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Efficient numerical techniques for perturbative lattice gauge theory computations

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Abstract

We discuss a set of methods and numerical tools, which are useful for a computer based approach to perturbative calculations in lattice gauge theory. The topics considered include the automatic generation of gluon vertex programs, a derivation of the Faddeev-Popov determinant on lattices with boundary, the use of a partially finite lattice with twisted boundary conditions as an infrared cutoff without zero modes, and finally the numerical extrapolation of lattice Feynman diagrams to the continuum limit. As an illustration of the methods we describe their implementation in the computation of the on-shell improved lattice action at weak coupling.

* Heisenberg foundation fellow

1. Introduction

In a recent article [1], we have presented our results on the computation of the action for on-shell improved lattice gauge theories at weak coupling, a calculation which essentially amounts to evaluate a number of one-loop Feynman diagrams with definite external momenta. The propagators and vertex functions from which Feynman diagrams in gauge theories are built are much more complicated on the lattice than they are in the continuum, especially so for improved lattice gauge theories (see e.g. the Appendix of Ref. [2]). Analytical manipulations of lattice diagrams are therefore time consuming and liable to errors. For this reason, we decided to follow a strategy where, apart from listing the diagrams and extracting the group theoretical factors, the whole calculation is done numerically on a computer. To guarantee the efficiency and reliability of the numerical computations, we have developed various adapted techniques, which we hope will prove useful for other perturbative calculations as well. It is thus our objective in this paper to describe these methods each in their own right in separate sections, which can be read and referred to independently from one another (common notations are summarized in section 2).

A computer program, which calculates the value of a lattice Feynman diagram, calls subprograms which compute the value of the relevant vertex functions given the momenta flowing into the vertices. Because of the above mentioned complexity of the lattice vertex functions, it is in general not easy to manufacture such vertex programs and to make sure that they are faultless.

If one approaches this problem straightforwardly, errors are likely to occur at two stages: firstly, when one derives an analytical formula for the vertex functions starting from a given lattice action S, and secondly, when this formula is coded into a computer program. In section 3, a method to produce vertex programs is described, which avoids the intermediary step of actually printing an analytical formula for the vertex functions on paper. The basic idea is simply to design an "algebraic" computer program, which requires as input the action S and the number of legs of the desired vertex function, and whose output is the vertex program *). In the course of our work on improved lattice gauge theories, we have found that the particular realization of this idea described in section 3 is foolproof and yields fast vertex programs. Moreover, simplifying features, e.g. when some of the momenta entering the vertex are external and hence fixed, can easily be taken into account to obtain even better performance of the generated programs.

Lattice gauge theory presents a framework in which the Faddeev-Popov determinant can be rigorously derived. We are of course aware of the existing treatments in the literature [4]. Nevertheless, we feel that a further discussion here would not be out of place, the aim being to derive a closed formula for the Faddeev-Popov determinant, which is valid for arbitrary linear gauge conditions and on lattices with or without boundary (section 4). Especially in the case with boundary, care must be

*) Algebraic computer programs have been used previously to check some of the rather involved algebra, which must be mastered to calculate Λ-parameter ratios (e.g. Ref. [3]).

paid to treat possible zero modes of the Faddeev-Popov operator correctly. With ordinary gauge fixing conditions, the Faddeev-Popov determinant turns out to be rather simple and is easily expanded by hand. Diagrams involving ghost loops are therefore negligibly complicated as compared to the diagrams with gauge boson loops, in particular, the numerical evaluation of these diagrams usually does not require special programming techniques.

Lattice Feynman diagrams are ultra-violet finite, of course, but infrared divergences may occur, especially if one aims at computing on-shell quantities. These divergences can be regulated by assuming a finite space-time volume, for example. However, with ordinary periodic boundary conditions, one then has to face an apparently difficult zero mode problem (the "torons" of Ref. [5]), which renders the normal Feynman diagram expansion invalid. As is described in detail in section 5, a better way to introduce an infrared cutoff is to compactify only two of the four space-time dimensions and to impose twisted periodic boundary conditions [6] in these directions. There are no torons in this case and the perturbation expansion is straightforward. Moreover, it turns out that the gluon propagator is completely massive, i.e. there are no singularities in the range of momenta admitted by the boundary conditions. In this twisted world, the integrands of Feynman diagrams are thus totally regular and the integrations over those momentum components, which are not quantized by the boundary conditions, can be done easily (an adapted exponentially convergent method of integration is described in subsection 5.3). In our calculation of the improved action, we used the formalism of section

5 merely as a tool, but we emphasize that the twisted world is interesting in itself and may prove useful to study the transition from the perturbative to the non-perturbative regime in non-abelian gauge theories.

In perturbative lattice gauge theory computations, one is often interested in the limiting behaviour of the diagrams as the lattice spacing "a" tends to zero. From Symanzik's work on the cutoff dependence of scalar field theories on the lattice [7], one expects that for any diagram D an asymptotic expansion of the form

$$(1.1) \qquad D \underset{a\to 0}{\sim} a^{-\omega} \sum_{n=0}^{\infty} \sum_{m=0}^{\ell} c_{nm}\, a^n (\ln a)^m$$

holds, where ℓ is the number of loops in the diagram and $\omega \geq 0$ depends on the convergence properties of D and of its sub-diagrams. In our numerical approach, the first few coefficients c_{nm} can be determined accurately by calculating the diagram for a sequence of lattice spacings and fitting the results with the asymptotic series (1.1). An adapted fit procedure together with a reliable estimation of the rounding and systematical errors is described in sub-section 6.2. It is based on a recursive blocking transformation, which takes into account the general form of the higher terms in the expansion (1.1) to increase the precision of the calculated first few coefficients c_{nm}. In this way, very accurate results can be obtained even if the diagram has only been evaluated for moderately small lattice spacings (very small lattice spacings usually require large amounts of computer time and are hence impractical).

The asymptotic expansion (1.1) is not only the basis of our numerical extrapolation procedure, but it is also of fundamental importance for lattice theories as it describes how precisely the continuum limit is approached in perturbation theory. It appears, however, that a rigorous proof of (1.1) has only been given for one-loop diagrams on the standard lattice $\mathbb{Z}^4$ [7] (Symanzik has given further reasons for the general validity of (1.1) by referring to Pauli-Villars regularized field theories, where he has earlier been able to prove the analogous expansion for any number of loops [8]). As an example of how a rigorous derivation of eq. (1.1) for lattices with boundary may look like, we here treat in detail the case of one-loop momentum sums over 4-dimensional Brillouin zones as they typically arise from Feynman diagrams with vanishing external momenta (sub-section 6.1). Diagrams with non-zero external momenta or momentum integrals instead of sums can be treated similarly [9].

It is only in the last section 7 that we give an illustration of the methods described in this paper by applying them to Symanzik's improvement programme. Although there is unavoidably some overlap with the material of Ref. [1], this section is meant as a technical supplement to that paper. We suggest that the reader, interested in this particular application, should read Ref. [1] first and consult Ref. [10] if an introduction to the programme is desired.

2. Notations

In this paper we will be dealing with various aspects of perturbative calculations in lattice gauge theory. We will work on a (4-dimensional) hyper-

cubic lattice $\mathbb{\Lambda}$ with spacing 'a', i.e.

(2.1) $\quad x \in \mathbb{\Lambda} \quad , \quad x = na \quad , \quad n \in \mathbb{Z}^4$.

For convenience we will often set a = 1. If desired the lattice spacing may always be reintroduced in these parts of the paper by dimensional analysis. $\hat{\mu}$ will denote the vector in direction μ of unit length. Lattice derivatives $\partial_\mu, \partial^*_\mu$ are defined by differences

(2.2) $$\partial_\mu f(x) = (f(x+a\hat{\mu}) - f(x))/a$$

(2.3) $$\partial^*_\mu f(x) = (f(x) - f(x-a\hat{\mu}))/a \ .$$

We limit ourselves to the case when the dynamical variables are SU(N) matrices $U(x,\mu)$ associated with links joining the points x and $x+a\hat{\mu}$. Often we will work with some directions compact; in this case the boundary conditions must be specified. $\mathcal{U}$ will denote the space of gauge fields.

The action S should be invariant under local gauge transformations

(2.4) $$U(x,\mu) \rightarrow \Lambda(x)\, U(x,\mu)\, \Lambda(x+a\hat{\mu})^{-1} \quad , \quad \Lambda(x) \in SU(N),$$

where the Λ's obey boundary conditions such that the transformation (2.4) is from $\mathcal{U}$ into itself. We denote by $\mathcal{G}$ the gauge group, the maximal set of such Λ's. Expectation values are given as usual by

(2.5) $$\langle O \rangle = \int \mathcal{D}[U]\, e^{-S[U]}\, O \ / \int \mathcal{D}[U] e^{-S[U]}$$

where $\mathcal{D}[U]$ is the Haar measure on $\mathcal{U}$.

We restrict attention to perturbative expansions around the classical vacuum and only to situations when the functional integral can be performed by substituting for the parallel transporter

(2.6) $$U(x,\mu) = \exp a g_0 A_\mu(x)$$

fixing the gauge, and expanding all entries in powers of the bare coupling g_0. In (2.6) the potential $A_\mu(x)$ is an element of the Lie algebra $\mathfrak{su}(N)$ of SU(N). The $A_\mu(x)$ have a Fourier decomposition appropriate to the boundary conditions. For the infinite volume case for example this takes the form

(2.7) $$A_\mu(x) = \$_{k,b}\ e^{ik\cdot(x+\frac{1}{2}a\hat{\mu})}\, \tilde{A}^b_\mu(k)\, T^b$$

where

(2.8) $$\$_{k,b} = \sum_{b=1}^{N^2-1} \prod_{\mu=0}^{3} \left(\int_{-\pi/a}^{\pi/a} dk_\mu \right)$$

and the T^b are matrices belonging to the fundamental representation of $\mathfrak{su}(N)$. The phase in (2.7) involves the coordinate of the mid-point of the link joining x and $x+a\hat{\mu}$. It has the consequence that the $\tilde{A}_\mu$ have the following periodicity properties

(2.9) $$\tilde{A}_\mu(k + 2\pi a^{-1}\hat{\rho}) = (-1)^{\delta_{\mu\rho}}\, \tilde{A}_\mu(k)$$

When performing lattice calculations it is useful to introduce the notation

(2.10) $$\hat{k}_\mu = \frac{2}{a} \sin \frac{a k_\mu}{2}$$

for any momentum k_μ.

Finally the class of actions we consider will be sums over closed curves $\mathcal{C}$ of terms of the form

(2.11) $$\mathcal{L}(\mathcal{C}) = \mathrm{Re}\ \mathrm{tr}\,[\mathbb{1} - U(\mathcal{C})]$$

where $U(\mathcal{C})$ is the parallel transporter around $\mathcal{C}$, starting at some arbitrary point on $\mathcal{C}$. Note $\mathcal{L}(\mathcal{C}) \geq 0$ for any $\mathcal{C}$. Extensions to actions involving higher characters of SU(N) are trivial. The standard Wilson action S_W involves only curves P surrounding single plaquettes, i.e.

(2.12) $$S_W[U] = \frac{2}{g_0^2} \sum_P \mathcal{L}(P)$$

3. Automatic generation of vertex programs

3.1 Definition of the vertices *

In this section we shall discuss how, for a given action, one can automatically generate programs which compute values of vertices appearing in the Feynman rules, for a given configuration of the external momenta.

Our formulae, in this section, refer to the infinite volume case, however,

* We set the lattice spacing a=1 throughout this section.

we stress that the reduced vertices we shall encounter (eq. (3.20)) are dependent only on the local nature of the action (the finite volume aspects having bearing on the allowed momenta). The action, of the general form discussed in Section 2, can be arbitrarily complicated and can include terms referring to many varieties of closed curves. It is of course sufficient to initially consider one general curve and finally sum over different curves.

Let $\mathcal{C}$ be an arbitrary closed path in $\mathbb{Z}^4$ of length ℓ. Further, let $\mathcal{C}_n$ be the path obtained by translating the path $\mathcal{C}$ through $n \in \mathbb{Z}^4$ and denote

(3.1) $$S(\mathcal{C}) = \sum_n \mathcal{L}(\mathcal{C}_n)$$

Vertex functions $V_r^{\mathcal{C}}$ are then defined in the perturbative expansion by *

(3.2) $$S(\mathcal{C}) = \sum_{r=2}^{\infty} \frac{1}{r!} g_0^r \sum_{k_1,a_1} \cdots \sum_{k_r,a_r} (2\pi)^4 \delta\Big(\sum_{i=1}^r k_i\Big) \cdot \tilde{A}_{\mu_1}^{a_1}(k_1) \cdots \tilde{A}_{\mu_r}^{a_r}(k_r) \cdot V_r^{\mathcal{C}}(k_1,a_1,\mu_1;\ldots;k_r,a_r,\mu_r)$$

and requiring them to be totally symmetric

(3.3) $$\sigma \cdot V_r^{\mathcal{C}} = V_r^{\mathcal{C}} \quad \text{for all} \quad \sigma \in \mathcal{P}_r ,$$

where $\mathcal{P}_r$ is the group of permutation of r elements, and the action of $\sigma \in \mathcal{P}_r$ on a function F of r arguments a_i is defined in the natural way by

(3.4) $$(\sigma \cdot F)(a_1, \ldots a_r) = F(a_{\sigma(1)}, \ldots, a_{\sigma(r)})$$

* The δ-function appearing is the periodic δ-function.

The vertex functions $V_r^{\mathcal{C}}$ are uniquely determined through eqs. (3.1)-(3.4) and the geometry of the curve $\mathcal{C}$. Our first task will be to derive an explicit expression for $V_r^{\mathcal{C}}$, which is suitable for programming.

3.2 Explicit representation for the vertices

The path $\mathcal{C}$ is completely specified by

(3.5) n(i): sequential vertices along $\mathcal{C}$ (i = 1,..,ℓ).

From these we can extract the following arrays s(i), μ(i) by

$$n(i-1) - n(i) = s(i)\cdot\widehat{\mu(i)} \quad , \tag{3.6}$$

which specify the directions of successive links along $\mathcal{C}$. In (3.6) set $i-1 \to \ell$ if i = 1, and s(i) takes values $\pm$ 1.

With this notation, the parallel transporter from n(i-1) to n(i) is given by $\exp g_0 X_i$ with

$$X_i = \begin{cases} A_{\mu(i)}(n(i)) & \text{if } s(i) = +1 \\ -A_{\mu(i)}(n(i-1)) & \text{if } s(i) = -1 \end{cases} \tag{3.7}$$

Thus, the action density associated with $\mathcal{C}$ becomes

$$\mathcal{L}(\mathcal{C}) = \frac{1}{2}\,\mathrm{Tr}\,\{2 - e^{g_0X_\ell}\cdots e^{g_0X_1} - e^{-g_0X_1}\cdots e^{-g_0X_\ell}\} \tag{3.8}$$

Expanding this expression in powers of g_0, we have

$$\mathcal{L}(\mathcal{C}) = \sum_{r=2}^{\infty} \frac{1}{r!}\, g_0^r\, \mathcal{L}_r(\mathcal{C}) \tag{3.9}$$

with

$$\mathcal{L}_r(\mathcal{C}) = (-1)^{r+1}\,\frac{1}{2} \sum_{1\le u_1\le\ldots\le u_r\le \ell} \frac{r!}{\alpha_1!\ldots\alpha_\ell!}\cdot \tag{3.10}$$

$$\cdot\,\mathrm{Tr}\,\{X_{u_1}\ldots X_{u_r} + (-1)^r X_{u_r}\ldots X_{u_1}\}$$

where α_i counts the factors associated to a given link:

$$\alpha_i = \sum_{a=1}^{r} \delta_{i,u_a} \qquad (i = 1\ldots\ell) \tag{3.11}$$

The Fourier representation of X_i is given by (see (2.7))

$$X_i = \$ \sum_{k,b} \sum_{\mu} \tilde{A}^b_\mu(k)\, T^b\, s(i)\, \delta_{\mu,\mu(i)}\, \exp\tfrac{i}{2}\, k\cdot a(i) \tag{3.12}$$

where a(i)/2 is the coordinate of the mid-point of the link joining n(i) and n(i-1),

$$a_\mu(i) = n_\mu(i) + n_\mu(i-1) \tag{3.13}$$

Inserting (3.12) in (3.10), we obtain (3.2) with

$$V_r^{\mathcal{C}}(k_1,a_1,\mu_1;\ldots;k_r,a_r,\mu_r) = \tag{3.14}$$

$$\frac{1}{r!} \sum_{\sigma\in\mathcal{P}_r} \sigma\cdot C_r(a_1,\ldots a_r)\,\sigma\cdot \hat{Y}_r^{\mathcal{C}}(k_1,\mu_1;\ldots;k_r,\mu_r)$$

$$\hat{Y}_r^e(k_1,\mu_1;\ldots;k_r,\mu_r) = \frac{1}{2}\sum_{1\le u_1\le\ldots\le u_r\le \ell} (-1)^{r+1}\frac{r!}{\alpha_1!\ldots\alpha_\ell!}$$

(3.15)

$$\cdot\, s(1)^{\alpha_1}\ldots s(\ell)^{\alpha_\ell}\cdot\{\delta_{\mu_1,\mu(u_1)}e^{\frac{i}{2}k_1\cdot a(u_1)}\ldots\delta_{\mu_r,\mu(u_r)}e^{\frac{i}{2}k_r\cdot a(u_r)}\}$$

where the Clebsch-Gordon coefficients C_r are defined by

$$C_r(a_1,\ldots,a_r) = \mathrm{Tr}(T^{a_1}\ldots T^{a_r}) + (-1)^r\,\mathrm{Tr}(T^{a_r}\ldots T^{a_1}) \tag{3.16}$$

They have simple properties under the subgroup $\mathfrak{Z}_r$ of permutations generated by cyclic permutations and the inversion ρ ($\rho(i) = r+1-i$), namely

$$\sigma\cdot C_r = \chi_r(\sigma)\cdot C_r \qquad , \quad \sigma\in\mathfrak{Z}_r \tag{3.17}$$

where χ_r is characterized by

$$\chi_r(\sigma\cdot\tau) = \chi_r(\sigma)\cdot\chi_r(\tau) \qquad , \quad \sigma,\tau\in\mathfrak{Z}_r$$

$$\chi_r(\sigma) = 1 \qquad \text{for } \sigma \text{ cyclic} \tag{3.18}$$

$$\chi_r(\rho) = (-1)^r \qquad \text{for inversion } \rho$$

Making use of property (3.17), we end up with

$$V_r^e(k_1,a_1,\mu_1;\ldots;k_r,a_r,\mu_r) = \tag{3.19}$$

$$\frac{1}{r!}\sum_{\sigma\in\mathfrak{S}_r/\mathfrak{Z}_r}\sigma\cdot C_r(a_1,\ldots,a_r)\,\sigma\cdot Y_r^e(k_1,\mu_1;\ldots;k_r,\mu_r)$$

where the reduced vertices Y_r^e are given by

$$Y_r^e(k_1,\mu_1;\ldots;k_r,\mu_r) =$$

$$\frac{1}{2}\sum_{1\le u_1\le\ldots\le u_r\le \ell}(-1)^{r+1}\frac{r!}{\alpha_1!\ldots\alpha_\ell!}\; s(1)^{\alpha_1}\ldots s(\ell)^{\alpha_\ell} \tag{3.20}$$

$$\cdot\sum_{\sigma\in\mathfrak{Z}_r}\chi_r(\sigma)\,\sigma\cdot\{\delta_{\mu_1,\mu(u_1)}e^{\frac{i}{2}k_1\cdot a(u_1)}\ldots\delta_{\mu_r,\mu(u_r)}e^{\frac{i}{2}k_r\cdot a(u_r)}\}$$

(the permutations σ act on the arguments $u_1,\ldots,u_r$ according to eq. (3.4)).

The reduced vertices have simple symmetry properties under permutations in $\mathfrak{Z}_r$:

$$\sigma\cdot Y_r^e = \chi_r(\sigma)\,Y_r^e \qquad \text{for } \sigma\in\mathfrak{Z}_r \tag{3.21}$$

Their reality properties are

$$Y_r^e(k_1,\mu_1;\ldots;k_r,\mu_r)^* = Y_r^e(-k_1,\mu_1;\ldots;-k_r,\mu_r) \tag{3.22}$$

Finally, for the curve $\tilde{e}$ obtained from e by inversion through the origin ($\tilde{n}(i) = -n(i)$), we have

$$Y_r^{\tilde{e}}(k_1,\mu_1;\ldots;k_r,\mu_r) = (-1)^r\,Y_r^e(-k_1,\mu_1;\ldots;-k_r,\mu_r) \tag{3.23}$$

In the following we will discuss only the automatic generation of the reduced vertices Y_r^e . Of course the Clebsch-Gordon coefficients C_r can also be programmed, but, at least for small r, these coefficients

are simply evaluated by hand.

When momentum is conserved *, $\sum_i k_i = 0$, the $a(u_j)$ in (3.20) can be replaced by translated coordinates $a'(u_j)$. This can be done separately for each configuration of the u_j's and hence we can use the translation invariance to get the exponents appearing in (3.20) into a standard form. Such a procedure is obviously useful to identify terms which have equal exponents and hence reduce the number of final independent $\{a(u_j)\}$ configurations appearing in (3.20). A particular realisation would be, for example

$$a'_\mu(u_j) = a_\mu(u_j) - s_\mu(\{u\}) \quad , \tag{3.24}$$

where

$$s_\mu(\{u\}) = (m_\mu - m_\mu(\mathrm{mod}\,2))/2$$

$$m_\mu = \max_j (a_\mu(u_j)) + \min_j (a_\mu(u_j)) \quad . \tag{3.25}$$

The "centralised coordinates" a' then obey the constraints

$$\max_j (a'_\mu(u_j)) + \min_j (a'_\mu(u_j)) \in \{0, 1\} \quad . \tag{3.26}$$

3.3 Generation of vertex programs

For the case when $\mathcal{C}$ is simply the curve around one plaquette and for reasonably small r ($\lesssim 5$), the terms in Eq. (3.20) can be quite easily

* As can be chosen without loss in Feynman diagram calculations.

collected by hand. However, for larger and more intricate curves the task becomes rather tedious, and the probability of making errors in the derivation of the analytical formulae is high. Another source of error is the subsequent transcription of the analytical expressions, which are algebraically complicated, into computer programs.

It is thus effort-saving and overall more reliable to generate vertex programs using algebraic computer techniques. One could employ for example standard routines such as REDUCE or SCHOONSCHIP. On the other hand, the expression (3.20) is ideally suited for programming in a language which is efficient in list processing, for example PL/I [11] with its facility of based storage.

We now proceed to describe the structure of a program whose sole function is, for a given curve (or set of curves), to write corresponding vertex programs. As explained in the introduction, the output of a vertex program is an array $YR(\mu_1,\ldots,\mu_r)$ equal to the numerical values of an r-point vertex function $\Upsilon^{\mathcal{C}}_r$ for a given input of external momenta. Such vertex programs can then be used as subprograms for the evaluation of Feynman diagrams, without reference to the programs which generated them.

The key to our method is to recognize that according to eq. (3.20), the reduced vertex function $\Upsilon^{\mathcal{C}}_r$ is a sum of terms of the form

$$\frac{1}{2} \oint e^{\frac{i}{2}\cdot(k_1\cdot v(1) + k_2\cdot v(2) + \ldots + k_r\cdot v(r))}$$

where f is an integer factor and $v_\mu(i)$ $(i = 1,\dots,r;\ \mu = 0,\dots,3)$ are integer vectors. For every combination of Lorentz indices $\mu_1,\dots,\mu_r$, the terms T contributing to $Y^e_r(k_1,\mu_1;\dots;k_r,\mu_r)$ can be found from eq. (3.20) and may be collected in a table $\mathcal{T}_r(\mu_1,\dots,\mu_r)$. Thus, each entry T in the list $\mathcal{T}_r(\mu_1,\dots,\mu_r)$ is just an integer f plus an integer array $v_\mu(i)$, and Y^e_r is simply given by

$$(3.27)\qquad Y^e_r(k_1,\mu_1;\dots;k_r,\mu_r) = \frac{1}{2}\sum_{T\in\mathcal{T}_r(\mu_1,\dots,\mu_r)} f\, e^{\frac{i}{2}(k_1\cdot v(1)+\dots+k_r\cdot v(r))}$$

Of course, since only the sum of all terms is required, the table $\mathcal{T}_r(\mu_1,\dots,\mu_r)$ may be reduced by adding up all those entries with equal shift vectors $v_\mu(i)$. If $\sum_{i=1}^{r} k_i = 0$, it is advantageous to perform this reduction only after the vectors $v_\mu(i)$ have been transformed to a normal form by a translation as explained at the end of subsection 3.2. Without further notice, we shall from now on assume that shift vectors $v_\mu(i)$ are normalized.

The main program for vertex generation calls two subprograms I and II, which perform distinct tasks. Subprogram I sets up the tables $\mathcal{T}_r(\mu_1,\dots,\mu_r)$ as follows. First, for the particular curve $\mathcal{C}$ under consideration, the integer arrays $a_\mu(i)$, s(i) and μ(i) (as defined by eqs. (3.6), (3.13)) are determined. Then, for a given r, sums over $1\le v_1\le v_2\le\dots\le v_r\le \ell$ and over permutations $\sigma\in\mathcal{Z}_r$ are made as in eq. (3.20). For each configuration of v_j's and σ, the rhs of eq. (3.20) defines a term T, i.e. a factor f and vectors $v_\mu(i)$. This term is then

added to the list $\mathcal{T}_r(\mu_1,\dots,\mu_r)$, where the Lorentz indices $\mu_1,\dots,\mu_r$ are given by $\mu_j = \mu(v_{\sigma(j)})$.

When adding a term, the table $\mathcal{T}_r(\mu_1,\dots,\mu_r)$ is first scanned to establish whether a term with the same vectors $v_\mu(i)$ already exists. If not, the new term is simply added to the list. If, on the other hand, a term with the same vectors $v_\mu(i)$ is found, the factors f of the new and the old term are added. In the case that the resulting factor is zero, the storage is freed. In this way one is economical with respect to the storage. The number of terms $n_{r,\ell}$ in the sum (3.20) for given r,ℓ is

$$(3.28)\qquad n_{r,\ell} = \frac{2}{(r-1)!}\,\ell(\ell+1)\dots(\ell+r-1)\ ,$$

e.g. for $r=6$, $\ell=6$ we have $n_{6,6} = 5544$. However, in practice the collection of lists have much fewer terms because of cancellations.

In certain applications, a general form for the vertices may not be required. The special properties of the momenta and Lorentz indices in such cases should then be incorporated at this stage to simplify the lists accordingly.

We finally remark that the subprogram I may be designed so that contributions from various curves with weight factors corresponding to the lattice action under investigation, can be added to the same tables in succession.

After subprogram I has run, the lists of terms described above exist in the core memory of the computer. It is the function of subprogram II to

convert these lists into ordinary vertex programs, which yield the vertices Y_r^e for given external momenta.

For each configuration $\mu_1,\ldots,\mu_r$ of Lorentz indices, subprogram II first locates the table $T_r(\mu_1,\ldots,\mu_r)$ in core memory. After that it runs through the list and for each term in the list prints an assignment statement on a print file. The assignment statements are of the form *

(3.29) $$YR(\mu_1,\ldots,\mu_r) = YR(\mu_1,\ldots,\mu_r) + TERM$$

where TERM is the mathematical expression corresponding to the term in the list, in the desired computer language (cp. eq. (3.27)).

In the final step the assignment statements in the print file are copied into an ordinary program file where they are completed with cards to make up an ordinary subprogram which can be compiled in the usual way. It is our experience that the vertex subprograms generated in this way are faultless and speed efficient.

Lastly we note that in most cases of interest a further simplification arises from the fact that the tables contain terms which come from a set

* Separate assignment statements are made for each term to avoid lengthy expressions, which could cause problems during compilation.

of loops $\{e_1,\ldots e_n\}$ which are mapped onto each other under inversion through the origin. Then the reduced vertex

(3.30) $$Y_r = \sum_{i=1}^{n} Y_r^{e_i}$$

satisfies (see (3.22) and (3.23))

(3.31) $$Y_r(k_1,\mu_1;\ldots;k_r,\mu_r)^* = (-1)^r\, Y_r(k_1,\mu_1;\ldots;k_r,\mu_r)$$

(3.32) $$Y_r(k_1,\mu_1;\ldots;k_r,\mu_r) = (-1)^r\, Y_r(-k_1,\mu_1;\ldots;-k_r,\mu_r)$$

It follows that each term with vector $v(i) \neq 0$ has a partner in the same list with $-v(i)$. These terms correspond then to exponentials which can be combined into a sine if r is odd or to a cosine if r is even. In the special case $v(i) = 0$, the term corresponds to a constant. Hence, the assignment statements (3.29) are written for pairs of terms rather than for single terms.

4. Linear gauge fixing conditions and the Faddeev-Popov determinant

Conventional perturbation theory involves a saddle point expansion around the classical vacuum configurations $U(x,\mu) = \Lambda(x)\Lambda(x+\hat{\mu})^{-1}$, $\Lambda \in \mathcal{G}$. The degeneracy of this saddle point requires that the gauge degrees of freedom are separated out before one expands the integrand in the functional integral in a power series of the coupling constant g_0. The separation of gauge variables from the other ("physical") degrees

of freedom amounts to choosing a special coordinate system in a neighborhood * of the classical vacuum manifold in such a way that a first set of coordinates parametrizes the gauge orbits and the remaining coordinates label the fields along the orbits. Only the latter are shifted by a gauge transformation, and gauge invariant quantities, in particular the action S, are independent of them. The integration over these variables is therefore trivial and may be factored out so that after that one will be left with the integrals over the "physical" coordinates and a non-degenerate saddle point.

Different coordinate systems of the above type correspond to different "gauge fixing conditions". We here consider a class of smooth parametrizations, which are geometrically motivated and which lead to particularly transparent formulae. Throughout this section, the lattice spacing is set equal to 1 for convenience, and we shall also assume that the lattice Λ is finite. If desired, the infinite volume limit may easily be taken at the end of all calculations.

For our derivation of the Faddeev-Popov determinant, a more detailed description of gauge fields and gauge transformations on the lattice Λ is needed. All commonly used boundary conditions may be accommodated in the following framework:

* In perturbation theory one effectively integrates only over an infinitesimally small neighborhood of the saddle point manifold. A parametrization of the gauge field manifold far away from this region is therefore not required here.

(a) Λ is a finite subset of the standard lattice $\mathbb{Z}^4$.

(b) Gauge fields $U(x,\mu)$ live on a fixed set $\mathcal{B}$ of bonds $(x, x+\hat{\mu}) \in \Lambda \times \Lambda$. $\mathcal{B}$ does not necessarily contain all the bonds on Λ, but we shall require that every $x \in \Lambda$ may be connected to any other point $y \in \Lambda$ by a sequence of bonds in $\mathcal{B}$. The gauge variables $U(x,\mu)$ are independent and unrestricted elements of SU(N).

(c) The action S is a continuous function of the gauge field variables $U(x,\mu)$ and the apriori measure in the functional integral is given by

$$\mathcal{D}[U] = \prod_{x,\mu} dU(x,\mu) \quad , \tag{4.1}$$

the product being taken over all bonds in $\mathcal{B}$ (dU denotes the invariant measure on SU(N)).

(d) The elements of the gauge group $\mathcal{G}$ are functions $V(x)$ on Λ with values in SU(N). In general, not all such functions are in $\mathcal{G}$, but only those for which the gauge transformation

$$U(x,\mu) \to V(x)\, U(x,\mu)\, V(x+\hat{\mu})^{-1}$$

is a symmetry of the action S.*

For example, a lattice with L sites on a side and periodic boundary conditions can be realized by choosing

$$\Lambda = \{ x \in \mathbb{Z}^4 \mid 0 \leq x_\nu \leq L \text{ for all } \nu ;\ x_\nu = L \text{ for at most one } \nu \}$$

*) If the group $\hat{\mathcal{G}}$ of all gauge transformations leaving the action fixed divides into several disconnected parts, the gauge group $\mathcal{G}$ is usually taken to be the identity component of $\hat{\mathcal{G}}$ (Gauss' law requires infinitesimal gauge invariance only). The discrete group $\hat{\mathcal{G}}/\mathcal{G}$ is then interpreted as a physical symmetry of the system.

$$\mathcal{B} = \{ (x, x+\hat{\mu}) \in \Lambda \times \Lambda \mid 0 \le x_\nu < L \text{ for all } \nu;\ \mu = 0,\dots,3 \}$$

$$\mathcal{G} = \{ V : \Lambda \to SU(N) \mid V(x) = V(y) \text{ if } x_\nu = y_\nu \ (\mathrm{mod}\, L) \text{ for all } \nu \}$$

Other boundary conditions (free, Dirichlet, twisted periodic, etc.) are also easily fit into the above framework so that in the following we shall assume that (a) - (d) hold. Note that (c) and (d) imply that $\mathcal{G}$ is a closed Lie subgroup of the group of all functions $V(x)$, $x \in \Lambda$, with values in $SU(N)$.

4.1 Infinitesimal fields

The basic idea of the parametrizations introduced in the next subsection is to first identify the gauge and non-gauge coordinate axes in an infinitesimal neighborhood of $U(x,\mu) = 1$, and then to use gauge transformations respectively the exponential mapping to extend the infinitesimal coordinate system to a finite neighborhood of the classical vacuum configurations. To prepare the ground for this construction, we here study the space $\mathcal{H}_1$ of infinitesimal gauge fields around $U(x,\mu) = 1$ and appropriate gauge fixing conditions.

$\mathcal{H}_1$ is equal to the linear space of all vector fields $a_\mu(x)$, which are defined on the bonds $(x, x+\hat{\mu}) \in \mathcal{B}$ and which take values in the Lie algebra $\mathfrak{su}(N)$ of $SU(N)$. A convenient inner product on $\mathcal{H}_1$ may be defined through

$$(4.2) \qquad (a,b) = -\sum_{x,\mu} \mathrm{Tr}\, \{ a_\mu(x)\, b_\mu(x) \}$$

where the summation is over all links in $\mathcal{B}$ and the trace is in the fundamental representation space of $\mathfrak{su}(N)$.

Infinitesimal gauge transformations $\omega(x)$ form a vector space $\mathcal{H}_0$ of scalar fields on the lattice, which also take values in $\mathfrak{su}(N)$. In general, $\mathcal{H}_0$ does not contain all possible such fields (i.e. there are usually some restrictions on $\omega(x)$ at the boundary of Λ). $\mathcal{H}_0$ may be identified with the Lie algebra of $\mathcal{G}$ and a scalar product may be defined by a formula analogous to (4.2). To every $\omega \in \mathcal{H}_0$, there corresponds an infinitesimal pure gauge field a_μ according to

$$(4.3) \qquad a_\mu(x) = \partial_\mu \omega(x) \quad \text{for all} \quad (x, x+\hat{\mu}) \in \mathcal{B}\ .$$

The set of all these modes a_μ is a linear subspace $\mathcal{H}_1^L$ of $\mathcal{H}_1$.

We now turn to discuss possible gauge fixing conditions for infinitesimal fields. Suppose $\mathcal{F} : \mathcal{H}_1 \to \mathcal{H}_0$ is a linear operator and let $\mathcal{H}_1^{\mathcal{F}}$ denote the kernel of $\mathcal{F}$, i.e.

$$(4.4) \qquad \mathcal{H}_1^{\mathcal{F}} = \{ a_\mu \in \mathcal{H}_1 \mid \mathcal{F}(a) = 0 \}\ .$$

We then say that $\mathcal{F}$ is an admissable gauge fixing operator, if the following criteria are satisfied:

(1) Every $a_\mu \in \mathcal{H}_1^{\mathcal{F}}$ has a unique decomposition

$$(4.5) \qquad a_\mu = a_\mu^{\mathcal{F}} + a_\mu^{L}\ ,$$

where $a_\mu^{\mathcal{F}} \in \mathcal{H}_1^{\mathcal{F}}$ and $a_\mu^{L} \in \mathcal{H}_1^{L}$.

(2) Let $\mathcal{G}_0$ be the group of constant (i.e. space-time independent) gauge transformations.* Then $\mathcal{H}_1^{\mathcal{F}}$ is invariant under the adjoint action of $\mathcal{G}_0$.

* $\mathcal{G}_0$ is a closed subgroup of $SU(N)$, which depends on the boundary conditions chosen. In the case of the twisted world of section 5, for example, $\mathcal{G}_0$ is equal to the centre of $SU(N)$.

In other words, if $a_\mu \in \mathcal{H}_1^{\mathcal{F}}$ and $V \in \mathcal{G}_0$, then $V a_\mu V^{-1} \in \mathcal{H}_1^{\mathcal{F}}$. Property (1) insures that the gauge fixing condition $\mathcal{F}$ leads to a clean separation of the gauge modes from the other "physical" degrees of freedom. The significance of property (2) will become fully clear later. At this point, we only mention that the vacuum manifold is isomorphic to $\mathcal{G}/\mathcal{G}_0$. To lift the degeneracy of the saddle point, it is therefore not necessary that the gauge fixing condition also breaks the invariance under $\mathcal{G}_0$.

A particularly natural choice for the gauge fixing operator $\mathcal{F}$ is the following. Let $d: \mathcal{H}_0 \to \mathcal{H}_1$ be defined by

$$(d\omega)_\mu(x) = \partial_\mu \omega(x) \qquad \text{for all } (x, x+\hat{\mu}) \in \mathcal{B}. \tag{4.6}$$

The adjoint operator $d^\dagger$ of d relative to the scalar products defined in $\mathcal{H}_0$ and $\mathcal{H}_1$ then maps $\mathcal{H}_1$ into $\mathcal{H}_0$. In the interior of the lattice, $d^\dagger$ is simply given by

$$(d^\dagger a)(x) = -\sum_\mu \partial_\mu^* a_\mu(x), \tag{4.7}$$

but near the boundary, the explicit form of $d^\dagger$ must be worked out taking into account the shape of Λ and the restrictions on $\omega(x) \in \mathcal{H}_0$ near the boundary. It is then easy to verify that the choice

$$\mathcal{F} = d^\dagger \tag{4.8}$$

has all the required properties. In this case, $\mathcal{H}_1^{\mathcal{F}}$ is simply the orthogonal complement of $\mathcal{H}_1^{\perp}$.

4.2 Parametrization of a neighborhood of the classical vacua

We are now in a position to set up a coordinate system around the classical vacua, which separates the gauge degrees of freedom from the physical ones as required for the saddle point expansion. To this end, choose some arbitrary admissable gauge fixing operator $\mathcal{F}$ as discussed above. Then, one can show that every gauge field $U(x,\mu)$, which is sufficiently close to a pure gauge configuration, can be represented by

$$U(x,\mu) = \Lambda(x) \exp q_\mu(x)\, \Lambda(x+\hat{\mu})^{-1}, \tag{4.9}$$

where $q_\mu \in \mathcal{H}_1^{\mathcal{F}}$ is small (say $\|q\| < \varepsilon$) and $\Lambda \in \mathcal{G}$. This representation is, however, not unique, because the rhs of eq. (4.9) is invariant under the substitution

$$\begin{aligned} q_\mu(x) &\longrightarrow V q_\mu(x) V^{-1}, \\ \Lambda(x) &\longrightarrow \Lambda(x) V^{-1}, \end{aligned} \tag{4.10}$$

where V is an arbitrary element of $\mathcal{G}_0$, the group of constant gauge transformations. Note that since $\mathcal{F}$ is an admissable gauge fixing operator, $V q_\mu V^{-1}$ is again an element of $\mathcal{H}_1^{\mathcal{F}}$.

The degeneracy (4.10) can be lifted by imposing a constraint on Λ. For example, one may realize the coset space $SU(N)/\mathcal{G}_0$ by some convenient subset of SU(N) and then require that for some fixed $y \in \Lambda$ the matrix $\Lambda(y)$ is in $SU(N)/\mathcal{G}_0$. Such a constraint defines a subset $\tilde{\mathcal{G}}$ of $\mathcal{G}$, which is

a smooth manifold except perhaps for a singular set of points, which is of zero relative measure and which may therefore be neglected in what follows. One may now prove, using property (1) of the gauge fixing operator $\mathcal{F}$ and the implicit function theorem, that the representation (4.9) is unique for $q \in \mathcal{U}_1^{\mathcal{F}}$, $\|q\| < \varepsilon$, and $\Lambda \in \tilde{\mathcal{G}}$.

To obtain an explicit parametrization of the gauge field manifold around the classical vacua, choose some orthonormal basis v^α in $\mathcal{U}_1^{\mathcal{F}}$ and some coordinates τ_A for $\tilde{\mathcal{G}}$. Then, the gauge field U(x,μ) parametrized by ξ_α and τ_A is given by eq. (4.9), where

$$q_\mu(x) = \sum_\alpha \xi_\alpha v_\mu^\alpha(x) \quad , \quad \sum_\alpha \xi_\alpha^2 < \varepsilon^2, \tag{4.11}$$

and Λ is the element of $\tilde{\mathcal{G}}$ with coordinates τ_A . Note that because the lattice $\mathbb{\Lambda}$ is finite, the total number of parameters ξ_α and τ_A is also finite.

4.3 The Faddeev-Popov determinant

We now proceed to work out the apriori measure (4.1) in the coordinates of the preceding subsection. Define a metric G in gauge field space by

$$G_{\alpha\beta} = \left(U^{-1}\frac{\partial}{\partial \xi_\alpha} U \, , \, U^{-1}\frac{\partial}{\partial \xi_\beta} U \right), \tag{4.12}$$

$$G_{\alpha A} = G_{A\alpha} = \left(U^{-1}\frac{\partial}{\partial \xi_\alpha} U, U^{-1}\frac{\partial}{\partial \tau_A} U \right), \tag{4.13}$$

$$G_{AB} = \left(U^{-1}\frac{\partial}{\partial \tau_A} U \, , \, U^{-1}\frac{\partial}{\partial \tau_B} U \right), \tag{4.14}$$

where the scalar product is given by eq. (4.2). The associated volume element

$$\prod_\alpha d\xi_\alpha \prod_A d\tau_A \, (\det G)^{1/2} \tag{4.15}$$

may be shown to have the same invariance properties as the apriori measure (4.1) and is hence proportional to $\mathcal{D}[U]$. We are thus left to calculate the determinant of G.

From the definition (4.9), (4.11) of our coordinate system, the derivatives of U with respect to ξ_α and τ_A can be worked out easily and one obtains

$$G_{\alpha\beta} = \left(J_q v^\alpha, J_q v^\beta \right) \tag{4.16}$$

$$G_{\alpha A} = -\left(J_q v^\alpha, d_q \omega^A \right) \tag{4.17}$$

$$G_{AB} = \left(d_q \omega^A, d_q \omega^B \right) \tag{4.18}$$

The notation here is as follows. The fields $\omega^A \in \mathcal{U}_0$ are defined by

$$\omega^A(x) = \Lambda(x)^{-1}\frac{\partial}{\partial \tau_A}\Lambda(x) \, . \tag{4.19}$$

J_q is a linear invertible operator acting in $\mathcal{U}_1$. Explicitly, it is given by

$$(4.20) \qquad (J_q a)_\mu(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(n+1)!} [\, Ad\, q_\mu(x) \,]^n \cdot a_\mu(x)$$

where $AdX \cdot Y = [X,Y]$ for all $X, Y \in \mathfrak{su}(N)$. The series in eq. (4.20) may also be written in the closed form

$$(4.21) \qquad [\, 1 - e^{-Ad\, q_\mu(x)} \,] / Ad\, q_\mu(x) \ ,$$

which should, however, be used with care, since AdX has always zero eigenvalues and is not invertible. Finally, the operator d_q occurring in eqs. (4.17), (4.18) maps $\mathcal{H}_0$ into $\mathcal{H}_1$ according to

$$(4.22) \qquad (d_q \omega)_\mu(x) = \partial_\mu \omega(x) + [\, 1 - e^{-Ad\, q_\mu(x)} \,] \cdot \omega(x)$$

In particular, $d_q = d$ if q vanishes.

We now use the following Lemma from linear algebra:

Lemma 4.1: Let w^i, $i = 1,2,3,\ldots$, be a basis in a Hilbert space $\mathcal{H}$ and suppose A is a linear operator in $\mathcal{H}$. Define matrices $a_{ij} = (w^i, Aw^j)$, $b_{ij} = (w^i, w^j)$.

Then, we have

$\det a = (\det A) \cdot (\det b)$

In our case, $\mathcal{H}$ is identified with $\mathcal{H}_1$ and the basis w^i with the vectors v^α and $J_q^{-1} d_q \omega^A$. For q = 0, this set of vectors is certainly a linear basis of $\mathcal{H}_1$, because ω^A plus the constant modes (i.e. the generators of $\mathcal{G}_0$) form a basis of $\mathcal{H}_0$ and the $d\omega^A$'s are hence a basis of $\mathcal{H}_1^L$, thus complementing the v^α's . For small q, the vectors $J_q^{-1} d_q \omega^A$ are just a little deformed so that we still have a basis. Choosing $A = J_q^\dagger J_q$, the Lemma yields

$$(4.23) \qquad \det G = (\det J_q^\dagger J_q) \cdot (\det \hat{G})$$

$$(4.24) \qquad \hat{G}_{\alpha\beta} = \delta_{\alpha\beta}$$

$$(4.25) \qquad \hat{G}_{\alpha A} = \hat{G}_{A\alpha} = -(v^\alpha, J_q^{-1} d_q \omega^A)$$

$$(4.26) \qquad \hat{G}_{AB} = (J_q^{-1} d_q \omega^A, J_q^{-1} d_q \omega^B) \ .$$

The next step is an application of

Lemma 4.2: For a matrix M with block structure

$$M = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}$$

we have

$$\det M = (\det A) \cdot (\det [\, C - B^T A^{-1} B \,])$$

Identifying M with $\hat{G}$ and using the completeness of the basis v^α in $\mathcal{H}_1^T$, one obtains

(4.27) $$\det \hat{G} = \det H$$

(4.28) $$H_{AB} = (J_q^{-1} d_q \omega^A , P J_q^{-1} d_q \omega^B)$$

where P denotes the (orthogonal) projector on the orthogonal complement of $\mathcal{H}_1^{\mathcal{F}}$. With the help of the adjoint operator $\mathcal{F}^\dagger$ of $\mathcal{F}$, which maps $\mathcal{H}_0$ into $\mathcal{H}_1$, we have

(4.29) $$P = \mathcal{F}^\dagger (\mathcal{F}\mathcal{F}^\dagger)^{-1} \mathcal{F}$$

Note that the zero modes (if any) of $\mathcal{F}\mathcal{F}^\dagger$ are orthogonal to the subspace $\mathcal{F}(\mathcal{H}_1)$ of $\mathcal{H}_0$, and the inverse of $\mathcal{F}\mathcal{F}^\dagger$ in eq. (4.29) has therefore a well-defined meaning.

Inserting (4.29) in (4.28), we have

(4.30) $$H_{AB} = (\Delta_{FP} \omega^A , (\mathcal{F}\mathcal{F}^\dagger)^{-1} \Delta_{FP} \omega^B) ,$$

(4.31) $$\Delta_{FP} = \mathcal{F} J_q^{-1} d_q$$

The Faddeev-Popov operator Δ_{FP} is a linear and in general non-hermitian operator acting in $\mathcal{H}_0$. An important property of this operator is now summarized by

Lemma 4.3: For small q, the zero modes of Δ_{FP} are exactly the constant fields $\omega \in \mathcal{H}_0$, and the range of Δ_{FP} is exactly the subspace $\mathcal{F}(\mathcal{H}_1)$ of $\mathcal{H}_0$.

Postponing the proof to Appendix A, we note that the Lemma implies in

particular that the fields $\nu^A = \Delta_{FP} \omega^A$ form a linear basis in $\mathcal{F}(\mathcal{H}_1)$. Applying Lemma 4.1 once more, we thus have

(4.32) $$\det H = (\det \hat{H}) \cdot (\det' \mathcal{F}\mathcal{F}^\dagger)^{-1} ,$$

(4.33) $$\hat{H}_{AB} = (\omega^A , \Delta_{FP}^\dagger \Delta_{FP} \omega^B) ,$$

where det' implies the determinant with zero modes omitted.

We finally introduce the space $\mathcal{H}_0'$ of all those modes $\omega \in \mathcal{H}_0$, which are orthogonal to the constant fields. Let P_0' be the corresponding orthogonal projector. By Lemma 4.3, $\hat{H}_{AB}$ may be then be written in the form

(4.34) $$\hat{H}_{AB} = (\mu^A , \Delta_{FP}^\dagger \Delta_{FP} \mu^B) , \quad \mu^A = P_0' \omega^A .$$

Since $\mu^{A'}$s are a basis of $\mathcal{H}_0'$, Lemma 4.1 applies and one obtains

(4.35) $$\det \hat{H} = (\det' \Delta_{FP}^\dagger \Delta_{FP}) \cdot (\det \Omega)$$

(4.36) $$\Omega_{AB} = (\omega^A , P_0' \omega^B)$$

Summarizing the results obtained so far, we have thus established the factorization

(4.37) $$\det G = (\det' \mathcal{F}\mathcal{F}^\dagger)^{-1} \det \Omega \det J_q^\dagger J_q \det' \Delta_{FP}^\dagger \Delta_{FP} .$$

Note that the first factor is independent of the coordinates ξ_α, τ_A,

the second one depends only on τ^A , and the last two factors depend only on ξ_α . In the functional integral (2.5) with gauge invariant observables $\mathcal{O}$, the first factor and the integral over the τ^A's therefore drops out and we are left with

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int_{\mathcal{H}_1^{\mathcal{F}}} \mathcal{D}[q] \{ \det J_q^\dagger J_q \det' \Delta_{FP}^\dagger \Delta_{FP} \}^{1/2} \mathcal{O}\, e^{-S}, \tag{4.38}$$

where in $\mathcal{O}$ and S the field U(x,μ) should be replaced by exp $q_\mu(x)$ ($\mathcal{D}[q]$ denotes the usual translation invariant measure in the vector space $\mathcal{H}_1^{\mathcal{F}}$). For perturbation theory, we finally substitute

$$q_\mu(x) = g_0 A_\mu(x), \tag{4.39}$$

and introduce (anti-commuting) Faddeev-Popov ghost fields c and $\bar{c}$:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int_{\mathcal{H}_1^{\mathcal{F}}} \mathcal{D}[A] \int_{\mathcal{H}_0'} \mathcal{D}[c] \int_{\mathcal{F}(\mathcal{H}_1)} \mathcal{D}[\bar{c}]\, \mathcal{O}\, e^{-S_{eff}} \tag{4.40}$$

$$S_{eff} = S - \frac{1}{2} \ln \det J_{g_0 A}^\dagger J_{g_0 A} - (\bar{c}, \Delta_{FP} c) . \tag{4.41}$$

As indicated in eq. (4.40), the ghost field c is not integrated over the whole space $\mathcal{H}_0$, but only over the space $\mathcal{H}_0'$ orthogonal to the zero modes of Δ_{FP}. Correspondingly, $\bar{c}$ is integrated over the range $\mathcal{F}(\mathcal{H}_1)$ of Δ_{FP}, which has the same dimension as $\mathcal{H}_0'$.

Eqs. (4.40) and (4.41) constitute our final result for the gauge fixed

functional integral on finite lattices Λ . From here on, perturbation theory simply proceeds by expanding $\mathcal{O}$ and S_{eff} in powers of g_0 and performing the resulting Gaussian integrals by Wick's theorem. For the measure term in S_{eff} and the Faddeev-Popov operator, the expansion in g_0 is easily worked out. For example, up to fourth order, we have

$$\frac{1}{2} \ln \det J_{g_0 A}^\dagger J_{g_0 A} = \sum_{x,\mu} \mathrm{Tr} \{ \frac{g_0^2}{24} (\mathrm{Ad}\, A_\mu(x))^2 - \frac{g_0^4}{2880} (\mathrm{Ad}\, A_\mu(x))^4 + O(g_0^6) \} \tag{4.42}$$

$$\Delta_{FP} = \Delta_0 + g_0 \Delta_1 + g_0^2 \Delta_2 + g_0^4 \Delta_4 + O(g_0^5) \tag{4.43}$$

$$\Delta_0 = \mathcal{F} d \tag{4.44}$$

$$\Delta_1 = \mathcal{F} \{ \frac{1}{2} \mathrm{Ad}\, A\, d + \mathrm{Ad}\, A \} \tag{4.45}$$

$$\Delta_2 = \frac{1}{12} \mathcal{F} (\mathrm{Ad}\, A)^2 d \tag{4.46}$$

$$\Delta_4 = \frac{1}{720} \mathcal{F} (\mathrm{Ad}\, A)^4 d \tag{4.47}$$

(in eq. (4.42), the sum is over all bonds in $\mathcal{B}$ and the trace is in the adjoint representation space of $\mathfrak{su}(N)$).

5. Perturbation theory on a lattice with twisted periodic boundary conditions

In this section we collect some results concerning SU(N) lattice gauge theories on a 4-dimensional lattice with 2 compact dimensions and twisted periodic boundary conditions for the gauge field (a "twisted tube" in other words)*. Compared to other lattices, the twisted tube has several technical advantages, in particular, the perturbation expansion is straightforward and the compact dimensions imply an infrared cutoff in the Feynman diagrams. Moreover, due to the special geometry, the summations over loop momenta are either finite (in the compact directions) or they are integrals over periodic analytic functions, a situation, which is favourable for numerical treatment. A further remarkable feature is that scattering processes of particles moving along the x_3-axis can be studied without ever running into infrared divergences (we have exploited this fact for our calculation of the on-shell improved action for lattice gauge theories, see section 7).

In subsection 5.1, we describe in some detail how to set up perturbation theory on the twisted tube. Since the discrete symmetries of the system are not immediately obvious from the Feynman rules, the transformation laws for the gauge potential $A_\mu(x)$ are derived in subsection 5.2. Finally, an efficient numerical integration program for periodic analytic functions, as they typically arise in Feynman diagrams, is described in subsection 5.3.

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* When more than two dimensions are compactified, the analysis can be carried through analogously.

5.1 Basic formalism

We consider a lattice of finite extent L in the x_1 and x_2-direction and infinite extent in the other two directions. The space $\mathcal{U}_\Omega$ of gauge fields on this lattice is identified with the set of fields $U(x,\mu) \in SU(N)$, $x/a \in \mathbb{Z}^4$, $\mu = 0,\ldots,3$, which are twisted periodic, viz.

$$U(x + L\hat{\nu}, \mu) = \Omega_\nu U(x,\mu) \Omega_\nu^{-1}, \quad (\nu = 1,2) \tag{5.1}$$

Here, the twist matrices Ω_ν are constant, gauge field independent elements of SU(N), which satisfy the algebra

$$\Omega_1 \Omega_2 = z \Omega_2 \Omega_1, \qquad z = e^{\frac{2\pi i}{N}}. \tag{5.2}$$

The corresponding gauge group $\mathcal{G}_\Omega$ consists of all fields $\Lambda(x) \in SU(N)$ with

$$\Lambda(x + L\hat{\nu}) = \Omega_\nu \Lambda(x) \Omega_\nu^{-1}, \quad (\nu = 1,2). \tag{5.3}$$

The twist algebra (5.2) insures the "integrability" of (5.1) (and (5.3)) in the sense that if x is shifted by several periods L in the x_1, x_2-plane, the resulting matrix U at the final point does not depend on the order in which the shifts are applied. In other words, if $U(x,\mu)$ is given arbitrarily for $0 \leq x_\nu < L$, $\nu = 1,2$, eq. (5.1) consistently defines a unique extension of $U(x,\mu)$ to all points x.

Examples of twist matrices Ω_ν have been given in the literature (e.g.

Ref.[12]), but since an explicit representation is never needed, we here only note that

(1) eq. (5.2) fixes the Ω_ν 's up to unitary transformations,

(2) they are irreducible, i.e. any matrix, which commutes with Ω_1 and Ω_2, is a multiple of the unit matrix, and

(3) $\Omega_\nu^N = (-1)^{N-1}\mathbb{1}$ for $\nu = 1,2$.

In particular, property (1) implies that all choices of twist matrices result in the same physical amplitudes.

For twisted periodic gauge fields, the action density is periodic in x_1 and x_2 and the total action S is defined by summing the density over an arbitrary periodicity cell (in the present formulation, there are no extra twist factors in the action, cp. Appendix B). Now suppose that $S \geqslant 0$ and $S = 0$ if and only if $\mathcal{L}(\mathcal{C}) = 0$ for every plaquette loop $\mathcal{C}$. Then, using properties (1) and (2) above, one readily shows that the only zero action fields are pure gauge configurations,

$$U(x,\mu) = \Lambda(x)\Lambda(x+a\hat{\mu})^{-1}, \qquad \Lambda \in \mathcal{G}_\Omega , \tag{5.4}$$

i.e. the toron manifold is trivial. It follows that for such actions, the perturbative expansion of the functional integral can be done straightforwardly by substituting

$$U(x,\mu) = e^{g_0 a A_\mu(x)} , \tag{5.5}$$

fixing the gauge and expanding all entries in powers of g_0. The gauge potential $A_\mu(x)$ in (5.5) satisfies

$$A_\mu(x)^\dagger = -A_\mu(x) , \qquad \mathrm{Tr}\, A_\mu(x) = 0 , \tag{5.6}$$

$$A_\mu(x + L\hat{\nu}) = \Omega_\nu A_\mu(x) \Omega_\nu^{-1} , \tag{5.7}$$

and an example of a gauge fixing condition, suitable for the calculation of on-shell quantities, is the familiar Coulomb gauge condition

$$\sum_{i=1}^{3} \partial_i^* A_i(x) = 0 . \tag{5.8}$$

The corresponding Faddeev-Popov ghost action is derived in section 4 and we shall therefore not repeat any details here. We only remark that in the present case the ghost fields c and $\bar{c}$ are also twisted periodic fields and the Faddeev-Popov operator Δ_{FP} has no zero modes.

Feynman rules are most conveniently formulated in momentum space. To this end, we would like to expand $A_\mu(x)$ into plane waves, which respect the periodicity (5.7). Now, it is not difficult to show that a basis of twisted periodic plane waves is given by

$$\Gamma_k\, e^{ik\cdot x} , \qquad -\pi/a < k_\mu \leqslant \pi/a , \tag{5.9}$$

where Γ_k is a (complex) $N \times N$ matrix, which solves the eigenvalue equations

(5.10) $$\Omega_\nu \Gamma_k \Omega_\nu^{-1} = e^{ik_\nu L} \Gamma_k \quad , \qquad (\nu = 1,2).$$

Actually, a non-zero solution of (5.10) exists if and only if the transverse momentum components k_1, k_2 satisfy

(5.11) $$k_\nu = m \cdot n_\nu \quad , \quad n_\nu \in \mathbb{Z} \quad , \quad m = \frac{2\pi}{LN} \quad ,$$

i.e. as expected, these momentum components are quantized, although the quantum m is smaller than the usual quantum $2\pi/L$. With (5.11), the solution of eq. (5.10) is unique up to a phase, which we may choose such that

(5.12) $$\Gamma_k = \Omega_1^{-n_2} \Omega_2^{n_1} z^{\frac{1}{2}(n_1+n_2)(n_1+n_2-1)} .$$

These matrices have previously appeared in the context of large N reduced models (see Ref. [13] and references therein). Besides eq. (5.10), the most relevant properties of the Γ_k's are

(5.13) $$\Gamma_k \in SU(N)$$

(5.14) $$\Gamma_{k'} = \Gamma_k \quad \text{if} \quad k'_\perp = k_\perp \ (\text{mod } N)$$

(5.15) $$\Gamma_k = \mathbb{1} \quad \text{if} \quad k_\perp = 0 \ (\text{mod } N)$$

(5.16) $$\text{Tr } \Gamma_k = 0 \quad \text{unless} \quad k_\perp = 0 \ (\text{mod } N)$$

(5.17) $$\Gamma_k^\dagger = z^{-\frac{1}{2}(k,k)} \Gamma_{-k}$$

(5.18) $$\Gamma_{k'} \Gamma_k = \Gamma_{k'+k} z^{\frac{1}{2}(\langle k',k\rangle - (k',k))}$$

In these equations, the notation $k'_\perp = k_\perp$ (mod N) means $n'_1 = n_1$ (mod N) and $n'_2 = n_2$ (mod N). Furthermore, the bilinear forms (k',k) and $\langle k',k\rangle$ are defined by

(5.19) $$(k',k) = n'_1 n_1 + n'_2 n_2 + (n'_1 + n'_2)(n_1 + n_2)$$

(5.20) $$\langle k',k\rangle = n'_1 n_2 - n'_2 n_1 .$$

Note that in view of eq. (5.14), there are exactly N^2 distinct Γ_k's. Also, one easily deduces from eqs. (5.15)-(5.18) that

(5.21) $$\frac{1}{N} \text{Tr} (\Gamma_{k'}^\dagger \Gamma_k) = \begin{cases} 1 \text{ if } k'_\perp = k_\perp \ (\text{mod } N) \\ 0 \text{ otherwise} \end{cases}$$

which implies that the Γ_k's form an orthonormal basis in the space of all complex NxN matrices.

After these lengthy preparations, we can now write down the Fourier representation, replacing eq. (2.7), of the gauge potential:

(5.22) $$A_\mu(x) = (L^2 N)^{-1} \sum_{k_\perp} \int_{-\pi/a}^{\pi/a} \frac{dk_0}{2\pi} \frac{dk_3}{2\pi} e^{ikx} \Gamma_k e^{\frac{i}{2} k_\mu a} \tilde{A}_\mu(k) .$$

The transverse momentum components are here summed over the discrete values (5.11) in the Brillouin zone. An interesting aspect of eq. (5.22) is that the color degrees of freedom of $A_\mu(x)$ are transformed into momentum degrees of freedom (note that as compared to a tube with ordinary periodic boundary conditions, the total number of possible values of transverse momentum is

enlarged by a factor of N^2). Using the properties of the Γ_k's listed above, eq. (5.6) translates to the following conditions on the Fourier amplitude $\tilde{A}_\mu(k)$:

$$\tilde{A}_\mu(k)^* = -z^{\frac{1}{2}(k,k)}\,\tilde{A}_\mu(-k) \tag{5.23}$$

$$\tilde{A}_\mu(k) = 0 \quad \text{if} \quad k_\perp = 0 \ (\text{mod } N)\ . \tag{5.24}$$

Correspondingly, the (free) gluon propagator is written as

$$\langle \tilde{A}_\mu(k)\,\tilde{A}_\nu(p)\rangle_{g_0=0} = \delta(k,-p)\,e^{-\frac{i}{2}(k_\nu+p_\nu)a} \cdot\left(-\tfrac{1}{2}z^{-\frac{1}{2}(k,k)}\right)\chi_k\,D_{\mu\nu}(k) \tag{5.25}$$

where $\delta(k',k)$ and χ_k are defined by

$$\delta(k',k) = L^2 N \delta_{n_1' n_1}\,\delta_{n_2' n_2}\,(2\pi)^2\,\delta(k_0'-k_0)\,\delta(k_3'-k_3) \tag{5.26}$$

$$\chi_k = \begin{cases} 0 \text{ if } k_\perp = 0 \ (\text{mod } N) \\ 1 \text{ otherwise} \end{cases} \tag{5.27}$$

(the δ-functions in eq. (5.26) should be interpreted as periodically extended, if k' and k are not in the same Brillouin zone). The propagator function $D_{\mu\nu}(k)$ is real and must be worked out from the given action and the gauge fixing condition. For the Coulomb gauge (5.8) and for small lattice

spacings we have the familiar expressions

$$D_{00}(k) = \frac{1}{\vec{k}^2}\ , \qquad D_{0j} = D_{j0} = 0 \tag{5.28}$$

$$D_{\ell j}(k) = \frac{1}{k^2}\left(\delta_{\ell j} - \frac{k_\ell k_j}{\vec{k}^2}\right) \tag{5.29}$$

All the considerations in section 3 on the gluon vertices go through unaltered, in particular, the reduced vertex functions $Y_r^e(k_1,\mu_1;\ldots;k_r,\mu_r)$ are the same as those appearing in the infinite volume case (eq. (3.20)). The only minor change is in the Clebsch-Gordan coefficients C_r (eq. (3.16)), which here become

$$C_r(k_1,\ldots,k_r) = \frac{1}{N}\left\{\mathrm{Tr}\left(\Gamma_{k_1}\ldots\Gamma_{k_r}\right) + (-1)^r\,\mathrm{Tr}\left(\Gamma_{k_r}\ldots\Gamma_{k_1}\right)\right\} \tag{5.30}$$

From eqs. (5.15)-(5.18), an explicit formula for C_r can be worked out and one finds in particular that

$$C_r(k_1,\ldots,k_r) = 0 \qquad \text{unless } (\textstyle\sum k_i)_\perp = 0 \ (\text{mod } N). \tag{5.31}$$

Actually, this result is a consequence of the invariance of the action under the group of transformations, isomorphic to $\mathbb{Z}_N \times \mathbb{Z}_N$, generated by

$$U(x,\mu) \to \Omega_\nu\,U(x,\mu)\,\Omega_\nu^{-1} \qquad \text{for all } x,\mu. \tag{5.32}$$

Together with translation invariance, it implies total momentum conservation (modulo $2\pi/a$) at each vertex. Note that the transformation (5.32) is not a gauge transformation, because $\Lambda(x) = \Omega_\nu$ does not satisfy the periodicity condition (5.3).

With all the ingredients ready, the perturbation expansion of the n-point correlation functions of $\tilde{A}_\mu(k)$ in terms of Feynman diagrams is derived as usual and we shall therefore not go into further details here. An important property of the resulting Feynman integrands is that they are completely regular, because the singularity at $k = 0$ of the propagator function $D_{\mu\nu}(k)$ is outside the range of possible momenta (cf. eqs. (5.24) - (5.29)). The physical significance of this observation becomes clear if we look for the poles of the propagator in the complex energy plane. For small lattice spacings, they are at

$$k_0 = \pm i \sqrt{k_\perp^2 + k_3^2} + O(a^2) \tag{5.33}$$

and since $k_\perp^2 \geq m^2$, it follows that the spectrum of the transfer matrix has a (mass) gap. We see therefore that the twisted compact dimensions make the theory massive in perturbation theory and thus provide for an infrared cutoff.

Starting from eq. (5.33), the particle spectrum of the theory can be worked out and scattering processes can be studied in perturbation theory (Ref. [1] and section 7). We emphasize that these excitations are truly physical

in the sense that they can be created from the ground state by applying gauge invariant operators, which are local in x_0 and x_3. In particular, their properties could also be studied by the strong coupling expansion and the Monte-Carlo simulation method. For the latter it is more convenient to use a formulation of twisted periodic boundary conditions, where the Ω_ν's do not appear explicitly and the twist is taken into account by a change of the action (cp. Appendix B).

5.2 Symmetry properties of the n-point functions

Due to the asymmetric shape of the twisted tube, the cubical symmetry of the infinite lattice $\mathbb{Z}^4$ is broken down to a smaller group of symmetries, which is generated by the following transformations:

(1) Reflection of x_0

(2) Interchange of x_0 and x_3

(3) Reflection of x_1

(4) Interchange of x_1 and x_2

For the symmetries (1) and (2), the associated transformation law for the link variables $U(x,\mu)$ is the ordinary one, which amounts to

$$\tilde{A}_\mu(k) \longrightarrow \sum_\nu R^{(i)}_{\mu\nu} \tilde{A}_\nu(R^{(i)}k) \,, \qquad (i = 1,2), \tag{5.34}$$

where $R^{(i)}_{\mu\nu}$ denotes the orthogonal matrix belonging to the transformation (i). The n-point correlation functions of $\tilde{A}_\mu(k)$ are invariant under (5.34),

provided this transformation is a symmetry of the action and the gauge fixing condition (as is usually the case).

For the transformations (3) and (4), the situation is more complicated, because they tend to conflict with the twisted periodicity (5.1) of the gauge fields, which must also be respected by a valid symmetry operation. However, as will be shown in detail below, the transformations (3) and (4) give rise to symmetries of the gauge theory too, provided they are combined with a charge conjugation. The corresponding transformation laws then read

$$\tilde{A}_\mu(k) \longrightarrow - z^{-n_1 n_2} \sum_\nu R^{(3)}_{\mu\nu} \tilde{A}_\nu(R^{(3)}k) \tag{5.35}$$

$$\tilde{A}_\mu(k) \longrightarrow - \sum_\nu R^{(4)}_{\mu\nu} \tilde{A}_\nu(R^{(4)}k) \tag{5.36}$$

(in eq. (5.35), the integers n_ν are defined by $n_\nu = k_\nu/m$).

We now proceed to derive the transformation law (5.35) (the derivation of (5.36) is similar and will be omitted). To this end, first note that the pair of matrices

$$\hat{\Omega}_1 = (\Omega_1^{-1})^* \quad , \quad \hat{\Omega}_2 = z\Omega_2^* \quad , \tag{5.37}$$

also satisfies the twist algebra (5.2) and is hence unitarily equivalent to the Ω_ν's, i.e. there exists $W \in SU(N)$ such that

$$\Omega_\nu = W \hat{\Omega}_\nu W^{-1} \quad , \qquad (\nu = 1,2). \tag{5.38}$$

Next, given a field $U(x,\mu) \in \mathcal{U}_\Omega$, we define the transformed field $\hat{U}(x,\mu)$ by

$$\begin{aligned} \hat{U}(x,\mu) &= W\, U(x',\mu)^* W^{-1} \qquad \text{if } \mu \neq 1, \\ \hat{U}(x,\mu) &= W\, U(x'-a\hat{\mu},\mu)^T W^{-1} \qquad \text{if } \mu = 1, \end{aligned} \tag{5.39}$$

where U^T denotes the transpose of U and x' is defined by

$$x' = R^{(3)}x = (x_0, -x_1, x_2, x_3). \tag{5.40}$$

The transformation (5.39) is the product of three operations, namely a reflection of x_1, a charge conjugation and a constant color rotation. These are usually symmetries of the action and it is also not difficult to check that $\hat{U}(x,\mu)$ is again twisted periodic so that altogether we have found a symmetry of the functional integral. The transformation law (5.35) is now obtained by working out the Fourier transform of the gauge potential $\hat{A}_\mu(x)$ associated with $\hat{U}(x,\mu)$, using

$$W \Gamma^*_{-k} W^{-1} = z^{-n_1^2 - n_2^2} \Gamma_k \, , \tag{5.41}$$

which follows from eqs. (5.37), (5.38) and the definition of Γ_k (eq. (5.12)).

5.3 Numerical evaluation of integrals of periodic analytic functions

As mentioned previously, due to the presence of the mass gap, the integrals

over loop momenta k_0, k_3 encountered in Feynman diagrams are integrals of periodic analytic functions. We shall consider below how such integrals can be numerically well approximated by appropriate sums. In particular, we will discuss the special refinements that have to be made in order to obtain sufficiently accurate results with modest computational effort, in situations when the mass gap is small.

For simplicity, we here only discuss how to integrate a periodic analytic function f(k) of a single variable $k \in \mathbb{R}$. Multiple integrals can be treated similarly, in particular, in our calculation of the improved action, we have merely iterated the procedure described below. Our aim is thus to calculate the integral

$$\mathcal{J} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} f(k) \qquad , \quad f(k+2\pi) = f(k) \ , \tag{5.42}$$

assuming that a subprogram exists, which computes f(k) for given k. The basic idea is to approximate $\mathcal{J}$ by the finite sums

$$I(T) = \frac{1}{T} \sum_{\nu=1}^{T} f\left(\frac{2\pi}{T}\nu\right) \qquad , \qquad T = 1,2,3,\ldots \tag{5.43}$$

For ordinary integrands, this method is not very efficient, but in our case, I(T) converges exponentially fast as $T \to \infty$. More precisely, we have

$$I(T) = \mathcal{J} + O(e^{-\varepsilon T}) \ , \tag{5.44}$$

where ε is the absolute value of the imaginary part of the singularity

of f(k) closest to the real axis. Eq. (5.44) is an easy consequence of contour integration and the representation

$$I(T) = \mathcal{J} + 2 \sum_{n=1}^{\infty} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \cos(nkT) f(k) \ , \tag{5.45}$$

which follows from the Poisson summation formula.

In various 1-loop diagrams (especially if the mass gap is small) one encounters situations in which ε is nearly zero. In such cases the rate of convergence can be drastically increased by making an appropriate change of variable, which maintains periodicity and moves the dominant pole away from the real axis. For example, if f(k) has a peak around k = 0 due to a pole at $k = i\varepsilon$, ε small, one could try .

$$k = k' - \alpha \sin k' \tag{5.46}$$

with

$$0 \leq \alpha(\varepsilon) < 1 \tag{5.47}$$

and α chosen close to 1 such as to move the singularity optimally away from the real axis in the k' plane. Then, we have

$$\mathcal{J} = \int_{-\pi}^{\pi} \frac{dk'}{2\pi} \hat{f}(k') \ , \tag{5.48}$$

with

$$\hat{f}(k') = (1 - \alpha \cos k') f(k(k')) \ , \tag{5.49}$$

and the corresponding approximations

$$\hat{I}(T) = \frac{1}{T} \sum_{\nu=1}^{T} \hat{f}\left(\frac{2\pi}{T}\cdot\nu\right) \tag{5.50}$$

converge significantly more rapidly to $\mathcal{I}$ than I(T), viz.

$$\hat{I}(T) = \mathcal{I} + O(e^{-\hat{\varepsilon}T}) \quad , \quad \hat{\varepsilon} = O(1) \, . \tag{5.51}$$

For the diagrams, which we have calculated, the rate of convergence achieved in this way typically was such that T = 32 was sufficient to obtain a relative accuracy of 14 digits. We finally note that since the convergence is known to be exponential, it is possible to control the error $|\mathcal{I} - \hat{I}(T)|$ by also calculating smaller sums, e.g. $\hat{I}(T/2)$ and $\hat{I}(T/4)$, and fitting the results with a constant plus exponential.

6. Asymptotic behaviour of Feynman diagrams for small lattice spacings and associated extrapolation procedures

6.1 Asymptotic behaviour of finite momentum sums

We here give a rigorous proof of the basic expansion (1.1) for a class of one-loop diagrams on finite lattices with periodic boundary conditions. Our objective is not so much to obtain the most general result, but to illustrate a strategy of proof, which appears to be more widely applicable. In particular, the proof can be easily adapted to the case of the partially compactified twisted lattice of section 5.

On a 4-dimensional LxLxLxL hypercubic lattice with periodic boundary conditions, the possible values of momentum are *)

$$k = \frac{2\pi}{L}\nu \quad , \quad \nu \in \mathbb{Z}^4 \quad , \quad -\pi/a < k_\mu \leq \pi/a \tag{6.1}$$

In the absence of masses and for vanishing external momenta, one-loop diagrams on this lattice assume the general form

$$D(f) = L^{-4} \sum_{k \neq 0} a^\delta f(ak) \, , \tag{6.2}$$

where δ denotes the engineering dimension of the Feynman integrand $f(q)$ and the summation is over the range (6.1). A simple example for the integrand is

$$a^\delta f(k) = |\hat{k}|^{-\delta} \, , \tag{6.3}$$

with $\hat{k}$ given by eq. (2.10). In general we expect that $f(q)$ has a singularity at q = 0, but is otherwise regular. More precisely, we shall assume that

(a) $f(q)$ is periodic with period 2π in all momentum components, i.e. if $q'_\mu = q_\mu \pmod{2\pi}$, then $f(q') = f(q)$.

(b) $f(q)$ is C^∞ for $q \pmod{2\pi} \neq 0$.

(c) The structure of the singularity of $f(q)$ at q = 0 is such that the

*) L has physical units with L/a being an integer.

function

$$\hat{f}(\varkappa, n) = \varkappa^{\delta} f(\varkappa n),$$

initially defined for $0 < \varkappa \leq \pi$ and $n \in S^3$, extends to a C^∞ function for all $\varkappa \in [0, \pi]$ (and all unit vectors n). Moreover, the Taylor coefficients of $\hat{f}$ at $\varkappa = 0$ are polynomials of n.

Functions f(q) having these properties are later referred to as elements of the class Φ_δ. According to property (c), every $f \in \Phi_\delta$ may be expanded around q = 0 in a series of the form

$$f(\varkappa n) \underset{\varkappa \to 0}{\sim} \varkappa^{-\delta} \sum_{m=0}^{\infty} \varkappa^m P_m(n), \tag{6.4}$$

where the P_m's are polynomials of the unit vector n.

The main result of this section is now summarized by the following

Theorem: For any $f \in \Phi_\delta$ we have

$$D(f) \underset{a \to 0}{\sim} a^{\delta-4}[A + B \ln(a/L)] + L^{\delta-4} \sum_{m=0}^{\infty} a_m (a/L)^m, \tag{6.5}$$

where the coefficients A, B and a_m are independent of L. Furthermore, B = 0 if $\delta \neq 4,5,6,\ldots$.

For actual Feynman diagrams, δ is always integer in which case the expansion (6.5) does indeed assume the general form (1.1). Note also that for superficially divergent diagrams (i.e. if $\delta < 4$), B vanishes and A is simply

given by

$$A = \int_{-\pi}^{\pi} \frac{d^4q}{(2\pi)^4} f(q) . \tag{6.6}$$

Thus, a possible application of the theorem is to calculate integrals of the type (6.6) by evaluating the finite sums D(f) for a range of lattice spacings and extrapolating to the limit $a \to 0$ using the method of subsection 6.2.

We now turn to the proof of the theorem. First, we simplify our notation by observing that apart from an explicit factor a^δ, the dependence of D(f) on the lattice spacing is only through the combination a/L. The limit $a \to 0$ at fixed L is therefore equivalent to $L \to \infty$ at fixed a. Taking the latter point of view, we may choose units such that a = 1. L is then an integer and (6.1), (6.2) and (6.5) become

$$k = \frac{2\pi}{L} \nu \quad , \quad \nu \in \mathbb{Z}^4 \quad , \quad -\tfrac{1}{2}L < \nu_\mu \leq \tfrac{1}{2}L \tag{6.7}$$

$$D(f) = L^{-4} \sum_{k \neq 0} f(k) \tag{6.8}$$

$$D(f) \underset{L \to \infty}{\sim} A - B \ln L + L^{\delta-4} \sum_{m=0}^{\infty} a_m L^{-m} \tag{6.9}$$

The proof of eq. (6.9) given below proceeds in three steps. First, by a partition of unity, the momentum cutoff implied by the Brillouin zone is replaced by a smooth cutoff function h(k). In the second step, the integrand f(k) is expanded according to eq. (6.4) and the cutoff function h is re-

placed by a Gaussian cutoff in each term. After that one is left with a set of momentum sums, whose integrands are analytically given and which are sufficiently simple to be tractable by ordinary techniques such as the Feynman parameter representation and the Poisson summation formula.

Suppose $h(k)$ is a C^∞ function of $k \in \mathbb{R}^4$ such that $0 \leq h \leq 1$ and

$$(6.10) \quad h(k) = \begin{cases} 1 & \text{if } |k| \leq \pi/4 \\ 0 & \text{if } |k| \geq \pi/2 \end{cases}$$

We then split the sum $D(f)$ into two parts according to

$$(6.11) \quad D(f) = D_1(f) + D_2(f)$$

$$(6.12) \quad D_1(f) = L^{-4} \sum_{k \neq 0} h(k) f(k)$$

$$(6.13) \quad D_2(f) = L^{-4} \sum_{k \neq 0} (1 - h(k)) f(k)$$

The following Lemma, which is proved in Appendix C, may now be applied to the second part $D_2(f)$.

Lemma 6.1: Let $g \in \Phi_\alpha$ and $\alpha < 4-2j$ for some integer j with $j \geq 3$. Then, for $L \longrightarrow \infty$ we have

$$(6.14) \quad D(g) = \int_{-\pi}^{\pi} \frac{d^4k}{(2\pi)^4} g(k) + O(L^{-2j})$$

Because the function $g = (1-h)f$ vanishes identically in a whole neighborhood of $k = 0$, it is an element of Φ_α for every α. It follows that $D_2(f) = D(g)$ only contributes to the coefficient A in the large L expansion

and all the non-trivial terms in (6.9) must therefore come from the first part $D_1(f)$.

For the further analysis of $D_1(f)$ we now make use of the expansion (6.4). Define polynomials $Q_m(n)$ through

$$(6.15) \quad Q_m(n) = \frac{1}{m!} \frac{\partial^m}{\partial x^m} \{ e^{x^2} x^\delta f(xn) \}_{x=0}$$

(the use of the factor e^{x^2} will become clear soon). Furthermore, set

$$(6.16) \quad f_m(k) = e^{-k^2} |k|^{m-\delta} Q_m(k/|k|), \quad (k \neq 0),$$

$$(6.17) \quad g_M(k) = h(k) \{ f(k) - \sum_{m=0}^{M} f_m(k) \}, \quad (|k_\mu| \leq \pi).$$

Note that g_M vanishes identically for $|k| \geq \pi/2$ so that we may periodically extend g_M to all $k \in \mathbb{R}^4$, excluding of course the singular points $k \pmod{2\pi} = 0$. From the definition (6.17) (and Taylor's theorem) we infer that $g_M \in \Phi_{\delta-M-1}$. Provided M is large enough, Lemma 1 therefore applies to g_M and we conclude that for $L \longrightarrow \infty$

$$(6.18) \quad D_1(f) = \sum_{m=0}^{M} D(h f_m) + \text{constant} + O(L^{\delta-M-3})$$

At this stage, the cutoff function h may be removed again. To this end, first note that hf_m vanishes for $|k| \geq \pi/2$ so that we are free to extend the summations over k to all $k \neq 0$ of the form $k = \frac{2\pi}{L}\nu$, $\nu \in \mathbb{Z}^4$. This is indicated symbolically by writing

$$(6.19) \quad D(hf_m) = D^\infty(hf_m) = \frac{1}{L^4} \sum_{k \neq 0}^{\infty} h(k) f_m(k)$$

Next, we observe that $(1-h)f_m$ is a C^∞ function, which together with its derivatives is rapidly falling off at infinity. As in the proof of Lemma 1, it may be shown that these properties imply

$$(6.20) \quad D^\infty((1-h)f_m) = \text{constant} + O(L^{-p})$$

for any power p. It follows that

$$(6.21) \quad D(hf_m) = D^\infty(f_m) + \text{constant} + O(L^{-p})$$

Summarizing the results obtained so far, we have for any fixed large M and $L \longrightarrow \infty$

$$(6.22) \quad D(f) = \sum_{m=0}^{M} D^\infty(f_m) + \text{constant} + O(L^{\delta-M-3})$$

We now proceed to prove that an expansion of the form (6.9) holds for each of the sums $D^\infty(f_m)$ individually. This will be achieved by a somewhat lengthy series of simple analytic manipulations.

We first remark that because of reflection symmetry, the polynomials Q_m may be replaced by

$$(6.23) \quad \hat{Q}_m(n) = \frac{1}{2}[Q_m(n) + Q_m(-n)]$$

without changing the value of $D^\infty(f_m)$. Next, let q_m denote an integer such that

$$2q_m \geq m - \delta$$

and such that $2q_m$ is also larger than the degree of $\hat{Q}_m$ (in particular, $q_m \geq 1$). Define

$$(6.24) \quad H_m(k) = |k|^{2q_m} \hat{Q}_m(k/|k|)$$

$$(6.25) \quad \alpha_m = q_m + \frac{1}{2}(\delta - m)$$

By construction, H_m is a homogeneous polynomial of k of degree $2q_m$. Furthermore, we have

$$(6.26) \quad D^\infty(f_m) = \frac{1}{L^4} \sum_{k \neq 0}^{\infty} |k|^{-2\alpha_m} H_m(k) e^{-k^2}$$

To obtain a more tractable expression, set

$$(6.27) \quad \varkappa = (2\pi/L)^2$$

$$(6.28) \quad F_m(z) = (2\pi)^{-4} \sum_{\nu \in \mathbb{Z}^4} H_m(\nu) e^{-z\nu^2}, \qquad (z > 0).$$

Then, eq. (6.26) may be rewritten in the form

$$D^{\infty}(f_m) = x^{-\frac{1}{2}(\delta-4-m)} \frac{1}{\Gamma(\alpha_m)} \int_0^{\infty} dt\, t^{\alpha_m-1} F_m(t+x) \tag{6.29}$$

(note that for $x>0$ the integral is absolutely convergent, because $\alpha_m>0$ and because F_m is a C^{∞} function, which is exponentially decaying at infinity). A good feature of this representation of $D^{\infty}(f_m)$ is that L enters only through the variable x, in particular, the function F_m is independent of L.

We now split $D^{\infty}(f_m)$ into two parts according to

$$D^{\infty}(f_m) = x^{-\frac{1}{2}(\delta-4-m)} \frac{1}{\Gamma(\alpha_m)} \{ I_1(x) + I_2(x) \} \tag{6.30}$$

$$I_1(x) = \int_0^1 dt\, t^{\alpha_m-1} F_m(t+x) \tag{6.31}$$

$$I_2(x) = \int_1^{\infty} dt\, t^{\alpha_m-1} F_m(t+x) \tag{6.32}$$

Because $F_m(z)$ and its derivatives are exponentially decaying at infinity, the integral I_2 is a C^{∞} function of x for $x > -1$. In particular, it may be expanded in an asymptotic power series at $x = 0$. It follows that the

contribution of I_2 to $D^{\infty}(f_m)$ has a large L expansion of the form (6.9) with $A = B = 0$.

To expand I_1, we need the following Lemma, which is proved in Appendix D.

Lemma 6.2: There exists a constant C_m such that the function $\hat{F}_m$ defined by

$$\hat{F}_m(z) = F_m(z) - C_m z^{-q_m-2}, \qquad (z>0), \tag{6.33}$$

extends to a C^{∞} function for $0 \leq z < \infty$.

Inserting (6.33) into the definition (6.31), we have

$$I_1(x) = C_m \int_0^1 dt\, t^{\alpha_m-1} (t+x)^{-q_m-2} + \hat{I}_1(x), \tag{6.34}$$

where $\hat{I}_1(x)$ is C^{∞} for $x \geq 0$ and can therefore be expanded in an asymptotic power series as $x \to 0$. Finally, to expand the explicit integral in eq. (6.34), we substitute $t = x/s$ and obtain the following contribution to $D^{\infty}(f_m)$:

$$\frac{C_m}{\Gamma(\alpha_m)} \int_x^{\infty} ds\, s^{-\frac{1}{2}(\delta-2-m)} (1+s)^{-q_m-2} \tag{6.35}$$

For small s, the integrand can be expanded in a convergent power series and this quickly translates into a small x expansion of the form (6.9). In particular, a logarithm is obtained if and only if $\delta - 2 - m$ is a positive even integer. Summing up, we have thus shown that $D^{\infty}(f_m)$ has a large L expansion of the proposed form.

The proof of the theorem is now completed by remarking that via eq. (6.27),

the expandability of $D^{\infty}(f_m)$ implies the validity of (6.9) up to terms of order $L^{\delta-M-3}$. Since M may be chosen arbitrarily large, the expansion in fact holds to all orders.

6.2 Extrapolation of lattice Feynman graphs

In the preceding subsection we have shown, for a class of one-loop Feynman diagrams, that as the lattice spacing tends to zero, one has an asymptotic expansion of the form

$$(6.36) \qquad D(a) \underset{a\to 0}{\sim} a^{-\omega} \sum_{n=0}^{\infty} a^n \left[c_{no} + c_{n1} \ln a \right]$$

We here discuss the question of how to extract the first few coefficients c_{ni}, when D(a) is known for a sequence of lattice spacings a_I, $I_{min} \leq I \leq I_{max}$. In order to keep the presentation of our method as transparent as possible, we shall make a few simplifying assumptions. First, the lattice spacings a_I are taken to be inversely proportional to I, i.e.

$$(6.37) \qquad a_I = 1/\mu I.$$

Secondly, we assume that only even powers of 'a' occur in the expansion (6.36) and that the leading coefficients c_{01} and c_{21} of the logarithmic terms are already known analytically. Actually, for the sum of diagrams which one needs to calculate for improvement, both conditions are met, in particular, c_{01} is proportional to the first coefficient of the Callan-Symanzik β-function and c_{02} vanishes because of tree improvement.

We now proceed to describe how to determine the leading coefficient c_{oo} accurately and how to control the rounding and systematical errors along the way. The extension of the method to subleading coefficients is trivial and will not be discussed any further. Using (6.37), we can define the dimensionless auxiliary function

$$(6.38) \qquad f_0(I) = \left\{ a^{\omega} \left[D(a) + (c_{01} + a^2 c_{21}) \ln I \right] \right\}_{a=a_I}$$

in terms of which the expansion (6.36) reads

$$(6.39) \qquad f_0(I) \underset{I\to\infty}{\sim} A_0 + A_1/I^2 + \sum_{n=2}^{\infty} (A_n + B_n \ln I)/I^{2n}$$

$$(6.40) \qquad A_0 = c_{oo} - c_{01} \ln \mu$$

A first approximation to the desired coefficient A_0 would thus simply be

$$(6.41) \qquad A_0 \simeq f_0(I_{max})$$

However, since a range of values of I is available, we can do better by defining an "improved" auxiliary function $f_1(I)$ through

$$(6.42) \qquad f_1(I) = \frac{(I+\delta_0)^2}{4\delta_0 I} f_0(I+\delta_0) - \frac{(I-\delta_0)^2}{4\delta_0 I} f_0(I-\delta_0) \ ,$$

where δ_0 is an integer parameter, typically $\delta_0 = 1$ or 2. Then, f_1 has an expansion of the form (6.39) with A_0 as before and A_1 missing.

f_1 is therefore more rapidly converging as $I \longrightarrow \infty$ and one expects that $f_1(I_{max} - \delta_0)$ is a better approximation to A_0 than the estimate (6.41) (note that $f_1(I)$ is only defined for $I_{min} + \delta_0 \leq I \leq I_{max} - \delta_0$).

The "blocking" transformation leading from the initial function f_0 to the improved function f_1 can be iterated and one obtains in this way a sequence of functions f_i such that

$$f_i(I) = A_0 + O(I^{-2i-2}) , \qquad i = 0,1,2,... \tag{6.43}$$

Actually, because of the logarithmic terms in eq. (6.39), the transformation $f_i \rightarrow f_{i+1}$ is a bit more complicated for $i \geq 1$ than for $i = 0$, namely

$$f_{i+1}(I) = w_1 f_i(I+\delta_i) + w_2 f_i(I) + w_3 f(I-\delta_i) \tag{6.44}$$

$$w_j = v_j / (v_1 + v_2 + v_3) , \qquad (j = 1,2,3) \tag{6.45}$$

$$v_1 = (I+\delta_i)^{2i+2} \ln(1 - \delta_i/I) \tag{6.46}$$

$$v_2 = I^{2i+2} [\ln(1+\delta_i/I) - \ln(1-\delta_i/I)] \tag{6.47}$$

$$v_3 = -(I-\delta_i)^{2i+2} \ln(1+\delta_i/I) \tag{6.48}$$

At each step, δ_i can be chosen freely and the range of values of I, where the new function is defined, shrinks. After a few iterations, further blocking is therefore often useless, because the available range of I is too small to observe the convergence of the improved function f_{i+1}.

To derive a reliable stopping criterion for the iteration described above, we need an estimate for the "systematical error"

$$s_i(I) = |f_i(I) - A_0| / |A_0| \tag{6.49}$$

To this end, we fit f_i with the function

$$\hat{f}_i(I) = \alpha + (\beta + \gamma \ln I) / I^{2i+2} \tag{6.50}$$

by minimizing the quadratic form

$$\sum_I I^{4i+8} [f_i(I) - \hat{f}_i(I)]^2 \tag{6.51}$$

with respect to the parameters α, β and γ. Of course, the fit function $\hat{f}_i$ is motivated by the large I expansion of $f_i(I)$ and the weight in (6.51) is chosen such as to minimize the effects of possible higher terms. Having determined α, β and γ, the systematical error is estimated by

$$s_i(I) \lesssim \hat{s}_i(I) / |f_i(I)| \tag{6.52}$$

$$\hat{s}_i(I) = \begin{cases} |\beta + \gamma \ln I| / I^{2i+2} & \text{if } \gamma/\beta \geq 0 \\ \max(|\beta|, |\gamma| \ln I) / I^{2i+2} & \text{if } \gamma/\beta \leq 0 \end{cases} \tag{6.53}$$

This formula avoids underestimating the error in case $\beta + \gamma \ln I$ happens to go through zero in or near the range of available values of I.

Before the systematical error determined in this way can be taken seriously, a test of the quality of the fit of f_i should be made. This is in general a rather subjective affair. Our criterion was to accept the fit if

$$(6.54) \qquad |f_i(I) - \hat{f}_i(I)| / |\hat{s}_i(I)| < \varepsilon \, I^2_{max} / I^2$$

where (say) $\varepsilon = 0.1$. If (6.54) was not satisfied, the systematic error was taken to be unestimable and f_i would then not be used to determine A_0.

So far we have assumed that the functions f_i are known with infinite numerical precision. Of course, since f_i is calculated on a digital computer, this is not actually the case, i.e. the computer approximates $f_i(I)$ by some number $\bar{f}_i(I)$ with a finite number of digits. If one uses 64 bit precision, the error

$$(6.55) \qquad \varepsilon_0(I) = (f_0(I) - \bar{f}_0(I)) / \bar{f}_0(I)$$

of the initial data can be rather small, e.g. $\varepsilon_0 \leq 10^{-14}$. However, through the blocking transformation the errors $\varepsilon_i(I)$ of the improved auxiliary functions f_i tend to increase significantly, a fact, which turns out to be one of the limiting factors to our method. To understand how these numerical errors evolve, we assume that the errors $\varepsilon_0(I)$ are random numbers with a Gaussian distribution of variance

$$(6.56) \qquad \langle \varepsilon_0(I) \, \varepsilon_0(I') \rangle = \delta_{II'} \, r_0(I)^2 \quad ,$$

where $r_0(I)$ is known. Because the blocking transformation is linear, it

follows that the errors $\varepsilon_i(I)$ are also distributed according to a Gaussian and the matrix $\langle \varepsilon_i(I) \, \varepsilon_i(I') \rangle$ can be calculated recursively. In particular, we may define

$$(6.57) \qquad r_i(I) = \langle \varepsilon_i(I) \, \varepsilon_i(I) \rangle^{1/2} \quad ,$$

which is a realistic estimate for the numerical precision of $f_i(I)$. It is our experience that with each blocking step, the significance loss thus determined is about 1 to 2 decimal places, slightly depending on the choice of the parameters δ_i.

As a result of the error discussion, the best possible estimate for A_0 may now be obtained by setting

$$(6.58) \qquad A_0 \simeq f_{i^*}(I^*) \quad ,$$

where i* and I* are chosen such as to minimize the total error. In addition, the (relative) precision of the estimate (6.58) can be predicted to be better than

$$(6.59) \qquad s_{i^*}(I^*) + r_{i^*}(I^*) \quad .$$

We have tested our extrapolation procedure in various cases where A_0 was known beforehand, for example by evaluating the diagrams directly in the continuum using dimensional regularization. In all cases, the error estimates were shown to be realistic (or even conservative), thus confirming our expectation that the method works reliably indeed.

7. Calculation of Symanzik's improved action[1]

The purpose of the present section is mainly to illustrate how the techniques introduced in this paper fit together in a concrete case. Besides that we want to provide further details on the calculation outlined in Ref. [1]. In order to avoid unnecessary repetitions, we shall here assume that the reader is familiar with Ref. [1], in particular, the notations of that paper on the improved action, the improvement coefficients $c_i(g_0^2)$, etc. are taken over.

7.1 Gauge fixing and the pole structure of the propagator

As explained in Ref. [1], the calculation of the coefficients $c_i(g_0^2)$ in perturbation theory proceeds by evaluating two on-shell quantities in the twisted world of section 5 and requiring the absence of $O(a^2)$ scaling violation terms. These on-shell quantities can be defined using gauge invariant (composite) interpolating fields (see subsection 7.2) and the choice of gauge one makes to perform the calculation is therefore of only practical importance. A convenient choice is e.g. the modified Coulomb gauge condition

$$\sum_{i=1}^{3} \partial_i^* A_i(x) = 0 \tag{7.1}$$

$$\partial_i^* = \{1 + a^2 (c_1^{(0)} - c_2^{(0)})(\partial_0^* \partial_0 + \partial_i^* \partial_i) + a^2 c_2^{(0)} \sum_\mu \partial_\mu^* \partial_\mu\} \partial_i^* \tag{7.2}$$

In momentum space, eq. (7.1) becomes

$$\sum_{i=1}^{3} s_{0i}(k)\, \hat{k}_i\, \tilde{A}_i(k) = 0 \ , \tag{7.3}$$

where the tensor $s_{\mu\nu}(k)$ is defined through

$$s_{\mu\nu}(k) = 1 - a^2 (c_1^{(0)} - c_2^{(0)})(\hat{k}_\mu^2 + \hat{k}_\nu^2) - a^2 c_2^{(0)} \hat{k}^2 \ . \tag{7.4}$$

This tensor also appears in the action, namely [14]

$$S\big|_{g_0=0} = (L^2 N)^{-1} \sum_{k_1} \int_{-\pi/a}^{\pi/a} \frac{dk_0}{2\pi} \frac{dk_3}{2\pi} \frac{1}{2} \sum_{\mu,\nu} s_{\mu\nu}(k) \left| \hat{k}_\mu \tilde{A}_\nu(k) - \hat{k}_\nu \tilde{A}_\mu(k) \right|^2 , \tag{7.5}$$

and the gauge condition (7.3) therefore implies the decoupling of the "static" potential A_0 from the transverse components A_i at $g_0 = 0$. For the propagator function $D_{\mu\nu}(k)$ defined in section 5, we thus have

$$D_{0i}(k) = D_{i0}(k) = 0 \ , \qquad (i = 1,2,3) \ , \tag{7.6}$$

$$D_{00}(k) = \Big(\sum_{i=1}^{3} s_{0i}(k) \hat{k}_i^2 \Big)^{-1} \ . \tag{7.7}$$

The other components are more complicated and explicit formulae are therefore deferred to Appendix E. Here we only note that

$$D_{ij}(k) = D_{00}(k)\, P_{ij}(\hat{k}) / Q(\hat{k}) \ , \tag{7.8}$$

where P_{ij} and Q are polynomials in $\hat{k}_0$ of degree 8 and 10 respectively.

In what follows, we assume that the coefficients $c_i^{(0)}$ are such that

$s_{\mu\nu}(k)$ is positive for all k and $\mu \neq \nu$. This insures the stability of the action (7.5) and is true for the values of $c_1^{(o)}$ and $c_2^{(o)}$, which are later found to be necessary for improvement. With this proviso, it is easy to show that the gauge fixing condition (7.1) is admissable in the sense of section 4 and the derivation of the Faddeev-Popov determinant given there therefore carries over to the present case. In particular, the Faddeev-Popov operator is given by

$$\Delta_{FP} = -\sum_{i=1}^{3} \partial_i^* \left\{ \frac{Ad\, q_i(x)}{1 - \exp - Ad\, q_i(x)} \partial_i + Ad\, q_i(x) \right\} , \tag{7.9}$$

where $q_i(x) = g_o a A_i(x)$. As already mentioned in section 5, the corresponding ghost fields are twisted periodic and from eq. (7.9) the Faddeev-Popov propagator is easily found to be equal to $D_{oo}(k)$.

The stability of the action (7.5) also implies that the polynomial $Q(\hat{k})$ is positive for real $\hat{k} \neq 0$. The only singularities of the propagator $D_{\mu\nu}(k)$ in the Brillouin zone are therefore at $k = 0$ (from the vanishing of Q) and at $\vec{k} = 0$ (from $D_{oo}(k)$). These latter singularities also occur in the ghost field propagator and are special to our choice of gauge. Since $\vec{k} = 0$ is excluded by the quantization of transverse momentum, the Feynman integrands actually encountered are completely regular as discussed in section 5.

For the physical interpretation of the theory, the poles of $D_{\mu\nu}(k)$ with complex k_o and real $\vec{k}$ are relevant. Because $D_{\mu\nu}(k)$ is even under $k_o \rightarrow -k_o$, such poles come in pairs with opposite signs of k_o. There are exactly

5 pairs stemming from the zeros of $Q(\hat{k})$ plus one additional pair from $D_{oo}(k)$. For small lattice spacings, two pairs converge to the relativistic locus

$$k_o = \pm i |\vec{k}| , \tag{7.10}$$

and the other poles move to infinity, i.e. the associated energies are of the order of the cutoff:

$$Im\, k_o = O(1/a) . \tag{7.11}$$

This behaviour is illustrated by Fig. 1, where the energy momentum relations corresponding to the 6 pairs of poles of $D_{\mu\nu}(k)$ are plotted for $k_1 = k_2$, $k_3 = 0$. Elsewhere in the 3-dimensional Brillouin zone the situation looks similar, in particular, the unphysical branches (those which are not approximately of the form (7.10)) are always far up in energy. Note that the physical branches closely follow the relativistic dispersion (7.10) up to rather large momenta ($|\vec{k}| \lesssim \pi/2a$) . This is partly due to tree level improvement as can be seen by comparing with the Wilson action, where the energy momentum relation starts to deviate from the relativistic formula already at $|\vec{k}| \simeq \pi/4a$. We finally observe that the two physical branches correspond to different (transversal) polarizations of the gluon. At tree level they are not exactly degenerate because of $O(a^4)$ scaling violation terms and at higher orders the degeneracy is completely lifted by the asymmetry of the lattice.

If we now take into account that the transverse momentum components k_1

and k_2 are quantized, we see that the energies k_o associated with the poles of $D_{\mu\nu}(k)$ cannot be arbitrarily close to zero. The family of poles with smallest energy is given by

$$k_1^2 + k_2^2 = m^2 \quad , \qquad m = \frac{2\pi}{LN} \quad ,$$

$$k_o = \pm i \sqrt{m^2 + k_3^2} + O(a^2) \quad , \tag{7.12}$$

i.e. these are the poles with the smallest amount of momentum in the transverse directions. As explained above, for each of these poles there are two possible polarizations. They can be distinguished by their parity under reflections of k_1 (or k_2). To see this, take for example $k_1 = 0$, $k_2 = m$. Then, $\tilde{A}_1(k)$ is even under a reflection (5.35) of k_1 and the other components $\tilde{A}_2(k)$ and $\tilde{A}_3(k)$ are odd. Correspondingly, one of the poles occurs in the $\tilde{A}_1(k)$ propagator and the other in the propagator of $\tilde{A}_2(k)$ and $\tilde{A}_3(k)$ (note that because of the gauge condition (7.3), these latter field components are linearly dependent so that there is only one degree of freedom associated to them). These symmetry considerations are also valid at higher orders of perturbation theory and the lowest lying poles of the full gluon propagator can therefore be unambiguously identified by specifying the momentum $\vec{k}$, the sign of Im k_o and the parity of the interpolating field under an appropriate reflection. Similarly, the next to lowest lying poles (those with $|k_1| = |k_2| = m$) can also be completely characterized by conserved quantum numbers.

7.2 Physical significance of the low lying poles of the gluon propagator

The physical interpretation of euclidean lattice gauge theories rests on the construction of a Hilbert space of physical states and the transfer matrix as described in detail for improved lattice gauge theories in Ref. [15]. The aim of the following discussion is to show that the poles (7.12) (and similarly the other poles of the propagator) are related to eigenvalues $e^{-\omega}$ of the transfer matrix through the familiar formula

$$\omega = a\,|\mathrm{Im}\, k_o| \quad . \tag{7.13}$$

This implies that although the gluon propagator is gauge variant, its low lying poles are associated with gauge invariant eigenstates of the transfer matrix and may therefore be interpreted as physical one-particle states. In fact, with little more work, the Hilbert space of physical states at $g_o = 0$ can be identified with a Fock space of an infinite tower of free particles as described in Ref. [1].

To establish (7.13) it is sufficient to construct, for each of the poles (7.12), a gauge invariant field $\mathcal{O}_k(x_o)$, which is composed from the link variables $U(x,j)$ at a fixed time x_o and which satisfies

$$\langle \mathcal{O}_k(x_o)^* \mathcal{O}_k(0) \rangle \Big|_{g_o=0} \underset{x_o \to \infty}{\propto} e^{-x_o |\mathrm{Im}\, k_o|} \quad . \tag{7.14}$$

As an example, consider the case with $k_1 = 0$, $k_2 = m$ and positive parity as explained above. Define a gauge invariant composite field $\varphi(x_o, x_2, x_3)$

through

$$\varphi(x_0,x_2,x_3) = \frac{1}{g_0}\,\mathrm{Tr}\{\Omega_1 \prod_{0\le x_1<L} U(x,1)\}\,, \tag{7.15}$$

which is just a Wilson loop winding around the twisted tube (in eq. (7.15), the matrix Ω_1 is needed to make the loop invariant under the gauge transformations (5.3)). Because of twisted periodicity, we have

$$\varphi(x_0,x_2+L,x_3) = z\,\varphi(x_0,x_2,x_3) \tag{7.16}$$

so that the Fourier transform

$$\mathcal{O}_k(x_0) = a^2 \sum_{x_2,x_3} e^{-i(k_2x_2+k_3x_3)}\,\varphi(x_0,x_2,x_3) \tag{7.17}$$

is well-defined. Noting $\Omega_1 = \Gamma_k^\dagger$, it is easy to show that

$$\mathcal{O}_k(x_0)\big|_{g_0=0} = \int_{-\pi/a}^{\pi/a} \frac{dp_0}{2\pi}\, e^{ip_0x_0}\,\tilde{A}_1(p_0,\vec{k})\,, \tag{7.18}$$

and the exponential decay (7.14) of the correlation function of $\mathcal{O}_k(x_0)$ thus follows from the residue theorem.

When the gauge coupling g_0 is turned on, the full gluon propagator not only has poles but also a cut in the complex k_0 plane, which comes from 2-particle intermediate states and which therefore starts at about $k_0 = \pm i\,2m$. The stable physical particles in the theory are thus the A mesons, which correspond to the lowest lying poles (7.12), and the B mesons, which belong to

the poles with $|k_1| = |k_2| = m$. In addition, there may be some poles just below the 2-particle threshold. As for $g_0 = 0$, the gauge invariant field defined above may be taken as an interpolating field for a positive parity A meson, and similar composite fields exist for the other A mesons and the B mesons. Because these fields are local in x_0 and x_3, an LSZ scattering theory can be formulated for them and a sensible definition of the scattering matrix for scattering processes involving A and B mesons can be obtained in this way *. One may then show that the scattering amplitudes so defined are in fact equal to the full propagator amputated n-point functions of the gauge potential A_i evaluated at the poles of the propagator and multiplied by polarization vectors and wave function renormalization constants as usual. In particular, the "phenomenological" coupling constant λ defined in Ref. [1] and the masses m_A and m_B of the A and B mesons have a well-defined physical interpretation and are therefore quantities suitable for the calculation of the improvement coefficients $c_i(g_0^2)$.

7.3 Calculation of $c_i(g_0^2)$ to one-loop order

The coefficients $c_i(g_0^2)$ are now determined order by order in perturbation theory by requiring the absence of $O(a^2)$ corrections to the mass m_A of a positive parity A meson and to the coupling constant λ. The leading terms in the expansions

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* The conceptually more satisfactory Haag-Ruelle scattering theory is presently unavailable for lattice theories.

$$m_A = m_A^{(0)} + g_0^2 m_A^{(1)} + O(g_0^4) \tag{7.19}$$

$$\lambda = g_0 \lambda^{(0)} + g_0^3 \lambda^{(1)} + O(g_0^5) \tag{7.20}$$

are obtained by locating the appropriate pole in the $\tilde{A}_1(k)$ propagator (cp. Appendix E) respectively by evaluating the 3-point vertex function at the momentum configuration where λ is defined. Skipping the trivial details, we note the result

$$m_A^{(0)} = m\{1 - (am)^2(c_1^{(0)} - c_2^{(0)} + \tfrac{1}{12}) + O(a^4)\}, \tag{7.21}$$

$$\lambda^{(0)} = -8m\{1 - \tfrac{1}{2}(am)^2[9(c_1^{(0)} - c_2^{(0)} + \tfrac{1}{12}) + 2c_2^{(0)}] + O(a^4)\}, \tag{7.22}$$

which implies

$$c_1^{(0)} = -\frac{1}{12} \quad , \quad c_2^{(0)} = 0 \tag{7.23}$$

for the improved action. From now on, the tree level coefficients $c_i^{(0)}$ are fixed to these values and the propagator and the vertices in Feynman diagrams refer to this tree level improved action, the vertices proportional to the one-loop coefficients $c_i^{(1)}$ (and the higher loop coefficients) being given a separate label (cp. Figs. 2,3).

At one-loop order, the calculation of m_A amounts to the evaluation of the self-energy diagrams drawn in Fig. 2, where the momentum flowing into the diagrams is given by

$$k = (im_A^{(0)}, 0, m, 0). \tag{7.24}$$

The terms proportional to $c_i^{(1)}$ are tree diagrams and can be easily computed by hand. If we define $\bar{m}_A^{(1)}$ to be the contribution of all other diagrams, we have

$$m_A^{(1)}/m = \bar{m}_A^{(1)}/m - (am)^2(c_1^{(1)} - c_2^{(1)}) + O(a^4). \tag{7.25}$$

Now it is important to note that apart from an overall factor of m^2, the self-energy diagrams to be calculated depend on N and L/a only. The small "a" expansion of $\bar{m}_A^{(1)}$ therefore assumes the general form

$$m_A^{(1)}/m \underset{a\to 0}{\sim} a_0 + (am)^2 a_1 + (am)^4[a_2 + b_2 \ln(am)] + \ldots, \tag{7.26}$$

where the coefficients a_i and b_i are dimensionless numbers depending on N. A logarithm of $O(1)$ is absent in eq. (7.26), because m_A is expected to have a limit at $a = 0$. There is also no logarithmic term of $O(a^2)$, because the action we use is improved at tree level [7]. Inserting (7.26) into eq. (7.25), we thus see that improvement at one-loop order requires the coefficients $c_i^{(1)}$ to be chosen such that

$$c_1^{(1)} - c_2^{(1)} = a_1 . \tag{7.27}$$

Using the techniques described in this paper, the coefficient a_1 can be calculated along the following lines. First, for every self-energy diagram

a computer program is written, which computes the value of the diagram given N and L/a. These programs perform the finite sums over the transverse components p_1, p_2 of the loop momentum p exactly and the integrations over the other two components p_0, p_3 are done using the integration method of subsection 5.3. The Feynman integrand for given p is computed by calling subroutines for the vertices as described in section 3 and a subroutine for the gluon propagator, which may be easily manufactured given the analytical expressions of Appendix E. The CPU time needed to compute a diagram is approximately proportional to $(L/a)^2$ and it is therefore important to make the programs efficient, in particular, factors of 2 can be gained by making use of the symmetry properties of the Feynman integrand (cp. subsection 5.2). When all the programs are ready, $\bar{m}_A^{(1)}/m$ can be calculated for fixed N and a range of L/a, for example, we have taken $10 \leq L/a \leq 36$ $(N = 2)$ and $6 \leq L/a \leq 30$ $(N = 3)$ with L/a even. The results are then fitted with the series (7.26) using the method of subsection 6.2. With an estimated initial numerical precision of 10^{-14} for individual diagrams, we have thus been able to extract the following numbers:

(7.28)
$$a_0 = -0.01682658(1) \quad , \quad a_1 = -0.011006(2) \quad , \quad (N=2),$$
$$a_0 = -0.03731598(1) \quad , \quad a_1 = -0.020799(4), \quad (N=3).$$

Incidentally, we note that we have also calculated the energy gap in a twisted world with 3 compact dimensions and obtained the more accurate result

(7.29) $$c_1^{(1)} - c_2^{(1)} = -0.01100879(1) \quad , \qquad (N=2),$$

(7.30) $$c_1^{(1)} - c_2^{(1)} = -0.02080086(2) \quad , \qquad (N=3),$$

which agrees with (7.27), (7.28) and also with the earlier calculation of Ref. [2].

The calculation of the coupling constant λ to one-loop order proceeds as for the mass m_A and, apart from the larger number of diagrams, no additional technical difficulties are encountered. The diagrams contributing to $\lambda^{(1)}$ are the vertex graphs listed in Fig. 3 plus the self-energy diagrams of Fig. 2, which give rise to a correction of order g_0^2 to the wave function renormalization constants Z_A and Z_B occurring in the definition of λ. Again, the diagrams proportional to the coefficients $c_i^{(1)}$ are easy to evaluate and we have

(7.31) $$\lambda^{(1)}/m = \bar{\lambda}^{(1)}/m + 36\,(am)^2(c_1^{(1)} - c_2^{(1)}) + 8\,(am)^2 c_2^{(1)} + O(a^4)$$

where (with new coefficients a_i, b_i)

(7.32) $$\bar{\lambda}^{(1)}/m \underset{a\to 0}{\sim} a_0 + b_0 \ln(am) + (am)^2 a_1 + (am)^4 [a_2 + b_2 \ln(am)] + \ldots$$

(7.33) $$b_0 = \frac{11N}{6\pi^2}$$

This value for b_0 is implied by the renormalization group and the tree level result (7.22). We have verified (7.33) from our data for $\bar{\lambda}^{(1)}$ to 6 significant decimal places and we have also checked that indeed there is no logarithm at order a^2 (as expected from tree improvement). Taking this into account, the fit of the data gave

(7.34) $a_0 = -0.8483231(3)$, $a_1 = 0.41988(3)$, $(N=2)$,

(7.35) $a_0 = -1.2877352(1)$, $a_1 = 0.78412(5)$, $(N=3)$.

Now for λ to be improved, we must have

(7.36) $$36\,(c_1^{(1)} - c_2^{(1)}) + 8c_2^{(1)} = -a_1 ,$$

so that together with eqs. (7.29), (7.30) we have two relations for the coefficients $c_i^{(1)}$, which can be solved and lead to the result quoted in Ref. [1].

We finally remark that individual diagrams contributing to $m_A^{(1)}$ or $\lambda^{(1)}$ in general have a small "a" expansion, which is not exactly of the form (7.26) or (7.32). Rather, there are usually also divergent terms and odd powers of the lattice spacing. In the sum of all diagrams, one may however show, using the gauge Ward identities, that these additional terms cancel out. That they do not show up in the numerical data for $m_A^{(1)}$ and $\lambda^{(1)}$ is thus another global check on our calculation.

Appendix A: Proof of Lemma 4.3

We first show that the constant ω's are zero modes of Δ_{FP}. Indeed, from eqs. (4.20)-(4.22), we have

(A.1) $$\Delta_{FP} = \mathcal{F} J_q^{-1} d + \mathcal{F} A d q$$

so that for constant modes ω

(A.2) $$\Delta_{FP}\omega = \mathcal{F}(A d q \cdot \omega) = -\mathcal{F}([\omega, q]) .$$

Now we note that ω is in the Lie algebra of $\mathcal{G}_0$ and $q_\mu \in \mathcal{H}^{\mathcal{F}}$. Hence by property (2) of $\mathcal{F}$, we have

(A.3) $$[\omega, q_\mu] \in \mathcal{H}_1^{\mathcal{F}} ,$$

and therefore $\Delta_{FP}\omega = 0$.

Next, we prove that for small q, there are no other zero modes. Because Δ_{FP} depends continuously on q, it is sufficient to show the absence of additional zero modes for $q = 0$. In this case, the equation

(A.4) $$\Delta_{FP}\omega = \mathcal{F} d\omega = 0$$

implies

(A.5) $$d\omega \in \mathcal{H}_1^{\mathcal{F}} \cap \mathcal{H}_1^{\perp} .$$

Thus, by property (1) of $\mathcal{F}$, we have $d\omega = 0$, and since the lattice Λ is linkwise connected, it follows that ω is constant.

We now proceed to show that the range of Δ_{FP} is equal to $\mathcal{F}(\mathcal{H}_1)$. For $q = 0$, this is certainly the case, because

(A.6) $$\Delta_{FP}(\mathcal{H}_0) = \mathcal{F}(\mathcal{H}_1^L) = \mathcal{F}(\mathcal{H}_1).$$

For $q \neq 0$, it follows from the definition of Δ_{FP} that

(A.7) $$\Delta_{FP}(\mathcal{H}_0) \subset \mathcal{F}(\mathcal{H}_1)$$

On the other hand, the codimension of $\Delta_{FP}(\mathcal{H}_0)$ is equal to the number of zero modes of Δ_{FP}, and since this is independent of q, we have

(A.8) $$\dim \Delta_{FP}(\mathcal{H}_0) = \dim \mathcal{F}(\mathcal{H}_1)$$

Together with (A.7), this relation implies $\Delta_{FP}(\mathcal{H}_0) = \mathcal{F}(\mathcal{H}_1)$, as was to be shown.

Appendix B: Form of the action suitable for Monte-Carlo calculations with twisted periodic boundary conditions.

In numerical simulations of lattice gauge theories, twisted periodic boundary conditions are usually implemented by a modification of the action, which amounts to multiply some plaquettes and (if present) other action pieces at the boundary by central elements of the gauge group (see e.g. Refs. [5, 12, 13]). In this formulation, the gauge fields $U(x,\mu)$ satisfy ordinary periodic boundary conditions rather than eq. (5.1).

We here show that through a simple change of variables in the functional integral (2.5), the realization of twisted periodic boundary conditions described in chap. 5 is mapped onto the modified action representation so that the two formulations are thus completely equivalent.

For the twisted tube of chap. 5, the independent link variables to be integrated over in the functional integral may be taken to be

(B.1) $$U(x,\mu) \quad , \qquad 1 \leq x_\nu \leq L \qquad (\nu = 1,2) \; ,$$

with x_0, x_3 and μ unrestricted. Using (5.1), the action $S[U]$ can be written as a function of these variables only. Note that some of the loops contributing to $S[U]$ cross the boundary and hence involve Ω_ν after the links not contained in the set (B.1) are replaced by their periodic images in (B.1).

We now choose new integration variables $U(x,\mu)$ according to

$$\text{(B.2)} \qquad \tilde{U}(x,\mu) = \begin{cases} U(x,\mu)\Omega_\mu & \text{if } \mu \in \{1,2\} \text{ and } x_\mu = L \\ U(x,\mu) & \text{otherwise.} \end{cases}$$

This transformation has unit Jacobian and when the action S[U] is expressed in terms of U, the Ω_ν's cancel. Actually, for loops crossing the boundary in the x_1- and x_2-direction (a plaquette loop passing through x and $x + a\hat{1} + a\hat{2}$ with $x_1 = x_2 = L$, for example), the Ω_ν's cancel only after a rearrangement using the twist algebra (5.2). These loops thus pick up central phase factors and one ends up with the modified action commonly used for Monte Carlo simulations with twisted periodic boundary conditions [13].

We finally remark that in the formulation of chap. 5, Wilson loops winding around the world require the inclusion of a matrix Ω_ν whenever the boundary at $x = L$ is crossed (otherwise the Wilson loop would not be invariant under the gauge transformations (5.3)). These Ω_ν's are also removed by the transformation (B.2).

Appendix C: Proof of Lemma 6.1

At $k = 0$, the singularity of $g(k)$ is integrable (in fact, $g(0) = 0$) and the integrals

$$\text{(C.1)} \qquad c_m = \int_{-\pi}^{\pi} \frac{d^4k}{(2\pi)^4}\, g(k)\, e^{ik\cdot mL}, \qquad m \in \mathbb{Z}^4,$$

are therefore well-defined. Furthermore, we have

$$(-\Delta_k)^\ell g(k) \underset{k\to 0}{\propto} |k|^{-\alpha-2\ell},$$

where Δ_k denotes the (4-dimensional) Laplace operator with respect to k. As long as $\ell \leq j$, the partial integrations in the following lines are therefore allowed:

$$(m^2L^2)^\ell c_m = \int_{-\pi}^{\pi} \frac{d^4k}{(2\pi)^4}\, g(k)\,(-\Delta_k)^\ell e^{ik\cdot mL}$$

$$= \int_{-\pi}^{\pi} \frac{d^4k}{(2\pi)^4}\, [(-\Delta_k)^\ell g(k)]\, e^{ikmL}$$

For $\ell = j$ and $m \neq 0$, this leads to the bound

$$\text{(C.2)} \qquad |c_m| \leq C\,(m^2L^2)^{-j},$$

where C is some constant independent of m and L. It follows that the sum

$$S(g) = \sum_{m \in \mathbb{Z}^4} c_m$$

is absolutely convergent and one easily shows that it is equal to D(g).

Indeed, we have

$$\begin{aligned} S(g) &= \lim_{\varepsilon \searrow 0} \sum_m e^{-\varepsilon \sum_\mu |m_\mu|} c_m \\ &= \lim_{\varepsilon \searrow 0} \int_{-\pi}^{\pi} \frac{d^4k}{(2\pi)^4} g(k) \prod_\mu \{ (1 - e^{-\varepsilon + ik_\mu L})^{-1} - (1 - e^{\varepsilon + ik_\mu L})^{-1} \} \\ &= \frac{1}{L^4} \sum_k g(k) \ , \end{aligned}$$

and since g(0) = 0, the last expression is equal to D(g). Summing up,

we have shown that

$$D(g) = c_0 + \sum_{m \neq 0} c_m \ ,$$

which together with (C.2) implies the Lemma.

Appendix D: Proof of Lemma 6.2

Starting from the well-known "duality" relation

$$(D.1) \qquad \sum_{\nu \in \mathbb{Z}^4} e^{-z\nu^2 + iw\cdot\nu} = (2\pi)^4 (4\pi z)^{-2} \sum_{\nu \in \mathbb{Z}^4} e^{-\frac{1}{4z}(w - 2\pi\nu)^2} \ ,$$

$(z > 0, w \in \mathbb{R}^4)$, we have

$$(D.2) \qquad F_m(z) = (4\pi z)^{-2} \sum_{\nu \in \mathbb{Z}^4} H_m(-i\nabla_w) e^{-\frac{1}{4z}(w - 2\pi\nu)^2} \Big|_{w=0}$$

Define

$$(D.3) \qquad C_m = (4\pi)^{-2} H_m(-i\nabla_w) e^{-\frac{1}{4}w^2} \Big|_{w=0}$$

$$(D.4) \qquad \hat{F}_m(z) = (4\pi z)^{-2} \sum_{\nu \neq 0} H_m(-i\nabla_w) e^{-\frac{1}{4z}(w - 2\pi\nu)^2} \Big|_{w=0}$$

Then, using the homogeneity of the polynomial H_m, one may show that for $z > 0$

$$(D.5) \qquad F_m(z) = C_m z^{-q_m - 2} + \hat{F}_m(z)$$

Furthermore, it is obvious from eq. (D.4) that $\hat{F}_m(z)$ together with all its derivatives vanishes as $z \to 0$, in particular, $\hat{F}_m(z)$ extends to a C^∞ function for $0 \leq z < \infty$.

Appendix E: Explicit expressions for the gluon propagator

Concise expressions for the functions Q and P_{ij} appearing in the gluon propagator (7.8) are given by

$$(E.1) \qquad Q = (\hat{k}^2)^{-2} \sum_{\mu} \Big[\hat{k}_\mu^2 \cdot \prod_{\rho \neq \mu} d_\rho^{-1} \Big]$$

$$(E.2) \qquad P_{ij} = \epsilon_{ikm}\, \epsilon_{jln}\, (\hat{k}_k s_{ok})(\hat{k}_l s_{ol})(\delta_{mn} d_m^{-1} + \hat{k}_m \hat{k}_n s_{oo}) ,$$

where the vector d_μ^{-1} is defined by

$$(E.3) \qquad d_\mu^{-1} = \sum_{\nu} s_{\mu\nu} \hat{k}_\nu^2 \quad .$$

For the calculations with the improved action

$$c_1^{(0)} = -\frac{1}{12} \quad , \quad c_2^{(0)} = 0 \quad ,$$

it is useful to have explicit expressions for Q, P_{ij} as polynomials in $\hat{k}_o^2$. Towards this end we define auxiliary quantities

$$(E.4) \qquad u_\mu = \frac{1}{12} \hat{k}_\mu^2$$

$$(E.5) \qquad X = \sum_{j=1}^{3} u_j \quad , \quad Y = \sum_{j=1}^{3} u_j^2 \quad , \quad Z = u_1 u_2 u_3 \, .$$

Then Q is a polynomial of degree 5 in u_o,

$$(E.6) \qquad Q = (12)^2 \cdot (u_o^5 + B u_o^4 + C u_o^3 + D u_o^2 + E u_o + F) ,$$

with coefficients given by

$$(E.7) \qquad B = 3 + X$$

$$(E.8) \qquad C = 3 + 4X + \tfrac{3}{2} X^2 + \tfrac{1}{2} Y$$

$$(E.9) \qquad D = 1 + 5X + \tfrac{7}{2} X^2 + \tfrac{5}{2} Y + 2XY + 7Z$$

$$(E.10) \qquad E = 2X + 3X^2 + 2Y + \tfrac{5}{2} XY + \tfrac{3}{2} X^3 + 3Z + \tfrac{3}{2} X^2 Y - \tfrac{1}{2} Y^2 + 4XZ$$

$$(E.11) \qquad F = (X + Y)(X + X^2 + Y + XY + 3Z) .$$

Q factorises for special configurations e.g. when one of the u_i's is zero or all three u_i's are equal.

Corresponding explicit formulae for the P_{ij} are:

$$(E.12) \qquad P_{11} = (12)^2 \cdot (A_{11} u_o^4 + B_{11} u_o^3 + C_{11} u_o^2 + D_{11} u_o + E) ,$$

with

$$(E.13) \qquad A_{11} = -u_1 + X$$

(E.14) $$B_{11} = -u_1(3+2X) + (3X + X^2 + Y)$$

(E.15) $$C_{11} = 3u_1^2 X - u_1\left(3 + 5X + \tfrac{7}{2}X^2 + \tfrac{3}{2}Y\right) + \left(3X + 3X^2 + 2Y + \tfrac{3}{2}X^3 + \tfrac{1}{2}XY\right)$$

(E.16) $$D_{11} = 3u_1^2(X+Y) - u_1\left(1+4X+\tfrac{11}{2}X^2+\tfrac{5}{2}Y+5XY+7Z\right) + \left(X+3X^2+Y+\tfrac{5}{2}X^3+\tfrac{5}{2}XY+\tfrac{5}{2}X^2Y+2XZ-\tfrac{1}{2}Y^2\right)$$

(E.17) $$E_{11} = -u_1\left[(X+Y)\left(1+2X+\tfrac{1}{2}X^2+\tfrac{1}{2}Y\right)+Z(3+X)\right] + (X+Y)\left[(1+X)(X+Y)+2Z\right].$$

The other diagonal elements are given by permutation of the momenta. The same comment applies to the off-diagonal elements which are given by the following formulae

(E.18) $$P_{23} = -12\,\hat{k}_2\hat{k}_3\left(u_0^4 + Bu_0^3 + C_{23}u_0^2 + D_{23}u_0 + E_{23}\right)$$

with B given in (E.7) and

(E.19) $$C_{23} = u_1 X + \left(3 + 3X + \tfrac{1}{2}X^2 + \tfrac{1}{2}Y\right)$$

(E.20) $$D_{23} = u_1^2 X + u_1(X - X^2 + Y) + \left(1 + 3X + \tfrac{3}{2}X^2 + \tfrac{3}{2}Y + XY + 7Z\right)$$

(E.21) $$E_{23} = u_1^2(X+Y) - u_1 X(X+Y) + \left[(X+Y)\left(1+X+\tfrac{1}{2}X^2-\tfrac{1}{2}Y\right) + Z(3+X)\right].$$

Finally we consider the free propagators of the A and B mesons. These take a particularly simple form, since, for general $c_i^{(o)}$

(E.22) $$D_{11}(k)\big|_{k_1=0} = d_1(k)\big|_{k_1=0}$$

(E.23) $$\tfrac{1}{2}\sum_{i,j=1}^{2} e_i e_j D_{ij}(k)\big|_{k_1=k_2} = d_1(k)\big|_{k_1=k_2}$$

where $e_1 = 1$, $e_2 = -1$.

The function d_1 has only two poles in the complex u_0 plane which can hence be determined analytically. The physical pole corresponds to an energy E(k) given by

(E.24) $$\cosh E(\underline{k}) = 1 - \frac{b_1}{4c_1^{(o)}}\left(1 - \sqrt{1 + 4c_1^{(o)} f_1 / b_1^2}\right),$$

where

(E.25) $$b_1 = 1 - (c_1^{(o)} - c_2^{(o)})\,a^2\hat{k}_1^2 - 2c_2^{(o)}a^2\hat{\underline{k}}^2$$

(E.26) $$f_1 = \hat{\underline{k}}^2\left(1 - c_2^{(o)}a^2\hat{\underline{k}}^2\right) - (c_1^{(o)} - c_2^{(o)})\,a^2\left(\sum_j \hat{k}_j^4 + k_1^2\underline{k}^2\right).$$

E(k) has a small-a expansion

(E.27) $$E(\underline{k}) = \sqrt{\underline{k}^2}\cdot\left[1 - \left(c_1^{(o)} - c_2^{(o)} + \tfrac{1}{12}\right)\cdot\tfrac{1}{2}a^2\left(\underline{k}^2 + \sum_j k_j^4/\underline{k}^2\right) + \ldots\right]$$

To obtain the energies of the A and B mesons of momentum p in the 3-direction we simply have to set $\underline{k}$ equal to $\underline{k}_A$ or $\underline{k}_B$ respectively where

(E.28) $$\underline{k}_A = (0, m, p) \quad , \quad \underline{k}_B = (m, m, p) \; .$$

In particular for the A meson with p = 0, Eq. (7.21) follows directly from (E.27).

The residue Z of d_1 at a physical pole

(E.29) $$d_1(k) = Z(\underline{k}) / (k_0^2 + E^2(\underline{k})) \quad + \text{regular}$$

is given by

(E.30) $$Z(\underline{k}) = -E(\underline{k}) \cdot \left[\sinh E(\underline{k}) \cdot 4c_1^{(0)} \sqrt{1 + 4c_1^{(0)} f_1 / b_1^2} \; \right]^{-1} .$$

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Figure captions

Fig. 1: Gluon energy momentum dispersion along the line $k_1 = k_2$, $k_3 = 0$ for the tree level improved action ($c_1^{(o)} = -1/12$, $c_2^{(o)} = 0$). The top level is doubly degenerate and all other levels to the left of the bifurcation points are not degenerate. All of them are purely imaginary, i.e. Re $k_o = 0$. The branches to the right of the bifurcation points represent complex energies (Re $k_o \neq 0$).

Fig. 2: Feynman diagrams contributing to the gluon self-energy at order g_o^2. Wavy lines denote gluon propagators and the broken lines represent the propagation of Faddeev-Popov ghosts. Diagram (e) stems from the measure term (4.42) and the diagrams (f) represent the contributions proportional to $c_i^{(1)}$ (i = 1,2).

Fig. 3: Feynman diagrams contributing to the 3-point vertex function at order g_o^3. The notation is the same as in Fig. 2, in particular, the diagrams (1) represent the contributions proportional to $c_i^{(1)}$.

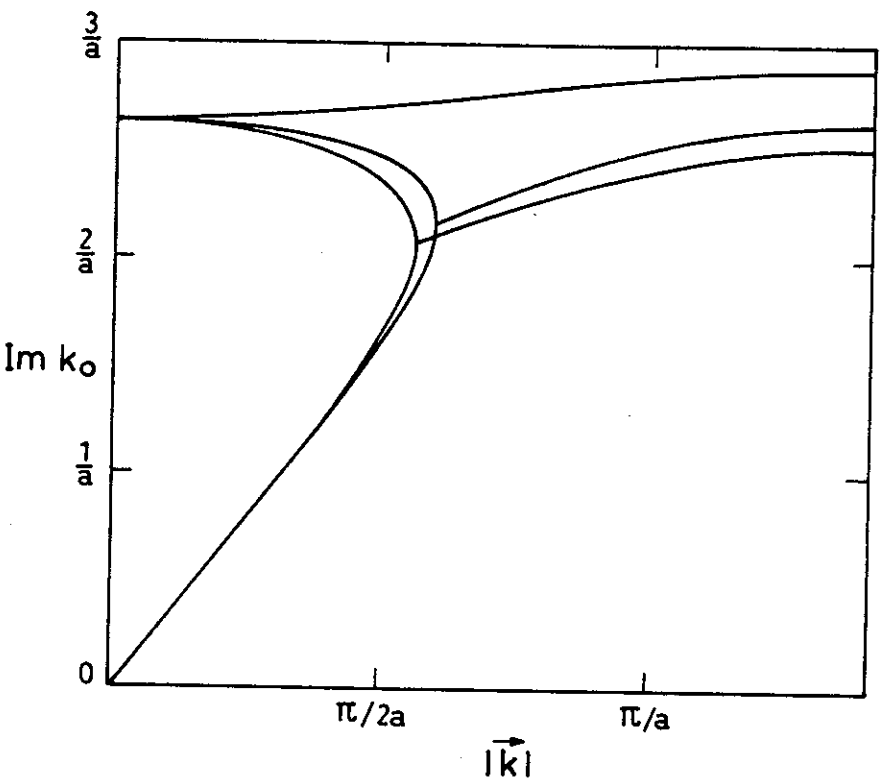

Fig.1

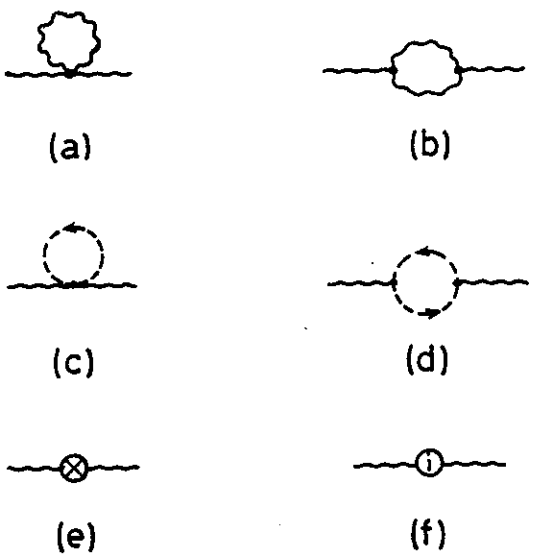

Fig. 2

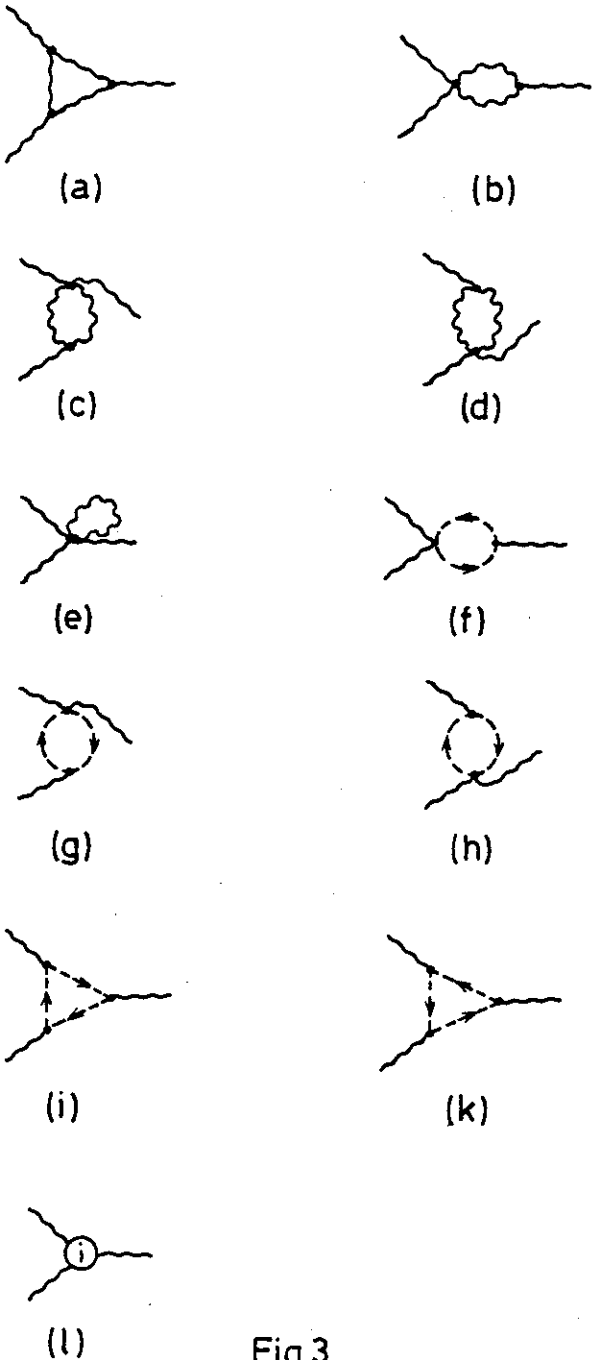

Fig.3