Summary and Outlook

In the year 2003 an intriguing paper was published: Frezzotti and Rossi realized that with the Wilson twisted mass formulation of lattice QCD at maximal twist $\mathcal{O}(a)$ improvement can be obtained without the need of additional improvement coefficients [42], which need to be computed non-perturbatively in the standard Symanzik improvement programme. Of course, such a theoretical proposition needs a check in practice and hence we performed a scaling test of maximally twisted mass QCD (mtmQCD), in the quenched approximation as a start. The results can be found in chapter 2 and the most important findings are the following:

- thanks to the twisted mass term playing the rôle of an infrared cut-off for the Dirac operator eigenvalue spectrum, it is possible to simulate pseudo scalar masses as low as 270 MeV without having problems with exceptional configurations.
- physical observables determined with mtmQCD show no $\mathcal{O}(a)$ lattice artifacts. With the PCAC definition of κ_{crit} also higher order lattice artifacts are small, even with scalar mass values as small as 270 MeV. (cf. figure 2.3 on page 43, figure 2.6 on page 46 and figure 2.7 on page 47)
- the effects of the explicit flavor symmetry breaking in mtmQCD are sizable when the charged/neutral pseudo scalar mass splitting is considered. Nevertheless, the splitting is a lattice artifact and we could show that it vanishes proportional to a^2, see figure 2.8 on page 49.
- while simulations with pseudo scalar mass values below 300 MeV are also possible with overlap fermions, a comparison of computational costs revealed that simulations with twisted mass fermions are a factor of 20 to 70 faster than simulations with overlap fermions.

Aiming at large scale simulations in full lattice QCD we developed – in addition to the investigation of mtmQCD as the potential formulation – a new variant of the Hybrid Monte Carlo algorithm in order to make full QCD simulations with light quark masses affordable. The new variant, a HMC with a combination of mass preconditioning and multiple time scale integration as presented in chapter 3, is based on the idea to precondition the fermion determinant in such a way that the most expensive part contributes the least to the total molecular dynamics force and can be therefore integrated on the largest time scale. It is applicable to a wide variety of lattice Dirac operators and moreover straightforward to implement.

Our simulations clearly show that with this new HMC variant (full dynamical) simulations with Wilson type fermions and realistic quark masses are possible with reasonable computational effort. This we could illustrate in an update of the so called "Berlin Wall" figure [105, 113]. With our HMC variant the "Wall" is shifted definitely towards smaller values of $m_{\mathrm{PS}}/m_{\mathrm{V}}$, see figure 3.4 on page 77.

Taking the results of these two chapters together, we have now a sound basis for performing large scale simulations with light quark masses. However, our first investigations in full lattice QCD revealed a surprising result: we have shown in chapter 4 that close enough to the continuum the phase structure of lattice QCD with Wilson type fermions and the Wilson plaquette gauge action exhibits the expected continuum phase structure distorted by lattice artifacts. Our investigation yielded that in a range of lattice spacings between 0.2 and 0.13 fm there exists a first order phase transition at the chiral point. This phase transition is characterized by a jump in the plaquette expectation value, the existence of meta-stabilities and most importantly by the fact that the minimal value of the charged pseudo scalar mass is significantly larger than zero. For the investigated lattice spacing the latter value lies well above 450 MeV.

This phenomenon finds its natural interpretation in terms of an effective potential model depicted in lattice chiral perturbation theory, where a first order phase transition is predicted as one of two possible scenarios emerging due to $\mathcal{O}(a^2)$ lattice artifacts. We stress here that the first order phase transition is a generic property of Wilson type fermions and it is not restricted to only the twisted mass formulation, which was mainly used for the simulations. The phase structure is summarized schematically in figure 4.8 on page 97.

This result on the one hand makes clear that indeed the knowledge of the phase structure is an essential pre-requisite before starting large scale simulations that was missing so far. On the other hand, the rather large minimal value of the charged pseudo scalar mass does not allow for simulations with realistic quark masses at affordable lattice spacings with mtmQCD and the Wilson plaquette gauge action. However, the size of the lattice artifacts and hence the size of for instance the minimal value of the pseudo scalar mass is certainly depending on the discretization of the gauge action. There were already hints for this in the literature and we could confirm that by adding a rectangular part to the Wilson plaquette gauge action the effects of the phase transition can be reduced when compared to the Wilson plaquette gauge action at equal lattice spacing. This means that for example with the DBW2 or the tree level improved Symanzik gauge action the minimal pseudo scalar mass value is significantly reduced and we are optimistic that at lattice spacings of about 0.15 fm dynamical simulations can be performed without being affected by the first order phase transition.

Recapitulating, we think the results of this work exhibit a sound basis for future large scale dynamical simulations with realistic masses and small enough lattice spacing. Of course, the next natural step is to repeat a scaling test for twisted mass QCD with $n_f = 2$ dynamical flavors of quarks, as we presented it in chapter 2 for the quenched approximation. In such a scaling test already some interesting continuum extrapolations should become possible. Then, in case of a positive outcome, we will proceed to $n_f = 2 + 1 + 1$ dynamical quark flavors, with up- and down-quark mass degenerate and strange- and charm-quark with different, non-degenerate masses. At the latest in these simulations such interesting items like ρ-decay, string breaking, π phase shift, or η and η' meson masses will be addressed.