3}\lambda^{1/3}\,. \tag{5.16}$$

Equation (5.15) differs from this result by a relative error of -0.95%.

We again emphasize the extreme triviality of this calculation. To understand why the result becomes more accurate for large n, we point out that this calculation is valid for short times (small h). Thus, by the uncertainty principle it is more sensitive to higher frequencies.

B. Asymmetric linear finite-element calculation

Let us repeat the above calculation for the asymmetric case where we leave α and β arbitrary but subject to the constraint $\alpha+\beta=1$. In place of (5.4) and (5.5) we have

$$q_1=q_0+p_0h-\beta\lambda q_0{}^3h^2+\cdots\,, \tag{5.17}$$

$$p_1=p_0-\lambda q_0{}^3h-3\alpha\lambda q_0p_0q_0h^2+\cdots\,. \tag{5.18}$$

Then, in place of (5.8) and (5.9) we find

$$\langle 1\,|\,p_1\,|\,0\rangle = \langle 1\,|\,p_0\,|\,0\rangle \left[1+i\tfrac{3}{2}h\lambda\gamma^4-\frac{3\alpha\lambda h^2\gamma^2}{2}+\cdots\right], \tag{5.19}$$

$$\langle 1\,|\,q_1\,|\,0\rangle = \langle 1\,|\,q_0\,|\,0\rangle \left[1+\frac{ih}{\gamma^2}-\tfrac{3}{2}\beta\lambda h^2\gamma^2+\cdots\right]. \tag{5.20}$$

Note that if we equate these to (5.10) and (5.11) to order h we obtain two equations which give precisely the same results as in (5.13) and (5.14). However, the order h^2 equations are inconsistent in general unless $\alpha=\beta=\frac{1}{2}$. This result is not surprising in view of our finding in Sec. IV that the effective lattice Hamiltonian $\mathscr{H}$ differs from the continuum Hamiltonian H by terms of order h unless $\alpha=\beta=\frac{1}{2}$.

C. Quadratic finite-element calculation

Let us extend the analysis of Sec. V A to the case of quadratic finite elements $r=2$. Since the effective lattice Hamiltonian for the case of quadratic finite-elements is accurate to order h^4, we now expand q_1 in terms of q_0 and p_0 to order h^4:

$$q_1 = q_0+p_0h-\tfrac{1}{2}\lambda q_0{}^3h^2-\tfrac{1}{2}\lambda q_0p_0q_0h^3 + \left[\tfrac{1}{8}\lambda^2q_0{}^5-\frac{\lambda}{4}p_0q_0p_0\right]h^4+\cdots . \tag{5.21}$$

It is not necessary to consider p_1 here, as it will produce redundant numerical results. We now construct a two-parameter normalized pair of states,

$$|\,\theta\rangle = |\,0\rangle\cos\theta+|\,2\rangle\sin\theta, \quad |\,\phi\rangle = |\,1\rangle\cos\phi+|\,3\rangle\sin\phi\ ,$$

such that for special values of the parameters the expectation value of q_1 oscillates with a single frequency ω. There are now four parameters, ω, γ, θ, and ϕ, to be determined by the four equations obtained by matching the matrix element of (5.21) with

$$\frac{\langle\phi\,|\,q_1\,|\,\theta\rangle}{\langle\phi\,|\,q_0\,|\,\theta\rangle}\simeq 1+i\omega h-\frac{\omega^2}{2}h^2-\frac{i\omega^3}{6}h^3+\frac{\omega^4}{24}h^4 . \tag{5.22}$$

They are

$$D\omega\gamma^2=\frac{1}{\sqrt{2}}\cos\phi\cos\theta-\cos\phi\sin\theta+\sqrt{3/2}\sin\phi\sin\theta\ ,$$

$$D\omega^2\gamma^4=\lambda\gamma^6\left[\frac{3}{2\sqrt{2}}\cos\phi\cos\theta+3\cos\phi\sin\theta+\frac{\sqrt{3}}{2}\sin\phi\cos\theta+\tfrac{9}{2}\sqrt{3/2}\sin\phi\sin\theta\right],$$

$$D\omega^3\gamma^6=\lambda\gamma^6\left[\frac{3}{2\sqrt{2}}\cos\phi\cos\theta-3\cos\phi\sin\theta+\frac{3\sqrt{3}}{2}\sin\phi\cos\theta+\tfrac{9}{2}\sqrt{3/2}\sin\phi\sin\theta\right],$$

$$D\omega^4\gamma^8=\lambda\gamma^6\left[\left[\frac{45}{4\sqrt{2}}\lambda\gamma^6-\frac{3}{\sqrt{2}}\right]\cos\phi\cos\theta+(\tfrac{135}{4}\lambda\gamma^6-6)\cos\phi\sin\theta + \left[\frac{15\sqrt{3}}{2}\lambda\gamma^6+3\sqrt{3}\right]\sin\phi\cos\theta+\left[\tfrac{285}{4}\sqrt{3/2}\lambda\gamma^6-\frac{9\sqrt{3}}{\sqrt{2}}\right]\sin\phi\sin\theta\right],$$

where

$$D=\frac{1}{\sqrt{2}}\cos\phi\cos\theta+\cos\phi\sin\theta + \sqrt{3/2}\sin\theta\sin\phi\ .$$

The procedure for solving these equations is straightforward. We eliminate the angles θ and ϕ and obtain a pair of simultaneous polynomial equations for γ and ω. The roots of these polynomials can be found by Newton's method. The lowest frequency is $\omega=1.082\,25\lambda^{1/3}$. This differs from the exact value of E_1-E_0 by -0.57%. Thus, going from linear to quadratic finite elements has reduced the relative error by a factor of 10. Unlike the linear finite-element calculation, this calculation supplies additional frequencies which we identify with E_3-E_0, E_1-E_2, and E_3-E_2, and which are accurate[7] to a few percent.

D. Eigenvalue calculation for the q^{2N} oscillator

This same procedure can be used to find the eigenvalues of the generalized anharmonic oscillator whose Hamiltonian H is given by

$$H=\tfrac{1}{2}p^2+\frac{1}{2N}\lambda q^{2N},\quad N=1,2,\ldots . \tag{5.23}$$

[Note that H in (5.1) is obtained from (5.23) by setting $N=2$.] The equations corresponding with (5.2) and (5.3) are

$$\frac{q_1-q_0}{h}=\tfrac{1}{2}(p_1+p_0) \tag{5.24}$$

and

$$\frac{p_1-p_0}{h}=-\lambda\left[\frac{q_1+q_0}{2}\right]^{2N-1}. \tag{5.25}$$

The generalizations of (5.4) and (5.5) are

$$q_1=q_0+p_0h-\tfrac{1}{2}\lambda {q_0}^{2N-1}h^2+\cdots \tag{5.26}$$

and

$$p_1=p_0-\lambda {q_0}^{2N-1}-\frac{\lambda}{2}(2N-1){q_0}^{N-1}p_0{q_0}^{N-1}+\cdots . \tag{5.27}$$

Following the procedure used to obtain (5.8) and (5.9) and making use of the identities

$$\langle 1\,|\,{q_0}^{2N-1}\,|\,0\rangle=\frac{2\gamma^{2N-1}(2N-1)!\sqrt{2}}{4^N(N-1)!}$$

and

$$\langle 1\,|\,{q_0}^{N-1}p_0{q_0}^{N-1}\,|\,0\rangle=\frac{2i\sqrt{2}\gamma^{2N-3}(2N-2)!}{4^N(N-1)!},$$

where γ is given in (5.6), we obtain the generalizations of (5.8) and (5.9) to arbitrary N:

$$\frac{\langle 1\,|\,q_1\,|\,0\rangle}{\langle 1\,|\,q_0\,|\,0\rangle}=1+ih\gamma^{-2}-\frac{2h^2\lambda\gamma^{2N-2}(2N-1)!}{4^N(N-1)!}+\cdots , \tag{5.28}$$

$$\frac{\langle 1\,|\,p_1\,|\,0\rangle}{\langle 1\,|\,p_0\,|\,0\rangle}=1+\frac{4ih\lambda\gamma^{2N}(2N-1)!}{4^N(N-1)!}-\frac{2h^2\lambda\gamma^{2N-2}(2N-1)!}{4^N(N-1)!}+\cdots . \tag{5.29}$$

If we compare the right-hand sides of (5.28) and (5.29) with

$$e^{i\omega h}\simeq 1+i\omega h-\omega^2h^2/2+\cdots ,$$

we obtain four equations for the two unknowns ω and γ. However, as before, two of these equations are redundant and we can solve unambiguously for the energy gap $\omega=E_1-E_0$:

$$\omega=\left[\frac{\lambda(2N-1)!}{4^{N-1}(N-1)!}\right]^{1/(N+1)}. \tag{5.30}$$

Note that when $N=1$ we obtain the *exact* answer $\omega=\sqrt{\lambda}$ (for the harmonic oscillator) and that when $N=2$ we obtain the result in (5.14) which is accurate to 5%. When N is large we can use the Stirling approximation

$$\Gamma(x)\sim x^{x-1/2}e^{-x}\sqrt{2\pi}\quad (x\to\infty)$$

to simplify (5.30):

$$\omega=\frac{N}{e}(2\sqrt{2}\lambda e/N)^{1/(N+1)}\quad (N\to\infty). \tag{5.31}$$

The results in (5.30) [and in (5.31)] become less accurate as N increases but they are quite good when $N\lesssim 5$. We have compared the exact value of ω with the prediction in (5.30) for various values of N in the range $\frac{1}{2}\le N\le 5$. When $N=\frac{1}{2}$ the relative error is 3.5% and when $N=1$ the error is 0. As N increases from 1 so does the error: at $N=\frac{3}{2}$ the error is 2.4%, at $N=2$ the error is 5.2%, at $N=\frac{5}{2}$ it is 10%, and at $N=3$ the error is 15%. The formula is only marginally useful when $N=5$ (the error is 36%); as $N\to\infty$ the result in (5.31) grows linearly with N while the exact value of ω approaches a constant.

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

[2]C. M. Bender, K. A. Milton, and D. H. Sharp, Phys. Rev. Lett. **51**, 1815 (1983).

[3]C. M. Bender, K. A. Milton, and D. H. Sharp, Phys. Rev. D **31**, 383 (1985).

[4]P. M. Prenter, *Splines and Variational Methods* (Wiley, New York, 1975).

[5]L. Durand, University of Wisconsin Report No. MAD/TH-210, 1984 (unpublished).

[6]C. M. Bender, F. Cooper, V. P. Gutschick, and M. M. Nieto, Phys. Rev. D **32**, 1486 (1985); F. Cooper, K. A. Milton, and L. M. Simmons, Jr., Phys. Rev. D (to be published); C. M. Bender, F. Cooper, J. E. O'Dell, and L. M. Simmons, Jr., Phys. Rev. Lett. **55**, 901 (1985).

[7]Repeating this calculation with the operator p instead of q in (5.21) and (5.22) gives nearly redundant numerical results: E_1-E_0 differs from the exact value by a relative error of -1.1%.