Variational estimate of the energy of an elementary excitation of the SU(2) lattice gauge theory

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We describe a variational estimate of the energy of an elementary excitation of the SU(2) lattice gauge theory. The vacuum state is modeled by a disordered trial wave function, which is optimized by the variational principle; and the excited state is constructed by letting a translation-invariant sum of plaquette operators act on the vacuum. The result does not have the proper continuum-limit behavior.

Lattice gauge theories can be formulated in the path-integral approach of Wilson[1] or the Hamiltonian operator approach of Kogut and Susskind.[2] The operator formulation deals directly with quantum states of the fields. For example, strong-coupling perturbation theory constructs approximate eigenstates by letting combinations of field operators act on the strong-coupling vacuum, the totally disordered state in which all field configurations are equally probable.[3] The challenge of the Hamiltonian formulation of lattice gauge theories is to construct weak-coupling approximations of the eigenstates; these are relevant to the continuum limit of the theory.

The variational principle offers a way to study the states of Hamiltonian lattice gauge theories.[4,5] We have described a variational estimate of the ground state of the SU(2) lattice gauge theory, based on a disordered trial wave function.[5] That work was partly motivated as a first step toward a study of the vacuum state by the Green's-function Monte Carlo method.[6] But the variational calculation is interesting in its own right.

The disordered trial wave function is a product of functions of the single plaquette variables. Thus it is gauge invariant, and has minimal coupling between the gauge fields on different links. The trial function depends on one variational parameter β. For $\beta=0$ the trial state is the strong-coupling vacuum; for large β the wave function is sharply peaked at field configurations for which every plaquette variable is small. For any β the state is disordered, in that the expectation value of the Wilson loop operator obeys an area law. It is an interesting question whether such a simple disordered state describes the vacuum; and if not, what is the nature of the difference between this state and the vacuum.

Our Monte Carlo calculations provide one way to study the difference between the disordered trial state and the vacuum state.[6] However, we find that the ground-state energy computed by the Monte Carlo method differs little from the variational energy obtained with this trial wave function. It does not follow that this naive disordered state is a good representation of the vacuum, because it may not describe other quantities accurately. Indeed the string tension in this variational state does not approach the weak-coupling limit derived from asymptotic freedom.[5]

The purpose of this paper is to describe an estimate of the energy of an elementary excitation of the gauge fields, based on the disordered state. The excited state is constructed in a way suggested by the strong-coupling expansion, by letting an operator act on the variational ground state. The operator that we use to create the excitation is a translation-invariant sum of single-plaquette operators. This construction is certainly a valid representation of the vacuum and its excitation in the strong-coupling region. But the point of the calculation is to check the behavior of this construction in the weak-coupling limit.

The Hamiltonian of the SU(2) lattice gauge theory is

$$H=\frac{g^2}{2}K+\frac{4}{g^2}V\ , \tag{1}$$

where

$$K=\sum_l E_a{}^2(l)\ ,$$
$$V=\sum_p\left[1-\tfrac{1}{2}\,\mathrm{Tr}U(l_1)U(l_2)U^\dagger(l_3)U^\dagger(l_4)\right]\ . \tag{2}$$

Here $U(l)$ is the element of SU(2) associated with link l. The electric field operator is defined by the commutator

$$[E_a(l),U(l)]=-\tfrac{1}{2}\sigma_a U(l)\ . \tag{3}$$

The first problem to solve regarding a quantum system with many degrees of freedom is to describe the ground state. We derived a variational estimate of the ground state of H, based on the trial wave function

$$\Psi_0=\exp(-\tfrac{1}{2}\beta V)\ , \tag{4}$$

where β is the variational parameter. We used Creutz's heat-bath Monte Carlo method to calculate the expectation value of the energy in this state.[5] The result is a set of magnetic and electric energies for various values of β, i.e., points on the curves

$$v(\beta)=\langle V\rangle\ ,\quad k(\beta)=\langle K\rangle\ , \tag{5}$$

where $\langle\ \rangle$ denotes the expectation value in the state Ψ_0. Then we fit these points with a function equal to a finite sum of orthogonal polynomials; the fits are shown in Figs. 1 and 2. The number of orthogonal polynomials in the

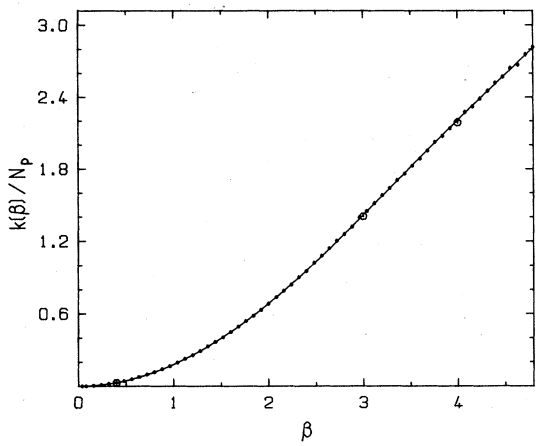

FIG. 1. The expectation value of the electric energy per plaquette in the trial wave function vs the variational parameter β. The points are for a $3\times3\times3$ (spatial) lattice; the three larger points are for a $6\times6\times6$ lattice. The solid curve is an orthogonal polynomial fit with 7 orthogonal polynomials.

sum is 6 for $v(\beta)$ and 7 for $k(\beta)$. The points in these figures are the energies *per plaquette* for a $3\times3\times3$ (spatial) lattice; the three larger points are for a $6\times6\times6$ lattice. There is very little dependence on the lattice size, because we use periodic boundary conditions, as shown by comparison of the 3^3 and 6^3 lattices. Also, both the large-β and small-β limits of v/N_p and k/N_p are independent of lattice size. Strictly speaking our results are for a 3^3 lattice, but they would not be very different for a larger lattice.

The variational estimate of the vacuum wave function is Ψ_0, with the value of β for which

$$0=k'(\beta)+\frac{8}{g^4}v'(\beta)\ , \tag{6}$$

where prime denotes differentiation. The energy bound is

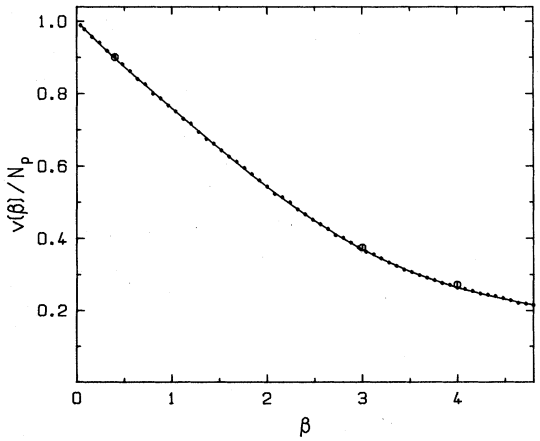

FIG. 2. The expectation value of the magnetic energy per plaquette vs variational parameter β. The points and curve have the same meaning as in Fig. 1. The fit uses six orthogonal polynomials.

$$E_0\le\frac{g^2}{2}k(\beta)+\frac{4}{g^2}v(\beta)\ . \tag{7}$$

To estimate the excitation energy we construct a state orthogonal to Ψ_0 by letting an operator act on Ψ_0. The operator is the sum of single plaquette variables, i.e., it is just V; this is gauge invariant and translation invariant. The reason for this choice is that it creates the elementary excitation in the strong-coupling expansion. Thus we consider the excited state

$$\Psi_1=c_1\Psi_0+c_2V\Psi_0\ , \tag{8}$$

where c_1 and c_2 are chosen such that Ψ_1 and Ψ_0 are orthogonal and have equal normalizations:

$$c_2=(\langle V^2\rangle-\langle V\rangle^2)^{-1/2}\ ,\quad c_1=-\langle V\rangle c_2\ , \tag{9}$$

where $\langle\ \rangle$ denotes the expectation value in the state Ψ_0.

In Eq. (9) we need to know $\langle V^2\rangle$. Fortunately, it is not necessary to calculate $\langle V^2\rangle$ from the Monte Carlo ensemble; it can be deduced from $v(\beta)$, since the form of Ψ_0 implies that

$$\langle V^2\rangle=v^2(\beta)-v'(\beta)\ . \tag{10}$$

This trick, computing expectation values in the state Ψ_0 by differentiation of $v(\beta)$ and $k(\beta)$, can be used for every expectation value in this calculation; as another example,

$$\langle KV\rangle=k(\beta)v(\beta)-k'(\beta)\ . \tag{11}$$

We believe that the polynomial fits to $v(\beta)$ and $k(\beta)$ shown in Figs. 1 and 2 are sufficiently good to allow us to compute such derivatives from the fitted function.

The first estimate of the energy of the elementary excitation of the SU(2) lattice gauge theory is simply the expectation value of H in the state Ψ_1. This naive excitation energy is

$$\Delta=(\Psi_0,\Psi_0)^{-1}[(\Psi_1,H\Psi_1)-(\Psi_0,H\Psi_0)]\ , \tag{12}$$

where the value of β is that determined in the original variational calculation. The expectation values in Eq. (12) are related to $v(\beta)$ and $k(\beta)$ by[7]

$$\frac{(\Psi_1,V\Psi_1)}{(\Psi_1,\Psi_1)}=v(\beta)-\frac{v''(\beta)}{v'(\beta)} \tag{13}$$

and

$$\frac{(\Psi_1,K\Psi_1)}{(\Psi_1,\Psi_1)}=k(\beta)-\frac{k''(\beta)+\frac{2}{\beta^2}k(\beta)}{v'(\beta)}\ . \tag{14}$$

Thus the estimated excitation energy is

$$\Delta=[-v'(\beta)]^{-1}\left[\tfrac{1}{2}g^2\left[k''+\frac{2}{\beta^2}k\right]+\frac{4}{g^2}v''\right]\ . \tag{15}$$

Note that the excitation energy is of order 1, whereas the vacuum energy is of order N_p, the number of plaquettes.

A second estimate is obtained by diagonalizing the Hamiltonian in the two-dimensional space spanned by Ψ_0 and Ψ_1. The energy matrix is

$$H_2=(\Psi_0,\Psi_0)^{-1}\begin{bmatrix}(\Psi_0,H\Psi_0) & (\Psi_0,H\Psi_1)\\ (\Psi_1,H\Psi_0) & (\Psi_1,H\Psi_1)\end{bmatrix}. \tag{16}$$

The diagonal components are given above; the off-diagonal components are obtained from

$$\frac{(\Psi_0,K\Psi_1)}{(\Psi_0,\Psi_0)}=-k'(\beta)[-v'(\beta)]^{-1/2} \tag{17}$$

and

$$\frac{(\Psi_0,V\Psi_1)}{(\Psi_0,\Psi_0)}=[-v'(\beta)]^{1/2}. \tag{18}$$

This alternative estimate of the energies is computed as follows. The value of β is chosen to minimize the smaller of the two eigenvalues of H_2; the minimum is the new variational bound on the vacuum energy. Then the new estimate of the excitation energy $\bar{\Delta}$ is the difference of the two eigenvalues of H_2 for that value of β.

The diagonal terms of H_2 are of order N_p, the number of plaquettes, and their difference is of order 1. The off-diagonal terms are ostensibly of order $\sqrt{N_p}$, but they are actually equal to zero for the original value of the variational parameter, by Eq. (6). These dimensions imply that the correction to the vacuum energy is only of order 1, negligible compared to the original variational bound which is of order N_p. On the other hand, the correction to the excitation energy is also of order 1, comparable to the first estimate of Eq. (15).

Figures 3(a) and 3(b) show our variational results on the vacuum energy and the excitation energy. Figure 3(a) gives the vacuum energy per plaquette obtained with the trial wave function Ψ_0. Curve (a) in Fig. 3(b) gives Δ, the naive estimate of the excitation energy; curve (b) gives $\bar{\Delta}$, the other estimate of the excitation energy obtained by diagonalizing H_2. The energies are plotted vs the parameter λ defined by

$$\lambda=\frac{8}{g^4}. \tag{19}$$

Rather than plot the energy itself, we have plotted the energy times $2/g^2$; this magnifies the strong-coupling region, and makes more clear the deviation from the strong-coupling limit. The sharp variations seen in curve (b) are presumably irrelevant artifacts of the inaccuracy of the polynomial fit.

The dashed curves in Figs. 3(a) and 3(b) are strong-coupling expansions ($\lambda\to 0$) for these energies, given by[8]

$$\frac{2E_0}{g^2N_p}=\lambda-\tfrac{1}{12}\lambda^2+O(\lambda^3),$$
$$\frac{2\Delta}{g^2}=3-\tfrac{71}{420}\lambda^2+O(\lambda^3). \tag{20}$$

The variational results agree with the strong-coupling results for small λ, because Ψ_0 and Ψ_1 approximate the strong-coupling eigenstates for small β. There is a slight difference between the strong-coupling excitation energy and the variational excitation energy; both approach 3 as $\lambda\to 0$, but from different directions: it can be shown that the small-λ limit of the variational excitation energy is

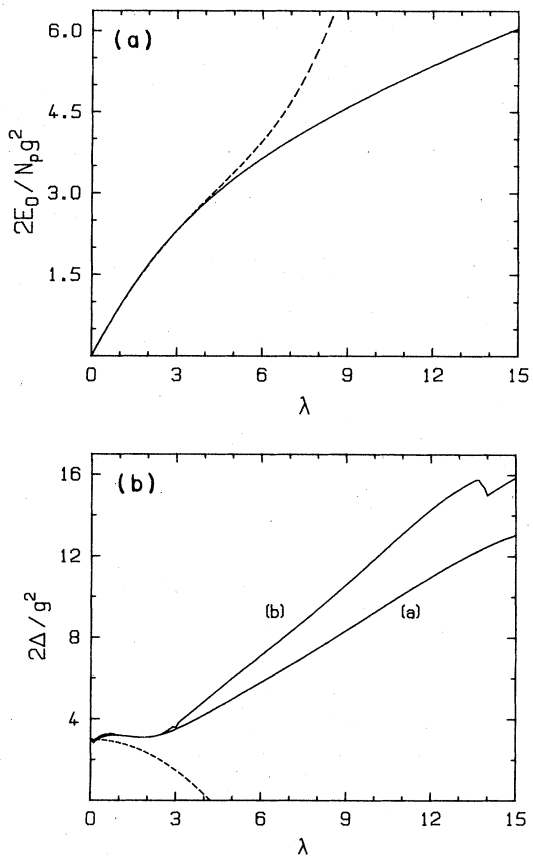

FIG. 3. (a) Variational bound on the vacuum energy per plaquette. The horizontal axis is $\lambda=8/g^4$. The vertical axis is the energy times $2/g^2$. The dashed curve is the strong-coupling limit in Eq. (20). (b) Variational estimates of the excitation energy. Curve (a) gives Δ and curve (b) gives $\bar{\Delta}$. The axes and the dashed curve have the same meaning as in (a).

$$\left[\frac{2\Delta}{g^2}\right]_{\text{variational}}=3+\tfrac{5}{36}\lambda^2-\tfrac{146}{3888}\lambda^4+O(\lambda^6), \tag{21}$$

and this λ dependence is visible in Fig. 3(b).

The *variational estimate* of the excitation energy approaches a nonzero constant in the weak-coupling limit ($\lambda\to\infty$). The asymptotic value can be deduced from the large-β limits of $v(\beta)$ and $k(\beta)$. It can be shown that as $\beta\to\infty$,

$$v(\beta)\cong\frac{1}{\beta},\quad k(\beta)\cong\tfrac{3}{4}\beta. \tag{22}$$

For large λ the variational parameter β is large, so these limits determine the variational estimates. They imply that

$$\Delta\to\sqrt{24} \tag{23}$$

in the limit $\lambda\to\infty$. Curve (a) in Fig. 3(b) is consistent with this asymptotic value.

The fact that the variational estimate of the excitation energy does not approach zero in the weak-coupling limit implies that the states Ψ_0 and Ψ_1 are not adequate approximations of the weak-coupling eigenstates. The excitation

energy Δ must approach zero as $\lambda \to \infty$ in order to have a proper continuum limit. The reason is that Δ is actually the energy in units of the lattice spacing, which is set equal to 1 in the definition of H. The mass of the particle associated with this excitation would be Δ/a for lattice spacing a. The continuum limit of the mass can be finite only if Δ approaches zero in the weak-coupling limit. In fact, the usual renormalization group analysis of a nonperturbative quantity[9] implies that Δ should decrease as $\exp(-24\pi^2/11g^2)$ as $\lambda \to \infty$; i.e., very rapidly on the scale of Fig. 3(b). Since the excitation energy obtained in this variational calculation does not approach zero, the trial states are not adequate representations of the weak-coupling eigenstates.

It is not surprising that the result of this variational calculation does not have the proper continuum-limit behavior. The trial states are not plain strong-coupling states, but they do resemble strong-coupling states in one regard. Specifically, there is no explicit correlation between the fields on different plaquettes in Ψ_0; this is also a property of the strong-coupling vacuum. It is true that Ψ_0 approaches an ordered state as $\beta \to \infty$, but this alone is evidently not enough to describe the weak-coupling limit. Correlations between fields on different plaquettes must be a significant aspect of the vacuum state of the SU(2) lattice gauge theory. In fact, in the weak-coupling limit the theory approaches a critical point, at which the correlation length is infinite. To describe continuum phenomena the trial function should incorporate correlations over lengths of order $a \exp(12\pi^2/11g^2)$.

The precise nature of the eigenstate in the weak-coupling limit remains elusive.

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[7]Equation (14) is derived by relating $(\Psi_0, VKV\Psi_0)$ to the derivative of $(\Psi(\beta_1), K\Psi(\beta_2))$ with respect to both β_1 and β_2.

[8]These can be derived by the methods described in the first paper in Ref. 3.

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