DEFINITION AND GENERAL PROPERTIES OF THE TRANSFER MATRIX IN CONTINUUM LIMIT IMPROVED LATTICE GAUGE THEORIES

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When operators of dimension 6 are added to the standard Wilson action in lattice gauge theories, physical positivity is lost in general. We show that a transfer matrix can nevertheless be defined. Its properties are, however, unusual: complex eigenvalues may occur (leading to damped oscillatory behaviour of correlation functions), and there are always contributions in the spectral decomposition of two-point functions that come with a negative weight.

1. Introduction

With the aim of reducing finite (ultraviolet) cutoff effects in lattice gauge theories, Wilson [1] and later Symanzik [2] proposed adding a set of judiciously chosen irrelevant operators to the standard one-plaquette action. These new terms also couple link variables separated by more than one lattice spacing, and consequently the old construction [3, 4] of the Hilbert space of physical states and of the Hamilton operator breaks down. From experience with higher derivative scalar field theories, one expects that, in one or the other way, physical positivity is in fact violated. The question then is to what extent it is violated and how exactly it is restored in the continuum limit.

In this paper, we show that a transfer matrix $T$ acting in a Hilbert space $\mathcal{H}$ (with positive definite scalar product) can always be defined (sect. 3). However, $T$ is in general not hermitian, and this leads to a number of complications, which are discussed in sects. 4–6. An important result is that a clean definition of the notion of "energy value" in continuum limit improved lattice gauge theories is obtained (it will be needed later for a new calculation of the coefficients of the dimension 6 operators.

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in the improved action \([5]\)). Furthermore, we find that near the continuum limit, positivity is only lost at energies of the order of the cutoff so that the effect becomes increasingly unimportant, when the bare coupling constant \(g_0\) is made smaller.

### 2. Improved lattice gauge theories

In this section we define the class of lattice gauge theories that we are going to consider. Thus, let \(\Lambda\) be a \(T \times L \times L \times L\) hypercubic, periodic lattice. Gauge fields living on \(\Lambda\) are conveniently identified with fields of matrices \(U(x, \mu) \in SU(N), \ x \in \mathbb{Z}^4, \ \mu = 0, \ldots, 3\), which are periodic:

\[
U(x + T\hat{\mu}, \mu) = U(x, \mu),
\]

\[
U(x + L\hat{\mu}, \mu) = U(x, \mu) \quad \text{for} \quad k = 1, 2, 3. \tag{1}
\]

Here, \(\hat{\mu}\) denotes the unit vector in the positive \(\mu\)-direction and the periods \(T\) and \(L\) are positive integers*. Instead of the periodic boundary conditions on the field implied by eq. \(1\), we could just as well assume twisted periodic boundary conditions in space-like directions without affecting any of the statements and formulae below.

To write down the "improved" action \(S[U]\) of a lattice gauge field \(U(x, \mu)\), some preparation is needed. First, we define 4 sets \(\mathcal{S}_i\) \((i = 0, \ldots, 3)\) of elementary closed loops \(C\) on \(\Lambda\) (see fig. 1). \(\mathcal{S}_0\) is the set of all loops (a), which wind once around a single plaquette. The set \(\mathcal{S}_1\) contains all loops (b) enclosing two coplanar plaquettes.

* For technical reasons, we shall actually assume \(T \geq 4\).
$S_2$ and $S_3$ are the sets of 3-dimensional loops (c) and (d), respectively. Loops that differ by orientation only, are considered equal, so that $S_i$ has $N_i T L^3$ elements, where

\[ N_0 = 6, \quad N_1 = 12, \]
\[ N_2 = 16, \quad N_3 = 48. \]  

Next, for any loop $C$ set

\[ \mathcal{E}(C) = \text{Re} \text{Tr}[I - U(C)], \]  

$U(C)$ being the ordered product of the link variables $U(x, \mu)$ along $C$. Note that $\mathcal{E}(C)$ is independent of the orientation of $C$.

The general form of the improved action considered here is [6]

\[ S[U] = \sum_{i=0}^{3} \sum_{C \in S_i} K_i \mathcal{E}(C), \]  

where the coefficients $K_i$ are supposed real*. They are to be determined from some improvement condition, but we shall not discuss this question any further, because the actual value of the $K_i$'s is irrelevant for the construction of the transfer matrix. Given the action, expectation values of gauge invariant combinations $\Theta$ of the field $U(x, \mu)$ are defined as usual:

\[ \langle \Theta \rangle = \frac{1}{Z} \int \prod_{x \in \Lambda} \prod_{\mu = 0}^{3} dU(x, \mu) \Theta[U] e^{-S[U]}, \]  

\[ Z = \int \prod_{x \in \Lambda} \prod_{\mu = 0}^{3} dU(x, \mu) e^{-S[U]}, \]  

($dU$ denotes the normalized Haar measure on SU($N$)).

Actually, actions $S[U]$ much more general than (4) allow the construction of a transfer matrix. In particular, other classes of loops $C$ may be added and $\mathcal{E}(C)$ could be replaced by any real gauge invariant and orientation independent function of $U(C)$.

3. Definition of the transfer matrix $T^{**}$

First, we must specify the Hilbert space $\mathcal{H}$ in which $T$ acts as a linear operator. In order to motivate our choice, consider the classical theory defined by the action (4).

* They are related to the bare coupling constant $g_0$ through $K_0 + 8K_1 + 8K_2 + 16K_3 = 2/g_0^2$.

** We assume that the reader is familiar with the transfer matrix formalism in ordinary lattice gauge theories (refs. [3, 4]).
In the $U(x,0) = 1$ gauge, the associated field equations assume the form of a fourth-order difference equation in the time coordinate $x_0$ (if $K_1 \neq 0$). To have a unique solution, initial data must therefore be given on 4 distinct equal time hyperplanes in $\Lambda$. This leads us to suspect that in quantum theory it is meaningful to talk about a transition amplitude to go from a given gauge field on a pair of consecutive equal time hyperplanes to some other gauge field on a later pair of hyperplanes. Wave functions $\psi$ that can be propagated with such an amplitude must be functions defined on the set of all lattice gauge fields $U$, which live on a fixed double layer of equal time hyperplanes in $\Lambda$ (see fig. 2). Thus, we make the ansatz

$$\psi = \psi[U_+, U_0, U_-],$$

where $U_+(x, k)$ and $U_-(x, k)$ are gauge fields on the top respectively bottom hyperplane of the double layer, and $U_0(x)$ sits on the time-like links connecting the two hyperplanes (we are no longer insisting on the temporal gauge $U(x, 0) = 1$).

A wave function of type (7) is called gauge invariant if

$$\psi[\bar{U}] = \psi[U]$$

whenever $\bar{U}$ and $U$ are gauge equivalent. In the course of the discussion, it will become clear that it is sufficient to consider gauge invariant wave functions only. A convenient gauge invariant scalar product of two wave functions $\varphi$ and $\psi$ is then given by

$$\langle \varphi, \psi \rangle = \int \mathcal{D}[U] \varphi[U] \ast \psi[U],$$

$$\mathcal{D}[U] = \prod_x dU_0(x) \prod_{x,k} dU_+(x,k) dU_-(x,k),$$

and the Hilbert space $\mathcal{H}$ is identified with the space of all gauge invariant wave functions $\psi$ of type (7), which have finite norm: $(\psi, \psi) < \infty$. 

Fig. 2. Side view of a double layer of equal time hyperplanes in $\Lambda$. 
We now proceed to define the transfer matrix $T$. The characteristic properties we want $T$ to have, are:

(i) $T$ is a bounded, linear operator in $\mathcal{H}$.

(ii) The partition function $Z$ (eq. (6)) is given by

$$Z = \text{Tr}\{T^T\},$$

where "Tr" means the trace in the Hilbert space $\mathcal{H}$.

(iii) Let $A[U]$ and $B[U]$ be two bounded gauge invariant functions of the double layer field $U = (U_+, U_0, U_-)$. Define an operator $\hat{A}$ (and similarly $\hat{B}$) through

$$(\hat{A}\psi)[U] = A[U]\psi[U], \quad (\psi \in \mathcal{H}).$$

Then, for any integer $t$ with $0 \leq t \leq T$, we have

$$\langle A, B_0 \rangle = \frac{1}{Z} \text{Tr}\{T^{T-t}\hat{A}T^t\hat{B}\}.$$  \hspace{1cm} (11)

Here, the euclidean observable $A_s$ (and similarly $B_s$) is equal to $A[U]$, where $U$ is identified with that part of the euclidean field integrated over in eq. (5), which lives on and between the $x_0 = s$ and $x_0 = s + 1$ hyperplanes.

It is not too difficult to guess an operator $T$ with the above properties (experience with ordinary lattice gauge theories and with an "improved" harmonic oscillator has been helpful at this stage). Thus, writing $T$ in the form of an integral operator,

$$(T\psi)[U] = \int \mathcal{D}[V] \mathcal{K}[U, V]\psi[V],$$

we have

$$\mathcal{K}[U, V] = e^{-\Delta S[U, V]} \prod_{x, k} \delta(U_-(x, k), V_+(x, k))$$  \hspace{1cm} (13)

($\delta(U, V)$ denotes Dirac's $\delta$-function relative to the Haar measure on $SU(N)$). The exponent $\Delta S$ in eq. (13) is given by

$$\Delta S[U, V] = \sum_{i=0}^{3} \sum_{\mathcal{C} \in \mathcal{S}_i} K_i \tau(\mathcal{C}) \mathcal{E}(\mathcal{C}),$$

where the sets of loops $\mathcal{S}_i$ are defined as the $\mathcal{S}_i$'s, but contain only those loops which can be drawn on the triple layer of equal time hyperplanes shown in fig. 3. The "time-factor" $\tau(\mathcal{C})$ is equal to 1, $\frac{1}{2}$ or $\frac{1}{3}$ depending on the time-like extent of $\mathcal{C}$, which can be 2, 1 or 0 lattice spacings.

Eqs. (12)--(14) define the transfer matrix. Since the kernel $\mathcal{K}$ is gauge invariant, $T$ maps gauge invariant wave functions onto gauge invariant ones. Furthermore, by the
Cauchy-Schwarz inequality, we have

$$|(T\psi)[U]| \leq C \left( \int \prod_x dV_0(x) \prod_{x,k} dV_-(x,k) \lvert \psi[V] \rvert_2^2 \right)^{1/2}$$

for some constant $C$. Hence

$$\lVert T\psi \rVert \leq C \lVert \psi \rVert$$

and $T$ is thus a bounded operator acting in $\mathcal{H}$. The properties (ii) and (iii) above are also readily verified. Note that the integral kernel of $T^T$ is gauge invariant in both arguments $U$ and $V$ separately. The trace of $T^T$ in the space of all wave functions is therefore equal to the trace in the Hilbert space $\mathcal{H}$, which contains only the gauge invariant wave functions.

4. Spectral properties of the transfer matrix

In ordinary lattice gauge theories, the transfer matrix is self-adjoint and can be diagonalized. Eq. (11) then yields the spectral representation for euclidean two-point functions, which is the conceptual basis for almost all modern calculations of the mass spectrum in lattice gauge theories. In particular, the eigenvalues $\lambda$ of the transfer matrix are interpreted as energy values through

$$E = -\frac{1}{a} \ln(\lambda/\Lambda)$$

($a$: lattice spacing, $\Lambda$: largest eigenvalue of $T$).

In improved lattice gauge theories, the transfer matrix is no longer hermitian. Rather, one finds from eqs. (12)–(14) that

$$T^\dagger = \theta T \theta,$$
where $\theta$ is a kind of time inversion operator:

$$(\theta \psi)[U_+, U_0, U_-] = \psi[U_-, U_0^+, U_+] .$$

Obviously,

$$\theta^+ = \theta , \quad \theta^2 = 1 ,$$

so that $\theta$ has eigenvalues $\pm 1$. Since $T$ is not hermitian (and not normal, i.e. $[T^+, T] \neq 0$), the usual spectral theory does not apply. However, $T$ is otherwise a rather well-behaved operator so that other results from the mathematical literature may be invoked to prove properties of the spectrum of $T$. In what follows, we shall not give detailed proofs of the statements made, because they can be derived easily from well-documented theorems (e.g. refs. [7–9]).

The spectrum $\sigma(T)$ of $T$ is defined to be the set of complex numbers $\lambda$, for which the operator $\lambda - T$ has no (bounded) inverse. A first series of results on $\sigma(T)$ derives from the fact that $T^2$ can be represented by a smooth integral kernel and is hence a compact operator. Thus, $\sigma(T)$ is a discrete set with $\lambda = 0$ being the only accumulation point. Furthermore, for any $\lambda \in \sigma(T)$, $\lambda \neq 0$, there are generalized eigenvectors $\psi \in \mathcal{H}$ satisfying

$$(T - \lambda)^k \psi = 0$$

for some $k = 1, 2, 3, \ldots$ The space of all such eigenvectors is denoted by $\mathcal{H}_\lambda$ and it is known that

$$m_\lambda = \dim \mathcal{H}_\lambda < \infty .$$

$\mathcal{H}_\lambda$ is invariant under the action of $T$, so that relative to a basis in $\mathcal{H}_\lambda$, $T$ is represented by an $m_\lambda \times m_\lambda$ matrix. If this matrix is transformed to the Jordan normal form, then eq. (20) implies that all its diagonal elements are equal to $\lambda$. It follows from this observation that there exists a smallest power $n_\lambda$ such that

$$(T - \lambda)^{n_\lambda} \psi = 0 , \quad \text{for all } \psi \in \mathcal{H}_\lambda .$$

Usually $n_\lambda = 1$ as in the hermitian case, but we have found examples (improved harmonic oscillator, strong coupling lattice gauge theories), where $n_\lambda > 1$ for some $\lambda$.

For any spectral value $\lambda \neq 0$, a projector $P_\lambda$ can be defined such that

$$\mathcal{H}_\lambda = P_\lambda \mathcal{H} ,$$

$$P_\lambda^2 = P_\lambda .$$

A convenient formula for $P_\lambda$ is

$$P_\lambda = \oint \frac{dz}{2\pi i} (z - T)^{-1} .$$
where the integration path encloses \( \lambda \), but no other spectral value. Further important properties of the \( P_\lambda \)'s are easily derived from eq. (24):

\[
[T, P_\lambda] = 0, \quad (25)
\]

\[
P_\lambda P_\mu = 0 \quad (\text{if } \lambda \neq \mu), \quad (26)
\]

\[
P_\lambda^t = \theta P_\lambda \theta, \quad (27)
\]

(note that since \( T \) is real, \( \lambda \in \sigma(T) \) implies \( \lambda^* \in \sigma(T) \)).

If \( T \) would be hermitian, we could now write down the spectral decomposition

\[
T = \sum_{\lambda \neq 0} \lambda P_\lambda. \quad (28)
\]

Such a relation is, however, not true for non-hermitian operators in general (there are difficult convergence and completeness problems). What can be established with little effort, is the following statement, which will be quite sufficient for our purposes. Let \( S \) be a finite subset of \( \sigma(T) \) not containing \( \lambda = 0 \). Then, the operator

\[
T_S = T - \sum_{\lambda \in S} TP_\lambda
\]

has spectrum

\[
\sigma(T_S) = \sigma(T) \setminus S. \quad (29)
\]

So, for example, if \( S \) is the set of all spectral values \( \lambda \) with \( |\lambda| \geq \lambda_0 \), \( T_S \) will have a spectral radius smaller than \( \lambda_0 \) and this implies

\[
\|T^k_S\| \leq C(\lambda_0)\lambda_0^k \quad (30)
\]

for some constant \( C(\lambda_0) \) and all \( k = 1, 2, 3, \ldots \). It follows that for fixed \( \lambda_0 \) and \( k \to \infty \), we have

\[
T^k = \sum_{|\lambda| \geq \lambda_0} T^k P_\lambda + O(\lambda_0^k), \quad (31)
\]

i.e. \( T^k \) can be well approximated by a spectral sum, provided \( k \) is large.

Another good property of the transfer matrix defined in the preceding section is that it preserves positivity. That is, if \( \psi[U] > 0 \) for all \( U \), then \( (T\psi)[U] > 0 \) for all \( U \). Actually, \( T^2 \) has the even stronger property of making an everywhere strictly positive smooth function out of any merely non-negative wavefunction \( \psi \) (not identically equal to 0). Under these circumstances, the Perron-Frobenius theorem
Fig. 4. Typical distribution of spectral values $\lambda$ of $T$. Spectral values always occur in pairs of complex conjugated numbers and there is a positive eigenvalue $\Lambda$, which is strictly larger than the absolute magnitude of any other spectral value. $\lambda = 0$ is the only point where spectral values accumulate.

applies and one can prove that $T$ has a real eigenvalue $\Lambda$ with

$$\Lambda > |\lambda| \text{ for all } \lambda \in \sigma(T), \quad \lambda \neq \Lambda. \quad (32)$$

Furthermore, the associated multiplicity $m_\Lambda$ is equal to 1 and the eigenfunction $\psi_\Lambda$ can be chosen positive. As we shall show in the next section, $\psi_\Lambda$ may be interpreted as the ground state wave function. Its non-degeneracy in particular implies that it must be invariant under the discrete symmetries of the system (translations, rotations and reflections, central conjugations).

Summarizing our results obtained so far, we expect a typical distribution of spectral values of $T$ to look as in fig. 4. Recall that we have always assumed the box size $L$ to be finite. In the large volume limit, the normalized spectral values $\lambda/\Lambda$ will be closely spaced and eventually form continuous lines.

5. Asymptotic decay of euclidean two-point functions

We are now going to show that the familiar relation between spectral values of the transfer matrix and the exponential falling off of euclidean correlation functions at large times holds as in ordinary lattice gauge theories. To this end, we must first send the time-like extent $T$ of our euclidean lattice to infinity. For the partition function
Z (eq. (9)), this limit can easily be determined with the help of Lidskii’s theorem (ref. [7], chap. XIII.17), which asserts that the naive formula
\[
Z = \sum_{\lambda \in \sigma(T) \setminus \{0\}} m_\lambda \lambda^T
\]  
(33)
is in fact rigorously true and that the sum on the r.h.s. of eq. (33) is absolutely convergent. In particular,
\[
\lim_{T \to \infty} Z/A^T = 1.
\]  
(34)

Next, consider the euclidean two-point function \( \langle A, B_0 \rangle \) (eq. (11)). Using the spectral decomposition (31) and the above result, one deduces that
\[
\lim_{T \to \infty} \langle A, B_0 \rangle = \Lambda^{-\epsilon} \text{Tr} \{ P_\Lambda \hat{A} T' \hat{B} \}.
\]  
(35)

Since the ground state wave function \( \psi_A \) is positive, it can be normalized such that
\[
(\psi_A, \theta \psi_A) = 1.
\]  
(36)
The projector \( P_\Lambda \) is then given by
\[
P_\Lambda = |\psi_A\rangle \langle \psi_A| \theta,
\]  
(37)
and eq. (35) may be rewritten as
\[
\langle A, B_0 \rangle_{T=\infty} = \Lambda^{-\epsilon} \langle \psi_A | \theta \hat{A} T' \hat{B} | \psi_A \rangle.
\]  
(38)

To evaluate the asymptotic behaviour of \( \langle A, B_0 \rangle_{T=\infty} \) at large times \( t \), we make use of eq. (31) once more to obtain
\[
\langle A, B_0 \rangle_{T=\infty} = \Lambda^{-\epsilon} \sum_{|\lambda| \geq \epsilon A} \langle \psi_A | \theta \hat{A} T' P_\lambda \hat{B} | \psi_A \rangle + O(\epsilon').
\]  
(39)

Because of eq. (22), the terms on the r.h.s. of this equation are actually explicit functions of \( t \) so that we end up with an asymptotic expansion
\[
\langle A, B_0 \rangle_{T=\infty} \sim \Lambda^{-\epsilon} \sum_{\lambda \in \sigma(T) \setminus \{0\}} \lambda p_\lambda(t),
\]  
(40)
where \( p_\lambda(t) \) is a polynomial of \( t \) with degree strictly less than \( n_\lambda \).

Eq. (40) establishes that (connected) two-point correlation functions always decay exponentially at large times. If the leading spectral value in eq. (40) is not real and positive, the exponential factor is multiplied by an oscillating amplitude. Such
anomalous behaviour has recently been observed at strong coupling and in the soluble 1-dimensional Ising model [10]. Also, the leading spectral value may have \( n_\lambda > 1 \), in which case the amplitude will be growing with a power of \( t \). This situation is realized in the “improved” harmonic oscillator for a special value of the frequency.

6. Recovery of the physical Hilbert space near the continuum limit

The technical Hilbert space \( \mathcal{H} \) that we have used so far contains many states with energies of the order of the cutoff, i.e. states, which are unimportant near the continuum limit. The point we wish to make in this section is that if we restrict ourselves to the subspace \( \mathcal{H}_{\text{phys}} \) of all those states, which have small energy relative to the cutoff (\( \lambda/\Lambda \) near 1 in other words), then the non-hermiticity of the transfer matrix can be transformed away by choosing a new scalar product and physical positivity is thus completely restored. A new scalar product relative to which \( T \) becomes hermitian, is suggested by eq. (17):

\[
(\varphi, \psi)_{\text{new}} = (\varphi, \theta \psi)_{\text{old}}.
\]

(41)

For the full Hilbert space \( \mathcal{H} \), this is not an acceptable scalar product, because \( \theta \) has eigenvalues \( \pm 1 \) and \( (\psi, \psi)_{\text{new}} \) is therefore indefinite. Now define the subspace

\[
\mathcal{H}_{\text{phys}} = \sum_{|\lambda| \geq \varepsilon \Lambda} \mathcal{H}_\lambda,
\]

(42)

where \( \varepsilon \) is to be determined (0 < \( \varepsilon < 1 \)). Studying the improved free field theory and lattice gauge theories in a finite (physical) volume at weak coupling [5,12], we found that \( \varepsilon \) can be chosen such that independently of the cutoff the following properties hold:

(i) All spectral values \( \lambda \) of \( T \) with \( |\lambda| \geq \varepsilon \Lambda \) are real and positive.

(ii) The new scalar product (41) is positive on \( \mathcal{H}_{\text{phys}} \), i.e. \( (\psi, \psi)_{\text{new}} > 0 \) for all \( \psi \in \mathcal{H}_{\text{phys}}, \psi \neq 0 \).

Thus, the new scalar product is acceptable on the physical subspace and the usual spectral theorem may be applied to show that \( n_\lambda = 1 \) for all \( \lambda \geq \varepsilon \Lambda \). Furthermore, the corresponding eigenfunctions can be chosen orthonormal relative to the new scalar product and the spectral representation (39) then assumes a form familiar from ordinary lattice gauge theories so that, for example, all terms contributing to the plaquette–plaquette correlation function are positive. Note that we have not rigorously proved the existence of an \( \varepsilon \) with properties (i) and (ii) for lattice gauge theories in a large (physical) volume. It is, however, suggested by our perturbative and free field calculations and could perhaps be further corroborated by studying the asymmetric continuum limit, where the time-like lattice spacing is made small compared to the spacing in other directions.
The actual value of the minimal $\epsilon$ with the above properties is of some practical interest, because it tells us up to what energy positivity may be expected to hold. An estimate of $\epsilon$ can be obtained in weak coupling perturbation theory by determining the location of unphysical (but gauge independent) poles in the propagator. For Symanzik improved actions [6] this yields

$$\epsilon = 0.127 \ldots ,$$

which is an encouragingly small number. It should, however, be noted that at intermediate values of the coupling constant $g_0$, a somewhat larger $\epsilon$ than (43) may be required.

### 7. Concluding remarks

The loss of physical positivity in continuum limit improved lattice gauge theories is a regrettable fact, but, as we have seen, it does not imply fundamental difficulties. For example, the mass spectrum can still be read off from the exponential decay of suitable correlation functions at large times, as in ordinary lattice gauge theories. On the other hand, care must be paid, when applying the variational method to extract the mass spectrum from short time correlation functions (for a review see ref. [11]). Strictly speaking, this method breaks down, but in cases where the correlation length is so large that the contribution of the high-energy states to the relevant two-point functions is negligible, it may anyhow be practical. We have studied this question in the improved massive free field theory and found that as soon as the correlation length is larger than one lattice spacing, the systematic error in a typical mass gap calculation due to the contamination by high-energy states would be a few percent only.

Recently, Parisi suggested the use of improved actions which contain only loops that extend over no more than one lattice in the time direction [13]. While this choice saves positivity, it spoils (discrete) euclidean invariance so that one will have to renormalize the speed of light.

### References


