Practical lower bound for scalar fields on a lattice

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A simple lower bound on the ground-state energy density is derived for a scalar field on a lattice. This bound is applied to ϕ^4 theory in one space and one time dimension and the results compared with available upper bounds.

I. INTRODUCTION

There has been in the last several years an increased interest in developing nonperturbative methods for computing the properties of field theory.[1] This is based on reservations one has about the applicability of perturbation theory in certain regions of choice of parameters, especially in regions where the theory in question may undergo a phase transition, and generally in any strong-coupling region. To this one may add the uncertainty regarding the existence of a convergent perturbation expansion for any value of the parameters. (As simple a problem as the anharmonic-oscillator Schrödinger equation fails to have a convergent expansion.) One general class of approaches to nonperturbative treatment begins with the simplification of placing the field theory on a discrete lattice. Within this class there are two broad subclasses. One may rotate the time axis into the complex plane and make both space and time dimensions discrete, achieving a certain similarity to lattice spin systems, about which a great deal has been said.[2] Or one may make only the spatial dimensions discrete, and leave time as a continuous parameter.[3] The latter approach seems more natural when the Hamiltonian is the central object of study, the former when considering generating functions. This paper is concerned with the second of these alternatives.

After the initial concession of the lattice approximation, it is up to one's ingenuity to obtain computational methods which exploit the simplification while giving up as little further ground as possible. Towards this end it is advantageous to have at one's disposal rigorous bounds against which one may compare one's latest favorite approximations. Some progress can be reported here. In a closely related paper, Drell, Weinstein, and Yankielowicz,[4] henceforth DWY, describe a variational upper bound on the ground-state energy density of ϕ^4 field theory in 1+1 dimensions. Here we shall describe its natural partner, a lower bound for the same quantity. In concert these bounds, at least for large values of the coupling, are capable of giving an absolute limit on the energy density of a few percent.

In Sec. II we will briefly introduce the notation and define the problem, and then derive the lower bound. In Sec. III we will describe some numerical results for the energy density.

II. THE LOWER BOUND

Suppose we are given two operators H and H^0 acting in the same Hilbert space. All of the eigenvalues of H^0 will be lower bounds to the corresponding, i.e., ordered, eigenvalues of H if their difference $\Delta = H - H^0$ is a positive-semidefinite operator. This is too strong a condition to be of use, though. Since we are concerned with the ground state the much weaker condition $\langle 0|\Delta|0\rangle \geq 0$ will give the bound $E_0 \geq E_0^0$, where $H|0\rangle = E_0|0\rangle$ and E_0^0 is the lowest eigenvalue of H^0. This is easily shown, for if $\langle 0|\Delta|\Delta\rangle \geq 0$ then

$$E_0 = \langle 0|H|0\rangle = \langle 0|H^0|0\rangle + \langle 0|\Delta|0\rangle \geq E_0^0. \tag{2.1}$$

We shall exploit the bound (2.1) by constructing an H^0 corresponding to the lattice Hamiltonian H in such a way that the degrees of freedom are separated into identical but uncorrelated blocks, and hence an H^0 which is diagonalizable by numerical methods. Before doing this we must set up the formalism of a field theory on the lattice.

We begin by setting up notation. Supposing that the spatial dimensions are discrete, we may associate a field strength $\phi_{\vec{n}}(t)$ with each site of a Cartesian lattice. The sites are labeled by a d-tuple of integers $\vec{n}$, with d the number of space dimensions. We will choose units such that the lattice spacing a is unity, so we may also identify $\vec{n}$ as the coordinate. The conjugate momenta to the field strengths will be denoted by $\pi_{\vec{n}}(t)$, which in the example we consider will be given by $d\phi_{\vec{n}}(t)/dt$. Quantization is to be accomplished by $[\pi_{\vec{n}}(t), \phi_{\vec{m}}(t)] = -i\delta_{\vec{n},\vec{m}}$. Since we are only interested in the static properties of the ground state, we will drop the time dependence after this.

The particular model we consider is ϕ^4 field theory, for which we choose the Hamiltonian in the

form

$$H=\sum_{\vec{n}}\left[\tfrac{1}{2}\pi_{\vec{n}}^2+\lambda(\phi_{\vec{n}}^2-f^2)^2\right]+\tfrac{1}{2}\sum_{\vec{n},\vec{m}}D^2_{\vec{n},\vec{m}}\phi_{\vec{n}}\phi_{\vec{m}}. \tag{2.2}$$

The D^2 term represents the gradient term in H. Following DWY we find the form

$$D^2_{\vec{n},\vec{m}}=D^2(\vec{n}-\vec{m})=\frac{1}{(2\pi)^d}\int_{-\pi}^{\pi}d\vec{k}\,\vec{k}^2e^{i\vec{k}\cdot(\vec{m}-\vec{n})} \tag{2.3}$$

to be most convenient. It possesses several desirable properties which are discussed elsewhere.[4,5] This leads in a natural way in the limit to the usual continuum form. When the cutoffs are removed (i.e., $a\to 0$) D^2 essentially becomes $-\nabla^2\delta(x-y)$. Happily, we may construct the analog of the usual momentum operator

$$\vec{P}=-i\sum_{\vec{n},\vec{m}}\pi_{\vec{n}}\vec{D}_{\vec{n},\vec{m}}\phi_{\vec{m}}, \tag{2.4}$$

$$\vec{D}_{\vec{n},\vec{m}}=\frac{1}{(2\pi)^d}\int_{-\pi}^{\pi}d\vec{k}\,\vec{k}e^{i\vec{k}\cdot(\vec{m}-\vec{n})} \tag{2.5}$$

and discover that it is the generator of, at least, discrete translations. One has

$$e^{-i\vec{P}\cdot\vec{n}}\phi_{\vec{m}}e^{i\vec{P}\cdot\vec{n}}=\phi_{\vec{m}+\vec{n}}. \tag{2.6}$$

This momentum is *not* generally conserved (it does not commute with the ϕ^4 term in H), but it is conserved up to integral multiples of 2π (or reciprocal lattice vectors). This will turn out to be important.

At this point we have a well-define problem to solve. The Hamiltonian (2.2) has an infinite number of degrees of freedom, though, and so some further approximation is needed. This approximation we now make by modifying the derivative term in H to give an H^0 satisfying the bound (2.1). Consider H^0 given by

$$H^0=\sum_{\vec{n}}\left[\tfrac{1}{2}\pi_{\vec{n}}^2+\lambda(\phi_{\vec{n}}^2-f^2)^2\right]+\tfrac{1}{2}\sum_{\vec{n},\vec{m}}\overline{D}^2_{\vec{n},\vec{m}}\phi_{\vec{n}}\phi_{\vec{m}} \tag{2.7}$$

or

$$\Delta=\tfrac{1}{2}\sum_{\vec{n},\vec{m}}(D^2_{\vec{n}-\vec{m}}-\overline{D}^2_{\vec{n},\vec{m}})\phi_{\vec{n}}\phi_{\vec{m}}, \tag{2.8}$$

where $\overline{D}^2$ is a real symmetric *block diagonal* matrix with identical blocks. In the remainder of discussion we will restrict ourselves to one space dimension for clarity. There is no restriction in principle, though, or in practice for one willing to do the calculations. This H^0 by design is numerically solvable (in principle at least) since it is the direct sum of "effective Hamiltonians" on a finite number of sites. If we can choose $\overline{D}^2$ in such a way that $\langle 0|\Delta|0\rangle\geq 0$, we are done. $\langle 0|\Delta|0\rangle$ depends on the two-point function $\langle 0|\phi_n\phi_m|0\rangle$. We can, by our previous discussions, write a spectral representation for this matrix element. Saturating in a complete basis of *momentum* eigenstates and demanding that the vacuum be invariant under *discrete* translations, one may obtain

$$\langle 0|\phi_n\phi_m|0\rangle=\int dp\,\rho(p)e^{-ip(m-n)},\quad \rho(p)\geq 0. \tag{2.9}$$

Thus $\langle 0|\Delta|0\rangle\geq 0$ if

$$\sum_{m,n}e^{ip(m-n)}(D^2_{m,n}-\overline{D}^2_{m,n})\geq 0. \tag{2.10}$$

This is probably not the weakest available condition on $\overline{D}$ that one may obtain. For free field theory one discovers that

$$\overline{D}^2_{n,m}=\frac{1}{2N+1}\sum_{\kappa}\kappa^2e^{i\kappa(n-m)},\qquad \kappa=2\pi j/(2N+1),\quad -N\leq j\leq N, \tag{2.11}$$

when n and m are in the same block of size $2N+1$ and zero elsewhere, will in fact satisfy $\langle 0|\Delta|0\rangle\geq 0$ by explicit construction of the spectral weight ρ, but fails to satisfy the inequality (2.10). Thus $\overline{D}^2$, moreover, gives better (higher) lower bounds as well as having interest as the natural generalization of (2.2) to a finite lattice. We have been unable to show under what conditions, if any, (2.1) provides a lower bound for an interacting field theory.

The program is now clear. One selects a block size for H^0 which one can deal with practically, and chooses the elements of $\overline{D}^2$ in order to satisfy (2.10). How to do this is a matter of numerical analysis, and taste, which we now discuss.

III. APPLICATIONS

One has complete freedom in choosing the matrix elements of $\overline{D}^2$, and in the most general calculation one could vary over the matrix elements subject to the constraint (2.10) so as to maximize the ground-state energy of H^0. We have chosen to consider a well-defined prescription for $\overline{D}^2$ which satisfies (2.10) and seems to be justified intuitively. In particular, we first suppose that within each block of size B $\overline{D}^2_{n,m}$ only depends on $|n-m|$. Equation (2.10) as a function of p is periodic 2π, and we only need to consider the interval $-\pi\leq p\leq\pi$. Thus it may be rewritten as

$$p^2\geq\overline{D}^2(0)+2\sum_{n=1}^{B-1}\frac{B-n}{B}\overline{D}^2(n)\cos(np),\quad 0\leq p\leq\pi \tag{3.1}$$

where the sum over D^2 may be done explicitly from (2.3), and $\overline{D}^2{}_{n,m} \equiv D^2(|n-m|)$. Supposing that for the ground state it is important to treat the small-p region as well as possible, we expand the right-hand side of (3.1) in a power series in p^2 of B terms and demand equality, thus fixing $\overline{D}^2$. The remainder in the expansion can be shown to be negative, and so this choice for $\overline{D}^2$ satisfies (2.10). In Table I we present for the first few values of B the matrix elements of $\overline{D}^2$ within a block.

The H^0 we have constructed may now be diagonalized numerically for different values of parameters giving lower bounds for the energy density in the ground state. The way in which this has been accomplished is to first diagonalize the "local" operators in H^0, i.e., those which only depend on the degrees of freedom at one site, in a large harmonic-oscillator basis so as to generate a basis of anharmonic-oscillator states, and compute in these states the matrix elements of the coordinates ϕ_n. This procedure is straightforward. The "local" Hamiltonian may be constructed as a matrix of size $N \times N$ directly from matrix representations of ϕ_n and π_n of size $(N+4)\times(N+4)$. This is necessary to eliminate wrong matrix elements from appearing on the edge of the matrix. The oscillator frequency may be considered a variational parameter. This procedure is very easily made to give precise results. If the oscillator frequency is adjusted correctly a 3×3 matrix will give a ground-state eigenvalue which is accurate to within 0.1% for all values of the coupling constant. In the numerical results here a 50×50 matrix was found to give the first 20 or so states (i.e., eigenvalues and eigenvectors) to about eight significant figures. The total effective Hamiltonian in a block is then rediagonalized in a basis of the first M anharmonic-oscillator states at each site. Its lowest eigenvalue is then studied as a function of M, and M is increased until it has converged to a desired accuracy. This lowest eigenvalue divided by B, the number of sites in a block, is then the desired lower bound on the energy density within the above-mentioned accuracy. In practice the lower bound was required to converge to within a small fraction of the distance of the lower bound to the best available upper bounds. For the one-site block one is already finished when the local Hamiltonian is diagonalized. For more sites in a block (here we have computed for $B=2$ and 3) the effective Hamiltonian is again constructed as a matrix which is a direct product of single-site operators. To obtain results which are accurate to three significant figures over the range of parameters considered it was necessary to keep four or five states per site in the two-site case and six or seven states per site in the three-site case. The contribution from states when all of the local oscillators are highly excited was not important, and comparable results were obtained in both cases when only states were kept for which the total number of excitations was limited, with much smaller matrices to diagonalize. The rate of convergence for this procedure was found to be very crudely exponential, with about two states per site per significant figure required in the three-site case. The methods for obtaining upper bounds to this particular problem have been discussed in detail by DWY.

In Fig. 1 we present a set of bounds for the Ham-

TABLE I. $\overline{D}^2{}_{ij}$'s for block lower bounds.

$B=1$: 0

$B=2$:
$$\begin{pmatrix} 2 & -2 \\ -2 & 2 \end{pmatrix}$$

$B=3$:
$$\begin{pmatrix} \frac{5}{2} & -2 & \frac{1}{4} \\ -2 & \frac{5}{2} & -2 \\ \frac{1}{4} & -2 & \frac{5}{2} \end{pmatrix}$$

$B=4$:
$$\begin{pmatrix} \frac{49}{18} & -2 & \frac{3}{10} & \frac{1}{15} \\ -2 & \frac{49}{18} & -2 & \frac{3}{10} \\ \frac{3}{10} & -2 & \frac{49}{18} & -2 \\ \frac{1}{15} & \frac{3}{10} & -2 & \frac{49}{18} \end{pmatrix}$$

$B=5$:
$$\begin{pmatrix} \frac{205}{72} & -2 & \frac{1}{3} & \frac{4}{63} & \frac{1}{112} \\ -2 & \frac{205}{72} & -2 & \frac{1}{3} & \frac{4}{63} \\ \frac{1}{3} & -2 & \frac{205}{72} & -2 & \frac{1}{3} \\ \frac{4}{63} & \frac{1}{3} & -2 & \frac{205}{72} & -2 \\ \frac{1}{112} & \frac{4}{63} & \frac{1}{3} & -2 & \frac{205}{72} \end{pmatrix}$$

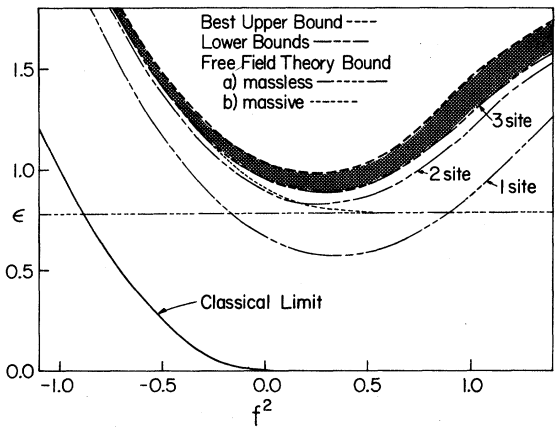

FIG. 1. Plots of bounds on the ground-state energy density of the Hamiltonian (2.2) for $\lambda=1$.

iltonian (2.2) as a function of f^2 with λ fixed at 1. The shaded region is that between the best upper and the best lower bound. Indicated as well are three trivial lower bounds for comparison. One is the classical minimum energy density, one is the ground-state density of massless free field theory, and last is the ground-state energy density of massive free field theory with a constant potential chosen so that $\lambda(\phi^2-f^2)^2 \geq \frac{1}{2}\mu^2\phi^2+C$. By computing with only three sites per block the energy density is constrained to within several percent of its value over the indicated range.

IV. CONCLUSIONS

The bound which has been presented is useful as a diagnostic tool for investigating other less conservative methods of computation. With considerably less justification one may attempt to extract information from the approximate ground-state wave function which results from the calculation. For example, the vacuum expectation value of local operators may be computed in the approximate ground state. Some further information of the same kind can be obtained by studying for both upper and lower bounds their dependence on a term like $JO(\phi)$ added to H, where O is some operator. This is because $\langle 0|O(\phi)|0\rangle_J = d\epsilon/dJ$, and by studying both bounds one may constrain $d\epsilon/dJ$.

The issue of renormalization is an important one, but has been ignored here. One must of course have some justification for computing on the lattice in a given range of parameters. The present method cannot shed any light in this direction, but rather comes into use after one has attempted to deal with this problem. One hope is that by appealing to renormalization-group arguments one can extrapolate to a strong-coupling regime where the approximations become valid.

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[1]This is a rapidly growing area; however, a small sampler of efforts which do not involve the lattice approximation is presented here. For bags see A. Chodos, R. Jaffe, K. Johnson, C. Thorn, and V. Weisskopf, Phys. Rev. D 9, 3471 (1974); W. Bardeen, M. Chanowitz, S. Drell, M. Weinstein, and T.-M. Yan, *ibid.* 11, 1094 (1975). For semiclassical approximation see S.-J. Chang, *ibid.* 12, 1071 (1975) and R. Jackiw, in *Theories and Experiments in High Energy Physics,* proceedings of the Second Orbis Scientiae, Univ. of Miami, 1975, edited by A. Perlmutter and S. M. Widmayer (Plenum, New York, 1975). For solitons and coherent excitations see R. Dashen, B. Hasslacher, and A. Neveu, Phys. Rev. D 11, 3424 (1975) and N. Christ and T. D. Lee, *ibid.* 12, 1606 (1975).

[2]A good reference is K. Wilson and J. Kogut, Phys. Rep. 12C, 75 (1974); see also K. Wilson, Phys. Rev. D 10, 2445 (1974).

[3]J. Kogut and L. Susskind, Phys. Rev. D 11, 395 (1975).

[4]S. Drell, M. Weinstein, and S. Yankielowicz, Phys. Rev. D 14, 487 (1976).

[5]R. Pearson, thesis, Stanford University (unpublished).