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IMPROVED CONTINUUM LIMIT LATTICE ACTION FOR QCD WITH WILSON FERMIONS

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Two possible ways of extending Symanzik's improvement programme to lattice fermions namely improvement to first and second order in the lattice spacing a are discussed. The corresponding lattice actions for fermions are constructed and tree-level improvement conditions are derived by considering "classical" improvement. The concept of "on-shell" improvement is generalized to the lattice fermions studied here and the free parameters are determined for $O(a)$ and $O(a^2)$ on-shell improved actions to all orders of perturbation theory. No evidence is found that the complicated structure of the $O(a^2)$ on-shell improved action, especially the arising fermion contact terms can be removed beyond tree level. The effect of terms in the action that explicitly break chiral symmetry and therefore remove the phenomenon of *species doubling* are investigated by considering the energy-momentum relations of the arising tree-level improved actions. Our main result is that the $O(a)$ improved action is a slightly modified Wilson fermion action which can still be written with only nearest-neighbour fermion interactions.

1. Introduction

Much effort has been spent in applying Symanzik's improvement programme [1] to lattice actions of various models. Originally developed by Symanzik in the framework of the Φ^4 theory [2] this procedure to systematically construct a lattice action with improved continuum limit approach has been applied to the non-linear σ-model in 2 dimensions [3, 4], the Gross-Neveu model [5, 6], pure Yang-Mills theory [7-10] and full QCD [11-13].

For the Φ^4-theory Symanzik was able to prove the consistency of the improvement programme to all orders of perturbation theory. To this end he demanded improvement of all (off-shell) Green functions. For lattice gauge theory this procedure is complicated because gauge-dependent terms have to be added to the action. A way of circumventing this problem is by demanding only the improvement of on-mass-shell quantities. This concept has been recently introduced by Lüscher and Weisz [14] in the context of pure Yang-Mills theory. The parameters in the action that are free, i.e. do not enter in spectral quantities are determined (to all orders of perturbation theory) by constructing a spectrum-conserving transformation of the action. The remaining constants have to be fixed order by order in perturbation theory by considering a suitable set of spectral quantities.

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In this paper we adopt this concept of on-shell improvement to Wilson lattice fermions. Previous work on the subject of improved lattice actions for fermions has been done by Eguchi and Kawamoto [11], Wetzel [12] and Hamber and Wu [13]. While these authors make a rather heuristic ansatz for the structure of their improved fermion action we present a somewhat more systematic approach. Improvement for lattice fermions can be considered on two levels. The first one is only to demand the cancellation of lattice artifacts to first order in the lattice spacing a which will be called $O(a)$ improvement in the following. To this end it suffices to use the standard one-plaquette Wilson action for the Yang–Mills part of the lagrangian. Furthermore the fermion part of the action has to be determined only up to operators of dimension five resulting in a fairly simple on-shell improved action. The second step, i.e. $O(a^2)$ improvement needs an improved action for the gluon part and additional operators of dimension six in the fermion part of the action including fermion contact terms.

In sect. 2 of this paper we set the stage for our investigations by constructing the most general lattice action for fermions including all possible operators up to dimension five and six respectively.

Classical improvement conditions are derived in sect. 3.

In sect. 4 we construct the isospectral transformation of the action and determine the free parameters of $O(a)$ and $O(a^2)$ on-shell improved lattice actions for fermions to all orders of perturbation theory.

Sect. 5 deals with the question of chirality breaking terms and species doubling by investigating the energy-momentum relations of suitable $O(a)$ and $O(a^2)$ on-shell improved actions. Throughout sects. 2–5 we give a separate discussion of $O(a)$ and $O(a^2)$ improvement and compare the results for both concepts at the end of each section.

In sect. 6 improvement beyond tree level is discussed and the results of a numerical calculation of the fermion contributions to the gluon self-energy are presented. Results for the second-order term obtained by Ukawa and Yang [15] are confirmed and comparison with the data for the gluon sector is made.

A discussion of our results is given in sect. 7.

2. General form of improved actions for Wilson fermions

As Symanzik's improvement programme requires the introduction of higher-dimensional terms into the action we construct lattice actions for Wilson fermions including (up to total derivatives) all possible gauge-invariant scalar operators of at most dimension five for $O(a)$ and six for $O(a^2)$ improvement that are invariant under discrete rotations, parity and charge conjugation transformations. To this end we first construct the invariant operators of the corresponding continuum effective lagrangians.

Postponing the introduction of flavour symmetry, we introduce Dirac fields $\bar{\psi}(x)$ and $\psi(x)$ and the gauge fields $A_\mu(x)$ which transform under the fundamental and adjoint representation of the colour group SU(N_c) respectively.

We shall use the shorthand notation $\bar{\psi}(x)$, $\psi(x)$, $A_\mu(x)$ for the N_c row and column matrices of the fermion fields with entries $\bar{\psi}_i(x)$, $\psi_i(x)$ (Dirac spinors) and the $(N_c \times N_c)$ matrix of the gauge fields with entries $A^a_\mu(x)t^a_{ij}$ where t^a are the generators of the fundamental representation of SU(N_c). Furthermore we set $D_\mu = (\mathbb{1}\partial_\mu + iA_\mu(x))$. Accordingly $\bar{\psi}(x)D_\mu\psi(x)$ will mean the product of the corresponding matrices.

2.1. O(a) IMPROVEMENT

Introducing a set of euclidean γ-matrices γ_μ with

$$\{\gamma_\mu, \gamma_\nu\} = 2\delta_{\mu\nu}\mathbb{1}\,,$$
$$\gamma_\mu^\dagger = \gamma_\mu\,, \tag{2.1}$$

we look for all operators up to dimension five that are invariant under gauge-, parity- and charge-conjugation transformations and discrete rotations. They are bilinear operators in the fermion fields and have the form $\bar{\psi}(x)O_i^b\psi(x)$. As we look for operators of at most dimension five the O_i^b can contain up to two derivatives. If Γ denotes a member of the 16-dimensional space to which our γ_μ belong (we choose γ_μ, γ_5, $\gamma_5\gamma_\mu$, $\mathbb{1}$, $\sigma_{\mu\nu} = \frac{1}{2}i[\gamma_\mu, \gamma_\nu]$ as a basis) discrete rotational invariance only allows O_i^b's of the following form:

$$\begin{aligned} \text{no derivatives:} \quad & O_0^b = \Gamma\,, \\ \text{1 derivative:} \quad & O_1^b = \Gamma_\mu D_\mu\,, \\ \text{2 derivatives:} \quad & O_2^b = \Gamma_{\mu\nu} D_{\mu\nu}\,. \end{aligned} \tag{2.2}$$

We can always choose all derivatives acting to the right-hand side $D_\mu = \vec{D}_\mu$. Terms that contain left-hand side derivatives $\overleftarrow{D}_\mu$ can always be expressed by terms containing only $\vec{D}_\mu$'s plus a total derivative. The operators $\bar{\psi}(x)O_i^b\psi(x)$ have to be invariant under parity and charge conjugation transformations.

We consider the effect of $\mathcal{P}$-parity:

$$\begin{aligned} \psi(x) &\to \psi'(x) = S(\mathcal{P})\psi(\mathcal{P}x)\,, \\ \bar{\psi}(x) &\to \bar{\psi}'(x) = \bar{\psi}(\mathcal{P}x)S(\mathcal{P})^{-1}\,, \\ D_\mu &\to D'_\mu = (\mathcal{P}^{-1})_{\mu\nu}D_\nu\,, \end{aligned} \tag{2.3}$$

with

$$\begin{aligned} S(\mathcal{P}) &= \gamma_\tau = S(\mathcal{P})^{-1}\,, \\ \mathcal{P}_{\mu\nu} &= \mathcal{P}^{-1}_{\mu\nu} = -(-1)^{\delta_{\mu\tau}}\delta_{\mu\nu}\,. \end{aligned} \tag{2.4}$$

Invariance of $\bar{\psi}(x)O_0^b\psi(x)$ entails $\gamma_\tau\Gamma\gamma_\tau=\Gamma$, i.e. $\Gamma=\mathbb{1}$. For $\bar{\psi}(x)O_1^b\psi(x)$ invariance means $\gamma_\tau\Gamma_\mu\gamma_\tau=-(-1)^{\delta_{\mu\tau}}\Gamma_\mu$ yielding $\Gamma_\mu=\gamma_\mu$.

If we demand linear independence among operators of the same dimension we derive the following set* of Γ's for the O_i^b:

$$\begin{aligned} O_0^b&: \quad \Gamma=\mathbb{1}\,,\\ O_1^b&: \quad \Gamma_\mu=\gamma_\mu\,,\\ O_2^b&: \quad \Gamma_{\mu\nu}=\delta_{\mu\nu}-i\sigma_{\mu\nu}\,, \quad \Gamma_{\mu\nu}=i\sigma_{\mu\nu}\,. \end{aligned} \tag{2.5}$$

One can check that charge conjugation

$$\psi(x)\to C\bar{\psi}^t(x)\,, \qquad \bar{\psi}(x)\to\psi^t(x)C\,,$$
$$C\gamma_\mu^tC^{-1}=-\gamma_\mu\,, \qquad C^{-1}=-C\,,$$

does not give any more restrictions on the O_i^b.

To incorporate an additional flavour symmetry with symmetry group $SU(N_f)$ and generators β^A we have to alter our shorthand notation in an obvious manner. As we shall assume flavour symmetry to be conserved the form of the operators bilinear in the fermion fields is not changed. We finally obtain the following set of independent invariant operators of dimension smaller than six ($F_{\mu\nu}=[D_\mu, D_\nu]$):

$$\begin{aligned} \text{dim 3:}&\quad O_0(x)=\bar{\psi}(x)\psi(x)\,,\\ \text{dim 4:}&\quad O_1(x)=\bar{\psi}(x)\not{D}\psi(x)\,,\\ \text{dim 5:}&\quad O_2(x)=\bar{\psi}(x)(D^2-\tfrac{1}{2}i\sigma_{\mu\nu}F_{\mu\nu})\psi(x)\,,\\ &\quad O_3(x)=\tfrac{1}{2}i\bar{\psi}(x)\sigma_{\mu\nu}F_{\mu\nu}\psi(x)\,. \end{aligned} \tag{2.6}$$

To put these operators on the lattice we define the following covariant lattice derivatives:

$$\begin{aligned} D_\mu^{\text{right}}\psi(x)&=\frac{1}{a}[U_\mu(x)\psi(x+\hat{\mu})-\psi(x)]\,,\\ D_\mu^{\text{left}}\psi(x)&=\frac{1}{a}[\psi(x)-U_\mu^\dagger(x-\hat{\mu})\psi(x-\hat{\mu})]\,,\\ D_\mu^{\text{L}}\psi(x)&=\frac{1}{2}[D_\mu^{\text{right}}+D_\mu^{\text{left}}]\psi(x)\,,\\ (D_\mu^2)^{\text{L}}\psi(x)&=\frac{1}{a}[D_\mu^{\text{right}}-D_\mu^{\text{left}}]\psi(x)\,,\\ \Delta^{\text{L}}\psi(x)&=\sum_\mu(D_\mu^2)^{\text{L}}\psi(x)\,, \end{aligned} \tag{2.7}$$

* The reason for this particular choice will become clear later.

where $U_\mu(x)$ denotes the link operator, a is the lattice spacing and $\hat{\mu}$ is a times the unit vector in the μth direction.

We then choose the following representations O_i^{L} of the operators O_i on the lattice:

$$O_1^{\mathrm{L}}(x) = \bar{\psi}(x)\gamma_\mu D_\mu^{\mathrm{L}}\psi(x)\,,$$

$$O_2^{\mathrm{L}}(x) = \bar{\psi}(x)(\Delta^{\mathrm{L}} - \frac{i}{2a^2}\sigma_{\mu\nu}P_{\mu\nu}(x))\psi(x)\,,$$

$$O_3^{\mathrm{L}}(x) = \frac{i}{2a^2}\bar{\psi}(x)\sigma_{\mu\nu}P_{\mu\nu}(x)\psi(x)\,, \tag{2.8}$$

where $P_{\mu\nu}(x)$ is the operator*

$$\begin{aligned} P_{\mu\nu}(x) = \tfrac{1}{4}(& U_\mu(x)U_\nu(x+\hat{\mu})U_\mu^\dagger(x+\hat{\nu})U_\nu^\dagger(x) \\ & - U_\nu^\dagger(x-\hat{\nu})U_\mu^\dagger(x-\hat{\mu}-\hat{\nu})U_\nu(x-\hat{\mu}-\hat{\nu})U_\mu(x-\hat{\mu}) \\ & + U_\nu(x)U_\mu^\dagger(x-\hat{\mu}+\hat{\nu})U_\nu^\dagger(x-\hat{\mu})U_\mu(x-\hat{\mu}) \\ & - U_\mu(x)U_\nu^\dagger(x+\hat{\mu}-\hat{\nu})U_\mu^\dagger(x-\hat{\nu})U_\nu(x-\hat{\nu}))\,. \end{aligned} \tag{2.9}$$

We can now write down the action suitable for $\mathrm{O}(a)$ improvement

$$S_{\mathrm{L}}^{\mathrm{F}_1} = -\frac{a^4}{g_0^2}\sum_{\substack{x \text{ all} \\ \text{lattice sites}}}\sum_{i=0}^{3} a^{(\dim O_i^{\mathrm{L}}(x)-4)}b_i(g_0^2, ma)O_i^{\mathrm{L}}(x)\,. \tag{2.10}$$

The coefficients $b_i(g_0^2, ma)$ are regular at $g_0 = 0$ and have to be determined order by order in perturbation theory. Reality of the action furthermore requires the coefficients b_i of the action (2.10) to be real.

2.2. $\mathrm{O}(a^2)$ IMPROVEMENT

For $\mathrm{O}(a^2)$ improvement we have to extend our considerations of subsect. 2.1 to operators of dimension six. Then bilinear operators of the form $O_3^b = \Gamma_{\mu\nu\rho}D_\mu D_\nu D_\rho$ have to be considered. As a new feature also quartic fermion operators of the form $(\bar{\psi}(x)O_i^q\psi(x))^2$ appear, where

$$O_0^q = \Gamma\,, \qquad O_1^q = \Gamma_\mu\,, \qquad O_2^q = \Gamma_{\mu\nu}\,. \tag{2.11}$$

The invariance considerations of subsect. 2.1 now yield

$$\begin{aligned} O_3^b\colon\quad & \Gamma_{\mu\nu\rho} = \delta_{\mu\nu}\delta_{\mu\rho}\gamma_\mu\,, \qquad \Gamma_{\mu\nu\rho} = \gamma_\mu\delta_{\nu\rho}\,, \qquad \Gamma_{\mu\nu\rho} = \gamma_\rho\delta_{\mu\nu}\,, \\ & \Gamma_{\mu\nu\rho} = 2\gamma_\nu\delta_{\mu\rho} - \gamma_\mu\delta_{\nu\rho} - \gamma_\rho\delta_{\mu\nu}\,, \\ & \Gamma_{\mu\nu\rho} = \gamma_\mu\gamma_\nu\gamma_\rho\,, \end{aligned}$$

* We have chosen this combination of plaquette operators with maximal symmetry as a lattice representation of $F_{\mu\nu}(x)$ for convenience.

$$O_0^q: \quad \Gamma = \mathbb{1}, \qquad \Gamma = \gamma_5,$$
$$O_1^q: \quad \Gamma = \gamma_\mu, \qquad \Gamma_\mu = \gamma_5\gamma_\mu,$$
$$O_2^q: \quad \Gamma_{\mu\nu} = \sigma_{\mu\nu}. \tag{2.12}$$

Introduction of a conserved flavour symmetry with generators β^A only affects the four fermion interactions. After making use of the Fierz identities and completeness relations we end up with twice as many contact terms and eventually find all invariant operators of dimension six:

(i) bilinear operators:

$$O_4(x) = \bar\psi(x)\gamma_\mu D_\mu^3\psi(x), \qquad O_5(x) = \bar\psi(x)D^2\not{D}\psi(x),$$
$$O_6(x) = \bar\psi(x)\not{D}D^2\psi(x), \qquad O_7(x) = \bar\psi(x)\gamma_\mu[D_\nu, F_{\mu\nu}]\psi(x),$$
$$O_8(x) = \bar\psi(x)\not{D}^3\psi(x), \tag{2.13}$$

(ii) contact terms:

$$O_9(x) = (\bar\psi(x)t^a\psi(x))^2, \qquad O_{10}(x) = (\bar\psi(x)\beta^A t^a\psi(x))^2,$$
$$O_{11}(x) = (\bar\psi(x)\gamma_5 t^a\psi(x))^2, \qquad O_{12}(x) = (\bar\psi(x)\gamma_5\beta^A t^a\psi(x))^2,$$
$$O_{13}(x) = (\bar\psi(x)\gamma_\mu t^a\psi(x))^2, \qquad O_{14}(x) = (\bar\psi(x)\gamma_\mu\beta^A t^a\psi(x))^2,$$
$$O_{15}(x) = (\bar\psi(x)\gamma_5\gamma_\mu t^a\psi(x))^2, \qquad O_{16}(x) = (\bar\psi(x)\gamma_5\gamma_\mu\beta^A t^a\psi(x))^2,$$
$$O_{17}(x) = (\bar\psi(x)\sigma_{\mu\nu}t^a\psi(x))^2, \qquad O_{18}(x) = (\bar\psi(x)\sigma_{\mu\nu}\beta^A t^a\psi(x))^2.$$

For the lattice representations of these six-dimensional operators we choose

$$O_4^{\mathrm{L}}(x) = \bar\psi(x)\gamma_\mu D_\mu^{\mathrm{L}}(D_\mu^2)^{\mathrm{L}}\psi(x), \qquad O_5^{\mathrm{L}}(x) = \bar\psi(x)\gamma_\mu\Delta^{\mathrm{L}}D_\mu^{\mathrm{L}}\psi(x),$$
$$O_6^{\mathrm{L}}(x) = \bar\psi(x)\gamma_\mu D_\mu^{\mathrm{L}}\Delta^{\mathrm{L}}\psi(x), \qquad O_7^{\mathrm{L}}(x) = \bar\psi(x)\gamma_\mu[D_\nu^{\mathrm{L}}, [D_\mu^{\mathrm{L}}, D_\nu^{\mathrm{L}}]]\psi(x),$$
$$O_8^{\mathrm{L}}(x) = \bar\psi(x)\gamma_\mu\gamma_\nu\gamma_\rho D_\mu^{\mathrm{L}}D_\nu^{\mathrm{L}}D_\rho^{\mathrm{L}}\psi(x). \tag{2.14}$$

As an extension of (2.10) we find the action suitable for $\mathrm{O}(a^2)$ improvement:

$$S_{\mathrm{L}}^{\mathrm{F}_2} = -\frac{a^4}{g_0^2}\sum_{\substack{x \text{ all} \\ \text{lattice sites}}}\sum_{i=0}^{18} a^{(\dim O_i^{\mathrm{L}}(x)-4)}b_i(g_0^2, ma)O_i^{\mathrm{L}}(x). \tag{2.15}$$

Reality of the action now requires

$$b_5(g_0^2, ma) = \bar b_6(g_0^2, ma),$$
$$b_i(g_0^2, ma) \text{ real}, \qquad i \neq 5, 6. \tag{2.16}$$

2.3. SUMMARY

Comparing the actions (2.10) and (2.15) we find that the task of also removing the $\mathrm{O}(a^2)$ lattice artifacts leads to a much more complicated action. Next-to-nearest

neighbour interactions have to be added and fermion contact terms appear, both features which yield considerable difficulties for numerical calculations. If no drastic simplification of (2.15) can be achieved via the introduction of suitable improvement conditions this action will be of little use for practical purposes.

3. Classical improvement

A suitable way to impose tree-level improvement conditions is the concept of *classical* improvement. It demands the vanishing of all corrections to the leading term $-(m\bar{\psi}(x)\psi(x)+\bar{\psi}(x)\not{D}\psi(x))$ in the small a expansion of the lattice action to the desired order (i.e. $O(a)$ or $O(a^2)$). As the classical action generates the tree-level vertex functions these should then be improved too to order $O(a)$ or $O(a^2)$ respectively.

To obtain the classical expansions of the operators $O_i^L(x)$ in (2.10) and (2.15) we note that these expansions always start with the corresponding continuum operator $O_i(x)$ plus corrections of classical dimension two higher.

To verify this we start with the expansion of our lattice derivative D_μ^L. Choosing a gauge with $A_\mu(x)=0\ \forall x$ it is easy to see that

$$D_\mu^L\psi(x)=(D_\mu+\tfrac{1}{6}a^2D_\mu^3+O(a^4))\psi(x)\,. \tag{3.1}$$

Furthermore

$$(D_\mu^2)^L\psi(x)=(D_\mu^2+\tfrac{1}{12}a^2D_\mu^4+O(a^4))\psi(x)\,, \tag{3.2}$$

$$P_{\mu\nu}(x)=a^2F_{\mu\nu}(x)+O(a^4)\,. \tag{3.3}$$

As only operators of dimension 3-6 appear in our actions (2.10) and (2.15) the only term whose expansion can give rise to combinations with a higher-dimensional operator of the action is $O_1^L(x)$ and we find

$$O_1^L=\bar{\psi}(x)\gamma_\mu(D_\mu+\tfrac{1}{6}a^2D_\mu^3+O(a^4))\psi(x)\,. \tag{3.4}$$

3.1. O(a) IMPROVEMENT

Classical improvement therefore entails for $O(a)$ improvement

$$b_0(0, ma)=ma\,,\qquad b_1(0, ma)=1\,,\qquad b_2(0,0)=b_3(0,0)=0\,. \tag{3.5}$$

This yields the *classical* improved lattice action

$$S^{CI_1}=-\frac{a^4}{g_0^2}\sum_{\substack{x\ \text{all}\\ \text{lattice sites}}}(mO_0^L(x)+O_1^L(x))\,. \tag{3.6}$$

3.2. $O(a^2)$ IMPROVEMENT

$O(a^2)$ *classical* improvement requires

$$b_0(0, ma) = ma\,, \qquad b_1(0, ma) = 1\,,$$
$$b_2(0, ma) = b_3(0, ma) = 0\,,$$
$$\tfrac{1}{6} b_1(0, ma) + b_4(0, 0) = 0\,,$$
$$b_i(0, 0) = 0\,, \qquad 5 \leq i \leq 18\,. \tag{3.7}$$

This yields the $O(a^2)$ *classical* improved action

$$S^{\mathrm{CI}_2} = -\frac{a^4}{g_0^2} \sum_{\substack{x \text{ all} \\ \text{lattice sites}}} (mO_0^{\mathrm{L}}(x) + O_1^{\mathrm{L}}(x) - \tfrac{1}{6} a^2 O_4^{\mathrm{L}}(x))\,. \tag{3.8}$$

3.3. SUMMARY

At least to lowest order in perturbation theory a drastic simplification of the $O(a^2)$ improved action occurs. The price to pay for also removing the $O(a^2)$ lattice artifacts is the introduction of one additional operator containing next to nearest-neighbour fermion interactions. We note that both actions (3.6) and (3.8) conserve chiral symmetry for bare mass zero and therefore show the phenomenon of "species doubling". In particular (3.6) is nothing but the so-called "naive" lattice fermion action. One way to avoid species doubling would be to add to the action irrelevant operators (i.e. of dimension seven) that break chiral symmetry. This has been done by Eguchi and Kawamoto and Wetzel for their tree-level $O(a^2)$ improved action. As *classical* improvement is consistent with tree-level *on-shell* improvement but *on-shell* improvement is meant to impose "minimal" improvement conditions we hope to be able to break chiral symmetry by an operator of dimension five.

4. Spectrum-conserving transformation of on-shell improved actions

We first want to give a more detailed description of the concept of on-shell improvement developed by Lüscher and Weisz in ref. [14]. Following Symanzik's approach of a perturbative construction of an improved action, suitable improvement conditions have to be imposed. For the Φ^4 theory Symanzik was able to prove that improvement of all Green functions could be achieved. In the case of the non-linear σ-model the situation turned out to be more complicated but Symanzik eventually showed that improvement of all Green functions is possible for a modified field operator. In the case of lattice gauge theory it has up to now not been proven that all Green functions can be improved. To this end it would be necessary to add gauge-dependent terms to the action at intermediate states of the calculation and

up to now no procedure has been given on how the gauge-invariant physical quantities can be eventually extracted. Lüscher and Weisz therefore proposed to introduce a minimal improvement scheme by demanding improvement only for low-lying (with momenta small compared to the cutoff) energy states, i.e. on-shell quantities. This allows one to keep gauge invariance manifest at all stages of the calculation but even for this case the existence of an on-shell improved action has not yet been proven but will nevertheless be assumed. Given one on-shell improved action other on-shell improved actions can be obtained by a local covariant transformation of the fields. Up to corrections of at least $O(a^2)$ for $O(a)$ improvement and $O(a^3)$ for $O(a^2)$ improvement this will amount to a shift in a certain set of coefficients of the original action. The maximal number of coefficients that can thus be varied independently by our transformation is the number of free parameters in the sense of on-shell improvement. Their values can be chosen zero or any other value which may be convenient for specific calculations. As has been pointed out by Lüscher and Weisz this argument applies to all orders of perturbation theory.

We have to find a spectrum-conserving transformation of the fermion and gauge fields and study its effects on a full QCD on-shell improved lattice action:

$$S_L = S_L^{YM} + S_L^F , \tag{4.1}$$

where S_L^{YM} denotes the pure Yang-Mills part of the action and S_L^F is the fermion action. For $O(a)$ improvement S_L^{YM} can be chosen the standard one-plaquette action and S_L^F has the form (2.10). For $O(a^2)$ improvement S_L^{YM} is the improved Yang-Mills action given in ref. [14] and S_L^F is given by (2.15).

Under the spectrum-conserving transformation we will have

$$S_L \to S_L' = S_L^{YM'} + S_L^{F'} . \tag{4.2}$$

In ref. [14] the part of the transformation giving rise to $S_L^{YM'}$ is discussed. We must therefore only study the part resulting in $S_L^{F'}$.

As the classical expansions of all lattice operators in the fermion part of the action start with their continuum analogue it is sufficient to consider the following transformations:

$$T_1: \quad A_\mu \to A_\mu + a^2(\tfrac{1}{2}\varepsilon \sum_\nu [D_\nu, F_{\mu\nu}] + \varepsilon' \bar\psi \gamma_\mu \psi) , \tag{4.3}$$

where $\bar\psi \gamma_\mu \psi = (\bar\psi_i \gamma_\mu t^a_{ij} \psi_j) t^a$ transforms as A_μ under $SU(N_c)$ and

$$T_2: \quad \begin{cases} \psi \to \psi + a\varepsilon_1 \not{D}\psi + a^2 \varepsilon_2 D^2 \psi + a^2 \varepsilon_3 \not{D}^2 \psi \\ \bar\psi \to \bar\psi + a\varepsilon_1' \bar\psi \not{\tilde D} + a^2 \varepsilon_2' \bar\psi \tilde D^2 + a^2 \varepsilon_3' \bar\psi \not{\tilde D}^2 . \end{cases} \tag{4.4}$$

This is the most general local covariant transformation of the fields up to $O(a^2)$. How does the action (4.1) transform under this substitution of the fields?

We are only interested in the lowest-order contributions (in g_0) to the transformed coefficients because for them the infinitesimal transformations can be integrated up yielding the redundant parameters of the on-shell improved action to lowest order. Given an on-shell improved action which is improved to order g_0^{2l} the same argument also provides the redundant coefficients to this order of perturbation theory. We simply have to choose the infinitesimal parameters ε_i' proportional to g_0^{2l} and the lowest-order part of our transformation will produce another g_0^{2l} on-shell improved action with shifted $b_i(g_0^{2l}, ma)$'s. The b_i's that thus can be varied to lowest order are therefore redundant to all orders of perturbation theory. To lowest order in g_0 we have the normalisation $b_1(0, ma) = 1$ and $b_0(0, ma) = ma$ which for the coefficients of the transformed action $b'(0, ma)$ can be imposed by a rescaling of the fields and the mass.

As shown in appendix A there is no contribution to $S_L^{F'}$ to first order in the infinitesimal parameters ε_i that is due to the transformation of the measure.

4.1. O(a) IMPROVEMENT

To this order only the fermion part of the lagrangian is affected so we only have to deal with the O(a) part of (4.4) (i.e. the ε_1, ε_1' parts). For $g_0 = 0$ we find

$$(g_0^2 \delta S_L^F)|_{g_0=0} = -a^4 \sum_{\substack{x \text{ all} \\ \text{lattice sites}}} [(\varepsilon_1 - \varepsilon_1') b_0(0, ma) O_1^L(x) + a(\varepsilon_1 - \varepsilon_1') b_1(0, ma) O_2^L(x) + O(a^2)] . \tag{4.5}$$

Reality of the transformed action demands $\varepsilon_1 - \varepsilon_1'$ real.

After performing the rescaling to first order in ε and separating higher-order terms in a we end up with

$$(g_0^2 \delta S_L^F)|_{g_0=0} = -a^4 \sum_{\substack{x \text{ all} \\ \text{lattice sites}}} [a(\varepsilon_1 - \varepsilon_1') O_2^L(x) + O(a^2)] . \tag{4.6}$$

For O(a) on-shell improvement we thus find the parameter $b_2(g_0^2, 0)$ to be redundant. This is why we made the particular choice for the operators O_2^b in (2.5). We may therefore use the operator $O_2^L(x)$ with an arbitrary coefficient to avoid the phenomenon of species doubling. This is not in contradiction to the on-shell improvement condition that low-lying states should not be affected because the low-lying energy states that are altered by the lifting of species doubling are at the edges of the Brillouin zone outside the range where improvement should be effective. This will be further discussed in the next section. The remaining coefficient $b_3(g_0^2, 0)$ which is not affected by the transformation has to be calculated perturbatively by considering suitable spectral quantities. As classical improvement is consistent with on-shell tree-level improvement we have $b_3(0, 0) = 0$.

4.2. O(a^2) IMPROVEMENT

Now T_1 and T_2 contribute to $S_L^{F'}$. We find

$$(g_0^2\delta_{T_2}S_L^F)|_{g_0=0} = -a^4 \sum_{\substack{x \text{ all} \\ \text{lattice sites}}} [(\varepsilon_1-\varepsilon_1')b_0(0,ma)O_1^L(x)$$
$$+ a((\varepsilon_1-\varepsilon_1')b_1(0,ma)+(\varepsilon_2+\varepsilon_2'+\varepsilon_3+\varepsilon_3')b_0(0,ma))O_2^L(x)$$
$$+ a(\varepsilon_2+\varepsilon_2')b_0(0,ma)O_3^L(x)+a^2(\varepsilon_1 b_3(0,ma)$$
$$+ \varepsilon_2' b_1(0,ma))O_5^L(x)-a^2(\varepsilon_1' b_3(0,ma)-\varepsilon_2 b_1(0,ma))O_6^L(x)$$
$$+ a^2((\varepsilon_1-\varepsilon_1')(b_2(0,ma)-b_3(0,ma))$$
$$+ (\varepsilon_3+\varepsilon_3')b_1(0,ma))O_8^L(x)+O(a^3)]\,. \tag{4.7}$$

Furthermore

$$(g_0^2\delta_{T_1}S_L^F)|_{g_0=0} = -a^4 \sum_{\substack{x \text{ all} \\ \text{lattice sites}}} a^2[\tfrac{1}{2}\varepsilon O_7^L(x)+\varepsilon' O_{13}^L(x)+O(a^2)]\,. \tag{4.8}$$

Whereas the Yang-Mills part of the action transforms as

$$S_L^{YM} \to S_L^{YM'} - \frac{a^4}{g_0^2} \sum_{\substack{x \text{ all} \\ \text{lattice sites}}} a^2[\varepsilon' O_7^L(x)+O(a^2)]\,. \tag{4.9}$$

Collecting all terms, considering only the $g_0 = 0$ parts of the coefficients and rescaling the fields as above yields

$$(g_0^2\delta S_L^F)|_{g_0=0} = -a^4 \sum_{\substack{x \text{ all} \\ \text{lattice sites}}} [a\{(\varepsilon_1-\varepsilon_1')$$
$$- ma((\varepsilon_1-\varepsilon_1')b_2(0,0)-(\varepsilon_2+\varepsilon_2'+\varepsilon_3+\varepsilon_3'))\}O_2^L(x)$$
$$- ma^2((\varepsilon_1-\varepsilon_1')b_3(0,0)-(\varepsilon_2+\varepsilon_2'))O_3^L(x)+a^2(\varepsilon_1 b_3(0,0)+\varepsilon_2')O_5^L(x)$$
$$- a^2(\varepsilon_1' b_3(0,0)-\varepsilon_2)O_6^L(x)+a^2(\tfrac{1}{2}\varepsilon+\varepsilon')O_7^L(x)$$
$$+ a^2((\varepsilon_1-\varepsilon_1')(b_2(0,ma)-b_3(0,ma))$$
$$+ (\varepsilon_3+\varepsilon_3'))O_8^L(x)+a^2\varepsilon' O_{13}^L(x)+O(a^3)]\,, \tag{4.10}$$

$$\text{reality of the transformed action demands} \quad \left.\begin{matrix}\varepsilon_1-\varepsilon_1' \\ \varepsilon_2+\varepsilon_2' \\ \varepsilon_3+\varepsilon_3' \\ \varepsilon \\ \varepsilon'\end{matrix}\right\} \text{real}\,. \tag{4.11}$$

The parameter ε performs the isospectral transformation in the Yang-Mills part of the action. It has been used by Lüscher and Weisz to consider the coefficient c_3 of the pure Yang-Mills improved action as a free parameter in the sense of on-shell

improvement. They proposed to set it to zero to all orders of perturbation theory. If we want this to persist only $b_7 + b_{13}$ can be varied independently, i.e. either b_7 *or* b_{13} can be chosen as a free parameter besides b_2, b_5, b_6, b_8. We note that the parameter b_3 can be kept unchanged by suitably rescaling the mass parameter. A possible choice for an on-shell $O(a^2)$ improved action would be to use the parameter b_2 as in the case of $O(a)$ improvement to break chiral symmetry and to set b_5, b_6, b_8, b_{13} to zero to all orders of perturbation theory. All other coefficients in particular those of the remaining contact terms have to be fixed by considering a suitable set of spectral quantities. To tree level however *classical* improvement sets them to zero. We have confirmed that this as expected also holds for $O(a^2)$ *on-shell* tree-level improvement by considering scattering amplitudes in the way proposed by Wetzel [12].

4.3. SUMMARY

The considerations of this section have been decisive on the question of what improvement concept should be pursued to higher orders of perturbation theory. For $O(a^2)$ improvement at most one of the disturbing fermion contact terms can be removed. Beyond tree level we are stuck with far too many operators whose coefficients would have to be determined by perturbative calculations. For $O(a)$ improvement the situation however looks favourable. We can use the redundant operator O_2^L to break chiral symmetry and only the coefficient $b_3(g_0^2, 0)$ has to be determined perturbatively. For numerical simulations this means a modification of the Wilson fermion action by one additional term. According to our opinion this is the improvement programme that should be pursued for QCD. By removing the first-order lattice artifacts in on-shell quantities considerable improvement might already occur.

5. Breaking of chiral symmetry and energy-momentum relations

In this section we try to get a better understanding of the effect of species doubling and its amendment by the introduction of chirality breaking terms into the lagrangian which was first proposed by Wilson [16]. Throughout this section we deal with fermions of zero bare mass.

5.1. O(a) IMPROVEMENT

For zero bare mass the $O(a)$ classical improved fermion action

$$S_F^{CI_1} = -\frac{a^4}{g_0^2} \sum_{\substack{x \text{ all} \\ \text{lattice sites}}} O_1^L(x) \tag{5.1}$$

has chiral symmetry and according to the no-go-theorem of Nielsen and Ninomiya [17] shows the phenomenon of species doubling. To cope with this problem of additional zeros of the energy-momentum relation at the edges of the Brillouin zone Wilson has proposed to add an extra term of higher classical dimension to the action thus explicitly breaking chiral symmetry. For the case of the naive fermion lattice action which coincides with (5.1) Wilson chose an operator of dimension five giving

$$S_{\mathrm{F}}^{\mathrm{W}} = -\frac{a^4}{g_0^2} \sum_{\substack{x \text{ all} \\ \text{lattice sites}}} [O_1^{\mathrm{L}}(x) - \tfrac{1}{2}\lambda a O_{\mathrm{W}}^{\mathrm{L}}(x)] \tag{5.2}$$

(with $O_{\mathrm{W}}^{\mathrm{L}}(x) = O_2^{\mathrm{L}}(x) + O_3^{\mathrm{L}}(x)$).

The concept of on-shell improvement as developed in the last section however allows to break chiral symmetry by an operator of dimension five, i.e. $O_2^{\mathrm{L}}(x)$ without violating the $\mathrm{O}(a)$ improvement of spectral quantities. We therefore choose as an $\mathrm{O}(a)$ tree-level on-shell improved action

$$S_{\mathrm{F}}^{\mathrm{OS}_1} = -\frac{a^4}{g_0^2} \sum_{\substack{x \text{ all} \\ \text{lattice sites}}} [O_1^{\mathrm{L}}(x) - \tfrac{1}{2}\lambda a O_2^{\mathrm{L}}(x)] . \tag{5.3}$$

Both actions (5.2) and (5.3) yield the same inverse propagator:

$$S_{\mathrm{F}}^{-1}(p) = \frac{1}{a} \sum_{\mu} (i\gamma_\mu \sin(p_\mu a) + 2\lambda \sin^2(\tfrac{1}{2} p_\mu a)) . \tag{5.4}$$

To get a better understanding of the relevance of the parameter λ in (5.4) we consider the emerging energy states. For improved actions these considerations have been first made by Lüscher [18] for a free scalar field.

The one-particle energy states are related to the poles of the time Fourier-transformed propagator. They are given by $E_i = -\ln z_i$ where z_i are the poles inside the unit circle. For the $\mathrm{O}(a)$ on-shell improved action (and the Wilson action which yields the same propagator) this investigation can be performed analytically. Here we give a qualitative discussion of the arising phenomena which for the $\mathrm{O}(a)$ improved action is shown in fig. 1 where the real parts of the resulting "energy states" are depicted (for unit lattice spacing). The momentum configurations chosen there are made for better comparison of the $\mathrm{O}(a)$ and $\mathrm{O}(a^2)$ on-shell improved actions. A more detailed survey of the used formulae is given in appendix B.

The main effect arising is the appearance of "unphysical" energy states besides the "physical" ones which approximate the continuum energy-momentum relation $E^2(\boldsymbol{p}) = \boldsymbol{p}^2 (\boldsymbol{p} = (p_1, p_2, p_3))$. The values of the parameter λ should then be chosen in such a way as to keep these unwanted effects sufficiently far away from the low-energy - low-momentum regime we are interested in. For the energy-momentum

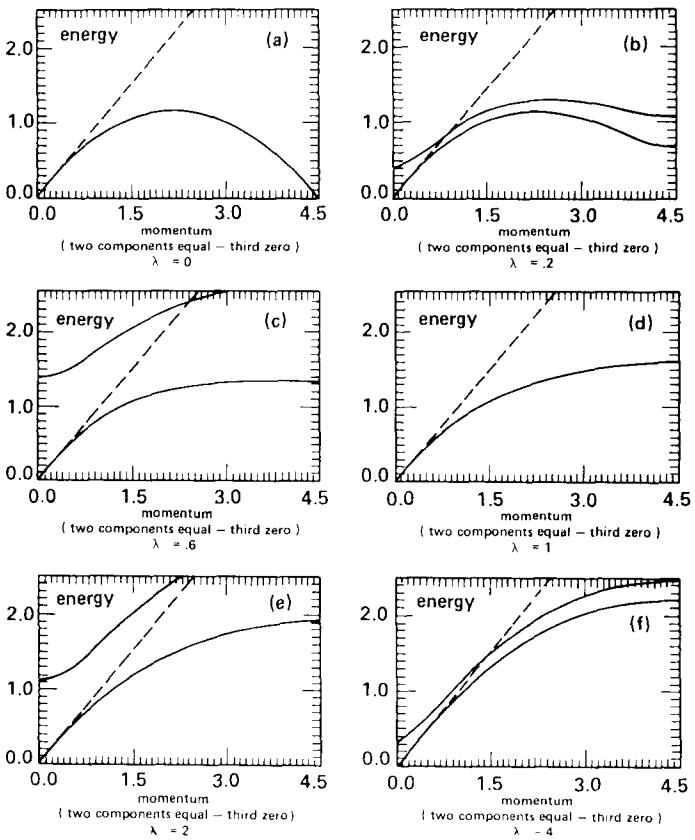

Fig. 1. Energy-momentum relations for the $O(a)$ tree-level on-shell improved fermion action (5.3) for values of (a) $\lambda = 0$, (b) $\lambda = 0.2$, (c) $\lambda = 0.6$, (d) $\lambda = 1$, (e) $\lambda = 2$, (f) $\lambda = 4$.

relation of the "physical" energy states we obtain a small-$\boldsymbol{p}$ expansion giving

$$E^2(\boldsymbol{p}) = \boldsymbol{p}^2 - \tfrac{1}{3}a^2\left((\boldsymbol{p}^2)^2 + \sum_{j=1}^{3} p_j^4\right) + a^4\left(\tfrac{8}{45}(\boldsymbol{p}^2)^3 + \tfrac{2}{9}\boldsymbol{p}^2 \sum_{j=1}^{3} p_j^4 + \tfrac{2}{45}\sum_{j=1}^{3} p_j^6\right)$$

$$+ a^6\left[\tfrac{1}{64}\lambda^2\left((\boldsymbol{p}^2)^2 + \sum_{j=1}^{3} p_j^4\right)^2 - \tfrac{289}{2835}(\boldsymbol{p}^2)^4 + \tfrac{28}{405}\boldsymbol{p}^2 \sum_{j=1}^{3} p_j^6\right.$$

$$\left. - \tfrac{34}{135}(\boldsymbol{p}^2)^2 \sum_{j=1}^{3} p_j^4 - \tfrac{73}{945}\sum_{j=1}^{3} p_j^8\right] + O(a^8)\,. \tag{5.5}$$

For $\lambda = 0$ there are two energy states, one real and one complex, whose real parts coincide. As only the real part of the energy is depicted in our figures just one curve is shown (fig. 1a). As a consequence of the chiral symmetry of the lagrangian there are additional zeros of the energy at $\boldsymbol{p} = \pi(\nu_1, \nu_2, \nu_3)$, $\nu_i = 0, \pm 1$. In the case of $\lambda \neq 0$

the "unphysical" second energy state has the small-$\boldsymbol{p}$ expansion

$$E(\boldsymbol{p}) = \frac{1}{a}\ln\left(\frac{\lambda+1}{\lambda-1}\right) + \frac{1}{4}a\frac{\lambda^2+1}{\lambda}\boldsymbol{p}^2 - \frac{1}{8}a^3\left[\frac{1}{8}\frac{\lambda^6-\lambda^4+7\lambda^2+1}{\lambda^3}(\boldsymbol{p}^2)^2 - \frac{1}{3}\frac{\lambda-2}{\lambda}\sum_{j=1}^{3}p_j^4\right]. \tag{5.6}$$

We see that for $\lambda < 1$ this solution is complex but its real part is shifted away to values way above the "physical" energy values as λ approaches 1 (figs. 1b, c). For $\lambda = 1$ this solution becomes infinite corresponding to a pole of the propagator at zero (fig. 1d) while for $\lambda > 1$ $E(\boldsymbol{p})$ is real and for $\lambda \gg 1$ again tends towards the physical energy-momentum relation (figs. 1e, f). The value of $\lambda = 1$ appears as the "natural" choice because the unphysical energy state is completely removed but also choices for λ between 0.6 and 1.6 appear reasonable.

5.2. O(a^2) IMPROVEMENT

Also for the O(a^2) *classical* improved fermion action

$$S_{\mathrm{F}}^{\mathrm{CI}_2} = -\frac{a^4}{g_0^2}\sum_{\substack{x \text{ all}\\ \text{lattice sites}}}[O_1^{\mathrm{L}}(x) - \tfrac{1}{6}a^2 O_4^{\mathrm{L}}(x)] \tag{5.7}$$

chiral symmetry has to be broken. Following the same line of argument as in subsect. 5.1 we choose an O(a^2) tree-level on-shell improved action as

$$S_{\mathrm{F}}^{\mathrm{OS}_2} = -\frac{a^4}{g_0^2}\sum_{\substack{x \text{ all}\\ \text{lattice sites}}}[O_1^{\mathrm{L}}(x) - \lambda' a O_2^{\mathrm{L}}(x) - \tfrac{1}{6}a^2 O_4^{\mathrm{L}}(x)], \tag{5.8}$$

yielding the inverse propagator

$$S_{\mathrm{F}}^{-1}(p) = \frac{1}{a}\sum_{\mu}(i\gamma_\mu \sin(p_\mu a)(1+\tfrac{2}{3}\sin^2(\tfrac{1}{2}p_\mu a)) + 4\lambda' \sin^2(\tfrac{1}{2}p_\mu a)). \tag{5.9}$$

However other choices for tree-level on-shell improved actions are possible. The parameter b_2 could be set to zero and chirality breaking can be performed by an "irrelevant" operator of dimension seven. This is exactly what Eguchi and Kawamoto [11] and Wetzel [12] do for their tree-level O(a^2) improved actions. For the chirality breaking term they take a judiciously chosen combination of the two lattice representations of the second derivative namely $D_\mu^{\mathrm{L}} D_\mu^{\mathrm{L}}$ and $(D_\mu^2)^{\mathrm{L}}$ so that in the classical expansion of this operator the leading terms (of dimension five) cancel.

This action yields the inverse propagator

$$S_{\mathrm{F}}^{-1}(p) = 2K\frac{1}{a}\sum_{\mu}(i\gamma_\mu \sin(p_\mu a)(1+\tfrac{2}{3}\sin^2(\tfrac{1}{2}p_\mu a)) + \tfrac{8}{3}r\sin^4(\tfrac{1}{2}p_\mu a)), \tag{5.10}$$

where we have used the same notation as Eguchi and Kawamoto.

As in the case of the $O(a)$ improved action we study the emerging energy states. In this case the poles of the propagator have to be determined numerically (see appendix B for details). As for the action used by Eguchi and Kawamoto with propagator (5.10) qualitatively the same effects arise as for the $O(a^2)$ on-shell improved action (5.8) we shall only discuss the latter. The real parts of the resulting energy states are depicted in fig. 2. The "physical" energy state now has the small-p expansion

$$E^2(p) = p^2 + \tfrac{1}{15}a^4\left((p^2)^3 - \sum_{j=1}^{3} p_j^6\right) + a^6\left[\tfrac{1}{126}\left((p^2)^4 + \sum_{j=1}^{3} p_j^8\right) + \tfrac{1}{144}\lambda'^2\left((p^2)^2 + \sum_{j=1}^{3} p_j^4\right)^2\right] + O(a^8). \quad (5.11)$$

We note that the $O(a^4)$ corrections in (5.11) vanish along the axis. This is why we

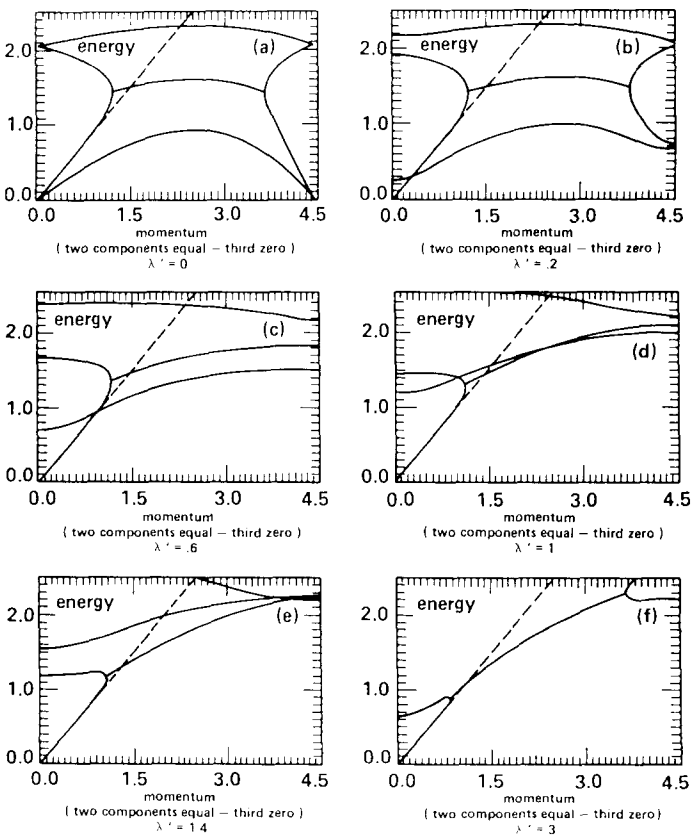

Fig. 2. Energy-momentum relations for the $O(a^2)$ tree-level on-shell improved fermion action (5.8) for values of (a) $\lambda = 0$, (b) $\lambda = 0.2$, (c) $\lambda = 0.6$, (d) $\lambda = 1$, (e) $\lambda = 1.4$, (f) $\lambda = 3$.

have chosen for our figures a momentum configuration with $p_1 = p_2 \neq p_3 \equiv 0$ in order to give a realistic picture of the small-$\boldsymbol{p}$ behaviour of the physical energy states.

We moreover note that after a suitable rescaling of the parameter r (namely $r = \frac{9}{2}\lambda'$) the small-a behaviour of the "physical" energy state arising from the poles of the propagator (5.10) of the action given by Eguchi and Kawamoto coincides up to $O(a^6)$ with that of the $O(a^2)$ on-shell improved action (5.9).

In addition to the "physical" energy state now three "unphysical" energy states appear. For $\lambda' = 0$ one of these "unphysical" states is complex with its real part being smaller than the physical energy value (fig. 2a). It has the small-$\boldsymbol{p}$ expansion

$$[\mathrm{Re}\,(E(\boldsymbol{p}))]^2 = \tfrac{9}{25}\boldsymbol{p}^2 - a^2\tfrac{216}{3125}(\boldsymbol{p}^2)^2 + a^4\left(\tfrac{7857}{390625}(\boldsymbol{p}^2)^3 - \tfrac{3}{125}\sum_{j=1}^{3} p_j^6\right) + O(a^6)\,. \tag{5.12}$$

For $\lambda' \neq 0$ the real part of this state is shifted away from the physical energy values so that the physical energy state eventually becomes the lowest-lying energy state (figs. 2b–d). At the same time as for the $O(a)$ on-shell improved action the additional zeros in the energy-momentum relations for $\boldsymbol{p} \neq 0$ disappear. On the other hand another "unphysical" state is shifted down the y-axis as λ' grows so no "natural" choice of λ' arises (figs. 2e, f). Values of λ' between 1 and 1.4 would however keep these unwanted effects sufficiently far away from the low-energy–low-momentum regime we are interested in.

5.3. SUMMARY

We have found that the concept of on-shell improvement allows for a consistent introduction of the chirality breaking terms needed to avoid the phenomenon of species doubling. For the tree-level on-shell $O(a)$ and $O(a^2)$ improved actions we have found that these additional terms can also be used to keep unwanted "unphysical" energy states away from the low-energy–low-momentum regime where improvement is supposed to work. For the $O(a)$ on-shell improved action this leads to the natural choice of $\lambda = 1$ which does away with the "unphysical" energy states. For the $O(a^2)$ improved action this cannot be accomplished but a reasonable range for the parameter λ' can nevertheless be given.

6. Improvement beyond tree level

According to Symanzik's programme the coefficients of the improved action have a perturbative expansion (in the case of QCD they are power series in the loop counting parameter g_0) and are to be determined by perturbative calculations. The concept of on-shell improvement simplifies the situation as only those coefficients have to be calculated that are not found to be free parameters by means of the isospectral transformation of the action.

Calculations of improvement coefficients to one-loop order have already been performed for the non-linear σ-model [4], the Gross-Neveu model [6], for pure Yang-Mills theory [8] and QCD [11].

For pure Yang-Mills theory a complete treatment following the concept of on-shell improvement will be given by Lüscher and Weisz [19].

In the one-loop calculation for QCD by Eguchi and Kawamoto the corrections to the fermion propagator were calculated. Since they obtain contributions from the operators $O_2^L(x)+O_3^L(x)$, $O_7^L(x)$ but also a small one from $O_5^L(x)$ and $O_6^L(x)$ which would have to be cancelled by special choices of the coefficients of these operators we would suspect that this quantity contains also off-shell parts because according to our investigations no contribution involving the operators $O_5^L(x)$ and $O_6^L(x)$ should occur when spectral quantities are considered.

Here we only present a calculation of the fermion contributions to the gluon self-energy thus extending the work of ref. [8] to the fermion sector to get an idea of its quantitative effects.

This calculation was performed using the tree-level improved action given by Eguchi and Kawamoto. As we wanted to confirm previous numerical results by Ukawa and Yang [15] for the part quadratic in the gluon momentum we used this $O(a^2)$ on-shell tree-level improved action rather than the one given by (5.8).

We write the fermionic part of the gluon self-energy Π_{dd} as (N_f: number of flavours)

$$\Pi_{dd}^f = N_f\left[\left(-\frac{2}{3}\frac{1}{(4\pi)^2}\ln k^2 + a_1\right)k^2 + a_2\sum_\rho k_\rho^4 + (a_3 + a_4 \ln k^2)(k^2)^2 + O(k^6)\right]. \quad (6.1)$$

On-shell improvement demands the absence of $\sum_\rho k_\rho^4 \ln k^2$ terms in (6.1) which we indeed find to be satisfied. Moreover also the coefficient a_4 is zero for this classical improved Wilson action. This is the same for the classical improved Yang-Mills part of the action but is not a consequence of on-shell improvement. This has been pointed out by Lüscher and Weisz in ref. [14]. Their argument also holds for the fermionic contribution to the gluon self-energy. On-shell improvement only demands improvement of the static potential $V(L)$. For the Fourier transformed static potential $V(k)$ this only means the absence of $\sum_\rho k_\rho^4 \ln k^2/(k^2)^2$ terms because only they are the origin of $a^2 \ln L/L^3$ contributions to $V(L)$ whereas terms like $\ln k^2$ only give rise to a^2/L^3 terms in $V(L)$. Considering the contribution of (6.1) to the static potential

$$V(k)^f = (\Pi_{dd}^f D_{dd}^2)|_{k_4=0} \approx \frac{1}{(\boldsymbol{k}^2)^2}\left[1 + 2(c_1 + \tfrac{1}{12})\frac{\sum_{\rho=1}^3 k_\rho^4}{\boldsymbol{k}^2} - 2(c_2 + c_3)\boldsymbol{k}^2\right]\Pi_{dd}^f, \quad (6.2)$$

where $\boldsymbol{k} = k|_{k_4=0}$, D_{dd} is the improved gluon propagator, one immediately verifies that only potential $\sum_\rho k_\rho^4 \ln k^2$ terms in (6.1) yield $a^2 \ln L/L^3$ contributions to $V(L)$

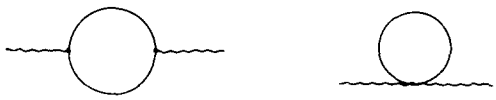

Fig. 3. Diagrams for the fermion contributions to the gluon self-energy.

as long as the tree-level improvement condition $c_1 = -\frac{1}{12}$ for the Yang-Mills part of the action holds.

To extract values for the coefficients a_i in (6.1) we evaluated the gluon self-energy contributions depicted in fig. 3 numerically to high precision. We first considered a configuration with only one component of the gluon momentum non-vanishing for lattice momenta ranging between 0.01 and 0.1. By repeating this calculation taking two components of the gluon momentum non-zero and fitting a behaviour of the form (6.1) to the data we were then able to separate $(k^2)^2$ and $\sum_\rho k_\rho^4$ contributions especially verifying the absence of $\sum_\rho k_\rho^4 \ln k^2$ terms. We did this for the three values of $r = 0.5$, 1 and 1.5 also chosen by Ukawa and Yang in [15] for their computations. We found the following results:

$$a_1 = \begin{cases} 0.0387357(2), & r = 0.5, \\ 0.02702288(3), & r = 1, \\ 0.0247816(1), & r = 1.5, \end{cases} \tag{6.3}$$

$$a_2 = \begin{cases} -0.00284(17), & r = 0.5, \\ -0.00086(5), & r = 1, \\ -0.00043(14), & r = 1.5, \end{cases} \tag{6.4}$$

$$a_3 = \begin{cases} -0.00057(9), & r = 0.5, \\ -0.00080(4), & r = 1, \\ -0.00174(9), & r = 1.5, \end{cases} \tag{6.5}$$

$$a_4 = 0, \qquad r = 0.5, 1, 1.5. \tag{6.6}$$

To compare our results (6.3) with those by Ukawa and Yang given in ref. [15] for their coefficients

$$c_F = 2b_0 \ln \frac{\Lambda^F_{\text{Improved}}}{\Lambda^F_{\text{Wilson}}},$$

$$b_0 = \frac{1}{(4\pi)^2}\left(\tfrac{11}{3}N - \tfrac{2}{3}N_f\right) \quad (N = \text{number of colours}),$$

we note the relation

$$c_F = N_f\left(a_1 + \frac{1}{(4\pi)^2}\left(\tfrac{2}{3}(\gamma_E - \ln 4\pi) - \tfrac{10}{9}\right) + \tfrac{1}{2}\mathscr{L}\right). \tag{6.7}$$

Here γ_E denotes Euler's constant $\gamma_E = 0.577215664\ldots$ and the constants $\mathscr{L}$ have been calculated by Kawai, Nakayama and Seo [20].

For the values of r chosen here they are

$$\mathscr{L} = \begin{cases} -0.02384\,, & r = 0.5\,, \\ 0.003107\,, & r = 1\,, \\ 0.01293\,, & r = 1.5\,, \end{cases} \tag{6.8}$$

so we obtain

$$c_{\mathrm{F}} = N_f \begin{cases} 0.01153 & (0.01152\,(2))\,, \quad r = 0.5\,, \\ 0.01329 & (0.01330\,(2))\,, \quad r = 1\,, \\ 0.01596 & (0.01596\,(2))\,, \quad r = 1.5\,, \end{cases} \tag{6.9}$$

the values in brackets are those given in ref. [15]. The number of digits quoted for our results are limited by the accuracy of the constants $\mathscr{L}(r)$ in ref. [20].

If we insert these results into the revised data for the Yang-Mills sector [8] (where $NN_f a_2$ (N = number of colours) and $NN_f a_3$ would have to be subtracted from the right-hand side of eqs. (4.34) and (4.33) of ref. [8] respectively) we find that the contributions from both sectors are of the same order of magnitude.

7. Conclusions

The concept of on-shell improvement has been found to be useful not only in the context of pure Yang-Mills theory but also for full QCD with Wilson fermions. It reduces the number of coefficients in the improved action whose perturbative expansions have to be calculated. Moreover it allows a somewhat "natural" incorporation of chirality breaking terms into the lagrangian needed to avoid the problem of species doubling.

Although the construction of an on-shell improved action removing in addition to the $\mathrm{O}(a)$ also the $\mathrm{O}(a^2)$ lattice artifacts in spectral quantities can be performed we do not see any possibility to exclude the arising fermion contact terms beyond tree level.

It should therefore be favourable to constrain improvement to $\mathrm{O}(a)$ on-shell improvement. Then the fermion part of the action is drastically simplified. The result is a slightly modified Wilson fermion action which still can be formulated with only nearest-neighbour fermion interactions:

$$\begin{aligned} S_{\mathrm{L}}^{\mathrm{O}(a)\ \text{improved}} = \frac{a^4}{g_0^2} \sum_{\substack{x\ \text{all} \\ \text{lattice sites}}} \frac{1}{2a} \Big\{ & -2[m(m_{\mathrm{R}}, g_0^2, a)a + d]\bar{\psi}(x)\psi(x) \\ & + \sum_{\mu} \bar{\psi}(x)[(1-\gamma_\mu)U_\mu(x)\psi(x+\hat{\mu}) + (1+\gamma_\mu)U_\mu^\dagger(x-\hat{\mu})\psi(x-\hat{\mu})] \\ & - \tfrac{1}{2} ic(g_0^2) \sum_{\mu,\nu} \bar{\psi}(x)\sigma_{\mu\nu}P_{\mu\nu}(x)\psi(x) \Big\}\,, \end{aligned} \tag{7.1}$$

$$c(g_0^2) = 1 + O(g_0^2)\,, \tag{7.2}$$

$$m(m_R, 0, a) = m_R(1 + \tfrac{1}{2} m_R a + O(a^2))\,. \tag{7.3}$$

Here $P_{\mu\nu}(x)$ is the operator given in (2.9) but any other lattice representation of $F_{\mu\nu}(x)$ can be chosen for convenience. The mass parameter is a function of the renormalized quark mass m_R, the bare coupling g_0 and the lattice spacing a. The new constant $c(g_0^2)$ has been introduced for $2(b_3(g_0^2) - b_2(g_0^2)) = 1 + 2b_3(g_0^2)$.

For the Yang-Mills part of the action the standard one-plaquette Wilson action can be used. This action should therefore be the improved action for lattice QCD most suitable for numerical calculations. Moreover the $O(a)$ chirality breaking term is one of the most disturbing lattice artifacts and its absence can be expected to produce considerably improved behaviour of the lattice simulation.

The discussion of the spectrum gives hints for a suitable choice of the parameters of the chirality breaking terms in the tree-level improved actions. Besides the well-known additional zeros in the energy-momentum relation at the edges of the Brillouin zone for lattice fermion lagrangians with chiral symmetry we also observed low-lying even complex energy states which have to be shifted away from the physical states by "finetuning" the parameters of the chirality breaking terms. For the $O(a)$ on-shell tree improved action this leads to the "natural" choice of $\lambda = 1$. This corresponds to the value of λ originally chosen by Wilson. For the $O(a^2)$ on-shell tree-level improved action no natural choice of the parameter λ' exists however values of λ' between 1 and 1.4 appear reasonable.

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Appendix A

Here we study the contributions to the action arising from the variation of the measure under the fermion part of the transformation T_1 in (4.3) and the transformations T_2 in (4.4).

In a concise notation the action on the lattice has the form

$$S_L = \sum_{\substack{x \text{ all} \\ \text{lattice sites}}} [\bar{\psi} h_x(U) \psi + \operatorname{Tr} f_x(U)]\,. \tag{A.1}$$

The action is a polynomial in the quark variables $\bar{\psi}_{if\alpha}(x)$ and $\psi_{if\alpha}(x)$ and the gluon fields $A_\mu^a(x)$ where i, f and α indicate N_c colour, N_f flavour and 4-spinor indices. The path integral is defined as

$$\int D\bar{\psi} D\psi DU \exp[-S_L[\bar{\psi}, \psi, U]]\,, \tag{A.2}$$

where

$$D\bar{\psi} = \prod_{x,i,f,\alpha} d\bar{\psi}_{if\alpha}(x),$$

$$D\psi = \prod_{x,i,f,\alpha} d\psi_{if\alpha}(x),$$

$$DU = \prod_{x,\mu} dU_\mu(x), \tag{A.3}$$

is the invariant Haar measure on $SU(N_c)$.

We first study the transformation T_1. The effect of the gauge part of T_1 has been studied in ref. [14]. When considering the transformation of the gauge field it is obvious to use the properties of the Haar measure for which the following relation holds:

$$\int dU F(U) = \int dU F(U_0 U), \tag{A.4}$$

where U_0 is an arbitrary but fixed group element. We choose $U_0 = \exp(\varepsilon'^a t^a)$ where ε'^a is an infinitesimal real number and the t^a are the generators of the group $SU(N_c)$. Then it is easy to see that if

$$\int dU_\mu(x) \exp[\bar{\psi} h_x(U_0 U_\mu(x))\psi + \mathrm{Tr} f_x(U_0 U_\mu(x))]$$

$$= \int dU_\mu(x) \exp[\bar{\psi} h_x(U_\mu(x))\psi + \mathrm{Tr} f_x(U_\mu(x))] \tag{A.5}$$

to first order in ε'^a the following relation must hold:

$$Q^a(\bar{\psi}, \psi) = \int dU_\mu(x) \exp[\bar{\psi} h_x(U_\mu(x))\psi + \mathrm{Tr} f_x(U_\mu(x))]$$

$$\times \left[\bar{\psi} t^a U_\mu(x) \frac{\partial h_x(U_\mu(x))}{\partial U_\mu(x)} \psi + \mathrm{Tr}\, t^a U_\mu(x) \frac{\partial f_x(U_\mu(x))}{\partial U_\mu(x)} \right] = 0. \tag{A.6}$$

If we now set

$$U_0(x) = \exp(a^3 \varepsilon'(\bar{\psi}_i(x) \gamma_\mu t^a_{ij} \psi_j(x)) t^a), \tag{A.7}$$

it is not *a priori* clear that this argument applies since Grassmann variables are involved and $U_0(x)$ is not an element of the group. But when we insert (A.7) into the path integral (A.2) we immediately verify that to first order in ε' we have

$$\int d\bar{\psi}(x)\, d\psi(x)\, dU_\mu(x) \exp[\bar{\psi} h_x(U_0(x) U_\mu(x))\psi + \mathrm{Tr} f_x(U_0(x) U_\mu(x))]$$

$$= \int d\bar{\psi}(x)\, d\psi(x)\, dU_\mu(x) \exp[\bar{\psi} h_x(U_\mu(x))\psi + \mathrm{Tr} f_x(U_\mu(x))]$$

$$+ a^3 \varepsilon' \int d\bar{\psi}(x)\, d\psi(x) (\bar{\psi}(x) \gamma_\mu t^a \psi(x)) Q^a(\bar{\psi}, \psi). \tag{A.8}$$

From (A.6) we see that the second term on the right-hand side of this equation vanishes. So we come to the conclusion that the functional integral (A.2) is invariant under the transformation (A.7).

Now we consider the transformation T_2. Using the lattice derivatives given in (2.7) we find (writing $\psi(x) = \psi_x$)

$$\psi_x = (\mathbb{1} + \boldsymbol{M})_{xy}\psi_y , \tag{A.9}$$

where the $(N_s \times N_s)$ matrix $\boldsymbol{M}$ (with entries $\boldsymbol{M}_{xy}$) is given by

$$\begin{aligned}\boldsymbol{M}_{xy} = [\, & a\varepsilon_1 \gamma_\mu (U_\mu(x)\delta_{(x+\hat{\mu})y} - U_\mu^\dagger(y)\delta_{(x-\hat{\mu})y}) \\ & + a^2\varepsilon_2 (U_\mu(x)\delta_{(x+\hat{\mu})y} + U_\mu^\dagger(y)\delta_{(x-\hat{\mu})y} - 2\delta_{xy}) \\ & + a^2\gamma_\mu\gamma_\nu\varepsilon_3 (U_\mu(x)U_\nu(x+\hat{\mu})\delta_{(x+\hat{\mu}+\hat{\nu})y} - U_\mu(x)U_\nu^\dagger(y)\delta_{(x+\hat{\mu}-\hat{\nu})y} \\ & - U_\mu^\dagger(x-\hat{\mu})U_\nu(x-\hat{\mu})\delta_{(x-\hat{\mu}+\hat{\nu})y} + U_\mu^\dagger(x-\hat{\mu})U_\nu^\dagger(y)\delta_{(x-\hat{\mu}-\hat{\nu})y})] . \end{aligned} \tag{A.10}$$

Using $\det \boldsymbol{A} = \exp \operatorname{Tr} \ln \boldsymbol{A}$ we find to first order in the infinitesimal parameters ε_i

$$\det(\mathbb{1} + \boldsymbol{M}) = 1 - 8N_c N_f N_S a^2 \varepsilon_2 . \tag{A.11}$$

As Grassmann variables are considered this contributes a factor $\det(\mathbb{1} + \boldsymbol{M})^{-1}$ which however only effects the normalisation of the measure and therefore can be neglected. In complete analogy we can conclude that the transformation of $\bar{\psi}(x)$ does not effect the measure to leading order.

Appendix B

In the case of the action (5.3) for the O(a) tree-level on-shell improved fermion action the task of finding the poles of the propagator (5.4) inside the unit circle can be done analytically.

Denoting (with $a = 1$ for convenience)

$$\begin{aligned} R_1(\boldsymbol{p}) &= 1 + \sum_{j=1}^{3} (1 - \cos^2 p_j) \geqslant 1 , \quad \boldsymbol{p} = (p_1, p_2, p_3) , \\ R_2(\boldsymbol{p}) &= 1 + \sum_{j=1}^{3} (1 - \cos p_j) \geqslant 1 , \end{aligned} \tag{B.1}$$

we have to find the roots of the polynomial

$$\begin{aligned} P(z) &= \sum_{\nu=0}^{2} a_\nu (z^{2+\nu} + z^{2-\nu}) , \\ a_0 &= \lambda^2 - 1 + 2R_1(\boldsymbol{p}) + 2\lambda^2 R_2^2(\boldsymbol{p}) , \\ a_1 &= -4\lambda^2 R_2(\boldsymbol{p}) , \qquad a_2 = \lambda^2 - 1 . \end{aligned} \tag{B.2}$$

We shall constrain ourselves to $\lambda \geqslant 0$ because all formulae depend only on $|\lambda|$. For

$\lambda^2 \neq 1$ we find with

$$a(p) = \frac{\lambda^2}{\lambda^2 - 1} R_2(p) ,$$

$$b(p) = \sqrt{\left(\frac{R_2(p)\lambda}{\lambda^2 - 1}\right)^2 - \frac{R_1(p)}{\lambda^2 - 1}} , \tag{B.3}$$

$$c^{\pm}(p) = a(p) \pm b(p) ,$$

the roots

$$z_{1,2} = c^{+}(p) \pm \sqrt{c^{+}(p)^2 - 1} ,$$

$$z_{3,4} = c^{-}(p) \pm \sqrt{c^{-}(p)^2 - 1} , \tag{B.4}$$

while for $\lambda^2 = 1$ the degree of the polynomial in (B.2) is reduced by one order now yielding the roots

$$z_0(p) = 0 , \qquad z_{1,2}(p) = a'(p) \pm \sqrt{a'(p)^2 - 1} , \tag{B.5}$$

where

$$a'(p) = \frac{R_1(p) + R_2^2(p)}{2R_2(p)} . \tag{B.6}$$

For all values of λ the "physical" energy state is $E(p)^{\text{physical}} = -\ln z_2(p)$ yielding the small-p expansion (5.5). For $\lambda < 0$ the "unphysical" energy state is given by $-\ln z_3(p)$ which is complex due to the fact that $z_3(p) < 0$. While for $\lambda = 1$ there is no "unphysical" energy state it is given by $-\ln z_4(p)$ for $\lambda > 1$ taking real values. For $\lambda \neq 0$ this "unphysical" state has the small-p expansion given by (5.6).

In the case of the $O(a^2)$ tree-level on-shell improved fermion action (5.8) the poles of the propagator (5.9) can in general only be determined numerically. If we denote by

$$R_1(p) = \sum_{j=1}^{3} \sin^2 p_j (1 + \tfrac{2}{3} \sin^2 \tfrac{1}{2} p_j)^2 ,$$

$$R_2(p) = 2 \sum_{j=1}^{3} \sin^2 \tfrac{1}{2} p_j , \tag{B.7}$$

the roots of the polynomial

$$P(z) = \sum_{\nu=0}^{4} a_\nu (z^{4+\nu} + z^{4-\nu}) ,$$

$$a_0 = -(216\lambda^2 (2R_2^2(p) + 4R_2(p) + 3) + 72R_1(p) + 65) ,$$

$$a_1 = 16(54\lambda^2 (R_2(p) + 1) + 1) , \qquad a_2 = -8(27\lambda^2 - 8) ,$$

$$a_3 = -16 , \qquad a_4 = 1 , \tag{B.8}$$

have to be found.

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