Flavours of Gauge Theories

Proefschrift

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An overview is given of flavour dynamics, with particular emphasis on the relevance of introducing dynamical flavours on the lattice. The importance of going beyond the inclusion of the lightest quarks, up and down, for phenomenology is stressed. Beyond QCD phenomenology, the Banks-Zaks fixed point and the concept of the conformal window are introduced. Both analytical and numerical results are presented for the determination of its lower bound, for quarks both in the fundamental and higher dimensional representations. This introduction is intended to provide context to the results of lattice studies of theories with a varying number of flavours, presented in the remainder of this thesis. At the end of this chapter, a concise overview of the content of this thesis will be given.
Quantum chromodynamics currently stands undisputed as the correct description of the strong interaction. The theory describes six flavours of elementary fermions, fundamentally charged under SU(3). Coupling to these charges are gauge bosons in the adjoint representation of the group, themselves charged under the gauge group. Phenomena such as confinement and parton scaling are very naturally explained in the framework of an SU(3) gauge theory, at least at a qualitative level. Quantitative predictions have been problematic, due to a crucial difference between the strong interaction and Abelian gauge theories such as quantum electrodynamics: Accurate phenomenological predictions cannot be derived from a perturbative expansion in the gauge coupling. Due to the running of the coupling constant, infrared observables coming from QCD are essentially non-perturbative and the historically very effective analytical arsenal developed for QED has to be expanded. A great number of creative approaches have been introduced over the course of the past 40 years. These usually tend to do particularly well for specific aspects of the theory, but falter for others.

The position that lattice field theory, and in particular lattice QCD, has in this set of approaches is exceptional. It takes the field equations underpinning the modern understanding of the strong interactions (QCD) and reformulates it in terms of the fundamental degrees of freedom on a finite size lattice of discretised space-time. Written in this form, the path integrals become accessible to numerical techniques. The smallest distance defined in the system is referred to as the lattice spacing and is usually written as $a$. In the limit of vanishing $a$ and infinite volume, the lattice and continuum formulation of QCD are identical. Away from that limit, any deviations from the continuum formulation are functions of the ultraviolet (the lattice spacing) and infrared (the finite volume of the lattice) regulators. The characteristic properties of QCD, asymptotic freedom and confinement, should guarantee a smooth convergence to the continuum limit. In this way, one has obtained a fully controlled approximation to QCD calculations from first principles. Rephrasing that: Arbitrarily accurate results can in principle be calculated, given enough computational resources.

A peculiar situation now arises. The complicated dynamics of the non-Abelian gauge field and its inherent non-perturbative properties are the main reason for invoking a numerical treatment. Integrating over the gauge fields in the path integral does in fact represent the bulk of the computational intensity. However, from an algorithmic point of view, it is not the non-perturbative gauge interaction that poses issues. Once the perturbative formulation of QCD in terms of generators of SU(3) is abandoned, the full gauge theory is naturally described on the lattice. It is the fermions, rather, that are problematic. Their fractional canonical dimension means there is no natural discretisation of quark fields. In addition, the fermion determinant occurring in the partition function can be exceedingly expensive to calculate; a cost that increases sharply as the mass decreases.

The complications of including fermions in numerical calculations have, for a long time, effectively forced physicists to opt for a lattice formulation that neglects the contribution of dynamical quarks to the vacuum. This approximation, known as quenched, tends to work surprisingly well for various quantities, as we will see
below. Of course, ignoring the effects of quarks on dynamics introduces a systematic error that limits precision on measurements. As both the quality and application of results from lattice calculations increased, these systematically biased results became less acceptable. Certain observables will be affected by quenching in particular, necessitating the inclusion of dynamical fermions in simulations to obtain any serious estimate at all. It is for this reason that all recent large scale simulations include at least two dynamical quark flavours. One can go further, though, and ask the question of principle. What happens when the fermion sector is enlarged up to the point that its effects become dominant?

In this thesis, we shall examine this question. This chapter will start out by focusing on those fermionic degrees of freedom that are relevant to the phenomenology of the Standard Model in section 1.1. We will discuss the quenched approximation, how it breaks down and in what way it can be connected to the full theory of QCD as contained in the Standard Model. Section 1.2 turns to questions on the physics of flavoured gauge theories that are relevant to physics beyond the Standard Model, focusing on the potential appearance of a so-called conformal phase transition. We describe the phase diagram of SU(3) Yang-Mills theories with a varying number of flavours and explain why a new phase would be expected to occur. The remainder of this chapter will discuss existing literature on this topic and present a general outline of the thesis.

1.1 Quarks and gluons

In its most general form, the partition function of QCD is written as

$$Z = \int DA_R \det[M]^{N_f} \exp \left[ -\frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a \right].$$  (1.1)

The determinant of the Dirac operator $M$ contains the full fermionic contribution to this partition function. It is a highly non-local object and consequently very computationally intensive. The quenched approximation mentioned earlier consists of the sweeping replacement $\det[M] \equiv 1$, which effectively removes all internal quark lines from the theory. Justification of its application in early lattice studies was based on some hand-waving arguments, but mainly on necessity of curbing the excessive costs of including dynamical fermions using algorithms available in the early eighties. Still, pure gauge theory would seem to exhibit all the crucial features of QCD. Analytical indications of confinement in Yang-Mills [1] were confirmed by numerical studies [2]. Pure SU(3) gauge theory on the lattice reproduces asymptotic freedom below a scale of $\Lambda_{\text{MOM}} = 170(50)$ MeV when converted to a perturbative regularization scheme [3]. Reasonable results could be obtained for fermionic observables as well, using both pure SU(2) and SU(3) Yang-Mills, though a non-physical $\eta-\pi$ degeneracy was found that would be broken only in the presence of internal quark loops. Notably, simulations did reproduce spontaneous chiral symmetry breaking and the hadronic spectrum showed acceptable agreement with phenomenology [4, 5]. Reports on small scale simulations implementing fermions as dynamical degrees of freedom were published early on [6–8]. But the limitations on volume and lattice
spacing imposed by the inclusion of the expensive fermion determinant were severe. Consequently, a large body of quenched results was compiled by the lattice community, a summary of which can be found in e.g. [9].

Even if the approximation appeared to work in practice, an uncontrolled source of systematic error had been introduced into the theory by quenching. An analytical study of the effects of quenching was made possible by development of a consistent quenched formulation of chiral perturbation theory [10–13], including ghost fields to cancel the contributions of the internal quark lines. The main impact of quenching turned out to rest on contributions from $\eta'$ towards the chiral limit. The physical $\eta'$ develops a large mass, because the anomaly in the singlet axial current [14,15] causes it to receive topological corrections. Figure 1.1 shows the first diagrams in an infinite series leading to the $\eta'$ propagator resummation

$$\sum_{n=0}^{\infty} \frac{1}{p^2 - m_{\pi}^2} \left( \frac{M^2}{p^2 - m_{\pi}^2} \right)^n = \frac{1}{p^2 - m_{\pi}^2 - M^2}. \quad (1.2)$$

The effective mass scale $M^2$ is being generated by instanton contributions according to [16–18]

$$M^2 = \frac{2N_f \chi_t}{f_{\pi}^2} = m_{\eta'}^2 + m_{\eta}^2 - 2m_{\pi}^2, \quad (1.3)$$

with $\chi_t$ representing the topological susceptibility.

Quenching erases contributions starting at diagram C in figure 1.1, since they contain sea quark contributions. Equation 1.2 is then truncated after $n = 1$, so the pole mass $m_{\pi}^2 + M^2$ is never generated. Instead, we have a single and a double pole

\[ \begin{align*}
A & \quad + \\
C & \quad + \\
D & \quad + \cdots
\end{align*} \]

Figure 1.1 Corrections to the $\eta'$ propagator from vacuum polarization diagrams in QCD. Quenching removes all diagrams starting from C, leaving $\eta'$ as an additional Goldstone boson in the limit $m \to 0$.

in the $\eta'$ propagator, with the particle becoming a Goldstone boson along with the pions as we approach the chiral limit. The regular logarithmic terms that are relevant at small quark masses in chiral perturbation theory [19,20] vanish for SU(3) in the absence of internal quark loops [21]. In their place come hairpin contributions from the now light $\eta'$, that can be constructed out of valence quark lines [11]. This means the low energy constants of quenched chiral perturbation theory are all modified, the effects of which show up already at relatively heavy quark masses [22].
1.1 Quarks and gluons

Whereas initial estimates seemed to indicate differences on most observables would be small [11], effects on particular measurements were found to be sizeable fractions of the result [13, 23]. Particularly damning, however, was the divergence of the logarithmic corrections coming from the $\eta'$ in the chiral limit. Those divergences are due to the double pole coming from the second term in equation 1.2 and signal the lack of unitarity of the theory. Since they will dominate the light mass regime, they completely foreclose the approach of the light quark limit – the quenched theory does not exist in the chiral limit [23]. Initial attempts at controlling the theory by resumming offending diagrams or redefining the quark mass [10, 24] were fruitless. While the double pole chiral logarithm could be largely absorbed in the low energy constants and thereby renormalised [25], essential divergences remained a prominent feature of a quenched theory in the chiral limit. The influence of quenching is most destructive in the determination of weak matrix elements. In the amplitude of important processes as $K^0 \rightarrow \pi^+\pi^-$ and $K^0 \rightarrow$ vacuum, quenching artefacts appear at leading order and are unconstrained [26–28]. This makes the quenched determination of fundamental weak quantities little more than an educated guess in certain cases.

The gradual switch to simulations using dynamical fermions was certainly motivated by the inherent limits on the precision and scope of quenched simulations described above. Another main component in the decision to extend simulations was also the growing feasibility of dynamical simulations allowed by massive technological improvements. There was obviously the hardware technology that outperformed Moore’s law during the eighties and nineties, but even more important were the algorithmic improvements over this period. Early estimates were that the computational burden was of the order of a petaflop-year [8] for such a simulation. Thanks to theoretical and algorithmic developments developments, fully dynamical simulations started appearing at costs less than a teraflop-year instead [29]. The understanding of the detailed behaviour of the theory led to the formulation of partial quenching approaches: strategies to make physical predictions while working in an otherwise non-physical space of parameters. By exploiting the freedom of varying fermions masses and flavours away from the physical point, one can extract physical results without the costly step of reaching physical sea quark masses.

Nowadays, large scale simulations with dynamical fermions at zero temperature are considered something of a benchmark of lattice QCD throughout the wider particle physics community. With the rising requirements on computing resources, a number of collaborations have been formed that tackle the costly Monte Carlo simulations collectively. With each fermion formulation having its particular strengths and drawbacks, these collaborations have typically chosen a specific formulation that suits their research goals particularly well. This fragmentation can complicate the interpretation of results obtained by different groups, but does have the fortunate consequence of allowing for independent checks on systematics. It would not be feasible to provide anything like a complete overview of the activities in this field, but the annual status reports presented at the Lattice conferences give an excellent impression of the different approaches [29, 30].

At the moment, the biggest challenge perhaps lies in reaching physical quark masses for the light $u$ and $d$ pair, but the remarkable results of [31] are likely to be
only the first of a new generation of simulations around the physical point. Note that physical light quark masses, which will remain an expensive affair, need not be a goal in and of itself. As long as simulations are sufficiently deep into the chiral regime for chiral perturbation theory extrapolations to be reliable, one can always settle for more efficient simulations at higher quark mass and extrapolate to the physical point. For what values of the quark masses that point is reached, depends upon the observable. The radius of convergence for the chiral expansion is rather large for the pion sector, but need not be so for other observables and in these cases, there may be few alternatives to brute forcing the mass dependence.

The results presented in chapter 2 have been obtained within this context by the European Twisted Mass Collaboration (ETMC). Here the particular variation of Wilson fermions known as twisted mass fermions is adopted. In the twisted mass formulation, a $\gamma^5$-twisted mass term is added to the standard, unimproved Wilson-Dirac operator, and the formulation becomes especially interesting when the theory is tuned to maximal twist [32]. The major advantage of the lattice theory tuned to maximal twist is the automatic $O(a)$ improvement of physical observables, independently of the specific type of operator considered, implying that no additional, operator specific improvement coefficients need to be computed. It is not yet computationally feasible to obtain these simulations at the physical point, but chapter 2 presents fits that demonstrate the reliability of the chiral extrapolation. The novelty of these results, however, lies in the presence of four distinct dynamical quark flavours.

To understand the relevance of this, one should first attempt to answer a more general question, that becomes important once one abandons the quenched approximation and decides to introduce dynamical quark flavours. Namely, how many flavours of quarks does one need to obtain physically accurate results? The most serious quenching artefacts relate to the approach of the chiral limit. Those are remedied effectively by the inclusion of light degrees of freedom. As to what constitutes those light quarks, physical intuition can guide us to some extent. QCD dynamically generates the scale $\Lambda_{\text{QCD}} \approx 200$ MeV, providing a natural cut-off on momenta relevant to the dynamics of gauge fields. The masses of the $b$ and $t$ quarks, coming in at about 4.2 GeV and 170 GeV, respectively [37], are far above this scale. Not only will their high mass suppress their occurrence in virtual quark loops, their coupling to QCD will be weak as the theory is highly perturbative at those energies. This freezes them effectively out of QCD dynamics at low energies, with residual contributions being readily absorbed in the matching of parameters to phenomenology. The situation is clearly opposite for the lightest $u$ and $d$ quarks, which weigh in at a meagre 2.5 MeV and 5 MeV, respectively [37]. Approaching the chiral limit as they are, the breakdown of the quenched approximation warrants their inclusion.

With the $s$ and $c$ quarks, a grey region is entered. The former is estimated to weigh about 80 MeV and would still be considered dynamical, but its isospin partner comes in an order of magnitude heavier, at 1.3 GeV [37]. Most modern large scale lattice QCD studies have therefore opted to include the strange as a dynamical flavour. Some collaborations have chosen to simulate at $N_f = 2$ for pragmatic reasons and comparison of results from $N_f = 2$ and $N_f = 2 + 1$ (as in [38,39], for example),
1.1 Quarks and gluons

Figure 1.2 A diagram of the flow of the unified effective field theory description of the weak and strong interactions, illustrating the hierarchy of scales in the theory. By applying operator product expansion [33, 34] and renormalisation group [35] techniques to the full standard model Lagrangian, one can systematically lower the energy scale and ‘integrate out’ the heavier particles. Successively, this will remove the top quark, the weak gauge bosons, the bottom quark and the charm quark. At this point, one reaches the chiral symmetry breaking scale $\Lambda_\chi$, at which the non-perturbative matching of chiral perturbation theory with QCD is performed. $N_f$ is the number of active flavours in a given theory. This diagram has been reproduced from [36].

shows that the quenching of the heavier quarks is in fact not the leading source of systematical errors, at least for the observables explored until now. One can therefore legitimately pose the question, if the effort of including the heavier flavours is a worthwhile investment.

A systematic answer to this question can be formulated by interpreting the quenching of quark flavours within the framework of formal effective field theory. Let us, following the approach of e.g. [36, 40], consider the separate flavours of quarks components of the larger unified description of weak and strong interactions. Then the reduction of that full description to the various effective field theories by means of renormalisation group flow and operator product expansion will naturally lead to
Introduction

the removal of heavier quarks as dynamical degrees of freedom. Their influence
becomes embedded, instead, in the effective theory at low energies in the form of
contact term operators and adjusted coefficients. The values of these coefficients can
be obtained through matching the high and low energy descriptions at each thresh-
old. The set of physical phenomena described by these effective field theories will be
restricted. Processes at energies above the scale of integration are not captured accu-
rately any longer. For those below that scale, the new operators will be suppressed
by powers of the integration scale and the particle masses.

Quenching, as in the complete neglecting of quantum corrections induced by
a particular flavour degree of freedom, could be interpreted as a rough approxi-
mation of this procedure. Its impact depends on the particular observables that
are investigated. To capture chiral dynamics, the typical scale of which is roughly
\( \Lambda_\chi = 4\pi f_\pi \simeq 1\text{GeV} \), the inclusion of the three lightest quarks – and in particular the
two lightest ones – as dynamical flavours is necessary. They cannot be integrated out
in the effective description, as they are dynamical well below \( \Lambda_\chi \). It is the neglect-
ing of these contributions that is typically referred to as quenching. The ignoring of
the charm and other heavier quarks amounts to the removal of additional operators
that are suppressed by powers of \( \Lambda_\chi \) and \( m_c \). Those corrections will typically be
minor for processes described within the framework of SU(2) and SU(3) chiral per-
turbation theory. But by that same reasoning, deviations should become apparent
for those processes that cannot be adequately captured by chiral perturbation theory
itself.

One field where the inclusion of the heavier quarks is highly relevant is the study
of finite temperature QCD phenomenology. An example is the chiral phase transi-
tion of QCD, which is an important process in the evolution of the universe. Lattice
results found the order of this phase transition depends on the number of quark
flavours and their masses. It should be first order for \( N_f \geq 3 \) \cite{41}, while a sec-
ond order transition appears for a two quark system \cite{42}. Since the physical case
calls in between these limits, a fully dynamical simulation is needed to resolve this
issue. The most recent results \cite{43} indicate the physical transition has, in fact, a
crossover nature. Weak interactions in particular are sensitive to the effects of heav-
ier flavours \cite{44}, and their presence as dynamical degrees of freedom is necessary
for obtaining accurate results. The ground for these effects lies in the GIM mecha-
nism \cite{45}, that generates flavour changing neutral currents in the Standard Model
proportional to the breaking of quark mass degeneracy. The mechanism depends
upon the inclusion of internal quark propagators and will therefore not function in
a partially quenched setup. Analysis based on partially quenched perturbation the-
ory \cite{46, 47} shows that the introduction of a dynamical charm is needed to reduce
quenching ambiguities in phenomenological predictions based on the GIM mecha-
nism. These would include the so-called \( \Delta I = 1/2 \) rule \cite{48}: The observation that
weak non-leptonic kaon decays much prefer the channel where the change in isospin
is 1/2 over the channel with a change of 3/2. The charm quark is not present as a
valence quark in \( K \rightarrow \pi\pi \), so the effect here would not usually be described as
quenching artefact. But the effects of charmed sea quarks on this process are not
negligible. The absence of the additional operators that distinguish three flavour
from four flavour simulations of the weak matrix elements might leave its mark on the results. A dynamical charm will remove all such ambiguities for weak observables. [46, 47]. With the lattice becoming an increasingly important tool in the calculation of elements of the CKM matrix [49], it will become crucial to account for flavour physics beyond chiral corrections.

In short, the increasing precision of lattice field theory and its ambition to contribute to the quantitative understanding of the Standard Model mandate the introduction of additional quark flavours. This is the motivation behind the ETMC’s efforts to introduce a dynamical third and fourth quark to the conventional $N_f = 2$ twisted mass setup. Another pioneering effort, using the highly improved staggered quark (HISQ) action [50], has been initiated by the MIMD Lattice Computation (MILC) collaboration, who have published some preliminary results [51–54]. These two projects are the first, and currently the only attempts to include a dynamical charm quark within lattice calculations, making the ETMC simulations unique in introducing a charm quark of the Wilson type. Further details can be found in chapter 2.

1.2 Phase diagram of flavoured theories

Beyond precision spectroscopy and phenomenology, we can ask a more general question as to the effects on gauge theories of the presence of fermions. Those issues are best framed in the context of lattice thermodynamics and the phases of gauge theories. Figure 1.3 gives an impression of the phase diagram of QCD, somewhat uncommonly projected onto the axes of temperature and number of massless flavours. Most research on lattice QCD can be said to focus on two regions within this diagram. A first focal point is the study of QCD at zero temperature referred to at the end of section 1.1, which would also cover the content of chapter 2. The physical theory of QCD does not, of course, lie in the projection plane used in figure 1.3. The presence of a quark mass hierarchy does not allow for a simple classification of the theory in terms of a single value $N_f$. Nevertheless, as was stressed above, the physical theory is fairly well approximated by an effective field theory having two dynamical quarks that are close to the chiral limit. We can therefore position the theory around $(T, N_f) = (0, 2)$, while keeping in mind that this is only approximately true.

The second main focal point in the diagram of figure 1.3 is the high temperature phase of physical QCD. Again, the existence of a mass hierarchy makes the positioning of this point somewhat approximate. As the point of interest here lies at the scale of deconfinement $\Lambda_{\text{QCD}}$, any quarks for which $m_q \ll \Lambda_{\text{QCD}}$ can be considered approximately massless. This would include not only the two lightest quarks, but also the strange quark that makes up a sizeable fraction of all sea quarks [57, 58]. Topics under investigation using finite temperature field theory include the QCD phase transition nature and critical temperature [43, 59–63] and the thermodynamical properties of QCD in general [64–69]. Many of these issues are conceptually intertwined with the technically highly complicated problem of simulating QCD at finite chemical potential. As such, they form a highly competitive and physically
Figure 1.3 A sketch of the phase diagram of an SU(3) Yang-Mills theory as a function of the temperature and the number of massless fundamental fermions present in the continuum. Three phases are indicated: a region of hadronic QCD, the phase relevant to spectroscopy where quarks are confined and chiral symmetry is spontaneously broken. Towards the top of the diagram we find the quark-gluon plasma, the deconfined but strongly interacting phase that has in the past decade become accessible to experiment (for a recent critical and comprehensive review, see [55]). At the right of the diagram is the location of the conformal phase, that will be extensively discussed in the remainder of this chapter. It exists properly at zero temperature only. This diagram does not display the QED-like region that appears at flavour numbers $N_f > 16.5$, where asymptotic freedom is lost. The line separating the hadronic and QGP phase indicates is envisaged as a line of chiral phase transitions; its shape is based on results from [56]. It is still unclear how the QGP and conformal phase are connected. Black stars indicate the approximate locations of two focal points of research into lattice QCD discussed in the text: The zero temperature and high temperature phases of physical QCD. Black dots indicate approximately the locations in the phase diagram that are sampled by the results presented in this thesis. The leftmost dot represents results for $N_f = 2 + 1 + 1$ simulations, that include the lightest four quarks as dynamical degrees of freedom. For the purpose of this diagram, they would be located around $N_f = 2$, as physical QCD is qualitatively well described as a theory with two approximately chiral quarks receiving small corrections from additional quark flavours. The middle dot represents measurements for $N_f = 8$, where a thermal phase transition was determined to a chirally symmetric phase. The rightmost dot represents zero temperature results at $N_f = 12$, a point that appears to lie just inside the conformal phase.
interesting class of problems. Moreover, given recent developments in quantitative cosmology (e.g. the results from the WMAP mission [70,71]) and the experimental access to the QGP provided by the current generation of particle accelerators (RHIC and LHC), results obtained from lattice calculations are increasingly confronted with and aiding the understanding of experimental data. For an overview of finite temperature field theory on the lattice and recent results, the reader is referred to recent reviews, some of which include [72–75]. The results presented in this thesis have no direct bearing on physical QCD at high temperatures. However, extensive use will be made of methods from finite temperature field theory from chapter 3 onwards.

A large part of this thesis will be dedicated to studies of the phase diagram of figure 1.3 away from the two focal points indicated by stars. Simulations have been performed at the locations of the black dots, to investigate the qualitative impact of increasing flavour numbers on non-Abelian dynamics. The Callan-Symanzik equations of QCD to two loops, where all coefficients are regularisation scheme independent, already hint at the possible existence of interesting physical phenomena as the number of light quark flavours is increased. This calculation was first done in [76] and the result reads

$$\beta(g) = -b_0 \frac{g^3}{(4\pi)^2} - b_1 \frac{g^5}{(4\pi)^4} + O(g^7). \quad (1.4)$$

It is important to note that the universal coefficients $b_0$ and $b_1$ depend upon the Casimirs $C_2(g)$ and $C_2(q)$ of the representations of SU(N) in which gluons and quarks are placed, as well as the trace $T(q)$ of the quark representation and the number of quark flavours $N_f$. We find

$$b_0 = \frac{11}{3} C_2(g) - \frac{4}{3} T(q) N_f,$$  \quad (1.5)

$$b_1 = \frac{34}{3} C_2^2(g) - \frac{20}{3} C_2(g) T(q) N_f - 4 C_2(q) T(q) N_f. \quad (1.6)$$

Values for $C_2$, and $T$ in different representations of SU(N) are summarized in table 1.1.

<table>
<thead>
<tr>
<th>$R$</th>
<th>$C_2$</th>
<th>$T$</th>
<th>$R$</th>
<th>$C_2$</th>
<th>$T$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fundamental</td>
<td>$\frac{N^2 - 1}{2N}$</td>
<td>$\frac{1}{2}$</td>
<td>$2S$</td>
<td>$\frac{(N-1)(N+2)}{N}$</td>
<td>$\frac{N+2}{2}$</td>
</tr>
<tr>
<td>Adjoint</td>
<td>$N$</td>
<td>$N$</td>
<td>$2A$</td>
<td>$\frac{(N+1)(N-2)}{N}$</td>
<td>$\frac{N^2 - 2}{2}$</td>
</tr>
</tbody>
</table>

Table 1.1 The Casimir $C_2$ and trace $T$ of different irreducible representations $R$ of the group SU(N): fundamental, adjoint, two-index symmetric (2S) and anti-symmetric (2A). This table is reproduced from [77]

We will momentarily focus on the specialization of equation 1.4 to the most physical case of $N = 3$ and fermions in the fundamental representation. In this form, equation 1.4 was instrumental in the establishing of asymptotic freedom [78,79]. The sign of the leading order coefficient $b_0$, in the case of QCD where gauge fields are in
the adjoint representation and quarks in the fundamental, is positive for values of $N_f < 16.5$. In this case, the theory will develop a UV fixed point at $g \to 0$. For a high number of flavours, the theory loses asymptotic freedom and flows towards the free limit in the IR. In a publication soon after those landmark papers, Caswell noticed that one could go beyond the leading order [76] and examine the sign of the second coefficient $b_1$. In the small and large flavour number limit of QCD, both coefficients agree in sign. But between the value of $N_f = 8.05$ and 16.5, there is a region in which the sign of $b_1$ is opposite to that of $b_0$. This opens up, to the extent that perturbation theory is valid, the possibility of an additional zero in the beta function. The consequences of this were first realised in [80]: an additional, non-trivial fixed point may develop in the theory. The authors of [80] assumed a phenomenologically inspired strong coupling limit as a completion of their perturbative analysis. Such a limit was derived for a latticised Yang-Mills theory in [81], giving a negative $\beta$ function for large values of $g$. Since this limit was introduced at all values of $N_f$, zeros of the beta function appeared for $N_f > 16.5$, as the two leading order terms of the perturbative expansion are strictly positive. While an additional UV fixed point at some large value of the coupling cannot be excluded \textit{a priori}, its existence is not obvious and still a matter of investigation. We will return to this question shortly.

To what extent is the above result of the appearance of an infrared fixed point in a perturbative expansion valid? Let us argue by, for a moment, assuming that a perturbative approximation is completely convergent and a full description of the theory. The two coefficients of the beta function responsible for the cancellation do not depend on the choice of regularisation scheme, while higher order terms are scheme dependent. This fact can be exploited through a redefinition of the coupling, such that all additional terms are cancelled systematically [82]. While we do not know exactly how to define this scheme, it can be shown to exist at least [83]. Since we assumed the theory to be fully described by its perturbative expansion, the change in sign of the beta function is now physically observable as a fixed point in this specific scheme. But a physical observable should be scheme independent, meaning that a change in sign of the beta function should persist to all orders in perturbation theory in any regularisation scheme – although the exact value of the coupling at which it appears remains scheme dependent.

The above argument obviously breaks down, because the initial assumption that the theory is fully described by its perturbative expansion is false in general. In those cases where perturbation theory fails to converge and non-perturbative physics dominates, the meaning of a zero in the two-loop beta function is limited. Specifically, the non-perturbative appearance of spontaneous chiral symmetry breaking introduces a mass gap for the fermions that will substantially alter the dynamics in the IR and cause the fixed point disappear altogether. But let us introduce an analytical continuation of $N_f$, which is straightforward, given that $N_f$ appears analytically in the partition function. Banks and Zaks now argue in [80] that the argument from perturbation theory does have direct implications for some (small) range values of $N_f$. This follows from the fact that, by moving close to the value $N_f^{AF}$ where asymptotic freedom is lost, the value $g^c$ at which the zero of the beta function appears can be made arbitrarily small. Hence, for some choice of $N_f$, perturbation theory should
be a wholly adequate description up to $g^c$ and the appearance of a Banks-Zaks fixed point should be a physical phenomenon. Of course, there is no reason to expect that this range of validity will include any integral values of $N_f$, which makes this point rather academic. Speaking generally, higher order corrections to equation 1.4 are expected to be large and perturbation theory will not be a particularly helpful tool. In fact, the authors of [82] point out the corollary to this argument: If no fixed point occurs for a value of $N_f$ where equation 1.4 does have a zero, this must be a consequence of essentially non-perturbative physics.

A phase diagram proposed in [80] is reproduced in figure 1.4. This diagram should be understood specifically in terms of a lattice regulated field theory. The theory enters different phases as the number of quark flavours $N_f$ and the input lattice coupling constant $g_L$ are varied. The latter is not really an independent parameter, because different values of the coupling in the discretised setup will correspond to a single continuum limit. We can interpret the systems at these different parameters as being discretisations of the continuum limit at different scales. Renormalisation Group (RG) transformations should connect the parameters describing these discretisations, with the inverse lattice spacing $a^{-1}$ providing an implicit momentum scale. As the continuum is approached, the RG flow will move towards fixed points in parameter space. At which fixed point one ends up, is uniquely determined by the RG curve on which one started. The fixed points therefore possess a basin of attraction, and a separation of phases is determined by a boundary between two such basins. Those regions not connected to the $g \to 0$ boundary will be phases without an asymptotically free continuum limit.

The diagram of figure 1.4 is a conjecture, that is supported by physical arguments, but also somewhat counter intuitive. Properties of the theory can be derived in the limit of both small and large $N_f$. The limit $N_f \to 0$ reduces to Yang-Mills theory, where no phase transitions will occur. Chiral symmetry is known to be broken for small values of $N_f$, though a strong coupling lattice transition may be present. Towards the strong coupling limit, the confining regime that is imposed by Banks and Zaks will introduce a UV fixed point for any value of $N_f$ where the theory has a deconfining phase. In the limit of $N_f > 1$ and $g^2 N_f < 1$, chiral symmetry can be shown to be preserved in the neighbourhood of the free limit. As argued in [80], a consistent perturbative expansion can be set up in the large $N_f$ limit, that will produce massless fermion propagators in some convergent neighbourhood of $g = 0$. Since a confining theory cannot be chirally symmetric [84–87], a chiral phase transition will be triggered at the location of the UV fixed point. The situation is more complicated just before the loss of asymptotic freedom. An expansion in $\epsilon = (N_f^{\text{AF}} - N_f)$, which in some neighbourhood of $\epsilon \to 0$ produces a reliable perturbative expansion due to the weak coupling IR fixed point, demonstrates the restoration of chiral symmetry at the IR fixed point. Not wanting to abandon phenomenology, Banks and Zaks assumed the continuing validity of the regular weak coupling limit $g \to 0$, including the induced mass gap from confinement. At the same time, chiral symmetry should be restored at the fixed point. To reconcile these two facts, a phase transition would need to occur at the location of the IR fixed point. Hence the curious and counter-
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Figure 1.4 Phase diagram of a generic SU(N) gauge theory with fundamental fermions, in the plane of flavour number versus bare coupling, as proposed in [80]. The area fill indicates the phase of the theory. The area filled with polka dots is confined and chirally broken, while the striped area is deconfined and chirally symmetric. The transition between the polka dot and striped phases coincides with the IR fixed point. The unfilled phase would be present in case of a separation between a confining and chiral transition. It would be chirally broken, but not confining.

intuitive re-entrant behaviour of theories above $N_f^{c1}$.

An important modification of the Banks-Zaks analysis was proposed in a series of studies by Appelquist and collaborators. These papers presented results on the pattern of chiral symmetry breaking in different gauge theories as a function of the number of flavours, using a ladder approximation to the Schwinger-Dyson gap equation [88]. Both in the context of QED in 2+1 dimensions [89–93] and regular QCD [82], a chiral phase transition was found as a function of the number of fermions. At the critical flavour number $N_f^c$, the effective fermion mass would be continuous [82,93], excluding a first order transition. However, no light scalar degrees of freedom were observed in the chirally broken phase close to the transition, also excluding a regular second order chiral phase transition [94]. Chivukula

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Note that one might perhaps envision the different lines in figure 1.4 not joining at a single point. We will assume they do, here and in subsequent depictions of the phase diagram, because it seems to be the most simple and plausible option. In fact, there is no obvious physical mechanism that would cause them to behave differently.
showed [95] that this peculiar property is a direct consequence of the presence of a fixed point. It breaks the effective low energy approximation, causing the scalar excitations to receive mass contributions from all momentum scales. This curious class of transitions was further studied in [96], where they were dubbed conformal phase transitions due to their association with the breaking of conformal symmetry. Their defining property was found to be an abrupt change in the spectrum of light excitations of the theory, but with a continuous chiral order parameter. With this insight, the assumed weak coupling limit in the original Banks-Zaks proposal could be modified as in figure 1.5. At a critical flavour number $N_f^c$, chiral symmetry is re-

![Figure 1.5](image_url)

Figure 1.5 Phase diagram of a generic SU(N) gauge theory with fundamental fermions, in the plane of flavour number versus bare coupling, as proposed in [96]. Area fill indicates the phase of the theory. The area filled with polka dots is confined and chirally broken, while the striped area is deconfined and chirally symmetric. The unfilled area is delimited to the left by a bulk chiral symmetry breaking transition, to the right by a bulk confinement transition. The transitions may well be entangled, in which case the lines will overlap and the unfilled phase will be absent. The dotted line in the striped area indicates the location of the line of fixed points. The line at $N_f^c$, separating the polka dot and striped areas, indicates the conformal phase transition described in [95,96].

stored and a conformal phase entered. The fixed point is now no longer associated with a phase transition, but is approached asymptotically from both stronger and weaker coupling. For a coupling $g = g^c$, there is no running of the coupling constant with the renormalisation scale $\mu$ and the theory becomes scale invariant and
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conformal\(^2\). In the neighbourhood of the fixed point, both above and below \(g^c\), this conformal symmetry will be perturbatively broken by the dynamics. Since the IR limit of both sides is identical, however, no phase transition will occur at the fixed point. The range of flavour values for which such a conformal phase exists is dubbed the conformal window \([82, 98]\).

The phase diagram of figure 1.4 implies the simultaneous appearance of an IR and UV fixed point in the theory by construction, but without any underlying physical cause. The phenomenon of the opening of a conformal window – or rather, its closing with decreasing flavour number – led the authors of \([99]\) to propose a scenario for conformal phase transitions based on the AdS/CFT correspondence \([100, 101]\). This duality holographically maps a string theory defined on anti-de Sitter space to a conformal field theory at the boundaries, and is well established for the supersymmetric variety of the latter. They analyse the mechanism by which a fixed point could disappear as a function of \(x_f = N_f / N_c\) and find three possibilities. Either the fixed point moves off towards the free or infinite coupling limits, or an IR fixed point is annihilated by a UV fixed point. This mechanism is well understood for the case of the so called Berezinskii-Kosterlitz-Thouless (BKT) phase transition \([102]\), a finite temperature phase transition for QCD with a defect in two dimensions. Here, the approach to the annihilation point from the non-conformal side induces a particular scaling behaviour, coined BKT scaling in \([99]\). Such scaling behaviour might identify a universality class for conformal phase transitions. In fact, the scaling predicted close to the conformal transition in \([96]\) is identical to it. The AdS/CFT derived fixed point merging might well be a framework for understanding the disappearance of the conformal window in large \(N_f\) QCD. This is particularly interesting, since it predicts the existence of a strong coupling UV fixed point inside the conformal window. Figure 1.6 provides a schematic overview of the proposed scenario. The theories defined at the fixed point on both branches (denoted QCD and QCD\(^*\)) would be the boundaries of a scalar theory in the bulk of a five-dimensional AdS space, from which mutual constraints on their anomalous dimension can be derived. For the sum of the dimensions of the chiral condensate operators on both branches, written as \(\Delta_+\) and \(\Delta_-\), one would obtain

\[
\Delta_+ + \Delta_- = D = 4. \tag{1.7}
\]

The dimension \(\Delta_+\) on the IR branch would then move from the engineering dimension 3 in the free limit to the dimension 2, at which point it would be annihilated by the UV branch. A schematic representation of this mechanism is shown in figure 1.6. A merger mechanism would naturally limit the value of the anomalous dimension on the IR branch to be smaller than 1 at the critical point. Notice that this limiting value is exactly the point at which the Fermi four-point interaction \((\bar{\psi}\psi)^2\) becomes a relevant operator, making it a natural bound for the occurrence of spontaneous chiral symmetry breaking. As we will see shortly, this critical value for the anomalous dimension has been independently used \([82]\) to determine a lower bound on

\(^2\)This may not be the case in two dimensions, where the conformal group becomes infinite dimensional \([97]\)
1.2 Phase diagram of flavoured theories

Figure 1.6 Schematic depiction of the merger mechanism for non-supersymmetric QCD, adapted from [99]. The solid line represents the IR fixed point, the dashed line its corresponding UV fixed point. The dimension of the $\bar{\psi} \psi$ operator at the fixed points is drawn versus $x_f = N_f/N_c$, with $x_c^f$ the onset of the conformal window. While a conformal QCD-like theory is defined at the IR line, a dual theory $\text{QCD}^*$ exists at the UV fixed point.

While not directly in the scope of this thesis, generalising to fermions in higher dimensional representations is in fact rather straightforward. There are four representations that have an asymptotically free phase for any number of colours $N_c$ [103]. Next to the fundamental representation, those are the adjoint, the two-index symmetric $(2S)$ and two-index anti-symmetric $(2A)$ representations. It is these four representations that are generally considered potentially physically relevant. The higher dimensionality of the non-fundamental fermions works towards a higher shielding efficacy. This, in turn, means that both the loss of asymptotic freedom and the onset of the conformal window are pushed down to lower flavour numbers. For example, perturbation theory (equation 1.4) suggests the appearance of a fixed point at flavour numbers as low as $N_f = 1.0625$ for adjoint fermions charged under SU(3). In contrast to fundamental fermions, where the critical flavour number lies above the phenomenologically speaking unnaturally high number of eight, the conformal window could be entered by theories with moderate flavour content. It is in this sense that theories with fermions in higher dimensional representations can be considered
the more natural extensions of the Standard Model.

Considering the phase diagram of theories with fermions in higher-dimensional representations, the main difference appears for the adjoint fermions. For fundamental fermions, confinement necessarily implies chiral symmetry breaking [84–87] and the two transitions are in practice found to occur simultaneously [104]. For adjoint fermions, this is not necessarily the case. Let us consider fermions charged under SU(3), for definiteness. If we write a discretised action for the usual case of fundamental fermions, one writes the gauge links as elements of SU(3). But for the higher dimensional adjoint fermions, the gauge links have to be placed in the eight-dimensional $U(8)$ representation of the group. Now the fermionic part of the action becomes [105, 106]

$$S_f = \int \bar{\psi} M \left[ U_{(8)} \right] \psi,$$

with $M$ the Dirac operator as a function of the gauge connections. The $U_{(8)}$ representation can in fact be written in terms of $U_{(3)}$, as

$$U_{(8)}^{ab} = \frac{1}{2} \text{Tr} \left( \lambda^a U_{(3)} \lambda^b U_{(3)}^\dagger \right),$$

where the $\lambda$s are the Gell-Mann matrices. The gluonic part of the action remains the same as for fundamental fermions and is a function of $U_{(3)}$ alone. The Polyakov loop

$$L(\vec{x}) = \text{Tr} \left[ \prod_{n=0}^{N_t-1} U_0(\vec{x}, n) \right]$$

is an order parameter of confinement in pure Yang-Mills, because it is sensitive to the spontaneous breaking of the global centre symmetry

$$U_0(\vec{x}, t) \rightarrow z U_0(\vec{x}, t), \quad z \in \mathbb{Z}_n$$

of the action by a confining gauge field. Adding fermions in the fundamental representation to this Yang-Mills action breaks the centre symmetry explicitly, so the Polyakov loop can no longer be used as an order parameter. But adding an adjoint term such as equation 1.8 preserves the symmetry, because the gauge elements in equation 1.9 occur in pairs with their hermitian conjugates. At the same time, the Polyakov loop expectation value is still a measure of the potential between two static charges$^3$. The scales at which confinement and chiral symmetry breaking occur are therefore independent for adjoint fermions and a confined chirally symmetric phase could in principle exist for some range of temperatures. No particular ordering of the two transitions is favoured theoretically, however. Quenched simulations [105, 108] indicate that the thermal scale of deconfinement actually lies below that of chiral symmetry restoration. It is for this reason that figure 1.7 depicts possible additional

$^3$It should be noted that this concerns charges in the fundamental $U_{(3)}$ representation. One can also define an adjoint Polyakov loop, which will in fact have a non-zero expectation value for any value of the coupling. This implies that adjoint fermions are always screened. See [105, 107] for details.
phases for values of $N_f > N_f^c$.

The appearance of a conformal phase transition and the restoration of conformal symmetry at the quantum level of QCD is an exciting development. One immediate consequence of the conformal window is a dramatic slowing of the running coupling constant at values of $N_f$ close to the conformal phase transition. This is an important ingredient of the modern incarnation of technicolour models, originally proposed in [109–111] and extended to in [112, 113]. These models tend to be plagued by large flavour changing neutral currents for interactions strong enough to produce realistic results for fermion masses [113]. Since no such currents are observed, naive technicolour models are excluded experimentally [37]. These issues are avoided if a slowly varying coupling exists for the technicolour gauge theory, because contributions to the mass over a large range of momenta can now accumulate [114–116]. Given that this effect is a consequence of the coupling constant “walking” rather than running, these theories are known as walking technicolour and several excellent reviews exist on this topic [117, 118]. The dynamics of the conformal window could a perfectly natural setting for the appearance of walking and the large scale quantitative investigation of these effects is currently under way [119].

While walking technicolour is usually considered the main reason for being interested in the existence of a conformal window, there are more theoretical questions to be answered. The way QCD deviates from conformality should provide valuable insight concerning the question if and how the AdS/CFT correspondence is realised for the strong interactions. The program for studying this connection is usually referred to as AdS/QCD and considerable progress has been made already (for a review, see [120]). The existence of a continuous transition into a conformal theory at zero temperature might serve as a basis for the systematic building of a correspondence between AdS and the QCD ground state. Along these lines, there may be an interesting relationship between the strongly coupled, but chirally symmetric quark gluon plasma and the conformal window [121–123].

### 1.3 Analytical bounds on the conformal window

Having determined the existence of a conformal window, a natural follow-up question it to ask for its bounds. The upper end of the conformal window will occur when asymptotic freedom and this point is determined exactly from perturbation theory. A number of analytical estimates for the lower end have been given in literature. We can distinguish a number of basic approaches to deriving this bound, all of which have in common that they provide an estimate of the end point of the chiral phase boundary. The first approach does so by means of an essentially perturbative estimate of the influence of chiral dynamics. A second approach employs non-perturbative methods, developed in the context of regular, hadronic QCD, to trace the chiral phase boundary. A final type of approach draws upon the similarities between QCD with an IR fixed point and $\mathcal{N} = 1$ supersymmetry and attempts to connect explicitly to a supersymmetric extension of QCD. We will now discuss the various results derived, using each of these basic approaches.
Figure 1.7 Conjectured phase diagram of a generic SU(N) gauge theory with adjoint fermions, in the plane of flavour number versus bare lattice coupling. The area filling indicates the phase of the theory. The phase structure is similar to that of figure 1.5, but richer since the scales of confinement and chiral symmetry breaking are detached. The polka dot filled area is confined and chirally broken, while the striped area is deconfined and chirally symmetric. The unfilled area is delineated by confinement and chiral symmetry breaking transitions, but the order of those is not constrained. Both lines might coincide, in which case the unfilled phase would simply be absent. Results from [105, 108] on the thermal phase transition in the quenched theory suggest this area would be deconfined, but chirally broken. The dotted line in the striped region indicates the location of the line of fixed points, that will always be in the deconfined and chirally symmetric phase. The solidly filled phase that appears above the conformal phase transition was proposed in [80]. It would be chirally symmetric, but confining. The deconfining transition separating the solidly filled and striped area might coincide with the conformal phase transition, in which case the former would be effectively absent. It might also coincide with the line of IR fixed points, though the theory should always be deconfining at the fixed points themselves. In this case, the theory would be confining for any value of $N_f < N_f^{AF}$. It is not clear, however, what mechanism would cause a deconfinement transition to occur when moving towards stronger coupling. This figure was adapted from [77].
1.3 Analytical bounds on the conformal window

1.3.1 Perturbative approaches
The first type of approach, in which one attempts to account for the chiral dynamics perturbatively, is conceptually the most straightforward. The earliest result on the lower bound of the conformal window, published in [82], uses this type of argument. Spontaneous chiral symmetry breaking, it says, would trigger the destruction of the IR fixed point. It is therefore natural to assume the conformal window opens the moment the IR fixed point $g^c$ drops below a critical value $g_{SB}$ where symmetry breaking is triggered. We have a perturbative estimate for the former, but we can also find one for the latter. One can therefore try to account for this physical reasoning manually. This improved estimate for the opening of the conformal window, which will of course still be perturbative in nature and truncated at two loops, will push $N_f^c$ towards higher values and IR fixed points at weaker coupling. To find $g_{SB}$, we perform a perturbative expansion of the anomalous dimension of the chiral order parameter $\langle \bar{\psi} \psi \rangle$. A mass gap is induced when the value of this anomalous dimension equals 1 [116], so again we can solve for the critical coupling. Alternatively, it can be found from a perturbative expansion of the Cornwall-Jackiw-Tomboulis effective action [124]. For fundamental fermions and a general gauge group SU(N), its result has been reported as [125, 126]

$$g_{SB}^2 = \frac{8\pi^2}{3} \frac{N_c}{N_c^2 - 1}. \tag{1.12}$$

Equating the perturbative IR fixed point $g^c$ to $g_{SB}$ and solving for $N_f$ gives

$$N_f^c = N_c \left( \frac{100N_c^2 - 66}{25N_c^2 - 15} \right). \tag{1.13}$$

For SU(3), this results in a critical flavour number of $N_f^c = 11.91$.

An interesting alternative angle was chosen, again by Appelquist and collaborators [127], in proposing an analogue to the 't Hooft anomaly matching condition. The anomaly referred to here is the residue of the pole of any correlation function. It only receives contributions from massless degrees of freedom and is an RG invariant quantity. The combination of these properties implies that the value of the anomaly can be used to connect the massless spectrum in the IR and the UV regime. When the theory one wants to study is asymptotically free, one can calculate the very straightforwardly in the UV regime. This value than places a constraint on the massless degrees of freedom in the strongly coupled IR limit, where the value of the anomaly must be reproduced. The anomaly matching condition is essentially a way of imposing the symmetries of the Lagrangian on the spectrum of composite particles. Although the procedure does not impose the absence of additional massless particles in the spectrum, there is no symmetry that will protect such particles from acquiring a mass. Their presence would therefore be unnatural and it is a customary assumption, when applying the anomaly matching procedure, that they will be absent. The authors of [127] propose promoting this assumption to a constraint. One consequence of such a constraint, is that one should reject any IR spectrum that contains more massless degrees of freedom than the free UV limit does. In a way,
one could say that the Lagrangian does not possess the necessary amount of symmetry to support such a spectrum. Applied concretely to QCD with a large number of flavours, this means that spontaneous chiral symmetry breaking should vanish for some value of \( N_f \). That value would be reached, the moment that the number of Goldstone bosons that would be produced exceeds the number of massless degrees of freedom in the free theory. Specialising to the fundamental representation, the well known expression for the number of Goldstone bosons in a spontaneously chirally broken theory reads

\[
\text{d.o.f}_{\text{IR}} = N_f^2 - 1. \tag{1.14}
\]

In the (free) UV limit, one can count the number of massless bosons and add number of independent fermionic degrees of freedom:

\[
\text{d.o.f}_{\text{UV}} = 2(N_c^2 - 1) + \frac{7}{2} N_c N_f. \tag{1.15}
\]

According to the constraint of \([127]\), the constraint should read \( \text{d.o.f}_{\text{IR}} \leq \text{d.o.f}_{\text{UV}} \), which translates into

\[
N_f \leq 4\sqrt{N_c^2 - \frac{16}{81}}. \tag{1.16}
\]

What makes this result of great potential interest, is that it provides an upper bound to the onset of the conformal window from symmetry considerations. For the case of SU(3), it would place \( N_f = 12 \) inside the conformal regime. Nevertheless, particular caution should be taken in interpreting these results, in spite of its basic assumption feeling rather natural and the reproduction of a number of known results \([127]\). Unlike for the ‘t Hooft anomaly matching condition itself, no rigorous arguments have been presented for its validity.

1.3.2 Non-perturbative approaches

The second line of arguments, based on non-perturbative models developed for hadronic QCD, was introduced in \([128]\). Here the critical number of flavours is found from the instanton liquid approach \([129]\). An onset of instability in the confining liquid is found for flavour numbers as small as \( N_f = 6 \). Note that this result contradicts the conclusion of \([130]\), co-authored by one of the authors, where small but finite sized pseudo-particles were observed for \( N_f = 10 \) and confinement was found to be absent only at \( N_f = 12 \). A study of the instanton effects \([131]\) specifically accounting for the presence of an fixed point, which should limit the strength of the coupling at the IR scales typical for instantons, put the critical flavour number at \( N_f^c \approx 3.7N_c \), or a potential \( N_f^c \approx 11.1 \) for SU(3). This value was derived in the context of SU(2), however.

Functional renormalisation group methods \([132, 133]\) are powerful tools in the analysis of phase transitions and provide a natural setting for studying the presence of spontaneous chiral symmetry breaking as a function of \( N_f \). This approach
starts by introducing an IR regulator on the full propagator that suppresses contributions below some momentum scale $k$. By means of a systematic expansion of the operators, a $k$-dependent effective action can be constructed. Renormalisation group relations are then used to connect the action at different scales [134]. These calculations are non-perturbative, though not exact, as the effective action usually needs to be truncated at some order. One such study [135] of QCD, extended with effective four fermion interactions to account for higher order corrections to the action, studied the coefficients of the four-fermion operators as function of the number of flavours. When approaching the critical flavour number from the chirally symmetric side, those coefficients should diverge, signalling the onset of the symmetry breaking. For SU(3), the authors of [135] obtained a critical flavour number of 10, with combined uncertainties producing a range roughly between 9 and 12 flavours. A very similar approach was used in [56, 136], but in the context of finite temperature field theory. The main goal of these papers was the calculation of chiral phase boundary of QCD as a function of $N_f$. While the focus is on the smaller flavour numbers relevant for QCD phenomenology, the authors find an estimate for the lower bound of the conformal window at the end point of the chiral phase boundary. Though this happens around $N_f = 12$, it is stressed that this results is quite sensitive to the truncation and consequently fully compatible with [135]. Interestingly, the authors define a consistent scale at each value of $N_f$ by equating the running coupling at the scale of the $\tau$ lepton. This introduces a certain arbitrariness to the shape of phase boundary and casts some aspersions on the ambition of the authors to determine scaling properties close to $N_c$. Nevertheless, very few schemes for setting the scale in these theories have been proposed and the possibility of connections to the quark gluon plasma might make this more than a cosmetic issue. As will become clear, these papers formed the direct inspiration for our lattice studies of the conformal window.

The research presented in [137] is somewhat hard to classify, but can be understood as an ingenious rewriting of QCD that allows for a direct study of the influence of fermionic degrees of freedom. In this case, the fermion determinant of equation 1.1 is rewritten in terms of an exponent of Wilson loops. This setup was discussed in [138] and is based upon the world-line formalism formulated in [139]. The argument of the exponent now becomes sum over all possible Wilson loop contours, such that we obtain schematically

$$\det [M]^{N_f} = \exp \left[ N_f \sum_c W \right] = \sum_n \left[ \frac{N_f}{n!} \left( \sum_c W \right)^n \right]$$

(1.17)

and $N_f$ moves from being the power of the determinant to being a natural part of the expansion. Equation 1.17 can be employed to write a systematic expansion of the full QCD action of equation 1.1. The leading order contribution to the expectation value of any observables calculated in this framework, being the $N_f = 0$ limit, will be the quenched, pure Yang-Mills result. Each higher order will add a Wilson loop to the configuration, which can be shown to carry a coupling factor $\lambda/N_c$ from an AdS/CFT mapping to a string theory. All in all, we will find an expansion in terms
where $\lambda$ is a constant that can be determined from, e.g. lattice simulations of Yang-Mills theory as the strength of the three glueball interaction vertex. The series that results will be geometrical and nicely convergent, as long as $N_f$ is small enough for the expression in equation 1.18 to be at most unity. Once the value $N_f^c$ where the expansion breaks down is reached, the expansion of the theory around a confining and non-chiral vacuum breaks down. The author of [137] associates this with the onset of the conformal window and writes the condition, for general gauge groups and representations of the fermions, as

$$N_f^c \frac{T(R)}{C_2} = \lambda^{-1}. \quad (1.19)$$

Given a numerical value of about 0.5 for $\lambda$ for Dirac fermions, we find $N_f^c = 4N_c$ for fundamental fermions, or $N_f^c = 12$ for $SU(3)$.

### 1.3.3 Supersymmetry inspired approaches

The final avenue to the lower bound of the conformal window attempts to use the availability of rigorous results in supersymmetric theories to derive properties of the closely related conformal phase. One possible way of exploiting the resemblance between the theories, is by using effective actions derived from supersymmetric QCD (sQCD). This approach was pioneered by Seiberg and Witten [140–143] and can be extremely powerful in deriving exact solutions, because of the underlying enhanced symmetries. Starting from sQCD, such an effective action for QCD was constructed in [144] by integrating out the gluinos and squarks below the scale of supersymmetry breaking. This action was valid for a number of flavours smaller than the number of colours, but the authors extend it to the large $N_f$ limit in [145]. Using a perturbative approximation to this effective theory, it is possible to calculate the anomalous dimension of various operators. As we saw before, chiral symmetry breaking will vanish when the anomalous dimension of the chiral condensate becomes 1. To determine the critical flavour number $N_f^c$, one can therefore solve the perturbative expression for this value. The result reported in [145] agrees with [82] and equals $N_f^c = 3.9N$.

The final type of approach to the Though the effective action itself is non-trivial, the result of [145] is still a perturbative estimate. But the interesting conjecture presented in [146] takes a flight forward and attempts to circumvent any expansions. It bases itself on the Novikov-Shifman-Vainshtein-Zakharov (NSVZ) supersymmetric beta function [147, 148]. For supersymmetric QCD, this beta function is an exact
1.3 Analytical bounds on the conformal window

The Ryttov-Sannino conjectured beta function mimics this form and proposes a closed form of the non-supersymmetric beta function

\[
\beta(g) = -\frac{g^3}{(4\pi)^2} \frac{\beta_0 + 2 T(R) N_f \gamma(g^2)}{1 - \frac{g^2}{8\pi^2} C_2(G)}, \quad (1.20)
\]

\[
\gamma(g^2) = -\frac{g^2}{4\pi^2} C_2(R) + \mathcal{O}(g^4). \quad (1.21)
\]

The Ryttov-Sannino beta function expands to the two loop beta function 1.4 by construction. It also reproduces lattice results in the \( N_f = 0 \) Yang-Mills and the large \( N_c \) limit, implying that it accounts for non-perturbative effects to some extent. These do not make for very stringent tests by any means, but one can conservatively treat equation 1.22 as a parametrization of the beta function. While the main application of an exact beta function would lie in the study of the fixed point itself, a lower bound on the conformal window can be derived from unitarity bounds. In a conformal theory, the dimensionality of the \( \bar{\psi}\psi \) operator should be equal to or larger than 1 in order to avoid states of negative norm and preserve unitarity [149]. As this operator has an engineering dimension of 3, this constrains the anomalous dimension at the fixed point to be at most 2. From the root of equation 1.22, one can obtain an expression for the value of \( \gamma(g^2) \) at the fixed point and determine the unitarity bound on \( N_f \) to be \( N_f^c \geq 8.25 \). This constraint is very mild, where the stronger \( \gamma = 1 \) bound produces a result comparable to the result of [114]. It should be noted that a similar NSVZ form for the closed beta function is found from the large-N limit of a quantum holographic effective action [150] for \( QCD_4 \), without the explicit imposition of supersymmetry. While this result is encouraging, it highlights a crucial problem of the Ryttov-Sannino conjecture. As pointed out in [77], the anomalous dimension of the gluons is fixed within the context of supersymmetry because of a series of subtle cancellations. Without those extensive symmetry constraints, there is no particular reason to believe a closed form along the lines of the NSVZ beta function should even exist. An expression such as the Ryttov-Sannino conjecture may be a useful and generally quite accurate parametrisation. But it is by no means a unique choice and its supersymmetric roots make it likely that it is missing certain features induced by the lack of cancellations in ordinary QCD.

Some of these features can be introduced by hand. Several refinements of the conjecture have in fact been proposed. A natural extension in the context of both phenomenology and lattice gauge theories is the addition of finite quark masses [151, 152]. Since masses are relevant operators, massive quarks will eventually decouple and the coupling will start to run. No true conformal window exist therefore, but
the proximity of a fixed point will cause the coupling to stall over a large range of scales and produce walking behaviour. Since a plateau in the strength of the coupling will be observed in practice, we can define a “quasi-conformal window”. The lower bound of this window, determined from a bound on $\gamma$ as in the massless case, will be a function of the mass and approach the conformal window from above in the chiral limit. The authors of [153] address the potential presence of an UV fixed point as proposed in [99], which is a feature that the Ryttov-Sannino conjecture does not reproduce. Using their modified expression in the large $N_c$ limit where conditions on the anomalous dimension derived in [99] are exact, they find a critical flavour number $N_f^c = 13.2$ for fundamental fermions in SU(3). This value is substantially larger than other predictions, but is lowered again to 12 when estimating $N_c^{-1}$ corrections. For any of these modifications, however, the fundamental problem remains. They may capture known features of the system we investigate to some (possibly good) degree, but their predictive power is limited.

1.3.4 Summary
A concise overview of analytical estimates – one that has rapidly become standard fare in any discussion of the topic – was provided in [103]. This discussion would not be complete without the inclusion of figure 1.8. The ranges plotted here for the four representations under consideration are based upon a number of criteria. The top line delimiting the predicted conformal regions is given by the perturbative loss of asymptotic freedom. By the large $N_c$ expansion argument of [80], these should be reliable estimates given by

$$N_f^{AF} = \frac{11}{4} \frac{D[G]C_2[G]}{D[R]C_2[R]}.$$

(1.24)

In this equation, $G$ denotes the adjoint representation of the gauge group, while $R$ is the representation of the fermions. The operator $D$ represents the dimensionality of the representation, $C_2$ is its quadratic Casimir. For the values of these quantities for different representations, see table 1.1. The dashed lines in figure 1.8 indicate the position of the perturbative Banks-Zaks fixed point. Barring exotic mechanisms, these could be considered a strict lower bound on the opening of the conformal window and are given by

$$N_f^{BZ} = \frac{D[G]C_2[G]}{D[R]C_2[R]} \frac{17C_2[G]}{10C_2[G] + 6C_2[R]}.$$

(1.25)

Taking into account the argument of [82] and using the ladder approximation calculation as an estimate for chiral symmetry restoration, the true lower bound of the conformal window is estimated by

$$N_f^c = \frac{D[G]C_2[G]}{D[R]C_2[R]} \frac{17C_2[G] + 66C_2[R]}{10C_2[G] + 30C_2[R]}.$$

(1.26)

This line is taken as the lower range of the conformal window in figure 1.8.
1.4 Numerical bounds on the conformal window

The only method to account for non-perturbative dynamics systematically from first principles is by means of lattice calculations. Lattice studies of the conformal window have an extensive history, being performed more or less in parallel to analytical analyses throughout. We will present a chronological overview of the developments.

Let us first note that these simulations have been done all but exclusively using staggered, or Kogut-Susskind fermions [154, 155]. This is due to a good match between the properties of this fermion discretisation and the requirements of the simulations. The interest in simulations at large $N_f$ has been predominantly qualitative and exploratory, giving rise to a need for a large number of runs with different parameters. This makes it undesirable to have to invest in the tuning of each run separately. Wilson-type fermions break chiral symmetry completely and consequently acquire an additive mass renormalisation. This introduces the need for tuning of the action and can complicate the study of chiral dynamics. The phase diagram of staggered fermions, on the other hand, is clean towards the chiral limit, because the staggered formulation preserves a non-trivial subgroup of the full chiral symmetry [156]. As a consequence, they do not require any tuning in particular. Finally and quite rele-
vantly, staggered fermions are exceedingly efficient compared to alternative formulations [29]. This enables even small scale studies to reach reasonably low masses and large volumes. It is for exactly these reasons, that the lattice simulations in the large $N_f$ limit reported upon in this thesis have been performed using staggered fermions, too. The staggered formulation does have some serious drawbacks, however. In the staggered formulation, the sixteen species of fermion from the naive discretisation of the fermion propagator get reduced to four different “tastes”. These tastes are degenerate in the continuum limit and are reduced to a single flavour by taking the root of the fermion determinant. It is not completely clear whether this procedure is completely well defined non-perturbatively [157–159]. Fortunately, the cases $N_f = 8$ (perturbatively walking), 12 (barely conformal according to most analytical predictions) and 16 (last integer flavour number before loss of asymptotic freedom) are particularly interesting for quarks in the fundamental representation. Most studies have been therefore been performed using multiple sets of unrooted quarks. But even then, lattice artefacts will break the taste symmetry of staggered fermions [160]. The upshot of this, is that one cannot simulate with perfectly degenerate quarks. This effect might have non-negligible consequences for the phase dynamics if taste breaking effects were to become too large.

The very first lattice study with a large number of quark flavours [161] was focused on the phase of the $N_f = 8$ theory as a function of the bare coupling. Due to the technical limitations of the time, the simulations had to be run on very small $4^3 \times 8$ lattices. Nevertheless, a first order chiral phase transition was observed, proving the feasibility of lattice studies in the large flavour number limit. These results were not sufficient for determining properties such as the sensitivity to volume effects. As a consequence, very little could be concluded about the zero temperature phase of the theory. The two studies first attempting to answer that question appeared in 1988 [162, 163]. Fukugita and collaborators [162] published results on the location and order of the confinement transition as a function of the number and mass of the quarks. The large $N_f$ limit was explored in simulations with $N_f = 10, 12$ and 18. At modest volumes of $8^3 \times 4$ and $8^4$ and bare quark masses down to a rather heavy $am = 0.1$, these data did present a marginal parametrical improvement over those of [161]. First order transitions were found in the Polyakov loop for each of the flavour numbers. The Polyakov loop is in fact the order parameter of confinement in pure Yang-Mills and not an order parameter in the presence of dynamical fermions, but the appearance of sharp transitions was attributed to the underlying chiral dynamics. Of course, it might also indicate that the input masses were too heavy to be fully dynamical. For $N_f = 18$, the authors assumed a bulk nature for the transition without further proof. But with the location for $N_f = 10$ and 12 of the transition showing some sensitivity to the change from $N_f = 4$ to 8, it was concluded that both were thermal and therefore in the regular phase of QCD. The combination of heavy masses and small temporal lattice size does limit the precision of these results, however. In [164], a study that could be considered a follow-up to [162], runs at $N_f = 8$ and 17 – bracketing the perturbative conformal window – were reported upon for much larger spatial volumes of $16^3 \times 4$. Again, a first order phase transition to a chirally broken and confined phase was observed. For $N_f = 8$, the transition turned
1.4 Numerical bounds on the conformal window

into a crossover for bare quark masses of $am = 0.25$ and heavier. As this puts the bare quark masses used in [162] within the regime of light masses, it indirectly bolsters those results. Unfortunately, no attempt was made to directly observe a shift in the location of the transition as a function of $N_t$. The presence or absence of apparent thermal sensitivity for $N_f = 17$ would have been a test of lattice artefacts interfering with the results of [162]. Nevertheless, one important conclusion from the data at $N_f > 16.5$ in both [162, 164] is a direct observation of lack of chiral symmetry at any number of flavours in the strong coupling limit, as envisaged in e.g figure 1.5. But the apparent thermal nature of the transition may be nothing but an artefact of $N_t = 4$ being an exceedingly small value. The other paper of 1988 by Kogut and Sinclair [163], a follow up to [161], covered a range of volumes (4$^4$, 6$^4$ and 8$^4$ being the largest) and included runs at $N_f = 8$ and $N_f = 12$. Here, too, first order transitions were found in the chiral condensate for both cases. Volume sensitivity, as a marker for a thermodynamics driven transition, was observed mainly in a comparison of 4$^4$ and 6$^4$. Some limited sensitivity to the volume was present beyond that for $N_f = 12$, but a vanishing Wilson line expectation value for the largest volumes was interpreted to indicate the absence of strong finite volume effects on the gauge dynamics. On balance, it was concluded that bulk transitions occurred at both flavour numbers, though the Polyakov loop appeared to be more sensitive to finite volume effects.

On balance, these early results were somewhat contradictory then. Finite volume systematics could easily be strong enough in either to invalidate any conclusions drawn. A group centred around Columbia university [165] set out to study the hadronic spectrum and chiral transition at $N_f = 8$. Employing volumes up to 16$^3 \times 32$ in combination with quark masses down to $am = 0.004$, these simulations were more mature in setup. A clear transition was observed for values of $N_t$ between 4 and 16, but conclusions were mixed. Sensitivity to the size of the lattice in the time direction was seen for small values of $N_t$, going up to $N_t = 8$. Above that value the position of the transition remained constant. The authors state that this would match the behaviour of a bulk transition, with enhanced finite volume effects for $4 < N_t < 8$. On face value, this would seem to imply the absence of a finite temperature transition and a fixed point at $N_f = 8$. It was noted, however, that the spectrum of particles in the chirally symmetric phase was very similar to that of the high temperature limit of QCD, while it did not exhibit signatures of conformal physics. This, and the contradiction with analytical predictions, led the authors to speculate a hadronic phase for $N_f = 8$ might still be preferred, but that lattice artefacts were too large for a definite conclusion.

In spite of the reservations expressed by the authors of the respective works, tentative conclusions from lattice analysis left room for the surprising conclusion that $N_f = 8$ might be inside the conformal window. Iwasaki and collaborators cemented these peculiar results by their investigations of large $N_f$ systems in the strong coupling limit [166]. Their simulations were, as an exception, performed using Wilson fermions and all performed in the rigorous strong coupling limit of $\beta = 0$ ($g_\Lambda \to \infty$). Lattices used here were asymmetrical, but comparatively large going up to a maximum size of 18$^2 \times 24 \times T$. The authors searched for a deconfining transition as a
function of the Wilson hopping parameter $k$, which implicitly determines the quark mass. This was done by studying the Polyakov loop, as well as the chiral limit of the pion mass that should indicate spontaneous chiral symmetry breaking. As the infinite mass limit is nothing but a confining regular Yang-Mills theory, this transition will exist for some value of $k$ if the theory is symmetric in the chiral limit. For $N_f$ down to values as low as 7, it was in fact found to occur. The location of this transition was further found to be independent of $N_t$, which would imply a true chiral symmetric zero temperature phase at $N_f = 7$ and up. Additional simulations were published over the course of several years [167, 168], using similar methodology. Here results were extended to extremely large flavour numbers, to obtain the limiting case of a chirally symmetric theory, and at finite coupling. The phase diagrams constructed on the basis of these give a fully symmetric chiral theory above a critical flavour number $N_f^c = 7$, even in the $\beta = 0$ limit.

It perhaps bears some stressing how counter-intuitive the appearance of a fixed point outside of the range predicted by the perturbation theory would be. The underlying mechanism for non-perturbative physics in the IR is the anti-shielding caused by gauge bosons coupling to themselves. Since fermion interactions are mediated by gauge bosons, an enhancement of the fermion sector would seem to imply a matching enhancement of the gauge bosons. For the shielding by fermions to overwhelm the anti-shielding of gauge bosons, it would seem they would have to interfere with the very mechanism that produces the shielding! Non-Abelian gauge theories are extraordinarily rich and such a mechanism may in fact exist, but it would have to be completely novel and no proposals for it have been made. At the same time, the absence of chiral symmetry breaking in the strong coupling $\beta \to 0$ limit – even away from the chiral limit – implies the absence of the confining bulk transition that is observed in simulations using staggered quarks. The latter is not particularly detrimental, since the bulk transition is a pure lattice artefact and its absence might be a consequence of the use of a Wilson action. Nevertheless, given their implications, the results of [166–168] should be put to scrutiny. Some potential issues are clearly present. For one, the expectation value of the Polyakov loop for different parameters constitutes the main part of the evidence, but this is not necessarily a useful observable in the presence of fermions. The papers do look at chiral symmetry, but use an extrapolation of the pseudo-scalar meson mass that is very susceptible to systematic errors. And it is exactly the magnitude of those systematic errors – the finite size and discretisation artefacts in this strong coupling limit – that remains unclear.

With the status of the lower bound of the conformal window unclear, it seemed advantageous to perform a detailed investigation of the theory far into the suspected conformal window. With a two-loop predicted IR fixed point $g^* \ll 1$ in combination with asymptotic freedom, the theory with $N_f = 16$ should be well described by perturbation theory. In [169], this setup was examined specifically. Not only was the location of a first order in both the chiral condensate and the string tension determined, but the spectrum of the theory in what was shown to be a chirally symmetric phase was studied. An innovative analysis was presented of the parameter dependence of the ratio of masses, which can be interpreted as an estimate of an effective beta function, and a change in sign of this beta function with respect to ordinary QCD
was found. Obviously, this effective beta function is both non-unique and measured away from the continuum limit, so lattice artefacts may well introduce spurious zeros. Nevertheless, data from simulations using the Schrödinger functional [170], which allows for studying the running of the coupling in a well defined scheme and in the chiral limit, corroborated the conclusions from [169]. The paper also presented an interesting comparison with the data from [165], providing a reanalysis of its data on the spectrum. The authors noted the apparent similarities between the dynamics found at $N_f = 8$ and 16, but in fact found an opposite sign of the beta function for both. At this point, the jury was still out on the extraordinarily low bound on the conformal window.

This confusing state of affairs was the backdrop of a second surge in lattice investigations of the conformal window. A window of potential progress had opened up by the rapid development of computer resources, but also remarkable strides on the algorithmic side. All lattice studies up to this point had been conducted using the Wilson plaquette action and naive staggered fermions. Through the use of improvement strategies, the accuracy of these results could be improved upon dramatically. At the vanguard of these results were papers on the running of the coupling at different flavour numbers [171, 172]. By means of a Schrödinger functional, these papers demonstrated a clear quantitative difference in the running of the coupling between $N_f = 8$ on the one hand and $N_f = 12$ and 16 on the other. For the former, a rapid increase of the coupling at larger distances $L$ was found. The latter showed an asymptotic approach to a fixed coupling from both above and below. These results are not scheme independent, however, so they cannot demonstrate the existence of an IR fixed point in themselves. But if not ironclad proof, the results of [171, 172] were strongly indicative of a conformal window being bounded by $8 < N_f^* < 12$. With this, lattice data appeared to come in line with analytical predictions.

Started before the publication of [171], the paper [173] included in this thesis as chapter 3 re-examined the setup of [165] at larger volumes and with an improved action and found results consistent with those of the Schrödinger function. Chapter 4 was published as [174] and extended some of the methodology pioneered in [169] to the $N_f = 12$ theory. As these papers will receive ample attention in coming chapters, we here only note their position in the time line of publications. Preliminary data from what amounted to a follow up study to [165] were shown in [175, 176]. The use of a highly improved action on larger volumes were intended to resolve the ambiguity of the previous paper and cast light upon the nature of QCD with twelve flavours. Agreement with the results of [171, 173] was found for $N_f = 8$. For the case of $N_f = 12$, strong finite volume effects complicated the analysis. Another noteworthy ongoing attempt at pinning down the chiral dynamics from a study of the spectrum is that of Fodor and collaborators [177–179]. In this program, an attempt was made to fully control systematics due to volume and taste symmetry breaking and account for these explicitly in the spectrum of meson masses and eigenvalues of the Dirac operator. Such efforts included the study of the system explicitly in the regime of small volumes. While this approach provides a radical solution for the issue of poorly controlled systematics first presented in [165], the move away from a continuum limit approximation complicates the interpretation of results. For both
these programs, chiral symmetry restoration was determined mainly from the mass spectrum of light mesons and their decay constants. Our understanding of these is grounded large in chiral perturbation theory and the applicability of results obtained in that framework may be limited in this context.

Another interesting approach is taken by A. Hasenfratz in a series of lattice studies of the RG flow, using Monte Carlo renormalisation group [180] calculations with a 2-lattice matching technique [181]. The gist of this technique lies in a blocking renormalisation in the spirit of Wilson. In the studies described here, a factor two blocking operation is defined according to

$$V_{n,\mu} = \text{Proj} \left[ (1 - \alpha) U_{n,\mu} U_{n+\mu,\mu} + \frac{\alpha}{6} \sum_{\nu \neq \mu} U_{n,\nu} U_{n+v,\mu} U_{n+\mu+v,\mu} U_{n+2\mu,\nu}^\dagger \right],$$

(1.27)

where the projection operator is onto elements of SU(3) and $\alpha$ presents an arbitrary parameter that can be tweaked for optimization. Using this operator, a new, blocked lattice can be produced from an existing one. Expectation values measured on this blocked lattice can be seen as results obtained from a momentum rescaled theory. By tuning input parameters to a separate run such that the blocked expectation values are reproduced, the effect of blocking on the parameters can be quantified. In principle, it possible to trace out the RG flow by these means and demonstrate a fixed point in the theory directly. Given a sufficient number of blocking steps, such a fixed point can eventually be connected to the perturbative, asymptotically free regime. A preliminary study [182] investigated the feasibility of this technique for known cases, examining $N_f = 4$ and 16, as well as pure Yang-Mills, using an aggressively improved gauge action. An effective massless limit was supposed at feasibly low quark masses. Using this effective limit, the complex procedure of tuning a multidimensional parameter space could be factorized: The coupling could be tuned by itself, followed by the mass at the fixed point away from the chiral limit to determine the anomalous dimension. For $N_f = 16$, indications of the presence an IR fixed point were found as expected. In addition, a measurement of the anomalous dimension of the mass at the fixed point was performed and it was found to be statistically vanishing. Preliminary data for the disputed case of $N_f = 12$, presented in [183], indicated the absence of a fixed point and indeed the absence of a bulk transition in the intermediate coupling regime. A later publication [184] actually retracted these conclusions, reporting that indications of the presence of a fixed point were found, though it was impossible to distinguish between slow walking behaviour and the presence of an actual fixed point. The anomalous dimension of the mass was again found to be vanishing. Here, too, the case of $N_f = 8$ was found to have no pseudo-conformal phase.

Summarizing, lattice studies of flavour-extended QCD, while initially conflicting with analytical predictions, have in the past few years been converging towards those. The lower bound of the conformal window has been all but unanimously found to be above $N_f = 8$, as one would expect from perturbation theory alone. While the case of $N_f = 12$ is somewhat disputed, those investigations drawing firm conclusions have found it to be (just) inside the conformal window. Barring surpris-
ing developments, the emphasis of lattice studies is set to move towards the inves-
tigation of the properties of the pseudo-conformal phase. It is perhaps unfortunate
that $N_f = 12$ should present an apparent boundary case, as one would perhaps pre-
fer to study a strongly coupled theory slightly deeper into the conformal window.
Unfortunately, the study of physics away from the natural multiples of four using
staggered fermions, possibly even at non-integer flavour numbers, would require
the rooting procedure mentioned earlier, which could introduce additional system-
atics [158].

1.4.1 Non-fundamental fermions
There has been quite some recent activity in the simulation of fermions in higher
dimensional representations, which has focused mainly on two cases where the con-
formal window is expected to open up at low flavour numbers. These are the two-
index symmetric (2S, or sextet) representation of SU(3) and the adjoint representa-
tion of SU(2).

Chiral symmetry breaking in theories including sextet fermions was first studied
in [185] using a staggered fermion formulation and matching gauge simulations to
predictions form random matrix theory [186, 187]. This approach was used again
in [178], but using overlap fermions that more faithfully reproduce the zero mode
spectrum. The pattern of chiral symmetry breaking in an SU(3) gauge theory with
sextet and fundamental fermions was compared, and it was concluded that no es-
sential differences existed between the representations in this respect. A previous
paper [179] had found similar results in the same setup, finding a topological charge
definition equivalent up to lattice artefacts from both fermion formulations. The rel-
evance of these observations lies in the functional equivalence of the higher dimen-
sional fermions in the modification of underlying gauge dynamics. As explained
above, there representation should be far more efficient and trigger the appearance
of an IR fixed point at much lower flavour numbers. Numerical support of this sce-
ario was first obtained in [188]. In an approach resembling [171], a Schrödinger
functional step scaling analysis was performed of an SU(3) gauge theory with two
sextet fermions in the Wilson formulation. Evidence was found for the existence of a
zero in the discrete beta function of the theory at rather weak coupling. This would
indicate the existence of an IR fixed point. The option was left open, however, of the
existence of a spurious zero in the discrete approximation due to the generation of
new non-perturbative degrees of freedom, as proposed in [189]. A direct investiga-
tion of the phase structure of this theory [190], used clover fermions on volumes up
to $12^4$. From measurements of the meson spectrum and the static potential, it pro-
vided evidence of a vacuum transition between a chirally broken strong coupling
and a chirally symmetric asymptotically free limit – again consistent with the exis-
tence of an IR fixed point in the theory. Interestingly, no indication was found for
the separation between a deconfinement and chiral transition, in contrast to the re-
sults of an early quenched study of sextet fermions [191] and the findings for adjoint
fermions mentioned below. Reported in a separate paper was the volume scaling of
the low lying eigenvalues for these runs, which was found to be atypical [192]. It was
hypothesised that the observed pattern of scaling was consistent with the existence
with an IR fixed point with a sizeable anomalous dimension.

For SU(2) theories, the two-index symmetric representation actually coincides with the adjoint representation. A number of papers published on SU(2) with adjoint fermions can therefore be seen as the smaller colour group analogues of the SU(3) sextet studies. Out of interest in the possible realisation of walking technicolour, Catterall and Sannino [193] compared the spectrum of SU(2) with two fundamental and two adjoint Wilson fermions. For the adjoint representation, the conformal window opens up perturbatively at $N_f = 1.0625$ already, but since the estimate of [103] raised this to $N_f = 2.075$, slow walking behaviour was expected for the latter. Qualitative differences in the $\pi$ and $\rho$ spectra were in fact observed at weak coupling, with the masses becoming very light for adjoint fermions. Some hints of an unexpected full restoration of chiral symmetry were actually found, though the $4^3 \times 8$ volumes used in these simulations might well be too small to obtain accurate results. Volumes were doubled in the follow up paper [194], where the authors, similar to the case of fundamental fermions, find a first order phase transition at strong coupling they identify as a lattice artefact. Even in this setup, however, it turned out to be ultimately impossible to distinguish between a slowly walking theory, or one generating an IR fixed point. An extensive study of the same spectrum was done by Del Debbio et al. [195–197], using Wilson fermions on a range of volumes up to $16^3 \times 32$ and investing heavily in controlling systematics. They concluded that it was natural to interpret the mass hierarchy they observed, with the glueball states lying well below the mesonic spectra, as being induced by conformal physics. Still, they postponed any definite conclusions to future studies aimed at simultaneously extrapolating to the chiral and continuum limit. Finally, the bulk transition observed in [194] was found as well in [198], at decidedly larger volumes up to $24^4$. To the weak coupling side of the transition, a restoration of chiral symmetry occurred, but the authors could not exclude this being due to enhanced finite volume effects. With these indications of non-trivial IR behaviour of the theory, the same authors performed a Schrödinger functional scaling study in [199]. The discrete beta function measured opposite signs around a scheme dependent critical value of the coupling, directly confirming the existence of the fixed point and vindicating the perturbative estimate. However, as the fixed point was found to lie at much weaker coupling than that predicted by perturbation theory, non-perturbative effects should be large in this region.

1.5 Outline of this thesis

In the following chapters, we will discuss work on what roughly amounts to a gradual increase of flavour numbers. Chapter 2 is phenomenology oriented. It describes an analysis of the initial results of the European Twisted Mass Collaboration $N_f = 2 + 1 + 1$ simulations, the first lattice calculations to attempt and include a physically accurate strange and charm quark. Previously, the research program of the ETMC used $N_f = 2$ simulations exclusively, rather than the now somewhat current $N_f = 2 + 1$ setup. As discussed above, this is due to the peculiar construction of the twisted mass action, that works only for isospin doublets. The technical
challenges of accurately simulating quarks with three non-degenerate mass values separated at vastly different mass scales, described in this chapter, necessitate careful checks of the viability of the results. To this end, chapter 2 presents chiral fits showing the consistency of the data and the impact of systematics.

Chapter 3 moves beyond phenomenology and presents results on the thermodynamics of QCD with eight flavours. Proof is presented of the occurrence of a first order phase transition using an $O(a^2)$ improved action on a range of lattice volumes. Not only is the location of this transition demonstrated to be sensitive to finite volume effects, the scaling properties of this sensitivity are investigated in detail. By an application of the two loop beta function, it is found that the shift can be related to a physical temperature. Having found a thermal phase transition, it is concluded no chirally symmetric vacuum exists at zero temperature. These results contrast with the ambiguous conclusions of [165] and are fully compatible with [171]. To our knowledge, these are the first studies showing thermal scaling in a theory with large flavour number.

In chapter 4, the approach of chapter 3 is extended to the case of twelve flavours. This peculiar value of $N_f$ is crucial, in that it is predicted to be sufficient to trigger a fixed point by most analytical approaches and results consistent with a fixed point here were found in [171]. We determine the location of the chiral symmetry breaking phase transition and demonstrate it has the hallmarks of a bulk phase transition. It is demonstrated that chiral symmetry is restored on the weak coupling side of the transition and that the approximation to the beta function first introduced in [169] produces a positive sign for the beta function. These properties are argued to be strongly suggestive of the existence of a fixed point.

Building on these findings, chapter 5 presents preliminary results on a range of observables for simulations with twelve quark flavours. The mass dependence of the bulk transition is investigated and it is found smooth transition found in chapter 3 turns from a crossover into a sharp first order phase transition as the chiral limit is approached. Somewhat surprisingly, a secondary transition appears as the crossover transition becomes first order. We provide arguments why this transition is in all likelihood a lattice artefact, without consequences for continuum physics. Data are also shown for the Polyakov loop and the static potential. The former does not produce a signal at zero temperature, but the mass dependence of the string tension gives a promising probe of conformal physics. Finally, the approach to the perturbative regime is studied from the plaquette expectation value, for which a stochastic estimate of the perturbative series is anticipated. It is found that non-perturbative effects dominate the results for the coupling constants at which results are currently available.

This thesis will conclude with a short, but critical discussion of the results presented and their position in the landscape of current literature. Suggestions are made for the continuation of this research program and the improvement of the results obtained from it so far.
Chiral properties of $N_f = 2 + 1 + 1$ twisted mass fermions

Accurate phenomenological predictions and their comparison with high precision experimental data are an important reason for studying lattice QCD in the context of the Standard Model (SM) and beyond the SM physics. Here the lattice formulation appears in a crucial supporting rôle, as it uniquely provides the quantitative access to strong interactions at all scales needed in the analysis of many strong and electroweak processes. As pointed out in chapter 1, the presence of the dynamical strange and in some cases also charm quarks is a requirement for a precise determination of electroweak processes. Our investigation of the effects of adding flavours naturally starts by considering lattice QCD phenomenology in the presence of an increased number of mass non-degenerate quarks, ultimately at their physical masses.

In this chapter, we present the first results of simulations including a dynamical charm with Wilson-like fermions. These runs are performed with $N_f = 2 + 1 + 1$ flavours of dynamical twisted mass fermions at maximal twist: a degenerate light doublet and a mass split heavy doublet. An overview of the input parameters and tuning status of our ensembles is given, together with a comparison with results obtained with $N_f = 2$ flavours. The problem of extracting the mass of the K- and D-mesons is discussed, and the tuning of the strange and charm quark masses examined. Finally we compare two methods of extracting the lattice spacings to check the consistency of our data and we present some first results of chiral perturbation theory fits in the light meson sector.

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1Based on ETM Collaboration (R. Baron et al.), Journal of High Energy Physics 1006, 111 (2010).
As was stated in chapter 1, the main strength of the twisted formulation lies in the automatic $O(a)$ improvement of physical observables. Detailed studies of the continuum-limit scaling in the quenched approximation [200–203] and with two dynamical quarks [204–207] have demonstrated that, after an appropriate tuning procedure to maximal twist, lattice artefacts not only follow the expected $O(a^2)$ scaling behaviour [32], but also that the remaining $O(a^2)$ effects are small, in agreement with the conclusions drawn in [208]. The only exception found so far is the neutral pseudo-scalar mass, which shows significant $O(a^2)$ effects. This arises from the explicit breaking of both parity and isospin symmetry, which are however restored in the continuum limit with a rate of $O(a^2)$ as shown in [32] and numerically confirmed in [204,209]. Moreover, a recent analysis suggests that isospin breaking effects strongly affect only a limited set of observables, namely the neutral pion mass and kinematically related quantities [210,211]. Other advantages worth mentioning are the fact that the twisted mass term acts as an infrared regulator of the theory and that mixing patterns in the renormalisation procedure are expected to be simplified.

Having been introduced in [32,212], the approach is by now well established. The ETMC has obtained many physical results with two light degenerate twisted mass flavours ($N_f = 2$) [204,205,207,213–227] and a review can be found in [228].

An extension of the twisted mass framework is realised by adding a heavy mass-split doublet $(c,s)$ to the light degenerate mass doublet $(u,d)$. This formulation was introduced in [32,229] and first explored in [230]. As for the mass-degenerate case, the use of lattice action symmetries allows to prove the automatic $O(a)$ improvement of physical observables in the non-degenerate case [229,231]. First accounts of our work were presented at recent conferences [232,233]. Recently, results with $N_f = 2 + 1 + 1$ staggered fermions have been reported in [51,52,54], while numerous studies are presently performed with $N_f = 2$ and $2 + 1$ flavours [31,37,53,234–239]. The inclusion of the strange and charm degrees of freedom allows for a most complete description of light hadron physics and eventually opens the way to explore effects of a dynamical charm in genuinely strong interaction processes and in weak matrix elements.

Here, we concentrate on results in the light-quark sector using the charged pseudo-scalar mass $m_{PS}$ and decay constant $f_{PS}$ as basic observables involving up and down valence quarks only. In figure 2.1 we show the dependence of (a) $m_{PS}^2/2B_0\mu_t$ and (b) $f_{PS}$ as a function of the mass parameter $2B_0\mu_t$, together with a fit to SU(2) chiral perturbation theory ($\chi$PT) at the smallest value of the lattice spacing of $a \approx 0.078 $ fm and lattice gauge coupling $\beta = 1.95$. We summarise the fit results for the low energy constants in table 2.1. These are the main results of this chapter.

A comparison between data obtained with $N_f = 2 + 1 + 1$ and $N_f = 2$ flavours of quarks - see sections 2.2.3 and 2.3, and [204] - reveals a remarkable agreement for the results involving light-quark observables such as the pseudo-scalar mass and decay constant or the nucleon mass. This provides a strong indication in favour of the good quality of our data in this new setup. In particular, barring cancellations due to lattice discretisation errors, these results would suggest that the dynamical strange and charm degrees of freedom do not induce large effects in these light-quark observables. In the $N_f = 2$ case, data collected at four values of the lattice
Figure 2.1 (a) The charged pseudo-scalar mass ratio \( \frac{m_{PS}^2}{2B \mu_l} \) and (b) the pseudo-scalar decay constant \( f_{PS} \) as a function of \( 2B \mu_l \) fitted to SU(2) chiral perturbation theory, see table 2.1. The scale is set by the value of \( 2B \mu_l \) at which the ratio \( f_{PS}^{[L=\infty]} / m_{PS}^{[L=\infty]} \) assumes its physical value [37] \( f_{\pi}/m_{\pi} = 130.4(2)/135.0 \) (star). The lattice gauge coupling is \( \beta = 1.95 \) and the twisted light quark mass ranges from \( a\mu_l = 0.0025 \) to \( 0.0085 \), see equation eq:sl for its definition, corresponding to a range of the pseudo-scalar mass \( 270 \lesssim m_{PS} \lesssim 490 \) MeV. The kaon and D meson masses are tuned to their physical value, see table 2.4. The lightest point (open symbol) has not been included in the chiral fit, see the discussion in section 2.2.1.

The rest of this chapter is organised as follows. In section 2.1 we describe the gauge action and the twisted mass fermionic action for the light and heavy sectors of the theory. The realisation of \( O(a) \) improvement at maximal twist is also presented. In section 2.2 we define the simulation parameters, describe the tuning to maximal twist as well as the tuning of the strange and charm quark masses and the relevance of discretisation effects. Section 2.3 includes a discussion of the fits to SU(2) \( \chi PT \) also for data on a slightly coarser lattice, \( a \approx 0.086 \) fm, and provides a first account of systematic uncertainties. Our conclusions and future prospects are summarised in section 2.4.
\[ \beta = 1.95 \]

| \( \bar{l}_3 \) | 3.70(7)(26) |
| \( \bar{l}_4 \) | 4.67(3)(10) |
| \( f_0 \) [MeV] | 121.14(8)(19) |
| \( f_\pi / f_0 \) | 1.076(1)(2) |
| \( 2B_0 \mu_{ud} / m^2_\pi \) | 1.032(1)(3) |
| \( \langle r^2 \rangle_\text{NLO} \) [fm\(^2\)] | 0.724(5)(23) |
| \( r_0^4 / a(\beta = 1.95) \) | 5.71(4) |
| \( r_0^4 (\beta = 1.95) \) [fm] | 0.447(5) |
| \( a(\beta = 1.95) \) [fm] | 0.0782(6) |

Table 2.1 Results of the fits to SU(2) \( \chi \)PT for the ensemble at \( \beta = 1.95 \). Predicted quantities are: the low energy constants \( \bar{l}_{3,4} \), the charged pseudo-scalar decay constant in the chiral limit \( f_0 \), the mass ratio \( 2B_0 \mu_{ud} / m^2_\pi \) at the physical point and the pion scalar radius \( \langle r^2 \rangle_\text{NLO} \). The first quoted error is from the chiral fit at \( \beta = 1.95 \), the second error is the systematic uncertainty that conservatively accommodates the best fitted central values of the three fits reported in table 2.9, section 2.3. The small error on the quoted lattice spacing comes exclusively from the fit at \( \beta = 1.95 \). The scale is set by fixing the ratio \( f_\text{PS}[L=\infty] / m_\text{PS}[L=\infty] = f_\pi / m_\pi = 130.4(2) / 135.0 \) to its physical value [37]. The chirally extrapolated Sommer scale \( r_0^4 \) is determined separately and not included in the \( \chi \)PT fits. For a comparison with the \( N_f = 2 \) ETMC results, see [233].

### 2.1 Lattice action

The general principle behind the numerical computation of QCD path integrals is the calculation of a weighted average of measurements to obtain expectation values of operators. In this setup, the measurements are of QCD operators on fixed background gauge field configurations and they are weighted by a Boltzmann factor \( \exp[-S] \), \( S \) being the action of the system. This construction will provide a stochastic approximation to a Euclidean (and discretised) path integral calculation for the operator under consideration. In general, we can write both the continuum and discretised action for QCD with four dynamical fermion flavours as

\[
S = S_g + S_l + S_h ,
\]

where \( S_g \) is the pure gauge action, \( S_l \) the fermion action for the light flavours \( u \) and \( d \) and \( S_h \) the action for the heavy flavours \( s \) and \( c \). We will describe each of these contributions separately for the case of our simulations, adding the standard derivations from literature for pedagogical purposes.
2.1 Lattice action

2.1.1 Gauge action

In the continuum formulation, the pure gauge action in Minkowski space is given by

\[ S_g = -\frac{1}{4} \int d^4 x \, F_{\mu\nu} F^{\mu\nu}, \quad (2.2) \]

where we suppress the coordinate dependence \( x \) for all fields. The field strength tensor \( F_{\mu\nu} \) can of course be written as a commutator of covariant derivatives

\[ D_\mu = \partial_\mu - ig t^a A^a_\mu, \quad (2.3) \]

where \( g \) is the coupling constant of the gauge field, \( t^a \) are the generators of SU(3) and \( A^a_\mu \) the associated gauge potential. The latter are not suitable as fundamental degrees of freedom on the lattice, as we cannot write a discretised action that preserves gauge invariance using a finite number of these. Instead, we introduce link variables \( U_\mu(x) \) that connect different sites on our lattice over a difference of the lattice spacing \( a \). These are matrix-valued finite elements of SU(3) and therefore have straightforward gauge transformation rules

\[ U_\mu(x) \rightarrow V(x) U_\mu(x) V^\dagger(x + \hat{\mu}), \quad (2.4) \]

where \( V(x) \) is a field of SU(3) matrices defining a local gauge transformation. A discretised gauge action should be written in terms of these discrete degrees of freedom \( U_\mu(x) \).

Since the field strength tensor is defined through a commutator of derivatives, it is natural to look for a discretisation of equation 2.2 in terms of a lattice analogue to the gauge invariant product of commutators \( F_{\mu\nu} F^{\mu\nu} \). It is easily seen from equation 2.4 that any closed loop of gauge links \( U_\mu \) (also known as a Wilson loop) will be gauge invariant, since every matrix \( V(x) \) will be multiplied by a complementary matrix \( V^\dagger(x) \). The smallest such Wilson loop

\[ W_{1,1,1}^{x,\mu,\nu} = U_\mu(x) U_\nu(x + \hat{\mu}) U_\mu^\dagger(x + \hat{\nu}) U_\nu^\dagger(x) \quad (2.5) \]

is known as a plaquette and is similar to a commutator of covariant derivatives in that it measures the local curvature of the gauge field. To insert it in the expression for the action, we take its trace (closing the indices \( \mu \) and \( \nu \)) and average over the plaquettes and their hermitian conjugates to obtain just the real part of equation 2.5. Inserting for the matrices \( U_\mu \) the identification \( U_\mu = \exp \left[ ig A_\mu(x + \hat{\mu}/2) \right] \), we find [240]

\[ \text{Re Tr} \, W_{1,1,1}^{x,\mu,\nu} = \text{Re Tr} \exp \left[ i g \left( A_\mu \left( x + \frac{\hat{\mu}}{2} \right) + A_\mu \left( x + \hat{\mu} + \frac{\hat{\nu}}{2} \right) - A_\mu \left( x + \hat{\nu} + \frac{\hat{\mu}}{2} \right) - A_\mu \left( x + \frac{\hat{\nu}}{2} \right) \right) \right]. \quad (2.6) \]
Note that the lattice is defined with a Euclidean metric, so the continuum limit of a correct lattice gauge action should provide the Wick rotated equivalent of equation 2.2. Expanding the expression of equation 2.6 around the centre of the plaquette $x + \hat{\mu}/2 + \hat{\nu}/2$ and using a finite difference approximation to the derivative gives us

$$\text{Re Tr } W_{x,\mu,\nu}^{1 \times 1} = 1 - \frac{a^4 g^2}{2} (\partial_\mu A_\nu - \partial_\nu A_\mu)^2 + \mathcal{O}(a^8) = 1 - \frac{a^4 g^2}{2} F_{\mu\nu}^2 + \mathcal{O}(a^6),$$  

(2.7)

with $F_{\mu\nu}^2$ the Euclidean analogue of $F_{\mu\nu} F_{\mu\nu}$. We can therefore write

$$S_g = \frac{a^4}{4} \sum_x \sum_{\mu,\nu} F_{\mu\nu}^2 = \frac{1}{g^2} \sum_x \sum_{\mu,\nu} \left(1 - \text{Re Tr } W_{x,\mu,\nu}^{1 \times 1}\right),$$  

(2.8)

which is usually referred to as the Wilson plaquette action. Its continuum limit is the SU(3) Yang-Mills action of equation 2.2, though it will differ by a value of $\mathcal{O}(a^2)$ from this action at any finite lattice spacing. The result of equation 2.8 is of course not a unique discretisation of equation 2.2. Any closed loop on the lattice with zero winding number will shrink to a single point in the continuum limit and reduce to a Yang-Mills action, though the expressions will differ at higher orders in $a$. This property is exploited in the so-called Symanzik improvement, where different Wilson loops are added together to obtain alternative lattice actions with reduced lattice spacing dependence. By tuning the coefficients of these different contributions suitably, an improved gauge action can be found that differs from the continuum action only by terms at higher order in $a$.

For the simulations of this chapter, we use a particular type of improved action known as the Iwasaki gauge action [241,242]. It includes, besides the plaquette term $W_{x,\mu,\nu}^{1 \times 1}$ also rectangular $(1 \times 2)$ Wilson loops $W_{x,\mu,\nu}^{1 \times 2}$

$$S_g = \frac{\beta}{3} \sum_x \left( b_0 \sum_{\mu,\nu=1}^{4} \{1 - \text{Re Tr } W_{x,\mu,\nu}^{1 \times 1}\} + b_1 \sum_{\mu,\nu=1}^{4} \sum_{\mu \neq \nu} \{1 - \text{Re Tr } W_{x,\mu,\nu}^{1 \times 2}\} \right),$$  

(2.9)

with $\beta = 6/g_0^2$ the bare inverse coupling, $b_1 = -0.331$ and the normalisation condition $b_0 = 1 - 8b_1$.

The choice for this action is motivated by the non trivial phase structure of Wilson-type fermions at finite values of the lattice spacing. The phase structure of the theory has been extensively studied analytically, by means of chiral perturbation theory [243–249], and numerically [250–255]. These studies provided evidence for a first order phase transition close to the chiral point for coarse lattices. This implies that simulations at non-vanishing lattice spacing cannot be performed with pseudoscalar masses below a minimal critical value.

The strength of the phase transition has been found [252,255] to be highly sensitive to the value of the parameter $b_1$ in the gauge action in equation 2.9. Moreover, in [230] it was observed that its strength grows when increasing the number of flavours in the sea from $N_f = 2$ to $N_f = 2 + 1 + 1$, at otherwise fixed physical
situation. Numerical studies with our \( N_f = 2 + 1 + 1 \) setup have shown that the Iwasaki gauge action, with \( b_1 = -0.331 \), provides a smoother dependence of phase transition sensitive quantities on the bare quark mass than the tree-level-improved Symanzik\(^{256,257}\) gauge action, with \( b_1 = -1/12 \), chosen for our \( N_f = 2 \) simulations.

Another way to weaken the strength of the phase transition is to modify the co-variant derivative in the fermion action by smearing the gauge fields. While the main results of this work do not use smearing of the gauge fields, we report in section 2.2.6 on our experience when applying a stout smearing\(^{258}\) procedure, see also\(^{259}\).

### 2.1.2 Action for the light and heavy doublet

The second component of the action contains the contribution of the light fermions. In Euclidean space, its continuum form reads

\[
S_L = \int d^4x \bar{\psi} (\mathcal{D} + m) \psi,
\]

the covariant derivative having been contracted with the Dirac \( \gamma \) matrices in their Euclidean form. It would seem straightforward to obtain a discretised expression by introducing a symmetric discrete derivative operator

\[
\left( \nabla_\mu + \nabla^*_\mu \right) = \frac{1}{2a} \left( U_\mu(x) \delta_{x,x+\hat{\mu}} - U^*_\mu(x-\hat{\mu}) \delta_{x,x-\hat{\mu}} \right),
\]

where \( \delta_{ij} \) indicates a Kronecker delta and the lattice spacing is set to 1 for notational convenience. This, however, will not work. If one sets all matrices \( U_\mu \) to the identity matrix to obtain a free fermion action and then Fourier transforms, one obtains the two-point Green’s function \( G(x,y) \) for this operator\(^{260}\)

\[
G(x,y) = \lim_{a \to 0} \pi/a \int_{-\pi/a}^{\pi/a} d^4p \frac{-i \sum_\mu \gamma_\mu \sin(a p_\mu) + m}{\sum_\mu \sin^2(a p_\mu) + m^2} \exp[ip(x-y)],
\]

where a trivial Kronecker delta on the colour indices is suppressed. The lattice spacing \( a \) functions as a UV regulator, because only momenta with a wavelength of at least twice that distance can be represented on the lattice and this limits the momentum \( p_\mu \) to values between \(-\pi/a\) and \(\pi/a\). Since the relevant range of momenta lies in the IR, the values of \( p_\mu \) thus removed are physically irrelevant for small values of \( a \). But while the factor \( \sin(ap_\mu) \) in equation 2.12 indeed becomes small for \( p_\mu = 0 \), it also vanishes at the edges of this first Brillouin zone, when \( ap_\mu = \pm \pi \). This implies that, next to the physical low energy modes, there are fifteen regions in momentum space contributing to the quark propagator. Since the edges of the first Brillouin zone move towards infinity in physical units as the continuum limit is approached, this limit of the expression represents the propagation of sixteen fermions in total, fifteen of which do so with infinite momentum. This problem is known as “fermion doubling” and it is an essential property of the theory, as it is due to the
CHAPTER 2  CHIRAL PROPERTIES OF $N_F = 2 + 1 + 1$

structure of the differential operators within the action and thereby the dimension of the fermion fields. Though it can be solved, the Nielsen-Ninomiya theorem [261] essentially states that it cannot be done with a local and translationally invariant operator while preserving chiral symmetry.

The Nielsen-Ninomiya theorem, its circumvention by reinterpreting the realization of chiral symmetry on the lattice [262] and the construction of lattice fermion operators in general are very rich topics, that cannot be done justice here. A unified overview of the myriad different approaches appears to currently be available only through the standard works on lattice QCD [240,260,263–266] and recent overviews on dynamical ensembles [29,267,268] and references contained therein. For now, we will focus on those formulations relevant to this thesis. The original proposal by Kenneth Wilson [269] was the inclusion of an additional, chiral symmetry breaking contribution to the fermion action. A Laplacian operator, which has dimensions of mass squared, is irrelevant in a RG sense when acting on fermions. It will carry an additional factor of the lattice spacing $a$ in a lattice formulation and therefore vanish in the continuum limit. We therefore find

$$S_l = a^4 \sum_x \left\{ \frac{1}{2} \bar{\psi}(x) \left[ \gamma_\mu \left( \nabla_\mu + \nabla_\mu^* \right) - a r \nabla_\mu^* \nabla_\mu + m \right] \psi(x) \right\}, \quad (2.13)$$

where an arbitrary Wilson coefficient $r$ is introduced that is conventionally set to one. This construction removes the “doublers” from the theory, as it modifies the Green’s function to

$$G(x,y) = \frac{\pi}{\sum_{\mu} \sin^2(p_\mu)} \int_{-\pi}^{\pi} \frac{d^4 p}{(2\pi)^4} \frac{-i \sum_\mu \gamma_\mu \sin(p_\mu) + \bar{m}(p)}{\sum_\mu \sin^2(p_\mu) + \bar{m}(p)^2} \exp[ip(x-y)], \quad (2.14)$$

with a momentum dependent effective mass $\bar{m}(p)$ defined as

$$\bar{m}(p) = a m + \frac{2r}{a} \sum_\mu \sin^2 \left[ \frac{ap_\mu}{2} \right]. \quad (2.15)$$

Though the momentum dependent part of this effective mass will vanish for fixed values of $p_\mu$, it will diverge at the corners of the Brillouin zone. This decouples the doublers, but of course at the expense of breaking chiral symmetry of the continuum action for $m = 0$. As a consequence, Wilson fermions have a number of complications. The quark mass will have an additive renormalization, that necessitates fine-tuning to reach small quark masses. It can also lead to the appearance of so-called exceptional configurations [270], where the current quark mass is driven to effectively negative values.

The basic construction of Wilson fermions outlined above can be refined further, in order to suppress lattice spacing artefacts and improve the properties of the operator towards the chiral limit. A particularly interesting type of improvement is achieved by adding a mass term of the form $i\mu \gamma^5 \tau^3$, where $\tau^3$ is the third Pauli matrix acting in flavour space. The lattice action for the mass degenerate light doublet
2.1 Lattice action

\((u,d)\), written in what is commonly referred to as the twisted basis reads \([32,212]\)

\[
S_l = a^4 \sum_x \{ \bar{\chi}_l(x) [D[U] + m_{0,l} + i\mu_l \gamma_5 \tau_3] \chi_l(x) \},
\]

(2.16)

where \(m_{0,l}\) denotes the untwisted bare quark mass, \(\mu_l\) is the bare twisted light quark mass and once again

\[
D[U] = \frac{1}{2} \left[ \gamma_\mu \left( \nabla_\mu + \nabla^*_\mu \right) - a \nabla^*_\mu \nabla_\mu \right]
\]

is the massless Wilson-Dirac operator. \(\nabla_\mu\) and \(\nabla^*_\mu\) are the forward and backward gauge covariant difference operators, respectively. Twisted mass light fermions are said to be at maximal twist if the bare untwisted mass \(m_{0,l}\) is tuned to its critical value, \(m_{\text{crit}}\), the situation we shall reproduce in our simulations. The quark doublet \(\chi_l = (\chi_u, \chi_d)\) in the twisted basis is related by a chiral rotation to the quark doublet in the physical basis

\[
\psi^\text{phys}_l = e^{i\frac{2}{3}\omega_l \gamma_5 \tau_3} \chi_l, \quad \bar{\psi}^\text{phys}_l = \bar{\chi}_l e^{i\frac{2}{3}\omega_l \gamma_5 \tau_3},
\]

(2.17)

where the twisting angle \(\omega_l\) takes the value \(|\omega_l| \to \frac{\pi}{2}\) as \(|m_{0,l} - m_{\text{crit}}| \to 0\). We shall use the twisted basis throughout this chapter.

We introduce a dynamical strange quark by adding a twisted heavy mass-split doublet \(\chi_h = (\chi_c, \chi_s)\), thus also introducing a dynamical charm in our framework. As shown in \([229]\), a real quark determinant can in this case be obtained if the mass splitting is taken to be orthogonal in isospin space to the twist direction. We thus choose the construction \([229,231]\)

\[
S_h = a^4 \sum_x \{ \bar{\chi}_h(x) [D[U] + m_{0,h} + i\mu_\sigma \gamma_5 \tau_1 + \mu_\delta \tau_3] \chi_h(x) \},
\]

(2.18)

where \(m_{0,h}\) is the untwisted bare quark mass for the heavy doublet, \(\mu_\sigma\) the bare twisted mass – the twist is this time along the \(\tau_1\) direction – and \(\mu_\delta\) the mass splitting along the \(\tau_3\) direction.

The bare mass parameters \(\mu_\sigma\) and \(\mu_\delta\) of the non-degenerate heavy doublet are related to the physical renormalised strange and charm quark masses via \([231]\)

\[
\frac{(m_s)}{R} = Z_p^{-1} \left( \mu_\sigma - \frac{Z_p}{Z_S} \mu_\delta \right),
\]

\[
\frac{(m_c)}{R} = Z_p^{-1} \left( \mu_\sigma + \frac{Z_p}{Z_S} \mu_\delta \right),
\]

(2.19)

where \(Z_p\) and \(Z_S\) are the renormalisation constants of the pseudo-scalar and scalar quark densities, respectively, computed in the massless standard Wilson theory. A chiral rotation analogous to the one in the light sector transforms the heavy quark doublet from the twisted to the physical basis

\[
\psi^\text{phys}_h = e^{i\omega_h \gamma_5 \tau_1} \chi_h, \quad \bar{\psi}^\text{phys}_h = \bar{\chi}_h e^{i\omega_h \gamma_5 \tau_1},
\]

(2.20)
CHAPTER 2  CHIRAL PROPERTIES OF $N_F = 2 + 1 + 1$

where the twisting angle $\omega_h$ takes the value $|\omega_h| \to \frac{\pi}{2}$ as $|m_{0,h} - m_{\text{crit}}| \to 0$.

2.1.3 $O(a)$ improvement at maximal twist

One of the main advantages of Wilson twisted mass fermions is that by tuning the untwisted bare quark mass to its critical value, automatic $O(a)$ improvement of physical observables can be achieved.

Tuning the complete $N_f = 2 + 1 + 1$ action to maximal twist can in principle be performed by independently choosing the bare masses of the light and heavy sectors $m_{0,l}$ and $m_{0,h}$, resulting, however, in a quite demanding procedure. On the other hand, properties of the Wilson twisted mass formulation allow for a rather economical, while accurate alternative [32, 231, 271], where the choice $m_{0,l} = m_{0,h} \equiv 1/2\kappa - 4$ is made, and the hopping parameter $\kappa$ has been introduced.

Tuning to maximal twist, i.e. $\kappa = \kappa_{\text{crit}}$, is then achieved by choosing a parity odd operator $O$ and determine $m_{\text{crit}}$ (equivalently $\kappa_{\text{crit}}$) such that $O$ has vanishing expectation value. One appropriate quantity is the PCAC light quark mass [208, 251, 252]

$$m_{\text{PCAC}} = \frac{\sum_x \left\langle \partial_0 A^a_{\mu,l}(x,t) P^a_l(0) \right\rangle}{2 \sum_x \left\langle P^a_l(x,t) P^a_l(0) \right\rangle}, \quad a = 1, 2,$$

(2.21)

where

$$A^a_{\mu,l}(x) = \bar{\chi}_l(x) \gamma_\mu \gamma_5 \frac{\tau_a}{2} \chi_l(x), \quad P^a_l(x) = \bar{\chi}_l(x) \gamma_5 \frac{\tau_a}{2} \chi_l(x),$$

(2.22)

and we demand $m_{\text{PCAC}} = 0$. For the quenched [201] and the $N_f = 2$ case [233], this method has been found to be successful in providing the expected $O(a)$ improvement and effectively reducing residual $O(a^2)$ discretisation effects in the region of small quark masses [208].

The numerical precision required for the tuning of $m_{\text{PCAC}}$ to zero has been discussed in [215]. Contrary to the $N_f = 2$ case [213, 215], where this tuning was performed once at the minimal value of the twisted light mass considered in the simulations, we now perform the tuning at each value of the twisted light quark mass $\mu_l$ and the heavy-doublet quark mass parameters $\mu_\sigma$ and $\mu_\delta$. This obviously leaves more freedom in the choice of light quark masses for future computations.

Although theoretical arguments tell us that $O(a)$ improvement is at work in our setup, a dedicated continuum scaling study is always required to accurately quantify the actual magnitude of $O(a^2)$ effects. In section 2.2.3 we provide a first indication that such effects are indeed small, at least for the here considered light meson sector; currently ongoing computations at a significantly smaller lattice spacing will allow for a continuum limit scaling analysis in this setup.

2.2 Simulation details

We performed simulations at two values of the lattice gauge coupling $\beta = 1.90$ and 1.95, corresponding to values of the lattice spacing $a \approx 0.086$ fm and $a \approx 0.078$ fm,
2.2 Simulation details

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<td></td>
<td>0.197</td>
<td>$24^3 \times 48$</td>
</tr>
<tr>
<td>A100.24s</td>
<td>0.1631960</td>
<td>0.0100</td>
<td></td>
<td></td>
<td></td>
<td>$24^3 \times 48$</td>
</tr>
<tr>
<td>B25.32</td>
<td>1.95</td>
<td>0.1612420</td>
<td>0.0025</td>
<td>0.135</td>
<td>0.170</td>
<td>$32^3 \times 64$</td>
</tr>
<tr>
<td>B35.32</td>
<td>0.1612400</td>
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<tr>
<td>B55.32</td>
<td>0.1612360</td>
<td>0.0055</td>
<td></td>
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<td>$32^3 \times 64$</td>
</tr>
<tr>
<td>B75.32</td>
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<td>$32^3 \times 64$</td>
</tr>
<tr>
<td>B85.24</td>
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<td>0.0085</td>
<td></td>
<td></td>
<td></td>
<td>$24^3 \times 48$</td>
</tr>
</tbody>
</table>

Table 2.2 Summary of the $N_f = 2 + 1 + 1$ ensembles generated by ETMC at two values of the lattice coupling $\beta = 1.90$ and $\beta = 1.95$. From left to right, we quote the ensemble name, the value of inverse coupling $\beta$, the estimate of the critical value $\kappa_{\text{crit}}$, the light twisted mass $a\mu_l$, the heavy doublet mass parameters $a\mu_\sigma$ and $a\mu_\delta$ and the volume in units of the lattice spacing. Our notation for the ensemble names corresponds to $X.\mu_l. L$, with $X$ referring to the value of $\beta$ used. The run A100.24s is used to control the tuning of the strange and charm quark masses.

respectively. The parameters of each ensemble are reported in table 2.2. The charged pion mass $m_{\pi}$ ranges from 270 MeV to 510 MeV. Simulated volumes correspond to values of $m_{\pi} L$ ranging from 3.0 to 5.8, where the smaller volumes served to estimate finite volume effects, see table 2.3. Physical spatial volumes range from $(1.9 \text{ fm}^3)$ to $(2.8 \text{ fm}^3)$.

As already mentioned, the tuning to $\kappa_{\text{crit}}$ was performed independently for each value of the mass parameters $a\mu_l$, $a\mu_\sigma$ and $a\mu_\delta$. The mass parameters of the heavy doublet $a\mu_\sigma$ and $a\mu_\delta$ reported in table 2.2 are related to the strange and charm quark masses. In particular, they are fixed by requiring the simulated kaon and D meson masses to approximately take their physical values, as discussed in section 2.2.2. The simulation algorithm used to generate the ensembles includes in the light sector, a Hybrid Monte Carlo algorithm with multiple time scales and mass preconditioning, described in [272], while in the strange-charm sector a polynomial hybrid Monte Carlo (PHMC) algorithm [271, 273, 274]; the implementation of [275] is publicly available.

The positivity of the determinant of the Dirac operator is a property of the mass-degenerate Wilson twisted mass action, which does not necessarily hold in the non degenerate case for generic values of the mass parameters $\mu_\sigma$ and $\mu_\delta$.\footnote{However, the positivity of the determinant is guaranteed for $\mu_\sigma^2 > \mu_\delta^2$ [229, 231].}
CHAPTER 2 CHIRAL PROPERTIES OF $N_F = 2 + 1 + 1$

<table>
<thead>
<tr>
<th>Ensemble</th>
<th>$m_{PCAC}/\mu_l$</th>
<th>$m_{PS}L$</th>
<th>$\tau_{int}(\langle P \rangle)$</th>
<th>$\tau_{int}(amps)$</th>
<th>$\tau_{int}(amp_{PCAC})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A30.32</td>
<td>-0.123(87)</td>
<td>3.97</td>
<td>118(55)</td>
<td>2.7(4)</td>
<td>46(19)</td>
</tr>
<tr>
<td>A40.32</td>
<td>-0.055(55)</td>
<td>4.53</td>
<td>103(48)</td>
<td>4.1(7)</td>
<td>51(21)</td>
</tr>
<tr>
<td>A40.24</td>
<td>-0.148(83)</td>
<td>3.48</td>
<td>132(57)</td>
<td>$\leq 2$</td>
<td>35(12)</td>
</tr>
<tr>
<td>A40.20</td>
<td>-0.051(91)</td>
<td>2.97</td>
<td>55(25)</td>
<td>2.9(7)</td>
<td>26(12)</td>
</tr>
<tr>
<td>A50.32</td>
<td>0.064(24)</td>
<td>5.05</td>
<td>50(19)</td>
<td>3.0(5)</td>
<td>21(7)</td>
</tr>
<tr>
<td>A60.24</td>
<td>-0.037(50)</td>
<td>4.15</td>
<td>28(8)</td>
<td>2.0(2)</td>
<td>13(4)</td>
</tr>
<tr>
<td>A80.24</td>
<td>0.020(19)</td>
<td>4.77</td>
<td>23(7)</td>
<td>2.4(3)</td>
<td>10(2)</td>
</tr>
<tr>
<td>A100.24</td>
<td>0.025(18)</td>
<td>5.35</td>
<td>18(5)</td>
<td>2.3(3)</td>
<td>13(3)</td>
</tr>
<tr>
<td>A100.24s</td>
<td>0.045(18)</td>
<td>5.31</td>
<td>18(5)</td>
<td>6.2(1.1)</td>
<td>18(5)</td>
</tr>
<tr>
<td>B25.32</td>
<td>-0.185(69)</td>
<td>3.42</td>
<td>65(25)</td>
<td>3.6(6)</td>
<td>26(9)</td>
</tr>
<tr>
<td>B35.32</td>
<td>0.009(34)</td>
<td>4.03</td>
<td>54(19)</td>
<td>5.5(8)</td>
<td>41(14)</td>
</tr>
<tr>
<td>B55.32</td>
<td>-0.069(13)</td>
<td>4.97</td>
<td>12(3)</td>
<td>$\leq 2$</td>
<td>8(2)</td>
</tr>
<tr>
<td>B75.32</td>
<td>-0.047(12)</td>
<td>5.77</td>
<td>14(4)</td>
<td>3.3(5)</td>
<td>13(3)</td>
</tr>
<tr>
<td>B85.24</td>
<td>-0.001(16)</td>
<td>4.66</td>
<td>15(4)</td>
<td>2.2(2)</td>
<td>11(2)</td>
</tr>
</tbody>
</table>

Table 2.3 For each ensemble, from left to right the values of $m_{PCAC}/\mu_l$, $m_{PS}L$, the integrated autocorrelation time of the plaquette, $m_{PS}$ and $m_{PCAC}$ in units of the trajectory length. Every ensemble contains 5000 thermalised trajectories of length $\tau = 1$, except A40.24 which contains 8000 trajectories.

itivity is monitored by measuring the smallest eigenvalue $\lambda_{h,min}$ of $Q_h^\dagger Q_h$, where $Q_h = \gamma_5 \tau_3 D_h$ and $D_h$ is the Wilson Dirac operator of the non-degenerate twisted mass action in equation 2.18. We observe that $\lambda_{h,min}$ is roughly proportional to the renormalised strange quark mass squared. Since we choose the mass parameters $\mu_\sigma$ and $\mu_\delta$ such that the strange quark takes its physical value, a spectral gap in the distribution of $Q_h^\dagger Q_h$ is observed, implying that the determinant of $D_h$ does not change sign during the simulation. This is sufficient for the purpose of this thesis, but a detailed discussion of this issue will be the topic of a forthcoming publication.

To generate correlators we use stochastic sources and improve the signal-to-noise ratio by using the “one-end trick”, following the techniques also employed in our $N_f = 2$ simulations [215]. We have constructed all meson correlators with local (L), fuzzed (F) and Gaussian smeared (S) sources and sinks. The use of smeared or fuzzed sources has stronger impact on the extraction of the kaon and $D$ meson masses; results for the latter are reported in section 2.2.2. The strategy for the technically involved determination of these masses in the unitary $N_f = 2 + 1 + 1$ Wilson twisted mass formalism is a topic in and of itself, an extensive discussion of which can be found in [276].

2.2.1 Tuning to maximal twist

To guarantee $O(a)$ improvement of all physical observables while also avoiding residual $O(a^2)$ effects with decreasing pion mass, the numerical precision of the tuning to maximal twist – quantified by the deviation from zero of $m_{PCAC}$ – has to satisfy $|Z_A m_{PCAC}/\mu_l|_{\mu_\sigma,\mu_\delta,\mu_\beta} \lesssim a \Lambda_{QCD}$ [213,215,233]. The left-hand side contains
2.2 Simulation details

Figure 2.2 The ratio $m_{\text{PCAC}}/\mu_1$ for the ensembles at $\beta = 1.90$ and 1.95 at the largest simulated volumes and as a function of $2B_0\mu_1$. For both ensembles the ratio $m_{\text{PCAC}}/\mu_1$ satisfies the 10% level criterion, except for the lightest point at $\beta = 1.90$ and $\beta = 1.95$ (open symbols), also affected by larger statistical errors. We assume $Z_A = 1$, while the actual value $Z_A \lesssim 1$ can only improve all tuning conditions.

the renormalised ratio of the untwisted mass over the twisted light-quark mass. A similar condition should be fulfilled by the error on this ratio. For the current lattice spacings, $a\Lambda_{\text{QCD}} \approx 0.1$, while the values of the axial current renormalisation factor $Z_A$ have not yet been determined. Nevertheless, since $Z_A$ enters as an $O(1)$ multiplicative pre-factor, and it is expected to be $Z_A \lesssim 1$ for our ensembles\(^3\), we adopt the conservative choice $Z_A = 1$ in verifying the tuning condition.

Satisfying this constraint clearly requires a good statistical accuracy in the determination of the PCAC mass. The values of $m_{\text{PCAC}}/\mu_1$ reported in table 2.3 and shown in figure 2.2 are well satisfying the tuning condition to maximal twist, with the exception of the lightest mass point at $\beta = 1.90$ and $\beta = 1.95$. We notice that the autocorrelation time of $m_{\text{PCAC}}$ reported in table 2.3 grows with decreasing values of the light quark mass $\mu_1$, thus rendering the tuning more costly for the two lightest points. For the ensemble B25.32, we are currently performing a new simulation aiming at a more accurate tuning to $\kappa_{\text{crit}}$. We are also testing a reweighting procedure [232] in $\kappa$ on the same ensemble, in view of applying it to the other not optimally tuned ensemble A30.32, and to future simulations. In what follows, we use the lightest mass points for consistency checks, and we exclude them from the final $\chi^2$ fits. We also remind the reader that the small deviations from zero of $a m_{\text{PCAC}}$ will only affect the $O(a^2)$ lattice discretisation errors of physical observables [215].

\(^3\)Preliminary determinations of $Z_A$ from ongoing dedicated runs with four degenerate light flavours, indicate that $Z_A \sim 0.7 - 0.8$ for the ensembles considered in this work.
Figure 2.3 (a): $2m_K^2 - m_{PS}^2$, and (b): $m_D$, as a function of $m_{PS}^2$, for $\beta = 1.95$ (dark) and $\beta = 1.90$ (light). The physical point is indicated by a star. The kaon and $D$ meson masses appear to be properly tuned at $\beta = 1.95$. The ensembles at $\beta = 1.90$, $\mu_\delta = 0.190$ have a larger value of the strange quark mass, while the red point at $\beta = 1.90$, $a\mu_\delta = 0.197$ appears to be well tuned. Data points have been scaled with the lattice spacing $a = 0.08585(53)$ fm for $\beta = 1.90$, and $a = 0.07820(59)$ fm for $\beta = 1.95$, obtained in this work and where the errors are only statistical.

2.2.2 Tuning of the strange and charm quark masses

The mass parameters $\mu_\sigma$ and $\mu_\delta$ in the heavy doublet of the action in equation 2.18 can in principle be adjusted so as to match the renormalised strange and charm quark masses by use of equation 2.19. In practise, in this work, we fix the values of $\mu_\sigma$ and $\mu_\delta$ by requiring that the simulated kaon mass $m_K$ and $D$ meson mass $m_D$ approximately take their physical values.

A detailed description of the determination of the kaon and $D$ meson masses is separately given in [276], while figures 2.3(a) and 2.3(b) show the resulting dependence of $(2m_K^2 - m_{PS}^2)$ and $m_D$ upon the light pseudo-scalar mass squared for both ensembles, and compared with the physical point. Table 2.4 summarises their numerical values, while the corresponding values for $a\mu_\sigma$ and $a\mu_\delta$ are given in table 2.2. Observe also that, in order to be able to properly tune the strange and charm quark masses to their physical values, $a\mu_\sigma$ must be chosen larger than $a\mu_\delta$, since (see equation (6)) the ratio $Z_P/Z_S$ is significantly smaller than one [276].

While the kaon and $D$ meson masses at $\beta = 1.95$ are sufficiently well tuned to their physical values, the ensembles at $\beta = 1.90$ with $a\mu_\delta = 0.190$ carry a heavier kaon mass. The latter is instead visibly closer to its physical value for $a\mu_\delta = 0.197$, as can be inferred from figure 2.3(a). We are currently performing simulations with $a\mu_\delta = 0.197$ for other light quark masses. Moreover, another set of values of $\mu_\sigma$ and $\mu_\delta$ are currently being used at $\beta = 1.90$ to generate ensembles with a slightly lower
2.2 Simulation details

<table>
<thead>
<tr>
<th>Ensemble</th>
<th>$\beta$</th>
<th>$am_K$</th>
<th>$am_D$</th>
</tr>
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<tbody>
<tr>
<td>A30.32</td>
<td>1.90</td>
<td>0.25150(29)</td>
<td>0.9230(440)</td>
</tr>
<tr>
<td>A40.32</td>
<td></td>
<td>0.25666(23)</td>
<td>0.9216(109)</td>
</tr>
<tr>
<td>A40.24</td>
<td></td>
<td>0.25884(43)</td>
<td>0.9375(128)</td>
</tr>
<tr>
<td>A40.20</td>
<td></td>
<td>0.26130(135)</td>
<td>0.8701(152)</td>
</tr>
<tr>
<td>A50.32</td>
<td></td>
<td>0.26225(38)</td>
<td>0.9348(173)</td>
</tr>
<tr>
<td>A60.24</td>
<td></td>
<td>0.26695(52)</td>
<td>0.9298(118)</td>
</tr>
<tr>
<td>A80.24</td>
<td></td>
<td>0.27706(61)</td>
<td>0.9319(94)</td>
</tr>
<tr>
<td>A100.24</td>
<td></td>
<td>0.28807(34)</td>
<td>0.9427(99)</td>
</tr>
<tr>
<td>A100.24s</td>
<td></td>
<td>0.26502(90)</td>
<td>0.9742(133)</td>
</tr>
<tr>
<td>B25.32</td>
<td>1.95</td>
<td>0.21240(50)</td>
<td>0.8395(109)</td>
</tr>
<tr>
<td>B35.32</td>
<td></td>
<td>0.21840(28)</td>
<td>0.8286(85)</td>
</tr>
<tr>
<td>B55.32</td>
<td></td>
<td>0.22799(34)</td>
<td>0.8532(62)</td>
</tr>
<tr>
<td>B75.32</td>
<td></td>
<td>0.23753(32)</td>
<td>0.8361(127)</td>
</tr>
<tr>
<td>B85.24</td>
<td></td>
<td>0.24476(44)</td>
<td>0.8650(76)</td>
</tr>
</tbody>
</table>

Table 2.4 For each ensemble, the values of the kaon mass and the $D$ meson mass as determined in [276].

$D$ meson mass and a third value of the kaon mass, in order to properly interpolate the lattice data to the physical strange quark mass.

2.2.3 Discretisation effects in light-quark observables

In this section we explore discretisation effects in the analysed light-quark observables. To this aim we also make use of the determination of the chirally extrapolated $r_0$ value for our data samples, as discussed in the following section 2.2.4.

In figures 2.4(a) and 2.4(b) we study the sensitivity of the charged pion mass and decay constant to possible discretisation effects, by comparing the $N_f = 2 + 1 + 1$ data at $\beta = 1.90$ and $\beta = 1.95$ and the results obtained in twisted mass simulations with two dynamical flavours [233]. The alignment of all data points at different values of $\beta$ is in itself an indication of small discretisation effects. The comparison and good agreement with the $N_f = 2$ data seems also to suggest no significant dependence upon the inclusion of dynamical strange and charm quarks for these light observables, at least at the present level of accuracy and provided that no cancellations occur due to lattice discretisation effects. However, only a more complete study at significantly different lattice spacings will allow to draw conclusions.

In the same spirit, we show in figure 2.5 an analogous ratio plot where the nucleon mass data points are included. The alignment of all data and the good extrapolation to the physical point is again evident. We defer to future publications the analysis of the baryon spectrum and the study of discretisation effects in strange- and charm-quark observables.
CHAPTER 2  CHIRAL PROPERTIES OF $N_F = 2 + 1 + 1$

Figure 2.4 The quantity $\alpha f_{ps}$ as a function of $(am^2_{PS})$, with (a) $\alpha = r_0^\chi$ and (b) $\alpha = 1/f_0$, for the $N_f = 2 + 1 + 1$ data at $\beta = 1.90$ and $\beta = 1.95$, and for the $N_f = 2$ data at $\beta = 3.90$, $\beta = 4.05$ and $\beta = 4.20$ in [233]. The values of $r_0^\chi$ for $N_f = 2 + 1 + 1$ are given in tables 2.1 and 2.9.

2.2.4 The Sommer scale $r_0$

The Sommer scale $r_0$ [277] is a purely gluonic quantity extracted from the static interquark potential. Since the knowledge of its physical value remains rather imprecise, we use the chirally extrapolated lattice data for $r_0/a$ only as an effective way to compare results from different values of the lattice spacing. In this work, the lattice scale is extracted by performing $\chi$PT inspired fits to the very precise data for $a f_{ps}$ and $a m_{PS}$, and by using the physical values of $m_\pi$ and $f_\pi$ as inputs.

Figures 2.6(a) and 2.6(b) display the data for $r_0/a$ at both values of the lattice coupling $\beta = 1.90$ and 1.95, and as a function of the bare lattice mass squared. The data are reasonably well described by a quadratic dependence, as also previously found for our $N_f = 2$ ensembles. For a more detailed discussion of the possible functional forms and their theoretical interpretation see [233]. To extrapolate to the chiral limit, we have performed fits using the largest available volume at each value of the pseudo-scalar mass. The chirally extrapolated values for our $N_f = 2 + 1 + 1$ ensembles are $r_0^\chi/a = 5.231(38)$ at $\beta = 1.90$ and $r_0^\chi/a = 5.710(41)$ at $\beta = 1.95$, where the lightest points of both ensembles have been excluded from the extrapolation, consistently with the fact that they do not satisfy our most stringent tuning condition to maximal twist.

In order to meaningfully compare the dependence upon the light quark mass at the two different lattice couplings $\beta = 1.90$ and 1.95, we estimated the slope of the functional form $r_0/r_0^\chi = 1 + c_r(r_0^\chi m_{PS})^4$, where the explicit lattice spacing dependence has been removed. We observe a mild dependence on the light quark mass and similar slopes $c_r[\beta = 1.90] = -0.0379(37)$ and $c_r[\beta = 1.95] = -0.0234(69)$. It
2.2 Simulation details

Figure 2.5 The ratio $m_{PS}^2/f_{PS}^2$ as a function of $m_{PS}^2/m_{N}^2$, for the $N_f = 2 + 1 + 1$ ensembles at $\beta = 1.90$ and $\beta = 1.95$, compared to the $N_f = 2$ data at $\beta = 3.90$, $\beta = 4.05$ and $\beta = 4.20$ [233]. The physical point is shown as a star.

is also worth noticing that the dependence upon the light quark mass of the $N_f = 2 + 1 + 1$ data and that observed in the $N_f = 2$ case [233] are not significantly different.

2.2.5 Effects of isospin breaking

A most delicate aspect of the twisted mass formulation is the breaking of the isospin symmetry. Clear evidence for this breaking has been found in the $N_f = 2$ simulations by ETMC when comparing the neutral with the charged pion masses. Indeed, while the discretisation effects in the charged pion were observed to be very small, significant $O(a^2)$ corrections appear when studying the scaling to the continuum limit of the neutral pion [233]. Notice, however, that similar effects have not been observed in other quantities that are in principle sensitive to isospin breaking but not trivially related to the neutral pion mass. These observations are supported by theoretical considerations detailed in [210,278].

In the $N_f = 2 + 1 + 1$ case, it turns out that the isospin breaking effect in the mass difference of charged and neutral pion masses is larger than for $N_f = 2$ at fixed physical situation, as can be inferred from table 2.5. This could be due at least in part, of course, to different gauge actions being used in the $N_f = 2$ and $N_f = 2 + 1 + 1$ cases. Still, the same theoretical considerations as in [278] do apply to the case of $N_f = 2 + 1 + 1$ flavours, and it is expected that the same class of physical observables as for $N_f = 2$ will not be significantly affected by isospin breaking corrections. Having said that, a careful measure of this effect for each observable or class of observables is anyway mandatory. The increase of the pion mass splitting with increasing the number of flavours in the sea is in line with the observation [230] of a stronger
first order phase transition when moving from \( N_f = 2 \) to \( N_f = 2 + 1 + 1 \), as discussed in section 2.1.1. Indeed, the endpoint of the phase transition \([243, 244]\) corresponds to the critical value of the light twisted mass \( \mu_{l,c} \) where the neutral pion mass vanishes. The mass difference can be described by
\[
\frac{r_0}{a} = \frac{c}{(a \mu_l)^2},
\]
where the coefficient \( c \) is related to \( \mu_{l,c} \)[246, 247] and it is therefore a measure of the strength of the first order phase transition. Hence, a larger value of \( c \) means that simulations are to be performed at smaller values of the lattice spacing to reach, say, the physical point. Table 2.5 reports on the values of \( m^\pm_{PS}, m^0_{PS} \) and \( c \) for some examples taken from the \( \beta = 1.95 \) ensemble and the \( N_f = 2 \) ensemble with the closest values of the lattice spacing and physical charged pseudo-scalar mass. As anticipated, the coefficient \( c \) increases in absolute value from \( N_f = 2 \) to \( N_f = 2 + 1 + 1 \).

We are currently performing simulations at a significantly different and lower lattice spacing than the present ensembles. They will allow to determine the slope \( c \) for \( N_f = 2 + 1 + 1 \) more accurately and to better quantify the conditions to approach the physical point.

### 2.2.6 Stout smeared runs

In addition to our main simulation ensembles, we also performed runs with stout smeared gauge fields in the lattice fermionic action. The stout smearing as introduced in [258] was designed to have a smearing procedure which is analytic in the unsmeared link variables and hence well suited for HMC-type updating algorithms. In an earlier work with \( N_f = 2 \) quark flavours [259] we showed that using smeared

Figure 2.6 The Sommer scale \( r_0/a \) as a function of \((a \mu_l)^2\) for (a) \( \beta = 1.90 \) and (b) \( \beta = 1.95 \). The lines represent a linear extrapolation in \((a \mu_l)^2\) to the chiral limit. The lightest point (open symbol) is not included in the fits and we have always used the largest available volume for a given value of the mass.
2.2 Simulation details

<table>
<thead>
<tr>
<th>Ensemble</th>
<th>$\beta$</th>
<th>$r_0^m_{PS}$</th>
<th>$r_0^m_{PS}$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>B35.32</td>
<td>1.95</td>
<td>0.7196(57)</td>
<td>0.388(40)</td>
<td>-12.0(1.1)</td>
</tr>
<tr>
<td>B55.32</td>
<td>0.8861(67)</td>
<td>0.679(40)</td>
<td>-10.6(1.8)</td>
<td></td>
</tr>
<tr>
<td>$B_6, N_f = 2$</td>
<td>3.90</td>
<td>0.7113(66)</td>
<td>0.585(43)</td>
<td>-4.6(1.5)</td>
</tr>
<tr>
<td>$B_2, N_f = 2$</td>
<td>0.9001(86)</td>
<td>0.712(54)</td>
<td>-8.6(2.2)</td>
<td></td>
</tr>
</tbody>
</table>

Table 2.5 Measurements of the masses of the charged and the neutral pion. We compare runs at $\beta = 1.95$ and $N_f = 2$ runs [233] with comparable lattice spacing and similar charged pion masses in physical units. All masses are reported in units of the chirally extrapolated $r_0$ for the same ensemble, see table 2.9, and $r_0^a / a = 5.316(49)$ for $N_f = 2$. We also report on the approximate value of $c$, giving the slope of the $a^2$ dependence of the pion mass splitting.

<table>
<thead>
<tr>
<th>Ensemble</th>
<th>$\beta$</th>
<th>$\kappa_{crit}$</th>
<th>$a\mu_I$</th>
<th>$a\mu_\sigma$</th>
<th>$a\mu_\delta$</th>
<th>$N_{traj.}$</th>
<th>$r_0^a / a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A_{st}40.24</td>
<td>1.90</td>
<td>0.145512</td>
<td>0.0040</td>
<td>0.170</td>
<td>0.185</td>
<td>1500</td>
<td>5.304(35)</td>
</tr>
<tr>
<td>A_{st}60.24</td>
<td>0.145511</td>
<td>0.0060</td>
<td></td>
<td></td>
<td></td>
<td>3100</td>
<td>5.300(37)</td>
</tr>
<tr>
<td>A_{st}80.24</td>
<td>0.145510</td>
<td>0.0080</td>
<td></td>
<td></td>
<td></td>
<td>2000</td>
<td>5.353(43)</td>
</tr>
</tbody>
</table>

Table 2.6 Parameters of the runs with stout smearing on $L/a = 24, T/a = 48$ lattices. The number of thermalised trajectories with length $\tau = 1$ is given by $N_{traj}$. The label “st” in the ensemble name refers to the use of stout smearing, compared to the non stout-smeared ensemble in table 2.2.

The definition of the stout smeared links can be found in [258], and for the parameter $\rho$ connecting thin to fat gauge links we choose $\rho = 0.15$. In principle, such smearing can be iterated several times, with the price of rendering the fermion action de-localised over a larger lattice region. We made a conservative choice to maintain the action well localised and performed a single smearing step. As shown in [259], this kind of smearing does not substantially change the lattice spacing, and for the sake of comparison we thus kept the same value of $\beta$ as in one of the non stout-smeared runs. On the other hand, the hopping parameter has to be tuned again, since the additive renormalisation of the quark mass is expected to be smaller. The parameters of our runs are given in Table 2.6. These runs have been done with the two-step polynomial Hybrid Monte Carlo (TS-PHMC) update algorithm [279]. Re-

<table>
<thead>
<tr>
<th>Ensemble</th>
<th>$a m_{PS}$</th>
<th>$a m_K$</th>
<th>$a m_D$</th>
<th>$m_{PCAC}/\mu_I$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A_{st}40.24</td>
<td>0.12600(93)</td>
<td>0.2479(18)</td>
<td>0.802(27)</td>
<td>0.0175(68)</td>
</tr>
<tr>
<td>A_{st}60.24</td>
<td>0.14888(78)</td>
<td>0.25338(67)</td>
<td>0.825(26)</td>
<td>0.0017(50)</td>
</tr>
<tr>
<td>A_{st}80.24</td>
<td>0.17156(69)</td>
<td>0.26198(80)</td>
<td>0.811(12)</td>
<td>0.0138(48)</td>
</tr>
</tbody>
</table>

Table 2.7 The masses in lattice units for the ensembles with one level of stout smearing.
sults for the hadron masses are collected in table 2.7, where the quoted errors include an estimate of the systematic error induced by variations of the fitting range. The method of estimating and combining statistical and systematic errors for the case of the kaon and $D$ meson masses is described in [276].

As the values of $m_{PCAC}/\mu_i$ in table 2.7 show, the hopping parameters are well tuned to maximal twist. The masses in the run with smallest light twisted mass $a\mu_i = 0.0040$ (ensemble $A_{st40.24}$) satisfy $r_0 m_{PS} = 0.668(10)$, $r_0 m_K = 1.315(13)$ and $r_0 m_D = 4.25(29)$. This means that the pion is lighter than in the corresponding run without stout smearing (see table 2.8 and the kaon and $D$ meson masses are closer to their physical value. The smaller pion mass should be interpreted as due to a quark mass renormalisation factor closer to one. For the same reason the tuned twisted masses in the heavy doublet $a\mu_c = 0.170$, $a\mu_d = 0.185$ are smaller than in the runs without stout smearing. It is also interesting to compare the mass splitting of the charged and neutral pion between runs with and without stout smearing. For the ensemble $A_{st60.24}$ we obtain a neutral pion mass $r_0^\chi m_{PS}^0 = 0.409(34)$ and a charged pion mass $r_0^\chi m_{PS}^\pm = 0.7861(56)$, in units of the chirally extrapolated value $r_0^\chi / a = 5.280(25)$, providing an estimate of the slope $c = -12.6(0.8)$. Notice that the mass dependence of $r_0^\chi / a$ in table 2.6 is reduced as compared to the runs with no stout smearing, and a quadratic dependence on the bare quark mass has been used for the extrapolation to the chiral limit, consistently with the analysis of section 2.2.4. For the corresponding ensemble $A_{st60.24}$ without stout smearing, using data in tables 2.8 and 2.9, we obtain instead $r_0^\chi m_{PS}^0 = 0.560(37)$, $r_0^\chi m_{PS}^\pm = 0.9036(71)$, and a slope $c = -13.8(1.2)$, slightly but not significantly different from the stout-smearred case.

The runs with stout-smearred gauge links show somewhat better characteristics than the ones without stout smearing, but the improvements are not dramatic, at least with one level of stout smearing. More iterations would further accelerate the approach to lighter masses and are expected to further reduce the charged to neutral pion splitting. However, it is a delicate matter to establish how physical observables other than the spectrum will be affected. Based on these considerations and given the present pool of data, the final results in this chapter are obtained with non stout-smeared simulations.

### 2.3 Results: $f_{PS}$, $m_{PS}$ and chiral fits

We concentrate in this section on the analysis of the simplest and phenomenologically relevant observables involving up and down valence quarks. These are the light charged pseudo-scalar decay constant $f_{PS}$ and the light charged pseudo-scalar mass $m_{PS}$.

The present simulations with dynamical strange and charm quarks, sitting at, or varying around, their nature given masses, should allow for a good measure of the impact of strange and charm dynamics on the low energy sector of QCD and the electroweak matrix elements. As a first step, one can determine the low energy constants of chiral perturbation theory ($\chi$PT). The values of $af_{PS}$ and $am_{PS}$ for our ensembles at $\beta = 1.95$ and $\beta = 1.90$ are summarised in table 2.8. In contrast to
2.3 Results: $f_{PS}$, $m_{PS}$ and chiral fits

Table 2.8 Lattice measurements of the charged pseudo-scalar mass $m_{PS}$, the charged pseudo-scalar decay constant $f_{PS}$ and the Sommer scale in lattice units $r_0/a$ for our two ensembles at $\beta = 1.90$ (A set) and $\beta = 1.95$ (B set). The value of the light twisted mass $a\mu_l$ and the spatial length $L/a$ are also shown. Quoted errors are given as (statistical)(systematic), with the estimate of the systematic error coming from the uncertainty related to the fitting range.

<table>
<thead>
<tr>
<th>Ensemble</th>
<th>$a\mu_l$</th>
<th>$m_{PS}$</th>
<th>$f_{PS}$</th>
<th>$r_0/a$</th>
<th>$L/a$</th>
</tr>
</thead>
<tbody>
<tr>
<td>A30.32</td>
<td>0.0030</td>
<td>0.12395(36)(14)</td>
<td>0.06451(35)(3)</td>
<td>5.217(30)</td>
<td>32</td>
</tr>
<tr>
<td>A40.32</td>
<td>0.0040</td>
<td>0.14142(27)(42)</td>
<td>0.06791(18)(4)</td>
<td>5.179(49)</td>
<td>32</td>
</tr>
<tr>
<td>A40.24</td>
<td>0.0040</td>
<td>0.14492(52)(34)</td>
<td>0.06568(34)(7)</td>
<td>5.178(44)</td>
<td>24</td>
</tr>
<tr>
<td>A40.20</td>
<td>0.0040</td>
<td>0.14871(92)(116)</td>
<td>0.06194(65)(23)</td>
<td>-</td>
<td>20</td>
</tr>
<tr>
<td>A50.32</td>
<td>0.0050</td>
<td>0.15796(32)(28)</td>
<td>0.07048(16)(4)</td>
<td>5.081(45)</td>
<td>32</td>
</tr>
<tr>
<td>A60.24</td>
<td>0.0060</td>
<td>0.17275(45)(23)</td>
<td>0.07169(22)(2)</td>
<td>5.209(58)</td>
<td>24</td>
</tr>
<tr>
<td>A80.24</td>
<td>0.0080</td>
<td>0.19875(41)(35)</td>
<td>0.07623(21)(4)</td>
<td>4.989(40)</td>
<td>24</td>
</tr>
<tr>
<td>A100.24</td>
<td>0.0100</td>
<td>0.22293(35)(38)</td>
<td>0.07926(20)(4)</td>
<td>4.864(21)</td>
<td>24</td>
</tr>
<tr>
<td>A100.24s</td>
<td>0.0100</td>
<td>0.22125(58)(119)</td>
<td>0.07843(26)(21)</td>
<td>4.918(50)</td>
<td>24</td>
</tr>
<tr>
<td>B25.32</td>
<td>0.0025</td>
<td>0.10680(39)(27)</td>
<td>0.05727(36)(8)</td>
<td>5.728(35)</td>
<td>32</td>
</tr>
<tr>
<td>B35.32</td>
<td>0.0035</td>
<td>0.12602(30)(30)</td>
<td>0.06074(18)(8)</td>
<td>5.634(43)</td>
<td>32</td>
</tr>
<tr>
<td>B55.32</td>
<td>0.0055</td>
<td>0.15518(21)(33)</td>
<td>0.06557(15)(5)</td>
<td>5.662(33)</td>
<td>32</td>
</tr>
<tr>
<td>B75.32</td>
<td>0.0075</td>
<td>0.18020(27)(3)</td>
<td>0.06895(17)(1)</td>
<td>5.566(44)</td>
<td>32</td>
</tr>
<tr>
<td>B85.24</td>
<td>0.0085</td>
<td>0.19396(38)(54)</td>
<td>0.06999(20)(5)</td>
<td>5.493(41)</td>
<td>24</td>
</tr>
</tbody>
</table>

Table 2.8 Lattice measurements of the charged pseudo-scalar mass $m_{PS}$, the charged pseudo-scalar decay constant $f_{PS}$ and the Sommer scale in lattice units $r_0/a$ for our two ensembles at $\beta = 1.90$ (A set) and $\beta = 1.95$ (B set). The value of the light twisted mass $a\mu_l$ and the spatial length $L/a$ are also shown. Quoted errors are given as (statistical)(systematic), with the estimate of the systematic error coming from the uncertainty related to the fitting range.

With standard Wilson fermions, an exact lattice Ward identity for maximally twisted mass fermions allows for extracting the charged pseudo-scalar decay constant $f_{PS}$ from the relation

$$ f_{PS} = \frac{2\mu_l}{m_{PS}^2} |\langle 0 | P_1^1(0) | \pi \rangle|, \tag{2.23} $$

without need to specify any renormalisation factor, since $Z_P = 1/Z_{\mu}$ [212]. We have performed fits to NLO SU(2) continuum $\chi$PT at $\beta = 1.95$ and $\beta = 1.90$, separately and combined. Results are summarised in table 2.9.

We thus simultaneously fit our data for the pseudo-scalar mass and decay constant to the following formulae, where the contributions $F$, $D$ and $T$ parametrising finite size corrections, discretisation effects and NNLO $\chi$PT effects, respectively, will be discussed below:

$$ m_{PS}^2(L) = \chi_{\mu} \left( 1 + \zeta_3 l_3 + D_{m_{PS}^2} a^2 + \zeta_2^2 T_{m_{PS}^2} \right) F_{m_{PS}^2}, $$

$$ f_{PS}(L) = f_0 \left( 1 - 2\zeta_4 l_4 + D_{f_{PS}} a^2 + \zeta_2^2 T_{f_{PS}} \right) F_{f_{PS}}, \tag{2.24} $$

with the pseudo-scalar mass squared at tree level defined as $\chi_{\mu} = 2 B_0 \mu_l$ and the chiral expansion parameter by $\zeta \equiv \chi_{\mu} / (4\pi f_0)^2$. The low energy constants $l_3$ and $l_4$ receive renormalization corrections according to $l_i = l_i + \ln \left[ \Lambda^2 / \chi_{\mu} \right]$, with $\Lambda$ the reference scale. During the fitting procedure, where all quantities are defined in
CHAPTER 2  CHIRAL PROPERTIES OF $N_F = 2 + 1 + 1$

lattice units, we set the reference scale to a single lattice spacing to let its constant logarithmic contribution vanish. Once the scale of the simulation has been set, the low energy constants are rescaled to the scale of the physical pion mass to recover the physical values $\bar{l}_3$ and $\bar{l}_4$.

Systematic errors can arise from several sources: finite volume effects, neglecting of higher orders in $\chi$PT and finite lattice spacing effects. These different corrections are accounted for explicitly in equation 2.24. Finite volume corrections are described by the rescaling factors denoted by $F_{m_{PS}}^2$ and $F_{f_{ps}}$, computed in the continuum theory. Notice that the discretisation effects present in the neutral pion mass, see section 2.2.5, generate peculiar finite volume corrections which have been recently analysed in [280]. We shall comment on them later. We investigated the effectiveness of one loop continuum $\chi$PT finite volume corrections, as first computed in [281], which do not introduce any additional low energy constants. However, the resummed expressions derived by Colangelo, Dürr and Haefeli (CDH) in [282] describe the finite volume effects in our simulations better, be it at the expense of the introduction of two new free parameters, and are thus adopted for this analysis. To $O(\xi^2)$, these corrections read

$$F_{m_{PS}}^2 = \left[ 1 - \sum_{n=1}^{\infty} \frac{\rho_n}{2\lambda_n} \left( \bar{\xi} I_m^{(2)} + \bar{\xi}^2 I_m^{(4)} \right) \right]^2$$

$$F_{f_{ps}} = 1 + \sum_{n=1}^{\infty} \frac{\rho_n}{\lambda_n} \left( \bar{\xi} I_f^{(2)} + \bar{\xi}^2 I_f^{(4)} \right), \quad (2.25)$$

with geometric contributions defined as

$$I_m^{(2)} = -2K_1(\lambda_n)$$

$$I_m^{(4)} = \left( \frac{101}{9} - \frac{13}{3} \pi + 8l_1 + \frac{16}{3} l_2 - 5l_3 - 4l_4 \right) K_1(\lambda_n) +$$

$$\left( -\frac{238}{9} + \frac{61}{6} \pi - \frac{16}{3} l_1 - \frac{64}{3} l_2 \right) \frac{K_2(\lambda_n)}{\lambda_n}$$

$$I_f^{(2)} = -4K_1(\lambda_n)$$

$$I_f^{(4)} = \left( \frac{29}{18} - \frac{29}{12} \pi + 4l_1 + \frac{8}{3} l_2 - 6l_4 \right) K_1(\lambda_n) +$$

$$\left( -\frac{307}{9} + \frac{391}{24} \pi - \frac{16}{3} l_1 - \frac{64}{3} l_2 \right) \frac{K_2(\lambda_n)}{\lambda_n}. \quad (2.26)$$

The $K_i$ are the modified Bessel functions and the low energy constants $l_1$ and $l_2$ again receive renormalisation corrections. Equations 2.25 and 2.26 use the shorthand notation $\lambda_n = \sqrt{nmt_{PS}L}$. The $\rho_n$ in equation 2.25 are a set of multiplicities, counting the number of ways $n$ can be distributed over three spatial directions$^4$. Because the finite volume corrections in the case of the volumes used in the chiral fits are fairly small to begin with and subsequent terms quickly decrease, the sums over $n$

$^4$These values are straightforwardly precomputed to any order, but are also given in, e.g., [282].
can be truncated rather aggressively without real loss of precision. It is therefore unnecessary, in practise, to go beyond the lowest contributions. The parameters $l_1$ and $l_2$, which are in fact low energy constants appearing at NLO in $\chi$PT, cannot be determined well from the small finite volume corrections alone. Priors are therefore introduced as additional contributions to the $\chi^2$, weighting the deviation of the parameters from their phenomenological values by the uncertainties in the latter. The values used as priors are -0.4(6) for $l_1$ and 4.3(1) for $l_2$ [282], as reported in table 2.9. We used the largest available volumes for each ensemble, in the $\chi$PT fits. For those points, the difference between the finite volume and the infinite volume values estimated via CDH formulae for $f_{PS}$ and $m_{PS}^2$ are within 1%, except for the runs B85.24 and A60.24 (see table 2.2 and table 2.8, where they are about 1.5% for both quantities.

Because of the automatic $O(a)$ improvement of the twisted mass action at maximal twist, the leading order discretisation artefacts in the chiral formulae of 2.24 are at least of $O(a^2)$, and $O(a^2\mu)$ for $m_{PS}^2$. The mass and decay constant of the charged pion have been studied up to NLO [243, 246, 249] in the context of twisted mass chiral perturbation theory ($tm\chi$PT). The regime of quark masses and lattice spacings at which we have performed the simulations is such that $\mu l \gg a^2\Lambda_{QCD}$. In the associated power counting, at maximal twist, the NLO $tm\chi$PT expressions for the charged pion mass and decay constant preserve their continuum form. The inclusion of the terms proportional to $D_{m_{PS}^2,f_{PS}}$, parametrising the lattice artefacts in equation 2.24, represents an effective way of including sub-leading discretisation effects appearing at NNLO. The finite lattice spacing artefacts can of course not be determined using only data from a single lattice spacing. In addition, including these terms when analysing data with an insufficient range in $a$, may lead to mixing of these degrees of freedom with continuum parameters and thereby destabilise the fits. Hence, these terms were neglected for the separate fits, but included to arrive at a qualitative estimate of these systematic effects in a combined fit to the data at both lattice spacings.

Finite size effects on our data at finite lattice spacing can be analysed in the context of twisted mass chiral perturbation theory as recently proposed in [280]. However, our present limited set of data with only a small number of different volumes all of them at a single value of the lattice spacing, is not sufficient to apply such an analysis. We plan, however, to perform dedicated runs on different volumes to confront our data to the finite size effect formulae of [280] and to estimate in particular the size of the pion mass splitting in this alternative way.

Finally, results from continuum $\chi$PT at NNLO can be included to examine the effect of the truncation at NLO. They are given by

$$T_{m_{PS}^2} = \frac{17}{102} (49 + 28 l_1 + 32 l_2 - 9 l_3) + 4 k_m$$

$$T_{f_{PS}} = -\frac{1}{6} (23 + 14 l_1 + 16 l_2 + 6 l_3 - 6 l_4) + 4 k_f. \quad (2.27)$$

Two new parameters $k_m$ and $k_f$ enter these corrections. Again, a limited range of input pion masses may lead to poorly constrained values of these newly introduced

\[5\text{Notice that, in principle, after performing the continuum limit at fixed physical volume, finite size effects can be analysed by means of continuum } \chi\text{PT.}\]
parameters, some degree of mixing among different orders and fit instabilities. To retain predictive power and stability, additional priors are given for $k_m$ and $k_f$, both priors set to $0(1)$, analogously to what is done for $l_1$ and $l_2$ in the CDH finite volume corrections.

To set the scale at each lattice spacing, we determine $a\mu_{\text{phys}}$, the value of $a\mu_l$ at which the ratio $\sqrt{m_{\text{PS}}^2(L=\infty)/f_{\text{PS}}(L=\infty)}$ assumes its physical value. We can then use the value of $f_{\text{PS}}$, or equivalently $m_{\text{PS}}$, to calculate the lattice spacing $a$ in fm from the corresponding physical value. We also perform a chiral fit combining the two different lattice spacings. With only two different values of $\beta$, that are in fact fairly close to each other, a proper continuum limit analysis cannot be performed. Instead, we treat this combined fit as a check on the presence of lattice artefacts and the overall consistency of the data. Without a scaling variable, such as the Sommer scale $r_0$, the data from different lattice spacings cannot be directly combined. Rather, the ratios of lattice spacings and light quark mass renormalisation constants ($Z_{\mu} = 1/Z_P$), as well as the renormalised $B_0$ parameter are left free in the fit.

In order to estimate the statistical errors affecting our fitted parameters, we generate at each of the $\mu_l$ values 1000 bootstrap samples for $m_{\text{PS}}$ and $f_{\text{PS}}$ extracted from the bare correlators, organised by blocks. For each sample, and combining all masses, we fit $m_{\text{PS}}^2$ and $f_{\text{PS}}$ simultaneously as a function of $\mu_l$. The parameter set from each of these fits is then a separate bootstrap sample for the purposes of determining the error on our fit results. By resampling $f_{\text{PS}}$ and $m_{\text{PS}}$ on a per-configuration basis, correlations between these quantities are taken into account.

Our final results for the separate and combined fits are summarised in table 2.9. The $\chi^2$PT fit ansätze provide a satisfactory description of the lattice data, with a $\chi^2$/d.o.f = 5.68/3 $\approx$ 1.9 at $\beta = 1.95$, $\chi^2$/d.o.f = 4.31/5 $\approx$ 0.9 at $\beta = 1.90$, and $16.9/11 \approx 1.5$ for the combined fit. We also predict the scalar radius of the pion at next to leading order

$$\langle r^2 \rangle_{\text{NLO}} = \frac{12}{(4\pi f_0)^2} \left( \bar{I}_4 - \frac{13}{12} \right).$$

The numerical values in table 2.9 for the combined fit show a very good agreement with the results from the separate fits, and with errors at the percent level throughout. The fits for $f_{\text{PS}}$ and $m_{\text{PS}}$ at $\beta = 1.95$ are displayed in figures 2.1(a) and (b), while in figures 2.7(a) and (b) we show the analogous fits at $\beta = 1.90$. Figures 2.8(a) and (b) show the results for the fit combining the two $\beta$ values.

The data presented here do not allow yet for a complete account of the systematic effects, but we extract estimates of their magnitude by extending the fits with additional terms as written down in equation 2.24. Checks were done for $\chi^2$PT NNLO terms and $O(a^2)$ corrections separately. Including NNLO corrections does not lower the total $\chi^2$ of the fit, while we do observe a shift of several standard deviations for the lower order parameters already present in the NLO fit. Using these shifted values to obtain the implied NLO approximation produces fits with much larger values of $\chi^2$. We conclude that the current data lack the precision and range in quark masses to constrain NNLO effects, the added degrees of freedom mix with NLO effects and
2.3 Results: \( f_{\text{PS}}, m_{\text{PS}} \) and chiral fits

| \( \beta \) | \( \bar{l}_3 \) | \( \bar{l}_4 \) | \( \bar{l}_1 \) | \( \bar{l}_2 \) | \( f_0 \) [MeV] | \( f_{\pi}/f_0 \) | \( 2B_0\mu_{u,d}/m_{\pi}^2 \) | \( \langle r^2 \rangle_{\text{NLO}}^{\text{NLO}} \) [fm\(^2\)] | \( r_0^\chi(\beta = 1.90) \) | \( r_0^\chi(\beta = 1.95) \) | \( a(\beta = 1.90) \) [fm] | \( a(\beta = 1.95) \) [fm] |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1.90 | 3.435(61) | 4.773(21) | -0.296(104) | 4.260(12) | 120.956(70) | 1.0781(18) | 1.029(16) | 0.7462(43) | 5.231(38) | - | 0.08585(53) | - |
| 1.95 | 3.698(73) | 4.673(25) | -0.430(93) | 4.329(15) | 121.144(83) | 1.0764(18) | 1.032(21) | 0.7237(51) | 5.710(42) | 5.231(37) | 0.08612(40) | 0.07775(39) |

| \( \beta \) | \( \bar{l}_3 \) | \( \bar{l}_4 \) | \( \bar{l}_1 \) | \( \bar{l}_2 \) | \( f_0 \) [MeV] | \( f_{\pi}/f_0 \) | \( 2B_0\mu_{u,d}/m_{\pi}^2 \) | \( \langle r^2 \rangle_{\text{NLO}}^{\text{NLO}} \) [fm\(^2\)] | \( r_0^\chi(\beta = 1.90) \) | \( r_0^\chi(\beta = 1.95) \) | \( a(\beta = 1.90) \) [fm] | \( a(\beta = 1.95) \) [fm] |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| combined | 3.537(47) | 4.735(17) | -0.309(139) | 4.325(10) | 121.031(54) | 1.0774(17) | 1.030(13) | 0.7375(34) | - | - | 0.07775(39) | - |
| priors | - | - | - | - | - | - | - | - | - | - | - | - | - |

Table 2.9 Results of the fits to SU(2) \( \chi \)PT for the ensembles at \( \beta = 1.95 \) and \( \beta = 1.90 \), separate and combined. The largest available volumes are used for each ensemble. Predicted quantities are: the low energy constants \( \bar{l}_{3,4} \) (while \( \bar{l}_{1,2} \) are introduced with priors), the charged pseudo-scalar decay constant in the chiral limit \( f_0 \), the mass ratio \( 2B_0\mu_{u,d}/m_{\pi}^2 \) at the physical point and the pion scalar radius \( \langle r^2 \rangle_{\text{NLO}}^{\text{NLO}} \). The scale is set by fixing the ratio \( f_{\text{PS}}^{[L=\infty]}/m_{\text{PS}}^{[L=\infty]} = f_{\pi}/m_{\pi} = 130.4(2)/135.0 \) to its physical value [37]. The chirally extrapolated Sommer scale \( r_0^\chi \) is determined separately and not included in the chiral fits. For a comparison with the \( N_f = 2 \) ETMC results, see [233].

destabilise the fit instead. In practise, we conclude that the systematic error from the truncation of \( \chi \)PT is unobservable at the current level of precision. Inclusion of \( O(a^2) \) corrections leads to similar observations, as the difference between the lattice spacings and the statistical accuracy of the data is too small to result in a stable fit. The fit mixes \( D_f_{\text{PS}} \) and \( D_{m_{\text{PS}}}^2 \) on the one hand and \( f_0, B_0 \) and the rescaling in the lattice spacing and the quark mass on the other.

The chirally extrapolated Sommer scale \( r_0^\chi \) has been determined separately, using a fit of \( r_0/a \) with quadratic dependence on the bare light quark mass, as shown in figures 2.6(a) and 2.6(b), and using the lattice spacing determined by the chiral fits. As also reported in table 2.9, the obtained values are \( r_0^\chi = 0.4491(43) \) fm at \( \beta = 1.90 \) and \( r_0^\chi = 0.4465(48) \) fm at \( \beta = 1.95 \), where only statistical errors are quoted. For consistency, we also verified that a combined chiral fit with the inclusion of \( r_0/a \), as data points and additional fit parameter, gives results anyway in agreement with the strategy adopted here.

For our final estimates of the low energy constants \( \bar{l}_{3,4} \) and the chiral value of the pseudo-scalar decay constant \( f_0 \) we use the predictions from the \( \beta = 1.95 \) ensemble based on two important observations. First, the strange quark mass in this ensemble is better tuned to the physical value. Secondly a reduced isospin breaking
is observed at this finer lattice spacing. The results for the $\beta = 1.90$ ensemble and the combined fits serve instead as an estimation of systematic uncertainties. As a result of the current $N_f = 2 + 1 + 1$ simulations we thus quote

$$\bar{I}_3 = 3.70(7)(26) \quad \bar{I}_4 = 4.67(3)(10),$$

(2.29)

and $f_0 = 121.14(8)(19)$ MeV, where the first error comes from the chiral fit at $\beta = 1.95$, while the second quoted error conservatively accommodates the central values from the $\beta = 1.90$ and combined fits as a systematic uncertainty. The predictions for $\bar{I}_3$ and $\bar{I}_4$ are in good agreement and with our two-flavour predictions [233] and with other recent lattice determinations [30, 283].

### 2.4 Conclusions and outlook

This chapter presented the first results of lattice QCD simulations with mass-degenerate up, down and mass-split strange and charm dynamical quarks using Wilson twisted mass fermions at maximal twist. This constitutes a first step in the effort of the ETMC to describe low energy strong dynamics and electroweak matrix elements by fully taking into account the effects of a strange and a charm quark.

We have considered ensembles at slightly different lattice spacings simulated...
2.4 Conclusions and outlook

Figure 2.8 (a) The charged pseudo-scalar mass ratio \( (m_{PS}/2B_0\mu_l)^2 \) and (b) the pseudo-scalar decay constant \( f_{PS} \) as a function of \( 2B_0\mu_l \), for the combined ensembles at \( \beta = 1.90 \) and \( \beta = 1.95 \), and fitted to equation 2.24. The scale is set as in figure 2.7 (indicated by the star). The light twisted masses used in the fit range from \( \mu_l = 0.0035 \) to \( 0.010 \). The lightest point at \( \beta = 1.90 \) (open light symbol) and at \( \beta = 1.95 \) (open dark symbol) lie outside our most conservative tuning criterion to maximal twist, and are not included in the fit.

with Iwasaki gauge action at \( \beta = 1.95 \) with \( a \approx 0.078 \) fm and \( \beta = 1.90 \) with \( a \approx 0.086 \) fm. The charged pseudo-scalar masses range from 270 to 510 MeV and we performed fits to SU(2) chiral perturbation theory with all data at a value of \( m_{PS}L \gtrsim 4 \). This analysis provides a prediction for the low energy constants \( \bar{l}_3 = 3.70(7)(26) \) and \( \bar{l}_4 = 4.67(3)(10) \), for the charged pseudo-scalar decay constant in the chiral limit \( f_0 = 121.14(8)(19) \) MeV and for the scalar radius at next-to-leading order \( \langle r^2 \rangle_{NLO} = 0.724(5)(23) \) fm\(^2\).

We have compared our results in the light meson sector with those obtained for \( N_f = 2 \) flavours of maximally twisted mass fermions, [233]. There, an extrapolation to the continuum limit, a study of finite size effects and checks against higher order \( \chi \)PT have been performed, leading to a controlled determination of systematic errors. The comparison we have carried through does not show any significant difference between \( N_f = 2 \) and \( N_f = 2 + 1 + 1 \) flavours, at least at the present level of accuracy. These results would suggest that effects of the strange and charm quarks are suppressed for these light observables, as it should be expected. The same comparison has also been used for a first investigation of lattice discretisation errors. As figures 2.4(a) and 2.4(b) show, the \( N_f = 2 + 1 + 1 \) data are completely consistent with the corresponding ones obtained for \( N_f = 2 \), where the discretisation effects have turned out to be very small. Thus, it can be expected that also for the case of \( N_f = 2 + 1 + 1 \) flavours the lattice spacing effects will be small, at least for the light meson sector considered here. Notice however that, at the present level of accuracy,
there is still the possibility that cancellations occur between physical contributions due to dynamical strange and charm quarks and lattice discretisation effects. A future more accurate study at a significantly lower lattice spacing will allow for drawing conclusions.

One aspect of the twisted mass formulation is the breaking of isospin symmetry. Its effect is likely to be most pronounced in the lightest sector, where lattice discretisation effects at $O(a^2)$, affecting the neutral pseudo-scalar mass only, generate a mass splitting between the charged and the neutral pseudo-scalar mesons. While this mass splitting for $N_f = 2 + 1 + 1$ flavours has been found here to be larger than in the $N_f = 2$ simulations at fixed physical situation, we do not find further effects in other quantities computed so far. This observation is supported by theoretical arguments [210,278] and consistent with the experience of the ETMC for the $N_f = 2$ flavour case.
From the case of QCD, with four quarks at their physical point, we move beyond the standard model and introduce eight degenerate flavours. With this, the emphasis of our studies shifts to the fundamental properties of the theory. Our goal is to reach a full understanding of the phase diagram of non-Abelian gauge theories, and in particular the emergence of a non-trivial IR fixed point. A perturbative analysis, while of limited validity in this context, indicates conformal physics should set in near this number of flavours. Most recent studies favour a higher flavour number instead, but older lattice data shows indications of behaviour consistent with restored conformal symmetry.

In our analysis, we use the occurrence of a thermal phase transition as a hallmark of the regular phase of QCD, as this is a feature strictly prohibited from occurring inside the conformal window. Given the conflicting body of results from literature, the case of eight flavour extended QCD provides an interesting ground for our methodology. We use an $O(a^2)$ improved action, to reduce systematic errors with respect to literature results and connect explicitly to the perturbative regime. As we move beyond physical QCD, the setting in which these methods have been shown to work, an explicit check on the stability of the results under removal of this improvement is needed. We show that the theory with eight flavours lies outside the conformal window and thus behaves as ordinary QCD.

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Analytical studies of QCD at large $N_f$ have recently been extended to finite temperature, and the line of phase transitions in the $T, N_f$ plane has been predicted on the base of a truncated renormalisation group flow calculation [56]. Note that the number of flavours can indeed be regarded as a continuous variable, since the Casimirs are polynomials in $N_f$ [169]. This means that the line of transitions found in [56] is in fact a true phase boundary between a conventional Goldstone phase and a chirally symmetric phase, the zero temperature limit of which is the onset of the conformal phase. We sketch the resulting phase diagram in figure 3. Lattice calculations provide a non-perturbative framework to attack this problem. The phase diagram of figure 3.1 suggests a natural strategy for finding the lower end point of the conformal phase: simply, find for which $N_f$ the finite temperature chiral symmetry breaking phase transition disappears. As a by-product, the numerically determined transition temperature as a function of $N_f$ can be compared with the analytic estimate of [56], and the nature of the phase transition investigated. There is, however,

![Phase Diagram](image_url)

**Figure 3.1** A projected view of the phase diagram of QCD-like theories in the temperature ($T$), flavour number ($N_f$) and bare coupling ($g$) space. In the $T - N_f$ plane, the line is a phase boundary between the chirally broken hadronic phase and the chirally symmetric quark gluon plasma, the zero end point of which is the onset of the conformal window. The zero temperature projected plane is inspired by the scenario in [82, 96].

one complication. Namely, it has been proposed – and to some extent proven – that the strong coupling limit of lattice QCD is always confining, regardless of the value
of \( N_f \) (see again e.g. [169]). A simple argument is that, at large enough coupling, \( N_f \) means nothing. For instance, the statement that at \( N_f = 16.5 \) asymptotic freedom is lost, is a statement of the continuum weak coupling regime, which has no special relevance at strong coupling. Even for those \( N_f \) which are supposed to fall deeply in the conformal phase, a strong coupling limit still exists which breaks chiral symmetry and confines.

This means that, even when the weak coupling continuum regime is conformal, a zero temperature ‘lattice’ phase transition will always take place between a strong and a weak coupling regime. In other words, for a fixed number of flavours, and for a given temporal extension of the lattice \( N_t \), we expect a phase transition to occur as a function of the lattice coupling to a ‘strongly coupled’ phase where chiral symmetry is broken, i.e. the chiral condensate is non zero in the chiral limit. This type of transition, called a bulk phase transition, has to be distinguished from a true thermal transition.

We can thus envisage two types of lattice behaviour as a function of the number of flavours. When \( N_f \) is such that QCD in the continuum and at zero temperature still breaks chiral symmetry and confines, i.e. when the continuum limit describes the ordinary phase of QCD, a transition to a symmetric phase has to be driven by thermal effects. As the zero temperature limit – or equivalently, the \( N_t \to \infty \) limit, given that \( T = 1/(N_t a)^2 \) – is approached, such a transition should get closer to \( \beta_c \to \infty \) and eventually disappear. Instead, for the values of \( N_f \) for which an infrared fixed point exists, the lattice phase transition should survive the \( N_t \to \infty \) limit, i.e. it is a bulk phase transition. The larger \( N_f \), the closer this bulk phase transition should get to the infinite coupling \( \beta \to 0 \) limit.

At a practical level, one should be able to distinguish between a bulk phase transition and a true thermal phase transition by studying the behaviour of the theory for a given \( N_f \) at different values of \( N_t \) and at varying lattice coupling \( \beta \). If the transition coupling remains non zero \( \beta_c \neq 0 \) when \( N_t \to \infty \) we have a bulk transition, thus providing a strong evidence that at the given \( N_f \) the continuum theory is chirally symmetric and falls into the conformal window. The alternative behaviour will point to a thermal transition happening at a given physical temperature \( T_c \). Note that in both cases, an additional bulk transition may still occur between two chirally broken phases.

As the overview of existing results presented in chapter 1 makes clear, results on the properties of the theory at \( N_f = 8 \) have been inconclusive. Older studies ([168], and to some extent [165]) suggested that the theory at \( N_f = 8 \) is already in the conformal window, while others confirmed analytic calculations [56, 80, 98, 146], indicating that \( N_f^c > 8 \), close to the upper limit for \( N_f^c \) calculated in [127]. The purpose of this study is to fully clarify the physics of eight flavours, as a first step towards the exploration of the phase diagram of QCD-like gauge theories at large \( N_f \).

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2That the size of the lattice in the temporal direction \( N_t a \) determines the temperature of the system, is a consequence of the similarities between quantum field theory and thermal field theory. A small value of \( N_t a \) will provide an IR cut off on the energy of the eigenmodes of the system and decrease the thermal correlation length, thereby raising the temperature. For a rigorous argument, see e.g. [260].
3.1 Simulation and Observables

The simulations in this chapter were performed using a slightly modified version of the publicly available MILC code\(^3\). A setup similar to the one used by MILC in their recent paper on the QCD equation of state [66] was employed.

We use an improved Kogut-Susskind fermion action, the “Asqtad” action which removes lattice artefacts up to $O(a^2 g^2)$ and a one-loop Symanzik improved [66, 284] and tadpole improved [285] gauge action. The complete action for $N_f$ mass degenerate flavours can be written as

$$S = -\frac{N_f}{4} \text{Tr} \ln M(am, U, u_0) + S_{\text{gauge}},$$

where

$$S_{\text{gauge}} = \sum_{i=p,r,pg} \beta_i(g^2) \sum_{\mathcal{C} \in S_i} \text{Re}(1 - U(\mathcal{C})), $$

with couplings defined as

$$\beta_p \equiv \beta = \frac{10}{g_0^2} \quad \beta_r = -\frac{\beta}{20u_0^2}(1 + 0.4805 \alpha_s) \quad \beta_{pg} = -\frac{\beta}{u_0^2} 0.03325 \alpha_s,$$

with $M(am, U, u_0)$ the fermion matrix for the Asqtad staggered action for a single flavour with mass $m$, and with $\alpha_s = -4 \log u_0 / 3.0684$. The $S_i$’s contain all the $1 \times 1$ plaquettes, the $1 \times 2$ and $2 \times 1$ rectangles and the $1 \times 1 \times 1$ parallelograms, respectively, that can be drawn on the lattice. The $U(\mathcal{C})$’s are the traces of the ordered product of link variables along $\mathcal{C}$, all divided by the number of colours. The tadpole parameter $u_0$ is defined in terms of the gauge invariant average plaquette as

$$u_0 = \langle U(\mathcal{C}) \rangle_{\mathcal{C} \in S_p}^{1/4}. $$

Exploiting the rather low sensitivity of the plaquette value to finite volume effects, the $u_0$ values for each run were determined by a self consistency procedure on $12^4$ and $16^4$ lattices for every $\beta$ investigated.

It has been proposed recently by members of the HPQCD collaboration [286] to include the effect of dynamical quarks into the one-loop improvement of the gauge action, the required coefficients of which they determined to first order through lattice perturbation theory. While it is true that a complete $O(a^2)$ improvement should fully account for gauge and quark loop contributions, the reliability of a one-loop truncated perturbative contribution from dynamical quarks at large $N_f$ becomes questionable. Since the coefficients found in [286] are sizeable and linear in the flavour number, a resummation would probably be called for, especially in the case of large $N_f$. Barring this, there is a risk that including a truncated series would

\(^3\)http://www.physics.indiana.edu/sg/milc.html
3.1 Simulation and Observables

severely overcompensate the actual quark loop effects and in fact worsen the $O(a^2)$ improvement, for values of $N_f \geq 3$. The scaling violations that are being observed for the heavy quark potential with the customary ‘partially’ improved action are not completely negligible, but well under control [287]. On the base of these considerations and the fact that observables employed in this study are less sensitive to scaling violation effects, we did not include these one-loop dynamical quark improvements.

The importance of improved actions in the study of QCD thermodynamics can be hardly overemphasized. A simple qualitative argument goes as follows. Remember that the physical temperature is $T = \frac{1}{N_t a}$, where $a$ is the lattice spacing. Let then $T^*$ be the physical transition temperature for $N_f = 8$, corresponding to the true thermal transition, which we are trying to detect working with $N_t$ time slices. This fixes the value of $a^* : a^* = \frac{1}{N_t T^*}$. For $N_t$ fixed, all lattice actions should give the same physical $a^*$. However, improved actions will have reduced lattice artefacts, and the results will be closer to the continuum limit. The reader might want to consult e.g. [288] and references therein, for more extensive discussions on how improved actions can effectively help controlling lattice artefacts, and several illuminating examples.

The determinant of the fermion matrix in equation 3.1 was rewritten using the conventional pseudo-fermion trick, which exploits the Gaussian functional integral identity

$$\det [M] = \int D\phi D\phi^* \exp \left[-\phi M^{-1} \phi^* \right],$$

where $\phi$ and its conjugate field are bosonic. Once integrated out of the action, fermions contribute the determinant of the Dirac operator to equation 3.1. By rewriting this determinant in terms of bosonic pseudo-fermions, one effectively exchanges fermions for bosons, that can be numerically dealt with, at the cost of a potentially expensive operator inversion. To generate our configurations with eight degenerate dynamical flavours, we used the rational hybrid Monte Carlo (RHMC) algorithm [289], which allows for simulating an arbitrary number of flavours through varying the number of pseudo-fermions used, i.e. it inherently uses an analytical continuation in the number of flavours. The staggered fermion Dirac operator produces fermions in mass-degenerate multiples of four, which one commonly – if somewhat controversially [158,290] – deals with by taking a root of the determinant. For our current purposes, rooting is unnecessary when using two pseudo-fermions. One could in principle choose a different number of pseudo-fermions, in combination with some rooting, in order to optimise performance. However, some experimentation showed that performance was in fact best using the most natural set up with two pseudo-fermions, conveniently also avoiding potentially troublesome fractional powers of the Dirac operator in the molecular dynamics.

To systematically investigate the character of eight flavour QCD under different thermodynamic conditions, simulations were run at two different values for the length of the temporal extent in lattice units $N_t$, namely 6 and 12. As was mentioned

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4Choosing alternative pseudofermion distributions can lead to large improvements in efficiency for non-degenerate masses, where ratios of contributions from light and heavy quarks can be introduced to precondition the inversions [291].
in the introduction, the scaling behaviour of the lattice coupling at the transition – defined according to equation (3.1) as $\beta_c = 10/g^2_{0c}$ – with $N_t$ is an indication of either the thermodynamic or bulk nature of the observed phase transition. To check for the influence of finite volume effects and deduce the scaling properties of observables, simulations were run for three spatial extents of the lattice $N_s = 12, 20, 24$ for $N_t = 6$, and $N_s = 24$ for $N_t = 12$. We chose a fixed value of the lattice degenerate quark mass $a m_l = 0.02$ to explore the region around the transition, and will describe how results can be modified by doing simulations at a lower quark mass in section 3.3. As it will be clear from the outcomes, the chosen masses are sufficiently light to clearly disentangle the behaviour around the transition temperature and establish the nature of the transition.

The Monte Carlo history was collected with trajectories of total length $\tau = 0.3$ to $0.4$, and time step $\delta \tau = 0.003$ to $0.007$ from the lowest to the highest $\beta$ values and from the smallest to the largest volume.

At each $\beta$, the expectation value of the real part of the Polyakov loop

$$L \equiv \frac{1}{3N_s^3} \sum_{\vec{x}} \Re \text{Tr} \prod_{x_4=1}^{N_t} U_4(\vec{x}, x_4)$$

was determined. It is important to remember that the real part of the Polyakov loop is a true order parameter only for the pure gauge theory, which is recovered in the infinitely heavy mass limit $m \to \infty$ of the theory with dynamical flavours. It is not an order parameter in all other cases, though a clear change in its value and its susceptibility can be observed at sufficiently heavy or sufficiently light values of the fermion masses. Where the theory does enter the regime of ‘light masses’ is based on empirical observations [292], it might shed light on the mechanism relating confinement to chiral symmetry breaking, and it depends on the flavour content of the theory.

The chiral condensate for $N_f$ degenerate flavours in lattice units

$$a^3 \langle \bar{\psi}\psi \rangle = \frac{N_f}{4N_s^3 N_t} \langle \text{Tr} \left[ M^{-1} \right] \rangle,$$

was determined by using a stochastic estimator with 20 repetitions. The chiral susceptibility, measuring the variation of the chiral condensate with varying the fermion mass $\chi = \partial \langle \bar{\psi}\psi \rangle / \partial m$ at fixed $\beta$ can be divided into a connected and disconnected component $\chi = \chi_{\text{conn}} + \chi_{\text{disc}}$, given in lattice units by

$$a^2 \chi_{\text{conn}} = -\frac{N_f}{4N_s^3 N_t} \langle \text{Tr} \left[ (MM)^{-1} \right] \rangle,$$

$$a^2 \chi_{\text{disc}} = \frac{N_f^2}{16N_s^3 N_t} \left[ \langle \text{Tr} \left[ M^{-1} \right] \rangle^2 - \langle \text{Tr} \left[ M^{-1} \right] \rangle^2 \right],$$

respectively. We have conveniently written the condensate and its susceptibilities in terms of traces of (products of) the staggered fermion matrix $M$ as they are actually
computed in the simulation. The connected and disconnected contributions to the chiral susceptibility are measured separately; more on this can be found in [293]. The connected contribution can also be measured in a partially quenched manner, performing a numerical derivative of the chiral condensate with respect to the valence quark mass

$$\chi_{\text{conn}} = \frac{\partial \langle \bar{\psi} \psi \rangle}{\partial m_V}.$$  \hspace{1cm} (3.7)

Both measurement methods were implemented, with results being in excellent agreement. The complete set of values reported on here have been found using the first method, since it has a lower computational overhead.

The disconnected chiral susceptibility is a non-local quantity that can be estimated from the variance of the bulk behaviour of the chiral condensate. However, such a variance for a condensate computed with stochastic estimators will automatically include part of the connected contributions, through random sources multiplying themselves. Following Bernard et al. [293], we straightforwardly eliminate those contributions by only considering the off-diagonal elements of the covariance matrix of the random sources introduced for the estimation of the chiral condensate.

We can use the chiral susceptibility and the chiral condensate to define two physically relevant quantities

$$\chi_\sigma \equiv \chi = \frac{\partial \langle \bar{\psi} \psi \rangle}{\partial m} = \chi_{\text{conn}} + \chi_{\text{disc}}$$ \hspace{1cm} (3.8)

and

$$\chi_\pi = \frac{\langle \bar{\psi} \psi \rangle}{m}.$$ \hspace{1cm} (3.9)

They are related through Ward identities [294] to the space time volume integral of the scalar ($\sigma$) and pseudo-scalar ($\pi$) propagators

$$\chi_{\sigma, \pi} = \int d^4x \, G_{\sigma, \pi}(x),$$ \hspace{1cm} (3.10)

thus implying that they should become degenerate when chiral symmetry is restored, following the degeneracy of the chiral partners. As a result, their associated cumulant $R_\pi \equiv \chi_\sigma / \chi_\pi$ should be, in the absence of explicit chiral symmetry breaking, one in a chirally symmetric regime, while it should be zero in the spontaneously broken phase. This dimensionless quantity is therefore a most useful physical observable in analysing chiral phase transitions, and we will employ it to compare results from simulations run at different temporal extents of the lattice.

3.2 Results at $N_t = 6$

The introductory discussion tells us that we must observe a phase transition between a phase where chiral symmetry is broken to a phase where chiral symmetry
is realized, for some value of the lattice gauge coupling $\beta_c$. There are basically two ways to assess a phase transition on a lattice. First, one can rely on obtaining infinite volume estimates of relevant quantities by performing simulations on lattices of different spatial extents. Whenever this is possible, the behaviour in the transition region is analogous to the one observed in the continuum. This strategy usually breaks down very close to the transition coupling, where the correlation length of the system grows large and becomes comparable to the lattice size. When this happens, it is mandatory to use finite size scaling techniques. The determination of the regime we are in can be made \textit{a posteriori}, by comparing results obtained from different volumes.

For the case at hand, results for the chiral condensate and the Polyakov loop are shown in figure 3.2. From the small differences found at different spatial extents, it was concluded that our results can indeed be considered infinite volume estimates for $\beta < 4.1$ and $\beta \geq 4.15$, and the $\beta$ dependence is smooth. The jump between the two branches is very clear for both observables and suggestive of a discontinuity.

These results allow us to immediately identify a transition region for $\beta$ between 4.1 and 4.15. In this region, one would expect to observe tunnelling between the two phases and enhancement of the associated susceptibilities. As mentioned above, the approach to the infinite volume limit should be slower here, because of the increasing correlation lengths. Indeed, volume dependence is observed, with the smaller of the lattices having a slightly higher $\beta_c$. This behaviour is consistent with known predictions for finite volume effects in first order phase transitions [295]. Since the shift is much less pronounced for the change of volume between $N_s = 20$ and 24, we concluded the infinite volume limit value for $\beta_c$ should be located at the lower parts of the designated transition region, and is bounded by $4.10 < \beta_c < 4.125$. For definiteness, we locate it at a value of 4.1125.

The chiral susceptibilities are shown in figure 3.3 and confirm our picture. The residual splitting is associated with the explicit breaking induced by the mass term, but the tendency towards degeneracy is very clear. Finally, we plot the cumulant $R_{n}$, defined earlier, in figure 3.3. In the chiral limit, the cumulant should be zero in the broken phase, and approach one in the chirally symmetric phase. The observed trend is consistent with all other findings, signalling a transition from a chirally broken to a chirally symmetric phase.

### 3.2.1 The transition region

Having bracketed off the relevant values for $\beta$, we investigated the area in which the phase transition occurs in more detail. Of specific interest here is the potential presence of meta-stabilities. Simulations were performed on $12^3 \times 6$ lattices starting from thermalised configurations at higher and lower values of $\beta$, but with identical parameters. The presence of metastable states could show up, either through the presence of hysteresis effects, or by appearance of tunnelling effects in the Monte Carlo history. The latter effect would be expected to be somewhat enhanced, because of the usage of a smaller spatial extent. However, for all of the values of $\beta$ that were examined near the threshold of the lattice of this size, a persistence of initial states was found after a large number of RHMC trajectories. This indicates the presence of
3.2 Results at $N_t = 6$

Figure 3.2 The chiral condensate (grey symbols) and Polyakov loop (open symbols) as a function of the lattice coupling $\beta$. Measurements were done for three different spatial extents of the lattice $N_s$: 12 (○), 20 (△) and 24 (□). The transition region has been indicated by vertical lines.

Finally, it is a matter of interest to what extent the behaviour of the Polyakov loop, as a signal of confinement, is intertwined with that of the chiral condensate. There are indications that the confinement/deconfinement transition is, in the presence of light quarks, driven by the chiral phase transition. Even though the signal of the Polyakov loop tends to be statistically weak for small numbers of measurements, it is possible to observe its change from the distribution of its phase. While the Polyakov loop tends to be distributed symmetrically in the complex plane for confining configurations, whenever fermions are present in a deconfined system, it will tend towards the real phase of its $Z(3)$ centre. In figure 3.5, we exhibit the Monte Carlo history of the phase of the Polyakov loop for a run at the threshold of
the transition region and at the largest spatial extent, i.e. $\beta = 4.1$ and $N_s = 24$. For comparison, the plot includes the equivalent part of the history at values of $\beta$ before and after the transition. Note the presence of a metastability close to the threshold, also for this largest volume. This shows that the Polyakov loop, though it is a true order parameter only in the pure gauge theory, retains transition behaviour close to the transition, even in the presence of eight degenerate flavours.

All data at $N_t = 6$ point towards a first order phase transition. The location of the jump of the chiral condensate and the Polyakov loop at all three spatial volumes considered, and the location of the hysteresis cycle at the smallest spatial extent, allows us to give the estimate of the broadest transition region, to be $4.10 < \beta_c < 4.15$. We take the occurrence of the jump of the chiral condensate and the Polyakov loop at our largest spatial volume $N_s = 24$, as the best indicator of the transition...
3.3 Results at $N_t = 12$

As explained in the introduction, the scaling of $\beta_c$ with varying the lattice temporal extension $N_t$ should distinguish between a thermal and a bulk transition. A thermal transition occurs at a physical temperature $T_c$ which we determine as

$$T_c = \frac{1}{a(\beta_c)N_t}$$  \hspace{1cm} (3.11)
Figure 3.5 Monte Carlo history for $\beta = 4.1$ and $N_s = 24$, at the threshold. The distribution flattens around zero in the deconfined phase, while it is randomly distributed between $\pm \frac{\pi}{2}$ in the confined phase. The same histories are shown for runs below and above the transition region (at $\beta = 4.0$ and 4.2) in lighter shades. The points are enumerated according to their trajectory number, disregarding the first 100 trajectories after the cold start for each.
3.3 Results at $N_t = 12$

for a given temporal extent $N_t$ and lattice spacing $a(\beta_c)$ at the transition coupling. Thus, performing simulations at different $N_t$, the transition coupling should rescale in order to give the same transition temperature $T_c$. Uncertainties in the determination of the transition temperature can be mainly introduced by lattice violations to the asymptotic scaling of observables. It is thus a possibility that past simulations leading to apparent scaling violations and indicating the presence of a bulk transition, might have been performed in a region of the lattice parameter space not sufficiently close to the continuum limit. Our highly improved lattice action should help us approaching the continuum limit and the correct scaling behaviour.

We have thus performed simulations at $N_t = 12$ with spatial volume $N_s = 24$ and at the same lattice mass $am = 0.02$, and looked for signals of the transition in the behaviour of the chiral condensate. The main result is shown in figure 3.6, where we observe a jump in the chiral condensate suggestive of a discontinuity, and slightly distorted and smoothed by the not so large spatial extent $N_s = 24$ as compared with the temporal extent $N_t = 12$. Notice also that effects of explicit chiral symmetry breaking due to the non zero physical mass are to be more pronounced at $N_t = 12$, for the same value of the lattice mass. The derivative of the condensate is also plotted in figure 3.6 to better locate the transition. The best fit value for the maximum of the derivative indicates a value for the transition coupling $\beta_c = 4.34 \pm 0.04$. This result allows us to place an upper and lower bound on the transition coupling $\beta$: $4.30 < \beta_c < 4.38$ at $N_t = 12$, with $N_s = 24$. While finite spatial volume effects will not effect our conclusion, we cannot quote this value as the infinite volume value, and we postpone a more refined analysis of finite volume effects to a future publication.

The combined results at $N_t = 12$ and $N_t = 6$ strongly suggest the occurrence of a first order thermal transition. To confirm this, an asymptotic scaling analysis is needed in order to verify that we are actually measuring a transition temperature in the continuum real world. We do so by means of the standard relation that connects the lattice cut-off $\Lambda_L$ to the gauge coupling $g$, $a\Lambda_L = R(g^2)$ with

$$R(g^2) = (b_0 g^2)^{-b_1/2b_0^2} e^{-1/2b_0 g^2},$$

(3.12)

where the two loop RG running of the $\beta$-function is accounted for, with the universal one- and two-loop coefficients given by

$$b_0 = \frac{1}{16\pi^2} \left( 11 - \frac{2}{3} N_f \right)$$

$$b_1 = \frac{1}{(16\pi^2)^2} \left( 102 - \frac{38}{3} N_f \right)$$

(3.13)

for $N_f$ massless flavours. Given a physical temperature $T_c$, equation (3.11) implies the scaling relation $N_t R(g_c(N_t)) = \text{const}$. Solving for $N_t = 6$ and $N_t = 12$, we can predict $\beta_c(g_c(N_t = 6))$ by knowing $\beta_c(g_c(N_t = 12))$. A strong discrepancy with the actual lattice determination might be suggestive of a bulk zero temperature transition, while a small discrepancy can indeed be expected and imputed to violations of asymptotic scaling and residual effects due to a non zero fermion mass. The ques-
Figure 3.6 The chiral condensate at $N_t = 12$ and $N_s = 24$ in lattice units as a function of the lattice coupling $\beta$. Best fit curves are superimposed and the vertical lines indicate the transition region. The absolute value of the finite difference between measured values of the condensate, as an approximation of its first derivative, is plotted in the bottom part of the figure with an arbitrary rescaling. It shows a peak at $\beta = 4.34$.

The most appropriate coupling $\beta_c(g_c)$ to insert in equation (3.12) in order to compare continuum perturbation theory with lattice calculations. Our simulations use a one-loop Symanzik improved and tadpole improved gauge action. These improvements are expected to ameliorate the agreement with the asymptotic scaling by correcting for up to and including $O(a^2)$ effects. In a finite temperature study this translates into the statement that the agreement with asymptotic scaling will set in at lower values of $N_t$ with respect to an unimproved lattice action.

Given these premises, we have predicted the transition coupling $\beta_c(N_t = 6)$ by using an effective coupling which relates the lattice $\beta$ and $g^2$ as $\beta = 6/g^2$ in equation (3.12). Notice that the lattice bare coupling, coefficient of the plaquette action in equation (3.1), is $\beta_{pl} = 10/g_0^2$ where the rescaling of the coefficients is due to the one-loop Symanzik improvement. The use of $\beta = 6/g^2$ in the RG formula is
meant to effectively take into account the tadpole and Symanzik one-loop improvement in our action. By using $\beta_c(N_t = 12) = 4.34 \pm 0.04$ we obtain the prediction

\[
\beta_c(N_t = 6) = 4.04 \pm 0.04,
\]
which deviates by less than 2% from the lattice determined $\beta_c$. We also verified that a rescaling of the effective coupling $\beta \rightarrow \beta u_{\lambda}^{-4}$ [284] improves the prediction by only 0.5% indicating that our effective coupling prescription is in fact already accounting for all the improvement. Further improvement of the lattice gauge action – e.g. the proper inclusion of quark loop corrections in the improvement program – and corrections for the non-zero fermion mass, should account for the tiny residual asymptotic scaling violations in this study. Figure 3.7 presents a comparison of our lattice results with the asymptotic scaling prediction. These results will be further elaborated upon in the final discussion.

In figure 3.8 we compare the transition at $N_t = 6$ and at $N_t = 12$ by means of the first derivative of the chiral condensate as a function of $T/T_c$ as predicted by the asymptotic scaling using the effective coupling $\beta = 6/g^2$. As before, the lattice determined $\beta_c(N_t = 12)$ corresponds to the point $T/T_c = 1$. The most important observa-
tion is that the transition at \( N_t = 6 \) is close to the predicted point \( T/T_c = 1 \), actually happening at \( T/T_c \approx 1.20 \). We show the data of the first derivative with a Gaussian fit superimposed. For the data at \( N_t = 6 \) we show, for the sake of comparison, the curves at the largest spatial extent \( N_s = 24 \) and the smallest \( N_s = 12 \). The lattice determined transition regions at \( N_t = 6 \) and \( N_t = 12 \) overlap at their boundaries. The amount of non-overlap is a measurement of the residual but small violations of asymptotic scaling. We did not observe any signal of discontinuity in the Polyakov

![Figure 3.8 'Scaling plot' for the finite difference approximation to the absolute value of the first derivative of the chiral condensate as a function of \( T/T_c \), determined using the effective coupling \( \beta = 6/g^2 \) in the RG formula. Data at \( N_t = 6, N_s = 24, 12 \) (open symbols) are compared with data at \( N_t = 12, N_s = 24 \) (grey symbols). The point \( T/T_c = 1 \) corresponds to \( \beta_c(N_t = 12) = 4.34 \). A Gaussian fit is superimposed to the \( N_t = 12 \) data, while indicative Gaussian curves are shown for \( N_t = 6 \). The baseline is subtracted and we only indicate data near the transition temperature. The lattice determined transition regions at \( N_t = 6 \) and \( N_t = 12 \) are indicated by vertical lines.

The Polyakov loop in our simulations at \( N_t = 12 \), with a lattice mass \( am = 0.02 \) and in the transition region of the chiral condensate. While the presence or absence of this signal is of no physical relevance below the infinite mass limit, given that the Polyakov loop is not an order parameter in the presence of dynamical fermions, we can still use
its behaviour at light quark masses to gain further insight into the mechanism that relates chiral symmetry restoration to deconfinement and the two limiting regimes of zero mass and infinite mass fermions. Here, we limited ourselves to verify that the presence or absence of a discontinuity of the Polyakov loop in coincidence with the discontinuity of the chiral condensate depends upon the physical fermion mass. By sufficiently lowering the fermion mass at \( N_t = 12 \) we expect that the picture of \( N_t = 6 \) will be restored.

The location and extent of the region of sufficiently light quark mass is a dynamical property of the \( N_f = 8 \) theory which cannot be judged a priori. A further refinement of this study can help in locating the critical end-points. The reader might want to review [292] for a pioneering study at \( N_f = 4 \). Here we focus on comparing between our results for the chiral condensate at \( N_t = 6 \) and those at \( N_t = 12 \). To this end, it is instrumental to recall how a finite mass affects the location and nature of the phase transition. In the chiral limit, standard universality arguments would predict a first order transition for \( N_f \geq 3 \) [41]. Since first order transitions should be robust under small perturbations, the transition is expected to persist at least for small mass values. In the infinite mass limit the transition becomes the deconfining transition of quenched (pure gauge) QCD, which is also a (weak) first order transition. For intermediate masses we can envisage two scenarios: the transition is of first order all the way from \( m = 0 \) up to the quenched limit, presumably becoming weaker as the quark mass increases. This is the simplest picture, but experience with lattice simulations with three flavours suggests differently. Here, the first order transition becomes a crossover for some critical value of the mass, say \( m = m_1 \), then the first order transition appears again at a larger mass \( m = m_2 \), and remains of first order until \( m \) approaches infinity and our theory resembles a pure gauge transition. In this second scenario, in addition to the two first order phase transitions, there are two second order transitions in the universality class of the 3D Ising model at the two endpoints \( m_1 \) and \( m_2 \), and a crossover in between. This crossover can be very weak, as is for instance the case in three flavour QCD [59].

The bare mass at \( N_t = 12 \) is the same as the one at \( N_t = 6 \), so the physical value of the mass at the transition coupling should be twice as big for \( N_t = 12 \). Because of this, and following the above discussion, we expect a smoother behaviour of the transition on the \( N_t = 12 \) lattice; either because the transition becomes weaker, or because we have reached the crossover domain. The actual nature of the phase transition is very much dependent on the precise value of the mass and one cannot draw any firm conclusions without studying this dependence. However, the above discussion allows us to conclude that the observed softening of the transition on the \( N_t = 12 \) lattice is certainly consistent with the behaviour expected on theoretical grounds and observed in three flavour QCD [59].

Considering the dependence of the location of the transition coupling or crossover on the mass, this should be linear for a first order transition according to

\[
\beta_c(m_q) = \beta_c(0) + \frac{\Delta \langle \bar{\psi} \psi \rangle}{\Delta S_G} m_q, \tag{3.14}
\]

where \( \Delta \langle \bar{\psi} \psi \rangle \) and \( \Delta S_G \) are the discontinuities of the chiral condensate and the gauge
action at $\beta_c$ [60]. This form should continue smoothly into the crossover domain. We have not estimated these values for $N_f = 8$, but by using the results available for $N_f = 3$ we can conclude that the variation of $\beta_c$ in the mass range [0.01, 0.02] should be even smaller than the error we quote and our conclusions on the location of the phase transition do not depend on the mass value. It would be of course interesting to perform simulations with different mass values. The present results allow us to firmly conclude that we are observing a true thermal transition, in other words $N_f = 8$ undergoes a chiral restoration transition at finite temperature and must be in the ordinary hadronic phase of QCD.

3.4 Tree level improved results

For a regular, asymptotically free theory, tadpole improvement enhances the convergence towards the perturbative limit in the weakly coupled region [296]. But an introduction of this scheme when asymptotic freedom is absent would introduce a non-physical background field contribution. It is conceivable that the interaction of the background field with a changing temperature would shift the transition coupling even for a bulk transition, potentially producing a non-physical thermal dependence in the theory.

To exclude such artefacts, additional simulations were run using a tree level Symanzik improved action. Concretely, this implies an identical action to that defined by equation 3.1, but with the gauge couplings redefined as

$$
\beta_p \equiv \beta = 10/g_0^2, \\
\beta_r = -\frac{\beta}{20}, \\
\beta_{pg} = 0.
$$

It is straightforward to obtain these couplings, as they are found by setting $u_0 = 1$. Remember that $u_0$ was introduced in a redefinition of the coupling, meant to absorb $O(g^2)$ (rather than $O(a^2g^2)$) tadpole contributions to the gauge field self-interaction [296]. The $O(a^2)$ improvement terms, which will need to cancel loop corrections, will all depend on the dominant loop correction $u_0$. Setting $u_0$ to its free field value of 1 therefore cancels all loop corrections, reducing the action to its tree level improved form. This is in fact a physically sensible consequence, as it is exactly the perturbative expansion at the scale of the lattice spacing that cannot be relied upon in the absence of asymptotic freedom.

The transition coupling for the appearance of spontaneous chiral symmetry breaking was determined at different values of the lattice size in the temporal direction $N_t$, in much the same way as was done in [165] and [241]. Reduced improvement will wash out the transition already for smaller values of $N_t$, so runs were performed for smaller values of $N_t = 4, 6, 8$ and 10. As there was no need for high accuracy, moderately sized lattices satisfying $N_s > N_t$ were deemed sufficient and the value $N_s = 12$ was used for all simulations.

For the order parameter of the chiral transition itself (see figure 3.9), a rapid change in value occurs. For $N_t \geq 6$, the nature of this change appears to be much
3.4 Tree level improved results

weakened with respect to the sharp first order transition observed for $N_t = 6$ in section 3.2. The value of the transition coupling, or rather the finite range of values, for which the transition occurs shows a clear shift towards higher values of $\beta$ as $N_t$ is increased. All other parameters remaining identical, this implies the expected

![Figure 3.9](image)

**Figure 3.9** The chiral condensate as a function of the bare lattice coupling constant $\beta$ for different values of the temporal lattice extent: from left to right, lines correspond to $N_t = 4, 6, 8$ and 10. The shift in the location of the onset of the restoration of chiral symmetry implies a direct influence on the dynamics of the system by the infrared degrees of freedom and demonstrates the compatibility of the results obtained with an action without tadpole improvement with a thermal origin of the observed phase transition.

persistence of spontaneous chiral symmetry breaking down to weaker coupling for a decrease in the lattice temperature. As expected, the effect becomes significantly weaker as $N_t$ is increased and the transition itself becomes more shallow. The data at $N_t = 4$ show a significant deviation from the other data points for each value of $\beta$ for which measurements were performed. This could reflect a very high temperature phase, but might also reasonably be due to lattice artefacts dominating the results with such a strong cramping in the temporal direction, as was observed for finite temperature measurements of regular QCD with and without quenching [242].

A direct comparison between results obtained with actions with and without tadpole improvement is not sensible, since the redefinition of the coupling introduced by the Lepage-Mackenzie tadpole scheme directly impacts all scales in which both the bare parameters and the observables are expressed. Most importantly, the input bare quark mass $m_q$ is kept identical for both theories, but the change in lattice spacing causes a shift in the quark mass in physical units, that will feed back into the results. In the chirally symmetric region of the theory, the differences in the measured
values of the chiral condensate at fixed coupling $\beta$ are typically of the order of 40%. Dimensional analysis implies an $O(a^3)$ factor for this particular observable, indicating a shift in the lattice spacing of the order of 12% when neglecting changes induced by the implicit change in lattice parameters. Indeed, comparing the dimensionless observable $R_\pi$, we observe a reduced change of about 7%. For the chirally broken phase, the numerical differences between results for both actions vary more considerably. This is probably due to discretisation artefacts, that may cause a cascade into a strong coupling bulk transition (without continuum limit) as the broken phase is entered. To confirm this, the behaviour under varying mass should be studied. Since we are currently only interested in the thermal sensitivity of $\beta_c$ as compared to the fully improved action, we will not pursue this matter here. Similar behaviour will be observed, and discussed more extensively, for a tree level improved action with $N_f = 12$ in chapter 5.

Interestingly, the position of the observed transition in terms of the bare coupling does not vary a great deal between the two actions. This lack of large changes in a dimensionless observable might be a consequence of the implicit rescaling is consistent over the set of parameters. The change in physical mass would lead to a change in physical temperature, but this could well be associated with a similar bare transition coupling. An explicit test would require some scale setting procedure, which is outside the scope of this study.

Both the shifting of the location of the transition and its widening are evident in the behaviour of the chiral cumulant $R_\pi$ in figure 3.10. The chiral limit of unity is approximated to varying degree by all systems at a coupling of $\beta = 4.4$, with values of 0.871, 0.935, 0.949 and 0.989 measured for $N_t = 10$, 8, 6 and 4, respectively. The curves here flow smoothly towards the free limit, where the cumulant reaches unity. To the strong coupling side, a sharp jump is observed for all values of $N_t$ towards a region where the value of the cumulant tends to a value around 0.1, implying strongly broken chiral symmetry for all. The largest value of $N_t = 10$ shows a fairly smooth rise of the cumulant over a large region, without any sharp alterations. This loss of a signal for what one would consider intermediate values of $N_t$ is not altogether unexpected, as this is exactly the type of amelioration of the signal quality that tadpole improvement ought to give [297, 298]. It does, however, complicate the direct comparison with the results reported in [165], as there a lack of scaling is observed exactly for larger values of $N_t$. A comparison with runs at a larger spatial volume of $N_s = 16$ (figure 3.11) shows perhaps a weak sensitivity of the location of the transition to the spatial volume of the system, at least at larger values of $N_t$. If so, this would suggest a first order phase transition is still occurring [295]. Such volume sensitivity is hard to discern at this level of precision, however, so its potential presence should be seen as demonstrating compatibility with the more obvious and varied signals of a first order phase transition measured using tadpole improvement.

Using the cumulant $R_\pi$ from figure 3.10, a sensible value of the transition coupling can be determined for all runs, allowing a scaling analysis similar to that performed in section 3.3. Somewhat limited by the coarse resolution of the scans, we tentatively set the transition couplings to the values provided in table 3.1. The tran-
3.4 Tree level improved results

Figure 3.10 The chiral cumulant as a function of $\beta$, for runs corresponding to the results in figure 3.9. Results are given for (lines from left to right) $N_t = 4$, 6, 8 and 10, all at a spatial volume of $N_s = 12$.

<table>
<thead>
<tr>
<th>$N_t$</th>
<th>$\beta_c$</th>
<th>$N_t$</th>
<th>$\beta_c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>3.850(50)</td>
<td>8</td>
<td>4.225(25)</td>
</tr>
<tr>
<td>6</td>
<td>4.125(25)</td>
<td>10</td>
<td>4.350(50)</td>
</tr>
</tbody>
</table>

Table 3.1 The transition coupling for several temporal lattice sizes $N_t$, as determined by bracketing the most rapid change in $R_\pi$ for the data plotted in figure 3.10.

The transition for $N_t = 10$ is smoothed out to such an extent that the resulting value of $\beta_c$ is somewhat arbitrary, while the value of the transition coupling is quite possibly influenced by finite volume effects for $N_t = 8$ (see figure 3.11). Because of its contrasting stability under changes in volume, we use $\beta_c$ for $N_t = 6$ as an anchor point in the analysis and observe the scaling of $\beta_c$ as predicted by equation 3.12. Between the adjacent and proximate values of $N_t = 6$ and $N_t = 8$, the scaling (figure 3.12) turns out to be quite adequate at the given level of precision. At the very strong coupling found for $N_t = 4$, the deviation from perturbative scaling is quite pronounced. This is not unreasonable, given the prominence of lattice artefacts noted before and the accelerated breakdown of perturbative scaling when entering the strong coupling regime without tadpole improvement.

Though the quality of the signal clearly deteriorates as tadpole improvement is removed, the results obtained with a tree level improved action are completely compatible with those using a fully $O(a^2)$ improved action.
Figure 3.11 The chiral cumulant as a function of $\beta$, for runs at $N_t = 6$ (lines to the left) and 8 (lines to the right), at an enlarged volume of $N_s = 16$. Results should be compared to that of figure 3.10, the relevant datasets of which have been reproduced using dashed lines. Some sensitivity of $\beta_c$ to the volume is expected for a first order transition [295].
Figure 3.12 Perturbative scaling of the transition coupling, anchored at the value of $\beta_c = 4.125(25)$ for $N_t = 6$. Points drawn as light squares are shown for the sake of completeness, but should be considered less significant. For $N_t = 4$, this is because lattice artefacts appear to be present – for one, figure 3.9 shows that, at beta $= 3.8$, measurements converge for $N_t \geq 6$, but $N_t = 4$ deviates quite significantly. On the other end of the range, the transition is largely smoothed $N_t = 10$. A transition region can be determined formally, which in fact appears to be nicely in line with expectations, but this might well be a fluke. The ribbon indicates the scaling region predicted by the two loop beta function. The perturbative approximation appears to work reasonably well over a small range of values in $N_t$, but in fact fails to describe behaviour for $N_t = 4$. 
3.5 Discussion

We find \( \beta_c(N_f = 8, N_t = 6, N_s = \infty) = 4.1125 \pm 0.0125 \), or \( 4.1 \geq \beta_c(N_f = 8, N_t = 6, N_s = \infty) \leq 4.125 \) and \( \beta_c(N_f = 8, N_t = 12, N_s = 24) = 4.34 \pm 0.04 \), or \( 4.30 \geq \beta_c(N_f = 8, N_t = 12, N_s = 24) \leq 4.38 \) and observe asymptotic scaling of the transition temperature within 20% by use of the perturbative scaling induced by asymptotic freedom, where the two loop beta function for an SU(3) gauge theory with \( N_f = 8 \) massless flavours has been used.

The occurrence of asymptotic scaling is a direct and strong indication that lattice artefacts are under control in the simulations presented in this paper. Earlier results, obtained by the Columbia group [165] in their work of the early 90’s, were attained from a non-improved action, and as such their results are not immediately comparable to ours. In any case, simulations performed at \( N_t = 8 \) without improvement in the action should be sensitive to lattice artefacts of at least \( O(a^2) \). Those artefacts are largely eliminated when using the improved action presented in section 3.1. The lack of asymptotic scaling at larger values of \( N_t \) observed in [165] may be partly due to the lack of such improvement. In figure 1 of this reference, to be compared directly to figure 3.7 in this chapter, the authors draw a dashed line whose existence they dub speculative, but that should in fact be reached by the current calculations. Of course, it would be very interesting to reach the continuum limit also without tadpole improvement, but this would require a much larger \( N_t \) and correspondingly low bare quark masses to improve the sharpness of the transition, as evidenced by the smoothing of the transition observed for the data obtained using a tree-level improved action on similar lattices. The latter, presented in section 3.4, while more crude and limited in accordance with their sensitivity to lattice artefacts, appear to show no significant qualitative deviations from those discussed in section 3.3, produced with a fully improved action. This simultaneously excludes action dependence of the results collected in this chapter and provides, through the observed deterioration of the signal, a handle on the effectiveness of the tadpole improvement scheme.

All evidence presented in this chapter is consistent with the occurrence of a true thermal transition. The emerging picture is in agreement with the conclusion of [171], as well as ladder calculations presented in [56], providing evidence that SU(3) gauge theory with eight flavours is in the normal, chirally broken phase of QCD at zero temperature and in the continuum limit. This study is an important step forward in our attempt to clarify the way SU(3) gauge theory with many flavours approaches the conformal phase [174] that precedes the loss of asymptotic freedom.
Evidence for a conformal phase in SU(N) gauge theories

Having established that N_f = 8 is still in the hadronic QCD-like phase, we shift our attention to larger numbers of fundamental flavours, in particular the interesting case of N_f = 12, in search of the conformal window. Many of the recent analytical studies predict a critical flavour number close to this integral value. That makes the investigation of the theory with twelve dynamical flavours highly relevant and possibly difficult at the same time, since a close proximity to the lower end of the conformal window makes it hard to discern between quasi-conformal behaviour and the regular phase of weakly interacting QCD near the end-point.

We observe a chiral phase transition and study the dependence of the transition coupling β_c on the lattice temperature scale N_t, finding that it persists in the limit of zero temperature, with no observable shift in the location of the transition coupling, in marked contrast to the behaviour found for the case with eight flavours described in chapter 3. Because a thermal transition occurring at low temperatures may be hard to discern, additional analysis is performed of the chiral extrapolation of the chiral condensate to establish restoration of chiral symmetry. As a final piece of evidence, the mass spectrum of the theory is used to deduce the behaviour of the non-perturbative beta function.

All evidence presented here points to a restoration of chiral symmetry at zero temperature and the presence of a Coulomb phase, implying the existence and onset of the conformal window for QCD-like theories having less than, but presumably close to twelve dynamical quark flavours.

1Based on A. Deuzerman, M.P. Lombardo and E. Pallante, Physical Review D 82, 074503 (2010).
This chapter is organized as follows. In section 4.1 we review previous theoretical work, in particular the scenario for conformality originally proposed in [82, 96], and define our strategy. Section 4.2 presents results on the chiral order parameter. It demonstrates the presence of a bulk transition and discusses the different systematics that may affect its measurement. These results are then used in section 4.3, that describes various theoretically motivated models for the a chiral extrapolation of the chiral condensate and the related fits. Section 4.4 addresses the spectrum, and it is organized in two subsections. The first one discusses the interrelation between the spectrum results and the pattern of chiral symmetry. The second subsection, similar in spirit to [169], argues that the lattice spacing increases when decreasing the coupling, as expected of a negative beta function; finally, it uses the numerical results combined with the perturbative input to argue in favour of the existence of a zero of the beta function. In section 4.5 we summarize the results, draw our conclusions.

4.1 A strategy for lattice conformality

A recent study of the SU(3) running coupling [171,172] by use of the lattice Schrödinger functional has concluded that \( N_f = 12 \) should already be in the conformal window. Other numerical studies, however, challenged this conclusion [176, 178, 182]. This is hardly surprising, given that \( N_f = 12 \) should be very close to the critical number of flavours [56, 127, 299, 300], making a numerical study particularly delicate. The strategy adopted in this thesis, complementary to that of [171,172], is inspired by the physics of phase transitions; it allows for the exploration of multiple aspects of the theory in different regimes and regions of the phase diagram, in order to probe the existence and properties of an IRFP inside and outside its basin of attraction.

The strategy of this study has received heuristic guidance by the scenario depicted in [82,96] and sketched in figure 4.1. We will implicitly assume the validity of that scenario. Following figure 4.1, at a given \( N_f > N_f^* \) and increasing the coupling from \( g = 0 \), one crosses the conformal line, location of the IRFP’s, going from a chirally symmetric (S) and asymptotically free phase (quasi-conformal phase) to a symmetric, but not asymptotically free one (Coulomb or QED-like phase). A phase transition need not be associated with the line of IRFP’s, differently from what was originally speculated in [80]. At even larger couplings, a transition to a strongly coupled chirally asymmetric (A) phase will always occur in the lattice regularised theory. The latter is referred to as a bulk phase transition. In the symmetric phases at non-zero coupling the conformal symmetry is still broken by ordinary perturbative contributions. They generate the running of the coupling constant which is different on the two sides of the symmetric phase. See [96] for a detailed discussion of this point. We emphasize that in the region considered in this paper conformal symmetry would still be broken by Coulombic forces.

A theory in the hadronic phase, \( N_f < N_f^* \), has a thermal phase transition in the continuum from a low temperature chirally broken phase to a high temperature chirally symmetric – quark gluon plasma – phase. Thus, as argued in chapter 3, the observation of a thermal transition in the continuum limit is incompatible with the existence of a conformal fixed point. It is also clear from figure 4.1 that the presence
4.1 A strategy for lattice conformality

Figure 4.1 Phase diagram of an SU(3) gauge theory with fundamental fermions in the $N_f$-$g$ plane after [96]. Theories for $N_f < N_f^*$ are QCD-like in the continuum, while for $N_f^* < N_f < N_f^c$ develop a conformal phase. $S$ and $A$ refer to chirally symmetric and asymmetric, respectively. The dashed line qualitatively indicates the location of the Banks-Zaks IRFP [80]. The dot-dashed line indicates a lattice bulk transition, which has been observed at $N_f = 12$ and $N_f = 16$. It stops at some small $N_f$ value. The line at $N_f = N_f^*$ represents the conformal phase transition [82,96], which is absent in the original Banks-Zaks scenario. The beta function on the conformal side is also sketched.
of a Coulomb phase next to the bulk transition at weaker coupling is a distinguishing feature of the conformal window. Here the non-perturbative beta function should be positive, implying a weakening of the effective coupling over increasing distances. The appearance of such a region is, in principle, a sufficient condition for the existence of an IRFP, since the perturbative beta function of $SU(3)$ with $N_f < 16\frac{1}{2}$ in the extreme weak coupling regime is known to be negative. Note, however, that the beta function is not universal away from fixed points with diverging correlation lengths and one can therefore not exclude a priori the appearance of spurious fixed points at intermediate values of the coupling constant [169].

The evidence presented here thus consists of a few components. First, it will be demonstrated that the location of the transition from the chirally symmetric to the broken phase is not sensitive to the physical temperature and is therefore compatible with a bulk nature. Subsequently, we will present a detailed study of the mass dependence of the chiral condensate on the weak coupling side of the bulk transition, which clearly favours exact chiral symmetry. Finally, the behaviour of the mass spectrum close to the bulk transition will be studied, and found to be compatible with a positive beta function, similarly to the observations of [169] for $N_f = 16$. These results are consistent with the scenario for conformality of figure 4.1.

We have simulated an $SU(3)$ gauge theory with twelve flavours of staggered fermions in the fundamental representation. We used a tree level Symanzik improved gauge action to suppress lattice artefacts, and Kogut-Susskind (staggered) fermions with the Naik improvement scheme, similarly to the action without tadpole improvement described in chapter 3. High statistics runs were performed at fixed bare quark mass $am = 0.05$ over an extended range of bare lattice couplings, on $16^3 \times 8$ and $16^4$ lattices. At two selected couplings, $6/g_L^2 = 3.9$ and $6/g_L^2 = 4.0$ we have performed runs on lattices $20^3 \times 32$, $24^4$, $32^4$ and five masses $am = 0.025, 0.04, 0.05, 0.06, 0.07$. The thermalisation of all runs was extensively verified by monitoring the stability of averages and uncertainties as a function of the discarded number of sweeps, and bin size. In addition, we have verified the decorrelation from initial conditions by performing simulations with ordered and random starts for a few selected couplings and masses. Runs were performed on the Huygens IBM Power6+ system at Sara supercomputing centre in Amsterdam and the IBM BG/P at the Rekencentrum of the University of Groningen. The largest volumes of $32^4$, needed for the bare quark mass of $am = 0.025$, were run on 512 nodes of the BG/P, corresponding to 2048 cores running at 850 MHz each. Obtaining sufficient statistics at those parameters required around 450 kCPU-hour. A more typical run, using a volume of $24^4$ for a bare quark mass of $am = 0.050$, would come in at around 100 kCPU-hour.

We have measured gauge and fermionic observables including the average plaquette, the Polyakov loop, the inter-quark potential, the chiral condensate and its susceptibility, the meson spectrum. We report here on our results for the chiral condensate and the meson spectrum. We underscore that staggered fermions have a remnant of exact chiral symmetry which allows a precise definition of the chiral order parameter – the condensate $\langle \bar{\psi}\psi \rangle$ – also on a coarse lattice.
4.2 The order parameter

Figure 4.2 shows our results for the chiral condensate at a fixed value of the bare quark mass $am = 0.05$ and for two volumes $16^3 \times 8$ and $16^4$, differing by a factor of two in their temporal extent $N_t$. The results display a sudden variation of the chiral order parameter as a function of the bare lattice coupling constant $g_L$, for both $N_t$. At this point one notices that the temperature of the system is related to the lattice temporal extent as $T = 1/a(g_L)N_t$, with $a(g_L)$ the lattice spacing for a given lattice coupling. From figure 4.2 one infers that the phase transition – or rapid crossover – happens at identical values of the transition coupling $g_c^L = 1.35(3)$, thus implying they occur at vastly different physical temperatures. Hence, one concludes that the observed transition (or crossover) is driven purely by the bare coupling constant itself and is therefore of bulk nature. Further information on this behaviour, with a refined scaling study, might shed light on the occurrence of a conjectured ultraviolet fixed point at strong coupling in the continuum theory [99]. The results of

![Plot of $\beta^3 \langle \bar{\psi} \psi \rangle$ vs $g_L$](image)

Figure 4.2 The bulk transition in the chiral condensate for $am = 0.05$ on lattices of $16^3 \times 8$ (circles), and $16^4$ (crosses) as a function of the bare lattice coupling $g_L$. Data are shown in the range $6/g_L^2 = 2.5$ to 4.7. The location of the transition is identical, while the curves describe physics at temperatures differing by a factor of two. Simulation errors are within symbol size.

...figure 4.2 beg for a detailed analysis of the behaviour of the chiral condensate at weaker couplings, in order to discriminate between a genuine phase transition to a chirally symmetric phase, and a rapid crossover to a phase where chiral symmetry is still broken.
In order to be able to extract information on the symmetry of the vacuum – chiral symmetry broken or restored – by extrapolating the condensate to the chiral limit, we need to measure it at infinite volume and at sufficiently light values of the quark masses. Light here means that the dynamics of the system is not yet dominated by the amount of explicit chiral symmetry breaking. This study, being of course extremely demanding from the point of view of numerical resources, was performed for two relevant selected couplings. We will first address the issue of systematic errors, then we will consider and compare several theoretically motivated parametrizations, appropriate for chirally broken or symmetric phases.

4.2.1 Finite volume effects

One major systematic effect potentially affecting analysis of the chiral order parameter and interpretation of the results is the finite volume at which simulations have been run. The reason for this can be ultimately found in the discretisation of the spectrum of eigenvalues that will necessarily occur at finite volume. One can write the chiral condensate in terms of the quark propagator \( S(x,y) \) as

\[
\langle \bar{\psi} \psi \rangle = \lim_{V \to \infty} \left( \frac{1}{V} \int_V dx S(x,x) \right).
\] (4.1)

One can write the propagator as a sum of eigenfunctions of the Dirac operator and integrate out the eigenvalues, to obtain [301]

\[
\langle \bar{\psi} \psi \rangle = \lim_{V \to \infty} \left( \frac{2m}{V} \sum_n \frac{1}{m^2 + \lambda_n^2} \right).
\] (4.2)

In the limit of infinite volume, the eigenvalues will become dense and the sum can be replaced by an integration

\[
\langle \bar{\psi} \psi \rangle = 2m \int_0^\infty d\lambda \rho(\lambda, m) \frac{\rho(\lambda, m)}{m^2 + \lambda^2},
\] (4.3)

where \( \rho(\lambda, m) \) is the density of eigenvalues within an infinitesimal range \( d\lambda \) around the eigenvalue \( \lambda \). A factor of the bare quark mass \( m \) multiplies the integral of equation 4.3, so only the IR divergent part of it will contribute to the condensate in the chiral limit. When the integral is regularised, one obtains from this the famous Banks-Casher relation [85]

\[
\lim_{m \to 0} \lim_{V \to \infty} \langle \bar{\psi} \psi \rangle = \pi \rho(0,0).
\] (4.4)

But finite volume corrections will lift the low lying eigenvalues, as the lowest eigenvalue is proportional to \( V^{-1} \neq 0 \). This removes the IR divergence and gives \( \rho(0,0) \to 0 \). An exactly chiral action will therefore give \( \langle \bar{\psi} \psi \rangle \to 0 \) for any finite size \( V \) of the lattice. Even away from the chiral limit, the contributions from the IR eigenmodes
4.2 The order parameter

may be so suppressed by a small lattice volume that all effects of spontaneous chiral symmetry breaking vanish. Generalizing, at any fixed volume, there exists a regime of finite masses that will go towards a chirally symmetric massless limit \[302\]. In fact, several groups have reported observing this regime at lattice sizes similar to ours \[176,178,179\], though using actions and bare quark masses different to the ones presented here. It is therefore necessary to explicitly exclude dominant finite volume effects.

When working at a particular finite quark mass, what volumes can be considered large enough? From the above derivation, we know the effects of spontaneous chiral symmetry breaking can be measured, provided that the integral of equation 4.3 can be introduced. The latter is sensible when the denominator in equation 4.2 varies slowly, in spite of the discretised values of \(\lambda\). Because the spacing of eigenvalues is inversely proportional to the volume, one can write

\[
\Delta \lambda \approx \frac{1}{V \rho(\lambda, m)} = \frac{\pi}{V \langle \bar{\psi} \psi \rangle}.
\] (4.5)

The last step is arrived at trivially by substituting in equation 4.4. When \(m\) is much larger than \(\Delta \lambda\), the term \(m^2 + \lambda^2 n\) will be a slowly changing quantity, and the form of equation 4.3 will be appropriate. Using equation 4.5, this gives us a condition

\[
Vm \langle \bar{\psi} \psi \rangle \gg 1.
\] (4.6)

Lattice results have been shown to reproduce the analytically expected behaviour accurately when this condition is satisfied \[303,304\]. Since this derivation only uses the form of the propagator, it is valid for each fermion flavour separately and therefore independent of the number of flavours altogether. Should the theory with \(N_f = 12\) possess a phase resembling regular QCD, in which case finite volume effects could interfere with observing spontaneous chiral symmetry breaking, then equation 4.6 should describe a range of safe parameters. It is easily seen from the numerical results in table 4.1, that there is no problem in satisfying this inequality for the results we obtained. The smallest value found is \(Vm \langle \bar{\psi} \psi \rangle = 7.28\) for \(am = 0.025\) and \(N_s = 16\) – a simulation that was excluded from further analysis.

We performed simulations for a succession of spatial lattice sizes and compared the value of the chiral condensate measured at each volume (see table 4.1). Finite volume effects are evident mainly for the smallest quark mass of \(am = 0.025\), and table 4.1 shows they follow the expected pattern. The effect shows up as a deviation of just over a percent between the smallest and largest volume and has not vanished completely even at \(N_s = 20\).

For each of the masses in table 4.1, the difference between the largest two volumes is smaller than both the difference between the smallest volumes and the combined statistical uncertainty, as graphically demonstrated in figure 4.3. The former ties in to the smoothness and monotony of the finite volume correction term of \[303\], in the sense that additional corrections would be expected to be even smaller in this declining series. The latter meant we could consider our largest volumes to be at infinite volume within their errors. The data set used for the extrapolation to the
Table 4.1 The volume dependence of the measured chiral condensate for $\frac{g^2}{\bar{g}^2} \equiv \beta = 3.9, 4.0$, for all masses used in the chiral approximation.

<table>
<thead>
<tr>
<th>$am$</th>
<th>$N_s$</th>
<th>$\langle \bar{\psi}\psi \rangle$, $\beta=3.9$</th>
<th>$\langle \bar{\psi}\psi \rangle$, $\beta=4.0$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.025</td>
<td>16</td>
<td>0.07592(22)</td>
<td>0.07113(11)</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>0.07638(22)</td>
<td>0.07212(13)</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td>0.07693(07)</td>
<td>0.07202(10)</td>
</tr>
<tr>
<td></td>
<td>32</td>
<td>0.07697(07)</td>
<td>0.07206(05)</td>
</tr>
<tr>
<td>0.040</td>
<td>16</td>
<td>0.12143(37)</td>
<td>0.11434(24)</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>0.12106(10)</td>
<td>0.11366(90)</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td>0.12092(17)</td>
<td>0.11360(10)</td>
</tr>
<tr>
<td>0.050</td>
<td>16</td>
<td>0.15004(26)</td>
<td>0.14090(52)</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>0.15018(17)</td>
<td>0.14093(19)</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td>0.15018(10)</td>
<td>0.14079(07)</td>
</tr>
<tr>
<td>0.060</td>
<td>16</td>
<td>0.17895(15)</td>
<td>0.16766(39)</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>0.17918(17)</td>
<td>0.16775(16)</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td>0.17897(14)</td>
<td>0.16787(11)</td>
</tr>
<tr>
<td>0.070</td>
<td>16</td>
<td>0.20705(65)</td>
<td>0.19469(42)</td>
</tr>
<tr>
<td></td>
<td>20</td>
<td>0.20776(19)</td>
<td>0.19476(11)</td>
</tr>
<tr>
<td></td>
<td>24</td>
<td>0.20768(10)</td>
<td>0.19470(13)</td>
</tr>
</tbody>
</table>

chiral limit consists therefore of the measurements at $N_s \times N_t = 24^3 \times 24$ and should allow for the observation of spontaneous chiral symmetry breaking, if present.

4.2.2 Mass effects

Evidence that we are considering sufficiently light quark masses is provided by the mass dependence of the condensate itself, and by our results for the spectrum in section 4.4, where we further elucidate this aspect. As for the issue of the continuum limit, we remind the reader that all the measurements are performed at a fixed value of the lattice spacing and no extrapolation to the continuum limit is considered. On the other hand, in the scenario of figure 1, there is only one symmetric phase at large $N_f$. Hence, once chiral symmetry is restored, it should stay so till the continuum. A preliminary study towards weak coupling has revealed no sign of further phase transitions, thus confirming this scenario. Being notoriously difficult to directly probe the IRFP with a lattice study, we are collecting precisely those measurements at finite lattice spacing and varying lattice coupling that can provide a combined evidence for the restoration of chiral symmetry and for the existence of the peculiar non asymptotically free regime that precedes the IRFP for decreasing coupling, a feature proper to non-Abelian gauge theories with a conformal phase. As we already noticed, if the bulk transition turns out to be a second order phase transition, this would signal the presence of an UVFP at strong coupling and the existence of a continuum limit for the strongly coupled theory, distinct from the ordinary continuum limit $6/g_{\text{L}}^2 \rightarrow \infty$ of the asymptotically free theory at weak coupling, see [99] for recent discussions on this point.
4.2 The order parameter

Figure 4.3 Observed finite volume effects in the chiral condensate, displayed as the difference $\Delta_{\text{FV}}$ between the measurements at the two largest available volumes ($24^3 \times 24$ and $32^3 \times 32$ for the lowest mass, $20^3 \times 32$ and $24^3 \times 24$ for the other masses) divided by their combined standard deviation $\sigma$. Triangles indicate results for $6/g_s^2 L = 3.9$, circles those for $6/g_s^2 L = 4.0$. A value of less than unity (within the band) implies that finite volume effects are within a single standard deviation of each other and therefore statistically irrelevant.

An indirect, but important influence of the finite bare quark mass on the chiral fitting procedure is the shifting of the transition coupling of the chiral transition. From an intuitive point of view, the effectiveness of the fermionic shielding is reduced with increasing bare mass as quantum contributions should be suppressed by $m^{-2}$ factors in the infrared. Spontaneous chiral symmetry breaking and the associated confinement will therefore set in at lower coupling. This intuition is corroborated by analytical approximations [305] for regular QCD and showing a large sensitivity in the limit of fairly small masses. On the lattice, the effect has been confirmed for finite temperature transitions [60]. The increased number of flavours present will work to enhance this effect [169].

The chiral extrapolation of the condensate close to a transition will be affected by this mass effect, with the measured condensate possibly showing an upwards deviation as a function of the mass. With increasing distance from the transition coupling, this upwards deviating trend will decay rapidly. Close to the transition coupling, however, it may be dominant. Fortunately, as such a deviation would be the only physically expected effect to introduce what appears like a negative exponent, it can be told apart. Figure 4.4 compares the mass dependence of the chiral condensate for a range of values of the coupling, starting at $6/g_s^2 = 3.5$, taken from figure 4.2 as the end point of the chiral transition for $am = 0.05$. With the mass effect shifting the transition towards weaker coupling, the condensates for $am = 0.06$ and 0.07
are expected to be raised considerably as $6/g^2 = 3.5$ should fall into the tail of the transition and the results confirm this. The effect disappears rapidly as the coupling decreases and seems to have all but vanished at this level once $6/g^2$ reaches a value of 3.7. At the level of accuracy needed for precision fits, however, the mass effect remains discernible. Allowing for an arbitrary power of the mass for the data in figure 4.4, i.e. $\langle \bar{\psi}\psi \rangle \propto am^\gamma$, gives a best fit of $\gamma = 1.004(6)$ for $6/g^2 = 3.7$, dropping to $\gamma = 0.976(4)$ only for $6/g^2 = 3.8$, with the quality of fit $\chi^2$ being 1.40 and 1.17, respectively. One might be tempted to stress the relevance of the measurements at $6/g^2 = 3.7$ as a consequence and assume large finite volume effects to be present at larger values of the coupling, as was done in [175,176]. But an additional measurement at $am = 0.025$ shows a deviation from the linear trend for lighter masses – finding 0.0892(2) for a predicted result of 0.0883. A fit of the full dataset will now find an optimal exponent $\gamma$ of 0.99(1). While not incompatible with the previous result as such, the qualitative change cautions against the assumption of a ‘sweet spot’, as the mass effect competing against other trends (anomalous dimension, finite volume effects) and rapidly decaying with the coupling will inevitably produce a region of the coupling in which something close to linear behaviour occurs. The shrinking of the usable range of the coupling due to the onset of dominant finite volume effects that is reported in [176] is therefore problematic, in that no separation of the different effects will be possible when remaining too close to the transition. For this study,
The order parameter

data sets at $6/g^2 = 3.9$ and 4.0 were selected, far enough from the transition region for mass effects to be strongly suppressed.

4.2.3 Correlation and thermalisation

An additional factor to take into account when safeguarding against the erroneous exclusion of spontaneous chiral symmetry breaking is the potential for underestimation of the errors because of the presence of correlations. The standard technique for removing these is the application of a blocking procedure to the date prior to its analysis. For a normally distributed observable in the absence of correlation, such blocking will leave the error essentially unchanged. If the original data were correlated however, the blocks will be increasingly less so, but the standard error in the mean (SEM) will increase as the influence of superfluous measurements declines. This procedure will work excellently for the type of correlations introduced by the Markov chain procedure used in generating configurations – the main property of these being a power law decline over a certain number of configuration. Inspecting the correlations for a thermalised large volume run at $am = 0.025$ in figure 4.5 shows the expected behaviour over short range. The autocorrelation should be integrated over to find an effective blocking size for the decorrelation of our data. Integrating over the local (i.e. lags up to 100) autocorrelation gives a result of 10.97 for the run depicted in figure 4.5, or 14.93 if the absolute autocorrelation is taken instead. From

![Autocorrelation R as a function of the lag τ for the Monte Carlo history at a volume of $32^3 \times 32$ and a quark mass $am = 0.025$. The local autocorrelation drops sharply over short distances, but weak correlations appear over long range.](image)
this, one concludes a blocking of twenty configurations suffices for local decorrelation. However, the weak autocorrelations over longer lags provide a less immediate problem for accurately determining the appropriate error budget. Once a sufficient number of domains has been found, a coarse enough blocking will provide a good estimate of the standard errors even here. However, at feasible simulation lengths, the total number of thermalised large fluctuations, that will span over 150 measured correlations or 750 updates, will be of the order of 10.

At the level of accuracy needed to distinguish between fits and for practical ensemble sizes, however, there may be an appreciable effect of the large scale correlations on the determination of the end of the thermalisation process. The criteria for deciding whether or not a particular Markov chain has reached a stable equilibrium are not always very sharp. Fortunately, with increasing statistics, the influence of any arbitrariness in the particular cut put on the ensemble of configurations should vanish. It is customary to apply a straightforward cut at a conservatively fixed number of trajectories and consider the data thermalised afterwards. With the comparatively large strides in parameter space taken in the simulation setup used for this study, such a construction would not produce optimal results, as the thermalisation process may slow considerably with lowering mass and increasing volume. As a consequence, one is forced to consider the Monte Carlo histories separately and look for stability of the measurements on observables.

The latter becomes complicated in the presence of the correlations observed earlier. While their amplitudes are relatively small, the combined effect of a fluctuation can shift the measured average by amounts of the order of a standard deviation for the numbers of trajectories that can reasonably be attained. These shifts can mimic thermalisation behaviour, such that a naive application of the stability criterion for the placing of a cut would lead to the incremental cutting of more and more data. In turn, this would successively diminish the available statistics, reinforcing the destabilizing effect of the remaining fluctuations. An ideal solution to this problem would be to enhance the available statistics by an order of magnitude and only then attempt the procedure, as none of these problems can occur in the limit of infinite statistics should. But it would be too conservative to assume nothing could be said about the observables – the fluctuations that do occur are within a very narrow band around a stable mean. An alternative view, and the one taken here, is that the error on the observable is underestimated. The cut dependence, and through it the fluctuations, could be quantified as a systematic error. When including such a systematic error, a realistic measurement of the chiral condensate can be given. Even with a slightly larger error, it might provide us with sufficient discriminatory power already.

To account for this systematic effect numerically, the data were in fact analysed with a range of cuts, starting from the first region of the Monte Carlo history dubbed stable and ending such that a statistically sufficient body of data would be present for each analysis. This fixed body of data entering every analysis we dub $O_i$ and, as the final part of the Markov chain, it should consist of fully thermalised data. This would be considered an extremely conservative choice of the thermalisation limit. From these analyses, we obtained a set of measured averages $\mu_i$ and associated standard errors $\sigma_i$. From these, a weighted global average $\bar{\mu}$ was calculated, with the inverse
squares of $\sigma_i$ functioning as weights. In the absence of systematic effects, this average would slightly overweight the data in $O_i$, but the increasing error would partially compensate for this. In general, $\bar{\mu}_i$ would be within equal within errors to the value found from a regular analysis. More crucial, however, was the determination of the error in this quantity. This was set to

$$\bar{\sigma}_i = \max \left[ \max [\mu_i + \sigma_i] - \bar{\mu}_i, \bar{\mu}_i - \min [\mu_i - \sigma_i] \right].$$  

(4.7)

By construction, the range $(\bar{\mu} - \bar{\sigma}, \bar{\mu} + \bar{\sigma})$ will cover $\mu_i$ and its associated error. In the limit of very high statistics, any cut dependence should vanish. This limiting property is guaranteed for the above procedure, as this would imply a dominant contribution to every average of $O_i$ limiting the spread of $\mu_i$ and, as a consequence, the amplitudes of $\sigma_i$. In addition, because of the clean Gaussian distribution appearing in the limit, the errors should be dominated by $\sqrt{N}$ behaviour and therefore determined by $O_i$ as the smallest data set in the analysis. Denoting the measurements associated with this set by $\mu_f$ and $\sigma_f$, one finds

$$\lim_{N \to \infty} \mu_i = \mu_f, \quad \lim_{N \to \infty} \bar{\mu}_i = \mu_f, \quad \lim_{N \to \infty} \bar{\sigma}_i = \sigma_f.$$  

(4.8)

Away from this limit, a conservative bound to the standard deviation from systematics is produced, that should decrease normally with added statistics.

### 4.3 Chiral extrapolation

Having obtained measurements of the bare quark mass dependence of the chiral condensate, one can attempt a chiral extrapolation. The appropriate way of doing this itself depends on the physical properties of the theory at the point of measurement, such as the phase of the theory and the proximity of a fixed point. To discriminate between the different scenarios, one therefore has to compare the extent to which different forms of the chiral extrapolation describe the data.

#### 4.3.1 Fits assuming the presence of a Goldstone boson

The functional forms discussed first would be appropriate if the bulk behaviour were not to be associated to a true chiral transition. For instance, it might just be due to a generic rapid crossover, or to a genuinely lattice transition between two phases with different ordering. In this case the range of couplings between $6/g_L^2 = 3.9$ and $6/g_L^2 = 4.0$ would still belong to the phase with broken chiral symmetry. We have thus considered the following functional form:

$$\langle \bar{\psi}\psi \rangle = Am + Bm \log(m) + \langle \bar{\psi}\psi \rangle_0,$$  

(4.9)

where the parameters were all left free, giving fits with two degrees of freedom, or in turn constrained to zero. The logarithmic mass dependence is typical of a chirally broken phase for a QCD-like theory in four dimensions at zero temperature.

The results of the fits to equation 4.9 are summarized in table 4.2. The linear
fits – case $B = 0$ also used in [176] – produce an intercept different from zero, but are highly disfavoured by their large $\chi^2$. The inclusion of the term $m \log(m)$ considerably improves the quality of the fits. Those with free intercept $\langle \bar{\psi}\psi \rangle_0$ gave an extrapolated value consistent with zero, and in agreement with the fit obtained by constraining $\langle \bar{\psi}\psi \rangle_0 = 0$. Both fits are satisfactory, and imply that the chiral condensate in the chiral limit is zero within errors. In conclusion, a conventional picture of the Goldstone phase seems not to be supported by our data.

<table>
<thead>
<tr>
<th>$6/g_L^2$</th>
<th>A</th>
<th>B</th>
<th>$\langle \bar{\psi}\psi \rangle_0$</th>
<th>$\sqrt{\chi^2}/\text{dof}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.9</td>
<td>2.70(3)</td>
<td>-0.103(13)</td>
<td>0.00013(54)</td>
<td>0.68</td>
</tr>
<tr>
<td></td>
<td>3.12(3)</td>
<td>0 (F)</td>
<td>0.0043(3)</td>
<td>3.12</td>
</tr>
<tr>
<td></td>
<td>2.682(5)</td>
<td>-0.107(2)</td>
<td>0 (F)</td>
<td>0.56</td>
</tr>
<tr>
<td>4.0</td>
<td>2.48(2)</td>
<td>-0.120(10)</td>
<td>-0.00091(42)</td>
<td>0.51</td>
</tr>
<tr>
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<td>2.73(1)</td>
<td>0 (F)</td>
<td>0.0041(5)</td>
<td>3.74</td>
</tr>
<tr>
<td></td>
<td>2.519(8)</td>
<td>-0.099(3)</td>
<td>0 (F)</td>
<td>0.56</td>
</tr>
</tbody>
</table>

Table 4.2 Fits to $\langle \bar{\psi}\psi \rangle = Am + Bm \log m + \langle \bar{\psi}\psi \rangle_0$

### 4.3.2 Fits with an anomalous dimension

We considered the functional form

$$\langle \bar{\psi}\psi \rangle = Am^{1/\delta} + Bm + \langle \bar{\psi}\psi \rangle_0,$$

containing an anomalous dimension, whose effect is parametrized by the exponent $\delta$. Since the fits described in subsection 4.3.1 already suggest that a curvature in the behaviour of the chiral condensate as a function of the mass is mandatory, we started by setting the linear term to zero. We note that analogous fits were used in the past to analyse QED in its symmetric phase, close to the strong coupling transition in [306], even if a more satisfactory account of the data requires the consideration of the magnetic equation of state, which is going to be discussed in the next section. Results for these fits are reported in table 4.3. All fits to equation 4.10 with $B = 0$ are satisfactory, with a chiral condensate compatible with zero in the chiral limit. This was checked, as before, by comparing fits with free intercept, and fits with $\langle \bar{\psi}\psi \rangle_0 = 0$.

One might still suspect that a fit combining a power-law term and a linear term, with a non zero intercept might still accommodate the data, hence indicating chiral symmetry breaking. For instance, a linear term can arise because of the additive renormalisation of the chiral condensate – see e.g. [69] for a discussion of this term in the context of the QCD thermal transition.

For completeness we have performed fits to equation 4.10 with the inclusion of a linear term. As expected from the near degeneracy between a power law with $1/\delta \approx 1$ and a linear term, the uncertainties coming from a Marquardt-Levenberg minimization of $\chi^2$ are huge – up to several times the fitted value itself. In table 4.3 we simply quote the central results, omitting the errors. Studies able to disentangle
4.3 Chiral extrapolation

The effect of linear scaling violations [69] were using an exact form for the scaling function which is not available here. In conclusion, the behaviour of the fits to equation 4.10 says that an additional linear term, or any analytic term in equation 4.10, is redundant for our data.

To acquire a feeling about the possible relevance of a linear term, we have also performed a sequence of fits, constraining the exponent to several values in the acceptable range given by the fit errors. The results are again summarized in table 4.3. It appears that the coefficient of the linear term smoothly changes from positive to negative, while the intercept - the chiral condensate in the chiral limit - remains consistent with zero throughout at $6/g_L^2 = 3.9$, and becomes slightly negative at $6/g_L^2 = 4.0$. We thus again conclude that our data point at exact chiral symmetry.

### 4.3.3 Fits motivated by the magnetic equation of state

Finally we considered fits motivated by the magnetic equation of state. The following equation is a satisfactory parametrization

$$ m = A\langle \bar{\psi}\psi \rangle + Bm + \langle \bar{\psi}\psi \rangle_0, $$

which would of course coincide with the simple power law when $A=0$. The coefficient of the linear term $A$ should vanish at a critical point, with $A \propto (\beta - \beta_c)$. This of

<table>
<thead>
<tr>
<th>$6/g_L^2$</th>
<th>A</th>
<th>$1/\delta$</th>
<th>B</th>
<th>$\langle \bar{\psi}\psi \rangle_0$</th>
<th>$\sqrt{\chi^2}/\text{dof}$</th>
</tr>
</thead>
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<tr>
<td>3.9</td>
<td>3.00 (F)</td>
<td>0.960 (F)</td>
<td>-0.30  (F)</td>
<td>-0.00002 (F)</td>
<td>0.96</td>
</tr>
<tr>
<td></td>
<td>2.700 (4)</td>
<td>0.9646 (4)</td>
<td>0.00 (F)</td>
<td>0.0000 (F)</td>
<td>0.55</td>
</tr>
<tr>
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<td>2.699 (25)</td>
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<td>0.00 (F)</td>
<td>-0.0000 (6)</td>
<td>0.68</td>
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<td>1.86 (24)</td>
<td>0.950 (F)</td>
<td>0.83 (26)</td>
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</tr>
<tr>
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<td>2.10 (27)</td>
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<td>0.68</td>
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<td>4.97 (64)</td>
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<td>-2.27 (66)</td>
<td>0.0000 (6)</td>
<td>0.68</td>
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<td>0.00 (F)</td>
<td>0.0000 (F)</td>
<td>0.87</td>
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<td>2.489 (18)</td>
<td>0.956 (3)</td>
<td>0.00 (F)</td>
<td>-0.0011 (4)</td>
<td>0.51</td>
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<tr>
<td></td>
<td>2.15 (17)</td>
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<td>0.33(18)</td>
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<td>0.06(21)</td>
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<td>0.960 (F)</td>
<td>-0.26(23)</td>
<td>-0.0011 (4)</td>
<td>0.51</td>
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<tr>
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<td>0.965 (F)</td>
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<td>0.970 (F)</td>
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<tr>
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<td>4.55 (36)</td>
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<td>5.74 (45)</td>
<td>0.980 (F)</td>
<td>-3.26(47)</td>
<td>-0.0010 (4)</td>
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Table 4.3 Fits to $\langle \bar{\psi}\psi \rangle = Am^{1/\delta} + Bm + \langle \bar{\psi}\psi \rangle_0$
course explains the smallness of $A$ close to the transition, while $\delta$ is the conventional magnetic exponent. The linear term in the condensate is implied by chiral symmetry, and guarantees that the ratio

$$\lim_{m \to 0} R_{\pi} = \frac{\partial \langle \bar{\psi} \psi \rangle / \partial m}{\langle \bar{\psi} \psi \rangle / m} = 1$$

approaches unity in the chiral limit and in the chirally symmetric phase. We can view equation 4.11 as a model for a theory with anomalous dimensions, which incorporates the correct chiral limit. Note that the linear term of equation 4.11 is of different origin than the one considered in equation 4.10. The latter describes violations of scaling and it is increasingly relevant at larger masses. In equation 4.11 instead, it is dominating at very small masses, away from the critical point.

Results for this case are given in table 4.4. The fit $m = m(\langle \bar{\psi} \psi \rangle)$ was performed with a least squares algorithm. Note that, as expected, the significance of the linear term is very low, closer to the bulk transition, and slightly larger by moving away from it. In table 4.5 we quote the numerical solutions of the equation $m(\langle \bar{\psi} \psi \rangle) = m_{\text{sim}}$, with $m_{\text{sim}}$ the simulation masses, to be compared with the simulation results for the condensate. The agreement is very good. All fits clearly favour a positive value for the coefficient of the linear term, as it should be in the chirally symmetric phase, and within the large errors the results for the exponent are compatible with the ones coming from the genuine power law fits. We conclude again in favour of chiral symmetry restoration.

### 4.3.4 Side-by-side comparison of the two simplest scenarios

The spirit of the analysis performed above is to see if any of the simplest physically motivated parametrizations can account for a condensate in the chiral limit different from zero, and we can conclude that all analyses favour a vanishing chiral condensate. In this subsection we directly compare in more detail the genuine linear fit, equation 4.9 with $B = 0$, as this is the only fit that produced a tiny non zero chiral condensate, and the genuine power law fit, equation 4.10 with $B$ and $\langle \bar{\psi} \psi \rangle = 0$, being it the simplest fit with a $\chi^2$ in an acceptable statistical range. In the rest of this section we refer to these fits as ‘linear’ and ‘power-law’, respectively.

The measured values of the chiral condensate and those predicted by the linear and power-law fits are shown in table 4.6. In figure 4.6 the measured data with superimposed fits are shown. Of course, since the range of variability of the chiral condensate is exceedingly larger than its errors, it is impossible to appreciate by eye the quality of the fits on this scale. A more effective description of the relative quality of the fits is offered by figure 4.7 and figure 4.8. In figure 4.7 we plot the difference

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|}
\hline
$6/\delta^2$ & $A$ & $B$ & $\delta$ \\
\hline
3.9 & 0.1(9) & 0.3(9) & 1.1(2) \\
4.0 & 0.3(1) & 0.077(9) & 1.3(1) \\
\hline
\end{tabular}
\caption{Fits to $m = A \langle \bar{\psi} \psi \rangle + B \langle \bar{\psi} \psi \rangle^\delta$}
\end{table}
### 4.3 Chiral extrapolation

<table>
<thead>
<tr>
<th>$6/g_L^2$</th>
<th>$am$</th>
<th>$\langle \bar{\psi}\psi \rangle$</th>
<th>$\langle \bar{\psi}\psi \rangle_{fit}$</th>
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<td>0.17897(14)</td>
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<td>0.070</td>
<td>0.20768(10)</td>
<td>0.20768</td>
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<tr>
<td>4.0</td>
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<td>0.11360(10)</td>
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<td>0.14079(07)</td>
<td>0.14083</td>
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<td></td>
<td>0.070</td>
<td>0.19470(13)</td>
<td>0.19469</td>
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</table>

Table 4.5 Comparison of the simulation results for $\langle \bar{\psi}\psi \rangle$ with the ones obtained from the fits to the Magnetic Equation of State.

Figure 4.6 Fits to the chiral condensate measured at $6/g_L^2 = 3.9$ (circles) and $6/g_L^2 = 4.0$ (triangles), with both linear fits and power-law fits drawn in.

between the chiral condensate predicted by the fits and the data, divided by the data themselves. The tension between fitted and numerical results for the linear form is quite evident. The pattern of the deviations in the linear fits indicates a significant curvature, which is reflected in the quality of the fit. The pattern of the residuals of the power law fit is instead far less structured and statistically insignificant throughout. figure 4.8 offers in our opinion the most clear way of visualizing the deviations by plotting the same difference as in figure 4.7, this time divided by the error $\sigma$. The horizontal band indicates the boundary of one standard deviation, and the points
Table 4.6 Measurements of the chiral condensate at $N_s \times N_t = 24^3 \times 24$ for two values of the coupling $6/g_s^2 = 3.9$ and 4.0, and a range of bare quark masses $m$, together with the values predicted by the fits to a linear and a power-law model.

<table>
<thead>
<tr>
<th>$6/g_s^2$</th>
<th>$m$</th>
<th>$a^3\langle \bar{\psi}\psi\rangle_{\text{measured}}$</th>
<th>$a^3\langle \bar{\psi}\psi\rangle_{\text{linear}}$</th>
<th>$a^3\langle \bar{\psi}\psi\rangle_{\text{power}}$</th>
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<tr>
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<td>0.070</td>
<td>0.19470(13)</td>
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</table>

obtained by a power law fit nicely fall within it, while again the tension with the linear form appears. These results thus confirm a strong preference for the restoration of chiral symmetry at the weak coupling side of the transition.

It is clear that additional data at even lighter masses will improve the discriminating power of these fits and eventually allow to significantly constrain the linear contributions. The presence of curvature in the data and the very good quality of the power-law fit, having barred finite volume effects, is also an indication that we are not in the heavy quark limit. In addition, one could also study the analogous of the GMOR relation of broken chiral symmetry, and variations of it in terms of the scalar meson mass, by also measuring the pion decay constant $f_\pi$ in the chiral limit and the scalar mass.

4.4 Spectrum analysis

An alternative approach to the study of the symmetry of a phase is offered by the spectrum analysis [294]. Particularly useful quantities for this type of study are the masses of the ground state excitations in the pseudo-scalar and vector channels, with slight abuse of nomenclature from QCD referred to as the $\pi$ and $\rho$ masses. We defer to future work the exploration of other interesting observables, such as the ratio of the scalar and pseudo-scalar masses or equivalently the ratio of transverse and longitudinal chiral susceptibilities.

4.4.1 Meson correlators and taste breaking

Because of the presence of temporal doublers, staggered fermions correlation functions show mixing of opposite parity states [307,308]. The interpolating fields for the pseudo-scalar and vector channels have dominant contributions from the respective particles and their excited states. The pseudo-scalar channel shows no discernible mixing with its parity partner. This is a usual result, as this parity partner is exotic
4.4 Spectrum analysis

Figure 4.7 Deviations $\Delta$ of the fitted value from the measured value $\bar{\mu}$ for the chiral condensate, rescaled by the measured value itself. Error bars represent the relative (rescaled by the data) standard deviation on the measured value. Deviations from the prediction with a fit to the linear form are given by open symbols, while those for a fit to a power-law are given by grey symbols. The top graph displays results for $6/g_L^2 = 3.9$, the lower graph those for $6/g_L^2 = 4.0$. The linear form shows tension with the data for both values of the coupling, which is quantitatively seen in the larger $\chi^2$ value.

and heavy [309]. For the vector channel, there is mixing of the vector meson (which would be $\rho$ meson in QCD) with its parity partner (which would be the $a_1$ meson in QCD) at an amplitude comparable to that of its first excited state. It was observed in [169] that the splitting between the energy levels of the excitations is not very large
Figure 4.8 Deviations $\Delta$ of the fitted value from the measured one for the chiral condensate, rescaled by the standard deviation $\sigma$ of each measurement. Results are shown for both $6/g_s^2 = 3.9$ (circles) and $6/g_s^2 = 4.0$ (triangles), with fits to the linear form shown using open symbols and fits to the power law drawn in with grey symbols. The data and corresponding fits are displayed on linear scales in the inset.
within the quasi-conformal phase. We too, observed a small separation between the different excitations. As a consequence of this, pure states were hard to isolate on the lattice volume of $16^3 \times 24$ that were used in these simulations. Instead, multi-state fits were used on the correlators, in general resulting in excellent fits except for the very lowest time points. The measurements of the correlators were relatively precise there, because of the large amplitudes. At the same time, those points contain contributions from rapidly decaying excited states.

Fits weighted in the usual way, i.e. with a weighting $\sigma^{-2}$ from the standard deviation $\sigma$, will weigh the low time points heavily result in bad overall fits. One way of dealing with this problem would be to exclude those specific points from the analysis, thereby sacrificing some of the capability to distinguish between the ground state and first excited state that dominate the remainder of the correlator. Alternatively, one can switch to relative weighting, minimizing the relative, instead of the absolute deviation. This removes the bias towards the lowest points, while still including all points to maximize the available information for the estimate of the ground state. Unfortunately, it clearly ignores the increasing amounts of noise as one measures increasing time separations. In practice, both methods produced very similar results. Since neither method could be said to be clearly superior, an average of both results was used as the final result, with a spread introduced as a systematic error component.

The generic form used for fitting staggered meson correlators can be written

$$C(t) = \sum_{i=1}^{N_e} A_i^e \cosh \left[ m_i^e \left( t - \frac{T}{2} \right) \right] + (-1)^t \sum_{j=0}^{N_o} A_j^o \cosh \left[ m_j^o \left( t - \frac{T}{2} \right) \right],$$

(4.13)

with $T$ the lattice size in the temporal direction and the indexed $A$ and $m$ the free parameters in the fit. Here $N_e$ is set to the number of ‘even’ modes, always referring to the dominant contribution to the correlator, and $N_o$ the number of ‘odd’ modes that mix in with opposite parity. In general, $N_o = N_e - 1$, with the number of odd modes set equal to zero manually for the pseudo-scalar correlator because of the lack of correlator mixing mentioned above. There were no correlators for which fitting to a formula with $N_o > 1$ produced constrained results. As figure 4.9 demonstrates, the described fitting procedures, with two even contributions for the $\pi$ and an additional odd contribution to account for the mixing with axial vector particle $a_1$ for the $\rho$, reproduced the data accurately. The alternating sign of the odd contributions, written customarily as $(-1)^t$, is by construction only defined at integer values of $t$ and was replaced by $\cos [\pi t]$ for numerical stability – this produces the smooth interpolation seen in figure 4.9.

As mentioned in chapter 1, lattice artefacts will break the taste symmetry of staggered fermions [160] and lift the original quark mass degeneracy. A full study of the magnitude of these effects would require the determination of the low lying eigenvalues of the Dirac operator, as was done in [310]. The presence of $O(a)$ improvement should reduce the effect and this has been explicitly shown to be the case [311]. We limited ourselves to an explicit check of the pion mass splitting by comparing the mass extracted from the pseudo-scalar correlator with the mass of the alternate
Figure 4.9 Meson correlators in the pseudo-scalar and vector channels for a representative run with \(6/g^2 = 3.7\), \(am = 0.05\) and a volume of \(N_s^3 \times N_t = 16^3 \times 24\). Fits with successively increasing number of terms in equations 4.13 are indicated by solid lines. For the pseudo-scalar correlator, the red line indicates a fit with a single cosine hyperbolic, the blue line a fit with a double cosine hyperbolic. For the vector correlator, the red line again indicates a single cosine hyperbolic, the purple line a cosine hyperbolic plus one of alternating signs, while the blue line represents the fit with a double cosine hyperbolic and a cosine hyperbolic of alternating sign.

pion appearing as the parity partner of the scalar \(\sigma\), similar in spirit to [312]. With the presence of the light pseudo-scalar contribution, the scalar correlator itself has an alternating sign. We folded the correlator with a \((-1)^t\) function to exchange even and odd contributions, then fitted the scalar correlator to a functional form identical to that of the vector, i.e. equation 4.13. For the representative ensemble from which the correlators in figure 4.9 were extracted, the lowest mass odd contribution to the scalar correlator was found to be \(am'_\pi = 0.759\), which should be compared to a value of \(am_\pi = 0.591\) from the pseudo-scalar correlator. This would imply a relative taste breaking of 28.6% for this particular run, though the splitting between the primary and secondary \(\pi\) mixing with the \(\sigma\) is not necessarily the largest of the multiplet. We can contrast this result with measurements at the lowest bare quark mass presented in this analysis, \(am = 0.025\), giving a pion mass splitting of only 14.3% that hints at roughly linear behaviour with the input bare quark mass. As expected from the level of improvement, the values found here are somewhat larger than those reported by other groups using staggered fermions with either stout smearing [177, 179] or a DBW2 gauge action [175].

But what are the consequences of the taste breaking in this system? Since the artefacts will vanish smoothly in the chiral and continuum limit, these is no issue in connecting to the continuum theory that interests us. At the level of the lattice regularised theory, the impact of the increased fermion masses caused by taste breaking could be described as lowering the effective flavour number. This would be a potential issue when simulating right at the edge of the conformal window. Here a (barely) conformal continuum theory could be pushed into the hadronic phase by the lattice regularisation. The results presented in this chapter, however, show no indications of this scenario. On a more quantitative level, we study the quasi-conformal phase
4.4 Spectrum analysis

<table>
<thead>
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<th>$6/g_L^2$</th>
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<th>value</th>
</tr>
</thead>
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</tr>
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<td>0.639(6)</td>
</tr>
<tr>
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</tr>
<tr>
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<td>$A$</td>
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</tr>
<tr>
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<td>$\sqrt{\chi^2/\text{dof}}$</td>
<td>0.70</td>
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</table>

Table 4.7 Results of fits to the functional form $(am_\pi)^2 = A(a^3\langle \bar{\psi}\psi \rangle)^{2\delta X}$. Fits are performed to the separate values of the coupling constant and the combined data set.

of the theory away from IR fixed point itself. There the value of the quark mass can be safely kept small with respect to the scales of the gauge field [184], at which point the exact values of the nearly degenerate masses are irrelevant. These considerations might obviously change for studies with a strong quantitative focus, but that is at any rate not in the scope of this investigation.

4.4.2 Spectrum and chiral symmetry

A powerful way to distinguish between symmetric and broken chiral symmetry [294] is to plot the pseudo-scalar mass as a function of the chiral condensate, as in figure 4.10. We have considered the same range of bare fermion masses used in section 4.3 for the chiral extrapolation of the condensate. The data are best fitted by a simple power-law form and the results are reported in table 4.7. They clearly suggest that chiral symmetry is restored and that the theory has anomalous dimensions. In the symmetric phase and in mean field [294], we expect a linear dependence with non negative intercept. The presence of anomalous dimensions is responsible for negative curvature - noticeably opposite to what finite volume effects would induce - and a zero intercept. The same graph in the broken phase would show the opposite curvature and extrapolate with a negative intercept.

This result gives also further confidence that the fermion masses used in this study are not too light, so that they do not significantly feel the finite volume, and not too heavy, so that they are not blind to chiral symmetry. In figure 4.11 we report on the measured values of $m_\pi$ and $m_\rho$ as a function of the bare fermion mass. Here the lightest point at $am = 0.025$ for the vector mass is absent, but a curvature can still be appreciated. Simulations were done on $16^3 \times 24$ volumes, while a set of measurements at larger volumes showed that finite volume effects were under control. The mass dependence shown in figure 4.11 hints again at a few properties of a chirally symmetric phase. We have fitted both the pion and the rho mass to a power law

$$m_{\pi,\rho} = A_{\pi,\rho}m_{\pi,\rho}^{\epsilon_{\pi,\rho}}$$

(4.14)
Figure 4.10 The relation between the chiral condensate and the pion mass, for $6/g_s^2 = 3.9$ (squares) and 4.0 (circles). The line represents a power law fit to the combined data, the results of which are reproduced in table 4.7.

with the results $A_\pi = 3.41(21), \epsilon_\pi = 0.61(2), A_\rho = 4.47(61), \epsilon_\rho = 0.66(5)$ at $6/g_s^2 = 3.9$, and $A_\pi = 3.41(21), \epsilon_\pi = 0.61(2), A_\rho = 4.29(11), \epsilon_\rho = 0.66(1)$ at $6/g_s^2 = 4.0$. The accuracies of these fits are not comparable with those achieved by the fits to the chiral condensate, however they allow to draw a few conclusions. First, the mass dependence of the vector and pseudo-scalar mesons is well fitted by a power-law. Second, it is also relevant that the exponents are not unity and $\epsilon_\pi \neq 1/2$. The latter result immediately tells that the pion seen here is not a Goldstone boson of a broken chiral symmetry. In addition, both mesons have masses scaling with roughly the same power, as it should be in a symmetric phase, and with increasing degeneracy towards the chiral limit. The exponent of the power law being not one, confirms that we are not in the heavy quark regime.

These results are confirmed in a more visual way by looking at the behaviour of the mass ratio. figure 4.12(b) shows the ratios of measured pseudo-scalar and vector masses, for a fixed coupling and as a function of the bare quark mass. We have superimposed the ratios of the best fits to the raw mass data, as explained in section 4.4.3. It is immediately clear that the ratio increases as the quark mass approaches zero, a behaviour opposite to what is expected for a Goldstone pion. Notice also that the mass ratio should be one for exact conformal symmetry in the chiral limit [197]: we do not yet observe that, since, as explained in Section 4.1, conformal symmetry is expected to be broken by Coulombic forces in the region of parameter space probed by this study. On the other hand, the trend towards unity as decreasing the lattice
4.4 Spectrum analysis

Figure 4.11 The relation between the bare quark mass and the masses of the pion (red) and rho meson (blue), for $6/g_L^2 = 3.6, 3.7, 3.8, 3.9$ and 4.0 from the uppermost line down. Power law fits to the separate values of beta are provided.

The coupling $g_L$ is evident, and certainly worth further exploration.

4.4.3 Spectrum, lattice spacing and the beta function

We used the spectrum results to determine the lines of “constant physics” in the two dimensional parameter space $g_L$ and $am$, the bare quark mass of degenerate fermions, following the same strategy which was successful for $N_f = 16$ [169]. Along these lines the coupling and masses are all functions of the lattice spacing $a$. Since all dimensionful quantities measured on the lattice will be expressed in terms of the lattice spacing and will therefore vary with $g_L$ even if they do not physically, a dimensionless quantity has to be taken as a reference. A convenient choice is the ratio of the $\pi$ and $\rho$ masses. Before continuing, let us specify that the same caveat as in Ref. [169] applies: since we are at strong coupling, there is no guarantee that the system can be described in terms of a one-parameter beta function. This implies, for instance, that the lines of “constant physics” determined by use of certain observables might not match those determined using other observables. If multiple bare couplings are needed, it might happen that the change of physics produced by changing only one bare coupling will not be compensated by a change of mass. So our lines of “constant physics” are, strictly speaking, lines of constant $m_\pi/m_\rho$ ratio. We will show in the following that in order to keep this ratio constant the bare parameters $am$ and $g_L$ controlling the simulations should be tuned as if we had a one parameter, positive beta function.
Figure 4.12 (a) Measurements of the pseudo-scalar (blue) and vector (red) masses versus lattice coupling at several values of the bare quark mass, from bottom to top $am = 0.04, 0.05, 0.06$ and $0.07$. Lines displayed represent a global parametrization, with a mixed $O(m)$ polynomial quark mass dependence and $O(\beta^2)$ polynomial dependence, with lattice parameter $\beta = 6/g_L^2$, and producing a reduced $\chi^2$ per degree of freedom just over unity for both channels. Errors include fitting systematics from combining several methods. (b) The measured $\pi$ to $\rho$ mass ratio as a function of the bare mass and decreasing coupling $g_L$, bottom to top $6/g_L^2 = 3.5$ to 4. The superimposed lines are ratios of the best fits in figure 4.12(a).

In figure 4.12(a) we report on the measured values of $m_\pi$ and $m_\rho$ as a function of the bare coupling, while figure 4.12(b) shows the ratios of measured pseudo-scalar and vector masses, for a fixed coupling and as a function of the bare quark mass. We have superimposed the ratios of the best fits to the raw mass data, confirming the good quality of the interpolations derived in figure 4.12(a) and used to produce figure 4.13.

It is immediately evident from figure 4.12(b) that, in order to keep the ratio constant, we should simultaneously decrease the lattice coupling $g_L$ and increase the bare mass. These results already indicate that the lattice spacing increases while decreasing the coupling. This is the same behaviour as observed for $N_f = 16$, and of the pion to sigma ratio in QED. It is also expected of a one parameter beta function with a positive sign.

To refine the analysis and express the result in terms of a physical observable instead of the unobservable bare quark mass, we proceed as follows. We fit the measured values of both masses to a polynomial parametrization, as shown in figure 4.12(a), then determine the value of the ratio of masses from the ratio of the two parametrizations. Because both masses are fitted separately, these fits are more robust against outliers in the separate measured values. Now, instead of only comparing points in parameter space at similar values of the ratio $R = m_\pi/m_\rho$, we can consider the ratio of interpolating functions

$$
\tilde{R}(g_L, am) = \frac{am_\pi(g_L, am)}{am_\rho(g_L, am)}.
$$

(4.15)

Given reference values for $g_L$ and $am$ and a different coupling $g'_L$ in the surroundings
of $g_L$, from

$$\tilde{R}(g_L, am) \equiv \tilde{R}(g_L', a'm')$$

(4.16)

one can determine the value $a'm'$ that keeps the ratio constant.

For this approach to be valid, no particular constraints need be put on the parametrizing function, other than that the data should be described to appropriate accuracy. We started from a polynomial expansion in both $\beta = 6/g^2$ and $am$ and performed a series of linear fits. The mass dependence was found to be approximately linear, while a second order polynomial provided a sufficient approximation of the behaviour with the coupling constant. A direct product of both expansions gave redundant degrees of freedom, producing values of $\chi^2$ below unity and some poorly constrained fitting parameters. Since the numerical values of the parameters are irrelevant – we just need them to describe the data – such a model might appear usable. But such an overly complete fit of the data implies we also fit the noise in the measurement, introducing statistical artefacts in the analysis. To eliminate some of the redundancy, a step-wise reduction of the polynomial was performed using Akaike’s Information Criterion (AIC), a measure of the trade-off between the gain in accuracy and loss of information to model complexity that is based on entropic principles [313]. For these regular $\chi^2$ fits, the AIC can be written as

$$AIC = 2k + \chi^2 + C,$$

(4.17)

with $k$ the number of free parameters in the fit and $C$ a constant that is ultimately irrelevant as only differences in the value of AIC for different models are relevant. Starting from the full direct product polynomial, fits were done removing each term present separately. If one or more of the reduced models provided a lower AIC, the most successful model was chosen and the procedure repeated. These iterations culminated in a model of the form

$$am_{\pi/\rho} (\beta, am) = c_0 + am \left(c_1 + c_2\beta + c_3\beta^2\right),$$

(4.18)

with only four degrees of freedom, $c_0$ to $c_3$, the fitted values of which are given in table 4.8, sufficient to describe the data as presented in figure 4.12(a).

| $c_0$ | $0.233$ | $0.245$ |
| $c_1$ | $56.96$ | $179.74$ |
| $c_2$ | $-22.25$ | $-81.96$ |
| $c_3$ | $2.371$ | $9.700$ |

Table 4.8 Results of fits to the masses of the pseudo-scalar and vector particles to the functional dependence of equation 4.18, as plotted in figure 4.12(a).

Having obtained a good approximation to the behaviour of the spectrum as a function of the two free parameters ($g_L$ and $am$) of our theory and the functional
Figure 4.13 Pseudo-scalar mass along lines of constant physics, for a model without inclusion of a term linear in the inverse coupling squared. The physical pion mass is identical along lines of constant physics, such that a decreasing pion mass in lattice units for increasing $g_L$, implies an increase of the lattice spacing for weaker couplings, signature of the Coulomb phase. The pseudo-scalar mass along lines of constant physics was constructed by interpolating along the isolines of the ratio of the separate interpolations of pseudo-scalar and vector masses, where the interpolating form chosen was always identical for both masses. The polynomial models shown here were found to be most appropriate by Akaike’s Information Criterion. Labels give the value of the ratio $m_\pi/m_\rho$ along the isolines.

dependence of the mass ratio within the region of our measurements, we can invert this relation and trace the isolines of the physical condition

$$R = m_\pi/m_\rho \equiv \text{const} \quad (4.19)$$

in parameter space. As $g_L$ and $am$ fully define our theory, this effectively provides us with a series of Renormalisation Group curves along which an identical physical system is described at differing lattice scales $a$. We will refer to these isolines as lines of constant physics. If one takes a dimensionful physical quantity, rather than the unobservable bare quark mass, and measures it along such a curve, any changes in the value measured should be a direct consequence of the changes in the scale itself. The pion mass is exactly such a physically fixed quantity, and tracing its value in lattice units along lines of constant physics will provide us with a direct non-perturbative measurement of the change in the scale $a$ as the coupling constant runs. Such an analysis is displayed in figure 4.13.

Generalizing, along the lines of “constant physics” the slope of the line of measured values of the pseudo-scalar mass is a direct measure of the sign of the beta function. Figure 4.13 provides evidence for the Coulomb-like phase, with a positive sign of the beta function, in full agreement with the more direct discussion of fig-
Since the beta function is known to be negative in the continuum limit, our results indicate a zero of the beta function at some intermediate coupling $g^*$. We emphasize that the location of this zero is regularization dependent, and we reiterate the caveat at the beginning of this section. Further, we do not claim to have directly studied the physics around the IRFP itself. The latter type of study is notoriously difficult, while the strategy presented here aims at probing the emergence of conformality in an indirect way.

4.5 Summary and Outlook

Summarizing the main findings of this chapter, we observed a lattice bulk transition (or crossover) which is clearly of non-thermal nature for an SU(3) gauge theory with three unrooted staggered fermions, corresponding to twelve continuum flavours. The realization of the chiral symmetry on the weak coupling side of this transition has been studied and the analysis of the order parameter favours a restoration of chiral symmetry. A study of the spectrum in the weak coupling phase close to the transition favours chiral symmetry restoration as well. Having derived the lines of constant physics, we inferred a positive sign of the beta function, implying the emergence of a Coulomb phase as envisaged in the scenario of [82,96].

The above results provide evidence towards the existence of a chirally symmetric, Coulomb-like phase on the weak coupling side of the lattice bulk transition. In the scenario of [82,96] and figure 4.1, such a Coulomb-like region must be entangled to the presence of a conformal infrared fixed point for the theory with twelve continuum flavours, without any further transition at weaker coupling. Such a Coulomb-like phase is not expected in ordinary QCD. We reiterate that the evidence provided is indirect, while we do not address the physics at the infrared fixed point.

A few directions are a natural extension of this work. An accurate chiral extrapolation of the chiral condensate in the strong coupling phase, would allow to determine the precise location of the chiral phase transition (or crossover). Establishing the nature of such a bulk transition might shed light on the possible emergence of an ultraviolet fixed point in the continuum theory at strong coupling [99]. It is also important to notice that a way to discriminate between the scenario of [82,96] and the one originally proposed in [80] is the presence of a chiral transition towards a broken phase at weaker couplings. While both scenarios share the presence of conformality and of a Coulomb-like phase, only in the first a range of theories exists – the conformal window – where confinement and chiral symmetry breaking do not occur at weak coupling. For a recent review on the subject, see Ref. [77]. In addition, more extended results on the mass spectrum, in particular an analysis of the chiral partners, would shed further light on the pattern of chiral symmetry breaking and restoration for this theory. Work in these directions is in progress. Alternative studies based on the Renormalization Group analysis as proposed in [314] will provide an independent and valuable tool to investigate these systems. Such studies aim to directly probe the existence of an infrared fixed point and complement indirect searches for conformal behaviour in SU($N$) gauge theories with matter content.
Having demonstrated the likely presence of a fermion induced fixed point of SU(3) Yang-Mills with twelve degenerate light quark flavours in the previous chapter, the question to its properties poses itself. It is important to remember that the scale invariance that characterizes the fixed point in the continuum theory cannot be directly observed in the setup that we have chosen. The mandatory explicit quark mass means conformal symmetry is always broken and a truly conformal phase will never be produced.

This does not imply that no further information on the conformal phase can be obtained from lattice simulations. In this chapter, we study the behaviour of the bulk transition with varying mass and determine its order. The nature of this transition is important, as it carries information on the potential existence of a UV fixed point. Complementary to the chiral dynamics, we examine the indicators of confinement, the Polyakov loop and static potential, for signs of the presence of the IR fixed point. Finally, a preparatory study of the perturbative expansion of the plaquette is presented, testing the approach of the perturbative regime.

The data reported here are largely preliminary and part of an ongoing research effort. We will therefore have to content ourselves with presenting first indications for physical properties of the theory, that will function to guide future studies into the curious case of QCD with twelve massless quarks.

\footnote{Manuscript in preparation.}
CHAPTER 5  FURTHER SIGNATURES

The bulk transition reported upon in chapter 4 was determined at a single value of the bare quark mass $a m$. Of course, no true conformal limit is in fact expected to develop away from the chiral limit and it is therefore crucial to determine the behaviour of the theory under changes in the quark mass. In fact, without any physical reference scale or well established results from chiral perturbation theory to guide us, it is not clear what range of finite quark masses can be considered small. Had we attempted an extrapolation to the continuum limit or assumed cut-off independence, no region of finite quark masses could be described as safe. In an RG sense, the quark mass is the only relevant operator in the system and it would be pushed towards infinity. This process would destabilize the original conformal fixed point and the theory should enter a phase resembling regular QCD. But even though no cut-off independent results can be obtained away from the asymptotically free limit, what is given as the bare coupling to the theory could be seen purely as an effective coupling at the given scale. Since they remain finite, it is implied our description will not be valid to arbitrarily high energies. However, though RG curves may not span the full range of lattice spacings, they can still be locally well defined.

This does not change the fact that no finite value of the mass will approach the continuum chiral limit of the theory. As such, the fixed point cannot be reached precisely within any of the simulations in their current setup. Fortunately, this does not imply they cannot be approached to a reasonable degree. The crucial realization in these is the connection the RG flow constructs between the measurement scale of the theory and the coupling. A vanishing beta function implies a coupling constant that is largely unchanged under large changes in that measurement scale. When simulating at a particular scale, as we approach the region of the IR fixed point, large changes in the physical scale are to be expected. That implies that, even at a small distance of the transition coupling, a well defined hierarchy of scales may be present on the lattice. Were the IR fixed point to be determined from a step scaling function, which is a natural translation of RG reasoning to lattice measurement, those scales would not immediately collapse in on each other. Rather, it is the continuing presence of the gluon induced lattice scale that will protect the gauge dynamics from large variations over sizeable scaling variations. A recent publication taking this approach in fact demonstrates this explicitly [184] for a range of quark masses similar to the ones used in our simulations.

The fact that a small mass regime exists does not by itself imply this regime is approached by the current simulations. In order to see if it is, we return to the bulk transition reported in chapter 4. We extend those data, obtained for a single bare quark mass, by measurements at a range of masses. This allows us to examine the behaviour of the order parameter and susceptibilities around the transition, under changes in both the bare quark mass and the volume of the lattice. From this, one can attempt to determine the order of the phase transition. As was pointed out in chapter 1, the nature of the transition can provide important information on the continuum limit of the theory. If the transition is associated with a UV fixed point, as predicted in [99], it should be second order. Observation of a first order phase transition, instead, would in principle exclude UV fixed point dynamics.

The presence of a conformal window could also, and complementary, be detected
5.1 Mass dependence of the bulk transition

As the shielding effect provided by dynamical quarks should be the main trigger of the transition, there should be a direct relation between the bare quark mass and the strength of the coupling. Since the shielding effect increases in strength as the quark mass lowers, chiral symmetry should be restored at stronger coupling towards the chiral limit. Figure 5.1 demonstrates that this is in fact the case and shows the direct relation between the dynamical quarks and the restoration of chiral symmetry at zero temperature. This vindicates our dismissal of chiral dependencies at those values of $\beta$ showing opposite curvature in chapter 4 (figure 4.4). Those were clearly present for the values $\beta = 3.5$ and 3.6, which figure 5.1 shows are within the broad transition region of the $am = 0.070$ system.

A peculiar feature of the figure 5.1, however, is the apparent appearance of a double transition at the two lowest value of the quark mass and the qualitative change in the transition associated with these. To fully understand the reason for this curious pattern, further analysis will be needed. In particular, there are strong indications of an as of yet not fully explored hysteresis cycle in the chiral condensate (shown later in this chapter) that complicate the determination of the transition location and might eventually connect what appear to be two separate transitions. Measurements in the region around $\beta = 3.0$ do, however, not show any two-state behaviour and a double transition remains a possibility. Unexpected as that might be, there are several scenarios in which it could occur. We will now discuss several such scenarios and assess their feasibility.

5.1.1 Scenarios for a double transition

A first possibility that needs to be considered, is the existence of a thermal transition that is masked by a bulk transition at higher masses. A strong coupling bulk transition – a lattice artefact – would take place at some $\beta_B^c$, separating two chirally broken phases. It would then be followed by a thermal transition, restoring chiral symmetry at some $\beta_T^c$. Upon increasing the mass, we enter a crossover region and both transitions merge. This scenario would directly undermine the conclusion drawn from the bulk transition in chapter 4. It draws upon one of the weaknesses
Figure 5.1 The chiral condensate in the transition region measured on volumes of $24^4$ for several values for the bare quark mass $am=0.020$ (purple), 0.025 (green), 0.040 (orange), 0.050 (blue) and 0.070 (red). The transition coupling was determined from the position of the peak in a finite difference approximation to the derivative of the condensate and is indicated by a vertical line of the appropriate colour for each value of the quark mass. Data for $am=0.040$ are preliminary, but appear to share traits of both the higher and lower masses: They currently show no clear discontinuity, but do sport a double peak in the derivative. All the data shown here were obtained from ordered starting configurations. Close to the transitions and as indicated by dashed lines, preliminary results from disordered starting configurations do not readily converge to the same value. This implies that the assignment of these values to a particular state is in fact somewhat arbitrary.

of the determination of the bulk transition in that chapter, in that we cannot exclude the occurrence of a thermal transition at an extremely low temperature, occurring immediately after the bulk transition itself and giving the appearance of a chirally symmetric zero temperature vacuum. As this is a matter of limiting behaviour that can always be pushed far enough to be just out of reach of the lattice simulation under consideration, it is in principle impossible to exclude it completely, though it can be made very unlikely by obtaining results at large volumes. However, once a clear transition is present, as there would then certainly be for $am = 0.02$ and 0.025, it should present a thermal signature. Fortunately, since a signal is found at the relatively large volume of $24^4$ used in these simulations, there is much room to examine thermal scaling. Such a study is of course only relevant for the transition at the weakest coupling, as a physically relevant thermal transition should connect to a chirally symmetric phase having a locally free continuum limit and this is the only
place where that could occur. As figure 5.2 shows, for small values of $N_{\tau}$, between

![Graph showing the chiral condensate for a constant bare quark mass of $a m = 0.025$ at different values of the temporal extent $N_{\tau}$: 6 (green), 8 (red), 10 (blue) and 24 (black). The location of the transition is sensitive to $N_{\tau}$ at small values, but then settles for $N_{\tau} \geq 10$.](image)

$N_{\tau} = 6$ and 10, the critical coupling indeed moves. This might be partially a thermal effect, though no perturbative scaling curve can be associated with the $N_{\tau} - \beta_c$ trajectory (figure 5.3). Within the resolution of $\Delta \beta_c = 0.025$ obtained for the scan, there is no remaining sensitivity to $N_{\tau}$ once it reaches a value of 10. With the transition as sharply defined as it is for the large volumes, a thermal signal could not be lost here – if anything, perturbative scaling should be more clearly approached. We therefore conclude that either small values of $N_{\tau}$ induce lattice artefacts that drive the system to chiral symmetry, or a UV driven bulk transition present in the zero temperature range is overtaken by thermal effects for very high temperatures. The latter would not be unexpected, as the dimensionally reduced infinite temperature limit of the theory does not break chiral symmetry.

Having established that a thermal transition is absent at lower masses as well – corroborating the conclusions from chapter 4 – the question remains as to the nature of both transitions and the mechanism that could trigger the appearance of a double transition as a function of the mass. A hypothesis would be that quark masses $a m \geq 0.05$ are too heavy to be truly dynamic, which implies they decouple and we observe an effectively quenched action dominated by a Yang-Mills confinement transition. At some critical value of the mass $0.025 < a m < 0.05$, a cross-over region would then be entered that induces the appearance of the second transition. Obviously, this scenario would be particularly damning for the results of chapter 4, but it
Figure 5.3 Transition coupling for a constant bare quark mass of \( am = 0.025 \) at different values of the temporal extent \( N_\tau \), as determined from a cold start. As the temperature is lowered, the transition coupling approaches a definite value and becomes insensitive to \( N_\tau \).

is exactly those results that exclude it. First of all, in the context of a pure Yang-Mills theory, a deconfining transition can only be triggered thermally, as we know bulk transitions are absent from the quenched theory. The absence of a thermal signature is therefore the first indication that the heaviest quark masses are not decoupling from the theory yet. An additional argument is found in the sensitivity of the value of \( \beta_c \) to the quark mass. As one would expect the dynamics around a critical point to be dominated by the phase transition itself, no effect of this magnitude should be expected from a degree of freedom that is essentially frozen out of those dynamics. Thirdly, features originating in pure gauge dynamics would be expected to become more prominent as the erosive effect of the shielding quark masses is tuned down by increasing the bare quark mass. What we observe instead, is a flattening and widening of the transition as we increase the quark mass from \( am = 0.04 \) to 0.07. Finally, we know an intermediate crossover region would have to be present due to results on the mass dependence in regular QCD [59]. Because in the limit of heavy quarks the number of flavours \( N_f \) is not relevant to dynamics, we should not expect large deviations from the behaviour observed there for values of \( N_f = 2 \) or 3. Instead, we find that it is in fact the heavy masses that produce a signature appropriate to crossover, in their extended transition region. Additionally, the eroding effect of an increase in the bare quark masses suggests that we would rather be at a region of relatively low quark mass in the crossover region.

Another interesting possibility is a separation between transitions associated with
5.1 Mass dependence of the bulk transition

chiral symmetry and confinement at low masses. As discussed already in chapter 3, for the regular phase of QCD and in the presence of massless fundamental fermions, confinement is lost the moment chiral symmetry is restored. Currently, there is no known compelling reason why this should be so, though explanations in terms of a transfer of criticality due to mixing between the glue ball and $\sigma$ channels have been proffered [315–317]. The arguments are more stringent for a weaker formulation of the conjunction of chiral symmetry breaking and confinement, in that a confined theory can be shown to break chiral symmetry. A formal argument for this, in the setting of the large-N expansion, was given in landmark paper by Coleman and Witten [86]. A physically more intuitive argument was presented earlier by Casher [84]. Here it is argued that a force with the generic properties of the strong interaction in a confining Hamiltonian cannot produce bound states while preserving chiral symmetry. Each eigenstate of the Hamiltonian will have to be localized and will therefore have to contain a superposition of field modes of opposite helicity. In the context of confining QCD, this implies a current quark mass will have to be induced, as each physical state will break conservation of the local chiral current. Because this argument is based on the properties of the colour charge interaction and the concept of confinement alone, it will carry over to a theory with any number of flavours. In the light of the above, if a separation of confinement and chiral transition were to occur by some mechanism – be it physical or pure lattice artefact – these transitions would have to appear such that the intermediate phase would be deconfined, but chirally asymmetric. The transition at the lowest value of $\beta$ should therefore be associated with deconfinement and checks should be made for the appearance of a non-zero Polyakov loop or string tension in the chiral limit of the intermediate region. These observables will be discussed later in this chapter, but the salient point is that the analysis of the bulk transition as performed in chapter 4 is not affected.

The scenario that will be the basis for our subsequent analysis assumes the presence of two bulk transitions at low masses, both of which are essentially lattice artefacts. One would connect a chirally symmetric to an asymmetric phase and is the essential observation, as it excludes a thermal transition. The second transition would be a strong coupling transition connecting two chirally broken phases. For higher values of the bare quark mass, either the strong coupling transition vanishes altogether, or the two merge into one extended crossover transition. As for the mechanism causing either the splitting or appearance of the second transition, it is not possible to draw a definite conclusion with the data currently available and one can only speculate. An important feature of the data presented is the continuity between the simulations at weak coupling, as evidenced for example by the smooth scaling towards the chiral limit reported upon in chapter 4. Towards the strong coupling limit, we again observe a rough convergence between the results at all values of the bare quark mass. This is completely consistent with the argument of [169] for the existence of a bulk transition, already presented in 3, that points out that in the $\beta \to 0$ (infinite coupling) limit the quarks are no longer good degrees of freedom for any finite value of the bare quark mass. This can be reformulated in terms of a lattice
hierarchy of scales. Lattice simulations should satisfy
\[ a < (\bar{m}_q)^{-1} < aN_s \]  
(5.1)
where \( \bar{m}_q \) represents the dressed quark mass, for which one could generally state
\[ \bar{m}_q \propto \langle \bar{\psi}\psi \rangle. \]  
(5.2)
In the infinite coupling limit, the current mass for a quark over any finite distance should diverge and by necessity
\[ (\bar{m}_q)^{-1} \ll a, \]  
(5.3)
implying that the discretised equations should no longer contain dynamical quarks as degrees of freedom. While this transition may in principle occur arbitrarily close to the \( \beta \rightarrow 0 \) limit, it does not seem unreasonable to assume the inversion of scales in fact occurs for the heavier bare quark masses. The chiral transition causes a sudden increase in the bare quark mass, which may be enhanced by an associated increase in the amount of taste breaking. This could lead to the newly formed bound states becoming sufficiently heavy to decouple as dynamic degrees of freedom from the theory. Since the processes of the development of a chiral quark condensate and the decoupling of the bound states would be mutually interfering, the transition thus found could be washed out. By lowering the bare quark mass, we also lower the mass of the bound states. By dropping below an as of now undetermined critical mass value, this mass could actually be lowered sufficiently to satisfy equation 5.1 even in the broken phase, at least initially. Of course, especially when remaining close to the critical bare quark mass, moving towards even stronger coupling should at some point trigger a similar hierarchy inversion as observed for the heavier masses and one arrives at a uniform infinite coupling limit. But because there is now a clear separation between both transitions, no interference takes place. Instead, we find the two sharply defined transitions of figure 5.2, which are much more similar to the thermal transitions observed for \( N_f = 8 \) in chapter 3.

To reiterate this point, the data presented here do not provide the evidence needed to verify this scenario. That could only be constructed from a far more detailed study of the separate phases observed, preferably around the critical value of the mass. It does provide us with a coherent setting for the interpretation of results, however, and we will take it as heuristic guidance in the continuation of this chapter. We will assume no separation between the confining and chiral transitions – and will indeed find no particular indications of this being the case – but the ordering of transitions indicated above would render such a phenomenon inconsequential to our further analysis.

5.1.2 Identification of the transitions
It is our intention to determine the order of the transition, for which we will need to examine its properties under variations of the parameters. Given the dissimilarities of the structure of transitions at low and high masses, care should be taken
5.1 Mass dependence of the bulk transition

in demonstrating the common origin of transitions. From our guiding scenario described above, it is natural to identify the transitions at high masses with the weak coupling transitions at low masses. In fact, our interest is in the onset of either confinement or chiral symmetry breaking, one of which will have to occur at the weak coupling transition. Nevertheless, a quantitative analysis of both high and low masses requires a continuous line of transitions. While the data are not currently sufficient for a definite proof, we here demonstrate that the assumption of the existence of such a line connecting these transitions is natural.

We plot the critical couplings for each of the transitions as a function of the bare quark masses in figure 5.4, from the numerical values reported in 5.1. In this double logarithmic plot, we in fact observe a natural power law for the critical coupling at low beta. That power law is largely meaningless and we do not want to imply any particular behaviour in the asymptotic strong coupling limit. What it does show, is a consistent tendency of the strong coupling transition to move towards lower $\beta$ for the values measured. The inflection points of the crossover transitions found for higher masses group naturally with the weak coupling transitions at low masses instead. Here the curvature in the log-log plot shows the absence of a power law here. Theoretically, a linear behaviour with potentially (depending on the order of the transition) an anomalous dimension would be expected. The superimposed fits, that we will return to shortly, demonstrate the possibility of such a fit.

An alternative way of identifying the appropriate transitions is by examining the chiral cumulant

$$R_\chi = \frac{\chi_\sigma}{\chi_\pi} = \frac{\chi_{\text{conn}} + \chi_{\text{disc}}}{\langle \bar{\psi}\psi \rangle/m},$$

which is a measurement of the second derivative of the free energy $F$ with respect to the mass divided by the first derivative. The behaviour of the free energy of a second order phase transition near the critical point is determined by the scaling length $t$ and the critical exponents. Any mass dependence of this function will be given by the generic scaling form [318]

$$F(t, m) \equiv F(t m^\omega),$$

with $\omega$ the relevant combination of critical exponents. As a consequence, the mass dependence of the cumulant around the critical point is described completely by the scaling functions. In the limit

$$t \to 0,$$

i.e. at the critical point itself, the mass dependence of the chiral cumulant will vanish and it will assume a universal value that is determined solely by the anomalous dimension $\delta$

$$R_\chi(m, t)|_{\beta_c} \equiv R_\chi(m, 0) = \frac{1}{\delta}.$$
Figure 5.4 Critical couplings determined from a finite difference approximation to the derivative of the chiral condensate and the plaquette as a function of the bare quark mass. Simulations were performed at a volume of $24^4$ and errors defined from the narrowness of the bracketing of the transition by separate runs. A certain amount of hysteresis would occur at small quark masses, but locations were defined consistently from ordered starts. Superimposed are fits to a pure power law (low beta values) and to a power law with intercept (high and single beta values). Results at $am = 0.04$ should be considered preliminary.

The cumulant will assume an identical value exactly at the location of the critical $\beta$, independent of any corrections coming from explicit chiral symmetry breaking. For a second order phase transition, this is the most accurate form of determining the position of the critical coupling of a chiral phase transition in the presence of explicit chiral symmetry breaking. It also serves as a consistency check on the critical value of $\beta$ determined by means of the power law extrapolation, the validity of which is of course based on similar considerations.

For the case of a first order transition, the constraints on the behaviour of the free energy around the critical coupling are less. By analogy to the first order deconfining transition in Yang-Mills theory [319], in the continuum we should find a discontinuity described by

$$
\Delta (F(\beta, m)) = 2\Delta(\langle \bar{\psi}\psi \rangle) \cdot m.
$$

(5.8)

The presence of a discontinuity in the free energy necessarily carries over to the chiral cumulant, which implies a crossing of the curves cannot be defined any more. In addition, since there is no critical scaling near the transition, no vanishing of the sensitivity to the external field, in this case the bare quark mass, would be expected.
to occur \textit{a priori}. Of course, the measurements on the bulk transition presented here and in chapter 4 are indicative of a crossover transition instead. Once a first order transition is broken down to a crossover transition, renormalization group analysis shows scaling behaviour in the relevant operator should be introduced \cite{320,321}. Now the critical exponent is replaced by a system dependent crossover exponent, which has limited physical meaning. But the core argument of \cite{318} will once again be valid and the cumulant should assume a unique value at the critical coupling.

Figure 5.5 The chiral cumulant $R_\chi$, defined in equation 5.4, calculated for all zero temperature volumes of $16^4$ at which simulations were available. Chiral symmetry restoration is signalled by the approaching the value 1 (identical masses for the $\pi$ and $\sigma$), while the broken phase produces a value approaching (identifying the $\pi$ as a Goldstone boson). Different bare quark masses are indicated by different colours: $am = 0.020$ (purple), 0.025 (green), 0.040 (orange), 0.050 (blue) and 0.07 (red). Where smooth, curves are expected to cross at the value of the critical coupling, which was determined to be around $\beta = 3.00(1)$ from an extrapolation of the critical couplings (see below). This behaviour is indeed found for the cumulants for the higher masses (and $am = 0.04$, in spite of its double peaks), while the cumulant at lower masses appears to converge to that value up until the discontinuity (dashed lines are added purely as guides to the eye, connecting the last measurement before the transition to the crossing point).

Generally then, the crossing of chiral cumulants from continuous transitions at a single critical coupling allows for their attribution to a single true chiral transition. Figure 5.5 shows that the cumulants determined over smooth transitions at heavy quark masses cross just below $\beta = 3$, at a value of $R_\chi = 0.086(2)$. The apparent discontinuities at lower masses are preceded by a similar curvature as the weak cou-
pling transition is approached coming from the free limit. We find it extrapolates towards the same critical values of $R_{\chi}$, implying similar dynamics for the transition in both cases. No clear connection is apparent for the trend in the chiral cumulant on either side of discontinuities. The intermediate region appears to share no properties with the measurements from heavy masses. In the strong coupling limit, we again find similar trends for all masses. This supports the conjecture of a merging of both transitions into a single crossover.

5.2 Order of the transition

To establish the order of the transition terminating the pseudo-conformal region, we need to take the different nature of the transition at high and low masses into account. We will focus on the low mass transition first and demonstrate it shows the hallmarks of a first order transition. Since our interest lies, eventually, in the chiral limit of the theory, these results alone are physically highly relevant. We will then provide an analysis of the mass dependence of the critical coupling, already alluded to in figure 5.4, connecting the crossover transition at higher masses to the low mass transitions and showing a natural interpretation in terms of a first order crossover. Finally, the order of the crossover transition will be determined directly from the high mass data alone.

5.2.1 Towards the chiral limit

It would seem a straightforward conclusion could be drawn directly from the appearance of the phase transition for $a m = 0.02$ and 0.025. The sharp change in value observed would be expected for a first order phase transition. Nevertheless, a sharp second order transition cannot be excluded. To corroborate our intuition here, we would hope to actually observe a bistable phase, producing in a single MC history values of the order parameter associated with the phase on both sides of the discontinuity. The smoothing of the crossover transition at higher values of the bare quark mass would prevent such a signal for $a m = 0.05$ and 0.07, but the sharpness of the signal at low quark masses may provide us with these. Though, as stated before, any fully ergodic Markov chain in a finite region around the pseudo-critical coupling should produce a bi-stability to some extent, its observation can be difficult in practice. The relatively large volumes used in this section would complicate this further, but even runs at small lattices of $12 \times 4$ around the transition did not produce any double peak structures in histograms of the Monte Carlo history.

An alternative to the direct observation of a double peak structure is the observation of hysteresis, as was done in the case of the thermal transition for $N_f = 8$. Figure 5.7 shows a comparison between a hot and cold start for a run with $a m = 0.025$ at $\beta = 3.175$, just inside the critical region. We find a separation between states that remains stable for at least 2000 thermalized trajectories.

The pseudo-critical values of $\beta$ plotted in figure 5.4 were, for consistency, measured from cold starts and should therefore present the lower bounds of the hysteresis loops, at least for the lower range of the quark masses. Below these values, no true bi-stabilities were observed yet. In the case of a first order phase transition, the
Figure 5.6 The plaquette measured as a function of the bare lattice coupling $\beta$, in the region around the double transition observed for the bare quark masses $am = 0.020$ (dark squares) and $0.025$ (light circles). Measurements were all on lattices of size $24^4$, with runs initialized consistently from cold starts to reduce potential ambiguity due to hysteresis effects. Vertical lines are guides indicating the location of the discontinuities observed for the order parameter. Discontinuities are observed for both masses at both locations, indicating that both transitions are in all likelihood of first order.

...
The chiral condensate measured for a coupling of $\beta = 3.175$ with a bare quark mass of $am = 0.025$ and for a volume of $24^4$. The lower data set results from a cold start, while the upper data set stems from a hot start. Results are plotted versus an equivalent of the trajectory number, calculated as the measurement number divided 4, which is equivalent to dividing by the number of measurements per configuration (20) and multiplying by the sampling interval (every 5 configurations). The trajectory length was fixed to 0.4, whereas the integration step-size was adjusted at intervals to maintain an acceptance rate close to 0.8. Counting from a rough thermalization in both cases from about 500 trajectories, this shows stability of both states over at least 2000 trajectories.

5.2.2 Connecting to the crossover regime

For the results presented above to connect physically to the transition observed at higher masses, the theory would need to have entered a crossover regime due to the heavier quark masses. Alternatively, we could be observing a different, second order phase transition hinting at a far more complicated phase diagram. Direct evidence for a true crossover nature can be obtained from the scaling behaviour of the system close to the pseudo-critical point. Let us use the definition

$$\chi_m = \frac{V}{N_f} \left[ \left\langle (\bar{\psi}\psi)^2 \right\rangle - \left\langle \bar{\psi}\psi \right\rangle^2 \right] = \frac{V}{N_f} \text{var} \left[ \langle \bar{\psi}\psi \rangle \right].$$

(5.9)

This underestimates the connected component, but is a good approximation to the total susceptibility in the critical region where this contribution is expected to remain analytical [323]. In the absence of long range ordering, the variance will scale inversely with the volume as it is effectively controlled by an increase in statistics. Because of the compensating volume factor, we find a scale invariant susceptibility.
5.2 Order of the transition

Figure 5.8 The chiral condensate measured for a coupling of $\beta = 3.150$ with a bare quark mass of $am = 0.025$ and for a volume of $24^4$. Results shown are produced from a cold start and plotted versus an equivalent of the trajectory number as defined for figure 5.7.

Near the critical coupling, however, the diverging correlation length associated with a second order phase transition implies a variance of the order parameter that scales sub-linearly with the volume. In this way, the scaling regime introduces a peak in the susceptibility, the height and width of which are dictated by a scaling function measuring the anomalous dimensions. For a first order transition at finite volume, the two state dynamics will produce a variance that is independent of the volume. A similar divergence should occur, but here the scaling of the peak width and height should be linear. For a crossover transition, however, neither mechanism would come into play. Even if a crossover exponent appeared as suggested in 5.1.2, the associated correlation lengths would not diverge and be irrelevant for all but very small lattices. The susceptibility should therefore be approximately invariant under changes in the volume, as argued in [43]. Figure 5.10 demonstrates a lack of scaling of the supposedly singular part of susceptibility. Even if the data over the critical region appear to be rather noisy, the difference in volume by almost an order of magnitude should lead to an observable signal. What is observed instead appears to be an opposite trend if anything, much like the continuum extrapolated data of [43].

Having found a true crossover regime at high masses, we would connect to our measurements at low masses through a fit to the mass dependence critical coupling. In a study of the finite temperature transition in QCD with two flavours in [323], which by current consensus seems to be of second order [41], an expansion in the

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$^2$Apparently this issue is still somewhat contended, given the results of [324, 325].
Figure 5.9 The connected susceptibility measured for bare quark masses of $am = 0.020$ (dark squares) and 0.025 (light circles), for volumes of $16^3 \times 24$ and $24^4$. Discontinuities, associated with first order phase transitions, are found in locations corresponding to those found for the order parameter.

The exponent $\beta\delta$ of the bare quark mass would be governed by that a universality class and one could therefore attempt to extract information on the critical exponents directly from this scaling behaviour. To do so, however, one needs to be aware of the contribution of the non-divergent remainder of the free energy, which at leading order would come in as a linear contribution to equation 5.10. On the other hand, if the chiral transition is of first order, such as has been found to be the case for $N_f = 3$, the scaling of the critical coupling with the mass is completely analytical. It is found again by expanding the divergent part of the free energy, as was done for the first order thermal deconfinement transition of pure Yang-Mills in [319], and given by [60]

$$\beta_c(am) = \beta^0_c + \Delta(\bar{\psi}\psi)\frac{\Delta S_G}{am},$$

(5.11)

which is in fact the form proposed in chapter 3. As stated there, the quantities $\Delta(\bar{\psi}\psi)$ and $\Delta S_G$ refer to the discontinuity in the chiral condensate and the plaquette action at the critical point, respectively. While it would be interesting to have an estimate of
5.2 Order of the transition

Figure 5.10 The disconnected susceptibility for a bare quark mass of $am = 0.05$ at volumes of $12^3 \times 24$ (red), $16^3 \times 24$ (green) and $24^4$ (blue). A first or second order phase transition at finite volume should produce a peak scaling with some power of the volume. With volumes differing by almost an order of magnitude, no clear volume dependence is observed, as would be expected for a crossover transition. A vertical line was added for orientation at the value of the pseudo-critical coupling as determined from the numerical derivative of the order parameter.

these quantities, our data are not sufficient to perform such an extrapolation and we have no obvious way to fix the renormalization constant required to find physical predictions. Instead, we simply look for the appearance of critical exponents appropriate for a second order transition. A fit to equation 5.10 of the pseudo-critical couplings is displayed in figure 5.1, the numerical values of which are given in table 5.1 for reference.

An error-weighted fit of the pseudo-critical couplings labelled $\beta_{c}^{\text{high}}$ to equation 5.10 produces a prediction of the critical coupling of $\beta_{c}^{0} = 2.8(2)$, with an associated exponent $\beta\delta$ equal to $0.6(3)$ and a residual error $\sqrt{\chi^2/d.o.f.}$ of 0.51. Since the errors in table 5.1 are derived from bracketing the transition, they cannot be interpreted as regular standard deviations. The alternative, unweighted fit results in $\beta_{c}^{0} = 2.91$ and $\beta\delta = 0.7(2)$. Both fits are compatible with linear behaviour and reproduce the critical coupling found from the crossing of cumulants in figure 5.5, but within rather large errors. Constraining the fit to a linear form increases the residual error only slightly to 0.67 and puts the critical coupling at $\beta_{c}^{0} = 3.00(1)$.

Using instead the values for $\beta_{c}^{\text{low}}$ for a fit to the same equation results in a residual error of 1.46, for $\beta_{c}^{0} = 0.6(4.7)$ and an exponent of 0.2(4). The relatively poor quality
Table 5.1 Pseudo-critical couplings determined from a finite difference approximation to the derivative of the chiral condensate for several values of the bare quark mass $a m$. Where a double peak in the derivative is present, the lower value of the pseudo-critical coupling is listed as $\beta_{c}^{\text{low}}$.

<table>
<thead>
<tr>
<th>$a m$</th>
<th>$\beta_{c}^{\text{high}}$</th>
<th>$\beta_{c}^{\text{low}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.020</td>
<td>3.106(06)</td>
<td>2.787(13)</td>
</tr>
<tr>
<td>0.025</td>
<td>3.163(13)</td>
<td>2.875(13)</td>
</tr>
<tr>
<td>0.040</td>
<td>3.250(50)</td>
<td>3.050(50)</td>
</tr>
<tr>
<td>0.050</td>
<td>3.313(13)</td>
<td>–</td>
</tr>
<tr>
<td>0.070</td>
<td>3.425(25)</td>
<td>–</td>
</tr>
</tbody>
</table>

of the fit, in spite of the comparatively large errors, combined with the non-physical central values for the parameters, indicate a strained fit. Figure 5.4 shows that the pseudo-critical values of the strong coupling transitions line up separately in a log-log plot. This would indicate their mass dependence might be described well by a power law. Such a functional dependence would imply the strong coupling transition moves towards $\beta = 0$ as the chiral limit is approached. Since this limit is in fact a (trivial) fixed point of the theory, the appearance of a scaling law would not be fully unexpected. A fit to such a power law gives an exponent of 0.132(4) with a small residual error of 0.18, though the diminutive error is of course partly due to the lack of precision on the result for $a m = 0.04$. To bolster this analysis, more precise data would be required at the existing points, in addition to observations of the strong coupling transition closer to the chiral limit. But a confirmation of the behaviour of $\beta_{c}$ at different masses would provide further support for the interpretation of the double transition set forth in 5.1.1.

5.3 The Polyakov loop

For a pure SU(3) Yang-Mills theory, the Polyakov loop is an order parameter signalling confinement, as at the critical coupling $\beta_{c}$, the U(1) symmetry is broken down to its discrete Z(3) centre. In chapter 3, it was already observed that the presence of dynamical fermions pushes the distribution towards the real root of this centre group, simplifying our observable to the real part of the Polyakov loop. But while it may exhibit pseudo-critical behaviour in the presence of fermions, there is no physical necessity for its occurrence. In addition to this, a signal in the Polyakov loop is not all that easily observed in large volumes. One classical alternative for the determination of the confining nature of a gauge theory is found in the string tension, but this observable needs both large statistics and volume and even then would be expected to be a relatively small quantity for the case of $N_{f} = 12$. Alternatively, one may examine the perturbative expansion of the plaquette. A confining theory is characterized by the presence of a non-perturbative gluon condensate [326] on top of a regular perturbative expansion starting at $\mathcal{O}(1/\beta)$. Fits to such a perturbative expansion on top of a constant term can be performed, such that the offset, which
represents the $\beta \to \infty$ free limit of such an expansion, gives an estimate of the magnitude of the gluon condensate. Both the Polyakov loop and gluon condensate are of limited utility in the determination of the nature of the theory. This is partly due to a limitation on the clarity of their observation, but mainly because confinement is not strictly a well defined property of the system. Nevertheless, we will discuss these two observables because of their usefulness in terms of observing positive signals, providing, if nothing else, a consistency check on our data.

Figure 5.11 displays measurements runs at volumes of $24^4$ for various values of the bare quark mass, at a range of values of $\beta$ including the observed chiral transitions for each of the masses. Note that, in spite of the marked change in the order parameter at these volumes, no signal is observed in the real component of the Polyakov loop. An inspection of the distribution of the measurement in imaginary space shows no deviations from full U(1) symmetry, showing the characteristic pattern of a confined system at each value of $\beta$ studied. The absence of a signal of deconfinement marks a difference from the system described in chapter 3. As stated above, this does not necessarily imply the presence of confinement, but could also be due to measurement insufficiencies. For that reason, it is instructive to examine results at smaller values of $N_\tau$. From the limiting behaviour of the bulk transition for $am = 0.020$ and 0.025, it was concluded that finite volume effects strongly influenced these systems. Nevertheless, the existence of a smooth limit for the chiral transition
towards the large volume limit would indicate the a certain amount of continuity for these systems, allowing for the inferring of properties from the small volume limit.

For the bare quark mass of \( am = 0.050 \), used for the study of the bulk transition in chapter 4, measured values of the Polyakov loop are displayed in figure 5.12. A signal appears for small values of the temporal extent \( N_\tau \), rapidly decaying for lower temperatures associated to larger values of the temporal period. One possible explanation of this behaviour, which was also observed in [176], would be the presence of a phase with very weakly broken chiral symmetry. The breaking down of the full U(1) symmetry of the Polyakov loop at what would amount to a second order phase transition at high temperatures should then be attributable to a regular thermal transition. Further support for this hypothesis could be found in the small shift in the value of \( \beta_c \) obtained from the slope of the Polyakov loop expectation value in the broken regime.

Several other properties of the data in figure 5.12 make this explanation unlikely, however. Note first of all the systematic differences in the curves for \( N_\tau = 4 \) on the one hand and \( N_\tau = 6 \) and 8 on the other. In particular, the presence of the non-zero expectation value of the Polyakov loop below what would be identified by the critical temperature is indicative of the presence of strong finite volume effects, rather than dynamics controlled by a physical critical temperature. The rapid decay in the signal as the value of \( N_\tau \) is increased is then conceivable attributable to the same effect. It could, of course, also be associated to the vanishing of thermal signals.

Figure 5.12 The real part of the Polyakov loop as a function of the bare lattice coupling \( g_L \), measured for the bare quark mass \( am = 0.05 \) at a spatial volume of \( 12^3 \) and four different values of the temporal lattice extent: \( N_\tau = 4 \) (purple), 6 (green) and 8 (red) and 24 (blue).
5.3 The Polyakov loop

for larger values of the lattice. This can only be judged against the backdrop of other observables, however. The most prominent of those is undeniably the transition in the chiral condensate, but its extension over a range of couplings complicates the definite association of the rise of the Polyakov with a critical coupling definitely before, after or at the chiral transition.

Such complications do not arise when going to lower masses. We previously saw the much sharper localization of the chiral transition at masses smaller than or equal to $am = 0.025$ and the presence of finite volume effects at lower values of $N_\tau$. Those are identified by the persistence and temperature insensitivity of the associated observable for larger volumes. One is tempted to attempt finding a similar correlation for the Polyakov loop. A comparison of the relative positions of the Polyakov loop

![Graph showing the real part of the Polyakov loop as a function of the bare lattice coupling $g_L$, measured for the bare quark mass $am = 0.02$ at a spatial volume of $24^3$ and three different values of the temporal lattice extent: $N_\tau = 6$ (green), 8 (red) and 24 (blue).](image)

transitions and their chiral counterparts indeed shows a strong correlation between the two. In particular, for those small values of $N_\tau$ where the Polyakov loop develops an expectation value, the location where this starts to happen shifts. These shifts in fact mirror the changing position of the discontinuity (at weakest coupling) in the chiral condensate. Since the behaviour of the latter at small $N_\tau$ was attributed to lattice artefacts, we conclude that the non-zero expectation value of the Polyakov loop for those particular runs is in all likelihood a lattice artefact itself.
5.4 The static potential

Finding no signal in the Polyakov loop at zero temperature, a natural alternative exists in the static potential. The binding energy between a heavy quark pair $V_{q\bar{q}}(r)$ as a function of the spatial separation $aR$ between them can be defined in several equivalent ways. One possibility is to extract the $R$ dependence from the correlation between Polyakov loops, which allows for an efficient measurement of the potential in a time coordinate independent manner [327, 328], which is especially useful at finite temperature [329]. In the zero temperature limit, however, the most common method for extracting this quantity is through the dependence of the Wilson loop expectation value which has been extensively used both in a quenched and dynamical fermion setting [277, 330–335].

An intuitive argument for the connection between the gauge invariant expectation of the Wilson loop and the potential between to heavy quarks can be painted as follows [260, 328]. We start from the non-relativistic Schrödinger equation, which should be an accurate description in the limit of heavy quark fields. A propagator can be derived from it by requiring

$$\left( D_t - \frac{\vec{D}^2}{2m} \right) G(x) = \delta^4(x). \tag{5.12}$$

The covariant derivative operators $D_t$ and $\vec{D}$ include the gauge fields in the regular manner, through

$$D_\mu \equiv \partial_\mu - igA_\mu(x). \tag{5.13}$$

Equation 5.12 reduces to a much simpler form in the limit of infinite mass, as the dependence on the spatial coordinates drops out of the left hand side of the equation altogether. The remaining simple differential equation admits the solution

$$G_\infty(x) \equiv \lim_{m \to \infty} G(x) = \left( \exp \left[ -i \int_0^t gA_0(x)dt \right] \right)_P \delta^3(\vec{x}), \tag{5.14}$$

where the subscript $P$ denotes path ordering. It is straightforward to see that the discretised equivalent of this propagator is given by a Wilson line

$$G_{\infty}^{\text{lat}}(x) = \prod_{t' = 0}^{T-1} U_0^t(\vec{x}, t'), \tag{5.15}$$

where $T$ denotes the discretised time coordinate with $T = a^{-1}t$. A quark-antiquark pair created at time $t = 0$ will therefore pick up an SU(3) phase factor up until its annihilation at a subsequent time $t = a \ast T$ without further dynamics. To complete our description of the heavy quark pair interaction, let us now fix the gauge by enforcing
the condition
\[ \vec{\nabla} \cdot \vec{A} = 0, \] (5.16)

which will bring us to the Coulomb gauge. This gauge breaks the manifestly gauge invariant form of our field equations, but is very natural for any non-relativistic description of quark interactions as it guarantees the satisfaction of Gauss' law and allows for the definition of an instantaneous quark potential that is itself an RG invariant quantity [336]. Immediate relevance to the current reasoning, however, lies in the implication of equation 5.16 that separate time-slices on the lattice will have constant gauge links, which are conveniently fixed numerically to unity in the regular gauge fixing procedure [327, 337]. The Wilson lines describing the propagation of heavy quarks can therefore be trivially connected at the initial and final time-slices and produce a Wilson loop, which as an observable is in fact a gauge invariant. At this point, the reasoning can be reversed and the Coulomb gauge fixing step in principle skipped. The gauge invariant expectation value of a Wilson loop can apparently, at a fundamental level, be identified with the correlation function of two infinitely heavy quarks in the Coulomb gauge, which is therefore itself a well defined quantity on the lattice in spite of its apparent non-relativistic and gauge dependent nature.

In the context of this chapter, the heavy quark potential holds an interest in two ways. First of all, one might attempt to use it in order to establish equivalent scales between different simulations. If one wishes, physical units could be assigned to the measurements as well, though this is mainly of cosmetic value as there is little merit in using the phenomenological models mentioned with theories that are ostensibly not QCD. However, this assumes the presence of a string tension – which should be absent for the deconfined theory we find for \( N_f = 12 \). A second, more directly interesting aspect of this observable lies in the dependence on distances introduced. The shape of the potential can be described analytically by merging a non-perturbative phenomenologically known component with regular perturbative contributions [338]. A string tension \( \sigma \), following from a string model of quark interactions, is introduced as a component linear in the separation \( R \). A perturbative calculation of Wilson loops on the lattice produces a Coulomb potential \( \epsilon R^{-1} \) and constant background \( V_0 \) for the potential at small values of \( R \) [338, 339]. For a continuum analysis, we therefore end up with a parametrisation according to

\[ V_{q\bar{q}}(R) = V_0 - \frac{\rho}{R} + \sigma R. \] (5.17)

Naively, when approaching a conformal fixed point, the potential should flatten out and become constant. The dynamical appearance of a conformal phase therefore requires

\[ \lim_{R \to \infty} \frac{\partial V_{q\bar{q}}(R)}{\partial R} = 0, \] (5.18)

at any value of the coupling in the basin of attraction of the fixed point. This constrains the string tension term \( \sigma R \) to a vanishing value. The presence of light, dy-
namical quarks will tend to weaken the string tension, so at this high number of flavours we should find a small result under any circumstances. With sufficiently high statistics, it may however be possible to demonstrate the existence of a small remaining string tension, which in the absence of systematics would indicate we find ourselves outside of the conformal window. Given the radically different setup, this observable is the closest we can come to the type of measurement done in [171, 172].

A crucial difference with our results lies in the the employment of the Schrödinger functional [340] in those investigations. This specific setup for measuring the scaling of the gauge coupling uses fixed boundary conditions that allow for simulating quarks in the massless limit [341]. Because of the explicit quark mass term being a relevant parameter under RG flow, our potential cannot be expected to show similar fully conformal behaviour over large distances. Instead, we will explicitly examine the behaviour of our potential towards the chiral limit.

5.4.1 Lattice considerations

The non-dynamical quarks are of course not eigenstates of the full lattice Hamiltonian, but will instead have overlap with a tower of excited states, as is generically the case for correlation functions measured on the lattice. And as usual in the Euclidean formulation, these will start to decay exponentially until only the ground state \( E_0 \) survives and it is exactly the dependence of this ground state on the spatial separation between the quarks that we identify with the static potential \( V_{q\bar{q}}(R) \). Concretely, we have

\[
\lim_{T \to \infty} \langle W(R, T) \rangle \propto C(R) e^{-\beta V_{q\bar{q}}(R) T},
\]

from which we conclude that the observable of interest is in fact given by the limit

\[
V_{q\bar{q}}(R) = \lim_{T \to \infty} \ln \left[ \frac{W(R, T - 1)}{W(R, T)} \right].
\]

The practicality of taking the limit in equation 5.20 might be questioned. Its convergence can be greatly improved by some form of averaging links over a local neighbourhood, known as smearing. This smoothens out short range fluctuations and increases overlap of creation and annihilation operators with the ground state, at the expense of information on the short distance behaviour of the potential. An alternative method of improving converge, that provides similar benefits of smoothing out short range volatility but does so in a manner that is well defined even away from the continuum limit, is the explicit numerical fixing of the Coulomb gauge. This method is commonly used by MILC [333] and the RBC/UKQCD collaborations [334], where the latter combined it with some smearing according to the APE smearing algorithm [342]. It is this technique that was adapted for the generation of the results reported on in this chapter, where gauge fixing was done according to the algorithm described in [337]. Results from the mentioned collaborations show that a stable results tend to be found for values of \( T \) as manageable as 4. Whether this property carries over to our simulations needs to be checked explicitly and results to
At small values of $R$, discretisation artefacts show up and cause a breaking of rotational symmetry [330]. With the improved staggered action used to obtain the results in this chapter, those artefacts are commonly observed [333] and our measurements provide no exception. These deviations from the continuum form can be attributed to the difference with the lattice one gluon exchange term that should approximate it. The explicit form of the latter is given by [331]

$$
G(\vec{R}) = 4\pi \int_{-\pi}^{\pi} \frac{d^3 k}{8\pi^3} \frac{e^{i\vec{k} \cdot \vec{R}}}{\sum_i \sin^2(k_i/2)}.
$$

(5.21)

Above expression might be used to account for the breaking of rotational invariance explicitly, if it is introduced numerically into equation 5.17. To do so, we note that the imaginary part of equation 5.21 is given by an odd integrand and therefore vanishes because of symmetry constraints. We have assumed an infinite volume lattice, which should have no consequences as we are interested in the effects near the UV cut-off. This does, however, introduce an artificial IR divergence that has to be regulated. The direct equivalent of the finite lattice size regulation would be to take the approximation

$$
G_{PV}(\vec{R}) = \lim_{\epsilon \to 0} \lim_{\eta \to 0} \left[ 8\pi \int_{\epsilon}^{\pi} \frac{d^3 k}{8\pi^3} \cos(\vec{k} \cdot \vec{R}) \right],
$$

(5.22)

leaving residual $O(\epsilon^{-2})$ contributions that can be absorbed by both normalization and the constant $V_0$ contribution to equation 5.17. Not only is the constant a mere shift in energy levels and therefore physically irrelevant, it is also divergent in the continuum limit and should therefore be cancelled in physically relevant quantities. The divergence does pose a numerical problem however and a more convenient scheme is found by additionally introducing a small gluon mass contribution $\eta$ according to

$$
G_M(\vec{R}) = \lim_{\eta \to 0} \lim_{\epsilon \to 0} \left[ 8\pi \int_{\epsilon}^{\pi} \frac{d^3 k}{8\pi^3} \frac{\cos(\vec{k} \cdot \vec{R})}{\eta^2 + \sum_i \sin^2(k_i/2)} \right].
$$

(5.23)

The limit in $\eta$ is smooth at any given small value of $\epsilon$ and kills off the $O(\epsilon^2)$ dependence efficiently. In practice, the value of the numerical integral stabilizes at the sub-percent level for $\eta \approx 10^{-3}$ for $\epsilon = 10^{-6}$. The result of equation 5.23 was tabulated for each of the discrete vectors $R$ for which the static potential was measured. These values were plotted in figure 5.14. For the potential at large distances, the difference in shape between both forms of the potential becomes insignificant. In this limit there is some ambiguity in the relative normalizations of the continuum and lattice Coulomb potentials, but this has no practical consequences as the normaliza-
tion can be absorbed in the fit coefficients.

Figure 5.14 Result of the numerical integration of $G_M$ as defined in equation 5.23 for all discrete vectors in an $8^3$ volume. To facilitate the comparison with a regular Coulomb potential, values were multiplied by $-R$. The breaking of rotational symmetry is clearly seen in the significant deviations between coaxial and off-axis contributions.

Replacing the Coulomb term in equation 5.17 by $g_2^2 G_M(R)$ would introduce the lattice Coulomb potential at tree level. Higher orders in lattice perturbation theory can be effectively absorbed in a redefinition of the coupling constant $g_L^2$ [296,339,343], suggesting that this form with a fitted coefficient should be essentially a full description of the perturbative regime. This does, however, not take into account the effects of improvement and smearing, that will drive the potential towards its smooth continuum form. In addition, emerging non-perturbative components of the potential may introduce rotational symmetry breaking cross terms not properly captured by the lattice Coulomb potential. It is therefore more appropriate to add a lattice correction term to the continuum Coulomb potential in equation 5.17, with a separate coefficient. In the absence of (strong) non-perturbative effects, as we expect is the case here, the magnitude of this coefficient will give an indication of the residual $O(a)$ effects.

The modified form of the potential from equation 5.17 used for performing fits to the lattice data is therefore

$$V_{\bar{q}q}^L(\vec{R}) = V_0 - \frac{\rho}{|\vec{R}|} + \sigma|\vec{R}| - \rho_{LCP} G_M(\vec{R}),$$

where the breaking of rotational symmetry makes $V_{\bar{q}q}^L$ dependent on $\vec{R}$ rather than
its magnitude. To clarify the presentation we will remove this controlled source of systematics by adding

$$\Delta(R) = -\rho_{\text{LCP}} \left( \frac{1}{|R|} - G_M(R) \right)$$

(5.25)

to the data, in principle restoring rotational symmetry artificially and introducing the effective Coulomb potential contribution $\rho_{\text{eff}} = \rho + \rho_{\text{LCP}}$.

As a direct test of the effectiveness of the lattice Coulomb potential corrections, we can examine data measured for a typical run and compensate with the fitted correction term. Figure 5.15 shows how a large part of short range deviations from the continuum Coulomb form are corrected for by taking into account a contribution proportional to $G_M$ as shown displayed in figure 5.14. In this plot the otherwise irrelevant constant contribution $V_0$ was subtracted, as well as the fitted string tension contribution $\sigma R$. The remainder should contain both the continuum and discretised Coulomb potential, as well as additional lattice artefacts and statistical noise. To show deviations more clearly, we multiply by the distance $R$ to obtain what should be a constant. At short range there are significant deviations from continuum Coulomb behaviour, but those are largely compensated for by the explicit addition of equation 5.23. The aforementioned normalization ambiguity, while of no consequence in the fits themselves, leads to a small shift in the overall strength of the Coulomb potential after correction. Since the magnitude of this parameter is of no direct interest here, this is a purely cosmetic effect. For these fits, the magnitude of these lattice artefacts relative to the continuum Coulomb term was found to be of $O(0.1)$. It should be noted that the short range heavy quark potential, as an observable, is expected to be particularly sensitive to lattice artefacts. Comparing the value of the reduced $\chi^2$ goodness of fit parameter confirms the improvement in the fit coming from the addition of this term, even if the naive fits to equation 5.17 can provide acceptable fits if a sufficient amount of data at large $R$ – where both formulations agree – is available.

5.4.2 The static potential for $N_f = 12$

Wishing to observe long range dynamics that is potentially quite sensitive to finite volume effects, there is need for simulations at reasonably large volumes. Because the potential is a noisy observable and signal quality should be sufficient up to distances large enough to probe the string tension as a dominant term, these large volumes need to be available with reasonably high statistics as well. We decided to exploit the availability of thermalized configurations at sizeable volumes due to the chiral extrapolation of the chiral condensate of chapter 4. We examined the convergence towards the $T \rightarrow \infty$ limit, the dependence of the potential on the bare quark mass and coupling and the effect of changes in the volume.

Our first concern was the identification of a plateau in the potential data. To obtain a good signal-to-noise ratio, it is useful to employ large volumes, where the intrinsic suppression of noise due to volume averaging of the Wilson loops is strongest. In figure 5.16 (and table 5.2), we therefore compare data obtained from different ra-
Figure 5.15 The effect of adding an explicit correction for leading order short range discretisation artefacts by including a contribution from the discretised one gluon exchange (figure 5.14). Displayed is the short range static potential measured on a volume of $32^4$ with a quark mass of $am = 0.025$ at $\beta = 3.9$. The result of fitting the data to equation 5.24 (see table 5.2) was used to eliminate the constant and linear contributions. The upper points give the remainder without further corrections – the component of the potential that would be identified with the continuum Coulomb potential naively – while the lower points show the effect of the correction of equation 5.25. Dashed lines indicate the respective averages.

tios of time-slices on a $32^4$ at a relatively low bare quark mass of $am = 0.025$ and starting at a distance $T = 4$, which MILC find works for their $N_f = 2 + 1$ ensembles [293]. Even for these large volume simulations, there is a rapid deterioration of the signal for higher values of $T$. This is of little consequence at shorter distances, where we find an identical effective Coulomb contribution $\rho_{\text{eff}}$ for all ratios. At larger distances, the values deviate and we find a shifting string tension $\sigma$ for each of the ratios. There is a downward trend for the three ratios, but one that appears to be convergent with the difference between $T = 5$ and 6 being close to negligible. As the statistical noise at smaller volumes is considerably larger, effectively killing the signal at $T = 6$ for the available ensembles, we decided to use the $T = 5$ data as the basis of our analysis.

One source of deviations that needs be accounted for is the finite volume. Of special interest here is also a report by the RBC and UKQCD collaborations [334] on a comparison of methods of measuring the static potential. They find that the Coulomb gauge fixing method, implemented the way it is for the results reported here, shows enhanced finite volume effects as compared to the alternative Bresen-
Table 5.2 Results of fitting the static potential measured for several ensembles to equation 5.24. Time-slice number $T$ refers to the particular ratio of time-slices the potential was determined from was measured on (notation as established in equations 5.20 and 5.24. The absence of a result for $\rho_{LCP}$ implies a fit without explicit lattice artefact correction (equation 5.17). Errors given are uncertainties produced by the fits.

<table>
<thead>
<tr>
<th>$\beta$</th>
<th>$a m$</th>
<th>$V$</th>
<th>$T$</th>
<th>$V_0$</th>
<th>$\rho$</th>
<th>$\rho_{LCP}$</th>
<th>$\sigma$</th>
<th>$\sqrt{\chi^2/dof}$</th>
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<tbody>
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<td></td>
<td>6</td>
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<td>0.0571(77)</td>
<td>0.0168(5)</td>
<td>0.88</td>
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</tbody>
</table>

The static potential

The explanation suggested for this by the author lies in the suppression of lattice mirror copy interference for the Bresenham method by the explicit connecting of points in the spatial volume. It is not quite clear why this should be so, as for the full ensemble gauge invariance should ensure no such physical effect should result from a gauge fixing procedure. On a per configuration basis, though, there might be an effect on the distribution of the errors though, possible creating an upwards bias on the large distance potential. The error suppression caused by a larger volume would then give the appearance of large finite volume effects, that should of course eventually vanish for very high statistics. As a side effect, the additional control over smearing introduced by alternatives, such as the Bresenham method, could reduce the amount of noise in the separate configurations. To be fully certain of control over this source of systematics, additional measurements would have to be gathered, replacing the Coulomb gauge fixing by some alternative routine. But even according to the results of [344], the smallest volume of $24^4$ considered here should be large enough to negate strong finite volume effects. Table 5.2 shows the influence on the string tension of a change in volume from $24^4$ to $32^4$ for several ensembles with otherwise identical parameters. We find stable results for $am = 0.025$ at $\beta = 4.0$ and $am = 0.020$ at $\beta = 3.9$, but a drop in the string tension by a significant 30% for $am = 0.025$ at $\beta = 3.9$. There is no clear indication why this should be so, but the latter result would appear to be an outlier in the context of the dataset as a
Figure 5.16 Approach to the $T \rightarrow \infty$ limit in equation 5.20. Data displayed are for $T = 4$ (red), 5 (blue) and 6 (purple) and measured on a $32^4$ volume for $am = 0.025$. The lattice Coulomb potential component was replaced by its continuum equivalent according to equation 5.25 to smoothen the presentation of the data, and a constant potential term was subtracted (see table 5.2). The data are shown multiplied by $R$, to provide a simple linear form as a function of $R^2$. The intercept is determined by the effective Coulomb potential coefficient $-\rho_{\text{eff}} = -(\rho + \rho_{\text{LCP}})$, while the slope is proportional to the string tension $\sigma$.

A crucial result observable related to the static potential is the mass dependence of the string tension. A recent paper [184] uses this relationship and its chiral limit to determine the nature of the vacuum for ensembles at different flavour numbers. The reasoning in that paper is based upon the appearance of confinement at heavy quark masses, where the effect of any potential infrared fixed point would be negated as the effectiveness of shielding is diminished. That particular limit is smoothly connected to the broken phase and the bulk transition, however, so this would not justify the assumption of a smooth extrapolation to the chiral limit. Perhaps a more natural setting is found when the residual string tension is connected to explicit chiral symmetry breaking. Like the Polyakov loop to which it is closely related, $\sigma$ is not an order parameter in the presence of light fermions. As mentioned before, it instead displays pseudo-critical behaviour triggered by the chiral dynamics. The explicit chiral symmetry breaking caused by the bare quark mass could therefore allow for a small string tension away from the chiral limit. Figure 5.17 shows the measured
5.4 The static potential

Figure 5.17 Mass dependence of the static potential, with mapping of the data following that of figure 5.16. Plotted are the potentials for am = 0.020 (green), 0.025 (blue), 0.040 (purple) and 0.050 (red). All measurements were performed at β = 3.9, on a volume of 32^4 for the smaller two and 24^4 for the larger two masses. Fit results can be found in table 5.2.

Potential for four different values of the bare quark mass at β = 3.9. At short range measurements agree, in accordance with the gluon domination of the potential here, resulting in a very comparable Coulomb structure of the data. The value of the string tension, however, is significantly impacted by the quark mass. We will attempt to extrapolate it to the chiral limit.

In [184], the chiral extrapolation is performed in terms of the bare quark mass. If the string tension is a consequence of the incomplete restoration of chiral symmetry, it is actually more appropriate to examine the behaviour of the string tension as the chiral condensate vanishes. Having found a power law description of the explicit chiral symmetry breaking at these values of the coupling in chapter 4, we would expect a similar form for this derived quantity. Fits should therefore be attempted to the general form

$$a^2 \sqrt{\sigma} = A \left( a^3 \bar{\psi} \psi \right)^{\xi} + C,$$

where ξ can be fixed to 1 or C to 0 for a linear or pure power law fit, respectively. Figure 5.18 displays both limits of the fit to equation 5.26. The goodness of fit found in table 5.3 indicates the most natural fit to the data is in fact a power law with a vanishing chiral limit, appropriate for a deconfining phase close to a crossover transition and fully consistent with the chiral symmetry restoration observed in chapter 4. At
Figure 5.18 Chiral extrapolation of the string tension $\sqrt{\sigma}$, measured at $\beta = 3.9$ on a volume of $32^4$ for the two lighter masses, $24^4$ for the larger two masses. Fit results can be found in Table 5.3.

At this point, the quality of the data are not yet sufficient to rule out a confining phase completely.

<table>
<thead>
<tr>
<th>$A$</th>
<th>$\xi$</th>
<th>$C$</th>
<th>$\sqrt{\chi^2/\text{dof}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.80(01)</td>
<td>1.00(F)</td>
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</tr>
<tr>
<td>0.63(01)</td>
<td>0.76(01)</td>
<td>0.000(F)</td>
<td>0.58</td>
</tr>
<tr>
<td>0.64(13)</td>
<td>0.81(20)</td>
<td>-0.001(26)</td>
<td>0.81</td>
</tr>
</tbody>
</table>

Table 5.3 Results of several fits of the string tension to equation 5.26. Errors are uncertainties in the fit.

At $\beta = 4.0$, Table 5.2 insufficient data are available to repeat the above analysis in full. Moving away from the bulk transition towards the weak coupling limit does produce a weakening of the string tension, beyond what would be expected from approaching the free limit of the theory or the effect of a change in lattice spacing. This can be seen by rescaling the string tension to obtain its strength relative to the potential at short distances. The coefficient of the Coulomb potential is dimensionless, so while it indicates the relative strength of the short range interaction, it will not cancel the change in lattice spacing. Instead, we turn to dimensionful constant
contribution $V_0$ to the potential to obtain the dimensionless ratio

$$\sigma_R = \frac{\sigma}{V_0^2}.$$  (5.27)

For the lighter $am = 0.025$ data available at both values of $\beta$, we obtain a value of $\sigma_R = 0.0065$ for $\beta = 3.9$, versus $\sigma_R = 0.0042$ for $\beta = 4.0$. Even if we found the differences between the two lattice spacings to be limited for other observables in chapter 4, we here conclude that the string tension decays rapidly. With only two different masses measured so far, a chiral extrapolation will have to be postponed at the weaker coupling. It is interesting to notice, however, that a linear extrapolation on the two known data points versus the bare quark mass produces a negative intercept of $-0.250$. Turning to the chiral condensate as a more natural independent for this linear extrapolation gives an intercept of $10^{-4}$, hinting at direct proportionality and a pure power law in the bare quark mass.

### 5.5 Plaquette

The plaquette, measure of the gluonic field strength, was shown earlier to display a discontinuity at both critical values of the coupling for the measured low quark masses (figure 5.6). Where the Polyakov loop does not present a signal, the plaquette can be used as a secondary observable, be it of a more indirect type. Given a confining vacuum, the plaquette (which we will denote here as the smallest Wilson loop $W_{11}$) should contain contributions given by a perturbative expansion on top of a non-perturbative gluon condensate $G$  

$$a^4 W_{11} = a^4 W_{11}^{\text{pert}} - a^3 \frac{\pi}{36} \left[ \frac{-b_0 g^3}{\beta(g)} \right] G.$$  (5.28)

This expansion can be used on our data in two ways. First, the existence of the gluon condensate is a property of a confining medium [346]. One possible check of confinement, then, is given by fitting a perturbative expansion function and observing the presence of a non-vanishing intercept. Unfortunately, the gluon condensate is notoriously difficult to observe, so the lack of an observed value can only be considered a sign of consistency, rather than proof of deconfinement. A second, more intricate approach would compare with results from a (semi-)analytical perturbative expansion. Since the coefficients of the expansion are scheme dependent, one would ideally compare to coefficients calculated directly using our lattice action. We will address this point below, but given such a set of coefficients, we would have a very powerful test of both confinement and the connection of our measurements to the weak coupling limit. The influence of the fermionic sector on a purely gluonic observable such as the plaquette is indirect. Because of this, the weak coupling limit of the plaquette should be stable under small changes in the bare quark mass, even if these fields exert a dominant influence of the chiral dynamics. Figure 5.19 confirms this, showing the results for different datasets agreeing at weak coupling, up until the region in which the approach of the pseudo-critical coupling causes the onset of
The plaquette expectation value, calculated as $\ln(a^4W_{11}^{-0.25})$ from the average of $a^4W_{11}$ over all directions and plotted versus the inverse of the bare lattice coupling $\beta$. Measurements are for a range of quark masses: $am = 0.020$ (red), 0.025 (blue), 0.050 (green) and 0.070 (orange). The black line is the result of a linear fit (up to third order in $\beta^{-1}$, without intercept), performed to the $am = 0.020$ data below the weak coupling transition. Data for different masses converge in the weak coupling limit and are apparently well described by the perturbative description for a deconfined phase.

transition behaviour. A fit without intercept term turns out to provide a good description of the data towards the weak coupling limit and the data in fact appear to be smooth up to the value found from a measurement at $\beta = 10.0$ where deconfinement should have occurred. A clearly difference in signal is found above the transition. For both of the heavier masses, this does seem to introduce the need for a non-zero intercept, implying the onset of confinement. It would be of particular interest to observe a similar pattern for the intermediate region at the lower quark masses. There is an obvious difference in slope above and below the transition, the result of a sudden change in dynamics, but this in itself does not imply the presence of a non-zero gluon condensate term. The limited extent of this region unfortunately means that an extrapolation towards the free coupling limit is very unconstrained. The results of figure 5.19 are encouraging, but a second look raises some questions. A perturbative description seems to be able to describe the data right up to the first bulk transition for $am = 0.020$. This is particularly surprising due to the absence of tadpole improvement, which was introduced specifically to improve convergence towards the perturbative limit. It leads one to suspect the straightforward expansion fit manages to account for curvature mainly due to the limited range of the coupling.
5.5 Plaquette

We can extract more information from the available measurements by using Ferrenberg-Swendsen reweighting [347]. Appendix A provides details on this technique that exploits the availability of a stochastic sampling of the full action, which means that estimates of observables for small deviations of the input parameters can be determined. Though the method has its limitations, which are also discussed in appendix A, it in principle allows us to obtain independent, non-perturbative estimates of the derivatives with respect to the coupling constant. Those can then be used in a simultaneous fit to both the plaquette expansion series and the derivative of this series, which should work well if we are in a perturbative regime.

One practical issue with this approach for our current dataset is the limited information we can extract on the errors associated with the derivatives. Not only will there be the usual correlation between successive configurations, but the assigning of weights will have the overall effect of lowering the amount of statistics. It also means a regular blocking analysis will not be appropriate to get an estimate of the decorrelated errors. On top of this, the calculation of the derivatives will introduce a systematic error due to the correlation between reweighted values calculated from a single distribution. While it is not immediately clear how to estimate the size of these effects, it is clear that the results of an uncorrelated bootstrapping analysis on the data will underestimate the errors on the data. A plot of the derivatives clearly demonstrates this, as the data are decidedly more noisy than the associated errors would suggest. Examining figure 5.20, it seems a peak structure appears around

![Figure 5.20 Derivatives of the plaquette with respect to the lattice coupling constant $\beta$, measured by means of reweighting. Zero temperature measurements for runs with $N_s \geq 24$ are plotted, for a range of masses covering $am = 0.020$ (red), 0.025 (green), 0.050 (blue) and 0.070 (purple).](image-url)
$\beta = 3$, which would resonate with the value of the critical coupling extracted from the linear chiral extrapolation of the pseudo-critical couplings. However, the data are obviously not normally distributed around this peak. Instead, errors seem to almost exclusively diminish the measured values. This can be explained by considering the effect of limited statistics on the reweighting measurement of a derivative. The configurations providing the main contribution to the corrections in the Taylor expansion of equation A.4 are those located in the tails of the Gaussian distribution of the action of the configuration making up the ensemble. Mapping out those tails smoothly requires high statistics studies, as even with 10 thermalized kilo-trajectories, we would only expect about 200 measured configurations at a distance of two standard deviations or more. The much better defined shape of the distribution around the central value, instead, will mainly contribute to the leading order term in equation A.4. Given limited statistics, we might happen to have an over-representation of eccentric values of the action, but we are much more likely to find an overly flat curve when approximating the Taylor expansion. The latter will always result in an underestimated value of the derivative, explaining the non-Gaussian deviations of figure 5.20.

When introducing derivatives to a fitting procedure based on minimizing $\chi^2$, it makes no sense to introduce errors that are both underestimated and not normally distributed. Instead of using the calculated errors, we introduce a homogeneous weighting factor $\lambda$ and only include the central values. The fitting procedure then consists of minimising

$$\chi^2 = \sum_i \left( \left( \mu_i^{\text{meas}} - \mu_i^{\text{pred}} \right)^2 \sigma_i^{-2} + \left( \partial_\beta \mu_i^{\text{meas}} - \partial_\beta \mu_i^{\text{pred}} \right) \lambda^{-2} \right).$$

(5.29)

This definition of $\chi^2$ changes the interpretation of the goodness of fit parameter and the choice of $\lambda$ introduces a certain level of arbitrariness to the procedure. We will therefore examine the effect of varying $\lambda$ around $O(\bar{\sigma})$, realising that the bare fit will be recovered for $\lambda \gg \bar{\sigma}$.

There have been only limited attempts to study the perturbative expansion of the plaquette at generic values for $N_f$, especially in the context of a staggered fermion lattice action. Because of the scheme dependence referred to earlier, this prohibits a fit of the lattice results to perturbation theory to a given order. Some results are available in literature. Of particular interest are calculations on the weak coupling expansion [335], providing results on the perturbation expansion for both the naive and Asqtad improved staggered fermion action. These, however, apply to an expansion in a renormalized coupling $a_V(q)$, defined at a typical momentum scale $q$ as

$$V(q) \equiv -\frac{4}{3} \frac{4\pi a_V(q)}{q^2}.$$
5.5 Plaquette

Figure 5.21 Fits to the plaquette data for $am = 0.020$ using equation 5.29 for the range $\beta > 3.5$, using $\lambda = 10^{-1}$ (red line), $\lambda = 10^{-3}$ (black line) and $10^{-5}$ (blue line), for an average value of the standard deviation on the plaquette of $\tilde{\sigma} = 2.6 \times 10^{-5}$. While the plaquette can be described by an expansion to $O(\alpha^3 L)$ up to the location of the bulk transition, the effect of the addition of data on the first derivative indicates a breaking down of the perturbative expansion at much weaker coupling.

In [335], the conversion from the bare lattice coupling

$$\alpha_L(q') = \frac{6}{4\pi \beta'},$$

(5.31)
defined at an intrinsic, $\beta$ dependent scale $q'$, to the renormalized coupling $\alpha_V$ at scale $q^*$ is done through a perturbative expansion of the $R \times T$ Wilson loop $W_{RT}$ in terms of $\alpha_V$, the plaquette obviously being the special case $W_{11}$. By matching the measured value of plaquette for a given value of $\alpha_L$ and solving, one obtains a result for $\alpha_V(q^*)$. Note that the momentum dependence is introduced by moving from the full non-perturbative measurement to the perturbative expansion and is contained explicitly in the perturbative coefficients [348]. As such, the value of $q^*$ associated with the plaquette is extrinsic to our lattice simulations, but needs to be compensated for between perturbative expansions of different quantities.

This approach would obviously need to be amended for our current investigation. To obtain information on the validity of the perturbative expansion of the plaquette, an alternate conversion between $\alpha_L(q')$ and $\alpha_V(q^*)$ is needed. One possibility is the direct determination of $\alpha_V(q^*)$ from measurements of the static potential as a function of the momentum $q$, but this would require computationally very intensive
large volume studies with high statistics for a large range of couplings. Alternatively, a matching between $\alpha_V(q)$ and the coupling $\alpha_{\overline{MS}}$ defined in the minimal subtraction scheme can be calculated using the perturbative expansion of the static potential presented in [349]. Separately, one can convert between $\alpha_L$ and $\alpha_{\overline{MS}}$ using long standing results from, e.g. [350]. After a perturbative renormalization step, using the expansion in [335], to move towards the energy scale $q^*$ we have obtained an independent, if slightly involved, determination of $\alpha_V(q')$.

Unfortunately, the action used in our simulations – Symanzik improved, but without tadpole improvement – does not correspond to either of the cases covered in [335]. While a report on the calculation of the plaquette expansion for a range of actions was to appear as a separate paper originally, this was apparently never published. Requests for this data to the authors were not responded to and so far this crucial and highly non-trivial component in the above approach is missing. An alternative and much more direct approach is the one employed by the authors of [351, 352]. They employ stochastic perturbation theory to derive the plaquette expansion in terms of $\alpha_L$ directly, in principle bypassing the need for additional perturbative conversion steps. Such calculations were not yet done for staggered fermions, but an effort to this end is under way at the time of writing. Results here will provide a direct check of the approach to the perturbative regime.

With only the literature results on the naive and Asqtad actions at our disposal, our capacity for analysing the measured plaquette expansion coefficients is limited. Table 5.4 reproduces the expansion coefficients given in [335]. While the coefficients are very significantly different between the naive and staggered action, there is a clear pattern. Because the action employed in the simulations includes part of the improvement of the Asqtad scheme and one would therefore expect the actual coefficients to lie between the values given in table 5.4. The increased flavour content induces a sign change in coefficient $c_3$, reflecting the behaviour of the perturbative beta function. Alternative actions might modify this signature, but the pattern will survive any change in perturbative scheme since no physical scheme can introduce a mapping to negative couplings. We can therefore attempt a check on the consistency of our data, even when expanding in the $\alpha_L$ scheme.

The results given in table 5.5 show remarkable deviations from the predictions in table 5.4. Moving away from the bulk transition gives us a rather consistent set of values for the three coefficients, with a clear positive sign for $c_2$. Since the result with
5.6 Conclusion

In this chapter, we have elaborated on our simulations using twelve quark flavours. In chapter 4, we established the existence of a bulk transition separating a chirally symmetric phase from a broken one. As this placed twelve flavour QCD within the conformal window, the natural follow up was to question the properties of this new phase of QCD. A study of the properties of the bulk transition under changes in the bare quark mass revealed the smooth transition observed in 4 as a crossover. Moving towards the chiral limit revealed a sharpening into a bona-fide first order phase transition and revealed the presence of an additional transition at strong coupling. We speculated that this transition is an artefact of discretisation and found indications of it moving towards the infinite coupling limit as the chiral limit is approached, though further simulations will certainly be needed to confirm this. A fit to the pseudo-critical couplings at finite mass revealed a connection between first order phase transition and the crossover transition observed at higher masses and

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<td>-3.2418</td>
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</table>

Table 5.5 Results for a fit of the measured plaquette value, in the form $-\frac{1}{4}\ln(W_{11})$, to the expansion of equation 5.29. Fits were performed on all zero temperature data available for $am = 0.05$ with spatial volumes at least equal to $12^3$ with couplings weaker than a specified limit $\beta_{\text{min}}$ and with three values of the scaling factor $\lambda$ that should be seen as relative to the average standard deviation on the plaquette measurements $\bar{\sigma} \approx 4 \times 10^{-5}$. No statistical errors are displayed, as they are meaningless in the absence of control over the systematical error.

generic $N_f$ for this quantity given in [335] for the unimproved action is in fact

$$c_2 = -1.2467(2) - 0.06981(5)N_f,$$

(5.32)

the sign cannot be readily attributed to an effect of the dynamical quarks. While it is not excluded that the sign inversion is a feature of our particular action, it is in fact more likely that we should interpret these results as a breakdown of the perturbative expansion. The inclusion of larger values of $\beta$ is therefore essential and such an extended dataset will be the basis of our comparison to the results of stochastic perturbation theory.
suggested a first order nature of the transition throughout. This would exclude the presence of a UV fixed point in addition to an IR fixed point, as was suggested in [99], at least at finite mass. However, the line of first order phase transitions at finite mass might terminate in a second order chiral limit, possibly leaving the AdS/CFT inspired scenario of [99] intact.

We subsequently examined the properties of the gauge sector, first turning to the Polyakov loop as an approximate order parameter for the deconfinement transition. No signal was found at zero temperature, confirming the results of [176]. It was indicated that this is most likely a property of the zero temperature phase, as was in fact already suggested in [98]. Instead, we examined the static potential and found a small remaining string tension that was very sensitive to the mass. Numerical evidence was presented that the string tension should vanish identically in the chiral limit, though further data will be required to build this case convincingly.

Finally, preparing for a further study using stochastic perturbation theory, the validity of the perturbative regime was tested. From a reweighting procedure, independent estimates were found for the derivative of the plaquette. No consistent perturbative expansion could be constructed in the region where data were available, though a missing prediction for the scheme dependent plaquette coefficients will be needed for a full numerical analysis. Nevertheless, preliminary results indicate a need for runs at weaker coupling to explicitly connect to the perturbation theory and the asymptotically free limit.
We conclude this thesis by tersely summarising the results of each research chapter and discussing them in the context of recent literature and ongoing developments. Weaknesses in the current data are pointed out and reflected upon, naturally introducing proposals for future extensions of the studies contained in this volume.
We set out work on this thesis with the goal of clarifying the influence of increasing quark content on the gauge dynamics and phase diagram of QCD-like theories. While this rich topic has of course not been exhaustively solved in the preceding pages, it is our hope that they may form a useful contribution to the scientific discourse on this topic, one that has become considerably more extensive over the past few years and that may yet branch out in currently unforeseeable directions. The material has been arranged in such a way that successive chapters deal with theories with increasing flavour content. This takes us from phenomenologically oriented simulations of twisted mass lattice QCD with dynamical strange and charm quarks to measurements of the suspected quasi-conformal phase at twelve flavour QCD. In this conclusive chapter, we critically summarize their content and highlight future perspectives.

The results of chapter 2 could be considered a sanity check on a new simulation setup designed by the European Twisted Mass Collaboration (ETMC). Presented are measurements of the light meson mass spectrum, coming from the first simulations using an \( N_f = 2 + 1 + 1 \) action with Wilson-like fermions. These simulations are the result of a large collective effort by lattice theorists all over the continent, putting to use the rapidly developing European supercomputing infrastructure. The inclusion of a dynamical charm quark is technical challenging and it is currently worked on by only two collaborations world-wide. The promise of these simulations lies in the possibility accurate simulations to answer open questions in flavour physics. The main results of this chapter include the adequate description of the mass dependence of the light mesons by SU(2) chiral perturbation theory. Scale setting by means of the pion decay constant gives results consistent with the gluonic length scale determined from the Sommer parameter \( r_0 \). As they stand, these results are incomplete. One important missing component is an extrapolation to the continuum limit. This was not yet possible, due to the availability of full ensembles at only two values of the lattice coupling \( \beta \). On top of that, those values – \( \beta = 1.90 \) and 1.95 – are fairly similar. The situation is set to improve in the near future, as simulations are under way to produce an ensemble at \( \beta = 2.10 \) and even weaker further values of the coupling. A proper continuum extrapolation will also require a determination of the renormalisation constants and they are currently being calculated.

Once a continuum extrapolation can be performed reliably, we can address the open question of the influence of isospin breaking induced by the twisted mass formulation. Frezzotti and Rossi have shown [210] that the isospin breaking at finite lattice spacing is an \( O(a^2) \) discretisation artefact when the simulation is tuned to maximal twist and it should therefore be possible to control it in principle. At current lattice spacings, however, it is important to take into account the presence of an anomalously light pion in the chiral dynamics. Calculations of the effect of isospin breaking on the chiral logs and finite volume effects have been recently performed autonomously [280, 353]. Those can be put to the test once ensembles at additional lattice spacings are available. A good quantitative description of the lattice spacing artefacts would indicate these systematic errors are well understood at least for this sector, though the influence on other observables may need to be established separately.
With the good match of simulation results to chiral perturbation theory, a second natural extension of the results of chapter 2 is a full analysis of the heavier mesons, in particular particles such as the kaon and the D meson that will be particularly sensitive to the impact of the dynamical strange and charm quark. What framework is most appropriate for that analysis is still an open question. While SU(3) chiral perturbation would seem a natural match, it has proven disappointing in describing the dynamics of other recent large scale simulation [354, 355]. A heavy quark extended SU(2) chiral perturbation theory seems more promising [356], but the framework of this analysis is not quite as well developed yet. Specifically, expressions for the finite volume effects of many of the observables have not yet been obtained, though they could be probably be adapted from recent work, such as [357]. The presence of non-negligible isospin breaking lattice artefacts should be accounted for in this analysis, as well. These will be the first steps towards exploring several unsolved puzzles of weak interactions, such as the mechanism behind the $\Delta = 1/2$ rule and the value of $\epsilon'/\epsilon$, where the charm is expected to play a crucial role. But the interest in lattice configurations without potential quenching artefacts lies also in broader applications of lattice QCD, such as the proposed program for the analysis of B-physics [225].

Chapter 3 shifts the focus of simulations from phenomenology to the fundamental question of the possible appearance of a non-trivial IR fixed point in Yang-Mills theories with a certain massless flavour content. It reports on simulations of the theory with eight quark flavours, by means of which a chiral phase transition is located. The observation of hysteresis shows this transition to be of first order at sufficiently high temperatures, but it starts to wash out as the temperature is lowered. This temperature is determined through the temporal lattice extent $N_t a$, with the lattice spacing denoted $a$ and $N_t$ the number of lattice spacings. Applying perturbative scaling formulae to connect a change in bare coupling to a rescaling of the lattice spacing reveals that the temporal lattice extent at the transition is almost constant, indicating that there is a well defined transition temperature $T_c$. Such a thermal transition cannot exist in the presence of an IR fixed point, so QCD with eight flavours should be in the regular hadronic phase.

At the time of publishing, the conclusions of chapter 3 contributed to the resolution of the open question of lattice results conflicting with analytical predictions. The papers by Iwasaki and collaborators [166–168] had drawn surprising conclusions – putting the opening of the conformal window as low as $N_f = 6$ – while the large study by the Columbia group [165] had unfortunately remained inconclusive. With contemporary and later papers corroborating the results of chapter 3 (see chapter 1) our understanding of this theory has improved dramatically. All recent reports on simulations with $N_f = 8$ fundamental fermions have been in broad agreement with each other and the general trend of analytical papers as described in chapter 1. Reception of the publication of chapter 3 has been rather positive accordingly. One weaker point in the results is the weakening of the transition at lower temperatures. This is a factor complicating the scaling analysis and the conclusions drawn could be strengthened by extending the data set. Two paths would appear to be open for doing so effectively. A simple approach would be to investigate the theory at intermediate values of $N_f = 8$ and 10, where the transition should still be sharper. An
alternative would be to lower the quark masses involved, which should increase the sensitivity to temperature and push the phase transition away from the crossover regime. If a sufficient range of quark masses would be sampled, this would also allow for studying the extrapolation of the theory towards the chiral limit.

Regardless of possible improvements, however, the conclusions drawn in chapter 3 should be solid. A phase transition is clearly identified at both temperatures. The observation of thermal scaling of this phase transition is definite, and unambiguously incompatible with the presence of a conformal phase. This fact, combined with the broad consensus that has now emerged in the lattice community on this topic, makes further investigations of the nature of the phase transition in $N_f = 8$ for purposes of excluding a conformal phase a low priority. Additional investigations are probably more productively performed in the broader context of a study of SU(3) Yang-Mills with fundamental fermions in the walking regime. This broadening of scope would first of all mandate a full study of the spectrum of these theories in the chiral and continuum limit, in a regime where the regular tools of QCD for obtaining those data are not fully applicable. Potentially more problematic even, a direct quantitative assessment of the influence of different fermion flavours on the gauge dynamics require the introduction of some scale setting scheme to mediate between essentially different theories. It seems inescapable that this would introduce a certain level of arbitrariness, such as the rather arbitrary equation of the interaction strength at energy scales of the $\tau$ lepton in [56]. One might therefore conclude that advances on the results of chapter 3 will be first and foremost challenging on a conceptual level.

Unlike the case of eight flavours, no general consensus can be said to have been reached for QCD with twelve fermion flavours. As this value lies close to the lower bound of the conformal window predicted by many of the analytical approaches, it stands to reason that the analysis would be less straightforward here. Chapter 4 presents evidence of this theory possessing a quasi-conformal phase. A chiral phase transition was found, the location of which was shown to be insensitive to the physical temperature. This implies a bulk nature of the transition, branding it a lattice artefact the importance of which lies in the fact that it would exclude the existence of a thermal transition. Approximate lines of constant physics were defined as trajectories in bare parameter space that keep the ratio of the pseudo-scalar and vector meson masses fixed. The change in lattice spacing along these trajectories provides a measurement of the sign of the beta function. In the region to the weakly coupling side of the chiral transition, this sign was found to be positive and therefore consistent with the Coulomb phase expected to the strong coupling side of an IR fixed point. As a direct test of the restoration of chiral symmetry, the extrapolation of the chiral condensate and pseudo-scalar mass to the chiral limit was studied. Curvature was found to be present in both, allowing for an extrapolated value compatible with zero and demonstrating the effective dynamical nature of quarks at the masses used in the study.

The results of chapter 4 are in full agreement with the earlier results based on an Schrödinger functional approach in [171, 172]. However, preliminary reports from other groups, notably those of [176,178,182], have challenged these conclusions. The
approaches of [176,178] are somewhat similar to those presented here, but with a different choice of action and parameters. Finding a particular combination of lattice action and parameters that approaches the continuum limit sufficiently but is still practically manageable is no easy task, and requires a certain amount of serendipity. As chapter 4 testifies, finite volume effects tend to increase rapidly for this theory as the quark mass is lowered. Simulations should in principle be performed as close to the chiral limit as possible, because mass effects interfere directly with quasi-conformal dynamics. But the volumes required to do so can quickly become very unwieldy, while correlation times grow rapidly at the same time. In the course of obtaining the results presented in this thesis, we found our lowest bare quark masses pushing the limits of feasibility. The parameters chosen in [176,178] may consequently be too ambitious to obtain data of sufficient quality.

Conversely, of course, concerns over the current results have been voiced in terms of the possible presence of finite size artefacts and the extent to which the chiral regime is probed by the quark masses used. For the former, the argument was already made in chapter 4 that the requirements for suppressed final volume effects in the regular hadronic phase of QCD have been satisfied, excluding a false positive on the appearance of a conformal phase due to finite size systematics. Explicit checks by varying the simulation volumes have been included in addition, demonstrating that finite volume effects are indeed under control even in this non-hadronic phase. Though some have concluded that this indicates the masses used are too heavy, the chiral extrapolation of the meson spectrum demonstrates directly that the fermions are dynamical and influencing the gauge dynamics. It should also be noted that there is no clear scenario in which quark masses being too heavy would lead to a restoration of chiral symmetry at intermediate masses if this symmetry is spontaneously broken in the chiral limit, as the opposite limit of a fully quenched theory (with infinite quark masses) will break this symmetry as well. In this sense, the fact that a phase transition is observed in the first place implies that fermion dynamics are influencing the phase structure. Quite independently of our results, [184] gives a numerical range of masses considered safe, for a quark action similar to the one used in this thesis. The quark masses upon which our results are based overlap with that region comfortably. It is interesting, in this context, to note that the conclusions of [184] on the $N_f = 12$ theory differ markedly from the earlier preliminary report [182] and now agree with ours. This demonstrates how crucial it is to await the final results also for other groups.

Additional observables for the simulations of chapter 4 are studied in chapter 5, to be discussed below. But other useful extensions of chapter 4 would include measurements at lower masses, which should magnify the difference in quality between a linear and a power-law fit. This should strengthen the indications of a chirally symmetric ground state and might constrain the fit sufficiently to isolate the linear and curvature terms that are both expected to be present in the chiral extrapolation of the condensate but can currently not be disentangled. With a more accurate determination of the exponent in the curvature term and information on its evolution with varying coupling, its origin could be established and the arguments of [314] for the absence of an anomalous dimension at the IR fixed point tested. Increasing
curvature when moving away from the bulk transition would imply an origin in the fixed point, while the opposite trend would point to a crossover exponent. The former would be exciting, since the trend of the exponent with coupling would be different on both sides of the fixed point and could therefore allow one to bracket its location. A study of the spectrum at slightly lower quark masses would also increase the overlap between our results and those of [176], allowing for a direct comparison and hopefully a convergence of results.

The final chapter 5 presents results of work in progress on $N_f = 12$ QCD. It is shown that a qualitative change occurs in the phase transition as the quark mass is lowered, as a crossover transition turns into a sequence of sharp first order transitions. Of these transitions, the one occurring at the weakest coupling is again shown to be of bulk nature and connected to the bulk transition at higher masses. No signals in the Polyakov loop are found at zero temperature either above or below the transition. However, a measurement of the static quark potential reveals a small residual string tension that vanishes in the chiral limit, in accordance with the expected behaviour for the quasi-conformal phase. Fits of plaquette measurements and numerical derivatives to a perturbative expression give indications of a sign change in the expansion coefficients that one would expect for a Coulomb phase. But a discrepancy between the fitting result to the direct plaquette data and its derivative implies the truncation of the perturbative series does not give an accurate description of the data.

One clear way in which these results can be improved upon is by adding measurements at weaker coupling. Though finite volume effects appear to increase strongly as one moves away from the region after the bulk transition and such additional simulations may be expensive as a result, it is important to connect to the perturbative regime. Such simulations should be combined with a set of perturbative coefficients computed directly for the current action, a calculation that is currently under way using stochastic perturbative techniques. Since the fermions are the critical component of the mechanism that triggers the appearance of the IR fixed point, it will be crucial as well to take into account explicitly the bare quark masses in these predictions. The hope is, that a change of sign in one of the coefficients would be triggered at the IR fixed point that could be observed even away from the massless limit. More generally, a precise quantitative comparison with perturbative coefficients may clarify the influence of the regularisation scheme on the various observables. This could be instrumental in understanding the relationship between results obtained in different settings.

The string tension component of the static potential does look like a most interesting probe of conformal physics as well and some results on smaller quark masses could allow for a more precise extrapolation towards the continuum limit. But the weakness of those measurements in the current setup will always be the numerical extrapolation towards a vanishing value, for which one can fundamentally never obtain more than an upper bound.

It is expected that the near future will show a convergence of results and a clarification of the extent of the conformal window. The real challenge in the future will be to find access to the quasi-conformal phase numerically and obtain quantitative
information on the behaviour of the spectrum. To achieve this, it is important that an effective description of the conformal phase is developed, in which the effects of the different scales distorting conformal dynamics, specifically the finite volume and non-zero quark mass, can be systematically estimated. The main problem plaguing the current programs for lattice simulations with many flavours is the absence of such a generally accepted framework, which tends to muddy the comparison and discussion of the various results and complicates the choice of parameters in the planning of further simulations.

It is a promising development that studies with a more direct focus on the physical application of theories in the walking regime are appearing [119,358]. Whether each of the separate efforts is ultimately successful or not, this shift marks a move of large-$N_f$ lattice simulations away from the realm of physical curiosity, towards direct utility in the construction of technicolour(-like) extensions of the Standard Model. One would hope that this will open up a new frontier where the lattice community can contribute essential qualitative and quantitative insights on physics beyond the Standard Model to the larger particle physics community. The latest generation of particle colliders is set to provide experimental data at unprecedented levels of quantity and precision. It will be up to theorists to provide similarly accurate predictions of experimental signatures for the many theoretical proposals that have been floated in recent years. As a mature field, providing the only known systematic option for dealing with non-perturbative field theory, the lattice should carve out a central role for itself in this process. The precise numerical analysis of the influence of flavour physics on gauge dynamics will be an important part of these efforts. Of course, this implies the need for the continued development of current lattice methods, probably including a move towards different actions and fermion formulations, novel observables and a consistent framework of analysis that provides non-ambiguous and quantitative control over systematics. In this sense, the quest to discover all the different flavours of gauge theories has only just gotten under way.
Ons moderne begrip van deeltjesfysica, waar dit proefschrift een kleine bijdrage aan probeert te leveren, is gebaseerd op een geïntegreerde set wiskundige modellen dat gezamenlijk bekend staat als het Standaard Model (SM). Om een indruk te krijgen van de inhoud van deze dissertatie, is het dan ook nodig om enigszins bekend te zijn met de opbouw van dit model. Vergelijkbaar met het periodiek systeem van elementen dat een ieder waarschijnlijk kent uit de scheikunde zoals die wordt gegeven op de middelbare school, ordent het SM alle ons bekende deeltjes in een regelmatig systeem. Zoals de chemie een onderscheid maakt tussen atomen als fundamentele bouwstenen en moleculen als samenstellingen van die atomen, zo maken fysici een onderscheid tussen wat elementaire deeltjes worden genoemd en samengestelde deeltjes die bestaan uit meerdere elementaire deeltjes. Het aantal elementaire deeltjes is – voor zover wij dat op dit moment in kunnen schatten – veel kleiner dan het aantal atomen. Kennen we zo’n honderd chemisch verschillende elementen, zo zijn er minder dan twintig fundamenteel verschillende elementaire deeltjes\(^1\). Deze beperkte groep elementaire deeltjes kent daarentegen wel een grote verscheidenheid aan interacties en de specifieke rol van de verschillende deeltjes loopt zeer ver uiteen.

Laten we daarom beginnen met het neerzetten van enkele fundamentele begrippen uit het SM. Een eerste, zeer belangrijk onderscheid is dat tussen de zogenaamde ‘fermionen’ en de ‘bosonen’\(^2\). De fermionen zijn deeltjes die misschien nog het meest

\(^1\)Natuurlijk met een slag om de arm – zo hebben bijvoorbeeld veel deeltjes een soort spiegelbeeldig anti-deeltje, dan in eigenschappen goeddeels identiek is, maar tegenovergestelde ladingen heeft. Ook zijn er twee soorten W-bosonen en maar liefst acht verschillende typen gluonen. Zou men deze alle apart meetellen, dan ligt het genoemde aantal natuurlijk hoger. Het precieze getal is voor de verdere redenatie echter van weinig belang.

voelden aan de klassieke voorstelling van deeltjes. Een belangrijk (en bekend) voorbeeld van een elementair fermion is het elektron: een deeltje met een elektrische lading dat een grote rol speelt in chemische processen en waarvan de bewegingen ten grondslag liggen aan alle elektronica, zoals dat woord al impliceert. Andere voorbeelden van fermionen zijn de ‘quarks’, die een belangrijk onderwerp van dit proefschrift zijn. Tegenover de fermionen staan de fundamentele bosonen. Binnen het SM zijn de bosonen de deeltjes die geassocieerd worden met interacties tussen verschillende deeltjes. In de relativistische en kwantummechanische beschrijving van de natuur kan een kracht tussen ladingen worden gezien als de uitwisseling van een bijzonder deeltje, specifiek geassocieerd met die kracht. Dit klinkt – en is – abstract, maar velen zullen toch bekend zijn met de zogenaamde ‘fotonen’, de deeltjes die geassocieerd zijn met zichtbaar licht\(^3\). Het foton is een elementair boson binnen het SM, dat de basis vormt van elektromagnetische interacties: de elektrische en magnetische krachten tussen twee elektrisch geladen deeltjes worden veroorzaakt door de onderlinge uitwisseling van fotonen. Een relevant voorbeeld van een ander boson is het ‘gluon’\(^4\). De uitwisseling van gluonen tussen deeltjes ligt aan de basis van een in het dagelijks leven minder duidelijk aanwezige interactie, namelijk de sterke kernkracht. Op deze uitwisseling komen we zo dadelijk nog terug.

Het diagram geeft een schematisch overzicht van de fermionen en bosonen in het SM. In dit overzicht zien we ook een onderscheid aangebracht tussen de reeds genoemde ‘quarks’ en de zogenaamde ‘leptonen’. Beide groepen bestaan uitsluitend uit fermionen, maar er is een cruciaal verschil in het type lading dat de twee groepen dragen. Het type lading van een deeltje bepaalt welke bosonen het deeltje uit kan wisselen, zodat bijvoorbeeld alleen elektrisch geladen deeltjes gevoelig zijn voor de elektromagnetische velden die het gevolg zijn van de uitwisseling van fotonen. Maar terwijl zowel de quarks als een deel van de leptonen elektrisch geladen zijn, zijn het alleen de quarks die de lading dragen die geassocieerd is met de sterke kernkracht en de uitwisseling van gluonen. Het zijn de speciale eigenschappen van de sterke kernkracht die de quarks tot een aparte groep maken.

Anders dan bij de elektromagnetische interactie gaat het bij de sterke kernkracht niet louter om een enkele soort (positieve of negatieve) lading, maar zijn er drie verschillende soorten lading. We zijn deze varianten ‘kleur’ gaan noemen, naar analogie van de manier waarop wij licht waarnemen, en de quarks kunnen dan ook een ‘groene’, ‘rode’ of ‘blauwe’ lading dragen. Het mag duidelijk zijn dat deze benamingen verder niets met de kleuren te maken hebben. Bij de enkele soort elektrische lading hoort ook maar één soort foton. Bij de gluonen ligt dat ingewikkelder: tussen quarks met verschillende soorten lading worden verschillende soorten gluonen uitgewisseld, waarbij we uiteindelijk acht soorten kunnen tegenkomen\(^6\). Deze merk-

\(^3\)Het woord ‘foton’ is dan ook afgeleid van het Griekse woord voor ‘licht’.
\(^4\)Naar het Engelse woord voor lijm, zoals we later zullen zien een treffende naam gegeven de specifieke rol die deze deeltjes spelen.
\(^6\)De exacte telling is wat ingewikkelder dan in deze schematische beschrijving duidelijk kan worden gemaakt. De verschillende combinaties die meegenomen dienen te worden zijn die tussen de drie verschillende ladingen en de tegenovergestelde ladingen van de anti-quarks, waarbij sommige combinaties geschreven kunnen worden als gecompliceerde samenstellingen van andere. Er blijven uiteindelijk acht onafhankelijke gluon soorten over.

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waardige constructie heeft grote gevolgen, want het betekent dat gluonen zelf ook een kleur lading dragen en dus op hun beurt nieuwe gluonen kunnen uitwisselen. En omdat ook die gluonen weer een kleur lading hebben, kan er een soort waterval van gluonen ontstaan.

Hoe meer deeltjes er worden uitgewisseld tussen geladen deeltjes, des te sterker wordt de interactie. Als je twee elektrisch geladen deeltjes uit elkaar trekt, kunnen er steeds minder fotonen uitgewisseld worden en wordt de aantrekkingskracht steeds kleiner. Maar bij quarks met een kleur lading, gebeurt precies het tegenovergestelde. Hoe verder de quarks uit elkaar getrokken worden, hoe meer gluonen er geproduceerd worden en hoe sterker de aantrekkingskracht. In dit opzicht lijkt het alsof de quarks met elkaar verbonden zijn middels een veer, die ook steeds moeilijker uit te rekken is. Hierdoor kun je nooit hard genoeg trekken om de quarks voorgoed uit elkaar te trekken en is het principieel onmogelijk om een enkele quark ooit te isoleren\(^7\). Dit verschijnsel staat bekend als ‘confinement’ (ofwel ‘opsluiting’) van de

\(^7\)Om iets preciezer te zijn: het is niet mogelijk om een quark voldoende energie mee te geven om het
Quarks. Quarks worden daardoor in de praktijk altijd gevonden als onderdeel van samengestelde deeltjes, waarvan de bekendste zonder twijfel het proton en neutron zijn, de bouwstenen van atoomkernen. Er bestaan echter veel meer van dergelijke composieten, die ‘hadronen’ worden genoemd. Alle quarks hebben een kleur lading en voor ieder soort quark bestaan er varianten met elk van de drie kleuren. Maar daarnaast zijn de zes soorten quarks – ook wel aangeduid als verschillende smaken, ofwel ‘flavours’ – wel degelijk van elkaar te onderscheiden. Hadronen bestaande uit verschillende quarks hebben andere massa’s, elektrische ladingen en levensduur.

De interacties tussen quarks die uiteindelijk de eigenschappen van de hadronen bepalen zijn niet eenvoudig om door te rekenen. Dat is een consequentie van het beschreven cascade-effect, waarbij de gluonen zelf weer nieuwe gluonen kunnen uitwisselen. Ook de interacties van fotonen zijn op dit kwantummechanische niveau niet eenvoudig, maar vaak kan via een wiskundige omschrijving van het model een eenvoudiger effectieve beschrijving worden gevonden. Voor de elektromagnetische kracht zijn dat op een hoog niveau bijvoorbeeld de wetten van elektriciteit en magnetisme zoals wij die leren op de middelbare school. Op laag niveau kennen we een efficiënte beschrijving, die gebruik maakt van het feit dat de interactie tussen twee elektrisch geladen deeltjes heel behoorlijk beschreven wordt door het uitwisselen van een enkel deeltje, terwijl het effect van het uitwisselen van een toenemend aantal deeltjes een steeds kleinere correctie geeft. Omdat er bij de sterke interactie over het algemeen zeer veel gluonen betrokken kunnen zijn, werkt deze zelfde aanpak daar veel minder goed. Ondanks een grote hoeveelheid onderzoek en enkele successen is er voor de wisselwerking tussen quarks en gluonen nog steeds geen goede beschrijving gevonden die het toelaat om accurate berekeningen uit te voeren met pen en papier. Daarom is in de afgelopen decennia een alternatieve aanpak gegroeid in populariteit: het berekenen van sterke interacties door middel van simulaties op (veelal) supercomputers.

De wiskundige structuur van de theorie is zodanig, dat het numeriek behandelen van de interacties van gluonen zeer efficiënt is. De quarks, daarentegen, zijn veel lastiger om mee te nemen in dergelijke simulaties. Het bleek gelukkig al snel dat men de quarks in eerste instantie kan verwaarlozen in de berekeningen om tot een min of meer correcte benadering van veel experimenteel meetbare resultaten te komen. Lange tijd werd dan ook gewerkt in de zogenaamde ‘quenched approximation’ – ofwel ‘onderdrukkende benadering’ – waarbij de quarks weggelaten worden. Maar de toegenomen precisie van en hogere eisen aan de resultaten van simulaties hebben recentelijk geleid tot de noodzaak van de introductie van zogenaamd ‘dynamische quarks’: quarks die volledig meetellen in de berekening. Het in dit proefschrift beschreven onderzoek kijkt naar het gedrag van simulaties van de sterke interactie wanneer meer en meer quarks meegenomen worden.

In hoofdstuk 1 wordt een samenvatting gegeven van de punten waarop de genoemde quenched approximation te kort schiet en de redenen voor de introductie van dynamische quarks. Ook wordt een overzicht gegeven van de recente litera-
tuur op het gebied van de invloed van meerdere quark flavours op simulaties van de sterke kernkracht. Hierbij wordt niet alleen gekeken naar het effect van de introductie van de quarks die we kennen uit het SM, maar ook naar de vorm van de theorie bij introductie van veel grotere aantallen flavours: tot zestien quark flavours of zelfs meer. Quarks in zulke grote hoeveelheden kunnen interfereren met het waternul effect van de gluonen dat ze normaal gesproken gevangen weet te houden. De hamvraag is hier wat er gebeurt met de sterke interactie wanneer er nog net niet genoeg quarks zijn om te ontsnappen, maar al teveel voor de gluonen om ze echt vast te kunnen houden. Met behulp van verschillende, soms zeer ingenieuze, analytische benaderingen zijn hier de afgelopen jaren een grote hoeveelheid voorspellingen over gedaan, maar alleen numerieke simulaties, zoals de berekeningen beschreven in dit proefschrift, kunnen achterhalen of de gebruikte benaderingen uiteindelijk hout snijden.

De resultaten beschreven in hoofdstuk 2 zijn onderdeel van een langlopend project van een samenwerkingsverband dat bekend staat als de European Twisted Mass Collaboration (ETMC). Dit initiatief verenigt een grote groep wetenschappers, werkzaam aan verschillende Europese universiteiten, die gezamenlijk grote (en kostbare) simulaties uitvoert. Tot zeer recent werkte het ETMC met simulaties waarin slechts de twee meest relevantelijke van de zes quarks in het SM (up en down) waren inbegrepen. Om te kunnen komen tot de bepaling van enkele bijzonder gevoelige waarden – en om de algemene betrouwbaarheid van resultaten te verhogen – probeert zij nu echter het aantal dynamische flavours te verhogen tot vier: up, down, strange en charm. Dit hoofdstuk is gebaseerd op een publicatie waarin wordt gedemonstreerd dat simulaties gedaan na het technisch gecompliceerde proces van het toevoegen van twee extra flavours resultaten produceren die consistent zijn met eerder behaalde resultaten. In het bijzonder laten de gegevens zien dat enkele bekende fysische wetmatigheden rond de massa’s van de verschillende quarks, die ook zeer belangrijk zijn voor de interpretatie van simulaties, precies gereproduceerd worden.

Hoofdstuk 3 gaat voorbij aan het SM zelf en begint te kijken naar het effect van het toevoegen van grote hoeveelheden quarks. Hier wordt specifiek gekeken naar het effect van acht flavours, waarover in de literatuur verwarring was ontstaan. In de jaren zeventig en tachtig was gespeculeerd dat in theorieën met specifieke aantallen quarks een dynamisch evenwicht zou kunnen ontstaan tussen de aantrekkende kracht van gluonen en het uitdijende effect van de quarks. In zo’n situatie zou de aantrekkingskracht tussen twee quarks altijd even groot zijn, onafhankelijk van de afstand. En omdat voor een elementair deeltje afstanden alleen gemeten kunnen worden in termen van de interacties met andere deeltjes, zou dat betekenen dat voor hen het hele concept van afstand eigenlijk niet meer zou bestaan. Een wereld die er op alle afstanden hetzelfde uitziet is symmetrisch op een bijzondere manier, die ‘conformeel’ wordt genoemd. Een eigenschap van zo’n wereld is dat ook een temperatuur niet meer goed gedefinieerd kan worden. Enkele vroege simulaties van dergelijke systemen met acht flavours hadden, zeer onverwacht, indicaties gegeven van de aanwezigheid van conforme symmetrie. In dit hoofdstuk worden echter resultaten gepresenteerd, die aantonen dat de theorie een fase overgang heeft bij een specifieke temperatuur, analoog aan het bevriezen van water bij nul graden Celsius.
Dat impliceert dat de quarks en gluonen wel degelijk weet hebben van het bestaan van zoiets als een temperatuur, zodat de theorie niet conformeel symmetrisch kan zijn.

In het daaropvolgende hoofdstuk 4 wordt gekeken naar simulaties met nog meer flavours, namelijk twaalf. De aanwijzingen voor het bestaan van conformele symmetrie zijn hier sterker, zowel vanaf de kant van analytische benaderingen als die van eerdere simulaties. De temperatuur afhankelijke fase overgang die eerder werd gevonden voor acht flavours bleek hier dan ook niet te vinden. Maar het daadwerkelijk aantonen van de afwezigheid van een afstandsschaal is nog niet eenvoudig. Het fundamentele probleem is het noodzakelijk introduceren van allerlei afstandsschalen tijdens de simulatie zelf. Zo kan er alleen gerekend worden aan een theorie in een afgebakend gebied, waardoor er een effectieve grootste afstand wordt geïntroduceerd. Daarnaast wordt in principe uitgegaan van quarks die zelf geen massa hebben, omdat ook een massa gebruikt kan worden om afstanden te simuleren. Binnen een computersimulatie is het echter onmogelijk om exact massaloze quarks te introduceren, zodat er in de praktijk met een zo klein mogelijke massa wordt gewerkt. Maar als er geen andere schalen zijn om de massa mee te vergelijken, is het ook niet mogelijk om te zeggen dat deze klein genoeg is. Om desalniettemin conclusies te kunnen trekken over de eigenschappen van de sterke interactie met twaalf quarks, is het nodig om het gedrag van de theorie onder kleine veranderingen in deze kunstmatige schalen te bepalen. De kennis van dat gedrag kan dan gebruikt worden om te extrapoleren naar de theorie die we daadwerkelijk willen bestuderen. Dit hoofdstuk maakt in een reeks van dergelijke extrapolaties aannemelijk dat de theorie met twaalf flavours inderdaad een conforme symmetrie kent.

Natuurlijk is het vinden van conformele symmetrie nog maar het begin. Zo zou het bijzonder interessant zijn om te zien waar de evenwichtstoestand precies ligt en hoe deze bereikt wordt. Met deze gegevens kan geprobeerd worden te bepalen hoeveel flavours er minimaal nodig zijn om conformele symmetrie te laten ontstaan. Daarom gaat hoofdstuk 5 in op manieren waarop deze eigenaardige toestand verder kan worden bestudeerd. De problemen die reeds beschreven werden in hoofdstuk 4 maken het nauwkeurig bepalen van eigenschappen geen sinecure. In dit hoofdstuk wordt daarom gekeken naar de manieren waarop aansluiting gevonden kan worden met alternatieve, analytische benaderingen. De resultaten zijn slechts ten dele positief. Zo blijkt het nog niet mogelijk om een verbinding te maken met de goed begrepen ‘storingstheorie’, die de interacties beschrijft als een serie correcties op een achtergrond van deeltjes die zich vrij kunnen bewegen. Deze beschrijving werkt goed – dat wil zeggen, er zijn slechts een klein aantal correcties nodig om een nauwkeurig antwoord te vinden – wanneer de koppeling tussen quarks en gluonen en gluonen onderling erg losjes is. De gesimuleerde koppeling blijkt echter nog te sterk te zijn. De vorm van de fase overgang, die in het algemeen afhangt van specifieke eigenschappen van het systeem, blijkt op opvallende wijze afhankelijk te zijn van de ingevoerde massa van de quarks. Dit is geheel consistent met de conclusies getrokken in hoofdstuk 4, maar bemoeilijkt de interpretatie van de fase overgang zelf. Een directe studie van de interactie tussen twee quarks als functie van de afstand blijkt voldoen aan de verwachtingen en geeft aanvullend bewijs voor het bestaan van een
exacte conformele symmetrie na extrapolatie.

Samenvattend wil dit proefschrift een kleine bijdrage geven aan het inzicht in de manier waarop de introductie van quarks het karakter van de sterke kernkracht wezenlijk kan veranderen. In een serie studies met toenemende aantallen quarks is aannemelijk gemaakt dat de introductie van flavours zoals die voorkomen in het Standaard Model leidt tot een consistente beschrijving van de fysische werkelijkheid. Voor grotere aantallen lichte flavours wordt bewijs gepresenteerd dat er een dynamisch evenwicht kan ontstaan tussen quarks en gluonen, van waaruit zich een interessant systeem met een uitzonderlijk hoge mate van symmetrie ontwikkelt. De studie van zo’n systeem met behulp van computersimulaties blijkt goed mogelijk, al blijft de interpretatie van de uitkomsten een technische uitdaging.
For the observables studied in this chapter, the functional dependence on the coupling is an important result. Unfortunately, scanning such a dependency by means of lattice simulations is in general an expensive affair. Each data point represents a separate run, requiring CPU time to both thermalise and gather statistics. Frankly, it would appear rather wasteful to expend these resources for the benefit of obtaining a single average. In addition, the limited prior information on the required resolution in the coupling can make this method time consuming.

This observation led Ferrenberg and Swendsen to propose a reanalysis technique on the partition function [347], now often referred to as Ferrenberg-Swendsen reweighting (FSR). As detailed in chapter 1, the Markov chain, by imposing detailed balance, produces configurations according to the Boltzmann distribution. A stochastic estimation of the thermodynamically weighted observables is then produced by the unweighted average over the measurements on the configurations. This distribution will be peaked around the values of the action appropriate to the parameters at which the simulation was run, but the produced configurations will have a non-vanishing probability of appearing within a small region around the original values in parameter space. From the distribution of the action, the shifts in the Boltzmann weight as a consequence of a small change in parameters can be calculated, providing the relative weights by which the given configurations would appear in a simulation at those new parameters.

In their original article, Ferrenberg and Swendsen propose it as a method for obtaining a smooth line of measurements passing through a phase transitions, the feasibility of which is demonstrated by means of simulations of two dimensional Ising and Potts models. The crucial difference between those models, each with a large but finite number of potential states, and full SU(3) lattice QCD, however, is the
sheer size of the phase space under consideration. This implies the spacing between subsequent values of the parameters that still allow for substantial overlap between the produced samples of phase space, a necessary condition for fully determining the expected value of the observations between the input parameters, will be far more restricted. In fact, this problem becomes larger as the volume of the simulation increases, as the obviously extensive nature of action reflects the associated increase of the phase space.

But even for those cases where overlap exists, concerns about the validity of the results remain. First of all, ergodicity remains a lingering issue. Unlike the case of a direct Monte Carlo integration, to which FSR could be compared otherwise, the Markov chain procedure can introduce a strong bias on the stochastic input to the integrand. Unless the space phase happens to have a very trivial structure at the point towards which one is reweighting – in which case the interest in doing FSR would be limited anyway – one is likely to sample only a small subset of the thermodynamically relevant regions in it by using only configurations compatible with parameters some distance to one side of the current one and from a strongly correlated source. This effect can be suppressed somewhat by simulating close to the desired parameters and accumulating a large amount of statistics, but this would largely defeat the purpose of introducing FSR in the first place. A second issue comes into play once the action used requires tuning. To obtain the correct results of macroscopic changes in the parameters, one would now have to trace the physical curve. This one would probably have to approximate linearly, introducing an additional source of systematic errors.

It might seem then that FSR can contribute little to the analysis of a data set the scale of those considered in this chapter. However, even with the limited range over which the FSR procedure is valid, it can produce valuable additional information. The original consideration of extracting additional information present in the ensemble distribution of the observable is valid, and it is important to realize this is in fact extra information that is lost when only a statistical reduction of the distribution is taken into consideration. Specifically, knowledge of the change in the observable as a function of a single parameter can be used to obtain partial derivatives. For a crude implementation, this could be done according to

\[
\langle \partial_{x_i} O[x] \rangle = \frac{O[x + \delta x_i] - O[x - \delta x_i]}{2\delta x_i} = \frac{\langle O[x] \rangle_S(\delta x_i) + \langle O[x] \rangle_S(-\delta x_i)}{2\delta x_i},
\]

(A.1)

where \( \langle O[x] \rangle \) denotes the ensemble average for the observable \( O \) as a function of the parameter set \( x \), \( \delta x_i \) represents a small variation in the \( i \)th parameter of such a set and
the notation

\[ \langle O[x] \rangle_{S(\delta x_i)} = \frac{\sum_n \exp \left[ - (S(x + \delta x_i, G_n) - S(x, G_n)) \right] O_n}{\sum_n \exp \left[ - (S(x + \delta x_i, G_n) - S(x, G_n)) \right]} \]

\[ \equiv \frac{\sum_n \left( W_n^{\delta x_i} O_n \right)}{W^{\delta x_i}} \]  (A.2)

was introduced for the ensemble average reweighted towards the shifted parameter set \( x + \delta x_i \), labelling the configurations in the ensemble by the index \( n \). Here the scalar value of the action \( S \) is written to stress its dependence on both the parameter set \( x \) and the generated gauge configuration \( G_n \). The reweighting factor for the \( n \)th configuration in the ensemble is denoted by \( W_n^{\delta x_i} \), while \( W^{\delta x_i} \) is introduced as a convenient shorthand notation for the sum over all weighting factors.

Whether the simple form of equation A.1 suffices depends mainly on the computational complexity of calculating the induced change in the action by a small shift in the parameter \( \delta x_i \). If one attempts to reweight in one of the quark masses, inversions of the Dirac matrix will be required for each of the masses, though one may gain some efficiency by using multi-mass inverters. A straightforward symmetric difference approximation to the partial derivative may then be satisfactory, especially given the existence of an inverse proportionality between the size of \( \delta x_i \) and the statistical accuracy of the reweighted observable \( \langle O[x] \rangle_{S(\delta x_i)} \) that stems from the roughly exponential decay in the number of significant observations \( O_n \). Because of this, smaller shifts that produce numerically and statistically appreciable change between \( \langle O[x] \rangle \) and \( \langle O[x] \rangle_{S(\delta x_i)} \) will tend to give more accurate end results. And as there is no pressing reason to push for large values of \( \delta x_i \), the error of \( O \left( \delta x_i^2 \right) \) can be kept under control.

If, on the other hand, the dependence of the action on a parameter is particularly straightforward, one may choose to extend upon the approximation of equation A.1 in order to more fully exploit the available data. Such a relatively simple dependence is found for the Symanzik improved action used in these simulations for the coupling. Recapitulating from earlier chapters, this action has the form

\[ S_{\text{gauge}} = \sum_{i=p,r} \beta_i (g^2) \sum_{C \in S_i} \text{Re}(1 - U(C)), \]

where the couplings for this particular case, without tadpole improvement factor \( u_0 \), was given by

\[ \beta_p = 10 / g_0^2, \]

\[ \beta_r = -\frac{\beta}{20}. \]  (A.3)

While the particular combination of generalized plaquette factors and multiplicities that make up the gauge contribution to the action are themselves not trivial, the de-
dependence on the coupling constant $\beta$ as an external parameter is through an overall multiplication. Because of this, the gauge component of the action can be extracted a single scalar factor for each configuration and a straightforward weighting function constructed from these. Since now the whole FSR procedure can be executed at the level of the measured averages per configuration, making it computationally fairly trivial, there is no need to restrict the number of reweighted measurements extracted. One could decide to move towards successively more accurate finite difference approximations to the derivative operator, but a different approach may be more efficient at this point.

First of all, boundaries can be set beyond which no further reweighting is done. These will always be slightly arbitrary, but should take into account the fact that at some finite distance from the original parameters, a single configuration will dominate the reweighted ensemble completely and the sampling will be exceedingly poor. A good quantifier of the ensemble size is given by the factor $W_{\delta x_i}$ as defined in equation A.2. If the maximum weight is normalized to one, the integration over the weighting factors $W_{\delta x_i}$ will produce the effective number of observations for the reweighted quantity. In order not to pollute the set of FSR samples, we set these to a particular minimum fraction of the original number of observations, usually 0.5. This generated two bounds $\beta_{\text{RW}}^{\text{min}}$ and $\beta_{\text{RW}}^{\text{max}}$, not necessarily symmetric, for the reweighting interval. Within this range, a certain number of reweighted ensembles were produced at regular intervals. Again, the sampling rate here was rather arbitrary, but in general 40 samples were generated.

In order to determine the moments of the distribution, a Taylor expansion was introduced for the observable around the original value of the coupling constant $\beta_0$ as

$$O[x, \beta] = O[x, \beta_0] + \frac{\partial O[x, \beta]}{\partial \beta} (\beta - \beta_0) + \frac{\partial^2 O[x, \beta]}{2 \partial \beta^2} (\beta - \beta_0)^2 + \ldots$$  \hspace{1cm} (A.4)

After performing a linear fit in the parameter $\beta - \beta_0$, the coefficients allow for an immediate determination of the partial derivative to any order. Obviously, the reliability of the determination will decrease rapidly if too many terms are fit to a small region of $\beta$. The stability of each of the coefficients under inclusion of additional terms should therefore be carefully checked. In addition, the strong correlation between the different reweighted ensembles can potentially lead to a severe underestimation of the errors. To counter this effect, one could perform a bootstrap analysis using independent samples for each point. As long as $W_{\delta x_i}$ is sufficiently large, the FSR will act to magnify the differences between the different samplings, thereby increasing the variability of fits to subsequent bootstrap samples and giving a better estimate of the uncertainties involved.
The time spent obtaining a Ph.D. is very intense and exciting and it certainly was so in my case. Eventual success is strongly dependent on the support of the people around you and I was fortunate enough to receive a lot of it. In this section of my dissertation, I want to express my gratitude towards a number of people in particular.

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1 Wejście do Polskiej rodziny mojej żony okazało się być wspaniałym doświadczeniem. Szczególnie pragnę podziękować rodzinom Asi, Ewie i Benkowi za serdeczność i goscinnośc dzieki, której miałem okazję poznać wiele polskich tradycji, a także za troskę i pomoc w trudnych chwilach. Adasiowi za okazywane zainteresowanie oraz pomocną dłoń, na którą zawsze można liczyć. Również serdecznie dziękuję, Jadwidge i Pawelowi za życliwość oraz sympatię z jaką się u nich nieustannie spotykam. Paulina, Przemek, Kasia oraz Piotr, chwile razem spędzone na wycieczkach, przy świątecznym stole oraz rozmowach zachowały się jako bardzo miłe wpomnienia w mojej pamięci.
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List of publications

- Albert Deuzeman, Maria Paola Lombardo and Elisabetta Pallante
  *The physics of eight flavours*

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