Wilson action in terms of the Kogut-Susskind Fermion Matrix *

B. KLEIHAUS, L. POLLEY, M.H. WENDEL, E.R. HILF

Fachbereich Physik, Universität Oldenburg, D-2900 Oldenburg, FRG
P.O.B.2503, FRG; (UO01 at DDAGSI3 in EARN).

PACS: 11.15.Ha; 02.70.+d

ABSTRACT

The Kogut-Susskind Fermion matrix D is the decisive ingredient of quantum Chromodynamics, as even the pure gauge action can be expressed by the trace of D^4. This is proven here in the first part. Secondly, an algorithm for the calculation of the action is presented, making use of the diagonal structure of the Kogut Susskind Fermion matrix.

INTRODUCTION

The Kogut Susskind [1] Matrix D in Physics is a nice example of a possibly huge (say 10^4 by 10^4) but very scarcely populated multidiagonal matrix. We will show that the Wilson action of Quantumchromodynamics [2], can be reformulated in terms of D. Even more, due to its multidiagonal structure, a rearrangement of elements will be given such that an actual calculation will be computationally at least comparable to the evaluation of the usual linkwise construction. In other words, the method presented here is mathematically and thus with regard to Physics intuition more clear and esthetic, with respect to numerical evaluation involving no further processing time.

Matrices of large dimensions, say $10^4 * 10^4$, are implicit e.g. in all calculations of SU(3) lattice gauge theory which is the modern theory of strong interaction (in contrast to mathematical instruments [3] necessary for models of nuclear structure). A space-time lattice serves as a numerical approximation of continous space and time. The typical size of these lattices is at least $10*10*10*10$ sites. The fundamental constituents of strong interacting matter (quarks) are described in terms of the relation between their "inner coordinates" in a 3 dimensional complex "colour space" on neighbouring sites of this lattice. This net of relations, or so called "gauge field", is represented by a matrix D, which consists of elements $D(S_1, C_1; S_2, C_2)$ transforming the colour component C_1 at lattice site S_1 into the colour component C_2 at lattice site S_2. For 3 colours and N_σ times N_τ lattice sites (where N_σ denotes the number of space directional links, N_τ the number of steps in time direction), the dimension of the complex matrix D is $(3N_\sigma N_\tau) * (3N_\sigma N_\tau)$. However, only as few as $4 * 3 * N_\sigma * N_\tau$ matrix elements are nonvanishing (depending on the boundary condition).

The dynamics of the gauge field which interacts with itself as well as with quarks is expressed in terms of a statistical weight $W(D)$, attributed to all possible matrices D,

$$W(D) = \text{const} * \det(D) * exp(-\text{const} * tr(D^4)). \tag{1}$$

For a Monte-Carlo simulation of strong interaction, a statistical ensemble of D-matrices is to be generated, yielding the weight function $W(D)$. The next step is then to calculate correlation functions. For instance masses of mesons and baryons are obtained from correlation functions of elements of the matrix inverse of D.

The existing programs which are storage-space optimized do not make use of the simple functional relation between weight factors, correlation functions, and the fermion matrix D, as in (1). They are therefore not easily reproduced. For a better understanding of the simple basic equations of lattice gauge theory it would thus be an advantage to reformulate the physics properties in terms of the Kogut Susskind matrix D, even though this may not improve the computational speed significantly.

First we have to show that the action S, occurring in the exponent of (1) is indeed given by the trace of the fourth power of the Kogut Susskind Fermion matrix which is the basic underlying conjecture. Next, our aim is to formulate an algorithm for the calculation of $tr(D^4)$ by explicit inclusion of the multidiagonal structure of the matrix.

---

*supported by Bundesministerium für Forschung und Technologie BMFT and Gesellschaft für Schwerionenforschung GSI

THE ACTION AS A FUNCTION OF THE KOGUT SUSSKIND FERMION MATRIX

PROOF. $S = tr(D^4)$

The covariant Dirac-operator D on the lattice can be written as a matrix, which acts on fermions in the following way. Represent the fermion-field as a $(N_\tau * N_\sigma)$-dimensional vector $(\psi(n))$. The n-th component of this vector is the field amplitude on the lattice site n. The covariant derivative of the fermion field at the site n is

$$\nabla_\mu \psi(n) = U_\mu(n)\psi(n+\hat{\mu}) - U_\mu^+(n-\hat{\mu})\psi(n-\hat{\mu}).$$

$\hat{\mu}$ means the unity vector in μ-direction. The SU(N)-matrix $U_\mu(n)$ represents the gauge transformation from the site n to the neighbour site n+$\hat{\mu}$ in μ-direction, and the matrix $U_\mu^+(n-\mu)$ the transformation from the site n to the neighbour site n-$\hat{\mu}$, respectively. The matrix representation of the covariant derivative is

$$\nabla_\mu(n,m) = U_\mu(n)\delta(n+\hat{\mu},m) - U_\mu^+(n-\hat{\mu})\delta(n-\hat{\mu},m).$$

The Dirac-operator D is now defined by the matrix

$$D(n,m) = \eta_\mu(n)\nabla^\mu(n,m).$$

The η_μ are

$$\eta_0(n) = 1, \eta_1 = (-1)^{n_1}, \eta_2 = (-1)^{n_1+n_2}, \eta_3 = (-1)^{n_1+n_2+n_3}.$$

We will now prove that the trace of the fourth power of the D-Matrix is up to an additive constant identical to the gluonic part of the Kogut-Susskind action

$$S = tr(D^4).$$

First let us calculate the square of the matrix

$$\sum_s D(n,s)D(s,m) =$$

$$\begin{aligned}
&\sum_s \sum_{\mu,\lambda} \eta_\mu(n)(U_\mu(n)\delta(n+\hat{\mu},s) - U_\mu^+(n-\hat{\mu})\delta(n-\hat{\mu},s))\\
&\quad *\eta_\lambda(m)(U_\lambda(s)\delta(s+\hat{\lambda},m) - U_\lambda^+(s-\hat{\lambda})\delta(s-\hat{\lambda},m))\\
&\quad = \sum_{\mu,\lambda}[\eta_\mu(n)\eta_\lambda(n+\hat{\mu})U_\mu(n)U_\lambda(n+\hat{\mu})\delta(n+\hat{\mu}+\hat{\lambda},m)\\
&\quad -\eta_\mu(n)\eta_\lambda(n+\hat{\mu})U_\mu(n)U_\lambda^+(n+\hat{\mu}-\hat{\lambda})\delta(n+\hat{\mu}-\hat{\lambda},m)\\
&\quad -\eta_\mu(n)\eta_\lambda(n-\hat{\mu})U_\mu^+(n-\hat{\mu})U_\lambda(n-\hat{\mu})\delta(n-\hat{\mu}+\hat{\lambda},m)\\
&+\eta_\mu(n)\eta_\lambda(n-\hat{\mu})U_\mu^+(n-\hat{\mu})U_\lambda^+(n-\hat{\mu}-\hat{\lambda})\delta(n-\hat{\mu}-\hat{\lambda},m)].
\end{aligned} \tag{2}$$

For the calculation of the trace of the fourth power

$$\sum_n \sum_s D^2(n,s)D^2(s,n). \tag{3}$$

it is not nessesary to calculate all products which will appear by inserting (2) into (3), if we look closely at the products of the δ. These products will be of the form

$$\begin{aligned}
&\delta(n+\epsilon_\mu\hat{\mu}+\epsilon_\lambda\hat{\lambda},s)\delta(s+\epsilon_\alpha\hat{\alpha}+\epsilon_\beta\hat{\beta},n)\\
&= \delta(n+\epsilon_\mu\hat{\mu}+\epsilon_\lambda\hat{\lambda},s)\delta(n-\epsilon_\alpha\hat{\alpha}-\epsilon_\beta\hat{\beta},s).
\end{aligned}$$

ϵ_i means sign of the unit vector $\hat{i}$. The products do not vanish if

$$\epsilon_\mu \hat{\mu} + \epsilon_\lambda \hat{\lambda} + \epsilon_\alpha \hat{\alpha} + \epsilon_\beta \hat{\beta} = 0.$$

This condition is fulfilled by two terms in the trace of the fourth power of D:
I

$$\delta(n + \hat{\mu} + \hat{\lambda}, s)\delta(s - \hat{\alpha} - \hat{\beta}, n) \neq 0$$

if $\mu = \alpha, \lambda = \beta$ or $\mu = \beta, \lambda = \alpha$,
II

$$\delta(n - \hat{\mu} + \hat{\lambda}, s)\delta(s + \hat{\alpha} - \hat{\beta}) \neq 0$$

if $\mu = \lambda, \alpha = \beta$ or $\mu = \alpha, \lambda = \beta$.
The resulting terms in the trace are
I

$$\sum_n \sum_{\mu,\lambda} (\eta_\mu(n)\eta_\lambda(n+\hat{\mu})\eta_\mu(n+\hat{\mu}+\hat{\lambda})\eta_\lambda(n+\hat{\lambda})U_\mu(n)U_\lambda^+(n+\hat{\mu}-\hat{\lambda})U_\mu^+(n-\hat{\lambda})U_\lambda(n-\hat{\lambda})$$

$$+\eta_\mu(n)\eta_\lambda(n+\hat{\mu})\eta_\lambda(n+\hat{\mu}+\hat{\lambda})\eta_\mu(n-\hat{\mu})),$$

II

$$\sum_n \sum_{\mu,\lambda} (\eta_\mu(n)\eta_\lambda(n+\hat{\mu})\eta_\mu(n+\hat{\mu}-\hat{\lambda})\eta_\lambda(n-\hat{\lambda})U_\mu(n)U_\lambda^+(n+\hat{\mu}-\hat{\lambda})U_\mu^+(n-\hat{\lambda})U_\lambda(n-\hat{\lambda})$$

$$+\eta_\mu(n)\eta_\mu(n+\hat{\mu})\eta_\lambda(n)\eta_\lambda(n-\hat{\lambda})).$$

The η-products in the second summands in the brackets do not depend on the lattice site n. Summation over the indicees μ, λ gives the value 4. Summation over the lattice sites gives a constant which depends on the lattice size.

For further calculations of the remaining terms in the sum let us look first at the case $\mu = \lambda$. The products of the U-matrices are the unit matrix and the η-products are independent of the lattice site and take the value 1. For $\mu \neq \lambda$ the sum over n, μ, λ is just the sum over all plaquettes. The SU(N) trace of the U-products equals the trace of the plaquette variables $U_{\mu\lambda}, U_{\mu\lambda}^+$

$$tr(U_{\mu\lambda}) = tr\big(U_\mu(n)U_\lambda(n+\hat{\mu})U_\mu^+(n+\hat{\lambda})U_\lambda^+(n)\big),$$

$$tr(U_{\mu\lambda}^+) = tr\big(U_\lambda(n)U_\mu(n+\hat{\lambda})U_\lambda^+(n+\hat{\mu})U_\mu^+(n)\big).$$

With the new summation index m=n+$\hat{\lambda}$ the second trace gets the form

$$tr\big(U_\lambda(n-\hat{\lambda})U_\mu(n)U_\lambda^+(n-\hat{\lambda}+\hat{\mu})U_\mu^+(n-\hat{\lambda})\big),$$

$$= tr\big(U_\mu(n)U_\lambda^+(n-\hat{\lambda}+\hat{\mu})U_\mu^+(n-\hat{\lambda})U_\lambda(n-\hat{\lambda})\big).$$

The η-products are independent of the lattice site and have the value -1. Now the trace of the fourth power of the matrix $D(n,m)$ can be written

$$tr(D^4(n,m)) = 6 * (N_\tau N_\sigma) + \sum_{n;\mu,\lambda} tr\big(2 - U_{\mu\lambda}(n) - U_{\mu\lambda}^+(n)\big). \tag{4}$$

this is up to a constant the gluonic part of the action.

The gluonic part of the action can be written as the trace of the fourth power of the fermion matrix, because the relevant contributing terms result from closed paths. This is a consequence of the rectangular and discrete structure of the lattice. The question, whether the action in the continuum case can also be written as a "trace" of the "fermion-matrix", is an open one. First one must define the matrix of the Dirac-operator and then take some trace, which could be a sum or an integral over a configuration space, replace Kroneckers delta symbol by Diracs delta function and the sum over lattice points by integration over space time. In the limit of vanishing lattice spacing the Dirac operator gets its continuum form. For the proof in the continuum case the calculations are similar to the proof for the lattice case and only those terms contribute which are due to closed loops. But they are all divergent even before the limit of vanishing lattice spacing is taken. So one might think the equality of the trace of the fourth power of the fermion matrix and the gluonic part of Wilsons action is a property of the lattice. On the other hand the continuum definitions of the Dirac operator and of the trace can be given in a less naive way. So the interesting question is what physical meaning has the trace of the fourth power of the Dirac operator in the continuum and in which way can it be connected to the lattice case. This will be worked out in a following paper.

THE ALGORITHM

Basic Idea. The structure of the Kogut-Susskind Fermion Matrix may be described by its main features: its huge size, its very scarce population located in 8 diagonals, its being antisymmetric. To access its physics consequences one has to learn how to handle it. A way, to surpass the directly unsurmountable obstacle of handling its huge size is given in this paragraph. First, instead of the two-dimensional indexspace, where a matrix element is given by its row-column position we use a new set of diagonal index K and position index L on the specific diagonal K. Each diagonal is characterized by a specific deviation Δ(diagonal index) from the main diagonal (for a matrix element positioned in row I and column J being an element of diagonal K the diagonal index is simply $J - I$). The range of the second new matrix index L is then

$$1 \ldots N_{DIM} - N_\sigma^{INT(|K-N_{DIA}-\frac{1}{2}|)}. \tag{5}$$

where N_{DIM} denotes the dimension of the matrix, N_σ stands for the number of lattice points in space direction, N_{DIA} is the number of diagonals below the main diagonal (in our case $N_{DIA} = 4$), INT denotes the function taking the integer part of a floating point number.

The matrix is constructed along its diagonals, starting in the lower left corner with the first diagonal $K = 1$ and ending up with the last one below the main diagonal (where $K = N_{DIA}$) making use of the antihermiticity of D. The elements are counted along each diagonal and stored sequentially in a large complex vector. Secondly, we note a specific property of the elements contributing to the trace of D^4 . In the traditional index terminology the trace of D^4 is given by

$$\sum_{ijmn} a_{ij} a_{jm} a_{mn} a_{ni}. \tag{6}$$

This sum can be now thought of as a sum over all rectangular combinations possible for any 4-element product of matrixelements

$$\sum_{ijmn} a_{ij} a^*_{mj} a_{mn} a^*_{in}, \tag{7}$$

This identity can be illustrated as

$$\begin{pmatrix}
a_{11} & \cdots & \cdots & \cdots & \cdots & \cdots & a_{1N} \\
\vdots & & & & & & \\
a_{i1} & \cdots & a_{ij} & \cdots & \cdots & \cdots & a_{iN} \\
\vdots & & & & & & \\
a_{j1} & \cdots & \cdots & a_{jm} & \cdots & \cdots & a_{jN} \\
\vdots & & & & & & \\
a_{m1} & \cdots & \cdots & \cdots & a_{mn} & \cdots & a_{mN} \\
\vdots & & & & & & \\
a_{n1} & a_{ni} & \cdots & \cdots & \cdots & \cdots & a_{nN} \\
\vdots & & & & & & \\
a_{N1} & \cdots & \cdots & \cdots & \cdots & \cdots & a_{NN}
\end{pmatrix}
=
\begin{pmatrix}
a_{11} & \cdots & \cdots & \cdots & \cdots & \cdots & a_{1N} \\
\vdots & & & & & & \\
a_{i1} & \cdots & a_{ij} & \cdots & a^*_{in} & \cdots & a_{iN} \\
\vdots & & & & & & \\
\vdots & & & & & & \\
\vdots & & & & & & \\
a_{m1} & \cdots & a^*_{mj} & \cdots & a_{mn} & \cdots & a_{mN} \\
\vdots & & & & & & \\
a_{N1} & \cdots & \cdots & \cdots & \cdots & \cdots & a_{NN}
\end{pmatrix}. \tag{8}$$

It is now useful to distinguish between double degenerated (eq. 9), single degenerated (eq. 10,11) and non-degenerated (eq. 12) contributions to the sum in (7) such that it desintegrates into the following parts

$$\sum_{i,j} |a_{ij}|^4 \tag{9}$$

$$2\sum_{\substack{j>l \\ i}} |a_{ij}|^2 |a_{il}|^2 \tag{10}$$

$$2\sum_{\substack{i>k \\ j}} |a_{ij}|^2 |a_{kj}|^2 \tag{11}$$

$$4Re\sum_{\substack{i>k \\ j>l}} a_{ij} a_{kj}^* a_{kl} a_{il}^* . \tag{12}$$

Realisation. The first term of double degenerated contributions can be easily calculated by summing over all "power four" - terms of single elements in the storage vector. The second and the third term are identical. One can calculate one of them by collecting the contributions from all two-point correlations with positions (I_{D1}, I_{P1}) and (I_{D2}, I_{P2}) in the new indices. The position of the second point on its diagonal (which lies exclusively below or above the first diagonal I_{D1}) has to be calculated including a characteristic shift depending on the position of both diagonals with respect to the main diagonal

$$I_{P2} = I_{P1} + \theta(N_{DIA} - I_{D1}) * (\Delta(I_{D2}) * \theta(N_{DIA} - I_{D2}) - \Delta(I_{D1})) \tag{13}$$

with the help of the step function

$$\Theta(x) = \begin{cases} 1, & \text{if } x \geq 0 \\ 0, & \text{otherwise,} \end{cases}$$

and where we used Δ(diagonal index) as defined above. However one has to realize that only the contributions from non- degenerated combinations are coming in from gauge-invariant quantities. On the other hand the degenerated terms only give rise to a change of a constant common factor.

In calculating the third (and only relevant) sum (eq. 12) the same procedure has to take place now also for the third corner point of the rectangle. Given the first (left upper) corner of the rectangle with diagonal index I_{D1} and position index I_{P1} on it, one has to perform the sum now over all diagonals that are allowed for the second (left lower) corner with position

$$I_{P2} = I_{P1} + \theta(I_{D1} - N_{DIA} - 1) * (-\Delta(I_{D2}) * \theta(I_{D2} - N_{DIA} - 1) + \Delta(I_{D1})) \tag{14}$$

and the third (lower right) corner with position

$$I_{P3} = I_{P2} + \theta(N_{DIA} - I_{D2}) * (\Delta(I_{D3}) * \theta(N_{DIA} - I_{D3}) - \Delta(I_{D2})). \tag{15}$$

To complete the rectangle the diagonal with index I_{D4} that fulfills the condition

$$\Delta(I_{D4}) - \Delta(I_{D3}) = \Delta(I_{D1}) - \Delta(I_{D2})$$

is selected; the position of the last (upper right) corner point is then given by

$$I_{P4} = I_{P1} + \theta(N_{DIA} - I_{D1}) * (\Delta(I_{D4}) * \theta(N_{DIA} - I_{D4}) - \Delta(I_{D1})). \tag{16}$$

A further analysis shows that only two kinds of terms in the non-degenerated case contribute

I

$$I_{D1} \leq N_{DIA}, I_{D2} < N_{DIA}, I_{D3} > N_{DIA}, I_{D4} > N_{DIA}$$

then

$$I_{P2} = I_{P1}, \tag{14a}$$

$$I_{P3} = I_{P2} - \Delta(I_{D2}), \tag{15a}$$

$$I_{P4} = I_{P1} - \Delta(I_{D1}), \tag{16a}$$

and

II

$$I_{D1} > N_{DIA}, I_{D2} \leq N_{DIA}, I_{D3} \leq N_{DIA}$$

then

$$I_{P2} = I_{P1} + \Delta(I_{D1}), \tag{14b}$$

$$I_{P3} = I_{P2} + \Delta(I_{D3}) - \Delta(I_{D2}), \tag{15b}$$

$$I_{P4} = I_{P1}. \tag{16b}$$

In both cases a summation over I_{P1} starting at $I_{P1} = 1$ with respect to the condition

$$0 < I_{P3} \leq \text{ length of diagonal 3}$$

is understood.

We studied the dependence of actual computing time for one calculation of $tr(D^4)$ of matrix dimension. The calculation of the total action for a $10^4 * 10^4$ lattice using the algorithm presented here (one iteration) is with 0.65 seconds even sligthly smaller than a reference calculation with the conventional one. Thus, apart from being technically competitive, one has gained a mathematically independent and more stringent formulation of the Wilson action as being just the trace of the fourth power of the Kogut Susskind fermion matrix.

ACKNOWLEDGEMENT

We are grateful to the Gesellschaft für Schwerionenforschung in Darmstadt for providing us with the service of their excellent computer facility.

REFERENCES

1. J.Kogut, L. Susskind, Phys.Rev. D11 (1975) 395
2. K.G. Wilson, Phys.Rev. D10 (1974) 2445
3. M.H.Wendel, and E.R.Hilf, Journ. of Math.Physics 26 (1985) 1570