Error estimate for the valence approximation and for a systematic expansion of full QCD

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We construct a systematic expansion for the lattice formulation of full QCD. The leading term is the valence (quenched) approximation. An error estimate for any truncation of this expansion is then obtained from a second expansion of full QCD, indexed by the number of virtual fermion loops included in each term. [S0556-2821(97)05507-0]

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I. INTRODUCTION

Several predictions obtained recently in the valence (quenched) approximation to the infinite volume, continuum limit of lattice QCD lie not far from experiment. For low-lying hadron masses [1], valence approximation results are within 6% $\pm$ 8% of experiment. For decay constants [2] the valence approximation differs from experiment by increments ranging from 12% $\pm$ 11% to 17% $\pm$ 6%. Missing from these calculations, however, is an independent theoretical estimate of the error arising from the valence approximation.

In the present article, we develop a systematic expansion for lattice QCD including the full effect of quark vacuum polarization. The leading term in this scheme is the valence approximation. If an infinite collection of higher terms is taken into account, full QCD is reproduced exactly. We then derive a formula which can be used to estimate the error in any vacuum expectation value obtained by truncation of this expansion to some finite number of terms.

In an exact treatment of QCD, virtual quark-antiquark pairs produced by a chromoelectric field reduce the field's intensity by a factor which depends both on the field's momentum and on its intensity. In the valence approximation this factor, analogous to a dielectric constant, is approximated by its zero-field-momentum zero-field-intensity limit [3]. The approximation which we consider here may be pictured as incorporating an inverse dielectric constant which is a sum of terms which progressively more accurately reproduce the correct dependence of the inverse dielectric constant on field momentum and field intensity. For this approximation to the inverse dielectric constant truncated to any finite number of terms, our error estimate is obtained from a second, independent expansion of full QCD, indexed by the number of virtual quark loops each term includes. A preliminary version of the present work was reported in Ref. [4].

The main motivation of the present article is to find a way of determining directly from QCD the errors arising in valence approximation calculations of hadron masses and decay constants. Our expansion of the inverse dielectric constant arising from quark-antiquark vacuum polarization itself plays no direct role in this error estimate. The expansion is included here largely because the mathematical machinery needed to construct the valence approximation error estimate leads naturally both to the complete expansion and to a corresponding error estimate.

A crucial question which we have not yet answered is whether in practice the determination of valence approximation errors using the form of our algorithm discussed here, or one of its possible variations, would be any faster than a direct comparison of valence approximation results with numbers found by the best present algorithms for full QCD. Whether or not the method we propose turns out to be useful in practice for quantitative error estimates, it appears to us that it may help provide a useful qualitative picture of the effect of vacuum polarization and of the physical mechanism underlying the relatively close agreement found in Refs. [1,2] between valence approximation predictions and the real world. The results we present in Sec. VIII are evidence that at least for moderately heavy quarks, the expansion we construct converges rapidly and the main effect of vacuum polarization is absorbed by the dielectric constant implicit in the valence approximation. How the expansion behaves as quark mass is decreased we hope to return to elsewhere.

We are aware of two other strategies for evaluating the relation between the valence approximation and full QCD. The application of chiral perturbation theory to estimating the errors introduced by the valence approximation has been considered by several groups [5–7]. The asymptotic behavior at small quark mass of a variety of predictions of the valence approximation has been shown to be qualitatively different from the behavior of full QCD. The quark mass below which these difficulties become quantitatively significant in the evaluation of low-lying hadron masses, however, appears to be well below the average of the up and down quark masses [8,9]. For physical values of quark mass, several unknown parameters enter chiral perturbation theory predictions of the errors in most valence approximation results. Quantitative determination of these errors is therefore not possible at present. Another method for evaluating the effect of virtual quark-antiquark pair production on QCD predictions is discussed in Ref. [10]. This calculation uses a weak-coupling expansion to leading order and is valid for small values of the gauge coupling constant and large values of the quark mass. The results we report in our trial calculation in Sec. VIII are qualitatively consistent with those described in Ref. [10]. Reviews of a variety of other recent valence approximation calculations are given in Ref. [11].

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In Sec. II we introduce definitions. In Sec. III we construct an expansion for the dependence of vacuum polarization on field momentum and field strength. In Sec. IV we derive an expression for the error in any vacuum expectation value arising from a truncation of the expansion of Sec. III. In Secs. V, VI, and VII we present an algorithm for evaluating the terms in the expansion and corresponding error estimates. In Sec. VIII we describe a trial calculation using our expansion and error estimates. The Appendix gives a calculation of a set of parameters needed by the algorithm in Sec. V.

II. DEFINITIONS

We consider Wilson's formulation of euclidean QCD on some finite lattice. A lattice gauge field consists of an assignment of an element $u(x_1,x_2)$ of the fundamental representation of SU(3) to each oriented nearest neighbor pair of sites (x_1,x_2) with the usual restriction that $u(x_1,x_2)$ is the adjoint $u(x_2,x_1)^\dagger$.

Define the Hilbert space $\mathcal{F}$ to consist of complex-valued functions f of the lattice gauge fields with finite value of the norm:

$$\|f\|^2=\zeta^{-1}\int d\mu |f|^2\exp(\mathcal{S}), \tag{2.1}$$

$$\zeta=\int d\mu\exp(\mathcal{S}).$$

The inner product on $\mathcal{F}$ is

$$(f,f')=\zeta^{-1}\int d\mu f^* f'\exp(\mathcal{S}), \tag{2.2}$$

$$\zeta=\int d\mu\exp(\mathcal{S}).$$

Here $\mathcal{S}$ is some real valued function of the field which is bounded in absolute value and invariant under all lattice translations, rotations, reflections, and gauge transformations. A useful choice for $\mathcal{S}$ will be discussed in Sec. III. A linearly independent basis for $\mathcal{F}$ consists of the collection $\{f_i\}$ of all possible products of matrix elements of irreducible representations of SU(3) including exactly one matrix element for each link, with links differing only by a flip of orientation identified. Distinct f_i are then orthogonal with respect to the inner product of Eq. (2.2) for $\mathcal{S}$ of 0. We choose the f_i to be normalized with respect to the inner product with $\mathcal{S}$ of 0.

Let d_i be the sum over all links of the dimension of the SU(3) representation assigned to that link by f_i. We assume the sequence $\{f_i\}$ is ordered in such a way that d_i is a nondecreasing function of i. Applying a Gram-Schmidt process to $\{f_i\}$ using the inner product of Eq. (2.2) for some nonzero choice of $\mathcal{S}$ gives an orthonormal basis $\{\hat{f}_i\}$ for $\mathcal{F}$.

Although the expansion to be constructed in Sec. III can be defined using only $\mathcal{F}$, for purposes of constructing an algorithm to evaluate this expansion it is slightly more convenient to work with the subspace $\mathcal{H}$ of $\mathcal{F}$ which is invariant under all lattice translations, rotations, reflections, gauge transforms, and complex conjugation. Let h_i be the projection of f_i onto $\mathcal{H}$. Since rotation, translation, reflection, gauge transformation, and complex conjugation leave the value of d_i unchanged, h_i will be a linear combination of a collection of f_j all of which have d_j equal to d_i. Most h_i obtained in this way will be linearly dependent on the set of h_j with $j<i$. Working upwards from i of 0, we eliminate any h_i which is dependent on surviving h_j with $j<i$. A Gram-Schmidt process on the surviving h_i gives an orthonormal basis $\{\hat{h}_i\}$ for $\mathcal{H}$.

Typical vectors in $\mathcal{H}$ are the function with value 1 for all gauge fields and the Wilson plaquette action

$$P=\sum_{(x_1,\ldots,x_4)}\mathrm{tr}[u(x_1,x_2)u(x_2,x_3)u(x_3,x_4)u(x_4,x_1)], \tag{2.3}$$

where the sum is taken over all oriented plaquettes $(x_1,\cdots,x_4)$ consisting of sequences of four successive nearest neighbors, with sequences related by a cyclic permutation identified. Any sum of traces of products of $u(x,y)$ over all rotations, translations, reflections and order reversals of some closed path gives yet another element of $\mathcal{H}$. The basis vector $\hat{h}_0$ is the function with constant value 1, and $\hat{h}_1$ is the normalized projection of P orthogonal to $\hat{h}_0$. The basis vectors $\hat{h}_2$, $\hat{h}_3$, and $\hat{h}_4$ are each found by continuing the Gram-Schmidt process on the three different sums of traces of products of $u(x,y)$ along one of the three distinct shapes of closed paths consisting of six lattice links.

We now define the lattice vacuum expectation value. We assume, for simplicity, quarks occur in degenerate pairs for some set of masses strictly greater than 0. Let M be Wilson's coupling matrix among half the quark fields, one from each degenerate pair. We impose periodic boundary conditions. For any function of the gauge fields G with bounded absolute value, a regulated form of the vacuum expectation value obtained after integrating out quark fields is

$$\langle G\rangle_R=Z^{-1}\int d\mu\ G\ \det(M^\dagger M+R)\exp\left(\frac{\beta}{6}P\right),$$

$$Z_R=\int d\mu\ \det(M^\dagger M+R)\exp\left(\frac{\beta}{6}P\right), \tag{2.4}$$

where β is $6/g^2$ for bare gauge coupling constant g, μ is the product of one copy of SU(3) Haar measure for each link variable on the lattice, and R a small non-negative parameter. The extension of Eq. (2.4) to vacuum expectations of products of quark and antiquark fields is not needed for the present discussion and will be omitted for simplicity. Since the determinant of the Wilson coupling matrix M is real, the expectation $\langle G\rangle_0$ is the usual vacuum expectation of lattice QCD. For any bounded G, $\langle G\rangle_R$ approaches $\langle G\rangle_0$ as R goes to 0.

We introduce the regulator R in the definition of $\langle G\rangle_R$ to provide a mathematically convenient rule for handling rare gauge configurations on which M becomes singular in the valence approximation. Monte Carlo valence approximation calculations often find averages of quantities involving M^{-1} at values of the quark mass for which some configura-

tions exist, such as all link variables close to the identity matrix, for which M has eigenvalues arbitrarily close to 0. These configurations are not encountered in practice because their total weight within the path integral is extremely small. It is generally believed that for any positive choice of quark masses, the total valence approximation measure of configurations with minimal $M^\dagger M$ eigenvalue below $O(m_q^2)$ goes to zero very rapidly in the limit of large lattice volume with lattice spacing held fixed. The expansion to be considered below will be done with some nonzero value of R much smaller than $O(m_q^2)$. After taking a limit of infinite volume of any vacuum expectation, a limit of zero R should leave the result essentially unchanged. For notational simplicity, the R subscript will be deleted from $\langle G\rangle_R$ and Z_R in the following.

The extension of Eq. (2.4) to QCD with one or more quark masses not in a degenerate pair follows from the preceding paragraph. For any coupling matrix N with all quark masses nonzero, the spectra of N and $N^\dagger$ are identical. Thus $\det(N)$ is real and non-negative unless N has a negative real eigenvalue. For κ less than 1/8, negative real eigenvalues of N cannot occur. Since the spectrum of N is a continuous function of κ, as κ is made larger than 1/8, negative real eigenvalues will occur with significant probability only once eigenvalues close to 0 become probable. As explained in the preceding paragraph, for the range of quark mass we consider and sufficiently large physical volume this probability is expected to be negligible. Thus for sufficiently large volume we can treat $\det(N)$ as real and non-negative. For a quark coupling matrix N with all quark masses positive but no other restrictions, a vacuum expectation value is therefore given by replacing $\det(M^\dagger M+R)$ in Eq. (2.4) with $\sqrt{\det(N^\dagger N+R)}$. With only minor changes, the expansion discussed in the remainder of this paper can then be adapted to QCD with one or more quark mass not in a degenerate pair.

The regulation parameter R is needed only for the Wilson quark coupling matrix. For Kogut-Susskind quarks the spectrum of $M^\dagger M$ is bounded from below by m_q^2 for all gauge configurations. For Kogut-Susskind quarks with positive quark mass, the probability of negative real eigenvalues of M can also be proved to be 0 in any volume.

III. EXPANSION

Any $\mathcal{S}$, bounded in absolute value and invariant under all lattice translations, rotations, reflections, and gauge transformations, can be chosen in Eq. (2.2) to define a space $\mathcal{H}$ to construct an expansion for $\ln[\det(M^\dagger M+R)]$. In the present section we will construct an expansion for QCD vacuum expectation values for any such $\mathcal{S}$. In Sec. IV we will be led to a choice of $\mathcal{S}$ which is likely to speed the convergence of this expansion.

Since M is a finite matrix with matrix elements bounded uniformly over all gauge fields, the spectrum of $M^\dagger M+R$ is bounded from above by some constant A. Thus $\det(M^\dagger M+R)$ has a finite value of the norm defined by Eq. (2.1) and is in $\mathcal{F}$. In addition $\det(M^\dagger M+R)$ is real valued and rotation, translation, reflection and gauge invariant. It is therefore in $\mathcal{H}$.

Since the spectrum of $M^\dagger M+R$ is bounded from below by R, $\det(M^\dagger M+R)$ is bounded from both above and below. Thus $\|\ln[\det(M^\dagger M+R)]\|$ is finite and $\ln[\det(M^\dagger M+R)]$ is also in $\mathcal{H}$. Using the orthonormal basis $\{\hat{h}_i\}$ of $\mathcal{H}$, we therefore have the convergent expansion

$$\ln[\det(M^\dagger M+R)]=\sum_i a_i\,\hat{h}_i, \tag{3.1}$$

$$a_i=(\hat{h}_i,\ln[\det(M^\dagger M+R)]). \tag{3.2}$$

An algorithm for the numerical evaluation of the coefficients a_i is presented in Sec. V.

For any G bounded in absolute value, an approximation to $\langle G\rangle$ can be obtained by combining Eqs. (3.1) and (3.2) with Eq. (2.4). The expectation value defined by Eq. (2.4) can be reexpressed as

$$\langle G\rangle=Z^{-1}\int d\mu\; G\;\exp\left(L_n+Q_n+\frac{\beta}{6}P\right),$$

$$Z=\int d\mu\;\exp\left(L_n+Q_n+\frac{\beta}{6}P\right), \tag{3.3}$$

where n is some positive integer and the partial sum L_n and remainder Q_n are

$$L_n=\sum_{i=0}^{n} a_i\,\hat{h}_i, \tag{3.4}$$

$$Q_n=\ln[\det(M^\dagger M+R)]-L_n=\sum_{i>n} a_i\,\hat{h}_i. \tag{3.5}$$

As n becomes large, Eq. (3.2) implies Q_n approaches 0 in $\mathcal{F}$. Thus it appears reasonable to try to approximate Eqs. (3.3) by omitting Q_n. We obtain

$$\langle G\rangle_n=Z_n^{-1}\int d\mu\; G\;\exp\left(L_n+\frac{\beta}{6}P\right),$$

$$Z_n=\int d\mu\;\exp\left(L_n+\frac{\beta}{6}P\right). \tag{3.6}$$

The expectation $\langle G\rangle_0$ is pure QCD with the quark determinant simply removed and no shift in β. The expectation $\langle G\rangle_1$ is the valence approximation including a shift in β. For any G bounded in absolute value, the approximate expectation $\langle G\rangle_n$ approaches $\langle G\rangle$ as n becomes large. This convergence holds for any admissible $\mathcal{S}$ in Eq. (2.2) defining the inner product of the space $\mathcal{H}$ and, in particular, does not require any particular relation between $\mathcal{S}$ and the action for QCD. A rigorous proof of this result is given elsewhere [12]. We will show below, however, that the choice of an $\mathcal{S}$ related to the QCD action is likely to help maximize the rate at which the expansion converges.

It may be useful to mention here that the hopping constant expansion for $\ln[\det(M^\dagger M)]$ expresses this quantity as a linear combination of Wilson loops formally similar to Eq. (3.1) and can be used to obtain an approximation to $\langle G\rangle$ similar to Eq. (3.6). In two crucial ways, however, the expansion of Eq. (3.1) differs from the hopping constant expansion, and approximation (3.6) differs from the corresponding approximation using the hopping constant expansion. First, the validity of expansion (3.1) and the accuracy of approximation (3.6) are not restricted to the range of large quark mass to which the hopping constant expansion and its related approximation apply. As we have already shown and as is discussed in more detail elsewhere [12], expansion (3.1) and approximation (3.6) apply as long as the quark mass is greater than 0. Second, even for values of quark mass at which the hopping constant expansion does converge, Eqs. (3.1) and (3.2) differ from the hopping constant expansion by an infinite rearrangement. That is, each term which appears in Eqs. (3.1) and (3.2) is a linear combination of an infinite set of the terms appearing in the hopping constant expansion and vice versa.

A crucial question concerning $\langle G\rangle_n$ is how large n must be made to obtain reasonably accurate results. In particular, it might seem that in analogy with the hopping constant expansion, an extremely large value of n will be needed to obtain accurate results for G which are sensitive to the low momentum components of the gauge field. For some G we believe this is likely to be the case. In particular, for any n there will almost certainly be some length scale above which all Wilson loops are given very inaccurately. On the other hand, relatively close agreement has been found between light hadron masses in the valence approximation, with n of 1, and hadron masses in the real world. This agreement suggests the expansion, or one of its variations, may converge fairly rapidly for light hadrons. We hope to return to this subject elsewhere. Examples for which n of 1 gives accurate results and n of 4 gives still more accurate results will be discussed in detail in Sec. VIII.

A wide range of other possible expansions and approximate vacuum expectation values similar to Eqs. (3.1) and (3.6), respectively, can be constructed by various choices of $\mathcal{S}$ or the expansion basis $\{h_i\}$. Yet another class of possibilities is to choose the a_i in Eq. (3.1) to force the first order error $\delta_{1n}(G)$, to be discussed in Sec. IV, to zero for a particular G or set of G, such as the π propagator or the ρ propagator. These alternatives to Eqs. (3.1) and (3.6) will not be discussed further here.

IV. ERROR ESTIMATE AND CHOICE OF $\mathcal{S}$

We now derive an estimate for the error in approximating any $\langle G\rangle$ by some $\langle G\rangle_n$. This estimate will then suggest a choice of $\mathcal{S}$ which will tend to lead to a small error in $\langle G\rangle_n$.

The difference between $\langle G\rangle_n$ and $\langle G\rangle$ arises from approximating $\ln[\det(M^\dagger M+R)]$ in the formula for $\langle G\rangle$ with L_n in the formula for $\langle G\rangle_n$. If the remainder in this approximation Q_n, defined by Eq. (3.5) as $\ln[\det(M^\dagger M+R)]-L_n$, is small, then we expect $\langle G\rangle_n$ to be close to $\langle G\rangle$. To estimate the difference between $\langle G\rangle_n$ and $\langle G\rangle$, we therefore to take Eqs. (3.3) for $\langle G\rangle$ and expand as a power series in Q_n. This is conveniently organized by replacing Q_n in Eqs. (3.3) by λQ_n, expanding $\langle G\rangle$ as an asymptotic series in powers of λ, and then setting λ to 1. We obtain

$$\langle G\rangle=\langle G\rangle_n+\sum_{p\geqslant 1}\delta_{pn}(G), \tag{4.1}$$

$$\delta_{1n}(G)=\langle(G-\langle G\rangle_n)(Q_n-\langle Q_n\rangle_n)\rangle_n, \tag{4.2}$$

$$\delta_{2n}(G)=\langle(G-\langle G\rangle_n)(Q_n-\langle Q_n\rangle_n)^2\rangle_n, \tag{4.3}$$

$$\delta_{3n}(G)=\langle(G-\langle G\rangle_n)(Q_n-\langle Q_n\rangle_n)^3\rangle_n-3\langle(G-\langle G\rangle_n)\times(Q_n-\langle Q_n\rangle_n)\rangle_n\langle(Q_n-\langle Q_n\rangle_n)^2\rangle_n, \tag{4.4}$$

$$\vdots$$

The term $\delta_{pn}(G)$ in this series is of order p in Q_n. Thus if Q_n is small, successive terms in this series should become progressively smaller. On the other hand, for a Monte Carlo evaluation it is not hard to show that the statistical dispersion of $\delta_{pn}(G)$ divided by its mean value will rise with system volume as volume to the power p. Thus succesive terms in this series will become progressively more expensive to evaluate. It is therefore our intention primarily to use $\delta_{1n}(G)$ as an estimate of the error in $\langle G\rangle_n$. If $\delta_{1n}(G)$ turns out to be a small fraction of $\langle G\rangle_n$, we would expect $\langle G\rangle_n$ to be a reliable approximation to $\langle G\rangle$ and $\delta_{1n}(G)$ to be a reliable approximation of the error in $\langle G\rangle_n$. Conversely, if $\delta_{1n}(G)$ is not a small fraction of $\langle G\rangle_n$, we can say only that $\langle G\rangle_n$ is not a reliable approximation to $\langle G\rangle$.

From the perspective of weak-coupling perturbation theory, the index p in Eq. (4.1) counts the number of internal quark loops entering each term of the expansion. In particular, $\delta_{11}(G)$ gives the corrections to the valence approximation arising from weak-coupling diagrams with a single quark loop, $\delta_{21}(G)$ gives the valence approximation error from diagrams with two quark loops, and so on. Thus while the expansion of Eq. (3.6) approximates the effect of vacuum polarization with a sequence of progressively less local effective actions, even the leading correction in Eq. (4.1), $\delta_{1n}(G)$ directly measures the difference between the effect of arbitrarily large virtual quark loops and their local approximation in Eq. (3.6).

Taking $\delta_{1n}(G)$ as an estimate of the error in $\langle G\rangle_n$ suggests a choice for $\mathcal{S}$ entering the norm defined in Eq. (2.1). From Eqs. (4.1) and (4.2) and the Cauchy-Schwarz inequality we obtain

$$(\langle G\rangle-\langle G\rangle_n)^2\approx(\langle(G-\langle G\rangle_n)(Q_n-\langle Q_n\rangle_n)\rangle_n)^2 \leqslant\langle(Q_n-\langle Q_n\rangle_n)^2\rangle_n\langle(G-\langle G\rangle_n)^2\rangle_n. \tag{4.5}$$

This relation suggests that the error in $\langle G\rangle_n$ will be minimized by a choice of $\mathcal{S}$ which minimizes $\langle(Q_n-\langle Q_n\rangle_n)^2\rangle_n$. But recall that Q_n is defined by Eq. (3.4) as the remainder $\ln[\det(M^\dagger M+R)]-L_n$ with L_n defined, in effect, to be the n term approximation to $\ln[\det(M^\dagger M+R)]$ which minimizes

$$\|Q_n\|^2=\zeta^{-1}\int d\mu\ |Q_n|^2\exp(\mathcal{S}), \tag{4.6}$$

$$\zeta=\int d\mu\exp(\mathcal{S}).$$

Since $\|Q_n\|^2$ has been minimized with respect to variations in L_n and since we would like to make $\langle(Q_n-\langle Q_n\rangle_n)^2\rangle_n$ small, it seems reasonable to try to turn the second expression into the first. If we choose $\mathcal{S}$ to be $L_n+\beta P/6$, then for n greater than 1, $\langle Q_n\rangle_n$ vanishes and we have

$$\langle(Q_n-\langle Q_n\rangle_n)^2\rangle_n=\langle(Q_n)^2\rangle_n=\|Q_n\|^2.$$

Thus for the calculation of $\langle G\rangle_n$ a good choice of $\mathcal{S}$ appears to be $L_n+\beta P/6$ itself.

The choice of $L_n+\beta P/6$ as $\mathcal{S}$ leads to a set of nonlinear equations for L_n. For the valence approximation, a single equation results which can be solved fairly easily. By a trick it can also be avoided completely. In the valence approximation, $\mathcal{S}$ becomes

$$\mathcal{S}=L_1+\frac{\beta}{6}P=\alpha+\frac{\beta'}{6}P, \tag{4.7}$$

with α and β' given by

$$\alpha=a_0+\frac{a_1\langle P\rangle_1}{\sqrt{[\langle P-\langle P\rangle_1]^2\rangle}},$$

$$\beta'=\beta+\Delta\beta,$$

$$\Delta\beta=\frac{6a_1}{\sqrt{[\langle P-\langle P\rangle_1]^2\rangle}}. \tag{4.8}$$

For any choice of β, the valence approximation value β' is the solution to

$$\beta'=\beta+\Delta\beta(\beta'). \tag{4.9}$$

With any reasonable number of flavors of quarks, less than 10 for example, it is easily confirmed numerically that $\Delta\beta(\beta')$ is a monotone increasing function of β' with derivative significantly less than 1. For two flavors of quarks with κ of 0.1600 considered in Sec. VIII, we find that $\Delta\beta$ rises from below 0.1 at β' of 0 to below 0.3 at β' near 6.0. Thus Eq. (4.9) can be solved by a fixed point iteration, taking β as an initial value of β'. A simpler procedure, however, is to choose the valence approximation β' first, then use Eq. (4.9) to determine the corresponding β for full QCD. This procedure will be adopted in the example to be discussed in Sec. VIII.

For the evaluation of $\langle G\rangle_n$ with n larger than 1, a $\mathcal{S}$ of $L_n+\beta P/6$ which minimizes $\langle(Q_n-\langle Q_n\rangle_n)^2\rangle_n$ could be found by iterating equations similar to Eq. (4.9). Just as an iteration of Eq. (4.9) converges rapidly, numerical experiments suggest that the equations for L_n would also converge rapidly. A simpler alternative, however, is to leave $\mathcal{S}$ fixed at its valence approximation value in Eq. (4.7). As mentioned above, the expansion we construct converges for a wide range of different $\mathcal{S}$, and Eq. (4.7) is certainly an admissible choice of $\mathcal{S}$ no matter what value of n we intended to use for $\langle G\rangle_n$. On the other hand, it appears to us unlikely that spending the computer time needed to find an improved $\mathcal{S}$ will decrease significantly the error in an expansion carried out to some n larger than 1. A more efficient use of computer time would probably be to work to higher n with $\mathcal{S}$ still fixed at its valence approximation value.

For an expansion with n larger than 1, we can still begin by specifying a value for the β' occuring in the valence approximation. The corresponding β parameter for full QCD, if needed explicitly, can then be found from β' using Eq. (4.9). The higher order terms entering the effective action L_n, however, do not depend on β and can be determined directly from Eq. (3.4). To test the accuracy of some approximation $\langle G\rangle_n$ and the corresponding error estimate $\delta_{1n}(G)$ an explicit value of β for full QCD is useful. In other calculations with n greater than 1, however, a determination of β is not necessary.

V. TRACE LOG ALGORITHM

The quantity $\ln[\det(M^\dagger M+R)]$ needed for Eq. (3.1) obeys the identity

$$\ln[\det(M^\dagger M+R)]=\mathrm{tr}[\ln(M^\dagger M+R)]. \tag{5.1}$$

We now consider an algorithm for finding $\mathrm{trln}(M^\dagger M+R)$. The algorithm exploits properties of the Chebyshev polynomials. Combined with Eq. (3.1), this algorithm gives the coefficients a_i. As discussed in Sec. II, we will assume the quark masses, lattice volume, and Monte Carlo ensemble size have been chosen in such a way that for all gauge configurations encountered the minimal eigenvalue B of $M^\dagger M$ lies well above R. The effect of R in $\mathrm{tr}[\ln(M^\dagger M+R)]$ is then negligible, and we omit R in the remainder of the paper.

It is perhaps useful to mention that the application of Chebyshev polynomials to an algorithm for the effect of quark-antiquark vacuum polarization in full QCD has also been discussed recently in Ref. [16]. The algorithm discussed in the present paper, however, and our use of Chebyshev polynomials are unrelated to the work in Ref. [16].

To evaluate $\mathrm{tr}[\ln(M^\dagger M)]$ we begin by generating an ensemble of Gaussian random complex-valued pseudoquark fields $\phi_i(x)$, where i is a multi-index ranging over all combinations of quark spin, color, and flavor and x ranges over lattice sites. For each i and x we choose $\phi_i(x)$ to be an independent random variable such that the average over this ensemble $\langle\langle\cdots\rangle\rangle$ gives

$$\langle\langle\phi_i(x)\ \phi_j(y)\rangle\rangle=0,$$

$$\langle\langle\phi_i^*(x)\ \phi_j(y)\rangle\rangle=\delta_{ij}\ \delta_{xy}. \tag{5.2}$$

We then have

$$\mathrm{tr}[\ln(M^\dagger M)]=\langle\langle((\phi,\ln(M^\dagger M)\phi))\rangle\rangle, \tag{5.3}$$

where $((\ldots,\ldots))$ is the inner product on the vector space of pseudoquark fields:

$$((f,g))=\sum_{ix} f_i^*(x)\ g_i(x). \tag{5.4}$$

Finding the inner product of two such vectors requires a comparatively small amount of arithmetic. The problem of evaluating the trace $\mathrm{tr}\,[\ln(M^\dagger M)]$ is thus reduced to finding $\ln(M^\dagger M)\phi$ for a large ensemble of ϕ.

For the evaluation of $\ln(M^\dagger M)\phi$ we combine properties of the Chebyshev polynomials with the restriction that the eigenvalues of $M^\dagger M$ lie between upper and lower bounds A and B, respectively. Define the operator Y and the parameter ϵ to be

$$Y=\frac{M^\dagger M}{A}, \tag{5.5}$$

$$\epsilon=\frac{B}{A}. \tag{5.6}$$

In the Appendix we will show that for any n greater than 1 there are a set of coefficients b_i, such that, for any number y between ϵ and 1,

$$\ln(y)=\sum_{i=0}^{n} b_i T_i^*\left(\frac{1-y}{1-\epsilon}\right)+\delta\ln(y), \tag{5.7}$$

$$|\delta|<2\ \exp(-2n\sqrt{\epsilon}), \tag{5.8}$$

where the T_i^* are Chebyshev polynomials. For large values of n, the inequality of Eq. (5.7) is nearly saturated. Since Y is a self-adjoint operator with all eigenvalues between ϵ and 1, for any vector ϕ,

$$\ln(Y)\phi=\sum_{i=0}^{n} b_i T_i^*\left(\frac{1-Y}{1-\epsilon}\right)\phi+\delta\ln(Y)\phi, \tag{5.9}$$

with δ bounded according to Eq. (5.7).

An iterative algorithm to evaluate the sum in Eq. (5.9) can be obtained from the recursion relation

$$T_{i+1}^*(z)=(4z-2)T_i^*(z)-T_{i-1}^*(z) \tag{5.10}$$

and initial values

$$T_0^*(z)=1,,$$

$$T_{-1}^*(z)=2z-1. \tag{5.11}$$

Define the sequences C_i and D_i for $0<i\leqslant n$ by

$$C_i=T_0^*(Y)\phi+c_i\left(\frac{2+2\epsilon-4Y}{1-\epsilon}C_{i-1}-D_{i-1}\right),$$

$$D_i=T_{-1}^*(Y)\phi+c_i C_{i-1}, \tag{5.12}$$

with initial values

$$C_0=T_0^*(Y)\phi,$$

$$D_0=T_{-1}^*(Y)\phi. \tag{5.13}$$

The coefficients c_i in Eq. (5.12) are found from the b_i in Eqs. (5.7) and (5.9) by

$$c_i=\frac{b_{n+1-i}}{b_{n-i}}. \tag{5.14}$$

Equations (5.10)–(5.14) imply that $b_0 C_n$ gives the sum in Eq. (5.9) and is therefore an approximation to $\ln(Y)\phi$ with relative error less than $|\delta|$.

The final result, by Eqs. (5.3) and (5.5), is

$$\mathrm{trln}(M^\dagger M)=\langle\langle((\phi,b_0 C_n))\rangle\rangle+d_M\ln(A), \tag{5.15}$$

where d_M is the dimension of the matrix M.

VI. MAXIMUM AND MINIMUM EIGENVALUES

Since for small values of δ the number of iterations required to obtain a fixed value of δ in Eq. (5.7) becomes a linear function of $\sqrt{A/B}$, the optimal choices for A and B become $\lambda_{\max}$ and $\lambda_{\min}$, respectively.

An efficient algorithm [14] for estimating the maximum and minimum eigenvalues of $M^\dagger M$ uses the Lanczos method to construct a tridiagonal approximation to $M^\dagger M$. Define the sequences of real numbers $\alpha_1,\ldots,\alpha_m$ and $\beta_0,\ldots,\beta_m$ and the sequences of pseudoquark fields $q_0,\ldots,q_m$ and $r_0,\ldots,r_m$ by

$$q_{i+1}=(\beta_i)^{-1}r_i,$$

$$\alpha_{i+1}=[(q_{i+1},M^\dagger M q_{i+1})],$$

$$r^{i+1}=M^\dagger M q^{i+1}-\alpha_{i+1}q_{i+1}-\beta_i q_i,$$

$$\beta_{i+1}=\sqrt{((r_{i+1},r_{i+1}))}, \tag{6.1}$$

with β_0 of 1, q_0 identically 0, and r_0 a randomly chosen pseudoquark field with norm 1. Here m is the number of distinct eigenvalues of $M^\dagger M$.

It can be shown that the sequence of pseudoquark fields $q_1,\ldots q_m$ generated by Eq. (6.1) is orthonormal, and the space spanned by these vectors is invariant under the action of $M^\dagger M$. The space spanned by $q_1,\ldots,q_m$ is smaller than the whole space of pseudoquark fields only if one or more of the eigenvalues of $M^\dagger M$ is degenerate. In the basis $q_1,\ldots,q_m$, $M^\dagger M$ is tridiagonal. All matrix elements of T_{ij},

$$T_{ij}=[(q_i,M^\dagger M q_j)], \tag{6.2}$$

vanish except

$$T_{i-1\,i}=\beta_{i-1},$$

$$T_{i\,i}=\alpha_i,$$

$$T_{i+1\,i}=\beta_i. \tag{6.3}$$

Each distinct eigenvalue of $M^\dagger M$ occurs exactly once as an eigenvalue of the matrix of Eq. (6.3). As n grows, the maximum and minimum eigenvalues $\lambda_{\max}^n$ and $\lambda_{\min}^n$ of the submatrix T_{ij}^n with $1\leqslant i,j\leqslant n$ approach the true maximum and minimum eigenvalues $\lambda_{\max}$ and $\lambda_{\min}$ of $M^\dagger M$ with errors falling exponentially in n.

To extract $\lambda_{\max}^n$ and $\lambda_{\min}^n$ from T^n, define the polynomial $p^n(\lambda)$ to be the determinant

$$p^n(\lambda)=\det(T^n-\lambda I^n), \tag{6.4}$$

where I^n is the $n\times n$ identity matrix. The $p^n(\lambda)$ can be calculated from the iteration

$$p^0(\lambda)=1,$$

$$p^{n+1}(\lambda)=(\alpha_{n+1}-\lambda)p^n(\lambda)-(\beta_{n-1})^2p^{n-1}(\lambda). \tag{6.5}$$

The eigenvalues T^n are the zeros of $p^n(\lambda)$. Thus we wish to find the largest and smallest of these zeros. It can be shown [14] that the number of zeros of $p^n(\lambda)$ lying below some λ is given by the number of sign changes in the sequence

$$p^0(\lambda),p^1(\lambda),\ldots,p^n(\lambda). \tag{6.6}$$

This relation can then be used to guide a search for the maximum and minimum zeros of $p^n(\lambda)$.

VII. PRECONDITIONER

With A and B given by $\lambda_{\max}$ and $\lambda_{\min}$, respectively, the amount of arithmetic required by the algorithm of Sec. V is proportional to $\sqrt{\lambda_{\max}/\lambda_{\min}}$. We now show how the calculation of $\mathrm{tr}[\ln(M^\dagger M)]$ can be converted into the calculation of $\mathrm{tr}[\ln(N^\dagger N)]$ for an operator N with a smaller value of $\sqrt{\lambda_{\max}/\lambda_{\min}}$. This change also tends to decrease the number of pseudoquark fields needed for a reliable evaluation of the trace.

The expression $\mathrm{tr}[\ln(M^\dagger M)]$ is gauge invariant since it is $\ln\det(M^\dagger M)$ and $\det(M^\dagger M)$ is gauge invariant. Prior to evaluating $\mathrm{tr}[\ln(M^\dagger M)]$ we can therefore transform to a lattice transverse gauge, defined to give a local maximum of the sum over all nearest neighbors x and y:

$$\sum_{x\,y}\mathrm{tr}[u(x,y)]. \tag{7.1}$$

Using, for example, the algorithm described in Ref. [1], the number of arithmetic operations required for gauge fixing is relatively small in comparison to the arithmetic needed to find $\ln(M^\dagger M)\phi$ for an ensemble of random pseudoquark fields ϕ.

Now define M_0 to be the fermion coupling matrix with hopping constant κ_0 and all $u(x,y)$ equal to 1. Since M has been transformed to a smooth gauge, if the bare gauge coupling constant g is made small and κ_0 is chosen optimally, we expect M_0 to be an approximation to M. Thus the preconditioned operator N,

$$N=(M_0)^{-1}M, \tag{7.2}$$

should be closer to the identity than is M. In particular, $\sqrt{\lambda_{\max}/\lambda_{\min}}$ for $N^\dagger N$ should be smaller than it is for $M^\dagger M$. Using the preconditioned operator we have the relation

$$\mathrm{tr}[\ln(M^\dagger M)]=\mathrm{tr}[\ln(N^\dagger N)]+\mathrm{tr}[\ln(M_0^\dagger M_0)]. \tag{7.3}$$

The additional term $\mathrm{tr}[\ln(M_0^\dagger M_0)]$ required to find $\mathrm{tr}[\ln(M^\dagger M)]$ by Eq. (7.3) does not depend on the gauge configuration and needs to be calculated only once. On the other hand, the operator M_0 is diagonal in momentum space. Thus fast Fourier transforms provide an efficient way to carry out the multiplication by negative powers of $M_0^\dagger M_0$ needed to determine $\ln(N^\dagger N)\phi$ by the algorithm of Sec. V. A rough guess might be that $\sqrt{\lambda_{\max}/\lambda_{\min}}$ for $N^\dagger N$ will go to a constant if the gauge coupling g is made small, while $\sqrt{\lambda_{\max}/\lambda_{\min}}$ for $M^\dagger M$ will progressively grow. Thus it seems plausible that for small enough g the additional cost of Fourier transforms required to apply the algorithm of Sec. V to the preconditioned operator will be more than made up for by the decrease in $\sqrt{\lambda_{\max}/\lambda_{\min}}$ and corresponding decrease in the number of iterations of Eq. (5.12). At least for the set of parameters at which we run the algorithm in the example described in the next section, this expectation turns out to be correct.

VIII. EXAMPLE

As a first test, we have applied the algorithms of Secs. V–VII to QCD with two flavors of quarks both with κ of 0.1600 on a 6^4 lattice. Taking from Ref. [1] the ρ mass in lattice units and critical hopping constant κ_c, and using the ρ mass to set the lattice scale, the quark mass for the calculations in this section is about 235 MeV, or about twice the strange quark mass. We calculated a variety of vacuum expectation values using Eq. (3.6) with n of 0, with n of 1, which is the valence approximation, and with n of 4, for which L_4 in Eq. (3.6) includes each of the three different six-link loops. We found also the corresponding error estimates for n of 1 from Eq. (4.2) and corrected vacuum expectations including these error estimates. All of the expectation values obtained from our algorithms we compared with direct calculations in full QCD.

The calculations in this section were done on an IBM RS/6000 workstation sustaining approximately 10 Mflops. The final production runs with our algorithm required about 1 week of machine time. The final comparison calculation with full QCD took about another 1 week. Another month or so of machine time was spent checking and exploring.

As discussed in Sec. III, rather than fixing β, we fixed β' given by the sum $\beta+\Delta\beta$. Our first task was then to calculate $\Delta\beta$. From β' and $\Delta\beta$ we determined β for full QCD. For β' we chose the value 5.700. Then $\langle\cdots\rangle_1$ becomes simply a pure gauge vacuum expectation with pure gauge β' of 5.700, and $\langle\cdots\rangle_0$ is a pure gauge vacuum expectation with the same β as used in full QCD, $5.700-\Delta\beta$.

To evaluate the expectations $\langle\cdots\rangle_0$ and $\langle\cdots\rangle_1$, ensembles of pure gauge configurations were generated using the Cabbibo-Marinari-Okawa algorithm. For $\langle\cdots\rangle_0$, β is comparatively small and we were not concerned with obtaining great precision. We found it sufficient to use 100 configurations with 100 sweeps to equilibrate and 100 sweeps between successive pairs. For $\langle\cdots\rangle_1$, however, we used 160 configurations with 1000 sweeps to equilibrate and 1000 sweeps between successive pairs. For all of the quantities for which $\langle\ldots\rangle_1$ was measured, we found 1000 sweeps to be more than sufficient to produce equilibrium values and to decorrelate successive values. The full QCD results were found using the hybrid Monte Carlo algorithm. Hamiltonian trajectories were generated using the algorithm of Ref. [13], which is faster than leapfrog by about a factor of 2. Vacuum

TABLE I. Comparison of work required to evaluate $\ln(\mathcal{O})\phi$ for different choices of $\mathcal{O}$.

$\mathcal{O}$	κ_0	$\langle\sqrt{\lambda_{max}/\lambda_{min}}\rangle$	Work/sweep	Work
$M^\dagger M$		58.1	1.0	58.1
$N^\dagger N$	0.091	22.1	2.0	44.2

expectations were taken over an equilibrium ensemble of 250 accepted trajectories, each of length 0.25 time units. Equilibrium was reached with 150 trajectories of 0.25 time units, each at β of 5.44, followed by 25 trajectories of 0.25 time units, each at β of 5.439.

To tune the algorithm of Sec. VI for $\langle\cdots\rangle_1$, we began by evaluating on each gauge configuration the ratio $\sqrt{\lambda_{max}/\lambda_{min}}$ for $M^\dagger M$. For the preconditioned operator $N^\dagger N$, we evaluated this ratio for a range of κ_0 and found the κ_0 which minimizes $\sqrt{\lambda_{max}/\lambda_{min}}$. Results are shown in Table I. The total work required to calculate $\ln(M^\dagger M)\phi$ is expected to be about 35% greater than the work required to find $\ln(N^\dagger N)\phi$ to the same accuracy. Trial calculations were consistent with this estimate. In the remainder of this section we therefore consider only the preconditioned operator and Eq. (7.3) to find $\mathrm{trln}(M^\dagger M)$.

Using the preconditioned operator N with the optimal κ_0, we then calculated the vacuum expectation value and correlation

$$V=\langle \mathrm{tr}[\ln(N^\dagger N)]\rangle_1,$$
$$C=\langle[\mathrm{tr}[\ln(N^\dagger N)]-\langle\mathrm{tr}[\ln(N^\dagger N)]\rangle_1][P-\langle P\rangle_1]\rangle_1, \tag{8.1}$$

for a range of different choices of the number of iterations of the Chebyshev algorithm, Eq. (5.12). The results are shown in Table II. The averages in Table II were found using a collection of 16 gauge configurations and 20 random ϕ for each configuration. For each configuration, we first calculated $\sqrt{\lambda_{max}/\lambda_{min}}$. The number of iterations of the Chebyshev algorithm, Eq. (5.12), was then chosen to be proportional to $\sqrt{\lambda_{max}/\lambda_{min}}$. The value of n_{Ch} shown in Table II is the number of iterations which would result for the average over all 160 configurations $\langle\sqrt{\lambda_{max}/\lambda_{min}}\rangle_1$. As n_{Ch} is increased above 50, the change in the two measured expectations shown in Table II is significantly less than the statistical errors in the expectations we found with our final, full ensemble of gauge configurations and ϕ. For the remaining calculations, we chose n_{Ch} to be 50.

TABLE II. Expectation values found from 16 gauge configurations each with 20 random ϕ, for various choices of the number of iterations of the Chebyshev algorithm used in the calculation of $\ln(N^\dagger N)\phi$.

n_{Ch}	V	C
10	390.22	6870
20	412.25	2733
50	412.74	2843
100	412.79	2848
200	412.79	2848

TABLE III. Expectation values and $\Delta\beta$ found from 160 gauge configurations for various choices of the number of random ϕ used in the evaluation of traces.

n_ϕ	V	C	$\Delta\beta$
10	416.8±2.1	2340±508	0.247±0.049
20	416.0±1.7	2343±387	0.248±0.029
30	415.8±1.5	2483±367	0.262±0.028
40	415.4±1.4	2531±343	0.267±0.026
50	414.7±1.3	2517±344	0.266±0.024
60	414.8±1.3	2499±318	0.264±0.023
70	414.9±1.2	2484±309	0.262±0.020
80	414.7±1.2	2470±294	0.261±0.018
90	414.7±1.1	2420±290	0.256±0.017
100	414.8±1.1	2483±307	0.262±0.017
110	414.8±1.1	2523±309	0.267±0.015
120	414.5±1.0	2501±296	0.264±0.014
130	414.2±1.0	2489±290	0.263±0.014
140	414.5±1.0	2472±288	0.261±0.014

Using the final ensemble of 160 gauge configurations and a range of values of the number n_ϕ of random ϕ for each gauge configuration we calculated V and C of Eq. (8.1). We also evaluated the dispersion $\langle[P-\langle P\rangle_1]^2\rangle_1$. We obtained the value $(5.68\pm0.61)\times10^4$. From C and $\langle[P-\langle P\rangle_1]^2\rangle_1$ we then found $\Delta\beta$. The results are shown in Table III. As expected, the values we obtained are consistent within errors as n_ϕ is varied while the size of the errors themselves tends to fall as n_ϕ increases. The optimal choice of n_ϕ producing the smallest statistical uncertainty in $\Delta\beta$ for a fixed amount of computation can be shown to be roughly 100.

The error bars on the numbers in these tables are statistical, found by the bootstrap method. From the ensemble of 160 data sets, each consisting of a gauge configuration and an associated collection of n_ϕ random ϕ, we randomly chose 160 new data sets to generate a bootstrap ensemble. On each bootstrap ensemble we then found V. In this way 100 bootstrap ensembles and 100 values of V were found. From these we evaluated the difference between the value of V larger than all but 15 results and the value of V smaller than all but 15 results. Half of this difference is shown as the statistical error. The errors for C and $\Delta\beta$ were found similarly. In the calculation of the error for $\Delta\beta$, $\langle[P-\langle P\rangle_1]^2\rangle_1$ was calculated independently on each bootstrap ensemble and used to determine the corresponding bootstrap value for $\Delta\beta$.

The most reliable value for $\Delta\beta$ is 0.261±0.014, obtained with n_ϕ of 140. Our algorithm then predicts that expectation values in full QCD with two flavors of quarks, κ of 0.1600

TABLE IV. Coefficients in the expansion of L_4 as a linear combination of $h_0,\ldots,h_4$.

i	a_i	$a_i/6^2$
0	414.5 (10)	11.513 (28)
1	10.4 (7)	0.288 (20)
2	2.9 (5)	0.079 (15)
3	1.9 (5)	0.053 (15)
4	0.7 (5)	0.020 (15)

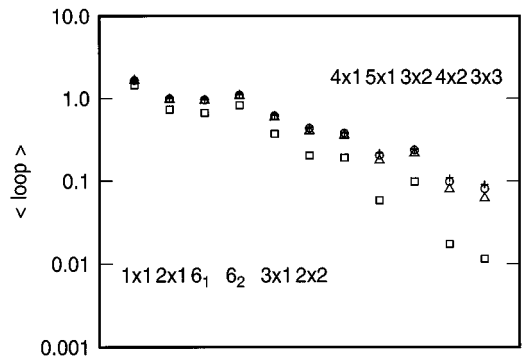

FIG. 1. Vacuum expectations of various Wilson loops found by four different methods. Boxes represent $n=0$ with $\beta=5.439$, triangles are the valence approximation $n=1$ with $\beta'=5.700$, circles are $n=4$ with $\beta'=5.700$, and plus signs are full QCD with $\beta=5.439$ and two quark flavors with $k=0.1600$.

and β of 5.439, will agree with $\langle\cdots\rangle_1$ at β' given by $\beta+\Delta\beta$ which is 5.700 ± 0.014. A still more accurate approximation to the full QCD expectation with two quark flavors, κ of 0.1600 and β of 5.439, is given by $\langle\cdots\rangle_4$ of Eq. (3.6) with L_4 including contributions from the plaquette and from each of the six-link closed paths. The coefficients in the expansion of Eq. (3.4) are found from the inner product of Eq. (2.2) with $\mathcal{S}$ of Eq. (4.7) and β' of 5.700. Table IV gives the coefficients $a_0,\ldots,a_4$ of $\hat{h}_0,\ldots,\hat{h}_4$ in Eq. (3.4). Here $\hat{h}_0,\ldots\hat{h}_4$, as discussed in Sec. II, are found by Gram-Schmidt orthonormalization applied to the sequence $h_0,\ldots,h_4$. The function h_0 is the constant 1, h_1 is Wilson's plaquette action Eq. (2.3), and h_2,h_3, and h_4, respectively, are the rotation- and translation-invariant linear combinations of the planar six-link loop, the loop six-consisting of the 6 link boundary of three orthogonal plaquettes joined to form half the surface of a cube, and the loop 6_2 consisting of the six-link boundary of a pair of orthogonal plaquettes joined on an edge. Having normalized the h_i to 1, each a_i with $i\geqslant1$ contains, in effect, a factor of the square root of the number of sites in the lattice. Table IV therefore lists also values for a_i divided by the square root of the number of lattice sites, 6^2. As i is increased, the a_i in Table IV fall rapidly. The coefficient a_4 is about 1.4 standard deviations away from 0.

Figure 1 shows vacuum expectations of a collection of different Wilson loops. All loops are rectangular with dimensions as shown except for the nonplanar six-link loops 6_1 and 6_2 we have just defined. The normalization of each loop is

$$\mathrm{tr}[u(x_1,x_2)u(x_2,x_3)\cdots u(x_n,x_1)], \tag{8.2}$$

so that if all link matrices $u(x,y)$ were given by the identity matrix, all loops would become 3. Each loop expectation shown in the figure is obtained in four different ways. Boxes indicate Eq. (3.6) with n of 0 and β of 5.439. Triangles represent the valence approximation, Eq. (3.6) with n of 1 and $\beta+\Delta\beta$ of 5.700. Circles give the vacuum expectation of Eq. (3.6) with n of 4 and $\beta+\Delta\beta$ of 5.700. Plus signs show full QCD with β of 5.439 and two flavors of quarks with κ of 0.1600.

For all but the 1×1 loop, clear differences can be seen in Fig. 1 between data points with n of 0 and β of 5.439 and points for the full theory with β of 5.439. For the largest loops these two results differ by as much as a factor of 10. For most loops, nearly all of this shift is correctly reproduced by the valence approximation, n of 1 and $\beta+\Delta\beta$ of 5.700. For the largest loops the valence approximation reproduces most of the shift due to vacuum polarization, but falls noticeably below the results of full QCD. The vacuum expectation, Eq. (3.6), with n of 4, with L_4 including a plaquette contribution and contributions from the three different six-link loops, agrees with full QCD within statistical errors for all but the three largest loops. Even for these, the expectation with n of 4 corrects more than 3/4 of the difference between the valence approximation and full QCD.

Since the error bars on all points in Fig. 1 are smaller than the symbols, in Table V we also give numerical values. In Table V we list, in addition to the data shown in the figure, Eq. (3.6) with n of 1 and $\beta+\Delta\beta$ of 5.700 but corrected by the error estimate of Eq. (4.2). This result is consistent with full QCD in all cases.

Overall, it appears that at least for the parameters considered here, the valence expansion of Eq. (3.6) converges rapidly to full QCD and the error estimate of Eq. (4.2) is quite reliable as a error estimate for the valence approximation. The difference between the valence approximation expectation $\langle\cdots\rangle_1$ and the expectation $\langle\cdots\rangle_4$ is almost as reliable as a valence approximation error estimate.

TABLE V. Vacuum expectation of various Wilson loops found by five different methods.

Loop	$n=0$ $\beta=5.439$	$n=1$ $\beta'=5.700$ (valence)	$n=4$ $\beta'=5.700$	$n=1$ + error $\beta'=5.700$ (valence + error)	Full QCD $\beta=5.439$ $\kappa=0.16$
1×1	1.4480 (15)	1.6503 (11)	1.6554 (17)	1.6504 (94)	1.6629 (5)
2×1	0.7313 (19)	0.9784 (16)	1.0013 (22)	0.9974 (138)	1.0090 (6)
6_1	0.6637 (19)	0.9426 (18)	0.9668 (26)	0.9620 (127)	0.9757 (6)
6_2	0.8243 (18)	1.0850 (16)	1.1013 (24)	1.0963 (113)	1.1099 (6)
3×1	0.3729 (16)	0.5898 (15)	0.6167 (22)	0.6107 (144)	0.6254 (7)
2×2	0.2033 (14)	0.4024 (16)	0.4367 (27)	0.4436 (142)	0.4480 (7)
4×1	0.1906 (12)	0.3563 (13)	0.3815 (21)	0.3747 (127)	0.3899 (6)
5×1	0.0584 (10)	0.1775 (12)	0.2042 (22)	0.2138 (99)	0.2166 (6)
3×2	0.0977 (9)	0.2160 (12)	0.2363 (16)	0.2322 (103)	0.2438 (6)
4×2	0.0172 (7)	0.0793 (10)	0.0978 (16)	0.1037 (66)	0.1085 (4)
3×3	0.0115 (8)	0.0618 (8)	0.0803 (18)	0.0922 (85)	0.0901 (4)

TABLE VI. Square of the distance between L_i and trln($N^\dagger N$). The calculation uses 160 gauge configurations each with 140 random ϕ.

i	$\langle[\mathrm{tr}[\ln(N^\dagger N)]-L_i]^2\rangle_1$
0	123.7 ± 17.4
1	16.0 ± 6.7
2	7.9 ± 7.8
3	4.2 ± 6.2
4	3.7 ± 4.6

As a further check of our method, we calculated expectation values of the squared differences

$$D_i=\langle[\ln(N^\dagger N)-L_i]^2\rangle_1, \tag{8.3}$$

for L_i given by Eq. (3.4) with i of $0,\ldots,4$. As a consequence of the definition of L_0, the term D_0 is just the squared dispersion

$$D_0=\langle\{\mathrm{tr}[\ln(N^\dagger N)]-\langle\mathrm{tr}[\ln(N^\dagger N)]\rangle_1\}^2\rangle_1. \tag{8.4}$$

To find D_0, we evaluated

$$E=\frac{1}{n_\phi}\left\langle\left[\sum_{i=1}^{n_\phi}((\ln(N^\dagger N)\phi_i,\ln(N^\dagger N)\phi_i))\right]\right\rangle_1,$$

$$D_0'=\frac{1}{n_\phi{}^2}\left\langle\left(\sum_{i=1}^{n_\phi}((\phi_i,\ln(N^\dagger N)\phi_i))-\sum_{i=1}^{n_\phi}\langle((\phi_i,\ln(N^\dagger N)\phi_i))\rangle_1\right)^2\right\rangle_1. \tag{8.5}$$

As in Sec. V, since for each i and x the $\phi_i(x)$ are Gaussian random variables with covariance given by Eq. (5.2), the averages over ϕ in the definition of E and D_0' can be evaluated analytically. For D_0 we then obtain

$$D_0=D_0'-\frac{E}{n_\phi}. \tag{8.6}$$

Other D_i were found similarly.

Results obtained from 160 gauge field configurations with n_ϕ of 140 are given in Table VI. As i increased the D_i fall rapidly to 0, with D_2, D_3, and D_4 all statistically consistent with 0. Thus as i increased, the L_i approachs tr[$\ln(N^\dagger N)$] rapidly in the norm of the Hilbert space $\mathcal{H}$ of Sec. II.

IX. COMPARISON WITH PERTURBATION EXPANSION

A calculation of the effect of quark-antiquark vacuum polarization using a weak-coupling perturbation expansion to leading order was reported recently in Ref. [10]. Staggered quarks are considered in Ref. [10] in place of our choice of Wilson quarks. The weak-coupling expansion in Ref. [10] is expected to be reliable for sufficiently small gauge coupling and sufficiently large quark mass. For two flavors of quarks with degenerate mass ma in lattice units ranging from 0.05 to 1.00 and a parameter corresponding to β' fixed at 5.68, the main effect of quark-antiquark vacuum polarization is found to be simply a coupling constant shift $\Delta\beta$. As ma ranges from 0.05 to 1.00, the shifted β for full QCD runs from 5.34 to 5.63.

For Wilson quarks, the mass is

$$ma=\frac{1}{2k}-\frac{1}{2k_c}. \tag{9.1}$$

Here k_c is the critical hopping constant at which the pion mass becomes 0. With our choice of 0.1600 for κ and with κ_c of 0.1694 [1] at β' of 5.700, ma becomes 0.1734. To a first approximation, corresponding versions of QCD with Wilson quarks and with staggered quarks should have equal values of quark mass and β. Thus the parameters of our trial calculation fall nearly within the range considered in the perturbative calculation of Ref. [10] and our results are qualitatively consistent with theirs. For two flavors of staggered quarks with ma of 0.1734 and β' of 5.68, the perturbative calculation predicts a $\Delta\beta$ of 0.226 in comparison to our prediction of 0.261 ± 0.014 for two flavors of Wilson quarks.

X. CONCLUSION

For the heavy quark mass used in the example of Sec. VIII, the computer time required to obtain an error estimate on loop expectation in the valence approximation by our algorithm was roughly comparable to that required to simply calculate these expectation values directly in full QCD. The crucial question which we have not yet answered is how much time would be required to apply the algorithm we have described to QCD and determine, from Eq. (4.2) with n of 1, the error in the valence approximation to hadron propagators for more realistic choices of quark mass, lattice spacing, and lattice volume than we chose in the test in the preceding section. If the algorithm can be run in reasonable time with n of 1, it might be possible to use larger n and obtain smaller errors in hadron propagators. If the error found in this way for some small value of n is itself small for at least one quantity from which the physical value of the lattice spacing can be determined, it will be possible to calculate $\alpha_{\overline{\mathrm{MS}}}$ for full QCD, where $\overline{\mathrm{MS}}$ denotes the modified minimal subtraction scheme.

A perturbation theory estimate, which we will not discuss here, suggests that the optimal number of random ϕ which our method requires will grow more slowly than a power of the inverse lattice spacing or the inverse quark mass. Similar estimates suggest similar growth rates for the number of independent gauge configurations needed to evaluate the expectation values entering the determination of the coefficients a_i in the expansion in Eq. (3.1). The remaining question is how large an ensemble of gauge configurations may be required for small values of lattice spacing and quark mass to find the valence approximation error in hadron propagators using Eq. (4.2). If the difference Q_n for some small value of n turns out to be quite small, as occurs for the parameter values in Sec. VIII, or if Q_n is sensitive only to low momentum fluctuations of the gauge field, the calculation of propagator errors may be possible with reasonable ensembles sizes. We do not know at present whether one of these conditions might be realized for values of lattice spacing and quark mass which would permit an extrapolation to the physical limit of hadron masses.

ACKNOWLEDGMENTS

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APPENDIX CHEBYSHEV EXPANSION

We now derive the coefficients n_i needed for the Chebyshev expansion of ln$y$ Eq. (5.7). From standard results on Chebyshev polynomials [15], it follows that

$$\frac{1}{y}\left[1+\rho T^*_{n+1}\left(\frac{1-y}{1-\epsilon}\right)\right]=\sum_{k=0}^{n} c_k T^*_k\left(\frac{1-y}{1-\epsilon}\right), \tag{A1}$$

where, for $1\leqslant k\leqslant n$,

$$c_k=2\frac{(1+\cosh\chi)\sinh[(n+1-k)\chi]}{\sinh\chi\cosh[(n+1)\chi]} \tag{A2}$$

and, in addition,

$$c_0=\frac{(1+\cosh\chi)\sinh[(n+1)\chi]}{\sinh\chi\cosh[(n+1)\chi]},$$

$$\rho=\frac{-1}{\cosh[(n+1)\chi]}, \tag{A3}$$

with χ defined by

$$\cosh\chi=\frac{1+\epsilon}{1-\epsilon}. \tag{A4}$$

Equation (A1) can be integrated from y to 1 using, for k greater than 1, the relation

$$\int T^*_k(x)dx=\frac{T^*_{k+1}(x)}{4(k+1)}-\frac{T^*_{k-1}(x)}{4(k-1)}, \tag{A5}$$

along with

$$\int T^*_1(x)dx=\frac{T^*_2(x)}{8}-\frac{T^*_0(x)}{8},$$

$$\int T^*_0(x)dx=\frac{T^*_1(x)}{2}+\frac{T^*_0(x)}{2}. \tag{A6}$$

We obtain

$$\ln(y)=\sum_{k=0}^{n+1} b_k T^*_k\left(\frac{1-y}{1-\epsilon}\right)+\delta\ln(y), \tag{A7}$$

where, for $1\leqslant k\leqslant n$,

$$b_k=-\frac{(1-\epsilon)(1+\cosh\chi)\cosh[(n+1-k)\chi]}{k\cosh[(n+1)\chi]} \tag{A8}$$

and, in addition,

$$b_{n+1}=-\frac{(1-\epsilon)(1+\cosh\chi)}{2(n+1)\cosh[(n+1)\chi]},$$

$$b_0=-\sum_{k=1}^{n+1}(-1)^k b_k. \tag{A9}$$

The bound, Eq. (5.8), on δ follows from the integral of Eq. (A1) combined with Eq. (A2) for ρ and the bound

$$|T^*_k(x)|\leqslant 1, \tag{A10}$$

for $0\leqslant x\leqslant 1$.

[1] F. Butler, H. Chen, J. Sexton, A. Vaccarino, and D. Weingarten, Phys. Rev. Lett. **70**, 2849 (1993); Nucl. Phys. **B430**, 179 (1994).

[2] F. Butler, H. Chen, J. Sexton, A. Vaccarino, and D. Weingarten, Nucl. Phys. **B421**, 217 (1994).

[3] D. H. Weingarten, Phys. Lett. **109B**, 57 (1982); Nucl. Phys. **B215** [FS7], 1 (1983).

[4] J. Sexton and D. Weingarten, in *Lattice '94*, Proceedings of the International Symposium on Lattice Field Theory, Bielefeld, Germany, edited by F. Karsch *et al.* [Nucl. Phys. B (Proc. Suppl.) **42**, 361 (1995)].

[5] A. Morel, J. Phys. (Paris) **48**, 111 (1987).

[6] S. Sharpe, Phys. Rev. D **41**, 3233 (1990); in *Lattice '89*, Proceedings of the International Symposium on Lattice Field Theory, Capri, Italy, 1989, edited by R. Petronzio *et al.* [Nucl. Phys. B (Proc. Suppl.) **17**, 146 (1990)]; Phys. Rev. D **46**, 3146 (1992); **30**, 213 (1993); J. Labrenz and S. Sharpe, in *Lattice '93*, Proceedings of the International Symposium, Dallas, Texas, edited by T. Draper *et al.* [*ibid.* **34**, 335 (1994)].

[7] C. Bernard and M. Golterman, in *Lattice '91*, Proceedings of the International Symposium, Tsukuba, Japan, edited by M. Fukugita *et al.* [Nucl. Phys. B (Proc. Suppl.) **26**, 360 (1992)]; C. Bernard and M. Golterman, Phys. Rev. D **46**, 853 (1992); C. Bernard and M. Golterman, in *Lattice '92*, Proceedings of the International Symposium on Lattice Field Theory, Amsterdam, The Netherlands, edited by J. Smit and P. van Baal [Nucl. Phys. B (Proc. Suppl.) **30**, 217 (1993)].

[8] D. Weingarten, in *Lattice '93* [6], p. 29.

[9] A. Duncan, E. Eichten, S. Perrucci, and H. Thacker, in *Lattice '96*, Proceedings of the International Symposium, St. Louis, Missouri, edited by T. Golterman [Nucl. Phys. B (Proc. Suppl.) (in press)], Report No. hep-lat/9608110 (unpublished).

[10] A. Hasenfratz and T. DeGrand, Phys. Rev. D **49**, 466 (1994); *Lattice '93* [6], p. 317.

[11] A. Ukawa, in *Lattice '92* [7], p. 3; D. Weingarten, in *Lattice '93*, [6], p. 29; C. Michael, in *Lattice '94*, [4], p. 147.

[12] D. Weingarten, Report No. IBM-HET-96-1, 1996 (unpublished).

[13] J. Sexton and D. Weingarten, Nucl. Phys. **B380**, 665 (1992).

[14] G. H. Golub and C. F. Van Loan, *Matrix Computations* (The Johns Hopkins University Press, Baltimore, 1989), p. 478.

[15] L. Fox and I. B. Parker, *Chebyshev Polynomials in Numerical Analysis* (Oxford University Press, London, 1968).

[16] M. Luescher, Nucl. Phys. **B418**, 637 (1994).