New approach to spectrum calculations in lattice Hamiltonian field theories: Introduction and application to $\lambda\phi^4$ theory in $1+1$ dimensions

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We introduce a finite-lattice technique for calculating the spectrum of fluctuating Bose theories in the continuum limit. The method gives the continuum spectrum to an estimated $\sim 1\%$ accuracy in $1+1$ dimensions using available computer memory. The spectrum of $\lambda\phi^4$ theory in $1+1$ dimensions is studied as a trial application; we find no bound states in the spectrum between m and $2m$.

I. INTRODUCTION

Recent advances in lattice quantum field theory have made possible the numerical solution of problems which had been studied for decades with little success. Of special note are the Monte Carlo calculations of the spectrum of gauge theories using techniques developed by Creutz,[1] which have recently been applied successfully to the determination of the hadron spectrum of QCD in $3+1$ dimensions.[2-4] Similar Monte Carlo techniques have been used to study properties of scalar theories in different numbers of space-time dimensions; fascinating results have been obtained in particular for the properties of $\lambda_0\phi^4$ theory in various dimensions.[5,6]

An essential limitation of Monte Carlo techniques is the determination of excited-state masses for given quantum numbers. This is because Monte Carlo techniques typically look at numerically evaluated propagators at large distances, where they become exponentials in the lowest-lying state's mass;

$$S(x-y)\sim\sum_i c_i e^{-M_i|x-y|}\sim c_0 e^{-M_0|x-y|}\ . \tag{1.1}$$

Although M_0 may be evaluated in this way, higher masses may not be separated unambiguously.

In this paper we develop a technique for determining all the rest-state ($\vec{P}_{\rm tot}=\vec{0}$) energies in a quantum field theory, using functional methods and lattice Hamiltonian field theory. The technique is explained in Secs. II and III of the paper, and in Sec. IV we discuss how the continuum limit of the lattice spectrum is obtained. Section V is a first nontrivial application, namely, the study of the renormalized "two-particle" mass ratio $m_2/m\equiv(E_2-E_0)/(E_1-E_0)$ in $\frac{1}{2}m_0^2\phi^2+\lambda_0\phi^4$ theory in $1+1$ dimensions. This theory is known to be nontrivial [in the sense that $\lambda\neq 0$ for suitable $\lambda_0\neq 0$ (Ref. 5)] but we nonetheless find that $m_2/m=2.0$ independent of λ_0. These results are consistent if the interaction is always repulsive so that no bound states may form, as was suggested by Lee[7] and Halliday[8].

The technique we use is to generate the lowest few eigenvalues of the Hamiltonian matrix, employing Paige's modification of the Lanczos technique.[9] We calculate the Hamiltonian matrix on a special basis of classical functions, suitably modified to span only $\vec{P}_{\rm tot}=\vec{0}$ wave functionals. This $\vec{P}_{\rm tot}=\vec{0}$ block diagonalization of H is important in that it eliminates all the redundant boosted states from the spectrum, and it also reduces computer-memory requirements by $\sim N_x^{-1}$ for large-N_x lattices.

The basis of classical functions is generated on a lattice in $\vec{x}$ space and in (classical) ϕ space, and the Hamiltonian matrix is determined by acting on this basis with the functional Hamiltonian operator. This gives diagonal terms which are the classical energies of the basis functions and off-diagonal terms ($\sim\hbar^2$) which drive the quantum fluctuations between the classical configurations in the physical energy eigenstates. Essentially we make function space discrete before evaluating the Hamiltonian. Removing the $\vec{P}_{\rm tot}\neq\vec{0}$ states from the basis has allowed us to treat problems with up to 5 space points and 14 ϕ points; this is equivalent to the brute-force diagonalization of a 14^5 square ($537\,824\times 537\,824$) dimensional Hamiltonian.

The finite Hamiltonian approach has previously been applied to the study of spin systems by Roomany *et al.*[10,11] and by Hamer and Barber.[12-15] Applications to continuous-x field theories include studies of the spectrum of the $(1+1)$-dimensional Schwinger model by Irving and Thomas[16] and Hamer *et al.*[17] and of $(1+1)$-dimensional SU(2) Yang-Mills theory by Hamer.[18]

Our approach differs from these earlier finite-lattice studies in two important aspects. First, we use a basis of classical functions rather than a basis of free-field-theory states. Second, we treat active (fluctuating) Bose fields rather than spin systems or fermions and nonfluctuating Bose fields. This requires an infinite number of states (N_ϕ) at each site as well as an infinite number of sites (N_x). Despite the forbidding distance from practical lattices to this limit, we find that we are able to obtain the low-lying spectrum of $(1+1)$-dimensional scalar field theories to an accuracy of $\sim 1\%$ at present.

II. LATTICE HAMILTONIAN FIELD THEORY USING WAVE FUNCTIONALS

An energy eigenstate of a quantum-mechanical problem is completely described by the wave function $\psi(\vec{x})$ at some fixed time t, this being the amplitude to find the particle at the point $\vec{x}$ in coordinate space. The wave function

$\psi(\vec{x})$ satisfies the time-independent Schrödinger equation.

Similarly, an energy eigenstate of a quantum field theory is described by a wave functional $\psi[\phi(\vec{x})]$, which is the amplitude to find the field at any specified function $\phi(\vec{x})$. The set of functions $\{\phi(\vec{x})\}$ may be thought of as points in function space at which the field may be detected, just as a particle may be detected at any of the points $\{\vec{x}\}$ in coordinate space. The wave functional $\psi[\phi(\vec{x})]$ satisfies a time-independent functional Schrödinger equation, which for a scalar field with a potential $V(\phi)$ is explicitly

$$\int d\vec{x}\left[-\frac{\hbar^2}{2}\frac{\delta^2}{\delta\phi(\vec{x})^2}+V(\phi(\vec{x}))\right]\psi[\phi(\vec{x})] \equiv H\psi[\phi(\vec{x})]=E\psi[\phi(\vec{x})]\ . \quad (2.1)$$

Examples of solutions of this Schrödinger equation, as well as the analogous equation for other Bose and Fermi fields, may be found in the literature.[19–21]

Numerical determination of energy eigenstates of quantum-mechanical problems requires the reduction of the continuum of points $\{\vec{x}\}$ to a finite lattice $\{\vec{x}_n\}$, following which the finite Hamiltonian matrix $H_{nn'}$ is diagonalized to give energy eigenvectors and eigenvalues. To treat quantum field theories similarly, we must restrict the continuum of functions $\{\phi(\vec{x})\}$ to a finite set of functions $\{\phi_n(\vec{x})\}$, $n=1,2,\ldots,N_f$. A finite-difference approximation to the functional Hamiltonian (2.1) is an $N_f\times N_f$ matrix, whose eigenvectors are the energy eigenstates and whose eigenvalues are the bound- and scattering-state energies of the quantum field theory.

To obtain a finite set of functions, we restrict ourselves to discrete values of both $\vec{x}$ and $\phi(\vec{x})$. The coordinate $\vec{x}$ (in one dimension) takes on the values $x_1=0$, $x_2=h_x$, $x_3=2h_x,\ldots,$ $x_{N_x}=(N_x-1)h_x$, and periodic boundary conditions are imposed by identifying x_{N_x+1} with x_1. The field $\phi_n=\phi(x_n)$ is also allowed only discrete values. For odd N_ϕ, these values are $\phi_n=0,\ \pm h_\phi,\ldots,$ $\pm(N_\phi-1)h_\phi/2$, with periodic ϕ boundary conditions, so that $\phi=(N_\phi+1)h_\phi/2$ is identified with $\phi=-(N_\phi-1)h_\phi/2$. The even-N_ϕ case can be made discrete using two schemes: (1) $\phi=\pm h_\phi/2,\ \pm 3h_\phi/2,\ldots,$ $\pm(N_\phi-1)h_\phi/2$, with $(N_\phi+1)h_\phi/2$ and $-(N_\phi-1)h_\phi/2$ identified as above, or (2) $\phi=0,\ \pm h_\phi,\ \pm 2h_\phi,\ldots,$ $\pm(N_\phi-1)h_\phi/2$, with the extreme points identified. We have used the first scheme in our example in Sec. III, but have employed the second scheme for our large-N_ϕ computations in Secs. IV and V. The spectra resulting from the two schemes are very close for large N_ϕ.

TABLE I. Finite-difference approximations.

Continuum	Discrete ($N_\phi-\phi$ by N_x-x)
x	$x_n=(n-1)h_x$
$\phi(x)$	$\phi(x_n)\equiv\phi_n$
$\frac{d\phi(x)}{dx}$	$\frac{\phi_{n+1}-\phi_n}{h_x}$
$\frac{\delta}{\delta\phi(x)}$	$\frac{1}{h_x}\frac{\partial}{\partial\phi_n}\Big\vert_{\text{lattice}}$ $=\frac{1}{h_x h_\phi}(\delta_{\phi_n',\phi_n+1/2h_\phi}-\delta_{\phi_n',\phi_n-1/2h_\phi})$ (only used as $\partial^2/\partial\phi^2$)
$\delta(x-x')$	$\frac{1}{h_x}\delta_{nn'}$
$\int_{-\infty}^{\infty}dx\,f(x)$	$h_x\sum_{n=1}^{N_x}f(x_n)$

After discretization, we have N_ϕ possible values for ϕ_n at each of the N_x points x_n. The total number of functions is

$$N_f=N_\phi^{N_x}\ . \quad (2.2)$$

The lattice for $N_\phi=5$ and $N_x=4$ and a typical function on this lattice are shown in Fig. 1.

We note that the number of points in function space represented on the lattice quickly becomes prohibitively large; for the $N_\phi=5$ field values and $N_x=4$ x sites shown in Fig. 1, we already have a $5^4=625$-dimensional function space and a 625×625-dimensional Hamiltonian to diagonalize. If we go to an $(N_\phi=7)\times(N_x=7)$ lattice, we find an 823 543-dimensional function space, and taking the 5×4 lattice to three space dimensions produces a truly astronomical $\sim10^{45}$-dimensional Hamiltonian.

Due to the large size of the Hamiltonian matrix in theories with fluctuating Bose fields, we are limited to models in only one space dimension. It is not practical to treat theories in higher dimensions or with more field degrees of freedom if one retains the complete basis of $N_f=N_\phi^{N_x}$ functions.

For purposes of illustration we shall consider the solution of a free scalar theory on a finite lattice. The continuum Hamiltonian is

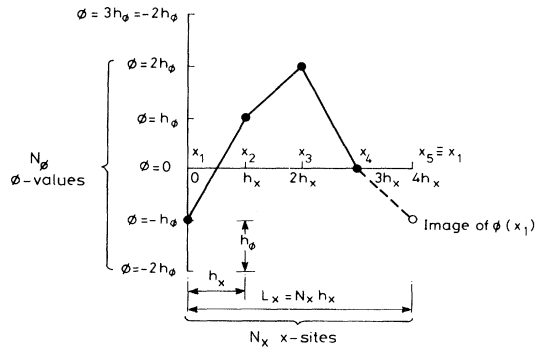

FIG. 1. Function-space lattice and a representative function for $N_\phi=5$ and $N_x=4$.

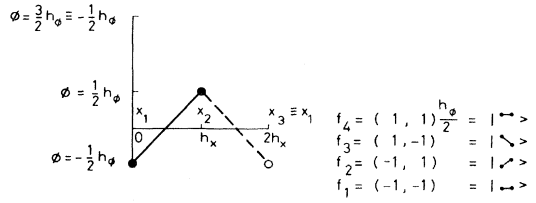

FIG. 2. The 2×2 lattice and its basis functions. [$f_2(\vec{x})$ is shown on the lattice.]

$$H=\int_{-\infty}^{\infty}dx\left[-\frac{\hbar^2}{2}\frac{\delta^2}{\delta\phi(x)^2}+\frac{1}{2}\underbrace{\left[\frac{d\phi(x)}{dx}\right]^2+\frac{1}{2}m_0{}^2\phi(x)^2}_{V(\phi(x))}\right]. \tag{2.3}$$

The mapping of continuum to discrete symbols we shall employ is as shown in Table I.

This maps the continuum Hamiltonian (2.3) into the following finite-difference operator:

$$H=\underbrace{-\frac{\hbar^2}{2h_x}\sum_{n=1}^{N_x}\frac{\partial^2}{\partial\phi_n{}^2}\Big|_{\text{lattice}}}_{H_{\text{fluctuations}}}+\underbrace{\frac{1}{2h_x}\sum_{n=1}^{N_x}(\phi_{n+1}-\phi_n)^2}_{H_{\text{kinetic}}}+\underbrace{\frac{h_x m_0{}^2}{2}\sum_{n=1}^{N_x}\phi_n{}^2}_{H_{\text{potential}}}. \tag{2.4}$$

We visualize this H as operating on a column vector whose entries are the N_f functions which serve as the basis for our wave functionals. Obviously, the $\frac{1}{2}(\vec{\nabla}\phi)^2$ term H_{kin} and the $\frac{1}{2}m_0{}^2\phi^2$ term H_{pot} are diagonal on this basis, and only the functional derivative $(-\hbar^2/2h_x)\times\partial^2/\partial\phi_n{}^2|_{\text{lattice}}$ in H_{fluc} produces off-diagonal terms in H. It is notable that an interaction $h_x\sum_{n=1}^{N_x}V_I(\phi_n)$ will only appear as a modification of the diagonal of H; the fluctuations are driven by H_{fluc}, which is the same in both free and interacting theories.

The finite-difference version of the partial derivative, $\partial^2/\partial\phi_n{}^2|_{\text{lattice}}$, requires some explanation. If we act on a given function $\phi(x)=(\phi_1,\phi_2,\ldots,\phi_n,\ldots,\phi_{N_x})$ with this operator, it returns a linear combination of functions which differ from $\phi(x)$ only at ϕ_n. The difference at ϕ_n depends on the finite-difference approximation used for the second derivative. The choice we have used connects functions which differ by ±1 or 0 units of h_ϕ:

$$\left.\frac{\partial^2}{\partial\phi_n{}^2}\right|_{\text{lattice}}\phi(x)=\frac{1}{h_\phi{}^2}[\phi_{\text{up}}(x)+\phi_{\text{down}}(x)-2\phi(x)]. \tag{2.5}$$

The functions ϕ_{up} and ϕ_{down} are equal to $\phi(x)$ everywhere except at x_n, where they are equal to ϕ_n+h_ϕ and ϕ_n-h_ϕ, respectively.

Only the $\partial^2/\partial\phi^2$ term in the Hamiltonian (2.4) produces off-diagonal terms in the Hamiltonian matrix on a classical function basis, just as it has coupled $\phi(x)$ to $\phi_{\text{up}}(x)$ here. This will be illustrated in the following example.

Consider a 2×2 lattice, with two space points $x_1=0$ and $x_2=h_x$, and two ϕ values $=\pm h_\phi/2$. This lattice and the four functions it allows are shown in Fig. 2. We write these four basis functions, which span the space of wave functionals on the 2×2 lattice, as a four-dimensional column vector:

$$\begin{bmatrix}|\ \bullet\!\!>\\ |\ \bullet\!\!>\\ |\ \bullet\!\!>\\ |\ \bullet\!\!>\end{bmatrix} \tag{2.6}$$

Assuming the functions are orthonormal in function space we easily find the matrix form of the diagonal parts of H,

$$H_{\text{kin}}=\frac{h_\phi{}^2}{h_x}\begin{bmatrix}0&&&\\&1&&\\&&1&\\&&&0\end{bmatrix},$$
$$H_{\text{pot}}=\frac{h_x m_0{}^2 h_\phi{}^2}{4}\begin{bmatrix}1&&&\\&1&&\\&&1&\\&&&1\end{bmatrix}. \tag{2.7}$$

The differential operator $\sum_n\partial^2/\partial\phi_n{}^2$ in H_{fluc}, when replaced by a finite-difference operator on the lattice, gives both diagonal contributions and off-diagonal terms. The off-diagonal entries connect function pairs which differ by one step in ϕ ($\Delta\phi=h_\phi$) at one x_n, and are equal at every other x point. On the 2×2 lattice, the matrix form of H_{fluc} is explicitly

$$H_{\text{fluc}}=-\frac{\hbar^2}{2h_x h_\phi{}^2}\begin{bmatrix}-4&1&1&0\\1&-4&0&1\\1&0&-4&1\\0&1&1&-4\end{bmatrix}. \tag{2.8}$$

For completeness, we note that an additional interaction $V_I(\phi(x))$ in the Hamiltonian (2.3) gives the diagonal contribution

$$H_{\text{int}}=h_x\begin{bmatrix}2V_I\left[\frac{h_\phi}{2}\right]&&&\\&V_I\left[\frac{h_\phi}{2}\right]+V_I\left[-\frac{h_\phi}{2}\right]&&\\&&V_I\left[-\frac{h_\phi}{2}\right]+V_I\left[\frac{h_\phi}{2}\right]&\\&&&2V_I\left[-\frac{h_\phi}{2}\right]\end{bmatrix}. \tag{2.9}$$

Returning to the free Hamiltonian, we may factor out the bare mass m_0 and write the entire lattice H in terms of three dimensionless parameters l_k, l_p, and l_f which control the relative strengths of the kinetic, potential, and fluctuation terms on the 2×2 lattice:

$$H=m_0\left\{2l_k\underbrace{\begin{bmatrix}0&&&\\&1&&\\&&1&\\&&&0\end{bmatrix}}_{\sim\frac{1}{m_0}\int\frac{(\vec{\nabla}\phi)^2}{2}dx}+l_p\underbrace{\begin{bmatrix}1&&&\\&1&&\\&&1&\\&&&1\end{bmatrix}}_{\sim\frac{1}{m_0}\int\frac{m_0^2\phi^2}{2}dx}+\hbar^2\frac{l_f}{2}\underbrace{\begin{bmatrix}4&-1&-1&0\\-1&4&0&-1\\-1&0&4&-1\\0&-1&-1&4\end{bmatrix}}_{\sim\frac{-1}{m_0}\int\frac{\hbar^2}{2}\frac{\delta^2}{\delta\phi^2}dx}\right\}, \tag{2.10}$$

where

$$l_k=\frac{h_\phi^2}{2m_0h_x}\,,$$

$$l_p=\tfrac{1}{4}m_0h_xh_\phi^2\,, \tag{2.11}$$

$$l_f=\frac{1}{m_0h_xh_\phi^2}=\tfrac{1}{4}l_p^{-1}\,.$$

Diagonalization of this H gives the four energy eigenstates and eigenvalues on the 2×2 lattice as functions of the mass parameter m_0 in the Lagrangian, Planck's constant $\hbar$, and the lattice parameters h_x and h_ϕ. As the results for general lattice parameters are complicated, we take for illustration particular values $h_x=m_0^{-1}$, $h_\phi=1$. [The general results are given in (2.17).]

Consider the classical-field-theory limit $\hbar\to 0$. In this limit the Hamiltonian is diagonal,

$$H=\begin{bmatrix}\frac{1}{4}&&&\\&\frac{5}{4}&&\\&&\frac{5}{4}&\\&&&\frac{1}{4}\end{bmatrix}m_0+O(\hbar^2) \tag{2.12}$$

and each function has a well-defined energy, which is just the classical energy

$$E_{\text{classical}}=\tfrac{1}{2}\int_{\text{lattice}}d\vec{x}[(\vec{\nabla}\phi)^2+m_0^2\phi^2]\,. \tag{2.13}$$

These classical eigenstates and energies are

State	Energy	Interpretation
$\lvert 2\rangle=\frac{1}{\sqrt{2}}\begin{bmatrix}-\sin\theta\\\cos\theta\\\cos\theta\\-\sin\theta\end{bmatrix}$	$E_2=\left[\frac{11}{4}+\frac{\sqrt{5}}{2}\right]m_0$	Rest 2-particle state,
$\lvert 1'\rangle=\frac{1}{\sqrt{2}}\begin{bmatrix}0\\1\\-1\\0\end{bmatrix}$	$E_1'=\frac{13}{4}m_0$	Boosted 1-particle state,

State	Energy
$\begin{bmatrix}1\\0\\0\\0\end{bmatrix}$	$\frac{1}{4}m_0$,
$\begin{bmatrix}0\\1\\0\\0\end{bmatrix}$	$\frac{5}{4}m_0$,
$\begin{bmatrix}0\\0\\1\\0\end{bmatrix}$	$\frac{5}{4}m_0$,
$\begin{bmatrix}0\\0\\0\\1\end{bmatrix}$	$\frac{1}{4}m_0$.

(2.14)

In this classical limit of the state vectors, the field has unit amplitude to be at one specific function, just as a particle in classical mechanics is found at only one point in coordinate space at a given time.

As we turn on the quantum fluctuations by bringing $\hbar$ up to unity, we find that the energy eigenstates are no longer diagonal in function space; there is instead an amplitude $\psi[\phi_i(\vec{x})]$ to find each of the $i=1,\ldots,4$ functions in a given state vector. For $\hbar=1$ and with the lattice parameters $h_\phi=1$ and $h_x=m_o^{-1}$, the states and spectrum for the 2×2 lattice are

$$|1\rangle=\frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\0\\-1\end{bmatrix} \qquad E_1=\tfrac{9}{4}m_0 \qquad \text{Rest 1-particle state,}$$

$$|0\rangle=\frac{1}{\sqrt{2}}\begin{bmatrix}\cos\theta\\\sin\theta\\\sin\theta\\\cos\theta\end{bmatrix}_{\theta=\frac{1}{2}\tan^{-1}(2)} \qquad E_0=\left[\frac{11}{4}-\frac{\sqrt{5}}{2}\right]m_0 \qquad \text{Vacuum.} \tag{2.15}$$

Some features of these state vectors which allow us to give them a physical interpretation will be discussed in Sec. III. Here we simply note a few features of the energy eigenstates on the 2×2 lattice which recur for larger lattices. One is the appearance of boosted states; on large-N_x lattices there are $\sim N_x$ times as many boosted states as rest states. Elimination of these redundant states from the basis results in a great reduction in the size of the Hamiltonian matrix to be diagonalized; this reduction of the basis to $\vec{P}_{\text{tot}}=\vec{0}$ states will be discussed in the next section. Another interesting feature is the unequal spacing of the vacuum, one-particle, and two-particle states. Although we must recover this equal spacing in the continuum limit, there is no reason to expect it on a finite lattice. For such a small lattice we need not have expected to find the continuum ordering $E_2>E_1>E_0$, though it does follow with the lattice parameters we have chosen.

We note that the mass parameter m_0 in the Lagrangian is not simply related to the spectrum of energies of the lattice except as an overall scale, and it is more intuitive to express the spectrum, relative to the vacuum energy E_0, as a multiple of the mass gap $m=E_1-E_0$. In these units, the 2×2 lattice spectrum becomes

State	Mass $=E-E_0$
$\|2\rangle$	$m_2=\dfrac{5+\sqrt{5}}{2}m,$
$\|1\rangle'$	(boosted $\|1\rangle$),
$\|1\rangle$	$\equiv m,$
$\|0\rangle$	$\equiv 0.$

(2.16)

For completeness, we quote below the 2×2 energies and mixing angle θ which follow from general lattice parameters h_ϕ and h_x:

$$\begin{aligned}
&\frac{1}{m_0}E_2=l_k+l_p+2\hbar^2 l_f+(l_k{}^2+\hbar^4 l_f{}^2)^{1/2}\,,\\
&\frac{1}{m_0}E_1'=2l_k+l_p+2\hbar^2 l_f\,,\\
&\frac{1}{m_0}E_1=l_p+2\hbar^2 l_f\,,\\
&\frac{1}{m_0}E_0=l_k+l_p+2\hbar^2 l_f-(l_k{}^2+\hbar^4 l_f{}^2)^{1/2}\,,\\
&\tan(2\theta)=2\hbar^2/h_\phi{}^4\,.
\end{aligned} \tag{2.17}$$

Finally the renormalized two-particle state mass on the 2×2 lattice is

$$m_2=2m/[1-1/(1+4\hbar^4/h_\phi{}^4)^{1/2}]\,. \tag{2.18}$$

This completes our explicit derivation of the states and spectrum on the 2×2 lattice.

III. THE $\vec{P}_{\text{tot}}=\vec{0}$ "REST" HAMILTONIAN H_R

As the number of states produced in diagonalizing the lattice Hamiltonian H, $N_f=N_\phi{}^{N_x}$, becomes very large for moderate values of N_ϕ and N_x, it is important to find ways of eliminating irrelevant parts of H. The reason H is so large is that it has *all* the energy eigenstates of the theory as eigenvectors. Most of these are boosted states, in which we have no interest. In this section we show how to eliminate all these boosted states from the Hamiltonian, which gives a much smaller "rest" Hamiltonian H_R. The eigenvectors of this H_R span the $\vec{P}_{\text{tot}}=\vec{0}$ subspace of the Hilbert space, and the eigenvalues of this matrix constitute the spectrum of rest states in the theory.

To eliminate $\vec{P}_{\text{tot}}\neq\vec{0}$ states from the Hamiltonian, we begin by constructing the momentum operator $\vec{P}_{\text{op}}$ in the continuum theory:

$$\vec{P}_{\text{op}}=\int d\vec{x}\;\vec{\nabla}\phi\dot{\phi}=-i\int d\vec{x}\;\vec{\nabla}\phi(x)\frac{\delta}{\delta\phi(\vec{x})}\,. \tag{3.1}$$

Operating on an arbitrary state $\psi[\phi(\vec{x})]$ with the exponentiated generator $\vec{P}_{\text{op}}$ gives

$$\begin{aligned}
(U[\vec{a}]\psi)[\phi(\vec{x})]&=e^{i\vec{a}\cdot\vec{P}_{\text{op}}}\psi[\phi(\vec{x})]\\
&=\psi[\phi(\vec{x}+\vec{a})]\,.
\end{aligned} \tag{3.2}$$

If ψ is an eigenstate of total momentum with eigenvalue $\vec{P}$, we conclude

$$\psi_{\vec{P}}[\phi(\vec{x}+\vec{a})]=e^{i\vec{a}\cdot\vec{P}}\psi_{\vec{P}}[\phi(\vec{x})]\,. \tag{3.3}$$

It immediately follows that rest wave functionals are translationally invariant.

To use this result to reduce H to its $\vec{P}_{\text{tot}}=\vec{0}$ part, we must project it onto a translationally invariant set of basis vectors. Constant functions already satisfy this requirement, but any nonconstant function $f_1(\vec{x})$ must be replaced by a basis vector which is the sum of all functions which are equivalent modulo translations:

$$\begin{aligned}
&|\vec{P}_{\text{tot}}=\vec{0}\text{ basis vector }f_1\rangle\\
&\quad=\frac{1}{\sqrt{N_a}}\sum_{\vec{a}}\delta(\phi(\vec{x})-f_1(\vec{x}-\vec{a}))\,.
\end{aligned} \tag{3.4}$$

On a lattice the sum over translations is discrete, and it is convenient to impose periodic boundary conditions.

Given this orthonormal $\vec{P}_{\text{tot}}=\vec{0}$ subbasis $\{|R_i\rangle, i=1,2,\ldots,N_R\}$, we may project the full H onto it to obtain the rest Hamiltonian H_R:

$$H_R=\sum_{i,j=1}^{N_R}|R_i\rangle\langle R_i|H|R_j\rangle\langle R_j| \ . \tag{3.5}$$

Diagonalization of H_R produces only $\vec{P}_{\text{tot}}=\vec{0}$ eigenvectors and eigenvalues.

An example will certainly help visualize this, so we recall the $N_\phi=2$ by $N_x=2$ lattice of Sec. II and its four basis functions:

$$f_1(x)=\begin{cases}\dfrac{-h_\phi}{2}, & x=0\\ \dfrac{-h_\phi}{2}, & x=h_x\end{cases}=|\ \text{—}\ \rangle\ ; \tag{3.6}$$

$f_2=|\ \diagup\ \rangle$; $f_3=|\ \diagdown\ \rangle$; $f_4=|\ \text{⟋—⟋}\ \rangle$.

The translationally invariant basis vectors are

$$|R_1\rangle=|\ \text{—}\ \rangle$$
$$|R_2\rangle=\frac{1}{\sqrt{2}}(|\ \diagup\ \rangle+|\ \diagdown\ \rangle) \tag{3.7}$$
$$|R_3\rangle=|\ \text{⟋—⟋}\ \rangle \ .$$

(Note that there is only one possible translation with periodic boundary conditions, $x_1=0\to x_2=h_x$ and $x_2=h_x\to x_1=2h_x\equiv 0$.)

The original function basis $\underline{4}$ decomposes into a $\underline{3}$ of $\vec{P}_{\text{tot}}=\vec{0}$ vectors and a $\underline{1}$ of $|\vec{P}_{\text{tot}}|=\pi/h_x$ vectors. The latter is

$$|P_1\rangle=\frac{1}{\sqrt{2}}(|\ \diagup\ \rangle-|\ \diagdown\ \rangle) \ . \tag{3.8}$$

Under the lattice translation this changes to

$$e^{ihP_{\text{op}}}|P_1\rangle=-|P_1\rangle=e^{ihp_1}|P_1\rangle \ , \tag{3.9}$$

so $p_1=\pm\pi/h_x$.

Using the set of $\vec{P}_{\text{tot}}=\vec{0}$ basis vectors (3.7) to reduce the full Hamiltonian (2.10) as in (3.5) we produce the following H_R:

$$H_R=\begin{bmatrix} l_p+2\hbar^2 l_f & -\dfrac{\hbar^2 l_f}{\sqrt{2}} & 0\\ -\dfrac{\hbar^2 l_f}{\sqrt{2}} & 2l_k+l_p+2\hbar^2 l_f & -\dfrac{\hbar^2 l_f}{\sqrt{2}}\\ 0 & -\dfrac{\hbar^2 l_f}{\sqrt{2}} & l_p+2\hbar^2 l_f\end{bmatrix} m_0 \ . \tag{3.10}$$

The single boosted state $|P_1\rangle$ we have excluded has an energy [using (2.10) and (3.8)] of

$$\langle P_1|H|P_1\rangle=(2l_k+l_p+2\hbar^2 l_f)m_0 \ . \tag{3.11}$$

Returning to the $\vec{P}_{\text{tot}}=\vec{0}$ rest Hamiltonian H_R (3.10), we may diagonalize it to find the following spectrum and rest states:

State	Energy
$\lvert 2\rangle=-\sin\theta\left\lvert\dfrac{\lvert R_1\rangle+\lvert R_3\rangle}{\sqrt{2}}\right\rangle+\cos\theta\lvert R_2\rangle$	$l_p+l_k+2\hbar^2 l_f+(l_k^2+\hbar^4 l_f^2)^{1/2}$,
$\lvert 1\rangle=\left\lvert\dfrac{\lvert R_1\rangle-\lvert R_3\rangle}{\sqrt{2}}\right\rangle$	$l_p+2\hbar^2 l_f$,
$\lvert 0\rangle=\cos\theta\left\lvert\dfrac{\lvert R_1\rangle+\lvert R_3\rangle}{\sqrt{2}}\right\rangle+\sin\theta\lvert R_2\rangle$	$l_p+l_k+2\hbar^2 l_f-(l_k^2+\hbar^4 l_f^2)^{1/2}$,

(3.12)

where

$$\tan(2\theta)=\frac{\hbar^2 l_f}{l_k}=\frac{2\hbar^2}{h_\phi{}^4} \ . \tag{3.13}$$

By inspection, these are the eigenvectors found earlier in Sec. II in diagonalizing the full Hamiltonian. The reduction of H to H_R might seem to be of only marginal value; we have reduced a 4×4 Hamiltonian on the 2×2 lattice to a 3×3 Hamiltonian, which is not much of an improvement. For larger $N_\phi\times N_x$ lattices, however, the reduction $H\to H_R$ becomes more economical. For example, the $N_\phi=5\times N_x=5$ lattice has an unreduced Hamiltonian of $5^5=3125\times 3125$ entries, and diagonalization produces a list of 3125 energies and eigenvectors. Only $629\approx 3125/N_x$ of these are rest states; the remaining 2496 are boosted copies of these rest states.

If we were to diagonalize the full $5^5\times 5^5$ Hamiltonian, we would somehow have to separate the boosted and rest state energies. This would be an involved procedure re-

TABLE II. Rest Hamiltonian dimensionality.

$N_x=$	2	3	4	5	6
$N_\phi=2$	3	4	6	8	14
3	6	11	24	51	130
4	10	24	70	208	700
5	15	45	165	629	2635
6	21	76	336	1560	7826

quiring knowledge of the corresponding eigenvectors. Constructing the rest Hamiltonian H_R initially both decreases storage requirements by $\sim(1/N_x)$ for large N_x and removes all these irrelevant boosted state energies from the spectrum.

The general result for the dimensionality of the rest Hamiltonian H_R, $N_R(N_\phi,N_x)$, is an interesting combinatoric problem. N_R may be visualized as the number of inequivalent circular necklaces which may be made from N_x equally spaced beads of N_ϕ colors, counting "flipped" necklaces as inequivalent. The number of such objects may be shown to be[22]

$$N_R=\sum_{\substack{n=1\\ n\mid N_x}}^{N_x}\frac{1}{n}\xi_n\ , \tag{3.14}$$

where $n\mid N_x$ means $n=$ all divisors of N_x and ξ_n is defined recursively by

$$\xi_n=N_\phi{}^n-\sum_{\substack{m=1\\ m\mid n}}^{n-1}\xi_m \tag{3.15}$$

and

$$\xi_1=N_\phi\ . \tag{3.16}$$

An equivalent result for the dimensionality N_R may be given in terms of Euler's totient function $\phi(d)$. [This is defined as the number of integers from 1 to d inclusive which are prime to d. For example, $\phi(4)=2$ because only 1 and 3 are prime to 4.] The expression for the dimensionality is[23]

$$N_R=\frac{1}{N_x}\sum_{\substack{n=1\\ n\mid N_x}}^{N_x}\phi(n)N_\phi{}^{(N_x/n)}\ . \tag{3.17}$$

For prime N_x the dimensionality is particularly simple:

$$\begin{aligned}N_R(N_\phi,N_x\text{prime})&=\frac{1}{N_x}\xi_{N_x}+\xi_1\\&=\frac{1}{N_x}N_\phi{}^{N_x}+\frac{N_x-1}{N_x}N_\phi\ .\end{aligned} \tag{3.18}$$

The explicit values of N_R for lattices up to $N_\phi=6$ by $N_x=6$ are given in Table II.

A further symmetry available here is the invariance of H under the discrete transformation $\phi(\vec{x})\rightarrow-\phi(\vec{x})$, which implies a definite ϕ parity (not to be confused with the more familiar spatial parity, to be discussed below) for the energy eigenstates;

$$\psi[-\phi(\vec{x})]=(\pm)\psi[\phi(\vec{x})]=\eta_\phi\psi[\phi(\vec{x})]\ . \tag{3.19}$$

This ϕ parity can be used to further reduce H_R. States composed of even or odd numbers of particles have plus or minus ϕ parity, respectively. In the list of states in (3.12), we use the negative ϕ parity of $[(|R_1\rangle-|R_3\rangle)/\sqrt{2}]$ to identify it as the one-particle state. The remaining two states both have positive ϕ parity and are identified with the vacuum and two-particle states. On such a small lattice only their energies distinguish them; on larger lattices, we may use the number of nodes to separate these states as well as their energies in the continuum limit.

Another discrete parity which commutes with H is spatial ($\vec{x}\rightarrow-\vec{x}$) parity. Nondegenerate eigenstates of H always have definite spatial parity

$$\psi[\phi(-\vec{x})]=(\pm)\psi[\phi(\vec{x})]=\eta_p\psi[\phi(\vec{x})]\ . \tag{3.20}$$

As the low-lying rest states (vacuum, one particle, and two particle) necessarily have $\eta_p=(+)$, this parity is not useful in distinguishing these states. It may be useful in further reducing the size of H_R, although we have not employed it here.

IV. APPROACH TO THE CONTINUUM SPECTRUM

It is very important to understand the asymptotic approach of the lattice spectrum to the continuum one for large N_ϕ and N_x. This is because we are limited by storage requirements to lattices of only moderate size; accurate determination of the continuum spectrum clearly requires identification and elimination of the spurious lattice contributions.

To understand the asymptotic approach to the continuum, we have studied the free scalar theory on the lattice in two limits; (1) $N_\phi\rightarrow\infty$, $N_x$fixed$=2$ (continuous ϕ limit) and (2) $N_\phi=3$, $N_x\rightarrow\infty$ (continuous x limit). In particular, we study the two-particle mass m_2/m in these limits, and show that our theoretical asymptotic behavior for large lattices agrees with explicit numerical results.

A. $N_\phi\rightarrow\infty$, $N_x=2$; continuous ϕ limit

Consider a lattice of $N_x=2$ space points and a very large number $N_\phi\rightarrow\infty$ of very closely spaced ϕ points. As ϕ_1 and ϕ_2 become continuous, the Hamiltonian approaches

$$\begin{aligned}H\simeq&-\frac{\hbar^2}{2h_x}\left[\frac{d^2}{d\phi_1{}^2}+\frac{d^2}{d\phi_2{}^2}\right]\\&+\frac{1}{2h_x}[(\phi_1-\phi_2)^2+(\phi_2-\phi_1)^2]\\&+\frac{h_x m_0{}^2}{2}(\phi_1{}^2+\phi_2{}^2)\ .\end{aligned} \tag{4.1}$$

We may diagonalize this H by going into Fourier space with

$$\begin{aligned}a_0&=\frac{1}{\sqrt{2}}(\phi_1+\phi_2)\ ,\\a_1&=\frac{1}{\sqrt{2}}(\phi_1-\phi_2)\ .\end{aligned} \tag{4.2}$$

These are the $N_x=2$ Fourier coefficients, generally given by

$$a_j=\frac{1}{\sqrt{N_x}}\sum_{i=1}^{N_x}\phi_i e^{ik_j x_i} . \tag{4.3}$$

This puts H in the separated form

$$H=-\frac{\hbar^2}{2h_x}\left[\frac{d^2}{da_0{}^2}+\frac{d^2}{da_1{}^2}\right]+\frac{h_x}{2}(\omega_0{}^2a_0{}^2+\omega_1{}^2a_1{}^2) , \tag{4.4}$$

$$\omega_0=m_0 , \quad \omega_1=[m_0{}^2+(2/h_x)^2]^{1.2} . \tag{4.5}$$

The $N_x=2$ lattice is thus a superposition of two independent momentum-space oscillators which satisfy the usual lattice dispersion relation

$$\omega(k)=\left[m_0{}^2+\frac{4}{h_x{}^2}\sin^2\left[\frac{kh_x}{2}\right]\right]^{1/2} . \tag{4.6}$$

On the $N_x=2$ lattice k takes on the values $k\equiv 2\pi/\lambda=0, \pi/h_x$.

The most general energy eigenstate of (4.4) is n_0 rest particles and n_1 particles of momentum π/h_x, with an energy of

$$E_{n_0,n_1}=\hbar[m_0(n_0+\tfrac{1}{2})+\omega_1(n_1+\tfrac{1}{2})] . \tag{4.7}$$

Note that only the even-n_1 states (with $p_{\text{tot}}=2\pi N/h_x\sim 0$) will appear in the spectrum of the rest Hamiltonian H_R.

The vacuum state in the continuous ϕ limit with $N_x=2$ is just a Gaussian function in a_0 and a_1. The explicit wave functional, which is an eigenfunction of (4.4), is

$$\psi[\phi(x)]=\left[\frac{c_0}{\pi}\right]^{1/4}\left[\frac{c_1}{\pi}\right]^{1/4}e^{-c_0a_0{}^2-c_1a_1{}^2} ,$$
$$c_i=\frac{\omega_i h_x}{\hbar} . \tag{4.8}$$

The rms fluctuation of a_i, the ith Fourier component of ϕ, is given by

$$\sigma_i=\frac{1}{\sqrt{2c_i}}=\left[\frac{\hbar}{2\omega_i h_x}\right]^{1/2} . \tag{4.9}$$

Now consider the effect of working on a large, fine-meshed ϕ lattice with N_ϕ points, rather than having ϕ continuous. We allow the ϕ grid size h_ϕ to shrink as $K_\phi/\sqrt{N_\phi}$ (K_ϕ is an adjustable number), so the full ϕ extent of the lattice, L_ϕ, grows as $\sqrt{N_\phi}$:

$$h_\phi=K_\phi/\sqrt{N_\phi} ,$$
$$L_\phi=N_\phi h_\phi=K_\phi\sqrt{N_\phi} . \tag{4.10}$$

There are two reasons why the lattice spectrum differs from the continuum result (4.7). First, the maximum value of the field ϕ on the lattice ($\sim L_\phi/2$) is finite, so the wings of the simple harmonic oscillator (SHO) wave functions such as (4.8) will be distorted. This gives an asymptotic energy defect for the vacuum state of

$$\delta E\equiv E_{\text{cont}}(\infty)-E_{\text{lattice}}(N_\phi)$$
$$\sim\frac{1}{L_\phi}e^{-cL_\phi{}^2}\sim\frac{1}{\sqrt{N_\phi}}e^{-c'N_\phi} \tag{4.11}$$

which falls very rapidly for large N_ϕ. This is *not* the source of the leading energy defect in $N_\phi{}^{-1}$ on our lattice. To avoid significant contributions due to this truncation, we must ensure that the ϕ lattice extent (L_ϕ) is much greater than the rms SHO full width $2\sigma_0$:

$$L_\phi=K_\phi\sqrt{N_\phi}\gg 2\sigma_0=2\left[\frac{\hbar}{2m_0h_x}\right]^{1/2} . \tag{4.12}$$

For an n-particle SHO state rather than the vacuum, we must increase the L_ϕ requirement to

$$L_\phi=K_\phi\sqrt{N_\phi}\gg 2\sqrt{2n+1}\sigma_0\sim 2\left[\frac{n\hbar}{m_oh_x}\right]^{1/2} . \tag{4.13}$$

The remaining source of differences between the continuum and lattice spectra is the effect of having a finite grid size in ϕ, h_ϕ. To make this effect perturbative, we must choose an h_ϕ much smaller than the rms width:

$$h_\phi=K_\phi/\sqrt{N_\phi}\ll 2\sigma_0=2\left[\frac{\hbar}{2m_0h_x}\right]^{1/2} . \tag{4.14}$$

The perturbative effect of using the finite-difference approximation to $\partial^2/\partial\phi^2$ may be seen by expanding it to $O(h_\phi{}^2)$. The finite-difference approximation introduces spurious terms of $O(h_\phi{}^2\partial^4/\partial\phi^4)$ in the Hamiltonian:

$$\frac{\psi(\phi+h_\phi)+\psi(\phi-h_\phi)-2\psi(\phi)}{h_\phi{}^2}=\frac{\partial^2\psi}{\partial\phi^2}+\frac{h_\phi{}^2}{12}\frac{\partial^4\psi}{\partial\phi^4}+\cdots , \tag{4.15}$$

so the lattice has a residual effective interaction of $O(h_\phi{}^2)$:

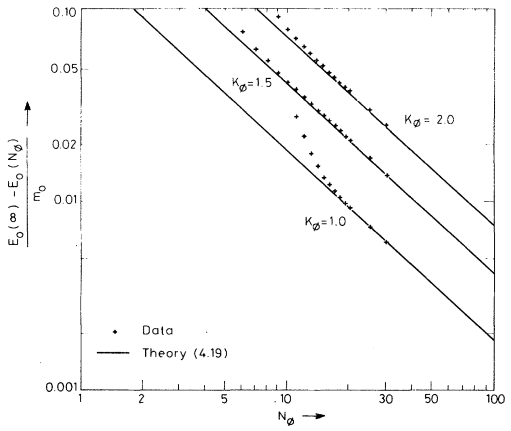

FIG. 3. Asymptotic approach to the zero-point energy E_0. ($N_x=2$, $K_x=\sqrt{8}$, $K_\phi=1.0$, 1.5, 2.0.)

$$\delta H=-\frac{\hbar^2 h_\phi{}^2}{24h_x}\left[\frac{\partial^4}{\partial\phi_1{}^4}+\frac{\partial^4}{\partial\phi_2{}^4}\right] . \tag{4.16}$$

This term gives the leading discrepancy between the continuum and lattice spectra. The matrix element of this effective interaction between free theory states with n rest particles and no moving ones for $N_x=2$ is

$$\langle n,0\,|\,\delta H\,|\,n,0\rangle = -\frac{\hbar^2 h_\phi{}^2}{64h_x}\{(c_0+c_1)^2+2nc_0[(n+1)c_0+2c_1]\} . \tag{4.17}$$

In the vacuum state, this gives an asymptotic vacuum energy for large N_ϕ of

$$E_0(N_\phi)=\tfrac{1}{2}\hbar(m_0+\omega_1)-\frac{h_\phi{}^2 h_x}{64}(m_0+\omega_1)^2+O(h_\phi{}^4) \tag{4.18}$$

$$=\underbrace{\tfrac{1}{2}\hbar(m_0+\omega_1)}_{E_0(\text{continuum})}-\underbrace{\frac{K_\phi{}^2 h_x(m_0+\omega_1)^2}{64}N_\phi{}^{-1}}_{\text{leading energy defect}}+O(N_\phi{}^{-2}) . \tag{4.19}$$

The $h_\phi{}^2\sim N_\phi{}^{-1}$ energy defect is characteristic of all the spectrum calculations we have studied numerically. An illustration of this is given in Fig. 3, which plots the vacuum energy defect against N_ϕ on a log-log scale. Three choices for K_ϕ (initial lattice size) are shown; the approach to the solid asymptotic curves is quite clear, and confirms (4.19).

Although choosing a small h_ϕ (that is, K_ϕ) reduces the energy defect in (4.19), it can significantly delay the onset of the $N_\phi{}^{-1}$ asymptotic behavior we are interested in by making the ϕ extent of the lattice, $L_\phi=K_\phi\sqrt{N_\phi}$, too small. This is the reason the $K_\phi=1.0$ energy defect curve in Fig. 3 departs from the asymptotic $N_\phi{}^{-1}$ behavior for $N_\phi\lesssim 15$. It is obviously preferable to have a larger error with a well-behaved N_ϕ dependence which can be isolated and subtracted off (as for $K_\phi=1.5$) than to have a smaller but nonasymptotic error of uncertain N_ϕ dependence (as for $K_\phi=1.0$, $N_\phi\lesssim 15$).

As a rule of thumb, one may choose the initial-lattice resolution K_ϕ to be the geometric mean of the maximum necessary extent in ϕ, L_ϕ (4.13) and the estimated required ϕ resolution h_ϕ (4.14). This gives a "reasonable" value for K_ϕ of

$$K_\phi\sim\sqrt{L_\phi h_\phi}\sim[2\sigma_0\sqrt{2n}\,2\sigma_0]^{1/2}\sim 2\sigma_0(2n)^{1/4} =(8n)^{1/4}[\hbar/(m_0h_x)]^{1/2} . \tag{4.20}$$

For the low-lying states, $n\sim 2$, and with h_x shrinking as $h_x=K_x/(m_0\sqrt{N_x})$ as we go to large N_x (4.29) and (4.32), this gives for our reasonable value of the lattice parameter K_ϕ

$$K_\phi\sim 2N_x{}^{1/4}/\sqrt{K_x} . \tag{4.21}$$

This is typically ~ 1.0 to ~ 1.5 for values of N_x and K_x we use in our large-N_x computations in Sec. V, which does indeed give rapid approach to the continuous ϕ spectrum.

As we have shown, the lattice spectrum with our choice of the finite-difference operator for the ϕ second derivative will approach the continuous ϕ spectrum as $h_\phi{}^2\sim N_\phi{}^{-1}$ for large N_ϕ:

$$E(N_\phi)=E(\infty)+e_1N_\phi{}^{-1}+e_2N_\phi{}^{-2}+\cdots . \tag{4.22}$$

For sufficiently large N_ϕ, therefore, we may take out the leading asymptotic approach to the continuum energy and accelerate convergence by forming the combinations

$$E^{(1)}(N_\phi)=(N_\phi+\tfrac{1}{2})E(N_\phi+\tfrac{1}{2}) -(N_\phi-\tfrac{1}{2})E(N_\phi-\tfrac{1}{2}) , \tag{4.23}$$

$$E^{(2)}(N_\phi)=\tfrac{1}{2}[(N_\phi+1)^2E(N_\phi+1)-2N_\phi{}^2E(N_\phi) +(N_\phi-1)^2E(N_\phi-1)] , \tag{4.24}$$

and so forth. (Note that the argument of $E^{(2n+1)}$ is half-integral.) The improved energies $E^{(n)}(N_\phi)$ converge to the continuous ϕ energies as

$$E^{(n)}(N_\phi)=E(\infty)+O(N_\phi{}^{-n-1}) . \tag{4.25}$$

Using (4.23) and (4.24), we obtain improved estimates of the continuous ϕ energy $E(\infty)$ for given N_ϕ. We then simply increase N_ϕ until the predicted values of $E(\infty)$ from $E^{(1)}$ and $E^{(2)}$ converge and stabilize to the desired accuracy, which occurs when the $O(N_\phi{}^{-2})$ corrections to $E^{(1)}$ become unimportant.

To illustrate this procedure, we have looked at the once- and twice-N_ϕ-improved two-particle masses $(m_2/m)^{(1)}(N_\phi)$ and $(m_2/m)^{(2)}(N_\phi)$ on the $N_x=2$ lattice, with $K_\phi=1.5$. These result from applying the convergence accelerations (4.23) and (4.24) to the raw two-particle mass ratio, which is given by

$$\frac{m_2}{m}(N_\phi)=\frac{E_2(N_\phi)-E_0(N_\phi)}{E_1(N_\phi)-E_0(N_\phi)} . \tag{4.26}$$

The raw data $(m_2/m)(N_\phi)$ and the once- and twice-N_ϕ-improved m_2/m are shown in Fig. 4 for $N_\phi=10$ to 28. The rapid convergence of the improved mass ratios to the continuous ϕ result $m_2/m=2.0$ is quite clear. Evidently, an accuracy of $\sim 10^{-3}$ is possible if we can accommodate N_ϕ values of $\gtrsim 15$.

Note that there is some "jitter" visible in the twice-N_ϕ-improved $(m_2/m)^{(2)}$ for large N_ϕ ($N_\phi\gtrsim 15$). This is due to rounding errors of $\sim 10^{-6}$ in the raw spectrum, which are magnified by $O(N_\phi{}^2)$ in removing the asymptotic

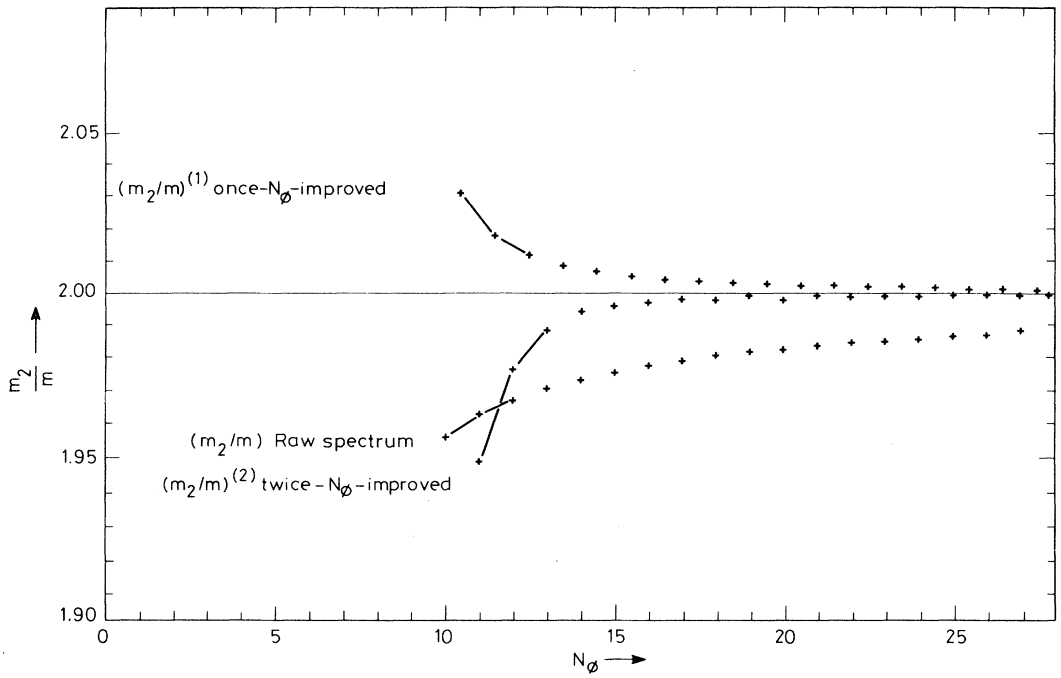

FIG. 4. Convergence of m_2/m to 2.0 in the free theory. ($N_x=2$, $K_x=\sqrt{8}$, $K_\phi=1.5$.)

behavior using (4.23) and (4.24). It is this rounding error which makes it impractical to accelerate the convergence of the spectrum in N_ϕ more than twice with present accuracy.

We could of course remove the $h_\phi{}^2 \sim N_\phi{}^{-1}$ asymptotic behavior initially by using a better approximation to $\partial^2/\partial\phi^2$ in Table I and (2.5), so that we obtain corrections only to $O(h_\phi{}^4)$ in (4.15). We have not done this because the off-diagonal terms in H would no longer all be equal (hence more difficult to code), and there would be twice as many of these terms (hence twice the run time). It is easier to just remove the $N_\phi{}^{-1}$ behavior from the spectrum by hand, as we have done in this paper.

B. $N_\phi=3$, $N_x\to\infty$; continuous-x limit

The continuum and lattice spectra also differ due to the finite-space lattice. The continuum of boosted states we find in the free theory, for example, is replaced by a discrete set of levels in momentum space, with a separation $\Delta k=\pi/L_x$ and a maximum momentum $k_{\max}=\pi/h_x$. These cutoffs in the IR and UV ensure that there are no divergences in our spectrum calculations, so that parameter renormalizations such as replacing m_0 by $m=(E_1-E_0)$ are finite.

Physically meaningful quantities such as the ratio of the two-particle state mass to the one-particle mass, m_2/m, are expected to approach the continuous-$\vec{x}$ limit on the lattice as we take $h_x\to 0$ and $L_x\to\infty$. As we are limited to small values of N_x sites, it is important to see how quickly we expect the lattice values of physical quantities to approach their continuum limits as a function of N_x.

We expect finite-size effects due to (a) replacing the continuum of states $\{\vec{k}\}$ by a discrete set, so momentum-space integrals become sums, (b) the modified dispersion relation for states on a lattice (4.6), and (c) replacing the continuous functional derivative in H (2.3) by a discrete set (2.4). The only effect we can estimate to our satisfaction is (b); fortunately, the evidence of our numerical calculation in Sec. V is that this effect gives the leading (in h_x) approach to the continuum spectrum.

For an example of (b), consider the energy of a single-particle state on the lattice in the free theory, with continuous ϕ and N_x large but finite, so that $|\vec{k}|h_x \ll 1$. The energy of this state relative to the vacuum is

$$E(\vec{k})-E_0=\left[m_0{}^2+\frac{4}{h_x{}^2}\sin^2\left[\frac{kh_x}{2}\right]\right]^{1/2} \tag{4.27}$$

$$=\underbrace{(m_0{}^2+\vec{k}^2)^{1/2}}_{\omega_{\vec{k}}}-\frac{1}{24}\frac{\vec{k}^4}{\omega_{\vec{k}}}h_x{}^2+O(h_x{}^4)\,. \tag{4.28}$$

Thus, the lattice dispersion relation gives an approach to the continuous-x spectrum as $\sim h_x{}^2$. Assuming we shrink the lattice with increasing N_x as

$$h_x=\tilde{K}_x/\sqrt{N_x} \tag{4.29}$$

we then expect for the renormalized spectrum with the zero-point energy removed, and expressed as a multiple of the mass gap $m=(E_1-E_0)$:

$$\delta(m_i/m)\,|_{\text{lattice}-\text{continuum}}=O(N_x{}^{-1})\,. \tag{4.30}$$

So, we generally expect the lattice spectrum to approach the continuum limit as $h_x{}^2$ as well as $h_\phi{}^2$ for small h_x and

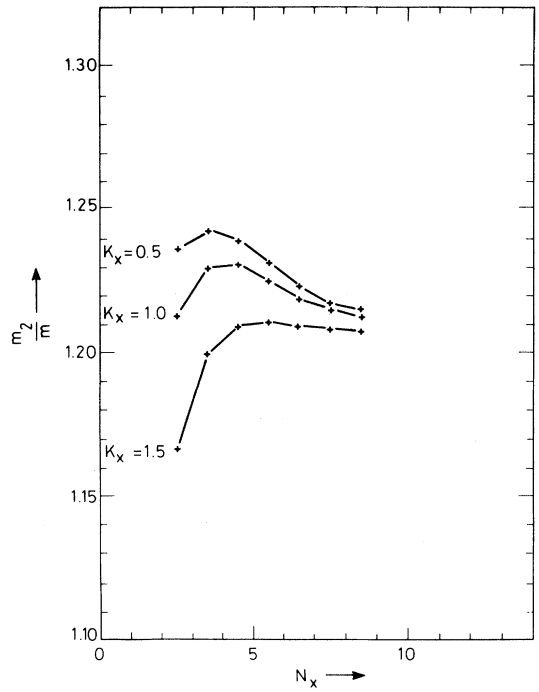

FIG. 5. Once-N_x-improved two-particle mass m_2/m. (Test case with $N_\phi=3$, $K_\phi=1.5$, K_x variable.)

h_ϕ. Note that in some special cases, such as *n rest* particles in the free theory, there are no $\vec{k}\neq 0$ states present. This means that results such as $m_2/m=2$ in the free theory are not effected by the lattice dispersion relation (4.6), and remain true for finite as well as infinite N_x.

Just as for ϕ discretization, in x space we must ensure that the lattice is large enough as well as fine enough to give an accurate spectrum. The natural scale of the problem on a small lattice with weak coupling is the bare mass m_0 in the Lagrangian. A physically plausible lattice must satisfy

$$L_x=\tilde{K}_x\sqrt{N_x}\gg\text{natural scale}\gg h_x=\tilde{K}_x/\sqrt{N_x}\ . \tag{4.31}$$

Taking m_0 as the natural length scale, a reasonable choice for $\tilde{K}_x$ is

$$\tilde{K}_x=K_x m_0{}^{-1}\ , \tag{4.32}$$

with K_x a dimensionless lattice parameter of order unity.

To test the expected $N_x{}^{-1}$ approach to the continuous-x spectrum (4.30), we have studied the spectrum of a spin system with only $N_\phi=3$ possible values for the field ϕ at each of the N_x sites. The allowed field values are $\phi=(h_\phi, 0, -h_\phi)$, where h_ϕ is chosen arbitrarily to be

$$h_\phi=\frac{K_\phi(=1.5)}{\sqrt{N_\phi(=3)}}=\frac{\sqrt{3}}{2}\ . \tag{4.33}$$

We have obtained the two-particle mass ratio m_2/m for $N_x=2\to 9$ for various values of K_x [recall $h_x=K_x/(m_0\sqrt{N_x})$]. As we expect the finite-lattice spectrum $(m_2/m)(N_x)$ to approach the continuum one as $N_x{}^{-1}$, we have removed this leading asymptotic behavior, analogously to (4.23):

$$(m_2/m)^{(1)}(N_x)=[N_x+\tfrac{1}{2}]m_2(N_x+\tfrac{1}{2})/m(N_x+\tfrac{1}{2}) -[N_x-\tfrac{1}{2}]m_2(N_x-\tfrac{1}{2})/m(N_x-\tfrac{1}{2})\ . \tag{4.34}$$

This once-N_x-improved m_2/m spectrum for various values of K_x is shown in Fig. 5. Approach to the continuous-x value of $m_2/m\sim 1.21$ is clear. It is evident that we could estimate the continuous-x m_2/m to an accuracy of $\sim 10^{-2}$ from the first three improved values of m_2/m, using $N_x=2\to 5$ and various values of K_x. This example leads us to believe that we can obtain the bound-state spectrum of (1 + 1)-dimensional theories to a similar accuracy of $\sim 10^{-2}$ at present.

V. $\lambda_0\phi^4$ SPECTRUM

We have discussed the techniques required to carry out lattice wave-functional spectrum calculations on small lattices and in the continuum limit in some detail. Now we shall present preliminary results on the spectrum of a nontrivial field theory, $\lambda_0\phi^4$, as a first application of our approach.

$\lambda_0\phi^4$ theory has been the subject of a number of lattice papers, and several remarkable results have been demonstrated analytically or through numerical experiments. The subject of many studies has been the behavior of the renormalized coupling constant λ as a function of λ_0 in the continuum limit in d space-time dimensions. The independent conclusion of Monte Carlo[5,6] high-temperature series[24,25] and strong-coupling studies[26,27] is that $\lambda=0$ independent of λ_0 in the continuum limit for $d\geq 4$. There

TABLE III. $\lambda_0\phi^4$ spectrum (m_2/m) for continuous ϕ, finite N_x.

$\lambda_0/m_0{}^2$ \ N_x	2	3	4	5
0.0	2.001	2.002	2.000	2.001
0.1	2.048	2.036	2.031	2.023
0.2	2.066	2.051	2.041	2.036
0.5	2.088	2.063	2.050	2.042
1.0	2.095	2.064	2.050	2.045
∞	2.140	2.092	2.068	2.059
Estimated error	±0.002	±0.002	±0.003	±0.005

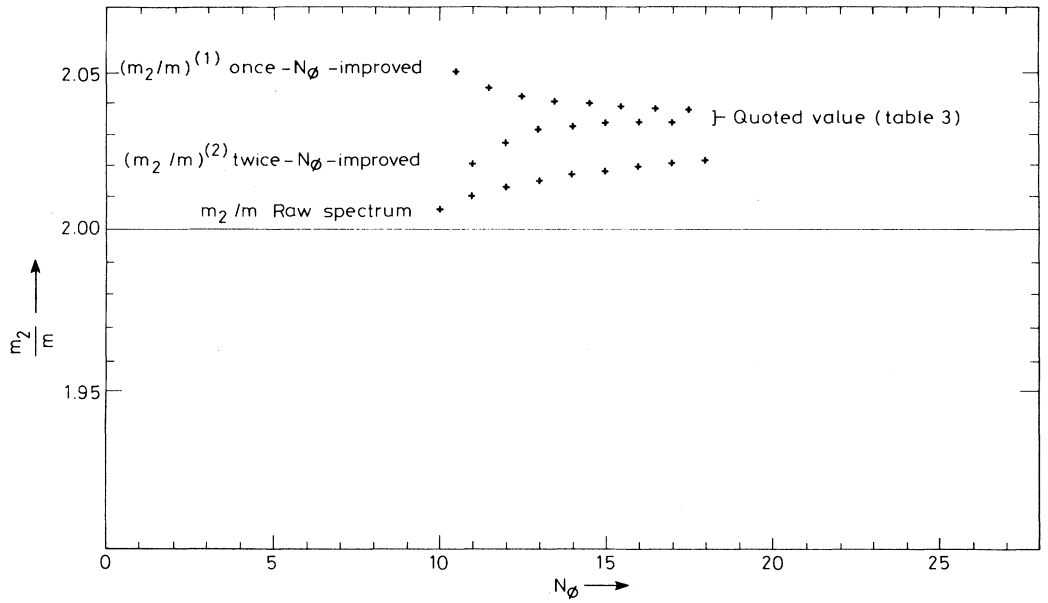

FIG. 6. A typical extrapolation of the lattice spectrum to continuous ϕ. ($N_x=3$, $K_x=\sqrt{8}$, $K_\phi=1.5$, $\lambda_0/m_0{}^2=0.1$.)

are proofs of this result for d greater than 4.[28–30] $d=3$ appears to be a complicated case with both interacting and noninteracting limits.[25,30] For the $d=2$ case we study here there is general agreement[5,24–27] that the continuum theory has nontrivial interactions, that is, it can support $\lambda>0$.

Although the existence of interactions in $d=2$ $\lambda_0\phi^4$ theory has been shown ($\lambda>0$), the question of the bound-state spectrum of this theory has not been studied numerically to our knowledge.

The particular question we shall study is the renormalized "two-particle" state mass $m_2/m\equiv(E_2-E_0)/(E_1-E_0)$ as a function of λ_0. We shall find that it is equal to 2.0, independent of λ_0 in the continuum limit, to within our estimated accuracy of ~ 0.01.

The continuum Hamiltonian for ϕ^4 theory is

$$H=\int d\vec{x}\left[-\frac{\hbar^2}{2}\frac{\delta^2}{\delta\phi(\vec{x})^2}+\tfrac{1}{2}|\vec{\nabla}\phi|^2+\tfrac{1}{2}m_0{}^2\phi^2+V_I(\phi)\right], \quad (5.1)$$

where

$$V_I(\phi)=\lambda_0\phi(\vec{x})^4 . \quad (5.2)$$

As discussed in Sec. II, the interaction (5.2) is a simple modification of the diagonal of the functional Hamiltonian matrix, as in (2.9). We then obtain the "two-particle" mass m_2/m in the continuum-ϕ limit for $N_x=2,3,4$, and 5, and for $\lambda_0/m_0{}^2=0,0.1,0.2,0.5,1.0$, and ∞, using the extrapolation technique discussed in Sec. IV. The results are given in Table III. A representative case of the extrapolation to $N_\phi=\infty$ for $N_x=3$ and $\lambda_0/m_0{}^2=0.1$ is shown in Fig. 6; the rapid convergence of the once- and twice-N_ϕ-improved values of m_2/m is evident. Taking these two values at large N_ϕ as upper and lower limits, we find m_2/m ($N_x=3$, $K_x=\sqrt{8}$, $N_\phi=\infty$, $\lambda_0/m_0=0.1$)$=2.036\pm 0.002$. This is the value quoted in Table III.

To extrapolate the values of m_2/m determined at finite N_x in Table III to the continuum limit, we have done a least-squares fit of the finite-N_x data to the expected asymptotic form:

$$\frac{m_2}{m}(N_x,\lambda_0/m_0{}^2)\cong\frac{m_2}{m}(\lambda_0/m_0^2)+\frac{e_1(\lambda_0/m_0{}^2)}{N_x} \quad (5.3)$$

for the accurately determined $N_x=2,3$, and 4 cases. Although one might reasonably be concerned that $N_x=2-4$ is not large enough to be in the asymptotic region for large N_x, we find empirically that the coefficient e_1 is of order 0.2 or less. Corrections of order $(e_1/N_x)^2$ can then be expected to modify our results by ~ 0.01.

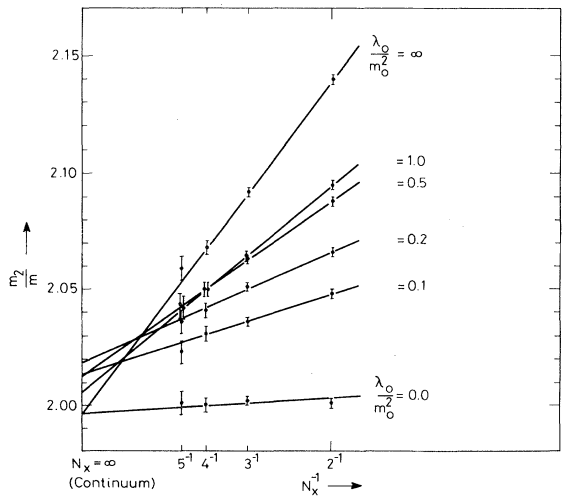

FIG. 7. Approach to continuum m_2/m in $\lambda_0\phi^4$.

TABLE IV. Renormalized two-particle mass in $\lambda_0\phi^4$.

$\frac{m_2}{m}(\lambda)$	$\frac{\lambda_0}{m_0^2}$
2.00	0.0
2.01	0.1
2.02	0.2
2.01	0.5
2.00	1.0
2.00	∞
all masses $\pm\sim 0.01$	

The result is shown in Fig. 7 and Table IV. We find that m_2/m in the continuum limit is consistent with the free-theory result $m_2/m=2$ independent of λ_0, to within the estimated error of ± 0.01 due to the extrapolation to $N_x=\infty$.

As we have covered the full positive range of $\lambda_0/{m_0}^2=0$ to ∞, it cannot be argued that this result depends on how the renormalized λ is defined on the lattice in the continuum limit. We find $m_2/m=2.0$, to within errors, for any positive value of λ_0.

This is a surprising but not unanticipated result; in perturbation theory, the four-ϕ contact tree diagram gives rise to a repulsive potential proportional to $\lambda_0\delta(\vec{x})$, which does not support bound states. Given this, Halliday[8] has argued that if the ϕ quanta experience a repulsive short-range interaction, they can just sit at infinite range, giving $m_2/m=2$. Certainly it cannot be >2 for this reason. What is nontrivial is that the full theory remains repulsive for all λ, so that no bound states form when all the higher-order effects beyond tree graphs are included. Lee[7] argues that this follows from the fact that the interaction Hamiltonian $\lambda\phi^4$ is positive, though his arguments are intuitive and do not constitute a proof.

We note that our result $m_2/m=2$ does not imply that $(1+1)$-dimensional ϕ^4 is a free theory; we have simply found that the interaction between quanta in the full theory does not appear to produce bound states with masses below $2m$, where m is the renormalized one-particle mass. This result says nothing about the presence of repulsive scattering in the continuum limit, although such scattering is consistent with our result.

VI. CONCLUSION

We have shown how to obtain the spectrum of energy eigenstates of an interacting quantum field theory using lattice and wave-functional techniques. Our method is to write the functional Hamiltonian operator as a matrix acting on a basis of classical functions on a lattice, which we then diagonalize using the Lanczos technique and extrapolate to the continuum limit.

Special techniques are introduced to project out irrelevant boosted states from the lattice, and to accelerate convergence of large lattice spectra to the continuum limit. These techniques allow the determination of the lowest few eigenvalues of a lattice field theory with a very large number of basis functions; in this paper we have presented results which would require the brute-force diagonalization of a $537\,824\times 537\,824$ (14^5 square) dimensional Hamiltonian.

As a preliminary application of this approach, we have obtained the first three energy levels of $\frac{1}{2}{m_0}^2\phi^2+\lambda_0\phi^4$ theory in $1+1$ dimensions. We find that this theory has a free spectrum ($m_2/m=2.0$), independent of λ_0, to within the estimated accuracy (± 0.01) of our method. We believe this result to be consistent with known results for ϕ^4 theory in $d=2$.

Since further interactions can be studied with a trivial modification of the diagonal of our Hamiltonian matrix, we hope to present studies of the spectra of a number of scalar field theories using these techniques in the near future.

Another important problem is the extension of this approach to $2+1$ and $3+1$ space-time dimensions. While it is impossible to do this and keep the full functional basis on the lattice, as we have done in $1+1$ dimensions, it may be possible to treat higher-dimensional problems with a representative sample of basis functions, rather than the full set. This possibility is currently under investigation.

Note added in proof. After completion of this work we learned that our results on the absence of bound states below $2m$ in $\lambda{\phi_2}^4$ theory (the test of Sec. V) was previously obtained by Spencer[31] and is discussed by Glimm and Jaffe.[32]

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