

A lattice approach to QCD in the chiral regime

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ABSTRACT: Non-perturbative lattice studies of QCD in the chiral thermodynamic regime, where chiral symmetry is spontaneously broken, require to deal with almost quark zero modes in a theoretically clean and computationally efficient way. We discuss the basic features and some realistic tests of a formulation, known as lattice tmQCD, that fulfills these requirements.

1. INTRODUCTION

Lattice field theory is known to provide a rigorous and systematically improvable way of studying QCD in the non-perturbative regime by means of Monte Carlo simulations. As in any numerical method, the coexistence of widely separated energy scales poses severe practical problems: for instance, the energy-momentum resolution a^{-1} , which is induced by the lattice regularization, should be kept much larger than both the typical hadron mass scale, say ~ 500 MeV, and the external momenta of the correlation functions that are computed. Moreover, the approximate and spontaneously broken flavour chiral symmetry that is exhibited by the strong interactions entails the need of performing at least a few simulations of lattice QCD in large volume and with small quark masses¹: a fully realistic setup would require a lattice of spatial volume L^3 , with $M_\pi L \geq 5$ and $M_\pi \sim 140$ MeV.

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¹This task is significantly alleviated by studying the renormalization problems in finite volume by means of renormalization group and finite-size scaling techniques, e.g. in the Schrödinger functional scheme.

The relevance of the approximate chiral symmetry for the low energy QCD amplitudes can hardly be overestimated: it determines many aspects of the dynamics, as shown by the chiral effective Lagrangian approach, and strongly constrains the operator mixings, which on the lattice may be particularly severe due to the dimensionful ultraviolet cutoff a^{-1} . The realization of the chiral symmetry on the lattice is known to be delicate since the pioneering work by Wilson [1] and in most cases the full flavour chiral symmetry is recovered only in the continuum limit. The highly remarkable exception is represented by those lattice formulations where the Dirac operator satisfies the Ginsparg-Wilson relation [2], which in turn entails an exact flavour chiral invariance at finite lattice spacing. The lattice regularizations with Ginsparg-Wilson quarks certainly simplify a lot the construction of renormalized operators, especially those relevant for the weak effective Hamiltonian, at the price however of a big overhead in the computational effort. In many cases one can avoid such an overhead by working within the framework of Wilson quarks, which seems to be more flexible and powerful than believed till few years ago, as we try to argue in the following. In general, the lattice regularization of the quark sector should be chosen with care depending on the physical applications and the related renormalization problems.

In this contribution we focus on a lattice formulation of QCD, based on Wilson quarks and known as twisted mass QCD (tmQCD), that is particularly suited for dealing with the u and d quarks. After discussing in Section 2 how the simulations of lattice QCD account for the contribution of quark zero modes, we illustrate in Section 3 the basic features of lattice tmQCD. In Section 4 we briefly report on an exploratory non-perturbative study of $O(a)$ improved lattice tmQCD, which reaches a pseudoscalar to vector meson mass ratio of $M_{PS}/M_V \simeq 0.47(1)$ and represents a successful test of several aspects of our approach.

2. Lattice QCD and physical quark zero modes

We assume that the reader is familiar with the lattice regularization of QCD introduced by Wilson [1] and for simplicity we consider the theory with two mass-degenerate quark flavours. In this case the lattice action with Wilson quarks reads

$$S = S_g[U; g_0^2] + a^4 \sum_x \bar{\chi}(x) \left[\left(\frac{1}{2} \gamma \cdot (\nabla + \nabla^*) - a \frac{1}{2} \nabla^* \cdot \nabla + m'_0 \right) \chi \right] (x), \quad (2.1)$$

where S_g is the pure gauge action, χ denotes the doublet of quark fields and $v \cdot w \equiv v_\mu w_\mu$, while $\nabla_\mu = \nabla_\mu[U]$ and $\nabla_\mu^* = \nabla_\mu^*[U]$ stand for the forward and backward covariant derivatives on the lattice. The hard breaking of the flavour non-singlet axial generators induced by the Wilson term can be compensated up to $O(a)$ effects by tuning the parameter m'_0 and the coefficients that parameterize any chirality-violating operator mixings [3]. The leading cutoff effects can be removed via the on-shell $O(a)$ improvement [4] à la Symanzik.

2.1 Valence and sea quarks

In any correlation function to be evaluated via Monte Carlo simulations, due to the huge dimensionality of the vector space spanned by the Grassmann variables in the Euclidean

path integral, it is customary to integrate out analytically the fermionic degrees of freedom. In the case of the correlator of two local pseudoscalar densities with isospin index $a = 1$,

$$C_{\text{PS}}^{11}(x-y) \equiv -\langle P^1(x)P^1(y) \rangle = -\mathcal{Z}^{-1} \int dU d\chi d\bar{\chi} \exp(-S) [\bar{\chi}\gamma_5 \frac{\tau^1}{2}\chi](x) [\bar{\chi}\gamma_5 \frac{\tau^1}{2}\chi](y), \quad (2.2)$$

this procedure yields

$$C_{\text{PS}}^{11}(x-y) = \int dU P[U; g_0^2, m'_q] \text{tr} \left\{ [D_{\text{W},c} + m'_q]^{-1}(x, y) \gamma_5 \frac{\tau^1}{2} [D_{\text{W},c} + m'_q]^{-1}(y, x) \gamma_5 \frac{\tau^1}{2} \right\} \\ P[U; g_0^2, m'_q] = \mathcal{Z}^{-1} \exp(-S_g[U, g_0^2]) \det(\{D_{\text{W},c} + m'_q\}[U]) \geq 0, \quad (2.3)$$

where² \mathcal{Z} denotes the Euclidean partition function and $D_{\text{W},c} = D_{\text{W},c}[U]$ is the critical (two-flavour) Wilson-Dirac operator:

$$D_{\text{W},c} = \frac{1}{2}\gamma \cdot (\nabla + \nabla^*) - \frac{a}{2}\nabla^* \cdot \nabla + m_c. \quad (2.4)$$

The parameter $m'_q = m'_0 - m_c$ is hence proportional to the renormalized quark mass that appears in the PCAC Ward identity: the massless theory is obtained for $m'_0 = m_c(g_0^2)$. Gauge configurations U are generated via suitable algorithms with probability $P[U; g_0^2, m'_q]$, and on each configuration U the quark propagator from the lattice site x to the site y , $[D_{\text{W},c} + m'_q]^{-1}(y, x)$, can be computed –for fixed x – by solving a linear system. By expanding the correlator (2.2) around the trivial perturbative vacuum, one can easily check that in eq. (2.3) the trace term involving quark propagators corresponds to valence quark diagrams dressed with any kind of purely gluonic corrections, whereas the term $\det(D_{\text{W},c} + m'_q)$ accounts for the sea quark corrections to the aforementioned dressed valence quark diagrams.

2.2 Quenched and partially quenched lattice QCD

It is well-known that with the established simulation techniques the simulation of the full theory, including the sea quark effects, has a very high computational cost, which quickly increases as the pion mass is decreased towards realistic values. On the other hand, it is technically trivial to choose different values for the parameter m'_q that appears in the fermionic determinant and its counterpart in the inverse Dirac operator: $m'_{q,\text{sea}} \neq m'_{q,\text{val}}$. A moment of thought reveals that such a modification of lattice QCD corresponds to a statistical model with extra spin-1/2 ghost fields, which is local and renormalizable by power counting but violates reflection positivity (see e.g. Ref. [5]). The general case $m'_{q,\text{val}} \neq m'_{q,\text{sea}}$ is referred to as partially quenched QCD, whereas the particular case $|m'_{q,\text{val}}| < |m'_{q,\text{sea}}| = \infty$ corresponds to the well-known quenched approximation.

It should be noted that these approximations in general break down as the valence quark mass $m'_{q,\text{val}} \rightarrow 0$ in the thermodynamic limit. In this regime the flavour chiral symmetry is spontaneously broken: if the chiral condensate is to be non-vanishing, the gauge configurations carrying zero modes of the Dirac operator must receive a finite weight in the Euclidean path integral, even in the limit (taken at infinite spatial volume) $m'_{q,\text{sea}} =$

²The symbol $\text{tr}\{\dots\}$ denotes the trace over flavour, colour and spin indices, whereas the symbol $\det\{\dots\}$ stands for the determinant with respect to all indices, including the space-time ones.

$m'_{q,\text{val}} \rightarrow 0$ [6]. It is clear that in the full theory the integration over the fermionic variables on any gauge background can not yield divergences: in presence of quark zero modes the infinities in the quark propagators must be compensated by the zeros in the fermion determinant, see eq. (2.3). Such a delicate compensation is no longer guaranteed if the condition $m'_{q,\text{sea}} = m'_{q,\text{val}}$ is violated: fermionic observables may hence diverge on gauge configurations carrying quark zero modes, which causes the breakdown of the quenched and partially quenched approximations.

However, when working sufficiently away from the thermodynamic chiral limit, the quenched –or partially quenched– approximation is expected to be reasonably accurate, at least for those quantities that are not very sensitive to sea quark effects. An example is given by the ratios of hadron masses [7], with the η' -meson mass being the most striking exception. Indeed, given the high computational cost of simulating the full theory, the quenched approximation has been widely used as a testbed for lattice techniques and for first non-perturbative estimates of quantities such as renormalized couplings, hadron masses and matrix elements, order parameters of phase transitions. The chiral effective Lagrangian for quenched QCD has also been worked out [5] with the aim of identifying and parameterising the deviations from the full theory close to the chiral limit.

Analogous remarks apply for the partially quenched approximation, the quality of which depends on the ratio $m'_{q,\text{sea}}/m'_{q,\text{val}}$. In particular, it has been remarked that the low-energy (Gasser-Leutwyler) constants of partially quenched QCD with N_f quark flavours coincide with those of the fully unquenched theory, provided that all the quark flavours are light enough for the chiral perturbation theory to be applicable [8]. In the physically relevant cases, which are $N_f = 3$ and –to some extent– $N_f = 2$, varying $m'_{q,\text{val}}$ while keeping fixed $m'_{q,\text{sea}}$ can then be very convenient, since it allows to investigate the dependence of the observables on $m'_{q,\text{val}}$ without performing many unquenched simulations.

3. Lattice tmQCD

Lattice tmQCD is an extension of the widely used formulation with Wilson quarks, from which it differs in that the physically non-vanishing quark mass term is in general not aligned with the Wilson term in the flavour chiral space. This simple modification brings definite advantages concerning the simulations with light quarks –especially in the quenched or partially quenched case– and the renormalization properties of some phenomenologically important quantities, such as the leptonic decay amplitude of pseudoscalar mesons or the mixing amplitude in the $K^0-\bar{K}^0$ system [9, 10, 11].

3.1 Lattice Wilson quarks and spurious zero modes

While the considerations of Subsections 2.1–2.2, apply to any sensible lattice regularization of QCD, working with Wilson fermions entails a further technical problem that renders particularly difficult –or even impossible– the simulations with light quarks. The problem arises whenever the quenched (or partially quenched) sample of configurations, as determined by a given choice of the bare parameters, includes gauge backgrounds on which the critical Wilson-Dirac operator $D_{W,c}$, eq. (2.4), has one or more eigenvalues with *negative*

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real part $\text{Re}(\lambda) < 0$ and (almost) zero imaginary part. Under these conditions, the massive Dirac operator $D_{W,c} + m'_{q,\text{val}}$ is singular for values of $m'_{q,\text{val}} > 0$ as soon as $m'_{q,\text{val}} + \text{Re}(\lambda) = 0$ for some of the real negative eigenvalues λ .

The fermionic observables, which involve $[D_{W,c} + m'_{q,\text{val}}]^{-1}$, may receive (almost) divergent contributions on the aforementioned gauge backgrounds, spoiling the expected decrease of the statistical errors with the number of independent measurements [12]. As an example of this phenomenon, we show in Fig. 1 the Monte Carlo history of the normalized relative standard deviation for the pion channel correlator $f \equiv f_P^{11}(x_0)$ at $x_0 = 24a = T/2$, see Section 4.1. The normalization of the standard deviation is such that it should approach a constant in the limit of infinite statistics: in the case of the standard Wilson regularization, which corresponds to the open symbols in Fig. 1, the problem is apparent. Via the combined effect of lattice artifacts and statistical fluctuations, "spurious" quark zero modes³ anticipate at non-vanishing values of m'_q the breakdown of the quenched or partially quenched approximation.

In practice, in the quenched case the rate of occurrence of gauge backgrounds with spurious quark zero modes –also called "exceptional configurations"– depends on the values of $m'_{q,\text{val}}$ and g_0^2 , on the physical linear size L of the lattice and on various details of the lattice regularization. The rate tends to increase when decreasing $m'_{q,\text{val}}$ and increasing g_0^2 and L/a , as well as when switching on the coefficient, $c_{\text{sw}}(g_0^2)$, of the counterterm that is needed for the on-shell $O(a)$ improvement of the fermionic action. For instance, in the regularization with plaquette gauge action and non-perturbatively $O(a)$ improved Wilson quarks, the problem is felt for $L \geq 1.5$ fm at values of g_0^2 corresponding to $a \sim 0.1$ fm and at valence quark masses that are about half the strange quark mass. A similar problem is also expected in partially quenched simulations, although with a lower rate depending on the ratio $m'_{q,\text{val}}/m'_{q,\text{sea}}$, and has indeed been observed, see e.g. Ref. [13].

In the fully unquenched case, one can expect troubles at the algorithmic level with light Wilson quarks on rather coarse lattices. This is because the state-of-the-art algorithms implement stochastically the fermion determinant that appears in the probability measure for the gauge configurations: almost exceptional configurations may hence be proposed, but are then almost certainly rejected. In this process however the simulation algorithm, e.g. the standard HMC one⁴, undergoes a severe slowing-down, due to a decrease in the acceptance rate and an increment of the condition number of the Dirac matrix before the accept/reject test.

3.2 Action and symmetries

As already known since 1989 [15], the problem with spurious quark zero modes is absent in the two-flavour theory if one considers the action

$$S_W[U, \bar{\psi}, \psi] = S_g + a^4 \sum_x \bar{\psi}(x) [(D_{W,c} + m_q + i\mu_q \gamma_5 \tau^3) \psi](x), \quad (3.1)$$

³These spurious quark zero modes should not be confused with the quark zero modes that play an important physical role in the thermodynamic chiral limit of renormalized QCD.

⁴Evidence for a large increase of the fermionic force at small quark mass values is reported in Ref. [14].

where ψ is a flavour quark doublet, the matrix τ^3 acts in the flavour space and the boundary conditions for finite-volume systems may remain unspecified for a while. Since m_c is known in practice with finite precision, the exactly known bare parameters are g_0^2 , μ_q and $m_0 = m_c + m_q$. It is easy to see that, as long as $\mu_q \neq 0$, on any gauge background the lowest eigenvalue of the Hermitean square of the matrix $(D_{W,c} + m_q + i\mu_q\gamma_5\tau^3)$ is bounded from below by $(a\mu_q)^2$.

The action (3.1) represents a sensible regularization of QCD with $N_f = 2$ mass-degenerate quark flavours, but in a quark field basis that is chirally twisted with respect to the standard one [9]. To illustrate this point, let us focus on the simple case $m_q = 0$, $\mu_q \neq 0$, and consider the very *same* lattice theory in the standard quark field basis, which is obtained by a suitable axial rotation with generator τ^3 :

$$\chi = \exp\left(i\omega\gamma_5\frac{\tau^3}{2}\right)\psi, \quad \bar{\chi} = \bar{\psi}\exp\left(i\omega\gamma_5\frac{\tau^3}{2}\right), \quad \omega = \arctan\frac{\mu_q}{m_q} = \frac{\pi}{2}. \quad (3.2)$$

The action (3.1) then reads

$$S_W[U, \bar{\chi}, \chi] = S_g + a^4 \sum_x \bar{\chi}(x)[(D_{\text{tmW},c} + \mu_q)\chi](x), \quad (3.3)$$

where

$$D_{\text{tmW},c} = \frac{1}{2}\gamma \cdot (\nabla + \nabla^*) + i\frac{a}{2}\gamma_5\tau^3\nabla^* \cdot \nabla - i\gamma_5\tau^3m_c. \quad (3.4)$$

The connection, eq. (3.2), between the two lattice quark bases makes obvious that the chiral limit is obtained for $m_q = \mu_q = 0$ with m_c being the usual function of g_0^2 . Inspection of the symmetries of the action (3.3) shows that in the chiral limit one vector and two axial generators –out of the six generators of the flavour chiral group– are preserved by the lattice regularization, while parity is preserved only up to a flavour exchange (P_F symmetry) and all other symmetries are as usual with Wilson fermions. It follows that μ_q is *multiplicatively* renormalized, $\mu_R = Z_\mu(g_0^2)\mu_q$, while $m_R = Z_m(g_0^2)m_q$. Power counting renormalizability and the recovery of the full flavour chiral symmetry in the continuum limit [3], together with the exact P_F invariance, imply that parity must also be recovered in the continuum limit. In contrast with other approaches based on the action (3.1) [12], the correlation functions of the massive QCD are obtained at finite μ_q , so that the problem with the spurious quark zero modes is certainly solved.

In the general case, where both m_q and μ_q are non-vanishing, the situation is fully analogous, but the relation between the two lattice quark bases involves an angle $\omega \neq \pi/2$. However, owing to the complications arising from the Wilson term, it is convenient to perform first the renormalization (and possibly the $O(a)$ improvement) of the correlation functions in a given quark basis and then transform to the "physical" basis, i.e. the one where the quark mass is coupled to the singlet scalar density. The first step implies that the continuum limit is approached at fixed values of g_R^2 , m_R , μ_R and the normalization conditions for the composite fields. Concerning the second step, for a wide class of renormalization schemes, the relation between the renormalized fields in two different bases that are related via a non-singlet axial rotation takes the same form as at the classical level [9].

In terms of polar quark mass coordinates,

$$\tan \alpha = \frac{\mu_R}{m_R}, \quad M_R = \sqrt{\mu_R^2 + m_R^2}, \quad (3.5)$$

the angle α identifies the quark basis and hence specifies the axial rotation with generator $\tau^3/2$ that allows to combine the renormalized correlation functions so to obtain finite correlators with given continuum quantum numbers⁵. On the latter correlators the partial breaking of isospin and parity is an effect of order $a\mu_R$ and represents no serious drawback.

If one identifies the two quark flavours with the u and d quark, the tiny mass difference between them can safely be taken into account by means of chiral perturbation theory. Alternatively, lattice tmQCD can also be formulated for a doublet of non-degenerate quarks, whilst retaining the protection against spurious quark zero modes [17]. Heavier flavours of Wilson quarks can be added e.g. in the usual way to the lattice tmQCD action for $N_f = 2$.

4. A test-study of lattice tmQCD with light quarks and in large volume

We present here some preliminary results of a high-statistics exploratory study of lattice tmQCD in the thermodynamic chiral regime. The study aimed at testing the absence of exceptional configurations, the computational cost and the magnitude of cutoff effects for a few typical observables. We adopt in the following the notation of Ref. [19], to the equations of which we refer with the prefix "I", and postpone many technical details to a forthcoming publication [20].

4.1 Observables and simulations

In this test-study we choose to work in the quark basis of action (3.1) and implement the *non-perturbative* $O(a)$ improvement of the action and the relevant operators along the lines of Ref. [18]. Attention is restricted to the pseudoscalar and vector meson masses, M_{PS} and M_V , the pseudoscalar (leptonic) decay constant, F_{PS} , and the polar quark masses, M_R and α , which are defined according to eqs. (I.3.3)–(I.3.20) for μ_R and m_R and eq. (3.5).

Set, β	$L/a, T/L$	# meas.	m_R/M_R	M_{Rr_0}	M_{PSr_0}	F_{PSr_0}	M_{Vr_0}
A1, 6.0	16, 2	650	−0.016(3)	0.2729(15)	1.711(7)	0.455(5)	2.662(40)
A1', 6.0	16, 3	650	−0.016(3)	0.2729(15)	1.714(6)	0.455(6)	2.656(42)
A2, 6.2	24, 2	535	−0.014(2)	0.2558(16)	1.623(8)	0.456(5)	2.557(32)
B1L, 6.0	24, 2	260	0.017(3)	0.1949(11)	1.452(6)	0.432(6)	2.517(35)
B1, 6.0	16, 2	535	0.001(3)	0.1949(11)	1.455(8)	0.428(5)	2.513(47)
B2, 6.2	24, 2	300	−0.004(4)	0.1962(12)	1.420(9)	0.436(7)	2.462(41)
C, 6.0	24, 2	260	0.083(5)	0.1205(7)	1.160(6)	0.401(6)	2.485(59)

Table 1: Statistics and renormalized quantities obtained in our simulations, which are identified by a label and the value of $\beta = 6/g_0^2$. The values of m_0 and μ_q can be found in Ref. [20].

⁵This point of view might lead to a reinterpretation of the "spontaneous breakdown of parity and isospin" in lattice QCD with Wilson fermions [16], which was observed by employing the action (3.1).

We work in the *quenched* approximation considering systems of physical size L^3T with L such that $M_{\text{PS}}L \geq 4.5$ to suppress finite volume effects. In practice we take $L = 1.5$ fm or $L = 2.2$ fm and $T/L = 2 \div 3$. Following Ref. [19], we impose boundary conditions of Schrödinger functional (SF) type and compute the SF correlators

$$f_A^{11}(x_0), f_P^{11}(x_0), f_V^{12}(x_0), k_V^{11}(x_0), k_T^{11}(x_0), k_A^{12}(x_0), f_1^{11}. \quad (4.1)$$

We hence construct the linear combinations of renormalized and $O(a)$ improved SF correlators that correspond to operator insertions (at time x_0) with well defined continuum quantum numbers, see eqs. (I.3.10)–(I.3.11) with α given by eq. (3.5). Namely, the correlators $[f_{A'}^{11}]_{\text{R}}(x_0)$ and $[f_{P'}^{11}]_{\text{R}}(x_0)$ correspond to the insertion of the isotriplet pseudoscalar operators $(A'_R)_0^1$ and $(P'_R)^1$, while the correlators $[k_{V'}^{11}]_{\text{R}}(x_0)$ and $[k_{T'}^{11}]_{\text{R}}(x_0)$ correspond to the insertion of the isotriplet vector operators $(V'_R)_k^1$ and $(T'_R)_{k0}^1$. In the limit of large x_0 and large $(T - x_0)$ and up to cutoff effects, these non-vanishing correlators are expected to be dominated by the lowest isotriplet pseudoscalar and vector meson states.

An overview of our simulation parameters, statistics and preliminary results for renormalized quantities is given in Table 1. The renormalized gauge coupling g_{R}^2 is eliminated in favour of the length scale r_0 [21], which is known to be about 0.5 fm, while the lattice spacing value corresponding to $\beta = 6$ (6.2) is $a \sim 0.093$ (0.068) fm. Our most critical simulation (set C, $\beta = 6$), where we employed a CGNE solver for the SSOR-preconditioned version of the Dirac matrix $(D_{\text{W,c}} + m_{\text{q}} + i\mu_{\text{q}}\gamma_5\tau^3)$, required ~ 230 GFlops \times day.

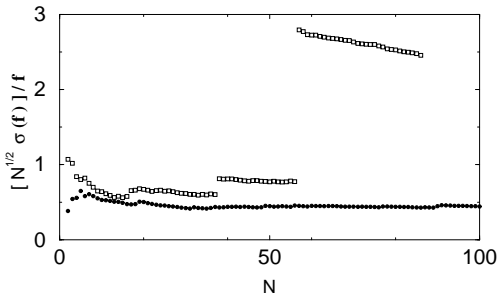


Figure 1: The square root of the relative a priori variance of $f = f_P^{11}(x_0 = 24a)$ versus the number of measurements N : data from the simulation C (filled symbols) and another simulation with the same values of β and M_{R} , but $\alpha = 0$ (open symbols).

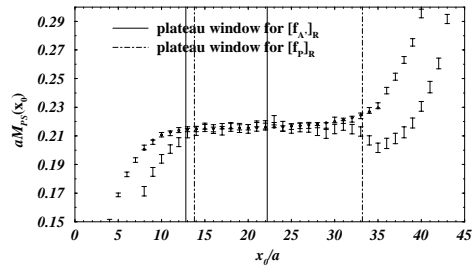


Figure 2: Pseudoscalar effective masses extracted from the correlators $[f_{P'}^{11}]_{\text{R}}$ and $[f_{A'}^{11}]_{\text{R}}$ for the simulation C. The tiny black circles denote our (good) fit to the effective masses from $[f_{A'}^{11}]_{\text{R}}$: at large x_0 a peculiar $O(a\mu_{\text{q}})$ contribution is present.

4.2 Results

We find that lattice tmQCD allows, as expected, to safely work in a region of parameters which would be inaccessible with ordinary Wilson quarks: see e.g. Fig. 1 as well as the findings of Ref. [24]. For a given number of independent measurements, the statistical errors on M_{PS} and M_{V} are comparable, up to a factor of one to three, to those found e.g. with domain wall quarks [22]. The CPU time effort, e.g. for the data sets A1, A1' and A2, is in line with the computational cost for ordinary Wilson quarks.

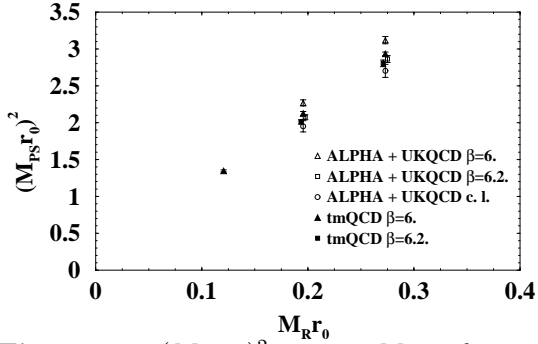


Figure 3: $(M_{\text{PS}}r_0)^2$ versus $M_{\text{R}}r_0$ from tmQCD and reanalysis of the data of Ref. [23], including a continuum extrapolation (c. l.).

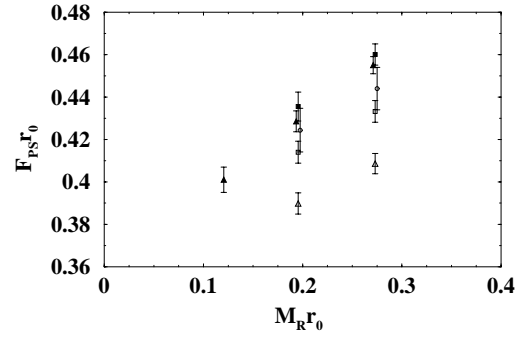


Figure 4: The analogous of Fig. 3 for $F_{\text{PS}}r_0$. Symbols are the same as specified in the legenda of Fig. 3.

The partial breaking of parity and isospin that is peculiar of lattice tmQCD is found to be a minor problem within our small statistical errors. In this respect it should be noted that we work at small values of $a\mu_{\text{q}}$, namely $0.0266 \geq a\mu_{\text{q}} \geq 0.0117$, and consider observables in physical channels where the lowest state is lighter than the lowest state of the corresponding channels with flipped parity and isospin. While deferring the details of our analysis to Ref. [20], we show in Fig. 2 an example of effective masses extracted from SF correlators, where the correlator $[f_{\text{A}'}^{11}]_{\text{R}}(x_0)$ receives contributions of order $a\mu_{\text{q}}$ that are visible at large x_0 . Analogous effects are expected and found to be negligible within statistical errors for both $[f_{\text{P}'}^{11}]_{\text{R}}(x_0)$ and the vector channel correlators.

As detailed in Refs. [18, 10], we expect the relations among our observables and the renormalized parameters r_0 and M_{R} to be $\mathcal{O}(a)$ improved. In particular, when working at $\alpha = \pi/2 + \mathcal{O}(a)$, which is the case of our study, the knowledge of a few counterterms (those with coefficients Z_{g} , m_{c} and c_{sw}) suffices to obtain an $\mathcal{O}(a)$ improved estimate of F_{PS} . In order to check for the residual scaling violations, we produced data at $\beta = 6.2$ (sets A2 and B2), while keeping α , M_{R} and r_0 fixed. The small mismatch in $M_{\text{R}}r_0$ for the set A2 was corrected by employing estimates of the dependence of our observables on $M_{\text{R}}r_0$.

We also reanalysed the data of Ref. [23], which were produced at $\beta = 6, 6.1, 6.2, 6.45$, by imposing precisely the same renormalization conditions as in this study of tmQCD. We then performed a continuum extrapolation of these data, assuming a purely quadratic dependence on $(a/r_0)^2$ and discarding the data at $\beta = 6$. However, the resulting estimate of F_{PS} is not fully $\mathcal{O}(a)$ improved, as for one of the necessary improvement coefficients, $b_{\text{A}}(g_0^2)$, only the one-loop estimate could be used. The outcome of this exercise is compared with the results from tmQCD in Figs. 3–4, omitting the case of $M_{\text{V}}r_0$ where cutoff effects are hardly visible within statistical errors. The estimators of M_{PS} and F_{PS} that are obtained from lattice tmQCD show rather small cutoff effects, which agrees with the findings of a scaling test [19] in intermediate volume ($L = 0.75$ fm).

5. Conclusions

Lattice tmQCD is well suited to perform non-perturbative studies of QCD in the chiral

(thermodynamic or finite-volume) regime for all cases where it is technically sufficient to recover chiral symmetry in the continuum limit. The framework has been successfully tested in the quenched approximation and can straightforwardly be extended beyond it.

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