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Test of a Hamiltonian variational method for SU(3) lattice gauge theory in 3 + 1 dimensions

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Abstract. We discuss a Hamiltonian variational procedure for lattice gauge theories, suitable for 3 + 1 dimensions, based on a trial state vector in terms of link variables. This method has been applied to the calculation of link and plaquette expectation values for the pure SU(3) lattice gauge theory. We find agreement with the Monte-Carlo data only in part of the weak-coupling and cross-over regions. Taking some two-link correlations in the trial state vector into account we improve the results in the cross-over region and smear out an unwanted phase transition.

1. Introduction

In recent times lattice quantisation has become a powerful tool for the non-perturbative study of gauge theories. Variational methods are one of several approaches to this. In the Hamiltonian formulation of the variational method (e.g., Patkoś and Deàk 1981, Patkoś 1982, Horn and Weinstein 1982, Hofsäss and Horsley 1983, Hari Dass *et al* 1983) the aim is to find a state vector ψ for the lattice such that the expectation value of the Hamiltonian

$$\langle H\rangle = \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} \tag{1}$$

becomes minimal. Usually a trial wavefunction constructed out of plaquette state vectors

$$\psi = \prod_{\text{plaquettes}} \psi_\square \qquad \psi_\square = \exp(\alpha(g^2)\mathrm{Tr}\, U_{\text{plaquettes}}) \tag{2}$$

is used (Patkoś and Deàk 1981, Patkoś 1982, Hofsäss and Horsley 1983, Hari Dass *et al* 1983); for this the expression $\langle\psi|H|\psi\rangle$ can be calculated relatively easily in 2 + 1 dimensions. However, due to Bianchi identities, this becomes more difficult in 3 + 1 dimensions even for Abelian groups (Hari Dass *et al* 1983). On the other hand, Horn and Weinstein (1982) used a link-dependent trial state vector to study some properties of the Abelian U(1) gauge theory. In the present paper we adopt a similar ansatz for the state vector to investigate the phase structure of the non-Abelian SU(3) gauge theory in 3 + 1 dimensions.

In § 2 we collect some necessary formulae for the variational Hamiltonian method. In § 3 a link-factorised trial state vector is considered. By inspecting the ground-state energy and link and plaquette expectation values we find that this very rough approximation produces an unwanted phase transition. In § 4 we discuss a possible way of improving the

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ansatz by using a trial state vector including link correlations. This correction smears out the phase transition. Finally, in § 5 we summarise our results.

2. Some necessary ingredients for our Hamiltonian variational method

In general, the state vector ψ of the lattice is constructed from functions $f(V)$, $V \in \mathrm{SU}(3)$, where V is a product of link variables along a closed or open contour, i.e. a loop or a string. Since the state vector has to be invariant under global gauge transformations,

$$f(V)=f(g^{-1}Vg) \qquad g \in \mathrm{SU}(3), \tag{3}$$

it is a class function on the group and therefore can be expanded in characters:

$$f(V)=\sum_{p,q=0}^{\infty} a_{p,q}\chi^{p,q}(V). \tag{4}$$

Here, as usual, the irreducible representations of the SU(3) group, $D^{p,q}(V)$, are numbered by two non-negative integers p and q so that, for example, $D^{1,0}(V)$ is the fundamental representation. $\chi^{p,q}$ is the trace (character) of the representation $D^{p,q}$. The dimension of the representations is given by

$$\dim(p,q)=\tfrac{1}{2}(p+1)(q+1)(p+q+2). \tag{5}$$

To avoid difficulties with the local gauge invariance of the state vector ψ, which is also necessary, the gauge on the three-dimensional lattice at a time t_0 is completely fixed so that no local gauge freedom is left (Batrouni 1982, Sharatchandra 1982). All links in the z direction carry link variables equal to unity; furthermore, the links in the x direction on the $z=0$ surface and the links in the y direction on the $x=z=0$ edge also have link variables equal to unity.

We use the Hamiltonian appropriate to the Wilson action (Kogut and Susskind 1975, Kogut *et al* 1979):

$$\begin{aligned} H &= \tfrac{1}{2}g^2 \sum_{\text{links}} E^2 - \frac{1}{g^2} \sum_{\text{plaquettes}} (\chi^{1,0}(U_1 U_2 U_3^{+} U_4^{+}) + \text{HC}) \\ &= H_{\text{elec}} + H_{\text{mag}}. \end{aligned} \tag{6}$$

Here the lattice spacing is set equal to one.

The eigenvalues of E^2 are those of the quadratic Casimir operator of the gauge group. Acting with E^2 on the representation $D^{p,q}$, one obtains

$$E^2 D^{p,q}(U)=\tfrac{1}{3}[(p+q)(p+q+3)-pq]D^{p,q}(U). \tag{7}$$

On the gauge-fixed lattice the single-plaquette Hamiltonian has to be averaged over different kinds of plaquettes: for every plaquette without gauge-fixed links one has to consider two plaquettes with two frozen links. As in every variational calculation, we consider a trial state vector depending on several variational parameters which are chosen to minimise the expectation value of the Hamiltonian.

3. First choice of the trial wavefunction

The simplest, mean-field-like ansatz for the ground state is

$$\psi = \prod_{\substack{\text{links}\\ l}} \varphi(U_l) \qquad \varphi(U) = \sum_{p,q=0}^{p_{\max}, q_{\max}} a_{p,q} \chi^{p,q}(U). \tag{8}$$

This extremely simple choice serves to illustrate the method and will be used as the starting point for corrections. Since the character expansion also contains the conjugate for every character in addition to the character itself, and the state vector has to be invariant under reversal of the orientation of the links, the coefficients $a_{p,q}$ can be chosen to be real and symmetric:

$$a_{p,q} = a_{q,p}. \tag{9}$$

The calculation of the expectation value $\langle H \rangle$ is possible without difficulties. The norm per link is given by

$$\langle \varphi | \varphi \rangle = \int_{\mathrm{SU}(3)} \mathrm{d}U \, \varphi(U) \varphi^*(U) = \sum a_{p,q}^2. \tag{10}$$

Then we immediately find the electric energy per link:

$$\tfrac{1}{2} g^2 \langle \varphi | E^2 | \varphi \rangle = \tfrac{1}{2} g^2 \sum_{p,q} \tfrac{1}{3} a_{p,q} [(p+q)(p+q+3) - pq]. \tag{11}$$

Because

$$\chi^{1,0}\left(\prod_{i=1}^{n} U_i \right) = \mathrm{Tr}\, D^{1,0}(U_1)\, D^{1,0}(U_2) \ldots D^{1,0}(U_n), \tag{12}$$

and since the state vector is factorised, we have to know the expectation value

$$\langle \varphi | (D^{1,0}(U))_{\alpha\beta} | \varphi \rangle \qquad \alpha, \beta = 1, 2, 3$$

to calculate the magnetic energy. The rules for group integrations and the orthonormality relations of the Clebsch–Gordan coefficients (de Swart 1964) give

$$\begin{aligned} \int_{\mathrm{SU}(3)} \mathrm{d}U \chi^{p,q}(U) \chi^{p',q'}(U)^* (D^{1,0}(U))_{\alpha\beta} &= \tfrac{1}{3} \sum_{c,d} \begin{pmatrix} p, q & p', q' \\ c & d \end{pmatrix} \Bigg| \begin{matrix} 0, 1 \\ \alpha \end{matrix} \Bigg) \begin{pmatrix} p, q & p', q' \\ c & d \end{pmatrix} \Bigg| \begin{matrix} 0, 1 \\ \beta \end{matrix} \Bigg) \\ &= \tfrac{1}{3} \delta_{\alpha\beta} \Delta(p, q, p', q') \end{aligned} \tag{13}$$

where

$$\Delta(p, q, p', q') = \begin{cases} 1 & \text{if the } (p', q') \text{ representation is part of the} \\ & \text{Clebsch–Gordan decomposition} \\ 0 & (p, q) \otimes (1, 0) = (p+1, q) \oplus (p-1, q+1) \oplus (p, q-1) \\ & \text{otherwise.} \end{cases}$$

As a result, we get

$$\langle \varphi | D^{1,0}(U))_{\alpha\beta} | \varphi \rangle = \tfrac{1}{3} \delta_{\alpha\beta} \sum_{p,q,p',q'} a_{p,q} a_{p',q'} \Delta(p, q, p', q'). \tag{14}$$

The minimum of the expectation value $\langle H \rangle$ is searched for numerically using a standard minimisation procedure. The coefficients $a_{p,q}$ with the symmetry property of equation (9)

are parametrised as

$$a_{p,q} = P(p, q)(\dim(p, q))^{1/2} \tag{15}$$

where $P(p, q)$ is a polynomial of third degree in $(pq)^{-1}$ and $(p+q)^{-1}$. With this parametrisation we determined the optimal state vector at different values of β ($\beta = 2Ng^{-2} = 6g^{-2}$). Other parametrisations have also been tested; they gave similar or worse results (higher ground-state energies). Figure 1 shows the calculated minimal ground-state energy. As in the mean-field calculations, a first-order phase transition is found at $\beta_c = 4.0 \pm 0.05$ (straight lines).

For $\beta < \beta_c$ no state vector with energy $\langle H \rangle < 0$ (lower than the perturbative vacuum) is found. Since we have used a link-factorised state vector, the amount of magnetic energy is smaller than the corresponding one with link correlations included. For strong coupling some correlations are necessary to obtain an amount of magnetic energy larger than the electric one so that a non-perturbative ground state exists.

The link state vector φ is, according to equation (8), a sum of $p_{\max} \times q_{\max}$ terms. We give here some of these (as yet unnormalised) terms to discuss their behaviour.

For $\beta = 4.5$ φ contains

$$1 + 0.669[3] + 0.408[6] + \ldots + 0.066[24] + \ldots + 0.00263[120] + \ldots,$$

for $\beta = 6.0$ φ contains

$$1 + 1.036[3] + 0.734[6] + \ldots + 0.209[24] + \ldots - 0.00930[120] + \ldots$$

and for $\beta = 7.5$ we obtain for φ

$$1 + 1.170[3] + 0.999[6] + \ldots + 0.373[24] + \ldots + 0.02843[120] + \ldots.$$

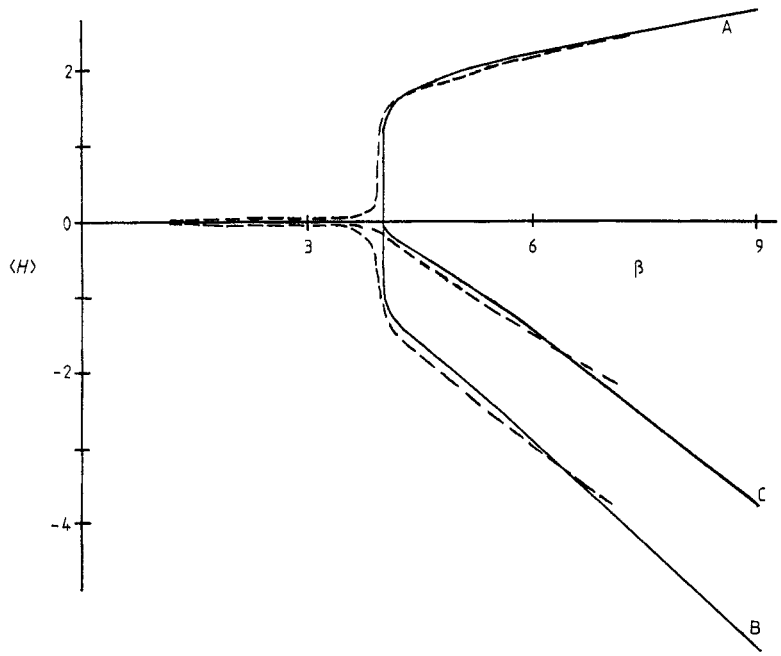

Figure 1. The electric (A), magnetic (B) and total (C) energy per plaquette as function of $\beta = 6g^{-2}$ (averaged over the two types of plaquettes) for the link-factorised (——) and the two-link (– – –) trial state vectors.

Here $[N]=(\dim(p,q))^{1/2}(\chi^{p,q}+\chi^{q,p})$ with $\dim(p,q)=N$. The first term is the coefficient of $\chi^{0,0}=1$ and corresponds to a freely fluctuating link variable. Therefore the electric energy vanishes. The influence of this term relative to the others decreases with increasing β. The link variables are straightened out more and more. So with increasing β the convergence of the character expansion gets worse. We proved that $p_{\max}=q_{\max}=5$ for $\beta<6$ and $p_{\max}=q_{\max}=7$ for $6<\beta<9$ are sufficient for the convergence of our calculations.

The link expectation value is defined as

$$\langle L\rangle=\langle\varphi|\chi^{1,0}(U)|\varphi\rangle/\langle\varphi|\varphi\rangle \tag{16}$$

and the plaquette expectation value of a plaquette with two gauge-fixed links is

$$\langle P\rangle=\langle\varphi(U_1)\varphi(U_2)|\chi^{1,0}(U_1U_2^{-1})|\varphi(U_1)\varphi(U_2)\rangle/\langle\varphi|\varphi\rangle^2. \tag{17}$$

Results for $\langle L\rangle$ and $\langle P\rangle$ with the ansatz of equation (8) are presented in figures 2 and 3, respectively (straight lines).

4. Improved trial state vector including some link correlations

In order to take correlations into account we propose to choose a more complicated state vector on part of the lattice (a local domain Γ), whereas all other links not shared by Γ carry the 'mean-field' state vector φ:

$$\psi=\Phi_\Gamma\prod_{\text{links}\notin\Gamma}\varphi(U_l). \tag{18}$$

This changes the energy of all plaquettes which share links with Γ. Therefore the following variational problem has to be solved:

$$\langle H_\Gamma+H_{\text{plaquettes with } l\in\Gamma}\rangle\to\text{minimum}. \tag{19}$$

For a large Γ the calculations would be very extensive because many different terms could contribute to Φ_Γ. As a first attempt we choose the domain Γ to consist of only one plaquette with two gauge-fixed links. Then the most general trial function of this domain would be

$$\Phi_\Gamma=\sum_{p,q,p',q',p'',q''}c_{p,q,p',q',p'',q''}\chi^{p,q}(U_1)\chi^{p',q'}(U_2)\chi^{p'',q''}(U_1U_2^{-1}). \tag{20}$$

Since this trial state vector already gives a rather extensive minimisation calculation, for simplicity we choose

$$\Phi_\Gamma=\sum_{p,q,p',q'}^{p_{\max},\ldots,q'_{\max}}c_{p,q,p',q'}\chi^{p,q}(U_1)\chi^{p',q'}(U_2). \tag{21}$$

The expectation value $\langle H\rangle$ can be calculated as described before. For the electric energy of one link of Γ we obtain

$$H_{\text{elec}}=\tfrac{1}{2}g^2\sum_{p,q,p',q'}\tfrac{1}{3}c^2_{p,q,p',q'}[(p+q)(p+q+3)-pq] \tag{22}$$

and for the magnetic energy of Γ we obtain

$$H_{\text{mag}}=-\frac{1}{g^2}\sum_{p,q,p',q',r,s,r',s'}c_{p,q,p',q'}c_{r,s,r',s'}\Delta(p,q,r,s)\Delta(p',q',r',s'). \tag{23}$$

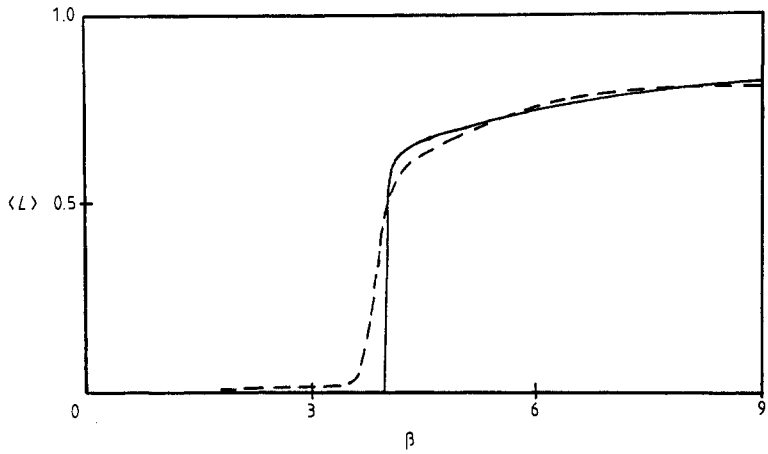

Figure 2. The link expectation value for the link-factorised (——) and the two-link (– – –) trial state vectors.

Different parametrisations of the $c_{p,q,p',q'}$ have been tested. We present here results for the parametrisation in the form of a polynomial of third degree in $(pq)^{-1}$, $(p+q)^{-1}$, $(p'q')^{-1}$, $(p'+q')^{-1}$, $(pp')^{-1}$, $(qq')^{-1}$, $(p+p')^{-1}$, $(q+q')^{-1}$. Since the expressions for the energy are rather complicated it was necessary to set $p_{\max}=q_{\max}=p'_{\max}=q'_{\max}=4$. Therefore for weak coupling (large β) we do not expect an improvement in our results. However, as can be seen from the broken curve in figure 1, for $\beta=4.2$ an energy 10% lower than that of the link-factorised trial state vector is obtained. For $\beta=6$ the energy is still 2% lower.

At about $\beta=4$ energy and link expectation values again decrease rapidly but tend to zero only slowly for lower β (figures 1 and 2). We have compared the plaquette expectation value for the domain Γ with the Monte-Carlo data of Creutz and Moriarty (1982) obtained on a four-dimensional Euclidean lattice (figure 3). In the cross-over region the agreement is better than for the link-factorised trial state vector.

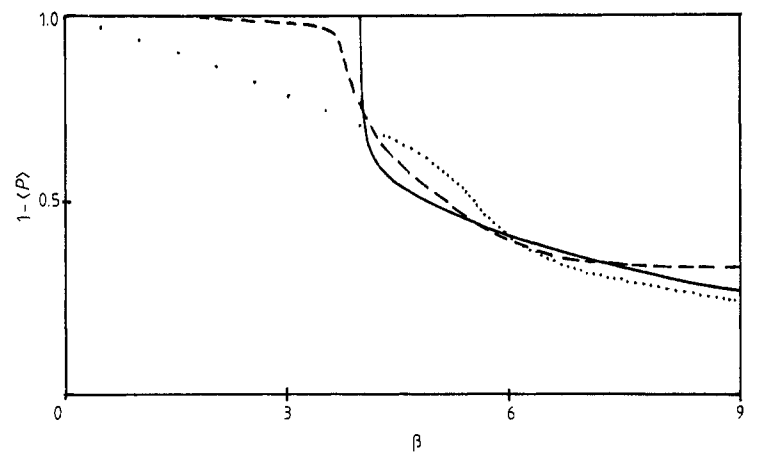

Figure 3. The expectation value of a plaquette with two gauge-fixed links for the link-factorised (——) and the two-link (– – –) trial state vectors compared with the Monte-Carlo data of Creutz and Moriarty (1982) (· · ·).

5. Summary

In this paper we have tested an ansatz for a Hamiltonian variational calculation of pure SU(3) lattice gauge theory. Contrary to a plaquette ansatz, our trial wavefunction allows us to calculate the expectation value of the Hamiltonian in 3 + 1 dimensions. Link and plaquette expectation values have been calculated for the state vectors obtained by minimising the ground-state energy. It turns out, as expected, that a link-factorised trial state vector does not reproduce the correct phase structure of SU(3) lattice gauge theory. A phase transition at $\beta = 4.0$ is found between weak and strong coupling, similar to that of mean-field calculations. Satisfactory agreement with the Monte-Carlo data exists only in part of the weak-coupling and cross-over regions. However, a simple correction, taking correlations of two links in the trial state vector into account, provides a better result. We find that the phase transition is smeared out; however, a very rapid cross-over is left. So further improvements are necessary and in principle feasible, but at the cost of very extensive variational calculations.

After completing our work we received a preprint from Horn and Karlinger (1983), who studied a similar mean link ansatz for the trial wavefunction in SU(2). However, unlike us they used a Monte-Carlo program to calculate the expectation value of the Hamiltonian.

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