Lanczos calculation of the spectrum of Hamiltonian lattice gauge theory

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(Received 17 August 1987)

The use of a generalized Lanczos technique for the accurate diagonalization of lattice-gauge-theory Hamiltonians is explored. The starting ansatz wave function is a Gaussian one which solves the theory exactly in the weak-coupling limit. Results are given for compact U(1) lattice gauge theory in $3+1$ dimensions, on 4^3 and 6^3 spatial lattices, and for a range of couplings in the continuum region. With 8 Lanczos states the precision for ground-state energies obtained ranges (depending on lattice size and coupling) from 1 part in 10^6 to 1 part in 10^8.

I. INTRODUCTION

Variational methods have long found a wide range of applications in a variety of areas of quantum physics, especially atomic and nuclear physics. More recently, a spate of publications[1] attest to the increasing interest in applying these methods to nonperturbative issues in quantum field theory. Another powerful technique which has been found to be useful in studying field theories is the Lanczos algorithm[2] for diagonalizing complicated eigensystems. In fact, the variational and Lanczos methods are intimately related—they can both be regarded as techniques for searching a subspace of the full quantum state space for the "closest" state to some desired exact eigenstate of the Hamiltonian. As we shall see below, the advantage of the Lanczos algorithm (suitably generalized) is simply that it is completely systematic: at zeroth order it coincides with the usual variational technique, but, when carried to higher order, the resulting spectral estimates are rigorously known to converge to the exact eigenvalues.

The Lanczos method has been successfully applied to various two-dimensional field theories, such as the O(3) σ model[3] and the Gross-Neveu model;[4] sufficient accuracy was attained in the computation of the spectra of the corresponding lattice Hamiltonians to demonstrate clearly the perturbative scaling of the mass gap in the continuum region of the theory. In all cases it is crucial to choose a starting ansatz for the ground-state wave function which is qualitatively correct in the continuum region of coupling. Such a choice is not particularly problematic for the two-dimensional theories mentioned above, but for four-dimensional gauge theory the choice of an exponential single-plaquette ansatz (p labels plaquettes)

$$\psi_0=\exp\left[\lambda\sum_p \mathrm{tr}(U_p)\right]|0\rangle \tag{1.1}$$

(where $|0\rangle$ is the strong-coupling vacuum), which would naturally generalize the ansatz used in Refs. 3 and 4, leads to difficulties. Technically, the matrix elements of typical operators with ψ_0 lead in $3+1$ dimensions to integrals which cannot be evaluated analytically. Moreover, even in $2+1$ dimensions (where the integrals may be evaluated in terms of Mathieu functions) the convergence based on any single-plaquette functional is too sluggish to be useful.[3] In this paper we show that a Gaussian ansatz, which exactly solves the lattice gauge Hamiltonian in the extreme weak-coupling region, leads to rapid convergence of the Lanczos eigenvalues in a range of weak to moderate coupling. Such an ansatz necessarily contains long-range plaquette-plaquette interactions (albeit of Coulomb type). But, as we shall see, the Lanczos algorithm builds in systematically all the relevant nonperturbative physics.

Our results are presented as follows. In Sec. II we give a brief, but essentially self-contained, review of the Lanczos procedure as we wish to apply it here. In Sec. III we discuss the problem of boundary conditions and nongauge-removable zero modes, which leads to some technical difficulties in the evaluation of matrix elements in the weak-coupling limit. Section IV describes the derivation of the weak-coupling ansatz. Finally, in Sec. V we explain how the Lanczos basis states are obtained and matrix elements evaluated, and give the results for compact $3+1$ U(1) lattice gauge theory. In particular, we show that at least six-place accuracy in the ground-state energy of a 6^3 lattice is obtainable over a range of couplings in the continuum region using only eight Lanczos basis states. Calculations for non-Abelian gauge theories are in progress.

II. REVIEW OF THE LANCZOS PROCEDURE

The Lanczos procedure[2] is often regarded as a technique for tridiagonalizing a large eigensystem. From our point of view, however, the procedure can provide (when suitably generalized) a rapidly convergent series of approximants to the spectrum of a complicated Hamiltonian in terms of a fairly small subspace of the full state space, so that the problems implicit in the diagonalization of very large eigensystems simply do not arise. The crucial precondition for the success of this approach is the choice of a physically appropriate ansatz as an approximate lowest-energy state in each sector of given conserved quantum numbers.

The basic idea of the Lanczos approach is simply stated: if $|\psi_0\rangle$ is any approximate trial state with a

nonzero overlap with the exact ground state $|\psi_{gs}\rangle$ of a Hamiltonian H (bounded below), then the states

$$|\psi_n\rangle \equiv H^n |\psi_0\rangle , \quad n=0,1,\ldots \tag{2.1}$$

span a subspace containing $|\psi_{gs}\rangle$, so that if

$$E_n \equiv \min_{|\psi\rangle=\sum_{i=0}^{n} c_i |\psi_i\rangle} \langle\psi|H|\psi\rangle , \tag{2.2}$$

the E_n converge monotonically to the exact ground-state energy E_{gs} from above. After much experimentation with a variety of quantum-mechanical and field-theory models, the following general features emerge.

(a) The Lanczos procedure can be tuned by including one or more variational parameters λ in $|\psi_0\rangle$. In fact, the choice of λ is crucial for rapid convergence. Use of a strong-coupling wave function in the weak-coupling region, for example, leads to disastrously slow convergence.[3] It should also be noted that the optimal values of λ may change considerably in higher order.

(b) In field theory especially, it is important[3,4] to further tune the Lanczos procedure by "dissecting" the states $H^n|\psi_0\rangle$ to obtain a larger list of basis states. This is done by treating each independent structure arising after the application of H as a new basis state provided it is separately compatible with the invariance (translation, rotational, gauge, etc.) of the system.

How may we apply this approach to a lattice gauge Hamiltonian in the weak-coupling region appropriate for the continuum limit? Here we are dealing with a Hamiltonian of the form [for U(N) theory]

$$H=K+\frac{1}{2g^2}\sum_p [N-\mathrm{tr}(U_p)] , \tag{2.3}$$

where the form of the kinetic energy K is not relevant for the present discussion. Evidently, for $g\to 0$, the potential energy forces the plaquette variable $U_p\to 1$ for all plaquettes p. After full gauge fixing (see Sec. IV for a potential trap here) this will imply that the link angles θ_l^α (l labels links, α group generators) appearing in each link variable $U_l=\exp(it_\alpha\theta_l^\alpha)$ are also forced to zero so that effectively H becomes harmonic. So we should expect that a suitable starting point for the Lanczos procedure in the weak-coupling region is to pick for $|\psi_0\rangle$ the exact ground state of the quadratic Hamiltonian obtained by taking the small-angle limit in (2.3). (A variational extension of this ansatz will be introduced in Sec. V.)

It should be strongly emphasized that although the proposed zeroth-order wave function $|\psi_0\rangle$ is just the one which we would use as the starting point of a Rayleigh-Schrödinger perturbation calculation, there is a profound difference in the two approaches. Anharmonic terms in the full Hamiltonian render weak-coupling perturbation theory divergent, whereas the Lanczos calculation always yields a monotone, rigorously convergent sequence of approximants to the exact spectrum. The *ingredients* of both Rayleigh-Schrödinger and Lanczos computations are similar: matrix elements of powers of the (kinetic and potential parts of the) Hamiltonian, but the resulting estimates lead in the former case to a divergent sequence of numbers. In the case of QCD, weak-coupling asymptotic expansions of the sort yielded by the Rayleigh-Schrödinger theory are useless as the low-energy spectrum is determined by self-consistent gap equations in which the effective coupling is driven to order unity in the physically important momentum regions (there is no external large mass to fix the effective coupling at a reasonably small value, as would be the case in toponium spectrum calculations, say). The calculation of the hadron spectrum in QCD requires a rigorously convergent, not merely asymptotic, expansion technique.

We close this section by giving a simple but striking illustration of the point raised in the last paragraph. Consider a one-dimensional anharmonic oscillator specified by the Hamiltonian

$$H=-\frac{1}{2}\frac{d^2}{dx^2}+\frac{1}{2}x^2+gx^4 . \tag{2.4}$$

We shall take $g=0.1$, moderately weak coupling, and compare the results of the Rayleigh-Schrödinger and Lanczos calculations up to ninth order. In both cases, the starting point is the weak-coupling Gaussian ansatz

$$\psi_0(x)=e^{-x^2/2} . \tag{2.5}$$

The results are presented in Table I. It is evident that whereas the Rayleigh-Schrödinger values oscillate around the correct result for a few orders (giving us a result correct to at most two significant digits) before diverging badly, the Lanczos numbers converge steadily, with geometrical increase of accuracy with order. After nine orders the ground-state energy is given to five significant digits. With an optimized coefficient in the Gaussian ansatz [see (5.15)], the Lanczos convergence is to eight digits after only six orders.

To summarize, the Lanczos approach allows us to circumvent neatly many well-known difficulties[5] arising in the reconstruction of the full nonperturbative information available in lattice Feynman diagrams. To the extent that we can compute sufficiently far in the algorithm, all of the nonperturbative information is automatically inserted. There is no need, for example, to carry out an explicit Borel resummation procedure (even if such a procedure were justified).

TABLE I. Comparison of Rayleigh-Schrödinger and Lanczos spectral convergence for an anharmonic oscillator.

Order	Rayleigh-Schrödinger	Lanczos ($\lambda=1.0$)	Optimized Lanczos ($\lambda=2.0$)
1	0.575	0.575	0.643 750 00
2	0.548 75	0.562 968 8	0.566 007 19
3	0.570 39	0.560 620 5	0.559 605 50
4	0.544 76	0.559 802 1	0.559 172 16
5	0.583 12	0.559 459 1	0.559 147 61
6	0.514 48	0.559 304 0	0.559 146 39
7	0.656 83	0.559 229 9	0.559 146 33
8	0.321 50	0.559 192 8	0.559 146 33
9	1.206 23	0.559 173 2	0.559 146 33

III. BOUNDARY CONDITIONS AND ZERO MODES

In this section we shall discuss the significance of an appropriate choice of boundary conditions on the spatial lattice of a Hamiltonian gauge theory in relation to the analytic calculation of matrix elements. As we shall see, zero modes present an obstacle for the evaluation of these matrix elements in the weak-coupling region—a removable obstacle in the event that all zero modes represent gauge degrees of freedom. However, it turns out that with some choices of boundary conditions on the gauge-link fields, not all zero modes may be removed simply by a choice of gauge, and we are forced to alter the physics of the model—albeit to a degree which should be ignorable in the continuum limit of many degrees of freedom.

The basic difficulty is illustrated by noting that we shall be dealing with a wave function of Gaussian form [l labels links, θ_l link angles in a U(1) gauge theory[6]]

$$\psi(\theta_l)=\exp\left[-\frac{1}{2g^2}\theta_l M_{ll'}\theta_{l'}\right], \tag{3.1}$$

where matrix elements will be obtained by integrating $|\psi|^2$ with various gauge-invariant combinations of the θ_l over the range $-\pi\le\theta_l\le\pi$. To perform these calculations we diagonalize the quadratic form $M_{ll'}$ in (3.1) by a change of variables ($\theta_n\equiv\sum_l O_{nl}\theta_l$)

$$\psi(\theta_n)=\exp\left[-\frac{1}{2g^2}\sum_n \mu_n\theta_n^2\right] \tag{3.2}$$

and, for small g, replace the finite range of the θ_n's by $-\infty<\theta_n<+\infty$ to obtain explicitly computable Gaussian integrals. This is correct to exponential accuracy $-e^{-\pi^2/2g^2\min(\mu_n)}$, but we are evidently in trouble if any of the μ_n's are zero. In fact, in these directions the wave function is flat, and we should really perform the integration first over these zero modes, leading to a complicated multinomial expression in the remaining nonzero modes. The expression is complicated because the original hypercubical integration range of the θ_l's has been replaced, after the orthogonal rotation to the θ_n's, by a much more complicated set of range restrictions.

The appearance of zero modes in (3.1) is, in fact, to be expected in any gauge theory where there are necessarily gauge directions in configuration space where the potential-energy function and, hence, the ground-state wave function is flat. One might at first expect that a complete gauge fixing (in which as many as possible of the θ_l's are set to zero, say) would eliminate all such zero modes. In fact, with the most common choice of boundary conditions for the lattice, toroidal (or periodic), this turns out not to be the case.

We shall illustrate the difficulty on a very simple example, a 2×2 lattice for a $(2+1)$-dimensional U(1) gauge theory (Fig. 1). (A completely general analysis of the zero modes will be given in Sec. IV.) With the links labeled as in Fig. 1, the potential energy in the weak-coupling region is proportional to

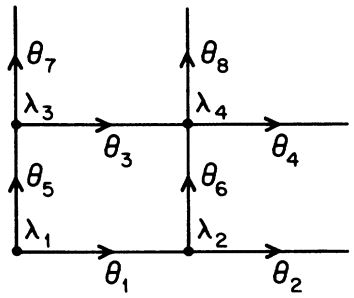

FIG. 1. A 2×2 spatial lattice for an Abelian lattice theory in $2+1$ dimensions.

$$V=\tfrac{1}{2}(\theta_1+\theta_6-\theta_3-\theta_5)^2+\tfrac{1}{2}(\theta_2+\epsilon\theta_5-\theta_4-\theta_6)^2 +\tfrac{1}{2}(\theta_3+\theta_8-\epsilon\theta_1-\theta_7)^2+\tfrac{1}{2}(\theta_4+\epsilon\theta_7-\epsilon\theta_2-\theta_8)^2 \tag{3.3}$$

invariant under the gauge symmetry

$$\theta_1\to\theta_1+\lambda_2-\lambda_1\ ,\quad \theta_2\to\theta_2+\epsilon\lambda_1-\lambda_2\ ,$$
$$\theta_3\to\theta_3+\lambda_4-\lambda_3\ ,\quad \theta_4\to\theta_4+\epsilon\lambda_3-\lambda_4\ ,\ \text{etc.} \tag{3.4}$$

In (3.3), $\epsilon=+1$ (-1) corresponds to periodic (antiperiodic) boundary conditions on the fields. In both cases (3.3) is exactly invariant under (3.4). However, if $\epsilon=-1$, the gauge symmetries (3.4) can be used to set, say, $\theta_5=\theta_6=\theta_7=\theta_8=0$, leaving a positive-definite quadratic form in $\theta_1,\theta_2,\theta_3,\theta_4$. If $\epsilon=+1$, on the other hand, at most three link angles can be set to zero, leaving *two* zero modes in V. The two remaining zero modes are readily understood as globally nontrivial connections—constant fields wrapping the torus in either the x or y directions but not removable by any local gauge transformation. In the language of differential forms, such a field evidently satisfies $dA=0$ *without* $A=d\lambda$ and is, hence, in one-to-one correspondence with the elements of the first cohomology group of the torus $(R\oplus R)$ (Ref. 7). The antiperiodic case $\epsilon=-1$ is analogous (though not precisely equivalent) to the case of the projective plane RP^2, known to be trivial at the level of first deRham cohomology.

In general, in d spatial dimensions, toroidal boundary conditions will lead to d zero modes which may not simply be gauged away. On an L^d lattice, there will in addition be $(d-1)(L^d-1)$ nonzero modes which evidently dominate the local physics as $L\to\infty$. So it is entirely reasonable that a modification of the original theory to a gauge-invariantly constrained one in which the troublesome zero modes are eliminated at the outset should leave the essential physics unaltered in the interesting limit of large L. In the Abelian case, the sum of all x links $(\equiv\theta_x)$ is evidently gauge invariant (similarly for y,z), so by taking as our theory the usual gauge-theory action together with the gauge- (and translation-) invariant constraint

$$\theta_x=\theta_y=\theta_z=0\ , \tag{3.5}$$

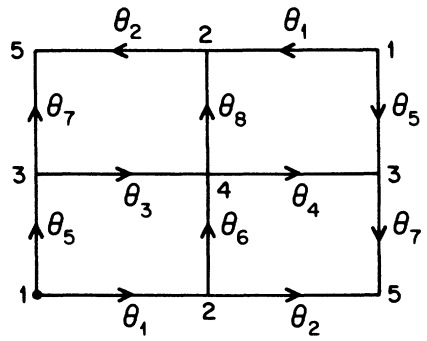

FIG. 2. Projective-plane boundary identification for an Abelian lattice theory in 2 + 1 dimensions.

we can completely eliminate all zero modes after gauge fixing in the toroidal case. Alternatively, one may elect antiperiodic or free boundary conditions in which the problem does not arise.

In the non-Abelian case, the constraint (3.5) on link angles [e.g., the Euler angles for each link in SU(2) gauge theory] would clearly not be gauge invariant. Setting a given spatial Wilson line to unity would represent a gauge-invariant constraint eliminating a zero mode in the linearized limit, but it would clearly spoil translation invariance. It might be thought that by setting up the theory on a projective manifold with trivial first cohomology the zero mode could be eliminated without loss of translation invariance. For example, in 2 + 1 dimensions, one might identify boundary lattice points as in Fig. 2 to produce a spatial manifold with the topology of RP^2 (the projective plane). The reader may easily verify that there are no zero modes in the potential energy after gauge fixing. Unfortunately, a conventional hypercubic lattice with projective plane (antipodal) identifications again seems to lead to a loss of discrete translational invariance: for example, in Fig. 2 site 3 has three independent nearest neighbors while site 1 has only two.[8] Again, with free boundary conditions, all zero modes are eliminated by gauge fixing, but one loses the discrete translational invariance present with toroidal boundary conditions. For the time being, free boundary conditions would nevertheless seem the most palatable choice in the non-Abelian case. In Lanczos calculations of the O(3) σ model in two space-time dimensions,[3] for example, asymptotic scaling of the mass gap was clearly demonstrated with just such boundary conditions.

IV. THE WEAK-COUPLING ANSATZ

In this section we shall provide a more careful discussion of the zero-mode question discussed above in the process of devising a suitable starting ansatz for the Lanczos procedure. The ansatz we shall use is determined by the requirement that it agree with the exact wave function in the $g \to 0$ limit. In particular, it is simply the exact ground state of the Hamiltonian corresponding to the noncompact version of the U(1) lattice theory, obtained by taking the small-angle limit of the compact version. It will be convenient to derive this Hamiltonian by a transfer-matrix technique,[9] starting from the contribution to the total Euclidean action arising from two adjacent spacelike planes

$$S=\frac{a}{2a_0g^2}\sum_{\mathbf{n}\mu}(\Delta\theta_{\mathbf{n}}+\psi_{\mathbf{n}}-\psi_{\mathbf{n}+\hat{\mu}})^2+\frac{a_0}{2ag^2}\sum_p\theta_p^2 . \quad (4.1)$$

In (4.1) a_0, a labels timelike and spacelike lattice spacings, respectively, $\mathbf{n}$ runs over lattice sites, μ over d spacelike directions, and p labels spacelike plaquettes. $\Delta\theta_{\mathbf{n}\mu}$ is the discrete time derivative of the spacelike link $\theta_{\mathbf{n}\mu}$, and $\psi_{\mathbf{n}}$ labels the timelike link connecting the two adjacent spacelike planes. The transfer matrix is obtained by integrating out these latter variables, a process simplified by going to lattice momentum space (L^d lattice)

$$\psi_{\mathbf{n}}=\frac{1}{L^{3/2}}\sum_{\mathbf{p}}e^{2\pi i\mathbf{p}\cdot\mathbf{n}/L}\psi_{\mathbf{p}} , \quad (4.2)$$

where

$$\psi_{\mathbf{n}}-\psi_{\mathbf{n}+\hat{\mu}}=\frac{1}{L^{3/2}}\sum_{\mathbf{p}}c_\mu(\mathbf{p})e^{2\pi i\mathbf{p}\cdot\mathbf{n}/L}\psi_{\mathbf{p}} , \quad (4.3)$$

where

$$c_\mu(\mathbf{p})\equiv 1-e^{2\pi ip_\mu/L} . \quad (4.4)$$

In the integral over timelike links a single zero mode appears, corresponding to the zero-momentum mode $\mathbf{p}=0$. This mode is clearly removable by gauge fixing (since a gauge transformation constant on spacelike surfaces leaves all $\theta_{\mathbf{n}\mu}$ unchanged and shifts precisely the mode $\psi_{\mathbf{p}=0}$). Thus we drop it when doing the $\psi_{\mathbf{p}}$ integrations and obtain

$$\int\prod_{\mathbf{p}\neq 0}d\psi_{\mathbf{p}}\exp\left[-\frac{a}{2a_0g^2}\left[\sum_{\mathbf{p}}\Delta_p|\psi_{\mathbf{p}}|^2+2\sum_{\mathbf{p}}\rho_{\mathbf{p}}^*\psi_{\mathbf{p}}\right]\right]$$
$$=\exp\left[\frac{a}{2a_0g^2}\sum_{\mathbf{p}\neq 0}\frac{1}{\Delta_p}|\rho_{\mathbf{p}}|^2\right] , \quad (4.5)$$

where we have introduced

$$\Delta_p\equiv\sum_\mu|c_\mu(\mathbf{p})|^2 \quad (4.6)$$

and

$$\rho_{\mathbf{p}}\equiv\sum_\mu c_\mu^*(\mathbf{p})\Delta\theta_{\mathbf{p}\mu} . \quad (4.7)$$

The kinetic contribution to the transfer matrix is thus

$$T_{\text{kin}}=\frac{a}{2a_0g^2}\sum_{\mathbf{p}}\left[\sum_\mu|\Delta\theta_{\mathbf{p}\mu}|^2-(1-\delta_{\mathbf{p}0})\frac{1}{\Delta_p}|\rho_{\mathbf{p}}|^2\right]$$
$$=\frac{a}{2a_0g^2}\sum_{\mathbf{p}\mu\nu}T_{\mu\nu}(\mathbf{p})\Delta\theta_{\mathbf{p}\mu}\Delta\theta_{\mathbf{p}\nu}^* \quad (4.8)$$

with

$$T_{\mu\nu}(\mathbf{p})\equiv\delta_{\mu\nu}-\frac{1-\delta_{\mathbf{p}0}}{\Delta_p}c_\mu^*(\mathbf{p})c_\nu(\mathbf{p}) . \quad (4.9)$$

The potential-energy contribution arises directly from the second term on the right-hand side of (4.1):

$$T_{\rm pot}=\frac{a}{2ag^2}\sum_{\mathrm{n},\mu<\nu}(\theta_{\mathrm{n}\mu}+\theta_{\mathrm{n}+\hat{\mu},\nu}-\theta_{\mathrm{n}+\hat{\nu},\mu}-\theta_{\mathrm{n}\nu})^2$$

$$=\frac{a_0}{2ag^2}\sum_{\mathrm{p},\mu,\nu}U_{\mu\nu}(\mathbf{p})\theta_{\mathrm{p}\mu}\theta^*_{\mathrm{p}\nu} \tag{4.10}$$

with

$$U_{\mu\nu}(\mathbf{p})=\Delta_p T_{\mu\nu}(\mathbf{p})\ . \tag{4.11}$$

Now, fix attention on a particular value of $\mathbf{p}$ ($\neq 0$). So far, we have avoided specifying boundary conditions (i.e., $\epsilon=\pm 1$ as in Sec. III). In the event $\epsilon=-1$, all allowed values of $\mathbf{p}$ are half-integral and the $\theta_{\mathrm{p}\mu}$ are complex. If $\epsilon=+1$, the $\mathbf{p}=0$ mode is to be removed by the explicit constraint (3.5). In this case we also assume for the time being that at least one component $p_\nu\neq 0$ or $L/2$, so that again $\theta_{\mathrm{p}\mu}$ is complex (the purely real modes are easily handled by an analogous procedure). We wish to choose a basis in which the quadratic forms $U_{\mu\nu}, T_{\mu\nu}$ [which are proportional, from (4.11)] are diagonal. Let

$$\theta_{\mathrm{p}\mu}=\frac{1}{\sqrt{2}}(\theta^c_{\mathrm{p}\mu}+i\theta^s_{\mathrm{p}\mu})\ ,\quad c_\mu(\mathbf{p})=\gamma_{\mathrm{p}\mu}+i\eta_{\mathrm{p}\mu}\ . \tag{4.12}$$

Then the potential energy may be written (in $d=3$)

$$\sum_{\mu\nu}U_{\mu\nu}(\mathbf{p})\theta_{\mathrm{p}\mu}\theta^*_{\mathrm{p}\nu}=\tfrac{1}{2}\Delta_p\sum_{a=1}^{4}\theta_p^{(a)2}\ . \tag{4.13}$$

The four nonzero modes $\theta_p^{(a)}$ (in $d=3$) are an orthogonal rotation of the original momentum-space modes and correspond to the transverse degrees of polarization for lattice photons of momentum $\mathbf{p}$ and $-\mathbf{p}$. Thus

$$\theta_p^{(a)}=\sum_{\alpha=1}^{6}O^{(a)}_{p\alpha}\theta_{p\alpha}\ ,\quad \theta_{p\alpha}\equiv(\theta^c_p,\theta^s_p)\ . \tag{4.14}$$

For each $\mathbf{p}\neq 0$ there are also two real zero modes (longitudinal polarization) arising from the single complex zero mode

$$\sum_\nu U_{\mu\nu}(\mathbf{p})c^*_\nu(\mathbf{p})=\sum_\nu(\Delta_p\delta_{\mu\nu}-c^*_\mu c_\nu)c^*_\nu$$

$$=\Delta_p c^*_\mu-\left[\sum c_\nu c^*_\nu\right]c^*_\mu=0\ .$$

These modes are eliminated by gauge fixing, in both the periodic and antiperiodic cases. The columns of the transformation matrix $O^{(a)}_\alpha$ are simply the real and imaginary parts of the two (in $d=3$) independent complex vectors perpendicular to c^*_ν [e.g., $\boldsymbol{\epsilon}\times\mathbf{c}^*_\nu$, $\mathbf{c}^*_\nu\times(\boldsymbol{\epsilon}\times\mathbf{c}^*_\nu)$ suitably normalized, with $\boldsymbol{\epsilon}$ an arbitrary polarization vector], and will not be written down explicitly here.

The lattice Hamiltonian is obtained from the transfer matrix[9] by standard techniques, taking $a_0\to 0$. After gauge fixing, we find

$$aH=-\frac{g^2}{2}\sum_{\mathrm{p},a}\frac{\partial^2}{\partial\theta^{(a)2}_{\mathrm{p}}}+\frac{1}{2g^2}\sum_{\mathrm{p},a}\Delta_p\theta_p^{(a)2}\ . \tag{4.15}$$

In (4.15) each independent mode is included once (thus, for $\epsilon=-1$, only one-half of the $\mathbf{p}$ values are summed over, say, those with $p_1>0$). The ground state of (4.15) is

$$\psi_0=\exp\left[-\frac{1}{2g^2}\sum_{\mathrm{p},a}\sqrt{\Delta_p}\,\theta_p^{(a)2}\right]\ . \tag{4.16}$$

This wave function will be the starting point of the Lanczos procedure used below to compute the spectrum of the *compact* U(1) lattice Hamiltonian.

Before proceeding to the Lanczos calculations of Sec. V, it will be convenient to introduce a more schematic (if somewhat less explicit) notation for the link variables. Thus, the pair $(\mathbf{p},a)$ labeling each independent real mode will be replaced by the single index n, and the ansatz (4.16) will be written more simply as

$$\psi_0=\exp\left[-\tfrac{1}{4}\sum_n\mu_n\theta_n^2\right]\ ,\quad \mu_n\equiv\frac{2}{g^2}\sqrt{\Delta_p}\ . \tag{4.17}$$

It will also be useful to introduce a matrix V_{pl} relating plaquette and link variables,

$$\theta_p=\sum_l V_{pl}\theta_l\ , \tag{4.18}$$

which will appear in transformed form as $\bar{V}_{pn}$ defined by

$$\theta_p=\sum_n\bar{V}_{pn}\theta_n\ . \tag{4.19}$$

Explicit analytic formulas for $\bar{V}_{pn}$ are easily obtained using the matrix $O^{(a)}_{p\alpha}$ introduced in (4.14), and will not be given here.

V. LANCZOS CALCULATION FOR U(1) LATTICE GAUGE THEORY

The calculation of the matrix elements required for the Lanczos procedure is completely straightforward in the Abelian case, once all zero modes have been removed by gauge fixing and, if necessary, by gauge-invariant subsidiary conditions. Using the simplified notation introduced at the end of Sec. IV, the compact U(1) Hamiltonian may be written

$$aH=-\tfrac{1}{2}g^2\sum_n\frac{\partial^2}{\partial\theta_n^2}+\frac{1}{g^2}\sum_p(1-\cos\theta_p) \tag{5.1}$$

with $\theta_p=\sum_n\bar{V}_{pn}\theta_n$. The starting ansatz is

$$\psi_0=\exp\left[-\tfrac{1}{4}\sum_n\mu_n\theta_n^2\right]\ . \tag{5.2}$$

By applying the kinetic and potential parts of H to ψ_0 separately, we obtain two additional states:

$$\psi_1\equiv\sum_p\cos(\theta_p)\psi_0\ , \tag{5.3}$$

$$\psi_2\equiv\sum_n(\mu_n^2\theta_n^2)\psi_0\ . \tag{5.4}$$

Thus, at $O(H)$ in the Lanczos scheme, the Hamiltonian will be diagonalized in a three-dimensional subspace, spanned by the states (5.2) and (3.4). A further application of H leads to the following five independent states:

$$\psi_3\equiv\left[\sum_p\cos\theta_p\right]^2\psi_0\ , \tag{5.5}$$

TABLE II. Lanczos estimates for ground-state energies of compact Abelian lattice theory in 3 + 1 dimensions (periodic boundary conditions).

Basis dimension \ $g^2\rightarrow$	4×4×4 lattice 0.2	0.3	0.4	6×6×6 lattice 0.2	0.3	0.4
1	149.3958	147.9812	146.6031	505.448	500.651	495.977
2	149.2893	147.7557	146.2296	505.103	499.951	494.869
3	149.2694	147.7045	146.1298	505.041	499.805	494.610
4	149.2673	147.6945	146.1020	505.025	499.722	494.403
5	149.2664	147.6896	146.0856	505.017	499.709	494.368
6	149.2628	147.6820	146.0735	505.006	499.689	494.343
7	149.2624	147.6806	146.0703	505.004	499.687	494.338
8	149.2623	147.6801	146.0682	504.997	499.651	494.251

$$\psi_4 \equiv \sum_n (\mu_n^2 \theta_n^2) \sum_p \cos(\theta_p)\psi_0 \ , \tag{5.6}$$

$$\psi_5 \equiv \sum_{pn} \sin(\theta_p)\bar{V}_{pn}\mu_n\theta_n\psi_0 \ , \tag{5.7}$$

$$\psi_6 \equiv \sum_n (\mu_n^3 \theta_n^2)\psi_0 \ , \tag{5.8}$$

$$\psi_7 \equiv \left[\sum_n \mu_n^2\theta_n^2\right]^2\psi_0 \ . \tag{5.9}$$

At $O(H^3)$ a further 12 states appear, bringing the total dimensionality of the Lanczos subspace to 20. In this paper we will present the spectral estimates obtained from the eight states given above, i.e., through $O(H^2)$.

The next step is to work out the action of the Hamiltonian on each of the Lanczos basis states defined above. For example, defining $K \equiv \sum_n \partial^2/\partial\theta_n^2$, one easily finds

$$K\psi_2 = 2\left[\sum_n \mu_n^2\right]\psi_0 - \tfrac{1}{2}\sum_n \mu_n\psi_2 - 2\psi_6 + \tfrac{1}{4}\psi_7 \ . \tag{5.10}$$

The only quantities appearing as coefficients in these expressions are the explicitly known eigenvalues μ_n and the transformed plaquette coefficients $\bar{V}_{pn}$. Finally, we must evaluate the Gaussian integrals arising in matrix elements such as

$$\langle\psi_0 \mid \psi_3\rangle = C\int d\theta_n \left[\sum_p \cos\theta_p\right]^2 \exp\left[-\tfrac{1}{2}\sum_n \mu_n\theta_n^2\right]$$
$$= \tfrac{1}{2}\sum_{pp'}\left[\exp\left[-\tfrac{1}{2}\sum_n \frac{1}{\mu_n}(\bar{V}_{pn}+\bar{V}_{p'n})^2\right] + \exp\left[-\tfrac{1}{2}\sum_n \frac{1}{\mu_n}(\bar{V}_{pn}-\bar{V}_{p'n})^2\right]\right] \tag{5.11}$$

(with $C \equiv \langle\psi_0 \mid \psi_0\rangle^{-1}$). Then, defining $(0 \le i,j \le 7)$

$$G_{ij} \equiv \langle\psi_i \mid \psi_j\rangle \tag{5.12}$$

and

$$H_{ij} \equiv \langle\psi_i \mid H \mid \psi_j\rangle \ , \tag{5.13}$$

one solves the generalized eigenvalue problem

$$Hv = \lambda G v \tag{5.14}$$

with the 8×8 real symmetric matrices G,H to obtain the spectrum $\{\lambda_i\}$ of H. As we see in (5.11), the computation of the matrix elements involves sum such as

$$\sum_{pp'} \exp\left[-\frac{1}{2\mu_n}\bar{V}_{pn}\bar{V}_{p'n}\right] \ .$$

In the worst case we have considered, we deal with sums over five plaquettes, such as

$$\sum_{pp'p''p'''p''''} V_{pn}V_{p'n}V_{p''n}V_{p'''n}V_{p''''n} \ .$$

Using translation invariance we can fix one of the pla-

TABLE III. Lanczos estimates for ground-state energies of compact Abelian lattice theory in 3 + 1 dimensions (antiperiodic boundary conditions).

Basis dimension \ $g^2\rightarrow$	4×4×4 lattice 0.2	0.3	0.4	6×6×6 lattice 0.2	0.3	0.4
1	149.9861	148.5604	147.1717	505.802	500.998	496.318
2	149.8787	148.3333	146.7956	505.457	500.298	495.209
3	149.8584	148.2811	146.6943	505.395	500.151	494.949
4	149.8563	148.2710	146.6661	505.378	500.067	494.742
5	149.8555	148.2660	146.6494	505.370	500.055	494.707
6	149.8515	148.2577	146.6363	505.359	500.035	494.682
7	149.8510	148.2563	146.6328	505.358	500.032	494.678
8	149.8510	148.2557	146.6307	505.350	500.000	494.589

TABLE IV. Variationally optimized estimates (periodic boundary conditions).

Basis dimension \ $g^2\rightarrow$	4^3 lattice 0.2 ($\lambda=0.959$)	4^3 lattice 0.4 ($\lambda=0.917$)	6^3 lattice 0.2 ($\lambda=0.959$)	6^3 lattice 0.4 ($\lambda=0.917$)
1	149.275 84	146.1216	505.0401	495.3400
2	149.275 80	146.1209	505.0399	494.3375
3	149.261 91	146.0615	504.9929	494.1377
4	149.261 91	146.0615	504.9928	494.1377
5	149.261 91	146.0614	504.9925	494.1377
6	149.261 91	146.0614	504.9925	494.1376
7	149.261 76	146.0604	504.9914	494.1343
8	149.261 71	146.0596	504.9913	494.1339

quettes and sum over the remaining four. This operation is $O((3L^3)^4)\approx O(81L^{12})$. With $L=6$, this is $\sim 10^{11}$ operations. We used the Cray XMP at the Pittsburgh Supercomputing Center to carry out these sums.

The results of the procedure outlined above are presented in Tables II and III for periodic and antiperiodic boundary conditions of the spatial lattice, respectively. Here we give the ground-state energies, in lattice units (aE_{gs}), of the lattice Hamiltonian for 4^3 and 6^3 lattices, for a variety of coupling (g^2) values. In both cases, the convergence is better for small coupling (in this limit our ansatz is exact) and for smaller lattices. In fact, the accuracy achieved with a 4^3 lattice and $g^2=0.2$ is about 1 part in 10^8 with the eight states appearing through $O(H^2)$. The relative accuracy achieved at each stage is roughly the same for periodic and antiperiodic cases: the precise numbers differ by quantities of order unity, whereas the energies given are extensive and order L^3.

So far, the Gaussian ansatz which we have used as a starting point for the Lanczos procedure was uniquely determined by the weak-coupling limit of the compact theory. So we have not really exploited the variational freedom available in the Lanczos approach. A glance at the second and third columns of Table I reveals that a considerable acceleration of convergence can be achieved by introducing a variational parameter λ in the ground-state ansatz,

$$\psi_0=e^{-\lambda x^2/2}, \tag{5.15}$$

for the anharmonic oscillator. Similarly, if we replace the ansatz (4.17) by

$$\psi_0=\exp\left[-\frac{\lambda}{4}\sum_n \mu_n\theta_n^2\right] \tag{5.16}$$

and vary λ, considerable improvement in the convergence rate is achieved. The results (for $g^2=0.2$ and 0.4, periodic boundary conditions), with optimal choices for λ, are displayed in Table IV. For the 4^3 lattice, for example, comparing Tables II and IV, we see that the results for $g^2=0.4$ achieved at $O(H)$ with $\lambda=0.917$ (with three basis states) are better (i.e., lower) than those achieved at the $O(H^2)$ level (eight states) with the original ansatz ($\lambda=1.0$). The improvement of convergence for $L=6$ is even more dramatic—we now obtain a six-place accuracy for the strongest coupling ($g^2=0.4$) with eight Lanczos states.

We should emphasize that the computational procedure used must be capable of extracting the spectrum to an accuracy of a small fraction of unity in lattice units, as the physically interesting mass gaps will be of this order of magnitude once the theory is tuned to the continuum region. For larger lattices (say $L=10$), the convergence will be slower, and it may be necessary to proceed to the $O(H^3)$ level with 20 Lanczos states. As the continuum limit of our compact U(1) lattice theory is a free Maxwell theory, we have not pressed these calculations further. Instead, the extension of the above techniques to the non-Abelian case, where one expects a physically interesting mass gap in the vacuum sector, is under active investigation.

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