Introduction

The notion of local gauge symmetries as introduced in 1929 by Weyl [1] turned out to be a cornerstone of modern field theory since so-called gauge theories describe fundamental interactions very successfully. The prototype of a gauge theory is quantum electrodynamics (QED), which describes nature with a so far unknown precision. An impressive example is the anomalous magnetic moment of the muon g_μ, where the experimental results deviate from the theoretical prediction for $a_\mu \equiv (g_\mu - 2)/2$ at the order of 10^{-9} by maximally 2 σ [2]. Our present understanding is that all fundamental interactions, strong interaction, electromagnetic interaction, weak interaction and gravitational interaction, are described by some form of a gauge theory.

Quantum chromodynamics (QCD), the theory of strong interactions, is based on a non-Abelian SU(3) gauge symmetry. The property of QCD that led directly to its discovery in 1973 [3, 4, 5] as a candidate theory of the strong interaction is asymptotic freedom [3, 6, 7, 8, 9], i.e. the coupling strength decreases at short distances and the quarks and gluons behave as effectively free particles. In turn, the coupling increases with the distance and at a distance of about 1 fm it assumes such large values that only bound states of quarks and gluons exits. The latter property, which is called confinement, together with asymptotic freedom imply that perturbative methods are applicable in QCD only at short distances, whereas they fail at large distances (low energies). Confinement, spontaneous breaking of chiral symmetry or the hadron mass spectrum are low-energy properties that can therefore not be described by perturbation theory and require a non-perturbative treatment of the theory.

With the framework of *lattice gauge theories* Wilson developed a non-perturbative tool to investigate the low-energy structure of QCD [10]. In this framework he was able to compute the non-relativistic quark/anti-quark potential in the static approximation showing that it increases linearly with the distance [10, 11]. Wilson proposed to regularize QCD with a discrete Euclidean space-time lattice with the inverse lattice spacing a^{-1} playing the rôle of an ultraviolet momentum cut-off. Then, in the course of renormalization the continuum is recovered by removing the cut-off, i.e. sending $a \to 0$. This approach can also be understood as replacing the continuum gauge theory by a discrete statistical mechanical system, an analogy that opens up the possibility to simulate QCD on computers by means of Monte Carlo methods. This framework facilitates investigations of low-energy properties of QCD from first principles with the quark masses as freely tunable parameters.

Unfortunately such computer simulations are only possible with an immense amount of computer resources. For this reason most of the current results have been obtained only in the so-called *quenched approximation*, where vacuum polarization effects of quark loops are neglected. However, even in this approximation simulations with small enough values of the quark masses are not affordable necessitating – besides the continuum extrapolation of physical quantities – an additional extrapolation in the masses to the point where the masses take their physical values. If the simulations can reach masses where chiral perturbation theory (χPT) is valid, then this last step of the extrapolation can be performed using the analytical results derived in χPT.

In QCD exist six flavors of quarks, whose (bare) quark masses are parameters that need to be tuned. But, aiming at investigations of the low energy structure of QCD, charm, bottom and top quarks can be considered as static to a good approximation due to their large mass values. Moreover, the two lightest quarks (up and down) are – when compared to the characteristic scale of QCD – to a good approximation mass degenerate. Hence, the targets of lattice QCD are simulations with a light doublet of mass degenerate quarks and one heavier quark, the strange quark.

While for the extrapolation in the quark mass χPT can be of essential help, the continuum extrapolation can only be performed by using small values of the lattice spacing a, such that one is close enough to the continuum limit. However, the computational costs increase approximately proportional to a^{-7} making it often infeasible to work at small enough lattice spacing. The way out is the fact that lattice QCD formulations are not unique and fortunately a formulation with genuine small lattice artifacts can be constructed by means of an effective field theory as worked out by Symanzik [12, 13, 14]. In this concept the lattice theory at finite values of a is mapped to an effective continuum theory. Lattice expectation values are then given by the corresponding continuum value plus correction terms proportional to powers of the lattice spacing. The *Symanzik improvement programme* then means to construct a discretization where at least the largest of those terms are absent. The simplest case in this approach is the $\mathcal{O}(a)$ improvement, where all terms linear in a vanish. However, lattice artifacts proportional to higher powers of a might still be large. This, together with the question for which values of a the effective theory is valid, is one of the crucial questions in lattice QCD and needs to be investigated through a detailed analysis of the scaling behavior in a of physical quantities.

All this illustrates the need for progress on the following topics:

- Formulations of lattice QCD with reduced lattice discretization errors are essential in order to control the continuum extrapolation reliably. Those formulations are available, but they need a test in practice, which concerns the size of residual lattice artifacts on physical observables. In addition, it is necessary to investigate how a lattice theory as such differs from its continuum counter part.

- A lattice QCD formulation should allow for simulations at small enough quark masses with affordable computational effort in order to make at least contact to chiral perturbation theory possible. Ideally, it would be desirable, of course, to work directly at the physical point. Moreover, simulations with two light mass degenerate quarks (up and down quark) and one heavier quark (strange quark) should be possible.

- Improvement and development of new algorithms is needed to reach small enough quark masses and small enough lattice spacings at possibly lower computational effort.

Motivated by these demands, we consider in this work the so-called *Wilson twisted mass* formulation of lattice QCD, which is expected to satisfy the requirements formulated above by the first two items. We present a detailed scaling test of this formulation in the quenched approximation and show that in fact lattice artifacts linear in a are absent and residual lattice artifacts are small (see chapter 2).

Then, in chapter 3, we introduce an algorithm for simulations of full QCD with scaling properties towards small quark masses that are significantly better than those of other presently used algorithms. This improvement is illustrated by comparing it to other state-of-the-art algorithms available in the literature.

In chapter 4 we finally present a study of the phase structure of lattice QCD with two flavors of Wilson twisted mass fermions and several discretizations of the gauge part in the action. This investigation is an essential preparatory work for any future large scale simulation and reveals evidence for the existence of a first order phase transition. A comprehensive understanding of the phase structure was missing so far, and became only possible with the Wilson twisted mass formulation of lattice QCD.