Strong-coupling field theory. I. Variational approach to ϕ^4 theory*

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Theoretical attempts to understand hadrons in terms of confined quark constituents lead naturally to the study of quantum field theory with methods that can be applied when strong interactions are present. In this paper nonperturbative, variational techniques are developed and applied to calculating the ground state and low-lying collective excitations ("kinks") of theories rendered finite on a discrete lattice. Particular application is made to a scalar theory with a self-coupling of the form $\lambda(\phi^2 - f^2)^2$ in two dimensions. Working in configuration space we reduce the theory to coupled Schrödinger problems and establish the conditions for the variational solution to exhibit a phase transition between ground states with $\langle\phi\rangle = 0$ and those exhibiting a spontaneously broken symmetry such that $\langle\phi\rangle \neq 0$. The phase transition is a second-order one in a simple trial state constructed in a single-site product basis. Low-lying excitations are constructed that are analogs of the classical "kink" solutions. The single-site basis is also generalized to form "blocks" of coupled lattice sites, and general properties of a block formalism are explored. The usual renormalization limit of cutoff$\to\infty$, or lattice spacing$\to 0$, is also studied as well as the relation of our approach to the conventional renormalization program.

I INTRODUCTION AND OUTLINE

The idea of quarks as fundamental constituents of matter continues to be remarkably successful in describing and predicting observed properties of hadrons, and so the challenge of incorporating these ideas within a calculable dynamical theory continues to grow in importance. This is a difficult challenge since one has to harmonize the fact that quarks behave as if they have a light mass and are bound together by relatively soft forces with the fact that single isolated quarks have never been observed.

Attempts to meet this challenge fall into two categories. There are those schemes which attempt to develop a calculable theory of confined quarks by starting from fundamentally new theoretical concepts,[1] and there are those schemes which seek to work within the more conservative framework of conventional local quantum field theory,[2,3] recognizing from the outset that weak-coupling perturbation calculations will be quite hopeless (at least for discussions of spectra).

In this paper we develop nonperturbative, variational techniques which can be applied to calculating the ground state and low-lying excitations of a class of quantum field theories that are rendered finite in terms of a cutoff. Our particular focus is on a scalar ϕ^4 theory in one space and one time dimension. The methods developed for this application are more general, however, as will be evident, and the introduction of a lattice equivalent to a cutoff field theory as well as the general variational techniques that we utilize are not limited to two dimensions. The virtue of using this particular two-dimensional example, besides its simplicity, is that the classical strong-coupling version of this theory possesses a solitonlike "kink" solution of low mass. Moreover, there is an exactly conserved "charge" which distinguishes this state from the vacuum state and so one might expect that the existence of this extended state will survive quantization. Hence this relatively simple model might be expected to possess a rich structure which cannot be adequately discussed by perturbative techniques. Our physical interest in this application as derived from the study of the "SLAC bag model" is to see if the naive semiclassical ideas survive once we go beyond the "tree approximation" and include quantum fluctuation corrections ignored in earlier studies. The results obtained for this test case lead us to hope that these methods will prove useful in the study of more general classes of theories, including in particular "asymptotically free gauge theories," although we have not given this question careful study to date.

The outline of our paper is as follows:

We consider the Lagrangian

$$L = \int \mathcal{L}\,dx, \tag{1.1}$$

$$\mathcal{L} = \frac{1}{2}\left(\frac{\partial\phi(x,t)}{\partial t}\right)^2 - \frac{1}{2}\left(\frac{\partial\phi(x,t)}{\partial x}\right)^2 - \lambda(\phi^2 - f^2)^2,$$

review the semiclassical analysis, and study its cutoff quantum field theory version—which in our formulation is equivalent to a discrete lattice theory— by carrying through detailed variational calculations.

Upper bounds on the energies of the ground state and "kink" states are constructed using different

trial forms. One approach is in terms of a momentum-space basis and is equivalent to an "average field" or Hartree-Fock approximation. However, we find that when the parameters of Eq. (1.1) are in the strong-coupling region, i.e., small f for fixed mass $\sqrt{\lambda}\, f$, the variational solution constructed by this approximation exhibits a behavior that violates a rigorous theorem due to Simon and Griffiths.[4] The specific problem encountered is that the theory exhibits "tricritical behavior." The resulting phase transition between ground states with $\langle \phi \rangle = 0$ and ground states with a spontaneously broken symmetry such that $\langle \phi \rangle \neq 0$ is a first-order one. Section II contains a detailed discussion of this problem.

A second approach to the variational calculation is in terms of configuration-space trial states. The development of this technique, and its particular application in terms of a single-site product basis to reduce the quantum field theory to a set of effective one-degree-of-freedom Schrödinger problems, is given in Sec. III. The equivalence of a cutoff field theory and of field theory on a discrete lattice is also explored. Working in this single-site basis for calculating upper bounds on the ground-state energy, we avoid the tricritical problem. Regions of coupling parameters such that these bounds are better (i.e., lower) than those obtained by the momentum-space method are explored. As the coupling parameters are changed, there occurs a second-order phase transition from the $\langle \phi \rangle = 0$ ground state to a spontaneously broken ground state with $\langle \phi \rangle \neq 0$. In particular, we exhibit an explicit solution for a limited range of parameters for which the analog of the semiclassical kink is found to be a low-lying excitation. Further numerical analysis and improvements in the energy upper bound, due to "configuration mixing" of low-lying excitations with the ground state, are also discussed.

In Sec. IV, we discuss the problem of taking the renormalization limit (cutoff $\to \infty$, or lattice spacing $\to 0$) and defining a finite version of our cutoff field theory. First, we investigate the relation of our approach with more conventional methods[5] applied in the renormalization program of quantum field theories. Then we extend our lattice formalism by setting up a systematic procedure for generalizing beyond a single-site basis to forming "blocks" of coupled lattice sites. Using the block wave-function formalism, we extend the region of the parameters λ and f in Eq. (1.1) to which our procedure can be expected to apply. We also show why the momentum basis fails, leading to tricritical behavior. Finally, we indicate how the "block formalism" provides a framework for developing resummation techniques which allow us to discuss the multiplicative renormalization of the Hamiltonian. These methods are reminiscent of the renormalization-group methods of Wilson and Kadanoff.[6] This last part of Sec. IV is more descriptive than actually substantiated by detailed calculations.

Detailed discussion of the application of these methods to theories including fermions and/or gauge fields is deferred to forthcoming papers. In Sec. V, however, we summarize the preliminary results we have obtained for the case of a theory of a fermion coupled linearly to the scalar field. We also indicate what we consider to be the most interesting problems which should be explored in the immediate future.

Four appendixes are included with specific calculational details.

II. ϕ^4 THEORY

In this section we review the semiclassical analysis of the theory specified by the Lagrangian (1.1) restricted to 1 space and 1 time dimension. We then study the quantum field theory based upon (1.1) by means of a momentum-space variational calculation.

The purpose of the semiclassical discussion is to exhibit the "kink" state and show that it is a low-mass configuration only in the strong-coupling regime of the theory. Hence, if this behavior is to survive quantization, we must face the strong-coupling quantum-field-theory problem when we go beyond the semiclassical tree approximation.

The purpose of the momentum-space variational calculation is to exhibit a practical method for going beyond perturbation theory. It is an explicit example of what it means to choose a trial ground state of a field theory and it exhibits general features as well as limitations of the method.

Since we wish to avoid any iterative weak-coupling expansions the implementation of an order-by-order Feynman graph renormalization procedure is not available to us. Thus, for the time being, we work with a cutoff version of the field theory and postpone the question of renormalization until Section IV. This cutoff can be introduced by cutting off the Fourier expansion of the field amplitudes at a maximum momentum or by formulating the theory on a lattice. Eventually we will explore both possibilities and their relationship. However, in this chapter, we exploit the first possibility. As implemented, the momentum-space calculation proves to have the serious defect of incorrectly predicting that the theory exhibits "tricritical behavior" in the strong-coupling limit. This is a prediction known rigorously to be false for this particular model.[4] This section closes

with an explanation of the nature of this difficulty, which we show how to avoid in Sec. III by using lattice methods and in Sec. IV by modifying the momentum method.

A. Semiclassical discussion

The Hamiltonian corresponding to (1.1) is

$$H=\int dx\left[\tfrac{1}{2}\pi^2(x,t)+\frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2+\lambda(\phi^2-f^2)^2\right], \tag{2.1}$$

with $f^2>0$ and $\pi\equiv\dot{\phi}$ the canonical field momentum,

$$[\pi(x,t),\phi(x',t)]=i\delta(x-x'). \tag{2.2}$$

Ignoring the quantum aspects of the theory, we drop the momentum π in (2.1) and treat $\phi(x)$ as a static classical field: $\phi\to g(x)\equiv\phi_{\rm cl}(x)$. Evidently the ground-state energy of the positive-definite classical Hamiltonian

$$H_{\rm cl}=\int dx\left[\frac{1}{2}\left(\frac{dg}{dx}\right)^2+\lambda(g^2-f^2)^2\right] \tag{2.3}$$

vanishes for a constant field

$$g^{(0)}=\pm f. \tag{2.4}$$

Equation (2.4) describes the doubly-degenerate ground state. The general solution of (2.3) satisfies the nonlinear Euler-Lagrange equation

$$\frac{d^2g}{dx^2}-4\lambda g(g^2-f^2)=0 \tag{2.5}$$

and substituting any solution of (2.5) in (2.3) gives the classical energy $E(g)$. The only time-independent solutions of (2.5) that give a finite value for the energy $H_{\rm cl}$ in addition to (2.4) are the one-parameter family of "kinks"[7]

$$g^{\pm}(x,x_0)=\pm f\tanh[(2\lambda)^{1/2}f(x-x_0)]. \tag{2.6}$$

Substituting (2.6) in (2.3) yields the classical energy

$$E^{\rm kink}=\tfrac{4}{3}(2\lambda)^{1/2}f^3. \tag{2.7}$$

We readily demonstrate that the kink describes a stable configuration even though its energy (2.7) lies above the ground-state value of $E^0=0$ for the constant configuration (2.4) by constructing a conserved "charge" from the current

$$j_\mu(x)=\epsilon_{\mu\nu}\frac{\partial\phi}{\partial x_\nu},\quad \mu,\nu=0,1$$
$$\epsilon_{\mu\nu}=-\epsilon_{\nu\mu},\quad \epsilon_{01}=1 \tag{2.8}$$

Evidently

$$\partial j_\mu/\partial x_\mu=0$$

and so

$$Q\equiv\int dx\, j_0(x)=\int dx\frac{\partial\phi}{\partial x}=\phi(\infty)-\phi(-\infty) \tag{2.9}$$

is a time-independent quantity. The conserved charge (2.9) vanishes for the vacuum state (2.4) since $g(\infty)=g(-\infty)$; for the kink (2.6) however, $Q^{\rm kink}=\pm 2f\neq 0$. Hence the kink is stable.

The usual way to construct the quantum analog of the kink is by expanding in a power series of the fluctuations about the classical solution

$$\phi(x,x_0)=g(x)+\phi'(x,x_0). \tag{2.10}$$

However, such an expansion converges, if it indeed converges at all, only in the weak-coupling regime, whereas the semiclassical treatment indicates that the strong-coupling regime is the one of interest to us. To make this point, introduce (2.10) into (2.1) so as to obtain

$$H=\int dx\left\{\left[\frac{1}{2}\left(\frac{dg}{dx}\right)^2+\lambda(g^2-f^2)^2\right]+\left[\tfrac{1}{2}\pi^2+\frac{1}{2}\left(\frac{\partial\phi'}{\partial x}\right)^2+\tfrac{1}{2}\phi'^2[4\lambda(3g^2-f^2)]\right]+(4\lambda g\phi'^3+\lambda\phi'^4)\right\}, \tag{2.11}$$

where we have used (2.5) to eliminate the terms linear in ϕ'. The usual weak-coupling approach to (2.1) is to expand ϕ about the constant $g=\pm f$ corresponding to the minimum in the classical energy. The quadratic terms in (2.11) lead to normal-mode motion for oscillators of mass

$$m_f=(8\lambda)^{1/2}f. \tag{2.12}$$

Since the classical kink energy is given by (2.7), we expect the kink to be a better approximation to the low-lying energy states of the theory than the perturbative result only if

$$E^{\rm kink}\ll m_f \tag{2.13}$$

or

$$f^2\ll 1. \tag{2.14}$$

The condition (2.13) corresponds to strong coupling according to (2.11) since, for fixed oscillator mass (2.12), it is equivalent to the conditions

$$\lambda\gg m_f^2\quad\text{and}\quad \lambda f\gg m_f^2. \tag{2.15}$$

In this regime the nonlinear cubic and quartic corrections in (2.11) will be large and their higher-order contributions important.

B. Iterative quantum mechanical procedure

A systematic application of the standard iterative techniques of renormalizable quantum field theory shows directly the importance of developing a strong-coupling approach for this regime of

parameters. Returning to (2.11), we already have computed the classical energy difference between a kink solution (2.6) in the $Q=2f$ sector and the classical ground-state energy of the constant $g(x)=f$ in the $Q=0$ sector. It is given by (2.7), i.e.,

$$[E^{\text{kink}}-E^0]_{\text{cl}}=\tfrac{4}{3}(2\lambda)^{1/2}f^3\,. \tag{2.16}$$

In order to evaluate the lowest-order quantum-mechanical energy difference between the kink and no-kink solutions, we must also include the zero-point energies due to quantum fluctuations computed from (2.11). In particular, these vacuum fluctuations are different in the two sectors for different values of $g(x)$ and this difference must be computed for us to know the true excitation energy of the kink state with $Q=2f$ relative to the $Q=0$ ground state.

An equivalent way of describing these corrections is as the sum over the loop corrections to the tree approximation. To lowest order, the one-loop correction to the zero-point energies due to quantum fluctuations is calculated by neglecting the cubic and quartic terms in (2.11). In particular, we must calculate the shift in the sum over the spectrum of zero-point energies for small oscillations about the kink solution (2.6) for $g(x)$, relative to the oscillations about the constant $g(x)=f$. This difference was computed by Dashen, Hasslacher, and Neveu.[3] For the constant solution, the sum over the zero-point energies is given formally by

$$\tfrac{1}{2}\sum_n \omega_n=\tfrac{1}{2}\sum_k (k^2+8\lambda f^2)^{1/2}, \tag{2.17}$$

which expresses the sum over plane-wave solutions with mass $m_f=(8\lambda)^{1/2}f$ as in (2.12). For the kink solution we expand the field in normal modes,

$$\phi'(x,t)=\sum_n \frac{1}{(2E_n)^{1/2}}\,[u_n(x,t)a_n+u_n^*(x,t)a_n^\dagger],$$

$$\dot\phi(x,t)\equiv\pi=-i\sum(\tfrac{1}{2}E_n)^{1/2}\,(u_n a_n-u_n^* a_n^\dagger), \tag{2.18}$$

$$[a_n,a_{n'}^\dagger]=\delta_{n;n'},$$

with u_n forming a complete basis of solutions to the Schrödinger equation derived from (2.11):

$$\left[\frac{d^2}{dx^2}-4\lambda(3g^2-f^2)\right]u_n=E_n^2u_n\,. \tag{2.19}$$

As shown by Dashen, Hasslacher, and Neveu, (2.19) can be solved in terms of known functions when g is given by the kink (2.6), and the shift of zero-point energy from (2.17) can be evaluated after performing a simple mass renormalization. They found

$$\Delta E^{\text{quantum mechanical}}=\tfrac{1}{2}\sum_n(E_n-\omega_n)$$

$$=\left(\frac{\sqrt{3}}{6}-\frac{3}{\pi}\right)(2\lambda)^{1/2}f, \tag{2.20}$$

i.e., the kink energy is shifted down by an amount of the order of m_f itself as a result of the quantum excitations being drawn into the potential well at the kink boundary. The conclusion to be drawn from (2.20) is that the shift in the fluctuation energy in the one-loop approximation is a very large one, much larger than the classical kink energy itself, which as shown in (2.16) is smaller by the factor $f^2\ll 1$. Evidently then, an expansion in fluctuations about the soliton solutions of the classical problem does not define a reliable iterative procedure for our purposes and we are faced inescapably with the challenge of strong-coupling theory.

C. Cutoff field theory: A variational calculation

In quantum field theory (2.1) leads formally to two kinds of infinities. The first is associated with the infinite extent (length or volume) of the system and the second is associated with the arbitrarily-high-momentum modes in the theory. In order to define a theory in which H is finite at each step, without resorting to infinite subtractions or renormalization prescriptions, we shall consider the field theory in a box of finite volume, V, and we shall terminate all momentum expansions of the fields at a finite maximum cutoff, $k_{\max}$. Eventually we will study limiting behavior for $V\to\infty$ and $k_{\max}$ arbitrarily large, but at each step we have a well-defined quantum-mechanical problem. Although this cutoff procedure costs us Poincaré invariance, we believe that we can ignore such violations when studying questions involving low-lying excitations, such as the existence of "bags" or coherent excitations, which are presumably built out of the long-wavelength structure of the theory.

Formally, the volume cutoff is introduced by integrating (2.1) over the range

$$-\frac{L}{2}\leq x\leq\frac{L}{2}\,.$$

A notation applicable for an arbitrary number ($p=1,2,3,\ldots$) of spatial dimensions is

$$\underline{x}=(x_1,\ldots,x_p) \tag{2.21}$$

and

$$-\frac{L}{2}\leq x_j\leq\frac{L}{2}\ \text{for}\ j=\{1,\ldots,p\},\quad V=L^p.$$

The Fourier expansion is written

$$\pi(\underline{x})=\sum_{\underline{k}} e^{i\underline{k}\cdot\underline{x}}\pi(\underline{k}),\quad \pi(\underline{k})=\frac{1}{V}\int d^p x\, e^{-i\underline{k}\cdot\underline{x}}\pi(\underline{x}),$$

$$\phi(\underline{x})=\sum_{\underline{k}} e^{i\underline{k}\cdot\underline{x}}\phi(\underline{k}),\quad \phi(\underline{k})=\frac{1}{V}\int d^p x\, e^{-i\underline{k}\cdot\underline{x}}\phi(\underline{x}), \tag{2.22}$$

where

$$\underline{k}=(k_1,\ldots,k_p),\quad k_j=\frac{2\pi}{L}n_j,$$

$$n_j=0,\pm 1,\ldots,\pm N,\quad k_{\max}=\frac{2\pi}{L}N,$$

and

$$[\pi(k_1,\ldots,k_p),\phi(-l_1,\ldots,-l_p)]=-i\delta_{\underline{k},\underline{l}}/V.$$

This gives for (2.1)

$$H=\sum_{\underline{k}=-\underline{k}_{\max}}^{\underline{k}_{\max}}[\tfrac{1}{2}\pi(\underline{k})\pi(-\underline{k})+(\tfrac{1}{2}k^2-2\lambda f^2)\phi(\underline{k})\phi(-\underline{k})]$$
$$+\lambda\sum_{\underline{k}_1,\underline{k}_2,\underline{k}_3,\underline{k}_4}[\delta_{\underline{k}_1+\underline{k}_2+\underline{k}_3,-\underline{k}_4}\phi(\underline{k}_1)\phi(\underline{k}_2)\phi(\underline{k}_3)\phi(\underline{k}_4)]$$
$$+\lambda V f^4. \tag{2.23}$$

The most obvious and simplest approach to a calculation of the ground state of (2.23) is to work in momentum space introducing for each mode $\underline{k}$:

$$\phi(\underline{k})=\frac{1}{(2\alpha_{\underline{k}}V)^{1/2}}(a_{-\underline{k}}+a_{\underline{k}}^\dagger),$$

$$i\pi(\underline{k})=\left(\frac{\alpha_{\underline{k}}}{2V}\right)^{1/2}(a_{-\underline{k}}-a_{\underline{k}}^\dagger), \tag{2.24}$$

$$[a_{\underline{k}},a_{\underline{k}'}^\dagger]=\delta_{\underline{k},\underline{k}'},$$

where the $\alpha_{\underline{k}}$ are arbitrary parameters to be varied.[8] For the trial state, we introduce a displaced Gaussian packet for each mode by defining

$$|S_{\alpha_{\underline{k}}};c\rangle\equiv e^{-icV\pi(\underline{k}=0)}|0_{\alpha_{\underline{k}}}\rangle, \tag{2.25}$$

where

$$a_{\alpha_{\underline{k}}}|0_{\alpha_{\underline{k}}}\rangle=0 \text{ for all } \underline{k}.$$

The variation parameter c provides a constant displacement of the field

$$\phi(\underline{x})|S_{\alpha_{\underline{k}}};c\rangle=e^{-icV\pi(\underline{k}=0)}[\phi(\underline{x})+c]\,|0_{\alpha_{\underline{k}}}\rangle. \tag{2.26}$$

For the ground-state energy, we compute from (2.23)

$$E_{(\alpha_{\underline{k}};c)}\equiv\langle S_{\alpha_{\underline{k}}};c|H|S_{\alpha_{\underline{k}}};c\rangle \tag{2.27}$$

and require

$$\frac{\partial E}{\partial\alpha_{\underline{k}}}=\frac{\partial E}{\partial c}=0 \tag{2.28}$$

to determine the extrema. We find in this way

$$\frac{1}{V}E(\alpha_{\underline{k}},c)\equiv\mathcal{E}(\alpha_{\underline{k}},c)$$
$$=\left[\frac{1}{V}\sum_{\underline{k}}\frac{1}{4}\left(\alpha_{\underline{k}}+\frac{k^2}{\alpha_{\underline{k}}}\right)+\lambda(3c^2-f^2)\frac{1}{V}\left(\sum_{\underline{k}}\frac{1}{\alpha_{\underline{k}}}\right)+\frac{3\lambda}{4}\left(\frac{1}{V}\sum_{\underline{k}}\frac{1}{\alpha_{\underline{k}}}\right)^2+\lambda(f^2-c^2)^2\right]. \tag{2.29}$$

The $\underline{k}$ sums extend over the interval $-2\pi N/L\leq k_j\leq 2\pi N/L$ for each component k_j. The extremum conditions give

$$\frac{\partial\mathcal{E}}{\partial c}(\alpha_{\underline{k}},c)=0:\quad 4\lambda c(c^2-f^2+\bar{f})=0, \tag{2.30}$$

$$\frac{\partial\mathcal{E}}{\partial\alpha_{\underline{k}}}(\alpha_{\underline{k}},c)=0:\quad \alpha_{\underline{k}}^2=k^2+4\lambda(\bar{f}-f^2+3c^2), \tag{2.31}$$

where we have introduced the definition

$$\bar{f}=\frac{3}{2V}\sum_{\underline{k}}\frac{1}{\alpha_{\underline{k}}}. \tag{2.32}$$

According to (2.31) we can write

$$\alpha_{\underline{k}}^2=k^2+\alpha_0^2 \tag{2.33}$$

in terms of a variational mass parameter

$$\alpha_0^2\equiv 4\lambda[\bar{f}(\alpha_0)-f^2+3c^2]. \tag{2.34}$$

Evidently we could have defined the $\alpha_{\underline{k}}$ introduced in (2.24) in terms of (2.33) and varied over the single mass parameter α_0 for all Fourier components. Henceforth we shall proceed in this way. In terms of α_0 and of the notation introduced for the sum

$$\bar{f}(\alpha_0)\equiv\frac{3}{2V}\sum_{\underline{k}=-\underline{k}_{\max}}^{+\underline{k}_{\max}}\frac{1}{(k^2+\alpha_0^2)^{1/2}}, \tag{2.35}$$

the energy density can be simplified to

$$\mathcal{E}(\alpha_0,c)=\frac{1}{2V}\sum_{\underline{k}}(k^2+\alpha_0^2)^{1/2}-\frac{\alpha_0^2}{6}\bar{f}$$
$$+\frac{2\lambda}{3}\bar{f}(3c^2-f^2)$$
$$+\frac{\lambda}{3}\bar{f}^2+\lambda(f^2-c^2)^2. \tag{2.36}$$

Equations (2.30) and (2.34) have two possible solutions

$$\text{(i)}\quad c=0 \text{ and } \frac{\alpha_0^2}{4\lambda}+f^2=\bar{f}(\alpha_0), \tag{2.37}$$

$$\text{(ii)}\quad c^2=f^2-\bar{f}(\alpha_0)>0 \text{ and } -\frac{\alpha_0^2}{8\lambda}+f^2=\bar{f}(\alpha_0), \tag{2.38}$$

Equation (2.35) shows that in the limit of large $\alpha_0 > k_{\max} = 2\pi N/L$, $\bar{f}$ decreases as $1/\alpha_0$ for any number of dimensions. For finite volume V, $\bar{f}(\alpha_0)$ diverges at $\alpha_0 = 0$ due to the $\underline{k} = 0$ term in the sum (2.35). Its rate of growth as $\alpha_0 \to 0$ can be computed by replacing the sum by an integral

$$\frac{1}{V}\sum_{\underline{k}} \to \frac{1}{(2\pi)^p}\int^{(k_{\max})} d^p k, \tag{2.39}$$

Figures 1 and 2 show that there is always a solution of (2.37) for $c = 0$ but that (2.38) will have two, one, or no solutions depending on values of f^2 and λ. In order to determine which of these roots corresponds to local minima or maxima of $\mathcal{E}(\alpha_0, c)$ we must also compute the second derivatives and calculate the trace and the determinant of the coefficients

$$\begin{Vmatrix} \frac{\partial^2 \mathcal{E}}{\partial \alpha_0^2} & \frac{\partial^2 \mathcal{E}}{\partial \alpha_0 \partial c} \\ \frac{\partial^2 \mathcal{E}}{\partial \alpha_0 \partial c} & \frac{\partial^2 \mathcal{E}}{\partial c^2} \end{Vmatrix} \tag{2.40}$$

and determine whether it is positive at the roots (2.37) or (2.38) indicating a local minimum, or negative for a local maximum. The straightforward differentiation is displayed in Appendix A. We find that the extremum (2.37) at $c = 0$ is *always* a local minimum. However, for the extremum (2.38) with $c \neq 0$ the condition for a local minimum is

$$\frac{\alpha_0}{4\lambda} > \left|\frac{\partial \bar{f}}{\partial \alpha_0}\right| = \frac{3\alpha_0}{2}\left(\frac{1}{V}\sum_{\underline{k}} \frac{1}{(k^2+\alpha_0^2)^{3/2}}\right). \tag{2.41}$$

These solutions are shown in Fig. 2.

What is the physical content of these results? In order to extract this most simply, we return to (2.36) and study $\mathcal{E}$ as a function of c for various values of the parameters f and λ. In particular, we vary f^2 for fixed λ. The extremum value $\alpha_0 \equiv \alpha_0(c)$ is determined from (2.34), which has a unique solution for every value of c since the left-hand side is monotonically increasing and the right-hand side is monotonically decreasing as a function of α_0. Figure 3 shows $\mathcal{E}(\alpha_0(c), c)$ for different values of f^2 and shows the same general behavior found in Fig. 2. In particular, there is always a local minimum at $c = 0$. As f^2 increases, for fixed λ, two local minima appear at $\pm c \neq 0$. In one-plus-one dimensions, i.e., $p = 1$, one finds num-

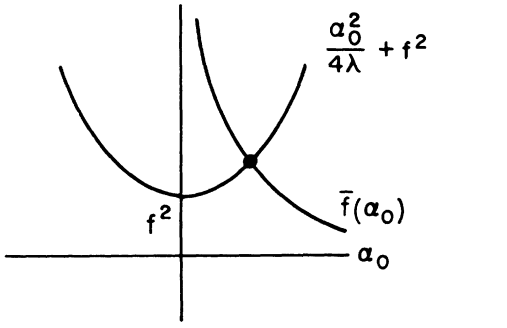

FIG. 1. Graphical solution to the momentum-space variational calculation [Eq. (2.37)] for the case $c = 0$.

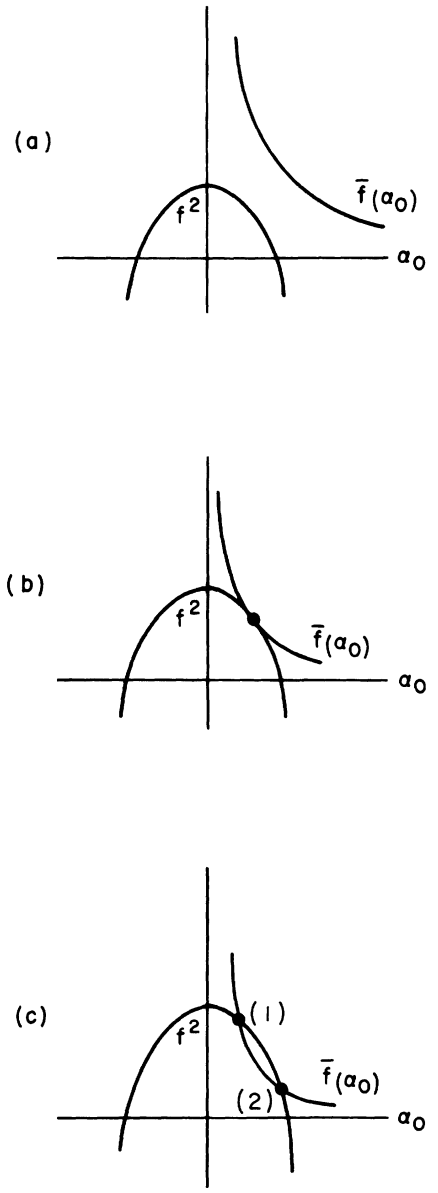

FIG. 2. Graphical solution to the momentum-space variational calculation [Eq. (2.38)]: (a) no solution; (b) tangency condition $\alpha_0/4\lambda = |\partial \bar{f}/\partial \alpha_0|$; (c) two solutions: (1) maximum at $c \neq 0$, (2) minimum at $c \neq 0$.

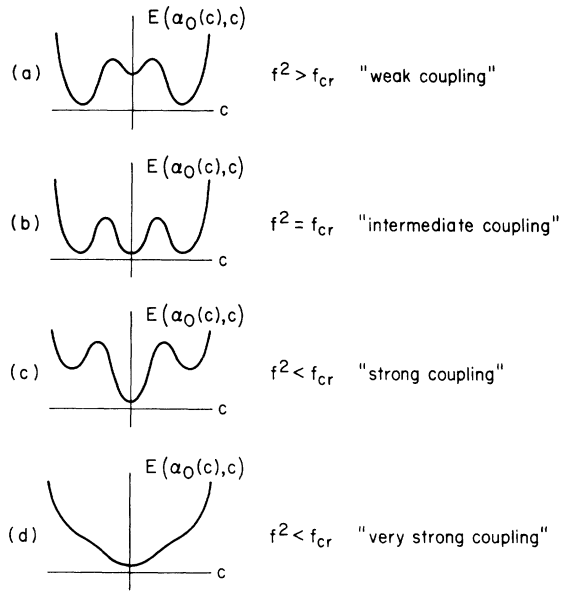

FIG. 3. The ground-state energy in the momentum-space variational calculation as a function of the vacuum expectation value c for fixed λ and different f^2: (a) $f^2 > \hat{f}_{cr}$ "weak coupling," $c \neq 0$ is the absolute minimum; (b) $f^2 = \hat{f}_{cr}$, the minima at $c = 0$ and $c \neq 0$ are degenerate; (c) $f^2 < \hat{f}_{cr}$ "strong coupling," $c = 0$ is the absolute minimum; (d) $f^2 \ll \hat{f}_{cr}$ "super-strong coupling". $c = 0$ is the only minimum.

erically that for the choice of the dimensionless parameter $\lambda/\Lambda^2 \sim 1$ these minima appear when $f^2 \sim 1$. For large enough f^2 the minima at $c \neq 0$ cross the one at $c = 0$. A numerical comparison of the energies of the $c = 0$ and $c \neq 0$ minima for $\lambda/\Lambda^2 = 1$ and a range of values for f are given in Table I. We conclude that they then become degenerate ground states of the theory, with $\langle \phi \rangle = +c$ or $-c$, respectively, because the overlap between them vanishes in the $V \to \infty$ limit, i.e.,

$$\langle S_{\alpha_k}; -c | S_{\alpha_k}; +c \rangle = \langle 0_{\alpha_k} | e^{-2icV\pi(k=0)} | 0_{\alpha_k} \rangle = e^{-\alpha_0 V^2 c}. \quad (2.42)$$

Thus either one of them, or any linear combination, is a satisfactory choice of a ground state of the theory if the variational calculation is any good. A specific choice of ground state is forced upon us if we add a small external source. Assuming that we always choose the one at $+c$ whenever the one at zero lies higher, Fig. 3 shows that as we vary λ and f the lowest eigenstate of the theory will jump discontinuously (i.e., a first-order phase transition) from a state such that $\langle \phi \rangle = c \sim f$ to $\langle \phi \rangle = 0$ at some critical values of the coupling parameters.

As intriguing as this behavior might seem, it can be shown that this form of $\mathcal{E}(\alpha_0(c), c)$ is a disease of the variational choice (2.26) for the form of the ground state. This behavior of $\mathcal{E}$ violates our intuition, which suggests that $\langle \phi \rangle$ should approach zero continuously, with the discontinuous change occurring in the rate of change of $\langle \phi \rangle$, i.e., its slope, in analogy to the observed behavior of spontaneous magnetization as a function of temperature. In addition, there is a much more serious problem, namely, that the behavior implied by (2.36) violates a rigorous theorem proved by Simon and Griffiths.[4] To explain the problem, let us add a linear source term to (2.1) of the form

$$H' = -J \int dV \phi = -J V \phi(k = 0), \quad (2.43)$$

which, following (2.26), adds the term $-Jc$ to the energy density (2.29). Since the added contribution is independent of α_0, the extremum value $\alpha_0 = \alpha_0(c)$ is the same as (2.34). Therefore,

$$\mathcal{E}'(\alpha_0(c), c) \equiv \frac{1}{V} \langle S_{\alpha_k;c} | H + H' | S_{\alpha_k;c} \rangle = \mathcal{E}_0(\alpha_0(c), c) - Jc. \quad (2.44)$$

$\mathcal{E}'$ is shown in Fig. 4, which is tilted by the linear term $-Jc$ relative to Fig. 3.

In the region of weak coupling, when the ground state lies at $\langle \phi \rangle = c \neq 0$ in the absence of a source term, the added contribution breaks the degeneracy between $\pm c$. Which of these states lies lower depends on the sign of J, and as one goes through $J = 0$, there is a sudden jump from one minimum to the other. This behavior is similar to what is known for a ferromagnetic medium in an applied magnetic field below the Curie temperature. However, in the strong-coupling region of $f^2 < \hat{f}_{cr}^2$, we see that a finite source strength

TABLE I. A table of values of $\mathcal{E}(c)$ at its local minima, obtained from the momentum-space calculation for $\lambda_0 = 1$ and a range of values for f_0. The asterisk indicates the region in which the $c \neq 0$ minimum crosses the $c = 0$ minimum and the dagger indicates those values of f_0 for which only the $c = 0$ minimum exists.

f_0	$\mathcal{E}(c_{min} = 0)$	$\mathcal{E}(c_{min} \neq 0)$	$c \neq 0$
1.5	4.1632	2.2251	1.3777
1.4	3.3469	2.0837	1.2568
1.3	2.6908	1.9408	1.1287
1.2	2.1714	1.7952	0.9892
1.1*	1.7704*	1.6446*	0.8258*
1.0*	1.4712*	1.4804*	0.5639*
0.9†	1.2588†	···†	···†
0.8†	1.1180†	···†	···†
0.7†	1.0341†	···†	···†

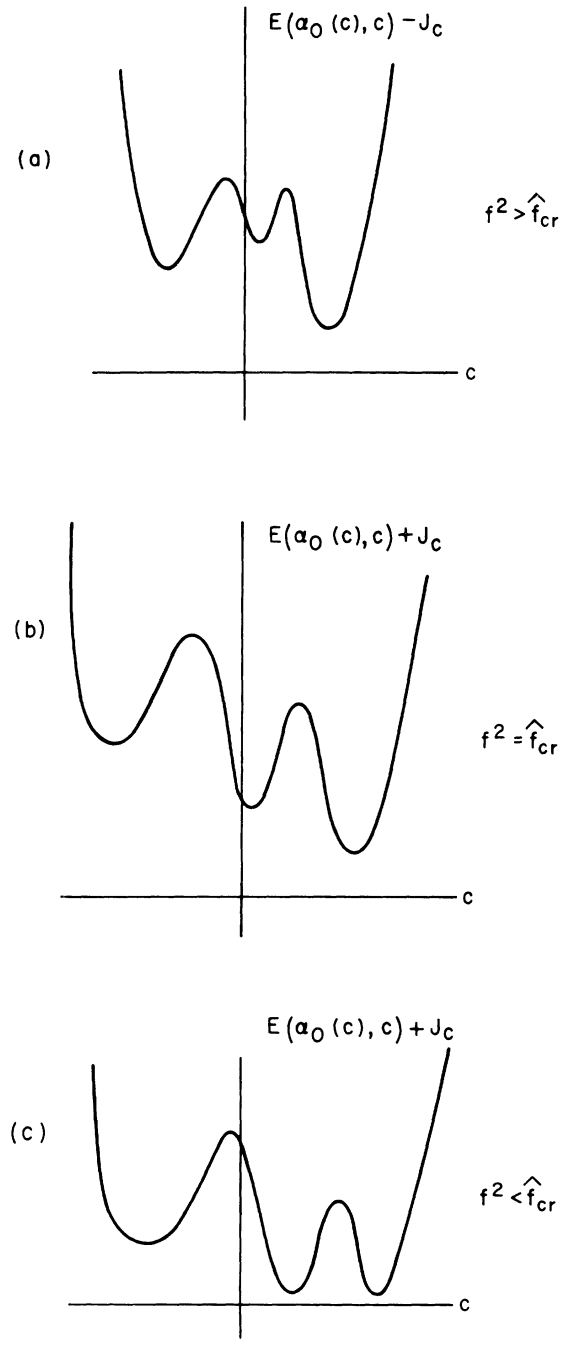

FIG. 4. The ground-state energy in the momentum-space variational calculation as a function of the vacuum expectation value c for fixed λ and different f^2 in the presence of an external source:

(a) $f^2 > \hat{f}_{cr}$. The minimum obtained from $c \neq 0$ of Fig. 3(a) is the absolute minimum.

(b) $f^2 = \hat{f}_{cr}$. The minimum obtained from $c \neq 0$ of Fig. 3(b) is the absolute minimum.

(c) $f^2 < \hat{f}_{cr}$. For strong enough J, the minimum obtained from $c \neq 0$ [Fig. 3(c)] can be made lower than the one obtained from $c = 0$ [Fig. 3(c)].

$J > J_{cr}(\lambda)$ can tilt the energy curves sufficiently so that the ground state becomes the minimum which develops from the solution with $c \neq 0$ when $J = 0$. As illustrated, a ground state developing from the $c = 0$ root when $J < J_{cr}(\lambda)$ jumps discontinuously to one developing from $c \neq 0$ when $J > J_{cr}(\lambda)$.

It is this behavior that is forbidden by the Simon-Griffiths theorem which proves that the particular theory described by Hamiltonian (2.1) plus (2.43) in $1x + 1t$ dimension leads to a ground-state expectation value for $\langle \phi \rangle$ that is a monotonic, analytic function of J for finite $J \neq 0$. Evidently the trial ground state is too crude for a study in this region, leading to an impossible shape for $\mathcal{E}(\alpha_0(c), c)$ and to a first-order phase transition. Actually, the crux of the difficulty lies in the local minimum in $\mathcal{E}(\alpha_0(c), c)$ at $c = 0$ which is entirely spurious, as we shall show in the Sec. III. In Sec. IV we construct a modification of the momentum-basis calculation which removes this difficulty and discuss its origin.

Although the Simon-Griffiths theorem is specific to this model in one space and one time dimension, this result suggests that these simple methods are inadequate for studying the strong-coupling region where the tricritical behavior sets in and phase transitions may occur. Unfortunately, it is precisely this region, with $0 < f^2 < 1$, that the semiclassical analysis suggests we must study in order for the kink to be a low-lying state [see Eq. (2.13)]. Note that if this calculation were valid, the kink could never exist as a low-lying state, since by the time the vacuum expectation value $\langle \phi \rangle$ decreases to the order of 1, it jumps discontinuously to zero. Thus, there is no region where $\langle \phi \rangle$ is small but different from zero which is a necessary condition for the existence of a low-mass kink.

The reason we so thoroughly discussed this incorrect momentum-space calculation is that it is the most straightforward application of the idea of doing a variational calculation for the ground state of a field theory. It also points out a virtue of this simple theory as a test case, namely, there exists an exact theorem due to Simon and Griffiths which provides a nontrivial constraint on the trial state one uses for the variational calculation. We conclude this section with three remarks:

(i) For weak coupling where $\mathcal{E}(c)$ is given by Fig. 3(a), there is no contradiction to any known theorem. Moreover, in this region there are reasons to believe that the momentum-space calculation correctly represents the ground-state energy.

(ii) The momentum-space calculation is just one example of a Hartree-Fock–type calculation. In Appendix B we derive the general Hartree-Fock

approximation from a more general variational calculation. This means, of course, that the Hartree-Fock calculation, which includes part of the two-loop contribution (the normal-ordering part), gives an upper bound on the ground-state energy.

(iii) The momentum-space calculation will be of importance to us when we discuss the renormalization limit in Sec. IV.

III. ϕ^4 FIELD THEORY ON A LATTICE

In this chapter we reformulate the cutoff theory discussed in Sec. II in terms of an equivalent lattice field theory which provides a natural language for constructing a new class of variational ground states. These are trial states expressed as products of wave functions at each of the individual lattice sites. A further extension of this approach to include trial states correlating neighboring sites is presented in Sec. IV.

The principal lessons to be learned from this analysis are the following:

(i) For a limited range of λ and f, the wave functions produce lower ground-state energies than the elementary momentum-space wave functions studied in Sec. II.

(ii) Within this range of parameters, we are able to use this variational procedure to study the region in which $\langle\phi\rangle \ll 1$. We show that the phase transition from the $\langle\phi\rangle \neq 0$ to the $\langle\phi\rangle = 0$ phase is, in fact, of second order and that one has no difficulties with the theorem of Simon and Griffiths.

(iii) Because we can get to a solution with $\langle\phi\rangle \ll 1$ by appropriate choices of the parameters λ and f, we are able to argue that kink states of arbitrarily low mass exist (no matter how large we choose the cutoff mass) and the mass of these states is much lower than the single-particle masses suggested by the perturbation expansion.

A. Field theory on a finite lattice

Introducing a maximum momentum cutoff $k_{\max}$ in (2.22), we developed a convenient language for working in $\vec{k}$ space with a finite number of degrees of freedom. If we now want to work in coordinate space, the analogous procedure is to replace the space continuum $\vec{x}$ by a discrete lattice of linear dimension L and minimum spacing $1/\Lambda$ defined so that there are $2N+1$ points on a side:

$$L = (2N+1)/\Lambda, \quad V = L^p. \tag{3.1}$$

The correspondence between languages is, as defined in (2.22),

$$k_p \equiv \frac{2\pi n_p}{L}, \quad k_{\max} = \frac{2\pi N}{L}, \tag{3.2}$$

where $n_p = 0, \pm 1, \ldots, \pm N$ now labels the lattice sites. The continuous coordinate $\underline{x}$ is replaced by a discrete lattice site label $\underline{j}$ such that for each component $j_p = 0, \pm 1, \ldots, \pm N$.

The volume integral in (2.1) becomes

$$\int d^p x \to \frac{1}{\Lambda^p} \sum_{\underline{j}} \tag{3.3}$$

and the fields at the lattice sites are defined by

$$\pi(\underline{x}) \to \pi_{\underline{j}} = \sum_{\underline{k}=-\underline{k}_{\max}}^{+\underline{k}_{\max}} e^{i\underline{k}\cdot\underline{j}/\Lambda} \pi(\underline{k}),$$

$$\pi(\underline{k}) = \frac{1}{(2N+1)^p} \sum_{\underline{j}} \pi_{\underline{j}} e^{-i\underline{k}\cdot\underline{j}/\Lambda},$$

$$\phi(\underline{x}) \to \phi_{\underline{j}} = \sum_{\underline{k}=-\underline{k}_{\max}}^{+\underline{k}_{\max}} e^{i\underline{k}\cdot\underline{j}/\Lambda} \phi(\underline{k}),$$

$$\phi(\underline{k}) = \frac{1}{(2N+1)^p} \sum_{\underline{j}} \phi_{\underline{j}} e^{-i\underline{k}\cdot\underline{j}/\Lambda},$$

where the $\pi(\underline{k})$ and $\phi(\underline{k})$ are the same as introduced in (2.22) and satisfy the commutation relations

$$[\pi(\underline{k}), \phi(-\underline{l})] = -i\delta_{\underline{k},\underline{l}}/V. \tag{3.5}$$

It follows that

$$[\pi_{\underline{j}}, \phi_{\underline{j}'}] = -i\Lambda^p \delta_{\underline{j},\underline{j}'}. \tag{3.6}$$

All of these transcriptions are entirely straightforward. The gradient operator in (2.1) is usually transcribed as a difference operator,

$$\nabla_l \phi = \Lambda(\phi_{l+1} - \phi_l). \tag{3.7}$$

Although this form is perfectly all right in the limit $\Lambda \to \infty$, it leads to undesirable difficulties with the introuduction of fermions for finite Λ. Since we are developing a formalism for very large but finite Λ, we choose an alternative definition that has the two desirable properties:

(i) For a free field theory it leads to an energy spectrum in accord with the relativistic form of the energy-momentum relation for all $k \leq k_{\max}$.

(ii) It automatically avoids doubling the fermion degree of freedom which results from (3.7) (see Kogut and Susskind, Ref. 2).

In terms of the program of this paper, these properties are not essential and we could just as well work with the familiar definition (3.7). However, for future applications (i.e., to gauge theories with fermions, and to a study of Lorentz transformation properties of the lattice theory), these properties are important and therefore we always adopt the following definition of the gradient: For

$$f_{\underline{j}} = \sum_{\underline{k}} e^{i\underline{k}\cdot\underline{j}/\Lambda} f(\underline{k}), \tag{3.8}$$

we define

$$\nabla f_{\underline{j}} \equiv \sum_{\underline{k}} i\underline{k} e^{i\underline{k}\cdot\underline{j}/\Lambda} f(\underline{k}) = \sum_{\underline{j}'} f_{\underline{j}'} \left(\frac{1}{V} \sum_{\underline{k}} e^{i\underline{k}\cdot(\underline{j}-\underline{j}')/\Lambda} i\underline{k} \right). \tag{3.9}$$

Note that (3.9) introduces long-range lattice correlations beyond the nearest neighbors. The kinetic term in (2.1) now becomes

$$\int d^p x \, \tfrac{1}{2}(\nabla\phi)^2 \to \frac{1}{\Lambda^p} \sum_{\underline{j}} \tfrac{1}{2}(\nabla\phi_{\underline{j}})^2 = \frac{V}{2} \sum_{\underline{k}} k^2 \phi(\underline{k})\phi(-\underline{k}) \equiv \frac{1}{\Lambda^p} \sum_{\underline{j},\underline{j}'} \tfrac{1}{2}\Lambda^2 \phi_{\underline{j}}\phi_{\underline{j}'} D(\underline{j}-\underline{j}'), \tag{3.10}$$

where

$$D(\underline{j}-\underline{j}') \equiv \frac{1}{(2N+1)^p} \sum_{\underline{k}=-\underline{k}_{\max}}^{+\underline{k}_{\max}} \left(\frac{k^2}{\Lambda^2} e^{i(\underline{j}-\underline{j}')\cdot\underline{k}/\Lambda} \right) \tag{3.11}$$

is a sum of correlation terms in each dimension of the lattice. In particular, for $p = 1$,[9]

$$D_{p=1}(j) = \begin{cases} \dfrac{4N(N+1)}{(2N+1)^2} \dfrac{\pi^2}{3} \xrightarrow{N\to\infty} \dfrac{\pi^2}{3} & \text{for } j = 0 \\ \dfrac{(2\pi)^2(-1)^j}{2(2N+1)^2} \dfrac{\cos(\pi j/2N+1)}{\sin(\pi j/2N+1)^2} \xrightarrow{N\to\infty} \dfrac{2(-1)^j}{j^2} & \text{for } j \neq 0. \end{cases} \tag{3.12}$$

For $p > 1$, we get a sum of such correlation terms in each dimension.

One important result is that with this definition of the gradient, the cutoff and lattice versions of *free field* theory are isomorphic, i.e., by (3.4) and (3.10)

$$H_0 = \frac{1}{\Lambda^p} \sum_{\underline{j}} \left[\tfrac{1}{2}\pi_{\underline{j}}^2 + \tfrac{1}{2}(\nabla\phi_{\underline{j}})^2 + \tfrac{1}{2}\mu^2\phi_{\underline{j}}^2 \right] = V \sum_{\underline{k}} \left[\tfrac{1}{2}\pi(\underline{k})\pi(-\underline{k}) + \tfrac{1}{2}(k^2+\mu^2)\phi(\underline{k})\phi(-\underline{k}) \right], \tag{3.13}$$

which is the familiar result for a cutoff Hamiltonian, and the commutators are the same as (3.5). Moreover, (3.13) leads to an energy spectrum of the form $(k^2+\mu^2)^{1/2}$ rather than one of the form $[\mu^2 + 4\Lambda^2 \sin^2(k/2\Lambda)]^{1/2}$ which would emerge from the prescription (3.7), and hence we have a relativistic form of the energy-momentum relation for all $k \leq k_{\max}$. Note that these results also apply to the case of a free fermion theory.

There is a difference between the cutoff and lattice versions of the field theory for the quartic term of (2.1). This arises from the fact that in the cutoff theory, by (2.22)

$$\int d^4x \, \phi^4(x) = V \sum_{\underline{k}_1,\underline{k}_2,\underline{k}_3,\underline{k}_4} \delta_{\underline{k}_1+\underline{k}_2+\underline{k}_3,-\underline{k}_4} \times \phi(\underline{k}_1)\phi(\underline{k}_2)\phi(\underline{k}_3)\phi(\underline{k}_4), \tag{3.14}$$

i.e., we must satisfy a true δ-function condition $\underline{k}_1+\underline{k}_2+\underline{k}_3+\underline{k}_4 = 0$. However, for the lattice theory, by (3.4)

$$\frac{1}{\Lambda^p} \sum_{\underline{j}} \phi_{\underline{j}}^4 = V \sum_{\underline{k}_1,\underline{k}_2,\underline{k}_3,\underline{k}_4} \left[\sum_{\underline{j}} e^{i(\underline{k}_1+\underline{k}_2+\underline{k}_3+\underline{k}_4)\cdot\underline{j}/\Lambda} \right] \times \phi(\underline{k}_1)\phi(\underline{k}_2)\phi(\underline{k}_3)\phi(\underline{k}_4) \tag{3.15}$$

and the factor in square brackets is a periodic δ function which equals unity for $(1/\Lambda)(\underline{k}_1+\underline{k}_2+\underline{k}_3+\underline{k}_4) = 0$ modulo 2π, for each component. Hence (3.15) conserves momentum in the Hamiltonian only up to "umklapps," in the language of solid-state physics. For quadratic terms, as in (3.13), in which the $\underline{k}$ are equal and opposite and limited by $\underline{k}_{\max}$ umklapps cannot occur. In (3.15), however, as in all terms of higher than quadratic power in the fields, it is possible to have an umklapp if two more of the momenta are of order of the reciprocal lattice spacing, i.e., for $k \sim 2\pi N/(2N+1) = k_{\max}$. Therefore, the difference between (3.14) and (3.15) can be expected to alter the high-momentum or short-distance behavior of H but have little or no effect on the low-momentum structure, viz., the mean field strength $\langle\phi\rangle$ in the ground states and low-lying coherent excitations. For simplicity, we choose to work with (3.15) and analyze the Hamiltonian:

$$H = \frac{1}{\Lambda^p} \sum_{\underline{j}} \left[\tfrac{1}{2}\pi_{\underline{j}}^2 + \tfrac{1}{2}(\nabla\phi_{\underline{j}})^2 + \lambda(\phi_{\underline{j}}^2 - f^2)^2 \right]. \tag{3.16}$$

Rescaling to dimensionless variables, we introduce

$$x_{\underline{j}} \equiv \Lambda^{(1-p)/2}\phi_{\underline{j}}, \quad p_{\underline{j}} \equiv \Lambda^{-(1+p)/2}\pi_{\underline{j}}, \quad [p_{\underline{j}}, x_{\underline{j}'}] = -i\delta_{\underline{j},\underline{j}'}. \tag{3.17}$$

Together with

$$\lambda_0 \equiv \lambda\Lambda^{p-3}, \quad f_0^2 \equiv f^2\Lambda^{(1-p)} \tag{3.18}$$

this gives

$$H = \Lambda \sum_{\underline{j}} \left[\tfrac{1}{2}p_{\underline{j}}^2 + \tfrac{1}{2}(\nabla x_{\underline{j}})^2 + \lambda_0(x_{\underline{j}}^2 - f_0^2)^2 \right]. \tag{3.19}$$

Although all subsequent discussions will be based upon (3.19), for completeness we observe that with the definition of the gradient in (3.9) there is a way to define the Hamiltonian so that the lattice theory is entirely equivalent to the cutoff theory and there are no umklapps.[10] This is accomplished by defining

$$H = \int_{-L/2}^{+L/2} d^p x \left(\frac{\pi^2(x)}{2} + \frac{(\nabla\phi)(x)^2}{2} + \lambda[\phi^2(x) - f^2]^2 \right), \quad \underline{P} = -\tfrac{1}{2}\int_{-L/2}^{L/2} d^p x [\pi(x)\underline{\nabla}\phi(x) + \underline{\nabla}\phi(x)\pi(x)], \tag{3.20}$$

where

$$\phi(\underline{x}) \equiv e^{i\underline{P}\cdot\underline{x}}\,\phi_{\underline{j}=0}e^{-i\underline{P}\cdot\underline{x}}$$
$$= \sum_{\underline{k}} e^{i\underline{k}\cdot\underline{x}}\phi(\underline{k})$$
$$= \sum_{\underline{j}} \phi_{\underline{j}}\left(\sum_{\underline{k}} \frac{1}{(2N+1)^p}\, e^{i\underline{k}\cdot(\underline{x}-\underline{j})/\Lambda}\right),$$
$$\pi(\underline{x}) \equiv e^{i\underline{P}\cdot\underline{x}}\,\pi_{\underline{j}=0}\,e^{-i\underline{P}\cdot\underline{x}} \tag{3.21}$$
$$= \sum_{\underline{j}} \pi_{\underline{j}}\left(\sum_{\underline{k}} \frac{1}{(2N+1)^p}\, e^{i\underline{k}\cdot(\underline{x}-\underline{j})/\Lambda}\right).$$

Substituting (3.21) into (3.20), we get

$$H = \sum_{\underline{j}}\left(\frac{\pi_{\underline{j}}^2}{2} - 2\lambda f^2\phi_{\underline{j}}^2 + \lambda f^4\right) + \tfrac{1}{2}\sum_{\underline{j}_1,\underline{j}_2} D(\underline{j}_1-\underline{j}_2)\phi_{\underline{j}_1}\phi_{\underline{j}_2} + \sum_{\underline{j}_1,\underline{j}_2,\underline{j}_3,\underline{j}_4} X(\underline{j}_1-\underline{j}_2,\underline{j}_1-\underline{j}_3,\underline{j}_1-\underline{j}_4)\phi_{\underline{j}_1}\phi_{\underline{j}_2}\phi_{\underline{j}_3}\phi_{\underline{j}_4}, \tag{3.22}$$

where the function

$$X(\underline{j}_1-\underline{j}_2,\underline{j}_1-\underline{j}_3,\underline{j}_1-\underline{j}_4)$$

can be calculated in a straightforward manner. All of the results and discussions based on the local Hamiltonian (3.19) can be obtained also from the Hamiltonian (3.22) with minor numerical modifications as can be readily shown.

Finally, we note that the interpolating field defined by (3.21) satisfies nonlocal equal-time commutation relations for finite N, i.e.,

$$[\pi(\underline{x}), \phi(\underline{y})] = \frac{-i}{V}\sum_{\underline{k}} e^{i\underline{k}\cdot(\underline{x}-\underline{y})}, \tag{3.23}$$

leading to a factor

$$-\frac{i\Lambda}{(2N+1)}\left\{\frac{\sin[\pi\Lambda(x-y)]}{\sin[\pi\Lambda(x-y)/2N+1]}\right\}$$

for each dimension p.[11]

B. Variational calculation with a single-site basis

Our trial state will be constructed in terms of a single-site basis introduced in terms of creation and annihilation operators for each lattice site, i.e.,

$$\phi_{\underline{j}} = \frac{1}{(2\alpha_{\underline{j}})^{1/2}}(a_{\underline{j}} + a_{\underline{j}}^\dagger),$$
$$i\pi_{\underline{j}} = \left(\frac{\alpha_{\underline{j}}}{2}\right)^{1/2}(a_{\underline{j}} - a_{\underline{j}}^\dagger), \tag{3.24}$$

$$[a_{\underline{j}}, a_{\underline{j}'}^\dagger] = \delta_{\underline{j},\underline{j}'}. \tag{3.25}$$

The vacuum at site $\underline{j}$ is defined by

$$a_{\underline{j}}|0_{\underline{j}}\rangle = 0. \tag{3.26}$$

Repeated application of $a_{\underline{j}}^\dagger$'s to form

$$|n_{\underline{j}}\rangle \equiv \frac{1}{(n_{\underline{j}}!)^{1/2}}(a_{\underline{j}}^\dagger)^{n_{\underline{j}}}|0_{\underline{j}}\rangle \tag{3.27}$$

permits us to build a complete set of product states spanning the Hilbert space:

$$|n_{-N}, \ldots, n_N\rangle = \prod_{\underline{j}=-N}^{N} |n_{\underline{j}}\rangle. \tag{3.28}$$

Our general trial state will be assumed to have the form

$$|\psi\rangle \equiv \prod_{\underline{j}} |\psi_{\underline{j}}\rangle, \tag{3.29}$$

where

$$|\psi_{\underline{j}}\rangle = \sum_{n_{\underline{j}}=0}^{\infty} c_{n_{\underline{j}}}^{\underline{j}}|n_{\underline{j}}\rangle.$$

Using (3.19) and the fact that

$$\langle\psi_{\underline{j}}|\psi_{\underline{j}'}\rangle = \delta_{\underline{j},\underline{j}'}$$

we find for the energy in this basis

$$\langle\psi|H|\psi\rangle = \Lambda\left[\sum_{\underline{j}}\langle\psi_{\underline{j}}|\tfrac{1}{2}p_{\underline{j}}^2 + \lambda_0(x_{\underline{j}}^2 - f_0^2)^2 + \tfrac{1}{2}D(0)x_{\underline{j}}^2|\psi_{\underline{j}}\rangle + \tfrac{1}{2}\sum_{\underline{j}_1\neq\underline{j}_2} D(\underline{j}_1-\underline{j}_2)\langle\psi_{\underline{j}_1}|x_{\underline{j}_1}|\psi_{\underline{j}_1}\rangle\langle\psi_{\underline{j}_2}|x_{\underline{j}_2}|\psi_{\underline{j}_2}\rangle\right], \tag{3.30}$$

where the diagonal terms with $\underline{j}_1 = \underline{j}_2$ have been separated in the expression for the gradient.

Assuming that the ground state is translationally invariant, we adopt the same $|\psi_{\underline{j}}\rangle$ for each site $\underline{j}$; i.e., in (3.29) $c_{n_{\underline{j}}}^{\underline{j}} = c_{n_{\underline{j}}}$, independent of $\underline{j}$. Equation (3.30) then simplifies further since

$$\langle\psi_{\underline{j}_1}|x_{\underline{j}}^1|\psi_{\underline{j}}\rangle \to \langle\psi|x^1|\psi\rangle \quad \text{and} \quad \langle\psi_{\underline{j}}|p_{\underline{j}}^2|\psi_{\underline{j}}\rangle \to \langle\psi|p^2|\psi\rangle$$

independent of $\underline{j}$. We can now use the identity, apparent from (3.11), that

$$\sum_{j_1} D(j_1 - j_2) = 0 \tag{3.31}$$

so that

$$\sum_{j_1 \neq j_2} D(j_1 - j_2) = -\sum_{j} D(0)$$

$$= -(2N+1)^p D(0)$$

and (3.30) becomes in this example

$$E_0(\psi) \equiv \langle \psi | H | \psi \rangle$$
$$= (2N+1)^p \Lambda [\langle \psi | \tfrac{1}{2} p^2 + \tfrac{1}{2} D(0) x^2 + \lambda_0 (x^2 - f_0^2)^2 | \psi \rangle$$
$$- \tfrac{1}{2} D(0) \langle \psi | x | \psi \rangle^2] . \tag{3.32}$$

Our problem now becomes one of varying the trial state $|\psi\rangle$ so as to minimize $E_0(\psi)$. Observe that (3.32) contains two kinds of terms: The first is the expectation value of a positive-definite Schrödinger Hamiltonian, and the second is the square of the expectation value of the mean field strength $\langle \psi | x | \psi \rangle$. This suggests choosing $\langle \psi | x | \psi \rangle$ as one of the variational parameters in any trial wave function. For example, a very simple choice is $|\psi\rangle \equiv e^{-ipc} |0\rangle$, where $|0\rangle$ satisfies (3.26) with α a variational parameter. Then we have $\langle \psi | x | \psi \rangle = c$ as the second parameter. This procedure is discussed in detail in Appendix C. We shall follow here, however, a more general procedure by first introducing a Lagrange multiplier, so that we can carry out the variation to minimize the energy with $\langle \psi | x | \psi \rangle$ held fixed, and then finding the lowest value to $E_0(\psi)$ by varying over all values of $\langle \psi | x | \psi \rangle$. To do this, define

$$\bar{H}(J) = \frac{p^2}{2} + \frac{D(0)}{2} x^2 + \lambda_0 (x^2 - f_0^2)^2 - Jx , \tag{3.33}$$

and let

$$\Gamma(J) = \langle \psi_0 | \bar{H}(J) | \psi_0 \rangle \tag{3.34}$$

be its ground-state eigenvalue. Evidently

$$\frac{\partial \Gamma(J)}{\partial J} = -\langle \psi_0 | x | \psi_0 \rangle \equiv -x(J) \tag{3.35}$$

for a normalized eigenstate[12] $|\psi_0\rangle$. Referring back to (3.32) and defining

$$\frac{1}{\Lambda (2N+1)^p} E(J) = \Gamma(J) + Jx(J) - \tfrac{1}{2} D(0) x^2(J) \equiv \mathcal{E}(J) , \tag{3.36}$$

the problem of minimizing $\langle \psi | H | \psi \rangle$ for the ground-state energy is reduced to finding the value of J such that

$$\frac{\partial \mathcal{E}(J)}{\partial J} = 0 . \tag{3.37}$$

Finding $\mathcal{E}(J)$ for arbitrary values of J is a formidable problem and can only be done numerically. Fortunately, however, for our purposes we only need to know $\mathcal{E}(J)$ for small J. This is because we are interested in exploring the region of small kink mass and the semiclassical discussion of Sec. II told us that this corresponded to having $\langle \psi | x | \psi \rangle \ll 1$.

If $J = 0$, the Schrödinger problem defined by (3.33) has a symmetrical potential and so $x(J=0) = 0$. Since the term $-Jx$ is an analytic perturbation on $\bar{H}(J=0)$, we know that for small J

$$x(J) = c_1 J (1 + c_3 J^2 + c_5 J^4 + \cdots) . \tag{3.38}$$

If $\mathcal{E}(J)$ minimizes for arbitrarily small values of $J \neq 0$, then we will also have a solution satisfying $x(J) \ll 1$ as desired. What we are looking for, then, is a regime of parameters λ_0 and f_0 in which the solution fulfills these criteria.

To demonstrate that such a region can be found, we perform a simple variational calculation. Observe first that (3.35) and (3.38) tell us that

$$\Gamma(J) = \Gamma(0) - \tfrac{1}{2} c_1 J^2 - \tfrac{1}{4} c_1 c_3 J^4 + \cdots \tag{3.39}$$

and so we can write (3.36)

$$\mathcal{E}(J) = \Gamma(0) + \tfrac{1}{2} c_1 [1 - c_1 D(0)] J^2$$
$$+ c_1 c_3 [\tfrac{3}{4} - c_1 D(0)] J^4 + \cdots . \tag{3.40}$$

For $J \ll 1$, (3.38) can be inverted

$$J(x) = \frac{1}{c_1} x - \frac{c_3}{c_1^3} x^3 + \cdots \tag{3.41}$$

and so we can express (3.40) as a function of $x(J)$, i.e.,

$$\mathcal{E}(x(J)) = \Gamma(0) - \frac{\eta}{2c_1} x^2 - \frac{c_3}{c_1^3} (\tfrac{1}{4} + \eta) x^4 + \cdots , \tag{3.42}$$

where

$$\eta \equiv -1 + c_1 D(0) . \tag{3.43}$$

Since c_1 is always positive according to (3.33) and (3.38), this will minimize for small x if

$$0 < \eta \ll 1 \quad \text{and} \quad c_3 < 0 , \tag{3.44}$$

with the minimum, x_c, occurring at

$$x_c^2 \simeq \frac{\eta c_1^2}{|c_3|} (1 - 4\eta) . \tag{3.45}$$

Hence we have $x_c^2 \ll 1$ if

$$\frac{\eta c_1^2}{|c_3|} \ll 1 \tag{3.46}$$

It now only remains for us to show that there exists a range of λ_0 and f_0 for which these conditions on c_1 and c_3 are satisfied. To do this by

analytic methods, we introduce a two-parameter trial state $|\psi\rangle$ of the form of a displaced Gaussian formed from (3.24) and (3.26),

$$|\psi_0\rangle = e^{-i\langle x\rangle p}|0\rangle\,, \quad \langle\psi_0|x|\psi_0\rangle = \langle x\rangle\,. \tag{3.47}$$

Taking the expectation value of (3.33) in this state and henceforth restricting ourselves to two dimensions, we find that

$$\langle\psi_0|\bar{H}(J)|\psi_0\rangle \equiv \Gamma_0(J)$$
$$= \frac{\alpha}{4} + \frac{D(0)}{4\alpha} + \lambda_0\left[\frac{3}{4\alpha^2} + \frac{3\langle x\rangle - f_0^2}{\alpha} + (\langle x\rangle^2 - f_0^2)^2\right]$$
$$+ \frac{D(0)}{2}\langle x\rangle^2 - J\langle x\rangle\,. \tag{3.48}$$

Differentiating (3.48) with respect to $\langle x\rangle$ and α gives the extrema as functions of J. Expanding in a power series for small J, using (3.38) for $\langle x\rangle$ and introducing

$$\alpha(J) = \alpha_0(1 + \alpha_2 J^2 + \cdots)\,, \tag{3.49}$$

we find directly

$$\alpha_2 = 6\lambda_0/[\alpha_0^3(\alpha_0^3 + 6\lambda_0)]\,,$$
$$c_1 = 1/\alpha_0^2 > 0\,, \tag{3.50}$$
$$c_3 = \frac{8\lambda_0}{\alpha_0^6}\left(\frac{6\lambda_0 - \alpha_0^3}{3\lambda_0 + \alpha_0^3}\right),$$

and

$$\frac{\alpha_0^2 - D(0)}{4\lambda_0} + f_0^2 = \frac{3}{2\alpha_0}\,. \tag{3.51}$$

In order to satisfy the condition $\eta \ll 1$, we see from (3.43) and (3.50) that

$$\alpha_0 = [D(0)]^{1/2}[1 - \tfrac{1}{2}\eta + O(\eta^2)]\,. \tag{3.52}$$

By (3.51) and (3.52) λ_0 and f_0 must then satisfy the constraint equation

$$f_0^2 = \frac{3}{2[D(0)]^{1/2}} + \frac{\eta D(0)}{4\lambda_0}\left(1 + \frac{3\lambda_0}{[D(0)]^{3/2}}\right) + O(\eta^2)\,. \tag{3.53}$$

Furthermore, in order to have $c_3 < 0$, it is necessary that $\alpha_0^3 > 6\lambda_0$ in (3.50). For $\eta \ll 1$ this becomes

$$\lambda_0 < \tfrac{1}{6}[D(0)]^{3/2}(1 - \tfrac{3}{2}\eta + \cdots)\,. \tag{3.54}$$

Since both of these conditions can be satisfied simultaneously, it is clear that we have established the desired result. Namely, we have $0 < x_c \ll 1$ when, by (3.53),

$$f_0^2 > f_{cr}^2 = \frac{3}{2[D(0)]^{1/2}} \xrightarrow[N\to\infty]{} \frac{3^{3/2}}{2\pi} = 0.83 \tag{3.55}$$

and, by (3.54),

$$\lambda_0 < \tfrac{1}{6}[D(0)]^{3/2} \xrightarrow[N\to\infty]{} \frac{\pi^3}{18\sqrt{3}} \sim 1.0\,. \tag{3.56}$$

With this choice of parameters, we find a reasonable second-order phase transition whose onset is characterized according to (3.45) and (3.53) by

$$\langle x\rangle = x_c \propto \left[\frac{\eta D(0)}{8\lambda_0}\right]^{1/2} \propto (f_0^2 - f_{cr}^2)^{1/2}\,. \tag{3.57}$$

The inequalities will be altered quantitatively by a more elaborate trial wave function but the general conclusions about the nature of the transition remain essentially unchanged.

Notice that throughout this analysis the term proportional to $D(0)$, which contains the effects of site-site recoupling in (3.32), plays an important role in eliminating tricritical behavior. Had $D(0)$ been zero, $\mathcal{G}(J)$ in (3.40) would have had the form

$$\mathcal{G}(J) = \Gamma(0) + \tfrac{1}{2}c_1 J^2 + \tfrac{3}{4}c_1 c_3 J^4 + \cdots\,.$$

Since $c_1 > 0$, we could only have obtained a minimum with $\langle x\rangle \neq 0$ if both $c_3 < 0$ *and* if the coefficient of the next higher term in $\mathcal{G}(J)$ of order J^6 was positive. However, there would again be a local *minimum* at $\langle x\rangle = 0$ leading to the tricritical problem encountered in the momentum-space calculation. The interesting question of what happened to the analog of the $D(0)$ term in the momentum-space calculation will be addressed in detail in Sec. IV.

To summarize, the main achievement of this calculation is that we have found that x_c in (3.45) can be made arbitrarily small by appropriate choice of λ_0 and f_0^2 without a spurious minimum at $\langle x\rangle = 0$. This is in contrast with the first-order phase transition found in the momentum basis between the $\langle\phi\rangle = 0$ and $\langle\phi\rangle = c \neq 0$ phases in Sec. II C. We have thus developed a variation procedure free of the tricritical problem and we have found that the spontaneous symmetry breaking of the ground state from the $\langle x\rangle = 0$ phase to $\langle x\rangle \neq 0$ can be established in accord with general principles. The possibility of finding a nonvanishing value of x_c that is arbitrarily small is of crucial importance for the study of low-lying kink solutions to this theory.

However, before discussing the kink solution, it is also important to compare the present bound, (3.42), on the ground-state energy with that obtained in (2.36) using the momentum basis. Although we have found that the trial state (3.47) removes the tricritical problem, we must also compare energy bounds in order to establish whether the single-site-basis approach as implemented here is a better variational approximation. In particular, we are interested in this comparison for parameters satisfying (3.53) and (3.54). Unfortunately, a numerical evaluation of (2.36) shows that, in the range of $\lambda_0 \lesssim 1$, as required in (3.56), the momentum calculation produces a lower bound

TABLE II. A table giving the single-site energies and $\langle x\rangle$ for $\lambda_0=3$ and a small range of f_0. The last column gives the values for the momentum-space calculation in this same region. (N.B. The momentum-space calculation has already gone through to the case where $c=0$ is the unique minimum.) This table shows that the single-site calculation provides a better description of what is going on all the way through the region of interest, i.e., $\langle x\rangle \to 0$.

f_0	$\langle x\rangle$	$\mathcal{E}_{\text{single-site}}$	$\mathcal{E}_{\text{momentum}}(c=0)$
0.8075	0.073	1.712 89	1.714 32
0.8060	0.018	1.707 43	1.708 66
0.805 94	0.011	1.707 21	1.7084
0.805 90	0.000 76	1.707 08	1.7083
0.805 902 5	0.0	1.707 08	1.7083

in the energy than the single-site calculation. However, this numerical constraint to $\lambda_0 \lesssim 1$ is only an artifact of our crude trial wave function, and one can do better.

Restricting ourselves to a single-site basis as in (3.29), we can numerically diagonalize the Hamiltonian to better than one part in 10^4 accuracy.[13] The results of this computer calculation show that if $\lambda_0=3$, the single-site wave function gives a lower ground-state energy than the momentum basis for all values of x_c such that $0 \leq x_c \ll 1$. Moreover, this calculation does not predict tricritical behavior. A numerical comparison of single-site and momentum-basis results for $\lambda_0=3$ and $0.8059 \lesssim f_0 \lesssim 0.8075$ is summarized in Table II. To recapitulate, we have developed techniques for a variational calculation free of illegal behavior and applicable in the strong-coupling regime $\langle x\rangle \ll 1$. Many avenues are open for improving both qualitative and quantitative predictions. One way would be to abandon the single-site basis approximation in (3.29) and build a procedure using blocks of neighboring lattice sites. This technique and its value for extending the realm of coupling parameters for which we can construct ground states will be discussed in Sec. IV, along with the relation of our method to renormalization theory.

C. Calculation of an upper bound on the kink mass

In order to compare with the semiclassical results of Sec. II A for a kinklike solution in one space and one time dimension, we now introduce a trial form that exhibits a dependence on the individual lattice sites j. We again work in a single-site basis (3.29) and compute an upper bound on the energy for the single-kink sector relative to the energy in the vacuum sector. Furthermore, if we can establish the accuracy of the ground-state energy, we can interpret our result as an upper bound on the single-kink mass and compare with the classical results of (2.6) and (2.7).

To carry out this calculation, it is simplest to modify (3.30) by adding and subtracting the diagonal term $j_1=j_2$ in the double sum, writing

$$E_{\text{kink}} \equiv \langle \psi_{\text{kink}} | \boldsymbol{H} | \psi_{\text{kink}} \rangle = \Lambda \Big[\sum_j \langle \psi_j | \tfrac{1}{2} p_j^2 + \lambda_0 (x_j^2 - f_0^2)^2 + \tfrac{1}{2} D(0)(x_j^2 - x_j \langle \psi_j | x_j | \psi_j \rangle) | \psi_j \rangle \Big] + \tfrac{1}{2} \sum_{j_1, j_2} D(j_1 - j_2) \langle \psi_{j_1} | x_{j_1} | \psi_{j_1} \rangle \langle \psi_{j_2} | x_{j_2} | \psi_{j_2} \rangle . \tag{3.58}$$

The double sum in the last term is essentially the classical gradient term in the energy expression (2.3), with the matrix element of the field replacing its classical strength. This is the only term coupling different lattice sites and therefore we can minimize the kink energy simply by imitating our procedure for the vacuum state, introducing a Lagrange multiplier $J(j)$ for each site and performing the variation subject to the condition that

$$\langle x_j \rangle \equiv \langle \psi_j | x_j | \psi_j \rangle$$

is held fixed. This state will automatically be orthogonal to the vacuum in the limit $(2N+1) \to \infty$ since the choice of a functional form for $\langle x_j \rangle$ as illustrated in Fig. 5 leads to $Q \neq 0$ for the conserved "charge" (2.9).

In analogy with (3.33) and (3.36), we introduce

$$\overline{H}(J(j)) = \frac{1}{(2N+1)} \sum_j \Big[\frac{p_j^2}{2} + \frac{D(0) x_j^2}{2} + \lambda_0 (x_j^2 - f_0^2)^2 - J(j) x_j \Big] \tag{3.59}$$

and define

$$\Gamma(J(j)) = \langle \psi_{\text{kink}} | \overline{H} | \psi_{\text{kink}} \rangle = \frac{1}{2N+1} \sum_j \Gamma_j(J(j)),$$

where $\Gamma_j(J(j))$ is the same function calculated in (3.39). The variational upper bound on the energy of the kink state is then computed by finding the local minima with respect to $J(j)$ of

$$\frac{1}{2N+1} E_{\text{kink}} = \frac{1}{2N+1} \sum_j \big[\Gamma_j(J(j)) + J(j) \langle x_j \rangle - \tfrac{1}{2} D(0) \langle x_j \rangle^2 \big] + \frac{1}{(2N+1)} \sum_{j_1, j_2} \tfrac{1}{2} D(j_1 - j_2) \langle x_{j_1} \rangle \langle x_{j_2} \rangle . \tag{3.60}$$

Since our goal here is to display an upper bound on the energy of a kink state that is low-lying, in the sense of the semiclassical energy (2.7), we now make a simplifying if crude approximation to esti-

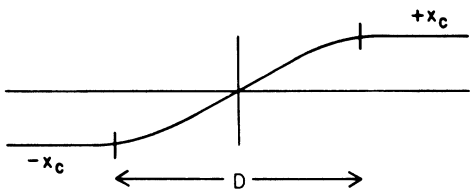

FIG. 5. The "kink" configuration.

mate the kink energy, and in particular to show its dependence on the parameters in the theory.

It is apparent that, except for an interval of finite length on the lattice, the value of $\langle x(j)\rangle$ must be arbitrarily close to $\pm x_c$, where x_c is the extremum determined by (3.45) for small J and $\langle x\rangle$. Otherwise, the excitation energy of the kink would be proportional to the total length of the lattice, $L=(2N+1)/\Lambda$, akin to the classical result that unless $g(x)$ makes the transition from $-f$ to $+f$ within a finite interval in (2.6), the total kink energy (2.3) would diverge as $\int_{-\infty}^{+\infty} dx$. Let us introduce as a parameter in the variational calculation the width, D, of the interval over which $x(j)$ changes from $-x_c$ to $+x_c$. We parametrize D in terms of the lattice sites by

$$D=(2j_0+1)/\Lambda\,, \tag{3.61}$$

where

$$\langle x_j\rangle=\begin{cases}+x_c & \text{for } j>j_0\,,\\ -x_c & \text{for } j<-j_0\,.\end{cases}$$

Using (3.61), we can write for the difference between the energy of the kink and vacuum states [recognizing $\Gamma(-J)=\Gamma(J)$]

$$E_{\text{kink}}(J)-E_0(J_c)=\Lambda\sum_{j=-j_0}^{+j_0}\left[\Gamma_j(J(j))+J(j)\langle x_j\rangle-\tfrac{1}{2}D(0)\langle x_j\rangle^2\right]-\frac{2j_0+1}{2N+1}E_0(J_c)+\Lambda\sum_{j_1,j_2}\tfrac{1}{2}D(j_1-j_2)\langle x_{j_1}\rangle\langle x_{j_2}\rangle\,. \tag{3.62}$$

The last term represents the "kinetic" energy due to the change of $\langle x_j\rangle$ in the transition region and is equal to

$$\Lambda\sum_{j_1,j_2}\tfrac{1}{2}D(j_1-j_2)\langle x_{j_1}\rangle\langle x_{j_2}\rangle\approx\Lambda(2j_0+1)\frac{x_c{}^2}{(2j_0+1)^2}=\frac{\Lambda x_c{}^2}{D\Lambda}\,. \tag{3.63}$$

This is evaluated by a linear approximation to $\langle x_j\rangle$ between $-j_0$ and j_0. Equation (3.63) is just the classical expression for the kinetic energy. Assuming that the ground-state energy has been evaluated accurately, we overestimate the energy difference in (3.62) if we simply set $J(j)=0$ in the transition region for calculating the difference of the first two terms. Using (3.42) and (3.61) this difference gives, to leading order in $x_c{}^2\ll 1$,

$$(2j_0+1)\Lambda\Gamma(0)-\frac{2j_0+1}{2N+1}E_0(J_c)=D\Lambda^2\frac{\eta}{2c_1}x_c{}^2\,. \tag{3.64}$$

Adding (3.63) and (3.64), we have

$$E_{\text{kink}}-E_0(J_c)=\Lambda\left[(D\Lambda)\frac{\eta}{2c_1}x_c{}^2+\frac{x_c{}^2}{(D\Lambda)}\right], \tag{3.65}$$

which is minimized at

$$(D\Lambda)=(2c_1/\eta)^{1/2}$$

to give

$$E_{\text{kink}}(J)-E_0(J_c)=2x_c{}^2\left(\frac{\eta}{2c_1}\right)^{1/2}\Lambda\,. \tag{3.66}$$

The constants can be expressed using (3.45) and (3.50) in terms of the coupling parameters. Using (3.56) and (3.18), we find

$$\begin{aligned}D&\sim(2\lambda_0{}^{1/2}x_c)^{-1}\Lambda^{-1}\\&\sim(2\lambda^{1/2}x_c)^{-1}\,,\\E_{\text{kink}}(J)-E_0(J_c)&\approx 4\lambda^{1/2}x_c{}^3[1+O(x_c)]\,.\end{aligned} \tag{3.67}$$

Equation (3.67) is the main result of this section. Assuming, as we remarked earlier, that the ground-state energy has been evaluated accurately, the one-kink energy is, aside from unimportant numerical factors, a rescaled version of the semiclassical result for the kink mass $\sim\sqrt{\lambda}\,f^3$ in (2.7). Thus (3.67) shows that the effect of the quantum corrections has been simply to rescale the classical field strength f to $x_c\equiv\langle\psi_j|x_j|\psi_j\rangle$ for sites outside of the kink region. No matter how large the cutoff Λ is made in (3.67), we are free to choose x_c small enough so that the kink mass

$$m_{\text{kink}}\sim 4\lambda_0{}^{1/2}\Lambda x_c{}^3 \tag{3.68}$$

is a finite and small mass. What we still face, of course, is the challenge of an accurate calculation for the ground state by going beyond the single-site lattice basis, but our principal point is now evident: *In the spontaneously broken theory for small values of $\langle x\rangle$ we find low-lying kink configurations in the quantum theory of (2.1) formulated on a lattice. Moreover, there is no reason to believe that this result is an artifact of having introduced a lattice since the kink represents a structure which extends over many lattice sites.* In particular, the kink extends over a number of

lattice sites given by

$$2j_0+1 \sim D\Lambda \sim \frac{1}{2\lambda_0^{1/2}x_c}.$$

IV. CONNECTION TO RENORMALIZED FIELD THEORY—THE BLOCK FORMALISM

In the previous sections we discussed two different attempts based on variational techniques for calculating bounds on the masses of the ground state and of the "kink" state for a lattice (or cutoff) field theory with a $\lambda_0(x^2-f_0^2)^2$ self-interaction. We saw that a calculation using a simple momentum-space basis for describing the ground state is adequate in the weak-coupling regime ($f^2 \gg 1$). For strong coupling ($f^2 \lesssim 1$), however, we encountered tricritical behavior and saw that such a calculation predicts a first-order phase transition (i.e., the vacuum expectation value $\langle x\rangle$ jumped discontinuously from $\langle x\rangle \sim 1$ to $\langle x\rangle = 0$). On the other hand, in the strong-coupling region we found a limited range of parameters for which a configuration-space basis provides a more appropriate description. The single-site calculation carried out in Sec. III exhibited a reasonable second-order phase transition with $\langle x\rangle \sim A(f_0^2-f_{cr}^2)^{1/2}$, as shown in (3.57). Moreover, this calculation allowed us to explore the region of coupling parameters in which $\langle x\rangle$ is arbitrarily small, and therefore to establish the existence of the kink configuration as a low-lying state.

Numerical studies also showed that for the region of parameters $\lambda_0 \sim 3$, $f_0^2 < 1$, the single-site basis produced lower upper bounds on the energy than the momentum-basis calculation all the way down to $\langle x\rangle = 0$. Unfortunately, for $\lambda_0 < 1$, i.e., $\lambda < \Lambda^2$, the momentum-space calculation, although manifestly incorrect, produced lower upper bounds on the ground-state energy than the single-site basis. We face, therefore, the following questions: "Why does the momentum basis win for $\lambda_0 < 1$?" "How can we extend our techniques to allow us to explore larger regions of λ_0 and f_0 without encountering forbidden behavior?" It turns out that the answers to these questions are intimately related to the general question of renormalization of this theory which we must now address.

We proceed as follows:

(1) First, we discuss the general problem of taking the lattice spacing to zero, i.e., $\Lambda \to \infty$, and defining a finite version of our Hamiltonian in order to establish contact with the usual renormalization procedure. This analysis shows simply why, for $\lambda_0 \ll 1$, the single-site calculation *must* lose to the momentum-space one.

(2) Next, we introduce a more general class of wave functions which correlate a finite number of neighboring sites to one another. We call these "block wave functions" and describe how they can provide a systematic way of extending the regions of parameters λ_0 and f_0^2 over which we can find bounds on the ground-state energies which are lower than those obtained in the momentum basis.

(3) Next, we develop a straightforward and practical scheme for working with the block wave functions. It is a hybrid method which uses a k-space momentum basis for performing the variational calculation within each of the individual blocks that are introduced using the site basis. With this technique we can explore the range of values of λ_0 and f_0^2 all the way into the usual renormalization region, with $\lambda_0 \to 0$ and $f_0^2 \to \infty$ in one space and one time dimension. As applied to this model, this technique has the virtue that it is capable of calculating exactly the parts of the ground- and excited-state energies which diverge as the cutoff $\Lambda \to \infty$, while at the same time completely avoiding tricritical behavior. The hybrid calculation also shows why the momentum-space calculation failed.

(4) Finally, we introduce scaling arguments and outline a procedure that indicates how the block formalism may give us a framework to improve further upon these calculations. These arguments are reminiscent of the resummation technique and renormalization-group ideas of Wilson and Kadanoff.[6]

A. On the connection to conventional renormalization theory

Our cutoff theory was defined in terms of the Hamiltonian density

$$\mathcal{H}^{\text{cutoff}} = \tfrac{1}{2}\pi^2(x) + \tfrac{1}{2}(\nabla\phi)^2(x) + \lambda[\phi^2(x) - f^2]^2 . \quad (4.1)$$

We now seek a way to redefine $\mathcal{H}$ so that it will be finite even as $\Lambda \to \infty$. As is well known, the only divergences in the ϕ^4 theory in one space and one time dimension are those associated with normal-ordering.[5] Normal-ordering the first two quadratic "free field" terms in (4.1) gives a term proportional to Λ^2, while the ϕ^4 term, as illustrated by the Feynman graphs of Fig. 6, contributes terms proportional to $\ln\Lambda$ and $\ln^2\Lambda$. Hence, once we define the Hamiltonian density $N(\mathcal{H}^{\text{cutoff}})$ to be normal-ordered with respect to an arbitrary mass, and require the coefficient of every term to be finite in the limit $\Lambda \to \infty$, the resulting Hamiltonian will define a finite theory. To carry out the normal-ordering we introduce a momentum basis

$$\phi(x) = \int dx\, e^{iqx}\phi(q) ,$$
$$\pi(x) = \int dx\, e^{iqx}\pi(q) , \quad (4.2)$$

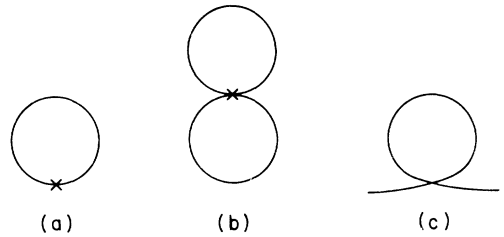

FIG. 6. Feynman graphs giving rise to logarithmic divergence in the Hamiltonian: (a) contribution to the vacuum energy ($\ln\Lambda$); (b) contribution to the vacuum energy ($\ln^2\Lambda$); (c) contribution to the coefficient of the term $N_{\mu^2}(\phi^2)$ ($\ln\Lambda$).

and define a_q and $a_q^\dagger$ by

$$\phi(q) \equiv \frac{1}{[2L\alpha_q(\mu^2)]^{1/2}}(a_{-q}+a_q^\dagger)$$

$$i\pi(q) \equiv \left[\frac{\alpha_q(\mu^2)}{2L}\right]^{1/2}(a_{-q}-a_q^\dagger) ,$$

where

$$\alpha_q(\mu^2) \equiv (q^2+\mu^2)^{1/2}$$

and μ^2 is arbitrary. We can then write the terms in (4.1) in normal-ordered form:

$$\begin{aligned}
&\phi^2(x) = N_{\mu^2}(\phi^2(x)) + \langle\phi^2\rangle_{\mu^2} ,\\
&\phi^4(x) = N_{\mu^2}(\phi^4(x)) + 6\langle\phi^2\rangle_{\mu^2} N_{\mu^2}(\phi^2(x)) + 3(\langle\phi^2\rangle_{\mu^2})^2 ,\\
&(\nabla\phi)(x)^2 = N_{\mu^2}((\nabla\phi)^2(x)) + \langle(\nabla\phi)^2(x)\rangle_{\mu^2} ,\\
&\pi^2(x) = N_{\mu^2}(\pi^2(x)) + \langle\pi^2(x)\rangle_{\mu^2} .
\end{aligned} \tag{4.3}$$

In the infinite-volume limit, with $k_{\max} = \pi\Lambda$, we find by straightforward calculation

$$\begin{aligned}
\langle\phi^2\rangle_{\mu^2} &= \frac{1}{2\pi}\int_0^{\pi\Lambda}\frac{dk}{(k^2+\mu^2)^{1/2}}\\
&= \frac{1}{2\pi}\ln\left\{\frac{\pi\Lambda}{\mu}+\left[1+\left(\frac{\pi\Lambda}{\mu}\right)^2\right]^{1/2}\right\} ,\\
\langle\pi^2\rangle_{\mu^2} &= \frac{1}{2\pi}\int_0^{\pi\Lambda} dk(k^2+\mu^2)^{1/2}\\
&= \frac{\pi\Lambda}{4\pi}(\mu^2+\pi^2\Lambda^2)^{1/2} + \tfrac{1}{2}\mu^2\langle\phi^2\rangle_{\mu^2} ,\\
\langle(\nabla\phi)^2\rangle_{\mu^2} &= \frac{1}{2\pi}\int_0^{\pi\Lambda}\frac{k^2dk}{(k^2+\mu^2)^{1/2}}\\
&= \langle\pi^2\rangle_{\mu^2} - \mu^2\langle\phi^2\rangle_{\mu^2} .
\end{aligned} \tag{4.4}$$

An important observation at this point is that from the point of view of rendering the theory finite, normal-ordering with respect to one arbitrary mass μ^2 is as good as normal-ordering with respect to any other mass. The difference is given by finite terms in the limit $\Lambda\to\infty$, as can be readily verified from (4.1) and (4.4). The Hamiltonian (4.1) can now be written as

$$\begin{aligned}
\mathcal{H}^{\text{cutoff}} &= N_{\mu^2}(\tfrac{1}{2}\pi^2 + \tfrac{1}{2}(\nabla\phi)^2 + \lambda\phi^4)\\
&\quad + (-2\lambda f^2 + 6\lambda\langle\phi^2\rangle_{\mu^2}) N_{\mu^2}(\phi^2)\\
&\quad + \langle\tfrac{1}{2}\pi^2 + \tfrac{1}{2}(\nabla\phi)^2 - 2\lambda f^2\phi^2\rangle_{\mu^2} + 3\lambda(\langle\phi^2\rangle_{\mu^2})^2 .
\end{aligned} \tag{4.5}$$

Defining a mass

$$m^2 \equiv -4\lambda f^2 + 12\lambda\langle\phi^2\rangle_{\mu^2} \tag{4.6}$$

we have

$$\begin{aligned}
\mathcal{H}^{\text{cutoff}} &= N_{\mu^2}(\tfrac{1}{2}\pi^2 + \tfrac{1}{2}(\nabla\phi)^2 + \tfrac{1}{2}m^2\phi^2 + \lambda\phi^4)\\
&\quad + \text{const}\times(\mu^2, \lambda, f^2) ,
\end{aligned} \tag{4.7}$$

which represents, up to a divergent c-number term, a finite normal-ordered Hamiltonian, provided m^2 and λ are finite in the limit $\Lambda\to\infty$. If we now introduce the dimensionless units as used earlier in (3.18), λ and m^2 may be chosen to be finite as $\Lambda\to\infty$ if and only if the dimensionless parameter λ_0 vanishes as

$$\lambda_0 = \frac{\lambda}{\Lambda^2} \to 0 \quad \text{as} \quad \Lambda\to\infty \tag{4.8}$$

and, in (4.6),

$$f^2 = f_0^{\,2} \cong 3\langle\phi^2\rangle_{\mu^2} \to \ln(\Lambda) \quad \text{as} \quad \Lambda\to\infty . \tag{4.9}$$

In other words, if we wish to study lattice theories corresponding to conventionally renormalizable theories we have to look at the region where $\lambda_0 \ll 1$ and $f_0^{\,2} \gg 1$. These conditions ensure that the dimensional parameters λ and m^2 are small with respect to the cutoff Λ. Clearly this is not the range we have been considering. Indeed, the single-site basis gave a lower upper bound on the ground-state energy than the momentum-space calcuation only when the coupling parameters were in the range $\lambda_0 \sim 3$, $f^2 \sim 1$. We emphasize, however, that even though the corresponding lattice Hamiltonian does not define a finite theory for this case in the limit $\Lambda\to\infty$, this example is of interest in itself. In particular, it possesses low-mass collective or quasiclassical-extended states as we saw in (3.68) for any arbitrarily large *finite* value of Λ.

Now we are in a position to answer the question raised in the introduction to this section: Why does the single-site calculation eventually lose to the momentum-basis calculation as λ_0 gets smaller ($\sim 1/\Lambda^2$)? The point is that the normal-ordering divergences of the theory, which in one space and one time dimension are the *only* divergences, are exhibited exactly by the momentum-space calculation as seen by comparing the quadratic (Λ^2) as well as the logarithmic ($\ln\Lambda$ and $\ln^2\Lambda$) terms in (4.4) and (4.5)

with (2.35) and (2.36) and observing the similarity of (2.37) with (4.6).

Hence we can write for the ground-state energy density calculated in the momentum basis

$$\mathcal{E}_{\text{momentum}} = A_0\Lambda^2 + B_0\ln\Lambda + C_0\ln^2\Lambda + \mathcal{E}^{\text{finite}}_{\text{momentum}} , \tag{4.10}$$

where the coefficients A_0, B_0, and C_0 are exactly what they should be for the true ground-state energy of $\mathcal{H}^{\text{cutoff}}$, in particular in terms of a cutoff $k_{\max} = \pi\Lambda$, $A_0 = \frac{1}{4}\pi$, which follows directly from (4.4) and (4.5). $\mathcal{E}^{\text{finite}}_{\text{momentum}}$ is larger than the true Λ-independent part of the ground-state energy density since the variational procedure gives an upper bound. As far as the single-site calculation is concerned, the energy density $\mathcal{E}_0(J)$, by (3.33), (3.36), and (3.48), has only a Λ^2 divergence and we can write

$$\mathcal{E}_{\text{single-site}} = A_0'\Lambda^2 + \mathcal{E}^{\text{finite}}_{\text{single-site}} . \tag{4.11}$$

In particular, for $\lambda_0 \to 0$ we can use (3.51) and (3.48) to evaluate the coefficient A_0', which is larger than the corresponding one in the momentum-basis calculation:

$$A_0' = \tfrac{1}{2}[D(0)]^{1/2} = \frac{\pi}{2\sqrt{3}} = \frac{2}{\sqrt{3}} A_0 > A_0 .$$

It is clear therefore that if we hold λ and f^2 fixed and take $\Lambda \to \infty$, eventually we must have

$$\begin{aligned}\mathcal{E}_{\text{single-site}} - \mathcal{E}_{\text{momentum}} &= (A_0' - A_0)\Lambda^2 - B_0\ln(\Lambda) - C_0\ln^2(\Lambda) \\ &\quad + (\mathcal{E}^{\text{finite}}_{\text{single-site}} - \mathcal{E}^{\text{finite}}_{\text{momentum}}) \\ &\to \left(\frac{2}{\sqrt{3}} - 1\right) A_0\Lambda^2 > 0 .\end{aligned} \tag{4.12}$$

The reason the single-site calculation with $\lambda_0 \sim 3$, $f_0^2 \sim 1$ produced a lower bound on the energy than the momentum-space one is that, for these parameters, the bare mass is comparable to the cutoff, and the cutoff-independent part of the energy density, i.e., the term we have called $\mathcal{E}^{\text{finite}}$, is comparable to the ones of order Λ^2, $\ln(\Lambda)$, and $\ln^2(\Lambda)$. Since in this region $\mathcal{E}^{\text{finite}}_{\text{single-site}} < \mathcal{E}^{\text{finite}}_{\text{momentum}}$, the single-site calculation wins. This, of course, tells us that when the finite part of the momentum-space energy gets smaller than the divergent parts, the momentum basis will win. Therefore, if we wish to extend our variational calculations in a site basis into the region of coupling parameters with $\lambda_0 \ll 1$ and $f^2 \gg 1$ and at the same time obtain lower bounds on the energy than the momentum-space approach, we must construct a class of trial functions that reproduce with arbitrarily high accuracy the coefficients A_0, B_0, and C_0 of the terms that diverge as $\Lambda \to \infty$. Only then can we claim that the comparison of the ground-state energy density in these trial states with the calculation in the momentum basis involved finite parts alone. Of course, we also demand that this class of trial states not produce any problem like the tricritical behavior found in the momentum-space calculation. It is the purpose of Sec. IV B to indicate a way toward accomplishing these goals.

B. Block wave function

The block wave-function formalism is a generalization of the single-site approach used in Sec. III which allows the correlation of a finite number of neighboring lattice sites to one another. It has the advantage of enlarging the space of variational trial states while still reducing the problem to a Schrödinger one with a finite number of degrees of freedom. Our starting point is to assume that the lattice is subdivided into B blocks, $B = (2b+1)$, of length $L_b = (2l+1)/\Lambda$ (see Fig. 7). The total length of the lattice will, therefore, be $L = BL_b$. The points on the lattice can be labeled either by $\{j\} = \{-N, N\}$, $L = (2N+1)/\Lambda$, as used thus far, or alternatively we can introduce j' and α such that $j' = \{-l, l\}$ and $\{\alpha\} = \{-b, b\}$ so that every j can be uniquely written as $j = j' + \bar{L}_b\,\alpha$; α labels the block we are in while j' labels the points within the block, and $\bar{L}_b = \Lambda L_b$. Adopting this notation we introduce a trial state as a product of block states:

$$\begin{aligned}|\psi^{\text{trial}}\rangle &= \prod_{\alpha=-b}^{+b} |\psi(\alpha)\rangle , \\ \langle\psi(\alpha)|\psi(\alpha')\rangle &= \delta_{\alpha,\alpha'} .\end{aligned} \tag{4.13}$$

$|\psi(\alpha)\rangle$ is a general trial state in the space of states generated by applying arbitrary polynomials in $a^\dagger(j' + \bar{L}_b\alpha)$ to the state $\Pi_{j'}|0_{j'+\bar{L}_b\alpha}\rangle$ [defined in Eq. (3.26)] for α fixed, and j' varying over $\{-l, l\}$.

Taking the expectation value of the Hamiltonian

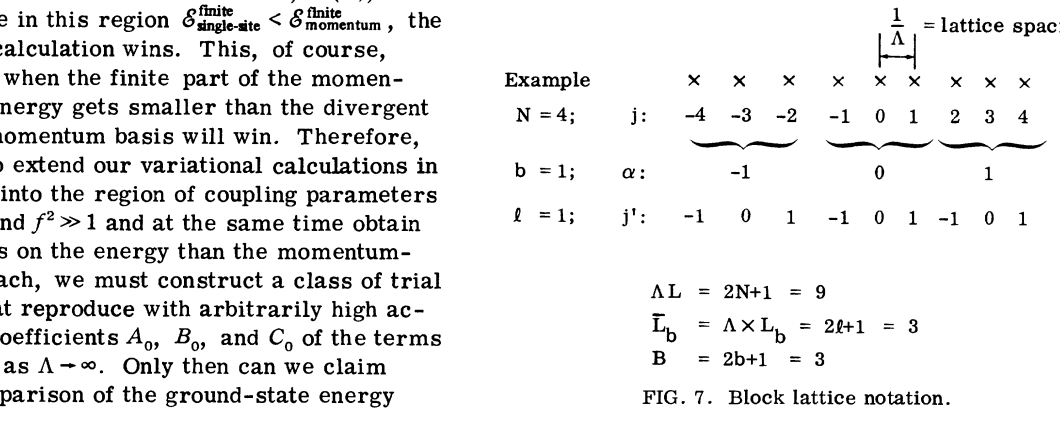

FIG. 7. Block lattice notation.

(3.19) in this trial state we obtain

$$\langle\psi^{\text{trial}}|H|\psi^{\text{trial}}\rangle=\Lambda\sum_{\alpha=-b}^{+b}\Big\langle\psi(\alpha)\Big|\sum_{j'=-l}^{+l}\left[\tfrac{1}{2}p_{(j'+\alpha\bar{L}_b)}{}^2+\lambda_0(x_{(j'+\alpha\bar{L}_b)}{}^2-f_0{}^2)^2\right]+\tfrac{1}{2}\sum_{j_1',j_2'}\left[D(j_1'-j_2')\,x_{(j_1'+\alpha\bar{L}_b)}\,x_{(j_2'+\alpha\bar{L}_b)}\right]\Big|\psi(\alpha)\Big\rangle$$
$$+\Lambda\sum_{\alpha_1\neq\alpha_1}\sum_{j_1',j_2'}\tfrac{1}{2}D(j_1'-j_2'+\bar{L}_b(\alpha_1-\alpha_2))\langle\psi(\alpha_1)|x_{(j_1'+\alpha_1\bar{L}_b)}|\psi(\alpha_1)\rangle\langle\psi(\alpha_2)|x_{(j_2'+\alpha_2\bar{L}_b)}|\psi(\alpha_2)\rangle\,. \quad (4.14)$$

Since we are interested in the ground state we assume that all of the $|\psi(\alpha)\rangle$ are constructed in an identical way. This construction preserves invariance under the translation from one block to another. To calculate the energy density we can suppress the α label, since summing over α produces B identical terms. This reduces our problem to finding the state which minimizes the following Schrödinger problem with $\bar{L}_b$ degrees of freedom:

$$\mathcal{H}^{\text{eff}}\equiv\frac{1}{\Lambda(2N+1)}\langle\psi|H|\psi\rangle=\Big\langle\psi\Big|\frac{1}{\bar{L}_b}\sum_{j=-l}^{+l}\left[\frac{p_j{}^2}{2}+\lambda_0(x_j{}^2-f_0{}^2)^2\right]+\frac{1}{\bar{L}_b}\sum_{j_1,j_2=-l}^{+l}\left[\tfrac{1}{2}D(j_1-j_2)\,x_{j_1}x_{j_2}\right]\Big|\psi\Big\rangle$$
$$-\frac{1}{\bar{L}_b}\sum_{j_1,j_2=-l}^{+l}\left[\tfrac{1}{2}D(j_1-j_2)\langle x_{j_1}\rangle\langle x_{j_2}\rangle\right]+\frac{1}{2N+1}\sum_{\alpha,j}\tfrac{1}{2}(\nabla\langle x_j\rangle)^2\,, \quad (4.15)$$

where we have used the fact that $\langle x_{j+\alpha L}\rangle=\langle x_j\rangle$ and introduced the notation

$$\sum_{\alpha,j}(\nabla\langle x_j\rangle)^2=\sum_{\substack{\alpha_1,\alpha_2\\ j_1,j_2}}D(j_1-j_2+\bar{L}_b(\alpha_1-\alpha_2))\times\langle x_{j_1}\rangle\langle x_{j_2}\rangle\,. \quad (4.16)$$

As in the single-site case the terms proportional to $\langle x_j\rangle^2$ complicate the minimization problem and so we introduce the Lagrange multipliers J_j and solve first for the ground state of

$$\bar{H}(J_j)\equiv\frac{1}{\bar{L}_b}\sum_{j=-l}^{+l}\left[\tfrac{1}{2}p_j{}^2+\lambda_0(x_j{}^2-f_0{}^2)^2-J_jx_j\right]+\tfrac{1}{2}\sum_{j_1,j_2=-l}^{+l}D(j_1-j_2)\,x_{j_1}x_{j_2} \quad (4.17)$$

for arbitrary J_j, with $\langle x_j\rangle$ held constant. Defining

$\Gamma(J_j)=$ ground-state eigenvalue of $\{\bar{H}(J_j)\}$

and noting as before [see (3.35)]

$$-\frac{\partial\Gamma}{\partial J_j}=\frac{1}{\bar{L}_b}\langle x_j\rangle\equiv\frac{1}{\bar{L}_b}x(J_j)\,, \quad (4.18)$$

our problem reduces to minimizing the function

$$\mathcal{E}(J_j)\equiv\Gamma(J_j)+\frac{1}{\bar{L}_b}\sum_{j=-l}^{+l}J_jx(J_j)+\frac{1}{2N+1}\sum_{\alpha,j}\tfrac{1}{2}(\nabla\langle x_j\rangle)^2-\frac{1}{2}\frac{1}{\bar{L}_b}\sum_{j_1,j_2}D(j_1-j_2)\,x(J_{j_1})\,x(J_{j_2})\,, \quad (4.19)$$

with respect to the $\bar{L}_b$ parameters J_j.

In principle, an exact solution for the ground state of $\bar{H}(J)$ will give a lower value for the upper bound on the ground-state energy than that given by the single-site basis. Therefore this will yield a better bound than the momentum-basis calculation for a large range of parameters λ_0 and $f_0{}^2$.

C. Hybrid calculation

In practice the general solution for the ground state of the $\bar{L}_b$ degree-of-freedom Schrödinger problem is difficult to obtain. In particular, each $\langle x_j\rangle$ and J_j will be a function of j due to end effects on each block. However, the $\langle x_j\rangle$ will, for most lattice sites, become independent of j as $\bar{L}_b\to\infty$. In other words, for the large-$\bar{L}_b$ limit we expect that the difference

$$\langle x_j\rangle-\frac{1}{\bar{L}_b}\sum_{j=-l}^{+l}\langle x_j\rangle\equiv x(J_j)-\bar{x} \quad (4.20)$$

will go to zero like $1/\bar{L}_b$ for most of the $\bar{L}_b\gg1$ sites within each block. With this in mind we minimize $\langle\psi|\bar{H}(J_j)|\psi\rangle$ only over states such that $\bar{x}=(1/\bar{L}_b)\sum_{j=-l}^{+l}\langle x_j\rangle$ is held fixed, and we construct $\mathcal{E}(J_j)$ by replacing $x(J_j)$ by $\bar{x}$. One accomplishes this technically by introducing a single Lagrange multiplier J to replace the individual J_j in (4.17):

$$\bar{H}(J)=\frac{1}{\bar{L}_b}\left\{\sum_{j=-l}^{+l}\left[\tfrac{1}{2}p_j{}^2+\lambda_0(x_j{}^2-f^2)^2\right]+\tfrac{1}{2}\sum_{j_1,j_2=-l}^{+l}D(j_1-j_2)x_{j_1}x_{j_2}\right\}-J\frac{1}{\bar{L}_b}\sum_{j=-l}^{+l}x_j\,. \quad (4.21)$$

Defining next

$$\Gamma(J) = \text{ground-state eigenvalue of } \{\overline{H}(J)\}, \tag{4.22}$$

we have

$$-\frac{\partial \Gamma}{\partial J} = \frac{1}{\overline{L}_b}\sum_{j=-l}^{+l}\langle x_j\rangle \equiv \overline{x}(J)\,. \tag{4.23}$$

We then construct

$$\mathcal{E}(J) = \Gamma(J) + J\,\overline{x}(J) - \frac{\Delta(\overline{L}_b)}{2}\overline{x}(J)^2\,, \tag{4.24}$$

where we have obtained (4.24) from (4.19) by replacing $\langle x(J_j)\rangle$ by $\overline{x}(J)$ and using the fact that (4.16) vanishes according to (3.31), i.e.,

$$\sum_{\alpha_1, j_1'} D(j_1' - j_2' + \overline{L}_b(\alpha_1 - \alpha_2)) = 0\,. \tag{4.25}$$

$\Delta(\overline{L}_b)$ is defined by

$$\Delta(\overline{L}_b) \equiv \frac{1}{\overline{L}_b}\sum_{j_1, j_2=-l}^{+l} D(j_1 - j_2) \tag{4.26}$$

and has the important property that[14] for $\overline{L}_b \gg 1$,

$$\Delta(\overline{L}_b) \to 0 \quad \text{as} \quad 1/\overline{L}_b\,. \tag{4.27}$$

It is of crucial importance to what follows that although $\Delta(\overline{L}_b)$ decreases with increasing $\overline{L}_b$ according to (4.27), at no stage is it actually zero.

Following a procedure similar to the single-site calculation, we note that the term $(J/\overline{L}_b)\sum x_j$ is, for small J and finite $\overline{L}_b$, an analytic perturbation of $\overline{H}(J=0)$; so we expand $x(J)$ as

$$x(J) = c_1 J(1 + c_3 J^2 + c_5 J^4 + \cdots)\,.$$

Repeating the steps leading to (3.40), with $\Delta(\overline{L}_b)$ replacing $D(0)$ there, we find

$$\mathcal{E}_{\overline{L}_b}(J) = \Gamma(0) + \tfrac{1}{2}c_1[1 - c_1\Delta(\overline{L}_b)]J^2 + c_1 c_3[\tfrac{3}{4} - c_1\Delta(\overline{L}_b)]J^4 + \cdots\,. \tag{4.28}$$

Minimizing with respect to J yields [see (3.43) and (3.45) for $x_c \ll 1$,

$$x_c^2 \cong c_1^2[c_1\Delta(\overline{L}_b) - 1]/|c_3| \tag{4.29}$$

when $[c_1\Delta(\overline{L}_b) - 1] > 0$; otherwise $x_c = 0$.

Note that we would incorrectly predict tricritical behavior, as in the momentum-space calculation, if we take the limit $\overline{L}_b \to \infty$ so that $\Delta(\overline{L}_b) \to 0$ without paying attention to what happens to the product $c_1\Delta(\overline{L}_b)$. In this limit, the sign of the coefficient of J^2 in (4.28) is positive independent of λ_0 and f_0; hence for all coupling strengths, $J=0$ becomes a local minimum and we run into the tricritical problem. However, the sign of the J^2 term in $E(J)$ does, in fact, depend on the parameters λ_0 and f_0, as we found earlier in the calculation of Sec. III B for the single-site basis. Care is required in taking the $\overline{L}_b \to \infty$ limit in such a way that $c_1\Delta(\overline{L}_b)$ is held fixed. We show how to do this in detail in Appendix D by bounding the energy eigenvalue (4.28) by means of a momentum-space calculation within each of the individual blocks; that is, we use the method of Sec. III, but keep $\overline{L}_b$ finite. We find that, as Λ and $\overline{L}_b \to \infty$, we can take $\lambda_0 \to 0$ and $f_0^2 \to \infty$ in such a way that x_c is held fixed and arbitrarily small. In particular, $\lambda_0 \to 0$ as $1/\overline{L}_b$ and $f_0^2 \to \infty$ as $\ln\overline{L}_b$, so that this limiting procedure also renders $H^{\text{cut-off}}$ in (4.7) finite if we make the association of $\overline{L}_b$ with the square of the cutoff, i.e., $\overline{L}_b \propto \Lambda^2$ in (4.8) and (4.9).

As $\overline{L}_b \to \infty$ the variational energy found by this hybrid method of a block basis, and within each block a momentum basis, converges to the momentum-space answer from above. Hence as shown in Appendix D, the block basis provides us with a technique of calculating which does not produce mathematically forbidden or unphysical behavior and at the same time yields bounds on energies that are as good as those obtained from the flawed (by tricritical behavior) momentum-space calculation. Our hope, which we shall try to motivate in Sec. IV D is that a more detailed use of the block formalism will enable us to do even better for the ground-state energy.

D. Extending the applicability of the block formalism; a scaling argument

We conclude this section by formulating a procedure for systematically improving on the variational calculation for the energies of low-lying states.

The nature of our approximation in the site basis can be stated as follows: An accurate treatment of the "potential terms" involving fields at the same lattice site, viz. $\lambda_0(x_j^2 - f^2)^2$, is possible, but the gradient terms coupling different sites are approximated only crudely. In the single-site basis the correlation between different sites is retained only in the fluctuations about the average field, i.e., the term $\frac{1}{2}D(0)(\langle x^2\rangle - \langle x\rangle^2)$, plus the classical derivative term for the kink energy in (3.58). With a generalization to the block basis for studying the ground-state energy we have included the correlations between sites within the individual blocks, but not between different blocks. Evidently the block procedure improves as the block size $\overline{L}_b$ increases. It is, therefore, of interest to determine how big the effect of the gradient terms is, how the accuracy of representing them improves with increasing $\overline{L}_b$, and how large a value of $\overline{L}_b$ is needed for reasonable accuracy as a function of the parameters λ_0 and f_0^2.

Note first that when the gradient terms are totally ignored, the Hamiltonian (3.19) becomes a sum of 1-degree-of-freedom operators at each site j, and the spectrum of eigenstates at each site is identical. The eigenstates of H are then characterized by specifying the different individual levels of excitation populated at each site. Barring additional degeneracies arising for specific values of λ_0 and f^2, the first excited state will be $(2N+1)$-fold degenerate corresponding to having the excited level at any one of the lattice sites. When the gradient terms are included in H, their effect is to lift this degeneracy; they also mix these states in general with the ground state and with the more-highly-excited spectrum. It is when these gradient-induced splittings are small relative to the spacing between the single-site excited states that the site basis is expected to provide a reasonable picture of the true ground state.

This feature can be displayed simply in the exactly soluble example of the quadratic Hamiltonian with positive mass:

$$H_0 = \Lambda\left\{\sum_j\left[\frac{p_j^2}{2}+\frac{1}{2}\left(\frac{\mu^2}{\Lambda^2}+D(0)\right)x_j^2\right] + \sum_{j_1\neq j_2}\frac{(-)^{j_1-j_2}}{(j_1-j_2)^2}x_{j_1}x_{j_2}\right\}, \tag{4.30}$$

where we use dimensionless canonical variables and measure energy in units of the cutoff Λ. H_0 is completely diagonalized in the momentum basis with ground-state energy

$$E_0^{ex} = \tfrac{1}{2}\sum_k (k^2+\mu^2)^{1/2} = \frac{\Lambda^2 L}{2\pi}\int_0^\pi dx(x^2+\mu^2/\Lambda^2)^{1/2}. \tag{4.31}$$

There is a gap of mass μ to the first excited (single-particle) state, i.e.,

$$E_1^{ex} - E_0^{ex} = \mu \tag{4.32}$$

and the splittings among the excited single-particle states are expressed by

$$E_1^{ex}(n) - E_0^{ex} = \left[\mu^2+\left(\frac{2\pi n}{2N+1}\right)^2\Lambda^2\right]^{1/2}, \quad \text{with } n=0,\pm1,\ldots,\pm N. \tag{4.33}$$

The single-site variational basis as in Sec. III gives a ground-state energy

$$E_0^{\text{one-site}} = \frac{\Lambda^2 L}{2}[D(0)+\mu^2/\Lambda^2]^{1/2} \tag{4.34}$$

and a gap to the first excited state

$$E_1^{\text{one-site}} - E_0^{\text{one-site}} = [\mu^2+\Lambda^2 D(0)]^{1/2}, \tag{4.35}$$

where $D(0)=\frac{1}{3}\pi^2$ in the $N\to\infty$ limit [see (3.12)]. The site calculation gives a result for the ground-state energy and for the first gap whose accuracy is measured approximately by the ratio

$$\Lambda^2 D(0)/\mu^2. \tag{4.36}$$

The quantity $[\mu^2+\Lambda^2 D(0)]^{1/2}$ measures the gap to the mean energy of the $(2N+1)$ degenerate 1-particle excitations of (4.30) and the gradient introduces splittings among levels of order $\approx(\Lambda^2/\mu^2N^2)\mu \approx (1/\mu^2L^2)\mu$, with the total splitting being $\sim[(\mu^2+\Lambda^2)^{1/2}-\mu]$.

Clearly the single-site basis gives an accurate result when $\Lambda^2 D(0)/\mu^2 < 1$, in which case the ground-state energy is accurate to better than 3% and the gaps between higher excitations in the single-site basis are large compared with the splittings among the degenerate one-particle levels and hence are relatively unimportant. The ratio

$$R = \frac{[\text{splittings among degenerate excitations at individual sites}]}{[\text{interval between excitation energies of single-site spectrum}]} \tag{4.37}$$

is a measure of how well the gradient is approximated by the single-site basis. When $R \ll 1$, the single-site basis is expected to be a very good approximation. However, if this ratio is not small, we require a more accurate treatment of the gradient terms.

This suggests using the formalism of the block functions, and working in a momentum basis within the individual blocks. In this way we lift the degeneracy among $\bar{L}_b$ single-site levels within a block and produce more accurate upper bounds on the ground-state energy. Couplings between the different blocks are introduced via the remaining terms of the gradient operator, but these couplings will induce smaller splittings since the "typical" separation between lattice sites in two different blocks is $\bar{L}_b > 1$ and the coupling strength between them is proportional to

$$D(j-j') \sim \frac{1}{(j-j')^2} \sim \frac{1}{\bar{L}_b^2}.$$

An iterative procedure based on working with larger and larger blocks formed by combining smaller block units and including site-site coupling via the gradient terms offers the promise of

a calculable and convergent procedure for a broad range of ratios R.

Returning once again to simple exactly soluble Hamiltonian H_0 in (4.30), we can illustrate the rapid convergence to the exact energies as the block size grows. It is easy to carry out the hybrid calculation if the lattice is divided into blocks that contain two sites each, and within which we use a momentum basis. The ground-state energy becomes

$$E_0^{\text{two-site}} = \Lambda^2 L \tfrac{1}{4}\{[D(0) - D(1) + \mu^2/\Lambda^2]^{1/2} + [D(0) + D(1) + \mu^2/\Lambda^2]^{1/2}\} \quad (4.38)$$

and the gap to the first excited state is

$$E_1^{\text{two-site}} - E_0^{\text{two-site}} = \{\mu^2 + \Lambda^2[D(0) + D(1)]\}^{1/2} \approx [\mu^2 + 0.4D(0)\Lambda^2]^{1/2}. \quad (4.39)$$

Comparing with (4.35) for the one-site result, the two-site basis is seen to converge for smaller values of μ^2.

More generally, we can abstract from these observations the following scaling argument for illustrating the value of the block formalism in extending the regime of parameters over which the site basis can be applied. First, we regroup the terms in (3.19), using (3.10) and the notation of Sec. IV B, i.e., the lattice is divided into $B = 2b+1$ blocks each of length $\bar{L}_b = 2l+1$ and we carry out the sum $j = j' + \alpha \bar{L}_b$ with $\{j'\} = \{-l, l\}$ and $\{\alpha\} = \{-b, b\}$:

$$\frac{1}{\Lambda} H = \sum_{\alpha} \left(\sum_{j'} \{\tfrac{1}{2} p_{j'}^2(\alpha) + \lambda_0 [x_{j'}^2(\alpha) - f_0^2]^2\} + \tfrac{1}{2} \sum_{j_1', j_2'} D(j_1' - j_2') x_{j_1'}(\alpha) x_{j_2'}(\alpha) \right)$$
$$+ \tfrac{1}{2} \sum_{\alpha_1 \neq \alpha_2} D(\bar{L}_b(\alpha_1 - \alpha_2)) \sum_{j'} x_{j'}(\alpha_1) x_{j'}(\alpha_2) + \tfrac{1}{2} \sum_{\substack{\alpha_1 \neq \alpha_2 \\ j_1' \neq j_2'}} D(j_1' - j_2' + \bar{L}_b(\alpha_1 - \alpha_2)) x_{j_1'}(\alpha_1) x_{j_2'}(\alpha_2), \quad (4.40)$$

where we have adopted the notation $x_{j'}(\alpha) = x(j' + \alpha \bar{L}_b)$. Rescaling the fields according to the canonical transformation

$$p \to \bar{L}_b^{-1/2} p, \quad x \to \bar{L}_b^{1/2} x \quad (4.41)$$

and using (3.12) so that for $\alpha_1 \neq \alpha_2$

$$D(\bar{L}_b(\alpha_1 - \alpha_2)) = \bar{L}_b^{-2} D(\alpha_1 - \alpha_2), \quad (4.42)$$

we obtain

$$H = \frac{\Lambda}{\bar{L}_b} (\mathfrak{h}_0 + \mathfrak{v}_0), \quad (4.43)$$

where

$$\mathfrak{h}_0 = \sum_{\alpha} \left(\sum_{j'} \{\tfrac{1}{2} p_{j'}^2(\alpha) + \tfrac{1}{2} \bar{L}_b^2 [-4\lambda_0 f^2 + D(0)] x_{j'}^2(\alpha) + \bar{L}_b^3 \lambda_0 x_{j'}^4(\alpha) + \bar{L}_b \lambda_0 f^4\} + \tfrac{1}{2} \bar{L}_b^2 \sum_{j_1' \neq j_2'} D(j_1' - j_2') x_{j_1'}(\alpha_1) x_{j_2'}(\alpha_2) \right.$$
$$\left. + \tfrac{1}{2} \sum_{\alpha_1 \neq \alpha_2} D(\alpha_1 - \alpha_2) \sum_{j'} x_{j'}(\alpha_1) x_{j'}(\alpha_2), \right.$$
$$\mathfrak{v}_0 = \sum_{\substack{j_1' \neq j_2' \\ \alpha_1 \neq \alpha_2}} \left\{ \frac{(-)^{j_1 - j_2} (-)^{\bar{L}_b(\alpha_1 - \alpha_2)} \bar{L}_b^2}{[j_1' - j_2' + \bar{L}_b(\alpha_1 - \alpha_2)]^2} \right\} x_{j_1'}(\alpha_1) x_{j_2'}(\alpha_2). \quad (4.44)$$

$\mathfrak{h}_0$ in (4.44) defined a theory of an interacting $\bar{L}_b$-component field $x_{j'}$ with a large coupling constant $\lambda_0 \bar{L}_b^3$ and a mass matrix

$$M_{j_1' j_2'}^2 = \bar{L}_b^2 [D(j_1' - j_2') - 4\lambda_0 f^2 \delta_{j_1' j_2'}].$$

This mass matrix can, of course, be diagonalized by an orthogonal transformation mixing the different components of $x_{j'}(\alpha)$ only within the individual blocks α. In general, the mixing only couples a finite number of neighboring field components as $\bar{L}_b$ grows large since the long-range order in $D(j_1' - j_2')$ decreases in coupling strength as $(j_1' - j_2')^{-2}$, according to (3.12). Moreover, it is important to notice in (4.44) that the block-block interaction in $\mathfrak{h}_0$ is given by the gradient term which has no powers of $\bar{L}_b$ in it. Therefore $\mathfrak{h}_0$, for large $\bar{L}_b$, is almost local within individual blocks. Furthermore, the "potential" $\mathfrak{v}_0$ contains no powers of $\bar{L}_b$. We conjecture, therefore, a good starting point to calculate the ground-state energy for large enough $\bar{L}_b$ is in terms of $\mathfrak{h}_0$ and a trial ground state constructed in a single-site basis. As we

argued earlier, this approximation gives a good bound on the ground-state energy when $\bar{L}_b^3\lambda_0 > \bar{L}_b^2$; i.e., the potential term is greater than the gradient term. For increasing $\bar{L}_b > 1$, this allows to us enter the regime of small λ_0 with this method, so long as we satisfy $\lambda_0 > 1\sqrt{\bar{L}_b}$.

This block-basis resummation argument is similar to our block-basis calculation of Sec. IV C; in both cases, the problem is reduced essentially to an $\bar{L}_b$-degree-of-freedom Schrödinger problem. Of course, for large $\bar{L}_b$, this is still a very complicated problem to actually solve and therefore we would like to do the regrouping into blocks in stages, with each step a small and readily computable problem. At each step we group the degrees of freedom into blocks of small length (with perhaps $\bar{L}_b$ equal 2 or 3), and introduce block degrees of freedom. Within each block, we want to lift the degeneracies in the single-site problem as already discussed. Although this could be accomplished in a k basis for the exactly soluble quadratic Hamiltonian, as we illustrated, in the general strongly coupled ϕ^4 theory a more accurate treatment of the single-site problem is required. We have not carried out a detailed analysis of this general problem, but in concluding this chapter we sketch a procedure which offers the promise of *systematically* improving the ground-state description.

Let us return to (4.40) which we group now into two terms, $H = H_0 + V$, where H_0 contains the single block terms and V contains all of the block-block coupling:

$$H = H_0 + V,$$
$$H_0 = \sum_{\alpha} H_0(\alpha), \tag{4.45}$$
$$V = \sum_{\alpha_1 \neq \alpha_2} V(\alpha_1, \alpha_2).$$

This grouping differs from (4.43) and (4.44), which included some of the block-block coupling in $\mathfrak{H}_0$ as defined. Stage one of our procedure is to construct a good variational basis and accurate energy eigenvalues for the low-lying states of $H_0(\alpha)$ for a single block α. We do this by choosing a small block size containing, for example, three sites only so that $\bar{L}_b = 3$. The variational calculation is performed by expanding in an orthonormal basis

$$x_{j'}(\alpha) = \sum_n u_n(j')x_n(\alpha),$$
$$p_{j'}(\alpha) = \sum_n u_n(j')p_n(\alpha), \tag{4.46}$$

if $\bar{L}_b = 3$, $j' = -1, 0, 1$, where $x_n(\alpha)$ and $p_n(\alpha)$ are conjugate operators $[p_{n'}(\alpha), x_n(\alpha)] = -i\delta_{n,n'}$ and the basis functions satisfy

$$\sum_n u_n(j)u_n(j') = \delta_{jj'}.$$

We perform the variational calculation for the "best" $u_n(j')$ by minimizing $H_0(\alpha)$ in a trial ground state containing the first $n = 1, 2, \ldots, \sigma$ excitations in the $u_n(j')$ eigenspectrum; see Appendix B for the general formalism. The cutoff at $n_{\max} = \sigma$ depends on one's strength in solving the $\bar{L}_b$-degree-of-freedom problem defined by $H_0(\alpha)$. Having thus constructed a trial basis, we rewrite H in terms of the truncated set of $n = 1, \ldots, \sigma$ solutions $u_n(j')$ and the $2\bar{L}_b \times \sigma$ operators $x_n(\alpha)$ and $p_n(\alpha)$.

As a second stage we now form new blocks, or "super blocks," each containing again three (or more generally $\bar{L}_b$) adjacent blocks of the first-stage decomposition. The terms in the newly constructed H are again regrouped into two terms,

$$\bar{H} = \bar{H}_0 + \bar{V},$$

where

$$\bar{H}_0 \equiv \sum_{\beta} \bar{H}_0(\beta)$$

contains single super-block terms and

$$\bar{V} \equiv \sum_{\beta_1 \neq \beta_2} \bar{V}(\beta_1, \beta_2)$$

contains all of the coupling between different super blocks. The summation indices are $\alpha = \alpha' + \bar{L}_b\beta$, with $\alpha' = -1, 0, 1$ when, for example, $\bar{L}_b = 3$. The number set

$$\{\beta\} = \left\{-\frac{(2N+1)}{\bar{L}_b^2}, \frac{(2N+1)}{\bar{L}_b^2}\right\}$$

labels the different super blocks. We again expand the canonical operators as in (4.46)

$$x_n(\alpha) \equiv x_{n,\alpha'}(\beta) = \sum_m \bar{u}_m(\alpha')x_{n,m}(\beta),$$
$$p_n(\alpha) = \sum_m \bar{u}_m(\alpha')p_{n,m}(\beta),$$

if $\bar{L}_b = 3$, $\alpha' = -1, 0, 1$, and repeat the process as before. This gives a rewrite of the original H in terms of the $(2\bar{L}_b\sigma)^2$ operators $x_{n,m}(\beta)$ and $p_{n,m}(\beta)$. The process may be repeated p times until the desired super-block length $\bar{L}_b = 3^p$ is achieved. In this way, a set of fields $x_{n_1,\ldots,n_p}$ and $p_{n_1,\ldots,n_p}$ will be constructed that in principle are free of degeneracies in their frequencies and include a reasonable approximation to the nonlinear effects contained in the $\lambda_0(x_j^2 - f_0^2)^2$ potential. Beyond a point in the calculation, more traditional iterative techniques are then expected to apply following the scaling argument constructed in (4.44). This,

at least, is the hope of the authors.

As outlined in this section, we have a procedure reminiscent of the techniques described by Wilson and Kadanoff[6] for extending the region of coupling parameters for which our site-basis variational methods can be applied. What remains to be provided is its implementation and substantiation as a rapidly converging, *practical* and systematic procedure.

V. REMAINING PROBLEMS

Our primary physical motivation in developing the nonperturbative variational techniques described in this paper is to understand quark confinement in the context of a local canonical quantum field theory with strong couplings. According to the current folklore, this implies solving a non-Abelian gauge theory of interacting fermion quarks and vector mesons. We have not yet applied the techniques used in this paper to this model and therefore have no idea whether or not there occur spontaneous breakdown of continuous symmetries and low-lying coherent variational states that represent confined color singlets. From a more fundamental point of view, the nonlinear self-coupled scalar field introduced in (1.1) may be nothing more than a phenomenological crutch in terms of which to exhibit the mechanism of spontaneous symmetry breaking. The nonvanishing vacuum expectation value $\langle \phi \rangle$ may in reality be products of fermion fields, viz. $\langle \bar{\psi}\psi \rangle$ or $\langle (\bar{\psi}\gamma_\mu \psi)^2 \rangle$ in the sense described in the earlier studies of Nambu and Jona-Lasinio.[15]

We have made a *preliminary* investigation based on the variational methods of this paper of the theory of a fermion field interacting linearly with the scalar field of (1.1) in one space and one time dimension. Results achieved thus far indicate that the fermion gives up a finite fraction ($\sim \frac{1}{2}$) of its mass when confined to the potential well it forms in the scalar field configuration in the ground state. The complete canceling of mass achieved in the classical kink state does not occur when the quantum fluctuations are included. These results will be described in a subsequent paper now in preparation.

In a fundamental way, we are of course limited by the very nature of our variational approach to establishing upper bounds only on the energy values. This makes it particularly important to *know* how accurate our ground-state calculations are since we wish to identify the difference of bounds on the energies of the ground state and of the low-lying kink states as excitation energies. Fortunately for the specific ϕ^4 model studied in this paper, new methods have been found by Pearson and Blankenbecler[16] which yield lower bounds on the energy. Thus the convergence of lower and upper bounds can be studied and the accuracy of the ground-state energy assessed.

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APPENDIX A

In Sec. II we stated the results of the variational analysis of the momentum-space calculation which led to the tricritical behavior in the strong-coupling regime. Here we shall elaborate a little more on this analysis.

In Eq. (2.36) we have derived the expression for the energy density

$$4\mathcal{E}(\alpha_0, c) = \frac{1}{V}\sum_k \left[2(k^2+\alpha_0^2)^{1/2} - \frac{\alpha_0^2}{(k^2+\alpha_0^2)^{1/2}} \right] + \frac{4\lambda}{3}\bar{f}(\alpha_0)^2 + \frac{8\lambda}{3}(3c^2 - f^2)\bar{f}(\alpha_0) + 4\lambda(c^2 - f^2)^2 , \tag{A1}$$

where

$$\bar{f}(\alpha_0) = \frac{3}{2V}\left(\sum \frac{1}{(k^2+\alpha_0^2)^{1/2}} \right) . \tag{A2}$$

The variation with respect to α_0 and c gives at the extremum

$$\frac{\partial(4\mathcal{E})}{\partial\alpha_0} = \frac{2}{3}\left(\frac{\partial\bar{f}}{\partial\alpha_0}\right)[-\alpha_0^2 + 4\lambda(\bar{f} - f^2 + 3c^2)] = 0, \tag{A3}$$

$$\frac{\partial(4\mathcal{E})}{\partial c} = 16\lambda c(\bar{f} - f^2 + c^2) = 0 . \tag{A4}$$

The analysis for the maxima and minima demands knowing all of the second derivatives

$$\frac{\partial^2(4\mathcal{E})}{\partial\alpha_0^2} = \frac{2}{3}\left(\frac{\partial\bar{f}}{\partial\alpha_0}\right)\left(-2\alpha_0 + 4\lambda\frac{\partial\bar{f}}{\partial\alpha_0}\right) + \frac{2}{3}[-\alpha_0^2 + 4\lambda(\bar{f} - f^2 + 3c^2)]\frac{\partial^2\bar{f}}{\partial\alpha_0^2} , \tag{A5}$$

where by (A3) the second term vanishes,

$$\frac{\partial^2(4\mathcal{E})}{\partial c^2} = 16\lambda(\bar{f} + 3c^2 - f^2) , \tag{A6}$$

$$\frac{\partial^2(4\mathcal{E})}{\partial\alpha_0\partial c} = \frac{\partial^2(4\mathcal{E})}{\partial c\partial\alpha_0} = 16\lambda c\frac{\partial\bar{f}}{\partial\alpha_0} . \tag{A7}$$

Direct differentiation shows that $\partial\bar{f}/\partial\alpha_0$ is absolutely negative. Returning to Eqs. (A3) and (A4) we see that $c=0$ *is always a solution.* Then α_0 is determined from

$$\frac{\alpha_0^2}{4\lambda}+f^2=\bar{f}(\alpha_0),$$

which always has one positive solution (see Fig. 1). The determinant of the matrix of second derivatives at this root is

$$\det\begin{pmatrix}\frac{\partial^2(4\mathcal{G})}{\partial c^2} & \frac{\partial^2(4\mathcal{G})}{\partial\alpha\partial c}\\ \frac{\partial^2(4\mathcal{G})}{\partial c\partial\alpha} & \frac{\partial^2(4\mathcal{G})}{\partial\alpha_0^2}\end{pmatrix}=\det\begin{pmatrix}16\lambda(\bar{f}-f^2) & 0\\ 0 & \frac{2}{3}\left(\frac{\partial\bar{f}}{\partial\alpha_0}\right)\left(-2\alpha_0+4\lambda\frac{\partial\bar{f}}{\partial\alpha_0}\right)\end{pmatrix}$$

$$=\det\begin{pmatrix}\frac{2}{3}\left|\frac{\partial\bar{f}}{\partial\alpha_0}\right|\left(2\alpha_0+4\lambda\left|\frac{\partial\bar{f}}{\partial\alpha_0}\right|\right) & 0\\ 0 & 4\alpha_0^2\end{pmatrix}>0 \tag{A8}$$

Hence $c=0$ corresponds always to a local minimum. For $f^2<0$ this is the *only* solution. However for $f^2>0$ there may be another solution according to (A6)

$$c^2=f^2-\bar{f}(\alpha_0), \tag{A9}$$

$$-\frac{\alpha_0^2}{8\lambda}+f^2=\bar{f}(\alpha_0). \tag{A10}$$

Next, we can calculate the determinant of the matrix of second derivatives at this root and get the condition for it being positive:

$$\frac{\alpha_0}{4\lambda}\geq\left|\frac{\partial\bar{f}}{\partial\alpha_0}\right|. \tag{A11}$$

The equality sign holds at the point of tangency of the two curves: $-\alpha_0^2/8\lambda+f^2$ and $\bar{f}(\alpha_0)$ [see in this respect Eq. (A10) and Fig. 2(b)].

Once f^2 becomes positive enough so that Eq. (A10) has two solutions [Fig. 2(c)], the solution which satisfies Eq. (A11) corresponds to a local minimum while the other corresponds to a local maximum. As drawn in Fig. 2(c), point 2 is the local minimum and point 1 is the maximum.

APPENDIX B: HARTREE-FOCK VARIATIONAL CALCULATION

In this appendix we review the general Hartree-Fock approximation *as a variational calculation.* We use the discrete lattice notation of Sec. III, starting from the Hamiltonian

$$H=\sum_j\{\tfrac{1}{2}\pi^2(j)+\tfrac{1}{2}[\nabla\phi(j)]^2+\lambda[\phi(j)^2-f^2]^2\}. \tag{B1}$$

The degrees of freedom $\phi(j)$ and $\pi(j)$ can be expanded in terms of a complete set of eigenfunctions $\{u_n\}$ of any Schrödinger problem. In the Hartree-Fock approach the "best" Schrödinger problem is determined self-consistently as follows. We expand

$$\phi(j)=\sum_n\frac{1}{(2\alpha_nV)^{1/2}}[u_n(j)a_n+u_n^*(j)a_n^\dagger],$$

$$i\pi(j)=\sum_n\left(\frac{\alpha_n}{2V}\right)^{1/2}[u_n^*(j)a_n^\dagger-u_n(j)a_n], \tag{B2}$$

$$[a_n,a_m^\dagger]=\delta_{n,m}.$$

The u_n's form a complete orthonormal set

$$\sum_j u_n^*(j)u_m(j)=V\delta_{n,m},$$
$$\sum_n u_n(j')u_n(j)=V\delta_{jj'}. \tag{B3}$$

The variational wave function is

$$|\psi^{\text{trial}}\rangle=\exp\left[i\sum_j\pi(j)g(j)\right]|0_{\{n\}}\rangle, \tag{B4}$$

where

$$a_m|0_{\{n\}}\rangle=0$$

and

$$\langle\psi|\phi(j)|\psi\rangle=g(j).$$

α_n, g, and $\{u_n\}$ will be our variational parameters. It is now easy to compute the expectation value of the Hamiltonian in this trial state:

$$E=\langle\psi|H|\psi\rangle$$

$$=\sum_j\left\{\frac{1}{V}\sum_n\frac{u_n^*(j)u_n(j)}{4}\alpha_n+\frac{1}{V}\sum_n\frac{\nabla u_n^*(j)\nabla u_n(j)}{4\alpha_n}+\frac{3\lambda}{4}\left[\frac{1}{V}\sum_n\frac{u_n^*(j)u_n(j)}{\alpha_n}\right]^2+2\lambda[3g^2(j)-f^2]\frac{1}{V}\sum_n\frac{u_n^*(j)u_n(j)}{2\alpha_n}\right.$$

$$\left.+\tfrac{1}{2}[\nabla g(j)]^2+\lambda(g^2-f^2)^2\right\}. \tag{B5}$$

Variation with respect to the α_n's and g gives

$$\sum_j u_n^*(j)[-\alpha_n{}^2-\nabla^2+4\lambda(\bar{f}-f^2+3g^2)]u_n(j)=0, \tag{B6}$$

$$[-\nabla^2+4\lambda(\bar{f}-f^2+g^2)]g(j)=0, \tag{B7}$$

where

$$\bar{f}\equiv\frac{3}{2}\left(\frac{1}{V}\sum_n\frac{u_n^*(j)u_n(j)}{\alpha_n}\right). \tag{B7'}$$

The variation with respect to the basis functions $\{u_n\}$ has to be done a little more carefully due to the orthonormality of the u_n's [Eq. (B3)]. It is therefore necessary to introduce Lagrange multipliers when varying over the u_n's in

$$\langle\psi|H|\psi\rangle-\sum_{n,m}\mathcal{E}_{n,m}u_n^*(j)u_m(j), \tag{B8}$$

obtaining

$$\sum_m(\alpha_n{}^2\delta_{nm}-4\alpha_n\mathcal{E}_{n,m})u_m(j)=[\nabla^2-4\lambda(\bar{f}-f^2+3g^2)]u_n(j). \tag{B9}$$

Multiplying Eq. (B9) by $u_n^*(j)$ and summing over j we get [using Eq. (B6)]

$$\alpha_n{}^2-4\alpha_n\mathcal{E}_{n,n}=-\alpha_n{}^2,$$
$$\mathcal{E}_{n,n}=\tfrac{1}{2}\alpha_n. \tag{B10}$$

The set of equations (B6) through (B10) is clearly very complicated. We can simplify the equations somewhat by looking at a particular set of solutions which are obtained if we specialize Eq. (B6) to

$$[-\alpha_n{}^2-\nabla^2+4\lambda(\bar{f}-f^2+3g^2)]u_n(j)=0. \tag{B11}$$

Clearly any solution to this equation is also a solution to Eq. (B6). Using this equation in Eq. (B9) we obtain

$$\mathcal{E}_{n,m}=\tfrac{1}{2}\alpha_n\delta_{n,m}. \tag{B12}$$

Therefore Eq. (B11) is consistent with Eq. (B9). Equations (B7) and (B11) give a set of self-consistent coupled eigenvalue equations. The solution can be, in principle, obtained by an iterative process. Starting with a given $\bar{f}(j)$ we can solve Eq. (B7) for $g(j)$ and then Eq. (B11) for the u_n's and α_n's which enable us to construct a new $\bar{f}(j)$ [Eq. (B7')]. Using these equations in the expression for the energy [Eq. (B5)] we find

$$\mathcal{E}=\frac{E}{V}=\mathcal{E}_{\text{class}}+\sum_n\tfrac{1}{2}\alpha_n+\frac{3\lambda}{4}\frac{1}{V}\sum_j\left(\frac{1}{V}\sum_n\frac{u_n^*(j)u_n(j)}{\alpha_n}\right)^2, \tag{B13}$$

where

$$\mathcal{E}_{\text{class}}=\frac{1}{V}\sum_j\{\tfrac{1}{2}[\nabla g(j)]^2+\lambda[g^2(j)-f^2]^2\}. \tag{B14}$$

For $\bar{f}=0$ the set of equations reduces to the Dashen, Hasslacher, and Neveu equations. Since $\bar{f}$ arises from the two-loop normal-ordering contribution, setting $\bar{f}$ to zero leaves us with the one-loop approximation. It is important to note that including the simple normal-ordering two-loop contribution yields an upper bound on the energy. Note also that the one-loop approximation $\bar{f}=0$ is not a good starting point for iterations. It is well known that owing to translation invariance Eq. (B11) with $\bar{f}=0$ and $g=f\tanh(2\lambda)^{1/2}f(x-x_0)$ [which is a solution of Eq. (B7) for $\bar{f}=0$] always has a zero eigenvalue $\alpha_0=0$ which in turn will make the new $\bar{f}$ [Eq. (B7')] divergent.

The momentum-space calculation in Sec. II is a particular solution to the Hartree-Fock set of equations for constant g and $\bar{f}$.

APPENDIX C: A SIMPLE VARIATIONAL CALCULATION

In this appendix we present the details of a calculation for variationally minimizing $E_0(\psi)$ in (3.32) using the trial state

$$|\psi\rangle=e^{-ipc}|0_\alpha\rangle, \tag{C1}$$

where $|0_\alpha\rangle$ satisfies (3.26), with α a variational parameter. Instead of introducing a Lagrange multiplier, the constant displacement c is introduced as a variational parameter:

$$\langle\psi|H|\psi\rangle\equiv E(\alpha,c)$$
$$=(V\Lambda)\left\{\frac{\alpha}{4}+\lambda_0\left[\frac{3}{4\alpha^2}+\frac{2(3c^2-f_0{}^2)}{2\alpha}+(c^2-f_0{}^2)^2\right]+\frac{D(0)}{4\alpha}\right\}. \tag{C2}$$

To minimize $E(\alpha, c)$ with respect to the variational parameters α and c we must solve the equations

$$\frac{\partial E}{\partial \alpha} = 0 = \frac{1}{4} - \lambda_0\left(\frac{3}{2\alpha^3} + \frac{3c^2 - f_0^2}{\alpha^2}\right) - \frac{D(0)}{4\alpha^2} \tag{C3}$$

and

$$\frac{\partial E}{\partial c} = 0 = 4c\lambda_0\left[\frac{3}{2\alpha} + (c^2 - f_0^2)\right]. \tag{C4}$$

According to (C4) the extrema are either at $c = 0$ or $c^2 = f_0^2 - 3/2\alpha$.

Case 1: $c = 0$. Substituting $c = 0$ into (C3) yields

$$\frac{\alpha^2 - D(0)}{4\lambda_0} + f_0^2 = \frac{3}{2\alpha}, \tag{C5}$$

which has a unique solution. In order to determine whether this is a local maximum, minimum, or saddle point, one must take the matrix of second derivatives and evaluate it at $c = 0$. Straightforward computation yields

$$\left.\frac{\partial^2 E}{\partial \alpha^2}\right|_{c=0} = \frac{2}{\alpha^3}\left[\frac{D(0)}{4} + \lambda_0\left(\frac{3}{2\alpha} - f_0^2\right)\right] + \frac{1}{\alpha^2}\left(\frac{3\lambda_0}{2\alpha^2}\right), \tag{C6}$$

which by (C5) is just

$$\left.\frac{\partial^2 E}{\partial \alpha^2}\right|_{c=0} = \frac{1}{2\alpha} + \frac{3\lambda}{2\alpha^4} > 0 \tag{C7}$$

In addition, one finds

$$\left.\frac{\partial^2 E}{\partial c \partial \alpha}\right|_{c=0} = \left.\frac{\partial^2 E}{\partial \alpha \partial c}\right|_{c=0} = 0 \tag{C8}$$

and

$$\left.\frac{\partial^2 E}{\partial c^2}\right|_{c=0} = 4\lambda\left(\frac{3}{2\alpha_0} - f_0^2\right) = [\alpha_0^2 - D(0)], \tag{C9}$$

where α_0 is the solution to (C5). Hence, if $\alpha_0^2 - D(0)$ is greater than zero the root at $c = 0$ is a local minimum; otherwise, it is a saddle point. Referring to the discussion of (3.51), where the identical equation arises in our discussion in terms of Lagrange multipliers, we see that $c = 0$ is a local minimum only when

$$f_0^2 < f_{cr}^2 = \frac{3}{2[D(0)]^{1/2}}. \tag{C10}$$

Hence, as discussed in the text the term $D(0)$ eliminates the problem of a local minimum occurring at $c = 0$ for $f_0^2 > f_{cr}^2$.

Case 2: $c^2 = f_0^2 - 3/2\alpha$. In this event direct substitution into (C3) yields

$$\frac{-\alpha^2 + D(0)}{8\lambda_0} + f_0^2 = \frac{3}{2\alpha}, \tag{C11}$$

which can have either two, one, or zero solutions depending upon the values of f_0^2 and λ_0. If f_0^2 is large enough, for fixed λ_0, (C11) has two solutions corresponding to the two intercepts in Fig. 2(c). In order to determine which of these is a local minimum, we take the matrix of second derivatives, finding that

$$\frac{\alpha}{4\lambda_0} \geq \frac{3}{2\alpha^2} \tag{C12}$$

is the condition for a local minimum. Graphically it is easy to convince oneself that only the root corresponding to the larger value of α is a local minimum.

We next want to determine whether this root can move smoothly toward $c^2 = 0$ when $f_0^2 \to f_{cr}^2$ so as to guarantee that the $c = 0$ root is not a minimum until $f_0^2 = f_{cr}^2$. Returning to Eq. (C12) it is easy to find the two roots in the two limits $\lambda \to \infty$ and $\lambda_0 \to 0$:

$$\begin{aligned} &\lambda_0 \to \infty: \quad \alpha_1^2 \approx 8\lambda_0 f_0^2, \quad \alpha_2 \approx \frac{3}{2f_0^2}; \\ &\lambda_0 \to 0: \quad \alpha_1 \approx D^{1/2}(0), \quad \alpha_2 \approx \frac{12\lambda_0}{D(0)}. \end{aligned} \tag{C13}$$

We are interested in α_1 which is the larger root corresponding to a local minimun. When $\lambda_0 \to \infty$,

$$c^2 = f_0^2 - \frac{3}{2\alpha_1} \to f_0^2,$$

while for $\lambda_0 \to 0$,

$$c^2 = f_0^2 - \frac{3}{2\alpha_1} \approx f_0^2 - \frac{3}{2D^{1/2}(0)} \xrightarrow[f_0^2 \to f_{cr}^2]{} 0.$$

There exists, therefore, a critical value λ_{cr} such that the $c \neq 0$ minimum obtained from the root α_1 moves smoothly toward zero for $f_0^2 \to f_{cr}^2$ so long as $\lambda_0 < \lambda_{cr}$. Since f_0^2 approaches f_{cr}^2 from above we already know that the $c = 0$ solution does not correspond to a minimum. Hence there is no tricritical behavior. It is easy to check that $\alpha = D^{1/2}$ and $f_0^2 = f_{cr}^2$ is always a solution of (C13). Substituting this solution in the minimum condition (C12) we observe that this solution corresponds to the local minimum moving smoothly toward zero only for

$$\lambda_0 \leq \lambda_{cr} = \frac{\alpha^3}{6} = \frac{D^{3/2}(0)}{6} < 1.$$

This is the same condition encountered in the

analysis of Sec. III. We have remarked there that we can relax this condition by allowing configuration mixing instead of using just a simple Gaussian.

If we drop the term proportional to $D(0)$ in (3.32) and in the development following Eq. (C2), we recognize that the problem being solved is simply that of the Schrödinger equation for the anharmonic oscillator. The familiar properties of the solution to that problem in both the weak- and strong-coupling limits can be traced simply in the above discussion, setting $D(0)=0$ everywhere.[17]

APPENDIX D: MOMENTUM BLOCK CALCULATION

In this appendix we give a simple variational block calculation of the ground-state energy where we use the momentum-space basis within the block itself. The block wave-function variation formalism described in Sec. IV leads to a Schrödinger problem as in (4.21) with a finite number of degrees of freedom:

$$\bar{H}(J)=\frac{1}{L_b}\left\{\sum_{j=-l}^{+l}\left[\tfrac{1}{2}p_j^2+\lambda_0(x_j^2-f_0^2)^2-Jx_j\right]+\tfrac{1}{2}\sum_{j_1 j_2}D(j_1-j_2)x_{j_1}x_{j_2}\right\}. \tag{D1}$$

$\Gamma(J)$ is defined as the lowest eigenvalue of $\bar{H}(J)$, and we shall determine an upper bound on $\Gamma(J)$ variationally by calculating in the momentum basis. An upper bound on the ground-state energy will then be found as in (4.24) by minimizing

$$\epsilon(J)=\Gamma(J)+J\bar{x}-\tfrac{1}{2}\Delta(\bar{L}_b)\bar{x}^2 \tag{D2}$$

with respect to the Lagrange multiplier J. The discrete set of allowed momenta within one block is

$$\{k\}=\left\{\frac{2\pi}{\bar{L}_b}j\right\},\quad -l\leq j\leq l. \tag{D3}$$

Next we introduce creation and annihilation operators through the Fourier expansion

$$\begin{aligned}x_j&=\sum_k e^{ikj}x_k\\&=\sum_k e^{ikj}\frac{1}{(2\omega_k\bar{L}_b)^{1/2}}(a_{-k}+a_k^\dagger),\\p_j&=i\sum_k e^{ikj}p_k\\&=\sum_k e^{ikj}p_k\left(\frac{\omega_k}{\bar{L}_b}\right)^{1/2}(a_{-k}-a_k^\dagger)\end{aligned} \tag{D4}$$

and the state $|0\rangle=\prod_k|0(k)\rangle$, where

$$a_k|0\rangle=0. \tag{D5}$$

For each fixed value J our variational wave function will be

$$|\psi^{\text{trial}}\rangle=e^{-i\pi(0)\bar{L}_b c}|0\rangle,$$

where the ω_k's and $c=\langle x\rangle$ are the variational parameters.

Using the notation

$$\begin{aligned}&\Gamma(\omega_k,c)=\langle\psi^{\text{trial}}|H(J)|\psi^{\text{trial}}\rangle,\\&x^2(k)=\sum_{j_1\neq j_2}\frac{2(-)^{j_1-j_2}}{(j_1-j_2)^2}e^{ik(j_1-j_2)},\\&\Delta=D(0),\\&\bar{f}=\frac{3}{2\bar{L}_b}\sum_k\frac{1}{\omega_k},\end{aligned} \tag{D6}$$

we calculate

$$\begin{aligned}\Gamma(\omega_k,c)&=\lambda(c^2-f^2)^2+\frac{\Delta(\bar{L}_b)}{2}c^2-Jc+\frac{1}{\bar{L}_b}\sum_k\left[\frac{\omega_k}{4}+\frac{4\lambda(3c^2-f^2)+\Delta}{4\omega_k}\right]+\frac{3\lambda}{4}\left(\frac{1}{L_b}\sum\frac{1}{\omega_k}\right)^2\\&\quad+\frac{1}{\bar{L}_b}\sum_k\left[\frac{1}{\bar{L}_b}\sum_{j_1\neq j_2}\frac{(-)^{j_1-j_2}}{(j_1-j_2)^2}e^{ik(j_1-j_2)}\right]\frac{1}{4\omega_k}\\&=\lambda_0(c^2-f^2)^2+\frac{\Delta(\bar{L}_b)}{2}c^2-Jc+\frac{1}{\bar{L}_b}\sum_k\left[\frac{\omega_k}{4}+\frac{4\lambda(3c^2-f^2)+\Delta}{4\omega_k}\right]+\frac{\lambda}{3}\bar{f}(\omega_k)^2+\frac{1}{L_b}\sum_k\left[\frac{x^2(k)}{4\omega_k}\right].\end{aligned} \tag{D7}$$

Varying with respect to ω_k and determining the extremum $\partial\Gamma/\partial\omega_k=0$ leads to

$$\omega_k^2=x^2(k)+\Delta+4\lambda(3c^2-f^2+\bar{f}). \tag{D8}$$

Defining $\bar{\omega}\equiv\omega(k=0)$ we get therefore

$$\omega_k^2=[x^2(k)-x^2(0)]+\bar{\omega}^2, \tag{D9}$$

where $\bar{\omega}$ satisfy the integral equation

$$\begin{aligned}\frac{\bar{\omega}^2-\Delta(\bar{L}_b)}{4\lambda_0}+f^2-3c^2&=\bar{f}(\bar{\omega})\\&\equiv\frac{3}{2\bar{L}_b}\sum_k\frac{1}{\{[x^2(k)-x^2(0)]+\bar{\omega}^2\}^{1/2}}\end{aligned} \tag{D10}$$

where we have used the fact that $x^2(0)+\Delta=\Delta(\bar{L}_b)$.

Varying with respect to c implies at the extremum $\partial\Gamma/\partial c=0$,

$$4\lambda_0 c\left[c^2 - f^2 + \bar{f}(\bar{\omega}) + \frac{\Delta(\bar{L}_b)}{4\lambda}\right] = J. \tag{D11}$$

Equations (D9) and (D10) are analogous to Eqs. (2.30) and (2.31) in the pure momentum calculation and Eqs. (C3) and (C4) in the single-site calculation. For $J=0$, $c_{J=0} = \langle x \rangle_{J=0} = 0$ due to the symmetry of the Hamiltonian. For small J we can follow the steps in the single-site calculation and expand

$$\begin{aligned} c(J) &= c_1 J(1 + c_2 J^2 + \cdots), \\ \bar{\omega}(J) &= \omega_0(1 + \omega_2 J^2 + \cdots). \end{aligned} \tag{D12}$$

Substituting these expansions into Eqs. (D10) and (D11) and equating coefficient of the same powers of J, we find

$$\begin{aligned} c_1 &= \frac{1}{\omega_0^2}, \\ c_3 &= \frac{2\lambda_0}{\omega_0^6}\left[\frac{\frac{4\lambda_0}{\omega_0}\left|\frac{\partial \bar{f}}{\partial \omega}\right|_{\omega_0} - 1}{\frac{4\lambda_0}{\omega_0}\left|\frac{\partial \bar{f}}{\partial \omega}\right|_{\omega_0} + 2}\right], \end{aligned} \tag{D13}$$

where ω_0 satisfies Eq. (D10) with $J=0$ and $c=0$:

$$\frac{\omega_0^2 - \Delta(\bar{L}_b)}{4\lambda_0} + f^2 = \bar{f}(\omega_0). \tag{D14}$$

In order for the ground-state energy to have a minimum at small J different from zero, the coefficient of the J^2 term in the expansion of (D2) must be small and negative. Recalling Eqs. (D2) and (D12)

$$\begin{aligned} \mathcal{E}(J) = \Gamma(0) &+ \tfrac{1}{2}c_1[1 - \Delta(\bar{L}_b)c_1]J^2 \\ &+ c_1 c_3[\tfrac{3}{4} - \Delta(\bar{L}_b)c_1]J^4 + \cdots, \end{aligned} \tag{D15}$$

this condition requires

$$\epsilon \equiv -1 + \Delta(\bar{L}_b)c_1 > 0 \tag{D16}$$

Using Eqs. (D13) and (D14), we obtain

$$\epsilon = \frac{4\lambda_0}{\omega_0^2}[f^2 - \bar{f}(\omega_0)]. \tag{D17}$$

The minimization of $\mathcal{E}(J)$ with respect to J for $\epsilon > 0$ and $c_3 < 0$ gives the critical value J_c and therefore the expectation value of the field in the ground state,

$$\begin{aligned} c(J_c) \equiv \langle x_c \rangle &= \frac{\epsilon c_1^2}{|c_3|} \\ &= [f^2 - \bar{f}(\omega_0)]\left|\frac{2 + \frac{4\lambda_0}{\omega_0}\left|\frac{\partial \bar{f}}{\partial \omega}\right|_{\omega_0}}{\frac{4\lambda_0}{\omega_0}\left|\frac{\partial \bar{f}}{\partial \omega}\right|_{\omega_0} - 1}\right|. \end{aligned} \tag{D18}$$

In order for c_3 to be negative

$$\frac{4\lambda_0}{\omega_0}\left|\frac{\partial \bar{f}}{\partial \omega}\right|_{\omega_0} < 1 \tag{D19}$$

while, from (D14) and (D17) we see that $\epsilon \ll 1$ if either

$$\frac{\lambda_0}{\omega_0^2} \approx \frac{\lambda_0}{\Delta(\bar{L}_b)} \ll 1 \quad \text{or} \quad f^2 \approx \bar{f}(\omega_0 = \Delta^{1/2}(\bar{L}_b))$$

For large $\bar{L}_b$ we can approximate

$$\frac{1}{\bar{L}_b}\sum_k \frac{1}{\omega_k} = \frac{1}{2\pi}\int_{-\pi}^{\pi} dk \frac{1}{(k^2 + \omega_0^2)^{1/2}} + O\left(\frac{1}{\bar{L}_b}\right), \tag{D20}$$

$$x^2(k) - x^2(0) = k^2 + O\left(\frac{1}{\bar{L}_b}\right), \tag{D21}$$

$$\bar{f}(\omega_0) \approx \frac{3}{2\pi}\ln\left[\frac{\pi}{\omega_0} + \left(1 + \frac{\pi^2}{\omega_0^2}\right)^{1/2}\right], \tag{D22}$$

$$\begin{aligned} \frac{1}{\omega_0}\left|\frac{\partial \bar{f}}{\partial \omega}\right|_{\omega_0} &\approx \frac{3}{2\omega_0^2(\pi^2 + \omega_0^2)^{1/2}} \\ &\approx \frac{3}{2\pi\omega_0^2} \\ &\approx \frac{3}{2\pi\Delta(\bar{L}_b)}. \end{aligned} \tag{D23}$$

Substituting Eq. (D23) into Eq. (D19) yields

$$\lambda < \frac{\pi}{6}\Delta(\bar{L}_b) \tag{D24}$$

while the substitution into Eq. (D18) gives

$$c(J_c) \equiv \langle x_c \rangle = [f^2 - \bar{f}(\Delta^{1/2}(\bar{L}_b))]\left|\frac{2 + (6/\pi)r}{(6/\pi)r - 1}\right|, \tag{D25}$$

where

$$r \equiv \frac{\lambda}{\Delta(\bar{L}_b)}.$$

Note that for $f^2 - \bar{f}(\Delta^{1/2}(\bar{L}_b))$ and r held fixed, $\langle x_c \rangle$ is constant. Of course as $\bar{L}_b \to \infty$ this means

$$\begin{aligned} &\lambda \sim \frac{1}{\bar{L}_b} \to 0 \quad \left[\text{recall} \Delta(L) \sim \frac{1}{L}\right], \\ &f^2 \sim \bar{f}(\Delta^{1/2}(\bar{L}_b)) \\ &\quad \sim \ln\left[\left(\frac{1}{\bar{L}_b}\right)^{-1/2}\right] \to \infty. \end{aligned}$$

This is precisely what is needed to define a finite Hamiltonian in the renormalization limit (see the first part of Sec. IV for details).

It is easy to be convinced that in the limit $\bar{L}_b \to \infty$, $\Gamma(0)$ converges to the momentum-basis energy density [Eq. (2.36)] for the case $\langle x \rangle = 0$. Therefore, keeping r fixed and small, in accordance

with Eq. (D25), so that the continuum momentum case is guaranteed to have its minimum at $\langle x \rangle = 0$, the energy converges (from above) in the limit $\bar{L}_b \to \infty$ to the momentum-space result. Since r and $f^2 - \bar{f}(\Delta^{1/2}(\bar{L}_b))$ are held fixed, we get the momentum-space result still having $\langle x_c \rangle \neq 0$, namely, without encountering any unphysical tricritical behavior.

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[9]If we adopt the usual definition of the gradient given in (3.7), we have $D_{p=1}(j) = 2\delta_{j1,0} - \delta_{j1,1} - \delta_{j1,-1}$, and all of our results follow through unchanged except for numerical coefficients.

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[11]Using the extension field $\phi(x)$ [see Eq. (3.21)] and constructing the usual operators $\theta_{\mu\nu}(x_1 t)$ and $M_{\nu\lambda}(x_1 t)$, one can also study the interesting questions of how large the corrections are to Lorentz invariance for large cutoff mass Λ and how Poincaré invariance is achieved in the $\Lambda \to \infty$ limit of the lattice theory. One can also study the time dependence of the "charges" associated with these operators for the system in specific physical states. For free field theory, this analysis is straightforward and one finds that lattice corrections are measured by the ratio of the momentum of the state relative to Λ. Hence Lorentz invariance is essentially preserved as long as we are dealing with states with low-enough momentum, i.e., states which do not resolve the lattice. Moreover, in the limit $\Lambda \to \infty$, the generators of "boosts" and "rotations" converge to conserved operators in the weak sense.

[12]Equation (3.35) is also true when the state $|\psi_0\rangle$ is determined by a variational calculation, $\langle H(J) \rangle \equiv \langle \psi_0(\alpha_n) | H(J) | \psi_0(\alpha_n) \rangle$, with the α_n's determined as a function of J from $\partial \langle H(J) \rangle / \partial \alpha_n = 0$.

[13]Note that for the computer calculation $f^2 \sim 0.64$ while the analytic calculation gives $f_{cr}^2 \sim 0.83$. However, the analytic calculation is done for $\lambda_0 < 1$ while $\lambda_0 = 3$ in the computer calculation (which allows for configuration mixing of up to the first fifty levels, although no more than the first 10 were required for one part in 10^4 accuracy).

[14]In fact, one can construct an upper bound of

$$\Delta(\bar{L}_b) < \frac{8 \ln 2}{\bar{L}_b} \quad \text{for } \bar{L}_b \gg 1.$$

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