Exact ground-state properties of SU(3) Hamiltonian lattice gauge theory

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We solve for the exact ground state of SU(3) Hamiltonian lattice gauge theory via the guided-random-walk algorithm. We show that the algorithm is effective in calculating the ground-state energy with excellent precision. By comparing exact and variational ground-state results in the case of SU(2) and SU(3), we further demonstrate that variational calculations based on the independent-plaquette trial function improve with increasing N from $N=2$ to $N=3$.

I. INTRODUCTION

In the Hamiltonian formulation of lattice gauge theory, physical observables such as glueball masses and string tension can be studied nonperturbatively via variational methods by evaluating only ground-state expectation values.[1-3] The required ground state can be evolved exactly via Hamiltonian Monte Carlo methods,[3-12] or further approximated by a variational trial function. The fact that a simple independent-plaquette trial function can produce evidence for a scaling 0^{++} glueball mass[13] in SU(5) and SU(6) strongly suggests that similar results in SU(3) can be obtained with a better trial function. Since all algorithms for evolving the exact ground state are computationally more intensive than merely sampling a trial function, finding an adequate variational ground state would greatly reduce the numerical efforts for determining physical observables. However, in order to assess the quality of the trial function directly, it is essential to know some properties of the exact ground state. In this work, we computed the exact SU(3) ground-state energy and the plaquette expectation value via the guided-random-walk[7,10,3] (GRW) algorithm. For future references, we give the exact ground-state energy numerically and in the form of a fitted polynomial. By comparing these results with those obtained variationally on the basis of the independent-plaquette trial function, as well as those obtained previously in the case of SU(2), we further demonstrate that the independent-plaquette trial function becomes increasingly better for larger N, at least in going from $N=2$ to $N=3$.

II. HAMILTONIAN LATTICE GAUGE THEORY

We consider the Kogut-Susskind SU(N) lattice Hamiltonian[14] in the form

$$H_{\rm KS}=\frac{g^2}{a}\{H\}=\frac{g^2}{a}\left\{\tfrac{1}{2}E_l^aE_l^a+\lambda\sum_p\left[1-\frac{1}{2N}\mathrm{Tr}(U_p+U_p^\dagger)\right]\right\}, \quad (1)$$

where $\lambda\equiv 2N/g^4$, l and p are link and plaquette labels, and where repeated indices imply summations. The color-electric field operators are to be regarded as first-order differential operators such that $E_l^aU_l=\delta_{l,l'}T^aU_l$, where $T^a=\frac{1}{2}\tau^a$ for SU(2) and $T^a=\frac{1}{2}\lambda^a$ for SU(3). For Monte Carlo calculation and other purposes, it is convenient to use the dimensionless Hamiltonian H with coupling λ as defined above. For example, in the strong-coupling limit of $\lambda\ll 1$, the dimensionless ground-state energy per plaquette defined by

$$e_0=E_0/N_p=\frac{1}{N_p}\frac{\langle\Psi_0|H|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle},$$

has the expansion

$$e_0=\lambda-\lambda^2/6+\cdots \quad (2)$$

for SU(2) and

$$e_0=\lambda-\lambda^2/48-\lambda^3/768-0.053\,888(\lambda/6)^4+\cdots \quad (3)$$

for SU(3). The fourth-order ground-state energy in SU(3) was previously computed in Ref. 15, but the explicit expression was never given. The above result is our independent determination. It also follows that the ground-state expectation value of the plaquette operator,

$$P=\frac{1}{N_p}\frac{1}{2N}\sum_p\mathrm{Tr}(U_p+U_p^\dagger), \quad (4)$$

can be obtained as

$$\langle P\rangle=\frac{\langle\Psi_0|P|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}=1-\frac{de_0}{d\lambda}. \quad (5)$$

It has been suspected for some time[16-20] that a reasonable trial ground state for (1) is the independent-plaquette wave function

$$\Phi_0=\exp(AN_pN^2P), \quad (6)$$

where P is the plaquette operator and A is the sole variational parameter. However, prior to the advent of Hamiltonian Monte Carlo methods for evolving the exact

ground state, there was no direct way of gauging the quality of this trial function, and no confidence was placed on its results. As we shall see, in comparison to the exact ground state, this trial function is an excellent first approximation.

Because of its directness in addressing the question of the spectrum, interest in Hamiltonian lattice gauge remains unabated. Aside from advances in exact Monte Carlo methods such as the GRW, momentum-space GRW (Refs. 2 and 12), variant GRW (Ref. 11), Green's-function Monte Carlo methods,[6,9] and projector Monte Carlo[8] methods, there are also notable developments in semianalytical methods of t expansion,[21–23] basis diagonalization,[24] and plaquette space integration.[25] In this work, we will concentrate on results obtained via the GRW algorithm. Since this algorithm, as applied to lattice gauge theories, has been extensively documented elsewhere,[7,10,3] we will be brief in summarizing its salient features.

III. THE GRW ALGORITHM

The exact ground state $|\Psi_0\rangle$ of H can be evolved from any initial trial state $|\Phi_0\rangle$ not orthogonal to $|\Psi_0\rangle$ via

$$|\Psi_0\rangle = \lim_{t\to\infty} e^{-t(H-E)}|\Phi_0\rangle \ . \tag{7}$$

In particular, the mixed product $\Phi_0|\Psi_0\rangle$ can be directly evolved as

$$\begin{aligned}\Phi_0|\Psi_0\rangle &= \lim_{t\to\infty}\Phi_0 e^{-t(H-E)}|\Phi_0\rangle \\ &= \lim_{t\to\infty} e^{-t(\tilde{H}-E)}\Phi_0|\Phi_0\rangle \ ,\end{aligned} \tag{8}$$

where $\tilde{H}=\Phi_0 H\Phi_0^{-1}$. By discretizing $t=N\Delta t$ and inserting complete sets of states between successive factors of $e^{-\Delta t(\tilde{H}-E)}$, the right-hand side (RHS) of (8) can be regarded as a path integral. To generate an ensemble of lattice configurations distributed according to $\Phi_0(x)\Psi_0(x)$, the GRW algorithm samples this path integral iteratively as follows: A population of $N_{\rm pop}$ lattice configurations is initially prepared with distribution $\Phi_0^2(x)$ using, for example, the Metropolis method. Successive generation of lattice configurations are then evolved stochastically according to the matrix element $\langle x_{n+1}|e^{-\Delta t(\tilde{H}-E)}|x_n\rangle$. To order Δt, this matrix element can be factored into two pieces corresponding to the kinetic (or electric) and the potential (or magnetic) part of the Hamiltonian $\tilde{H}$. The kinetic piece can be sampled by multiplying each link matrix of each lattice configuration sequentially by a stepping SU(3) matrix Gaussian distributed near the identity with step size $\approx\sqrt{\Delta t}$ but slightly biased (i.e., guided) by Φ_0. The potential piece can be sampled by replicating an entire lattice configuration according to its expectation value of

$$\exp\{-\Delta t[\Phi_0^{-1}(x)H\Phi_0(x)-E]\} \ .$$

After the ensemble has evolved long enough to reach the stationary distribution $\Phi_0(x)\Psi_0(x)$, the ground-state energy E_0 can be determined as that value of E which keeps the ensemble population stable, usually around $N_{\rm pop}$, in successive generations. Alternatively, E_0 can be calculated directly from the ensemble configurations via

$$E_0=\frac{\langle H\Phi_0|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle} \ . \tag{9}$$

Note that in this case, if Φ_0 were the exact ground state, then the above direct determination would yield E_0 exactly irrespective of any Monte Carlo errors. In general, significant reduction of statistical errors in the ground-state energy can be achieved with any reasonable trial functions. By repeating the calculation several times using different values of Δt, the residual error of order Δt can be eliminated by a simple linear extrapolation. The values of E_0 determined by these two methods are usually in excellent agreement with each other after the time-step extrapolation.

Since the GRW algorithm only generates an ensemble of lattice configurations with distribution $\Phi_0(x)\Psi_0(x)$, the ground-state expectation values of operators other than the Hamiltonian can be obtained most conveniently via a simple perturbative estimate:[4]

$$\begin{aligned}\frac{\langle\Psi_0|0|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle} &= 2\frac{\langle\Phi_0|0|\Psi_0\rangle}{\langle\Phi_0|\Psi_0\rangle}-\frac{\langle\Phi_0|0|\Phi_0\rangle}{\langle\Phi_0|\Phi_0\rangle} \\ &\quad +O((\Psi_0-\Phi_0)^2) \ .\end{aligned} \tag{10}$$

To the extent that the trial function is a reasonable approximation to the exact ground state, this perturbative estimate can be quite accurate.

IV. GROUND-STATE RESULTS

For uniformity in comparing results for different SU(N) gauge groups, it is more useful to introduce the dimensionless Kogut-Susskind ground-state energy per plaquette per gluon degree of freedom defined by

$$\epsilon_0=\frac{a\langle H_{KS}\rangle}{N_p(N^2-1)} \ , \tag{11}$$

and to employ the coupling constant $\xi\equiv 1/Ng^2$, where ξ is related to λ via $\xi=\sqrt{\lambda}/2N^3$ and $\epsilon_0=e_0/[\xi N(N^2-1)]$. Figure 1 shows the SU(2) ground-state energy taken from Ref. 10 and plotted in this manner. The variational results are ground-state energies calculated with the trial function (6) and minimized with respect to A. The average configuration population maintained in the exact GRW calculation was $N_{\rm pop}=10$. The lower solid curve is the second-order strong-coupling result given by (2). In the weak-coupling limit, the energy ϵ_0 has the simple expansion

$$\epsilon_0(\xi)=C_0-C_1/\xi-C_2/\xi^2-\cdots \ . \tag{12}$$

The constant C_0 is universal for all SU(N) gauge groups but has a slight dependence on lattice size. For lattice sizes of 4^3, 6^3, and ∞^3, the values for C_0 are, respectively, 0.793 43, 0.795 42, and 0.795 87. The constant C_1 appears also to be universal, although it has never been explicitly calculated except in the case of U(1) (Ref. 19). As

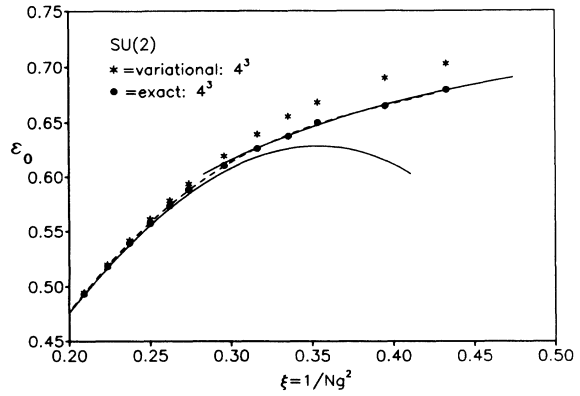

FIG. 1. The dimensionless ground-state energy per plaquette per gluon degree of freedom ϵ_0, as a function of the coupling constant $\xi=1/Ng^2$ for a 4^3 lattice. The lower and upper curves are strong- and weak-expansion results. See text for details.

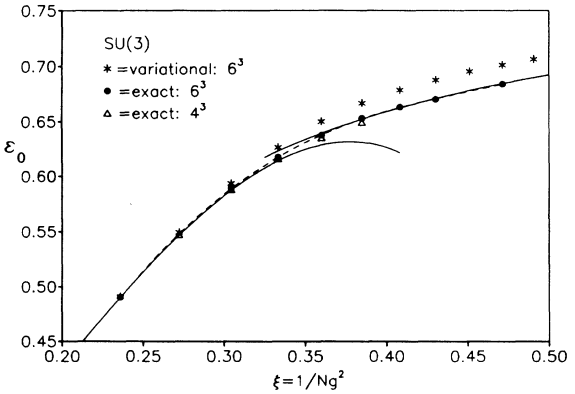

FIG. 2. The dimensionless ground-state energy ϵ_0, as a function of the coupling constant $\xi=1/Ng^2$ for the case of SU(3). See text for details.

we shall see, the SU(2) and SU(3) values for C_1 are numerically found to agree well with the U(1) value of $C_1=C_0^2/16$ ($=0.039\,34$, $0.039\,54$, $0.039\,59$, respectively, for the previous lattice sizes). As was first done in Ref. 10, by simply fitting a few data points at high values of ξ, one finds that $C_1\approx 0.041$ and $C_2\approx 0.004$. The resulting weak-coupling expansion with these constants is plotted as the upper solid curve in Fig. 1. As a succinct summary, we also give the following low-order polynomial fit to the exact ground-state energies between $0.6\le\lambda\le 3.0$:

$$e_0=-0.029\,463+1.090\,682\lambda-0.253\,427\lambda^2 +0.029\,705\lambda^3\ . \tag{13}$$

The fitted results, reexpressed in terms of ϵ_0 and ξ, are plotted in Fig. 1 as a dashed line. We have chosen to fit e_0 in terms of λ because the plaquette expectation value can then be estimated easily via (5). We caution that a good fit for the energy may not be good enough for estimating its derivative.

Figure 2 contains our new results for SU(3). As in Ref. 10, the GRW algorithm is initiated by sampling Φ_0^2 with the optimal value of A via the Metropolis algorithm. The number of hits per link ranges from 1 to 5 depending on A and 1500 sweeps are typically used for equilibration. An average population of $N_{\rm pop}=20$ configurations are maintained in the exact GRW algorithm for both the 6^3 and the 4^3 calculation. Each complete calculation at a single value of λ, with four runs of different time-step size for the 4^3 lattice and three runs for the 6^3 lattice, requires ~ 2 Cyber 205 hours. The largest step size used in the 6^3 lattice calculation ranges from $\Delta t=0.06$ for $\lambda=5$ to $\Delta t=0.02$ for $\lambda=10$. For each step size Δt, after equilibrated for 200–300 generations, expectation values are computed in blocks of 100 generations (~ 2000 configurations), and averaged over 8–15 blocks. The plotted variational results have the same meaning as in the SU(2) case and are taken from Ref. 13. The lower curve is the strong-coupling result given by (3). The upper solid curve is the fitted weak-coupling expansion with $C_1\approx 0.040$ and $C_2\approx 0.006$. The numerical values of the plotted ground-state energies are tabulated in Table I. The dashed curve is the polynomial fit to data between $3\le\lambda\le 12$:

$$e_0=-0.313\,249+1.214\,438\lambda-0.067\,631\lambda^2 +0.001\,862\lambda^3\ . \tag{14}$$

In the case of the ground-state energy, finite-size effects appear to be small, as is evident from the close agreement

TABLE I. Numerical values for the optimal variational parameter A, the SU(3) exact ground-state energy e_0, and the plaquette expectation value evaluated according the perturbative estimate (10). Uncertainties in the last digit are enclosed in parentheses.

λ	A	e_0 (6^3)	$\langle P\rangle_{\rm pert}$ (6^3)	$\langle P\rangle_{\rm pert}$ (4^3)
3	0.13	2.775(0)	0.1605(5)	
4	0.18	3.575(1)		0.231(1)
5	0.225	4.304(2)	0.298(5)	0.305(3)
6	0.27	4.939(2)	0.377(3)	0.383(5)
7	0.315	5.510(3)	0.449(4)	0.449(4)
8	0.35	6.034(5)	0.491(5)	0.503(5)
9	0.38	6.50(1)	0.539(3)	
10	0.41	6.92(1)	0.576(5)	
12	0.44	7.74(1)	0.616(5)	

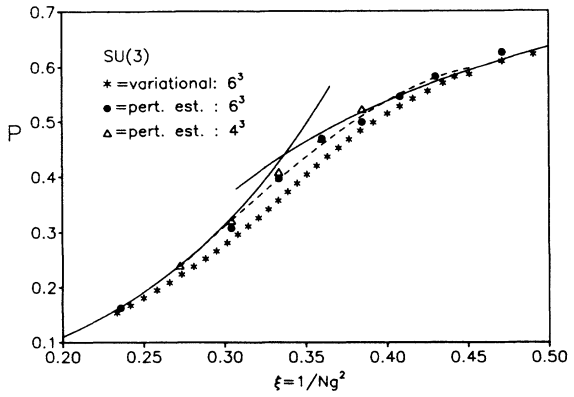

FIG. 3. The SU(3) ground-state plaquette expectation value as a function of the coupling constant $\xi=1/Ng^2$. See text for details.

between the 4^3 and the 6^3 data. The SU(3) ground-state energy has also been computed via the t expansion method;[22] unfortunately, because Ref. 22 only presented results in graphic forms, we were unable to make a direct comparison.

Figure 3 gives the SU(3) expectation value of the plaquette operator P. The numerical values for both the 6^3 and the 4^3 calculations are given in Table I. The importance of this expectation value is that it is essentially the derivative of the ground-state energy. The lower solid, upper solid and the middle dashed curves are obtained by differentiating the strong-coupling, the weak-coupling and the fitted ground-state energy, respectively. The direct perturbative evaluations of $\langle P \rangle$ according to (5), despite greater time-step extrapolation errors, remain in good overall agreement with the above results. In comparison, the variational estimates are generally lower, and appear to have less of a bend, than the exact expectation. These characteristics of the variational calculation are also similar to those found previously[10] in the case of SU(2).

From Figs. 1 and 2, it is clear that the independent-plaquette trial function is capable of reproducing the bulk behavior of the exact energy. Its major failing appears to be that of being higher than the exact energy in the weak-coupling regime by a roughly constant amount. In SU(2), from the last two data points in Fig. 1, we find $\Delta\epsilon=\epsilon_0(\text{var})-\epsilon_0(\text{exact})\approx 0.024$. However, in SU(3), over that same range of ξ, this difference has diminished to $\Delta\epsilon\approx 0.016$; a 33% improvement. It is thus highly suggestive that Φ_0 is becoming a better trial ground state as N increases.

V. CONCLUSIONS

In this work, we have shown that the GRW algorithm is effective in computing the exact ground-state energy. Our numerical value for the exact energy can serve as a useful reference point for future improvements of the variational ground-state wave function. Since our experience has been that a GRW run requires at least an order of magnitude more CPU time than a corresponding variational calculation, finding an adequate trial function would greatly reduce the numerical efforts needed to evaluate physical observables. Already we have some evidence that a sufficiently good trial ground state for SU(3) may not be too difficult to devise.[26]

By comparing the exact and the variational ground-state energy in both SU(2) and SU(3), our work has not only shown that the independent-plaquette wave function is a very good first approximation to the exact ground state, but also provided the first direct evidence that it actually improves with increasing N.

The current GRW algorithm is less effective in computing expectation values of operators other than the Hamiltonian. In evaluating the plaquette expectation value, due to the fact that we are limited to only three or four Δt values for performing the $\Delta t\rightarrow 0$ extrapolation, the resulting extrapolation errors are quite large. All errors noted in Table I are errors of this type. Moreover, we have noticed considerable bias in $\langle P \rangle$ as we go from $N_{\text{pop}}=15$ to $N_{\text{pop}}=20$. We would have preferred to do the calculation, resources permitting, with a population size of $N_{\text{pop}}=30-50$ instead. A possible improvement of the GRW algorithm, that would alleviate some of these difficulties, would be to develop a second-order GRW algorithm that has only a residual error of $(\Delta t)^2$. As pointed out elsewhere,[3] the guided walk part of the GRW algorithm is exactly the same as the Langevin algorithm. It is very likely that recent advances in developing the second-order Langevin algorithm[27–29] for solving Euclidean pure gauge theory can lead to similar improvements in the GRW algorithm.

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