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Finite-Element Lattice Hamiltonian Matrix Elements. Anharmonic Oscillators

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Abstract

The finite-element approach to lattice field theory is both highly accurate (relative errors $\sim 1/N^2$, where N is the number of lattice points) and exactly unitary (in the sense that canonical commutation relations are exactly preserved at the lattice sites). In this paper we construct matrix elements for the time evolution operator for the anharmonic oscillator, for which the continuum Hamiltonian is $H = p^2/2 + \lambda q^{2k}/2k$. Construction of such matrix

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elements does not require solving the implicit equations of motion. Low order approximations turn out to be quite accurate. For example, the matrix element of the time evolution operator in the harmonic oscillator ground state gives a result for the $k = 2$ anharmonic oscillator ground state energy accurate to better than 1%, while a two-state approximation reduces the error to less than 0.1%. Accurate wavefunctions are also extracted. Analogous results may be obtained in the continuum, but there the computation is more difficult, and not generalizable to field theories in more dimensions.

I. INTRODUCTION

For over a decade now, the finite-element method has been developed for application to quantum systems. (For a review of the program see [1].) The essence of the approach is to put the Heisenberg equations of motion for the quantum system on a Minkowski space-time lattice in such a way as to preserve exactly the canonical commutation relations at each lattice site. Doing so corresponds precisely to the classical finite-element prescription of requiring continuity at the lattice sites while imposing the equations of motion at the Gaussian knots, a prescription chosen to minimize numerical error. We have applied this technique to examples in quantum mechanics and to quantum field theories in two and four space-time dimensions. In particular, recent work has concentrated on Abelian and non-Abelian gauge theories [2–6], especially on issues of chiral symmetry breaking.

Because it is the equations of motion that are discretized, a lattice Lagrangian does not exist in Minkowski space. This is because the equations of motion are in general nonlocal, involving fields at all previous (but not later) times. Similarly, a lattice Hamiltonian does not exist, in the sense of an operator from which the equations of motion can be derived.

However, because the formulation is unitary, a unitary time-evolution operator must exist which carries fields from one lattice time to the next. For linear finite elements this operator in quantum mechanics has been explicitly constructed [7]. Construction of this operator requires solving the equations of motion, which are implicit. Therefore, it is most useful, and perhaps surprising, that when matrix elements of the time evolution operator are constructed in a harmonic oscillator basis, they do not require the solution of the equations of motion [8]. Although these general formulas were derived some years ago, it seems they have not been exploited. Our purpose here is to study, in a simple context, the matrix elements of the evolution operator, and see how accurately spectral information and wavefunctions may be extracted.[1] Our goal, of course, is to apply similar techniques in gauge theories, for example, to study chiral symmetry breaking in QCD.

II. REVIEW OF THE FINITE-ELEMENT METHOD

Let us consider a quantum mechanical system with one degree of freedom governed by the continuum Hamiltonian

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

from which follow the Heisenberg equations

$$\dot{p} = -V'(q), \quad \dot{q} = p. \tag{2.2}$$

These equations are to be solved subject to the initial condition

$$[q(0), p(0)] = i. \tag{2.3}$$

It immediately follows from (2.2) that the same relation holds at any later time

$$[q(t), p(t)] = i. \tag{2.4}$$

Now suppose we introduce a time lattice by subdividing the interval $(0, T)$ into N subintervals each of length h. On each subinterval ("finite element") we express the dynamical variables as rth degree polynomials

[1]A preliminary version of this work appears in [9].

$$p(t)=\sum_{k=0}^{r}a_k(t/h)^k,\quad q(t)=\sum_{k=0}^{r}b_k(t/h)^k, \tag{2.5}$$

where t is a local variable ranging from 0 to h. We determine the $2(r+1)$ operator coefficients a_k, b_k, as follows:

1. On the first finite element let

$$a_0=p_0=p(0),\quad b_0=q_0=q(0). \tag{2.6}$$

2. Impose the equations of motion (2.2) at r points within the finite element, at $\alpha_i h$, $i=1,2,\ldots,r$, where $0<\alpha_1<\alpha_2<\cdots<\alpha_r<1$. This then gives

$$p(h)\approx p_1=\sum_{k=0}^{r}a_k,\quad q(k)\approx q_1=\sum_{k=0}^{r}b_k. \tag{2.7}$$

3. Proceed to the next finite element by requiring continuity (but not continuity of derivatives) at the lattice sites, that is, on the second finite element, set

$$a_0=p_1,\quad b_0=q_1, \tag{2.8}$$

and again impose the equations of motion at $\alpha_i h$, and so on.

How are the α_i's determined? By requiring preservation of the canonical commutation relations at each lattice site,

$$[q_1,p_1]=[q_0,p_0]=i, \tag{2.9}$$

one finds

$$r=1\quad\text{(linear finite elements)}:\qquad \alpha=\frac{1}{2} \tag{2.10a}$$

$$r=2\quad\text{(quadratic finite elements)}:\qquad \alpha_\pm=\frac{1}{2}\pm\frac{1}{2\sqrt{3}} \tag{2.10b}$$

$$r=3\quad\text{(cubic finite elements)}:\qquad \alpha_{1,3}=\frac{1}{2}\mp\frac{\sqrt{3}}{2\sqrt{5}},\quad \alpha_2=\frac{1}{2} \tag{2.10c}$$

These points are exactly the Gaussian knots, that is, the roots of the rth Legendre polynomial,

$$P_r(2\alpha - 1) = 0. \tag{2.11}$$

Amazingly, these are precisely the points at which the numerical error is minimized. It is known for classical equations that if one uses N rth degree finite elements the relative error goes like N^{-2r}, while imposing the equations at any other points would give errors like N^{-r}.

Let us consider a simple example. The quartic anharmonic oscillator has the continuum Hamiltonian

$$H = \frac{1}{2}p^2 + \frac{1}{4}\lambda q^4, \tag{2.12}$$

for which the equations of motion are

$$\dot{q} = p, \quad \dot{p} = -\lambda q^3. \tag{2.13}$$

If we use the linear ($r = 1$) finite-element prescription given above, the corresponding discrete lattice equations are

$$\frac{q_1 - q_0}{h} = \frac{p_1 + p_0}{2}, \quad \frac{p_1 - p_0}{h} = -\frac{\lambda}{8}(q_1 + q_0)^3. \tag{2.14}$$

(Notice the easily remembered mnemonic for linear finite elements: Derivatives are replaced by forward differences, while undifferentiated operators are replaced by forward averages.) By commuting the first of these equations with p_1+p_0 and the second with q_1+q_0 the unitarity condition (2.9) follows immediately. These equations are implicit, in the sense that we must solve a nonlinear equation to find q_1 and p_1 in terms of q_0 and p_0. Although such a solution can be given, let us make a simple approximation, by expanding the dynamical operators at time 1 in powers of h, with operator coefficients at time 0. Those coefficients are determined by (2.14), and a very simple calculation yields

$$\begin{aligned} q_1 &= q_0 + hp_0 - \frac{\lambda}{2}h^2 q_0^3 + \dots, \\ p_1 &= p_0 - \lambda h q_0^3 - \frac{3}{2}\lambda h^2 q_0 p_0 q_0 + \dots. \end{aligned} \tag{2.15}$$

We can define Fock-space creation and annihilation operators in terms of the initial-time operators

$$q_0 = \gamma\frac{(a+a^\dagger)}{\sqrt{2}}, \quad p_0 = \frac{(a-a^\dagger)}{i\sqrt{2}\gamma}, \tag{2.16}$$

which satisfy

$$[a, a^\dagger] = 1. \tag{2.17}$$

Here we have introduced an arbitrary variational parameter γ, which represents the width of the corresponding harmonic oscillator states. The Fock-space states (harmonic oscillator states) are created and destroyed by these operators:

$$|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle, \tag{2.18}$$

which states are not energy eigenstates of the anharmonic oscillator. We can now take matrix elements in these states of the dynamical operators at lattice site 1, using (2.15):

$$\begin{aligned}\langle 1|p_1|0\rangle &\approx \langle 1|p_0|0\rangle(1 + i\frac{3}{2}h\lambda\gamma^4 - \frac{3}{4}h^2\lambda\gamma^2 + \ldots) \\ &\approx \langle 1|p_0|0\rangle(1 + i\omega h - \frac{1}{2}\omega^2 h^2 + \ldots),\end{aligned} \tag{2.19}$$

and

$$\begin{aligned}\langle 1|q_1|0\rangle &\approx \langle 1|q_0|0\rangle(1 + i\frac{h}{\gamma^2} - \frac{3}{4}h^2\lambda\gamma^2 + \ldots) \\ &\approx \langle 1|q_0|0\rangle(1 + i\omega h - \frac{1}{2}\omega^2 h^2 + \ldots),\end{aligned} \tag{2.20}$$

where we have assumed approximately exponential dependence on the energy difference ω. Equating the coefficients of the terms through order h^2 constitutes four equations in two unknowns. These equations are consistent and yield

$$\omega = \frac{3}{2}\lambda\gamma^4 = \frac{1}{\gamma^2}, \tag{2.21}$$

so the energy difference between the ground state and the first excited state is approximately

$$\omega = \left(\frac{3}{2}\lambda\right)^{1/3} \approx 1.145\lambda^{1/3} \tag{2.22}$$

which is only 5% higher than the exact result $E_{01} = 1.08845\lambda^{1/3}$. A similar calculation using quadratic finite elements ($r = 2$) reduces the error to 0.5%.

Numerical results for a large number of energy differences can also be obtained by taking the discrete Fourier transform of the time sequence $\{\langle 0|q_n|1\rangle\}$. For example, for 1000 finite elements, energy differences are computed at the 2–3% level [10].

III. THE TIME-EVOLUTION OPERATOR

Because the canonical commutation relations are preserved at each lattice site, we know that there is a unitary time evolution operator that carries dynamical variables forward in time:

$$q_{n+1} = U q_n U^\dagger, \quad p_{n+1} = U p_n U^\dagger, \tag{3.1}$$

For the system described by the continuum Hamiltonian (2.1) in the linear finite-element scheme, we have found [7] the following formula for U:

$$U = e^{ihp_n^2/4} e^{ihA(q_n)} e^{ihp_n^2/4}, \tag{3.2}$$

where[2]

$$A(x) = \frac{2}{h^2}[x - g^{-1}(4x/h^2)]^2 + V(g^{-1}(4x/h^2)), \tag{3.3}$$

$$g(x) = \frac{4}{h^2}x + V'(x). \tag{3.4}$$

The implicit nature of the finite-element prescription is evident in the appearance of the inverse of the function g.

Given the time evolution operator, a lattice Hamiltonian may be defined by $U = \exp(ih\mathcal{H})$. For linear finite elements $\mathcal{H}$ differs from the continuum Hamiltonian by terms of order h^2. For example,

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[2]A misprint occurs in (2.21b) of [1].

$$V=\frac{1}{2}m^2q^2: \quad \mathcal{H}=\frac{2}{mh}\tan^{-1}\left(\frac{mh}{2}\right)\left[\frac{1}{2}p^2+\frac{1}{2}m^2q^2\right], \tag{3.5a}$$

$$V=\frac{\lambda}{3}q^3: \quad \mathcal{H}=\frac{1}{2}p^2+\frac{1}{3}\lambda q^3+h^2\left[\frac{\lambda}{12}pqp+p^3\right]+\ldots, \tag{3.5b}$$

$$V=\frac{\lambda}{4}q^4: \quad \mathcal{H}=\frac{1}{2}p^2+\frac{1}{4}\lambda q^4+h^2\left[-\frac{\lambda^2}{24}q^6-\frac{\lambda}{8}qp^2q\right]+\ldots. \tag{3.5c}$$

If one uses quadratic finite elements $\mathcal{H}$ differs from the continuum Hamiltonian by terms of order h^4, etc.

IV. MATRIX ELEMENTS OF DYNAMICAL VARIABLES

Remarkably, it is not necessary to solve the equations of motion to compute matrix elements of the dynamical variable. Introduce creation and annihilation operators as in (2.16). Then, in terms of harmonic oscillator states (2.18) the following formula is easily derived [8] for a general matrix element of q_1:

$$\langle m|q_1|n\rangle = -\frac{\gamma}{\sqrt{2}}(\sqrt{m}\delta_{n,m-1}+\sqrt{n}\delta_{m,n-1})$$
$$+\frac{e^{-i\theta(m-n)}}{R\sqrt{\pi 2^{n+m}n!m!}}\int_{-\infty}^{\infty}dz\, ze^{-g^2(z)/4R^2}g'(z)H_n(g(z)/2R)H_m(g(z)/2R), \tag{4.1}$$

where g is given by (3.4), $H_n(x)$ is the nth Hermite polynomial, and we have introduced the abbreviations

$$R^2=\frac{4\gamma^2}{h^4}+\frac{1}{h^2\gamma^2}, \quad e^{-i\theta}=\frac{2\gamma}{Rh^2}+\frac{i}{Rh\gamma}. \tag{4.2}$$

For the example of the harmonic oscillator, this formula gives for the ground state–first excited state energy difference $\omega=(2/h)\tan^{-1}(h/2)$, consistent with (3.5a), while for the anharmonic oscillator (2.12) if we expand in h we obtain precisely the expansion (2.20).

V. MATRIX ELEMENTS OF THE TIME EVOLUTION OPERATOR

A similar formula can be derived for the harmonic oscillator matrix elements of the time evolution operator. (There is an error in the formula printed in [8].)

$$\langle m|U|n\rangle = \frac{1}{2R}\frac{1}{\sqrt{\pi 2^{n+m} n! m!}} e^{-i(n+m+1)\theta}$$
$$\times \int_{-\infty}^{\infty} dz\, g'(z) H_n(g(z)/2R) H_m(g(z)/2R) e^{[ihV(z)+ih^3V'(z)^2/8-h^2 g(z)^2 e^{-i\theta}/8\gamma R]}, \qquad (5.1)$$

which again is expressed in terms of g not g^{-1}.

For the harmonic oscillator, where $V = q^2/2$, (5.1) gives for the ground-state energy

$$\langle 0|U|0\rangle = e^{i\omega_0 h}, \quad \omega_0 = \frac{1}{h}\tan^{-1}\frac{h}{2}, \qquad (5.2)$$

which follows from (3.5a). For the general anharmonic oscillator, $V = \lambda q^{2k}/2k$, again we expand in powers of h, with the result, for the harmonic oscillator ground state,

$$\langle 0|U|0\rangle = 1 + ih\lambda^{1/(k+1)} f(\alpha) - \frac{h^2}{2}\lambda^{2/(k+1)} s(\alpha)$$
$$\approx 1 + i\omega_0 h - \frac{1}{2}\omega_0^2 h^2 + \ldots, \qquad (5.3)$$

where $\alpha = \lambda\gamma^{2k+2}$ and

$$f(\alpha) = \frac{1}{4\alpha^{1/(k+1)}}\left(1 + \frac{2\alpha}{k}\frac{\Gamma(k+1/2)}{\Gamma(1/2)}\right) \qquad (5.4a)$$
$$s(\alpha) = \frac{1}{16\alpha^{2/(k+1)}}\left(3 - 4\alpha\frac{2k-1}{k}\frac{\Gamma(k+1/2)}{\Gamma(1/2)} + \frac{4\alpha^2}{k^2}\frac{\Gamma(2k+1/2)}{\Gamma(1/2)}\right). \qquad (5.4b)$$

This result also derivable from (3.5), using (2.16), but with considerably more labor. Equating powers of h in (5.3) gives us two equations, which are to be solved first for the dimensionless number α. Once the number α is determined, the value of ω_0 is expressed as

$$\omega_0 = \lambda^{1/(k+1)} f(\alpha). \qquad (5.5)$$

For a first estimate, we use only the $O(h)$ equation (5.5) and employ the "principle of minimum sensitivity" (PMS) [11] that is, use the stationary value of α,

$$f'(\alpha) = 0 \Rightarrow \alpha = \frac{2^{k-1}}{(2k-1)!!} \Rightarrow f(\alpha) = \frac{k+1}{4k}\frac{[(2k-1)!!]^{1/(k+1)}}{2^{(k-1)/(k+1)}}. \qquad (5.6)$$

Specific examples are

$$f(\alpha) = \begin{cases} 0.4293, & k=2, \\ 0.4639, & k=3, \\ 0.5230, & k=4, \end{cases} \qquad (5.7)$$

which are higher than the exact values [12] of 0.420805, 0.43493, and 0.46450 by about 2%, 7%, and 13%, respectively. In fact, when we solve (5.3) for α, that is solve $f(\alpha)^2 = s(\alpha)$, we find complex values, for example, for $k=2$

$$\alpha = \frac{1}{2} \pm \frac{i}{2\sqrt{3}} \Rightarrow f(\alpha) = 0.4178 \mp 0.0077i. \tag{5.8}$$

The imaginary part is small, and the real part is only 0.7% low. The corresponding result for $k=3$ is $f(\alpha) = 0.4453 \mp 0.0352i$, where the real part is now only 2% high. However, for $k=4$, $f(\alpha) = 0.5171 \mp 0.0713i$, and the real part is still 11% high. The failure of (5.8) to be real does not indicate any breakdown of unitarity, but only that the one state approximation is not exact.

We do much better by making a two-state approximation, where we must diagonalize the 2×2 matrix

$$\begin{pmatrix} U_{00} & U_{02} \\ U_{20} & U_{22} \end{pmatrix}. \tag{5.9}$$

For $k=2$ we then find the following relation between $\omega_{0,2}$ and $\alpha = \lambda\gamma^6$:

$$\omega_{0,2} = \frac{\lambda^{1/3}}{16}\alpha^{-1/3}[12 + 21\alpha \mp 2\sqrt{3}(8 + 16\alpha + 33\alpha^2)^{1/2}], \tag{5.10}$$

which, for the $-$ sign, is plotted in Fig. 1. This graph shows that the ground-state energy is very insensitive to the value of α for a broad range of values. The principle of minimum sensitivity gives

$$\omega_0 = 0.42124\lambda^{1/3}, \tag{5.11}$$

in spectacular agreement with the exact result, being only 0.1% high, while it gives a value for the third state, $\omega_2 = 2.992\lambda^{1/3}$, accurate to 1%. (The exact value is $2.959\lambda^{1/3}$ [13].) Solving for α from the eigenvalues of (5.9) gives even better results:

$$\omega_0 = \lambda^{1/3}(0.42054 \pm 2\times 10^{-6}i), \quad \omega_2 = \lambda^{1/3}(2.9433 \pm 0.0220i), \tag{5.12}$$

where the ground state energy is now low by 0.06%, the imaginary part being negligible. The real part of the energy of the third state is low by only 0.5%. These results for the ground state are much better than those resulting from the WKB approximation [13].

The corresponding PMS values for the $k = 3$ and $k = 4$ oscillators are similarly impressive: $\omega_0 = 0.43913\lambda^{1/4}$ (+0.9%) and $\omega_0 = 0.47718\lambda^{1/5}$ (+2.7%), respectively. Using the $O(h^2)$ data to compute α gives truly outstanding agreement:

$$k = 3: \quad \omega_0 = (0.43284 \pm 0.00259i)\lambda^{1/4} \tag{5.13a}$$

$$\omega_2 = (3.4532 \pm 0.1271i)\lambda^{1/4} \tag{5.13b}$$

$$k = 4: \quad \omega_0 = (0.46347 \pm 0.01463i)\lambda^{1/5} \tag{5.13c}$$

$$\omega_2 = (4.0186 \pm 0.3081i)\lambda^{1/5} \tag{5.13d}$$

where the real parts of the ground-state energies are now low by 0.5% and 0.2%, respectively.

VI. WAVEFUNCTIONS

In the process of diagonalizing (5.9) we find the corresponding wavefunctions in the two-state approximation, that is, the wavefunctions are taken to be linear combinations of $n = 0$ and $n = 2$ harmonic oscillator states of width γ. The real parts of these wavefunctions are plotted in Figs. 2 and 3. (The imaginary parts amount to only 2% for the ground-state wavefunction and 5% for the excited-state wavefunction.) These are normalized to unity at the origin to facilitate comparison with [13].

When these are compared with the exact wavefunctions given in [13], we see that the approximate ground-state wavefunction is nearly indistinguishable from the exact one, and is much better that the WKB wavefunction given there. The excited-state wavefunction is quite good, but deviates slightly from the exact wavefunction, and in particular, the minimum at $x \approx 1.1$ should be about 10% deeper. This deviation is not surprising, since the exact excited-state wavefunction must contain a substantial mixing with the $n = 4$ harmonic oscillator state. The error in the excited-state wavefunction is also manifested in that fact that in this approximation the two wavefunctions are not quite orthogonal, the magnitude of the overlap being 5%.

VII. CONCLUSIONS

The simple calculations given here for quantum-mechanical anharmonic oscillators are the beginning of a program to develop use of lattice Hamiltonian techniques to explore gauge theories in the finite-element context. The numerical results presented in Sec. V and VI also hold in the continuum, by virtue of (3.5), but the calculations are much more tedious without the use of the finite-element formula (5.1). It is in two or more space-time dimensions that the essential nature of the lattice in such calculations comes into play [4,5,14]. The high accuracy contrasted with the simplicity of the approach leads us to expect that we can extract spectral information, anomalies, and symmetry breaking from an examination of the time-evolution operator in gauge theories.

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FIGURES

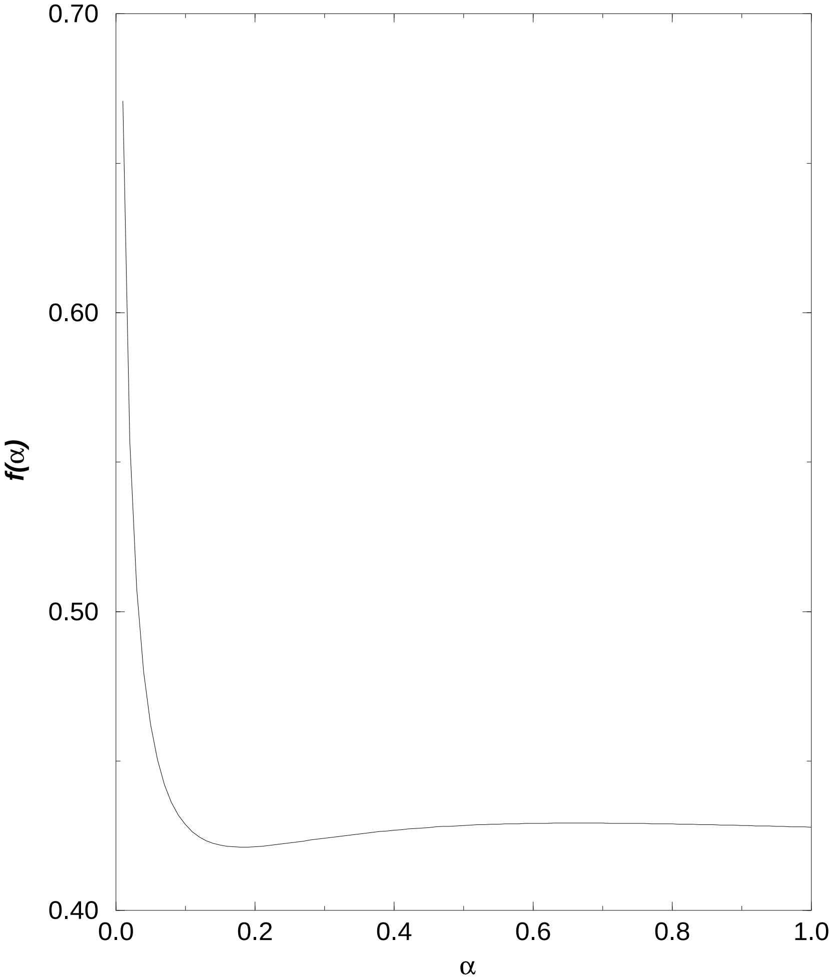

FIG. 1. Ground-state energy for the quartic anharmonic oscillator as a function of $\alpha = \lambda\gamma^6$, in the second approximation. Here $\omega_0 = \lambda^{1/3} f(\alpha)$, $f(\alpha)$ given by (5.10).

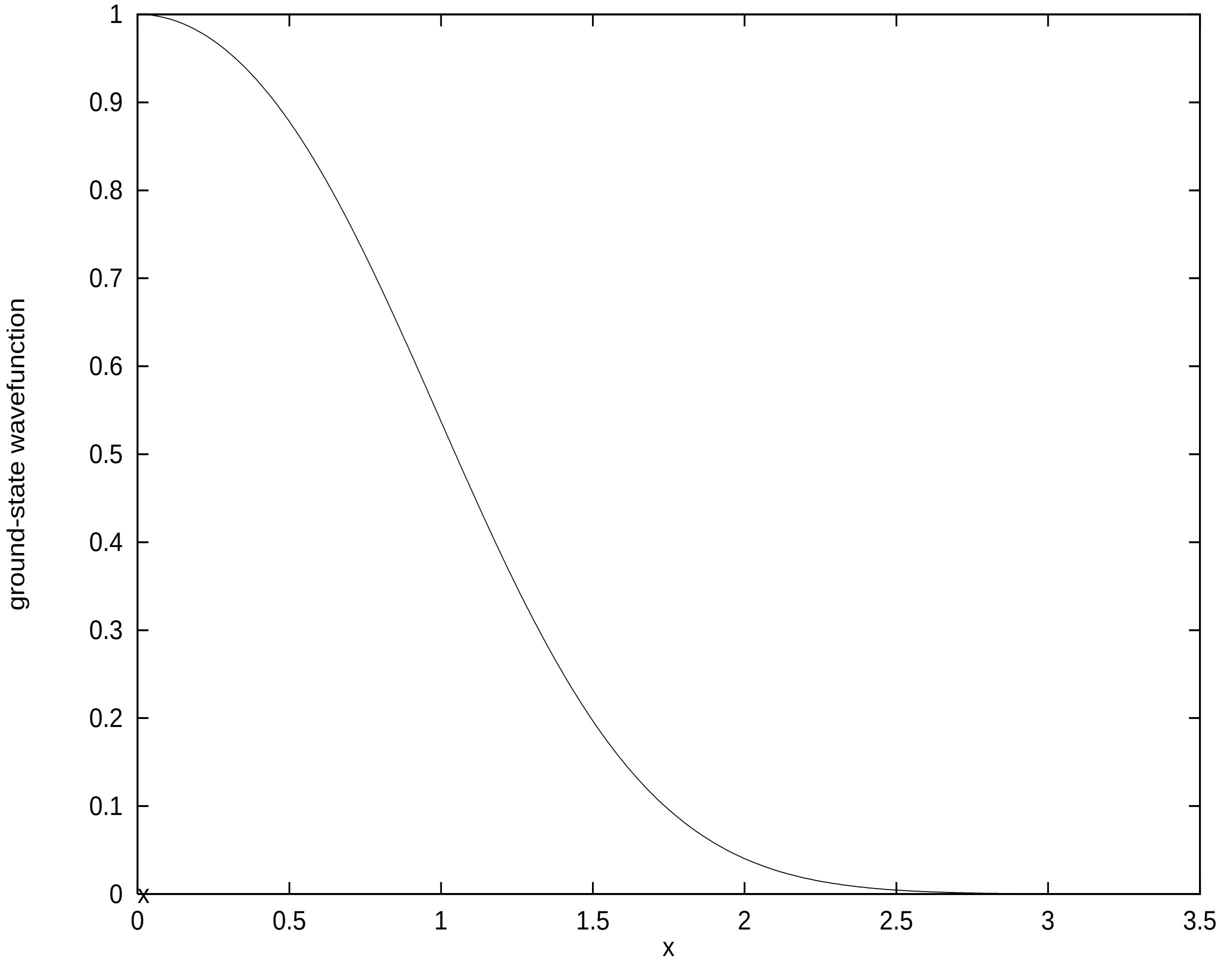

FIG. 2. Ground-state wavefunction in the two-state approximation.

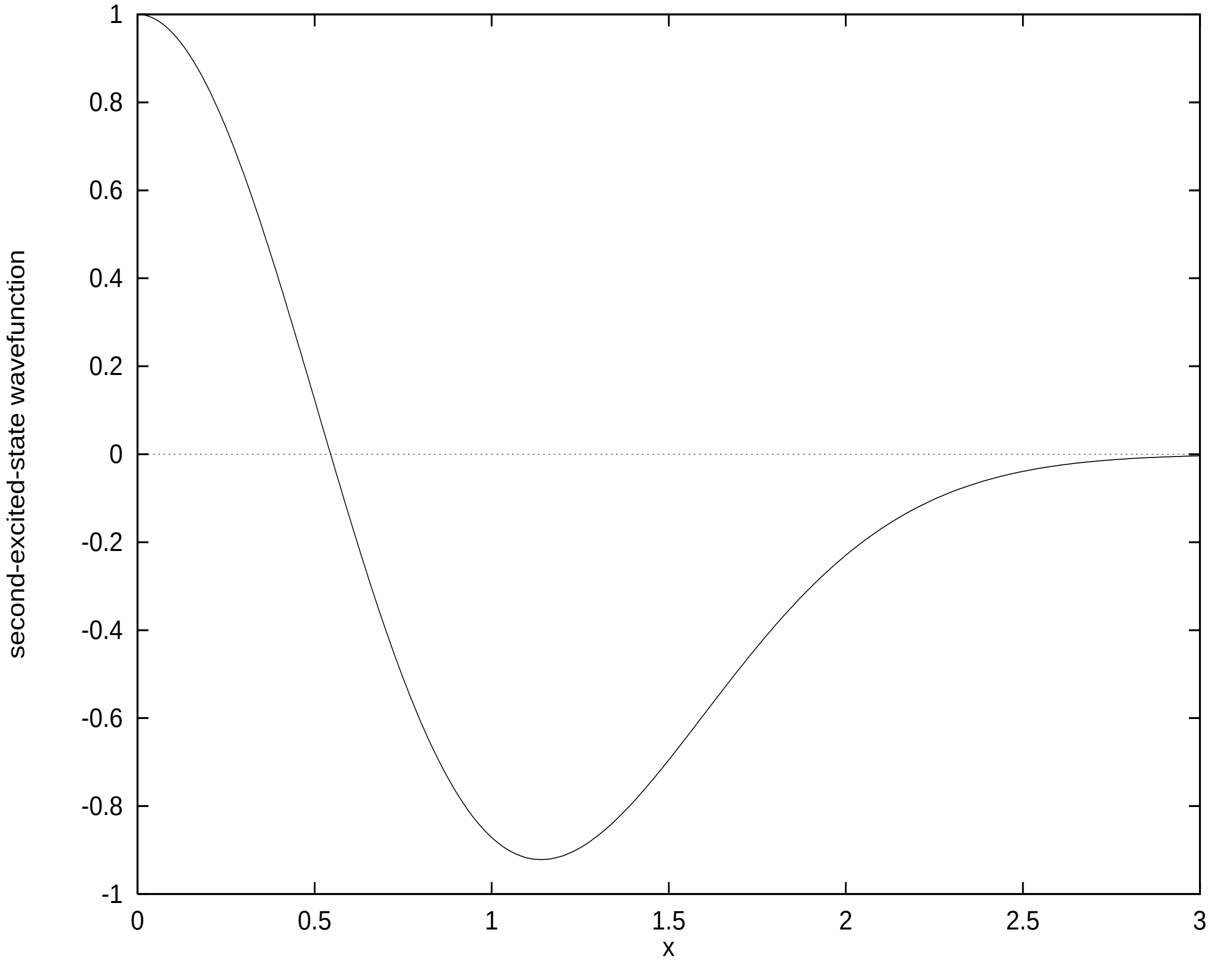

FIG. 3. Second-excited state wavefunction in the two-state approximation.