$\mathcal{N} = 1$ Super-Yang-Mills theory on the lattice with twisted mass fermions

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ABSTRACT: Super-Yang-Mills theory (SYM) is a central building block for supersymmetric extensions of the Standard Model of particle physics. Whereas the weakly coupled subsector of the latter can be treated within a perturbative setting, the strongly coupled subsector must be dealt with a non-perturbative approach. Such an approach is provided by the lattice formulation. Unfortunately a lattice regularization breaks supersymmetry and consequently the mass degeneracy within a supermultiplet. In this article we investigate the properties of $\mathcal{N} = 1$ supersymmetric SU(3) Yang-Mills theory with a lattice Wilson Dirac operator with an additional parity mass, similar as in twisted mass lattice QCD. We show that a special 45° twist effectively removes the mass splitting of the chiral partners. Thus, at finite lattice spacing both chiral and supersymmetry are enhanced resulting in an improved continuum extrapolation. Furthermore, we show that for the non-interacting theory at 45° twist discretization errors of order $\mathcal{O}(a)$ are suppressed, suggesting that the same happens for the interacting theory as well. As an aside, we demonstrate that the DD α AMG multigrid algorithm accelerates the inversion of the Wilson Dirac operator considerably. On a $16^3 \times 32$ lattice, speed-up factors of up to 20 are reached if commonly used algorithms are replaced by the DD α AMG.

KEYWORDS: Lattice QCD, Lattice Quantum Field Theory, Supersymmetric Gauge Theory

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1 Introduction

The standard model (SM) of particle physics very successfully describes all processes mediated by the electromagnetic, weak and strong forces — but several open questions remain unanswered. For example, the Higgs boson with mass $m_H = (125.18 \pm 0.16)\text{GeV}$ [1] is unreasonably light since the mass is quadratically divergent and a mass of the order of the Planck mass is expected. The situation improves considerably in a supersymmetric theory,

where every bosonic particle has a fermionic superpartner with the same quantum numbers (besides the spin) and vice versa. In a supersymmetric standard model a small Higgs mass is easier to accommodate since in leading order bosonic and fermionic divergences cancel and there is no quadratic divergence [2, 3]. Another urgent problem of modern physics is the large amount of dark matter seen in our universe. It outweighs the visible matter by a factor of six, making up about 27 percent of the universe. Supersymmetric models naturally provide a dark-matter candidate, the so-called lightest supersymmetric particle (LSP). This particle is stable and can not decay if R -parity is conserved [3, 4].

A straightforward extension of the SM is the minimal supersymmetric standard model (MSSM). The present work deals with non-perturbative phenomena of the strongly coupled subsector of the MSSM which is $\mathcal{N} = 1$ Super-Yang-Mills (SYM) theory with gauge group $SU(3)$. It is the supersymmetric extension of pure Yang-Mills (YM) theory describing gluons in interaction with their superpartners, the so-called gluinos. As members of the same $\mathcal{N} = 1$ vector super-multiplet the gluons and gluinos are (in perturbation theory) massless. Both are in the adjoint representation of the gauge group $SU(3)$ and on-shell the degrees of freedom match. The latter statement holds true since the gluinos are Majorana fermions. The theory is asymptotically free and shows confinement, similar to QCD.

Our analytical and numerical investigations aim for a better understanding of the low-energy properties of this confining theory. Unfortunately almost all lattice regularizations break supersymmetry explicitly and as a result of this breaking one observes a mass-splitting within a given supermultiplet. In the present work we shall present a novel lattice formulation which considerably reduces the mass-splitting of the chiral partners in the Veneziano-Yankielowicz supermultiplet of $\mathcal{N} = 1$ SYM. As a result the difficult fine-tuning problem to the chiral and supersymmetric continuum limit is less severe.

Early analytic studies of supersymmetric lattice systems go back to Dondi and Nicolai [5], who studied the discretized Wess-Zumino model. Subsequently the restoration of supersymmetry in the continuum limit and the spectrum of particles have been studied for these Yukawa-type lattice models [6–10] or in related supersymmetric non-linear sigma-models [11]. Early simulations of four-dimensional $\mathcal{N} = 1$ SYM theory with quenched fermions were performed in [12, 13]. Clearly, dynamical fermions are an integral part in any supersymmetric field theory and the inclusion of light dynamical fermions in simulations is essential.

Extensive investigations and simulations of $\mathcal{N} = 1$ SYM with gauge group $SU(2)$ and with dynamical fermions were performed by the DESY-Münster collaboration during the past 20 years. In [14] the chiral symmetry breaking was investigated and two ground states have been spotted. A comprehensive lattice study including the mass spectrum was first presented in [15] and concluded with [16]. Later, those results were refined with the help of a variational analysis [17]. Ward Identities were exploited in [18] to determine the gluino mass as well as the mixing coefficient of the supercurrent. An investigation of the theory at finite temperature revealed that deconfinement and chiral symmetry restoration occur at the same temperature [19]. This insight was confirmed recently using the gradient flow [20]. The lattice studies are supplemented with an one-loop calculation of the supersymmetric Ward identities [21], the analysis of the adjoint pion within partially quenched chiral perturbation theory [22] and the perturbative calculation of the clover coefficient [23].

More recently the spectrum of the low lying bound states [24] and supersymmetric Ward identities [25] have been calculated for $\mathcal{N} = 1$ SYM with gauge group $SU(3)$. Besides these studies with Wilson fermions, first investigations and simulations with domain wall fermions and overlap have been presented in [26–28] and [29, 30]. With Ginsparg-Wilson fermions no fine-tuning should be necessary to end up with a supersymmetric continuum theory [31].

A dimensional reduction of $\mathcal{N} = 1$ SYM theory from $d = 4$ to $d = 2$ spacetime dimensions leads to the $\mathcal{N} = (2, 2)$ SYM theory and the two theories have supermultiplets of identical length. The mass spectrum of the reduced theory [32], the Ward identities [33], the dynamical breaking of supersymmetry [34] and the large N behavior [35] were investigated in detail. Certain field theories with extended supersymmetry can be formulated such that some (nilpotent) supersymmetry transformations are preserved exactly on the lattice [36]. In this context the four-dimensional $\mathcal{N} = 4$ SYM theory was studied e.g. in [37] and its cousin, the two-dimensional $\mathcal{N} = (8, 8)$ SYM in [38].

In the present work we propose and carefully study a deformation of the $\mathcal{N} = 1$ SYM lattice action by twisting the mass term. We will argue by analytic and numeric means that this twisting leads to a sizable reduction of the mass splitting (caused by a breaking of supersymmetry by lattice artifacts) within the Veneziano-Yankielowicz supermultiplet. Actually, the concept of a twisted mass was first introduced to lattice QCD in [39] with the aim to remove exceptional configurations. Later, $\mathcal{O}(a)$ improvement at (maximal) twisting angle $\pm\pi/2$ was recognized as particularly interesting for measuring physical quantities [40]. Also a study of the two-dimensional Wess-Zumino model with a twisted lattice action revealed a dramatic suppression of the discretization errors for an optimal twist angle [7]. In the present work the IR improvement of the mass degeneracy in the Veneziano-Yankielowicz supermultiplet at optimal twist angle $\pi/4$ is crucial. At the same time the $\mathcal{O}(a)$ discretization errors are reduced at this twist angle.

This paper is structured as follows: in the following section we summarize basic facts about $\mathcal{N} = 1$ SYM theory in the continuum and on the lattice, which are relevant for our work. Section 3 further elaborates on some aspects in more detail analytically. The results of our numerical calculations are presented in section 4. Our conclusion and a summary is given in section 5.

2 Basics

In this section we recall relevant facts about $\mathcal{N} = 1$ SYM theory and thereby fix our notation. In section 2.1 the continuum formulation, symmetries and effective field theory predictions are addressed. Afterwards, the Wilson Dirac operator with twisted mass term is introduced (section 2.2.1) and the main differences to the standard formulation are discussed (section 2.2.2). In section 2.2.3 we finally introduce all lattice observables whose numerical results are discussed then in section 4.

2.1 $\mathcal{N} = 1$ Super-Yang-Mills theory in the continuum

In Minkowski spacetime the on-shell action of $\mathcal{N} = 1$ SYM theory reads

$$S_{\text{SYM}}^{\text{M}} = \int d^4x \, \text{tr} \left(-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{i}{2} \bar{\lambda} \not{D} \lambda - \frac{m}{2} \bar{\lambda} \lambda \right), \quad (2.1)$$

1 bosonic scalar	$s = 1, l = 1, 0^{++}$	gluinoball	$a\text{-}f_0 \sim \bar{\lambda}\lambda$
1 bosonic pseudoscalar	$s = 0, l = 0, 0^{-+}$	gluinoball	$a\text{-}\eta' \sim \bar{\lambda}\gamma_5\lambda$
1 majorana-type	$s = \frac{1}{2}, l = 1, \frac{1}{2}^{i+}$	gluino-gluonball	$\tilde{g}g \sim F_{\mu\nu}\Sigma^{\mu\nu}\lambda$

Table 1. Veneziano-Yankielowicz supermultiplet.

and looks similar to the action of Quantum Chromodynamics (QCD) with a single flavor. In the supersymmetric theory the fermion and gauge boson are members of the same vector supermultiplet such that the former (called gluino) is described by a Majorana field $\lambda(x)$ and transforms in the same adjoint representation as the gauge potential $A_\mu(x)$. This way, fermionic and bosonic degrees of freedom match as dictated by supersymmetry. The supersymmetry transformations are further discussed in section 3.2.

The action in eq. (2.1) contains a finite gluino mass m which breaks supersymmetry softly. On the lattice this mass is fine-tuned such that after continuum extrapolation a supersymmetric limit is reached which at the same time is chirally symmetric.

At high energies or high temperatures, $\mathcal{N} = 1$ SYM can be considered as a gas of free gluons and gluinos. More interestingly, at low energies it is a confining theory similar to non-supersymmetric gauge theories and has a rich spectrum of low lying color-singlet bound states. This spectrum has been investigated with the method of effective field theory based on the theory's symmetries and applying anomaly matching. Three different types of bound states are expected to arise: pure glueballs, pure meson-like gluinoballs and gluino-gluonballs.

Supersymmetry arranges these bound states in supermultiplets of $\mathcal{N} = 1$ supersymmetry. As long as supersymmetry is unbroken, the states within a supermultiplet have equal mass. Veneziano and Yankielowicz predicted a chiral supermultiplet [41] of bound states listed in table 1. The names of the particles are chosen in analogy to QCD, with the prefix “a-” indicating the adjoint representation. As usual, the quantum numbers J^{PC} specify the total angular momentum J , the parity P and the charge conjugation C .

Subsequently Farrar, Gabadadze and Schwetz suggested the existence of a second supermultiplet [42] consisting of the particles listed in table 2. Based on symmetry arguments they suggested the more general effective Lagrangian

$$\mathcal{L}^{\text{eff}} = \frac{1}{\alpha}(S^\dagger S)^{1/3}\Big|_D + \gamma \left[\left\{ S \log \left(\frac{S}{\mu^3} \right) - S \right\} \Big|_F + \text{h.c.} \right] + \frac{1}{\delta} \left(-\frac{U^2}{(S^\dagger S)^{1/3}} \right) \Big|_D \quad (2.2)$$

with chiral superfield S , real tensor superfield U , dynamically generated scale μ and further low-energy constants α , γ and δ .¹ In the limit $\delta \rightarrow \infty$ the effective action of Veneziano and Yankielowicz is recovered. The effective Lagrangian (2.2) describes propagating massive fields, for example the scalar and pseudoscalar glueball. The physical states will be mixtures of states from these two multiplets with equal quantum numbers [42].

The chiral symmetry of $\mathcal{N} = 1$ SYM theory has a different breaking pattern compared to QCD. For vanishing gluino mass and gauge group $SU(N_c)$ the classical theory has

¹In [43], the same authors suggest an alternative formulation with two chiral superfields.

1 bosonic scalar	$s = 0, l = 0, 0^{++}$	glueball	$0^{++} \sim F_{\mu\nu} F^{\mu\nu}$
1 bosonic pseudoscalar	$s = 1, l = 1, 0^{-+}$	glueball	$0^{-+} \sim \epsilon_{\mu\nu\rho\sigma} F^{\mu\nu} F^{\rho\sigma}$
1 majorana-type	$s = \frac{1}{2}, l = 0, \frac{1}{2}^{(-i)+}$	gluino-glueball	$\tilde{g}g \sim F_{\mu\nu} \Sigma^{\mu\nu} \lambda$

Table 2. Farrar-Gabadadze-Schwetz supermultiplet.

a global $U(1)_A$ symmetry² $\lambda \mapsto e^{i\alpha\gamma_5/2}\lambda$. The axial anomaly reduces this $U(1)_A$ to the discrete subgroup $\mathbb{Z}_{2N_c}$,

$$\lambda \mapsto e^{2\pi i n \gamma_5 / 2N_c} \lambda \quad \text{with} \quad n \in \{1, \dots, 2N_c\}. \quad (2.3)$$

A gluino condensate $\langle \bar{\lambda}\lambda \rangle \neq 0$ spontaneously breaks this remnant symmetry further to a $\mathbb{Z}_2$ symmetry. Therefore N_c physically equivalent vacua are expected.

To construct the lattice formulation one first switches from Minkowski to Euclidean theory [44]. In Euclidean spacetime the continuum on-shell action has the form

$$S_{\text{SYM}}^E = \int d^4x \, \text{tr} \left(\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} \bar{\lambda} \not{D} \lambda + \frac{m}{2} \bar{\lambda} \lambda \right). \quad (2.4)$$

This continuum action is the point of departure for the lattices studies presented below.

2.2 $\mathcal{N} = 1$ Super-Yang-Mills theory on the lattice

To study the mass spectrum and in particular the confinement of color charges, a non-perturbative method is required. We choose the ab-initio lattice method although it breaks supersymmetry explicitly.³ Different lattice formulations are feasible, depending on the discretization of the continuum action and in particular on the choice of lattice fermions.

In the present work we shall use the lattice formulation with Wilson fermions introduced by Curci and Veneziano [45]. At finite lattice spacing, supersymmetry and chiral symmetry are broken simultaneously by the discretization and Wilson term. This breaking leads to a relevant counter-term, which is proportional to the gluino mass term. To compensate this, an explicit gluino mass term is added and fine-tuned such that the (renormalized) gluino becomes massless in the continuum limit. Since the gluino mass term is the only relevant operator, supersymmetry and chiral symmetry will be restored in the continuum limit.

Unfortunately, confinement prevents the direct measurement of the gluino. Here we follow Veneziano and Yankielowicz who proposed to monitor instead the (unphysical) adjoint pion mass, defined in a partially quenched approximation, similarly as in 1-flavor QCD [41]. Its mass squared

$$m_{a-\pi}^2 \propto m^R \quad (2.5)$$

is proportional to the physical gluino mass, which can be calculated in partially quenched chiral perturbation theory [22]. This quantity requires only low statistics and is easy to

²Usually the angle of the chiral rotation is α . We chose $\alpha/2$ since in section 3.1 the bilinear condensates are investigated and with our choice they transform with the angle α .

³For $\mathcal{N} = 1$ SYM there is no partially supersymmetric formulation as for the theory with 32 supercharges.

compute. By fine-tuning to the critical gluino mass m_{crit} we are able to recover in the continuum limit simultaneously supersymmetry as well as chiral symmetry.

In contrast to QCD, where the Dirac fermions give rise to a fermion determinant, in $\mathcal{N}=1$ SYM theory the Pfaffian of the Dirac operator enters the path integral after integrating out the Majorana fermions. Since the Pfaffian is proportional to the square root of the determinant, the *rational* hybrid Monte Carlo algorithm (RHMC) [46] is used in our simulations.

2.2.1 Lattice formulation

Different lattice formulations of a continuum theory vary in their discretization errors and how fast the correct continuum limit is reached. In our simulations the gauge part of the lattice action $S_{\text{lat}} = S_g + S_f$ is given by the Symanzik-improved Lüscher-Weisz action

$$S_g[\mathcal{U}] = \frac{\beta}{3} \left(\frac{5}{3} \sum_{\square} \text{tr}(\mathbb{1} - \text{Re}\mathcal{U}_{\square}) - \frac{1}{12} \sum_{\square\square} \text{tr}(\mathbb{1} - \text{Re}\mathcal{U}_{\square\square}) \right), \quad (2.6)$$

and the action for the Majorana field (the gluino part)

$$S_f[\lambda, \bar{\lambda}, \mathcal{U}] = a^4 \sum_{x,y \in \Lambda} \bar{\lambda}(x) D_W(x, y) \lambda(y) \quad (2.7)$$

contains the Wilson Dirac operator with an additional twisted mass term,

$$D_W^{\text{mtw}}(x, y) = (4 + m + im_5 \gamma_5) \delta_{x,y} - \frac{1}{2} \sum_{\mu=\pm 1}^{\pm 4} (\mathbb{1} - \gamma_{\mu}) \mathcal{V}_{\mu}(x) \delta_{x+\hat{\mu}, y}. \quad (2.8)$$

Here the gauge links $\mathcal{V}_{\mu}(x)$ are in the adjoint representation. They are constructed from the gauge link $\mathcal{U}_{\mu}(x)$ in the fundamental representation and the generators, T^a , of the Lie algebra using the relation

$$[\mathcal{V}_{\mu}(x)]^{ab} \equiv 2 \text{tr} \left[\mathcal{U}_{\mu}^{\dagger}(x) T^a \mathcal{U}_{\mu}(x) T^b \right]. \quad (2.9)$$

Furthermore, we define $\gamma_{-\mu} \equiv -\gamma_{\mu}$ and $\mathcal{V}_{-\mu}(x) \equiv \mathcal{V}_{\mu}^{\dagger}(x - \hat{\mu})$ for simplicity.

At finite lattice spacing (with or without twisted mass term) supersymmetry and chiral symmetry are explicitly broken and only a fine-tuning of the gluino mass, $m \rightarrow m_{\text{crit}}(\beta)$ while taking the limit $\beta \rightarrow \infty$, assures a simultaneous restoration of both symmetries in the continuum limit. After the critical point at $(m_{\text{crit}}, m_5 = 0)$ is determined via a parameter scan, the mass parameters can also be specified by their distance $\delta m = m - m_{\text{crit}}$, $\delta m_5 = m_5$ with respect to the critical point. A useful variant are polar coordinates centered at the critical point with distance M from this point and twist angle α ,

$$m - m_{\text{crit}} = M \cos \alpha \quad \text{and} \quad m_5 = M \sin \alpha. \quad (2.10)$$

We added a parity-breaking mass term $im_5 \gamma_5 \delta_{x,y}$ to the Wilson Dirac operator

$$D_W(x, y) = (4 + m) \delta_{x,y} - \frac{1}{2} \sum_{\mu=\pm 1}^{\pm 4} (\mathbb{1} - \gamma_{\mu}) \mathcal{V}_{\mu}(x) \delta_{x+\hat{\mu}, y}, \quad (2.11)$$

to reduce the explicit susy-breaking by lattice artifacts in the two-point functions of the supermultiplet partners. This term is similar as for twisted-mass lattice QCD but for one Majorana fermion flavor.⁴ A special feature of $\mathcal{N} = 1$ SYM motivates it: if we had twisted not only the mass but also the Wilson term (which becomes an irrelevant term in the continuum) we would have a double-twisted Wilson Dirac operator

$$D_W^{\text{dtw}}(x, y) \equiv \left(4e^{i\varphi\gamma_5} + Me^{i\alpha\gamma_5}\right)\delta_{x,y} - \frac{1}{2} \sum_{\mu=\pm 1}^{\pm 4} \left(\mathbb{1}e^{i\varphi\gamma_5} - \gamma_\mu\right)\mathcal{V}_\mu(x)\delta_{x+\hat{\mu},y}. \quad (2.12)$$

For identical twist angles $\varphi = \alpha$, the standard and double-twisted Wilson Dirac operators are related by a chiral rotation,

$$e^{i\alpha\gamma_5/2}D_W e^{i\alpha\gamma_5/2} = D_W^{\text{dtw}}. \quad (2.13)$$

The chiral rotation can be undone by a variable transformation of the Majorana fields

$$\lambda \mapsto e^{i\alpha\gamma_5/2}\lambda, \quad \bar{\lambda} \mapsto \bar{\lambda}e^{i\alpha\gamma_5/2}, \quad (2.14)$$

and, if no anomaly enters through the measure, we obtain for Grassmann integrals of Majorana bilinears (i.e., the scalar and pseudo-scalar bilinears)

$$\int \mathcal{D}\lambda e^{-\lambda^T C D_W^{\text{dtw}} \lambda} \begin{pmatrix} \bar{\lambda}_x \lambda_x \\ i\bar{\lambda}_x \gamma_5 \lambda_x \end{pmatrix} = \int \mathcal{D}\lambda e^{-\lambda^T C D_W \lambda} \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} \bar{\lambda}_x \lambda_x \\ i\bar{\lambda}_x \gamma_5 \lambda_x \end{pmatrix}. \quad (2.15)$$

At twist angles $\alpha = \varphi = \pi/4$, the chiral and parity condensate $\langle \bar{\lambda}\lambda \rangle$ and $\langle \bar{\lambda}\gamma_5\lambda \rangle$ thus have equivalent magnitudes. In addition, two-point correlators of adjoint mesonic states are mass degenerated by construction and their operator basis can be combined by an arbitrary rotation.⁵ This means that the double-twisted formulation with $\alpha = \varphi = \pi/4$ has a continuum limit with mass-degenerated scalar and pseudoscalar mesonic states. Actually we shall see below that the mass degeneracy is seen at finite lattice spacing even for the twisted-mass Wilson Dirac operator, D_W^{mtw} , that is the operator D_W^{dtw} with $\varphi = 0$ and $\alpha = \pi/4$. The chiral and the parity condensates differ, though.

Before proceeding with the properties of the twisted Dirac operator, a few notes are in order: whereas in twisted-mass lattice QCD simulations the twisted basis is rotated back to the physical basis for the calculation of observables, we interpret the m_5 -mass term as a deformation which vanishes in the chiral limit $m \rightarrow m_{\text{crit}}$, $m_5 \rightarrow 0$.⁶ In section 3.1 the correlators of the chiral partners $a\text{-}\eta'$ and $a\text{-}f_0$ are studied analytically and in section 4.3

⁴In contrast to 2-flavor twisted-mass QCD, where the twist term contains the Pauli matrix τ_3 , $\mathcal{N} = 1$ SYM theory contains only one flavor and thus τ_3 is absent.

⁵See for example [42], where the $a\text{-}f_0$ and $a\text{-}\eta'$ are described by one common complex field A of the chiral multiplet S .

⁶In contrast to QCD, where the quark masses are tuned to obtain the physical meson masses, the bare mass of the fermionic gluino m is tuned via eq. (2.5) to the point, where the renormalized gluino becomes massless, $m^{\text{R}} = 0$, in the continuum limit. At finite lattice spacing, this point is characterized by a minimal adjoint pion mass, which can not fall below the lattice cut-off. Hence all numerical values of m_{crit} mentioned in this paper are determined numerically this way.

	D_W of eq. (2.11)	D_W^{mtw} of eq. (2.8)
γ_5 -hermiticity	$(\gamma_5 D_W)^\dagger = \gamma_5 D_W$ $(D_W^{-1})^\dagger = \gamma_5 D_W^{-1} \gamma_5$	$(\gamma_5 D_W^{\text{mtw}}(m_5))^\dagger = \gamma_5 D_W^{\text{mtw}}(-m_5)$ $((D_W^{\text{mtw}})^{-1})^\dagger = (D_W^{\text{mtw}} + 2im_5 \gamma_5) \cdot (\gamma_5 D_W^{\text{mtw}} \gamma_5 D_W^{\text{mtw}} + 4m_5^2)^{-1}$
$\mathcal{C}$ -antisymmetry	$(\mathcal{C} D_W)^T = -\mathcal{C} D_W$	$(\mathcal{C} D_W^{\text{mtw}})^T = -\mathcal{C} D_W^{\text{mtw}}$
eigenvalues	double degenerated in complex conjugated pairs	complex
det	$\mathbb{R}^+$	$\mathbb{C}$
Pf	$\mathbb{R}$	$\mathbb{C}$

Table 3. Properties of the untwisted and twisted Wilson Dirac operator.

different “directions” in the (m, m_5) -plane for the extrapolation to the critical point are analyzed numerically. Both investigations reveal an optimal twist angle, for which the chiral partners have equal masses. This reduces the breaking of chirality and supersymmetry at finite lattice spacing considerably.

In contrast to Ginsparg-Wilson fermions, which preserve a variant of chiral symmetry even at finite lattice spacing [31], twisted fermions still break chiral symmetry. But since our main focus is on spectroscopy, the mass-degeneracy of chiral partners provides an improvement for the extrapolation to the critical point. In addition, the twisted formulation has the same computational costs as Wilson fermions which are much smaller than for Ginsparg-Wilson fermions with the overlap Dirac operator [26, 30] or the domain-wall formalism [27, 47].

A similar twist was used in [7] for the supersymmetric Wess-Zumino model in two dimensions. There, a modified Wilson term was tuned such that the discretization errors in the eigenvalues of the free lattice Dirac operator are reduced to $\mathcal{O}(a^4)$. For the $\mathcal{N} = 1$ SYM theory, we perform an analogous calculation for the twisted Wilson Dirac operator in section 3.3. As one option, we will also increase the freedom of finding a suitable action further by choosing the twist angles α, φ entering D_W^{dtw} independently. Then no direct connection between the action and the observables exist anymore, but $\mathcal{O}(a)$ improvement may be possible.

2.2.2 Properties of the Wilson Dirac operator

In table 3 we compare the relevant properties of the Wilson Dirac operator with and without mass twist. Most differences result from the loss of γ_5 -hermiticity when a mass twist is added and only a modified γ_5 -hermiticity involving $\pm m_5$ holds. As a consequence, the complex eigenvalues do not come in complex-conjugated pairs and the determinant as well as the Pfaffian may have non-zero imaginary parts. Nevertheless, we shall demonstrate in section 4.9 that only a very mild sign problem emerges. As we have seen for the particular choice $\alpha = \varphi$ in the double-twisted Wilson Dirac operator (2.12), the chiral phase can be removed by a change of variables and therefore the Pfaffian becomes real again.

2.2.3 Lattice observables

The simulations are performed with the action $S[\mathcal{U}, \lambda] = S_B[\mathcal{U}] + S_F[\mathcal{U}, \lambda]$, where the Lüscher-Weisz action $S_B[\mathcal{U}]$ was defined in eq. (2.6) and the fermionic action is given by

$$S_F[\mathcal{U}, \lambda] = \frac{1}{2} \text{tr}(\lambda^T \mathcal{C} D[\mathcal{U}] \lambda) = \frac{1}{2} \text{tr}(\lambda^T \tilde{D}[\mathcal{U}] \lambda), \quad (2.16)$$

with Wilson Dirac operator $D[\mathcal{U}]$ without twist (2.11) or with twisted mass (2.8). The effective action after integrating out the Majorana fermions is $S_{\text{eff}}[\mathcal{U}] = S_B[\mathcal{U}] - \log(\text{Pf}(\tilde{D}[\mathcal{U}]))$.

For hadron spectroscopy, interpolating lattice operators for the particles of interest are required. The interpolating operators for mesons are bilinears of the form

$$O(x) = \bar{\lambda}(x) \Gamma \lambda(x). \quad (2.17)$$

Specifically the interpolating operators for the adjoint mesonic states $a\text{-}\eta'$ and $a\text{-}f_0$ are [45]

$$O_{a\text{-}\eta'}(x) = \bar{\lambda}(x) i\gamma_5 \lambda(x) \quad \text{and} \quad O_{a\text{-}f_0}(x) = \bar{\lambda}(x) \lambda(x). \quad (2.18)$$

After integrating over the fermion field the correlators of these bilinears are given by gauge averages of products of the fermion lattice propagator

$$G_{xy} = \langle x | D^{-1} | y \rangle. \quad (2.19)$$

In particular, the correlators between the source at $y = (0, \vec{y})$ and the sink at $x = (t, \vec{x})$ contain connected and disconnected contributions

$$\begin{aligned} C(t) &= \langle O(t, \vec{p} = \vec{0}) O^\dagger(0, \vec{p} = \vec{0}) \rangle = \frac{1}{|\Lambda_3|^2} \sum_{\vec{x}, \vec{y} \in \Lambda_3} \langle O(t, \vec{x}) O^\dagger(0, \vec{y}) \rangle \\ &= \frac{1}{|\Lambda_3|^2} \sum_{\vec{x}, \vec{y} \in \Lambda_3} \langle \text{tr}(\Gamma G_{xx}) \text{tr}(\Gamma G_{yy}) \rangle_{\mathcal{U}} - \frac{2}{|\Lambda_3|^2} \sum_{\vec{x}, \vec{y} \in \Lambda_3} \langle \text{tr}(\Gamma G_{xy} \Gamma G_{yx}) \rangle_{\mathcal{U}}, \end{aligned} \quad (2.20)$$

where $\Gamma \in \{\mathbb{1}_4, \gamma_5\}$. For the connected⁷ two-point correlator, the contribution of the position-independent vacuum expectation value

$$\frac{1}{|\Lambda_3|^2} \sum_{\vec{x}, \vec{y} \in \Lambda_3} \langle \text{tr}(\Gamma G_{xx}) \rangle_{\mathcal{U}} \langle \text{tr}(\Gamma G_{yy}) \rangle_{\mathcal{U}} \quad (2.21)$$

must be subtracted from the correlator in eq. (2.20) [48]. Instead of fitting the constant vacuum contribution (2.21), it is beneficial to calculate the large cancellations between $\langle \text{tr}(\Gamma G_{xx}) \text{tr}(\Gamma G_{yy}) \rangle$ and $\langle \text{tr}(\Gamma G_{xx}) \rangle \langle \text{tr}(\Gamma G_{yy}) \rangle$ numerically. This procedure is further stabilized when y is consistently described by point sources and x is averaged over the whole

⁷We encounter a misuse of language. Here “connected” is understood in the sense of QFT calculations, where $W = \ln Z$ is used to compute connected Feynman diagrams approaching zero at large spatial separation. This must not be confused with the term “connected” to distinguish between contributions like the last term of eq. (2.20) compared to the “disconnected” contributions of the first term.

lattice with the stochastic estimator technique. In parameter sets with small ensemble sizes these signals are too noisy and we use instead the (unphysical) correlators

$$C_{a-\pi}(t) = \frac{2}{|\Lambda_3|^2} \sum_{\vec{x}, \vec{y} \in \Lambda_3} \langle \text{tr}(\gamma_5 G_{xy} \gamma_5 G_{yx}) \rangle_{\mathcal{U}} \quad \text{and} \quad C_{a-a}(t) = \frac{2}{|\Lambda_3|^2} \sum_{\vec{x}, \vec{y} \in \Lambda_3} \langle \text{tr}(G_{xy} G_{yx}) \rangle_{\mathcal{U}}, \quad (2.22)$$

which contain just the connected contributions.⁸

In $\mathcal{N} = 1$ SYM theory there exist also mixed states containing bosonic and fermionic building blocks. To measure the gluino-glueballs we define the interpolating operator⁹

$$[O_{\tilde{g}g}(x)]_{\alpha} = [\Sigma_{ij}]_{\alpha\beta} \text{tr}_c \left(F^{ij}(x) \lambda^{\beta}(x) \right) \quad (2.23)$$

with $\Sigma_{ij} \equiv [\gamma_i, \gamma_j]$ and the spatial clover plaquette $F_{ij}(x)$. Then, the corresponding correlator with source at y and sink at x including a matrix Γ to contract the indices is

$$\begin{aligned} C_{\tilde{g}g}(x, y) &= \langle \Gamma^{\mu\delta} [O_{\tilde{g}g}(x)]_{\mu} [\bar{O}_{\tilde{g}g}(y)]_{\delta} \rangle \\ &= - \left\langle [\Gamma^T]^{\delta\mu} [\Sigma_{ij}]_{\mu\beta} \text{tr}_c(F^{ij}(x) T^a) (G_{xy})_{ab}^{\beta\rho} \text{tr}_c(F^{lm}(y) T^b) [\Sigma_{lm}]_{\rho\delta} \right\rangle_{\mathcal{U}}. \end{aligned} \quad (2.24)$$

The gluino-gluon correlator has a time-symmetric and a time-antisymmetric component. By expanding the correlator in the spinor-space of complex 4×4 matrices, those are identified as the components of $\Gamma = \gamma_4$ and $\Gamma = \mathbb{1}_4$ respectively. In our simulations those two variants as well as the combinations $\Gamma = \frac{1}{2}(\mathbb{1}_4 \pm \gamma_4)$ are measured. It is reported that the antisymmetric component has a longer plateau in the effective mass and thus should be preferred for the determination of the ground state mass. On the other hand, the symmetric component is expected to have a better signal for the excited states [49, 50]. Although this correlator has no disconnected contribution, it requires high statistics because of sizable gauge field fluctuations.

Besides those states with gluino content, there exist glueballs states in the Farrar-Gabadadze-Schwetz (FGS) supermultiplet. In the continuum, bosonic states transform under tensor representations of the rotation group $SO(3)$, but the lattice discretization breaks this symmetry to the finite cubic group. With the help of the irreducible representations of the cubic symmetry group the eigenstates can be classified and a restoration of the rotation group in the continuum limit can be achieved [51]. For the scalar glueball $F_{\mu\nu} F^{\mu\nu}$ with quantum numbers $J^{PC} = 0^{++}$ we use the interpolating operator [52]

$$O_{0^{++}}(x) = \text{Re} \left(\text{tr}(\mathcal{U}_{12}(x) + \mathcal{U}_{23}(x) + \mathcal{U}_{31}(x)) \right). \quad (2.25)$$

The pseudoscalar glueball $\tilde{F}_{\mu\nu} F^{\mu\nu}$ with quantum numbers $J^{PC} = 0^{-+}$ can be measured with the operator

$$O_{0^{-+}}(x) = \text{Re} \sum_R (\text{tr}(\mathcal{W}(\mathfrak{C}_R)) - \text{tr}(\mathcal{W}(P\mathfrak{C}_R))) \quad (2.26)$$

⁸The connected correlators (2.22) as two-flavor states do not allow any vacuum contribution as in (2.21).

⁹The trace runs only over the color degrees of freedom and the indices i, j run only over the spatial directions to avoid any contributions of multiple time-slices [13].

Here we assumed that a, b are real, which is the case for the mesonic states under investigation. Without twist the operators for $a\text{-}f_0$ and $a\text{-}\eta'$ (compare to eq. (2.18)) have the form

$$a\text{-}f_0 : \quad \bar{\lambda}_x \lambda_x = O_{1,0}(x), \quad (3.2)$$

$$a\text{-}\eta' : \quad i\bar{\lambda}_x \gamma_5 \lambda_x = O_{0,1}(x). \quad (3.3)$$

Adding a chiral rotation as in eq. (2.14) to the spinors, those bilinears become

$$a\text{-}f_0 : \quad \bar{\lambda}_x e^{i\alpha\gamma_5} \lambda_x = O_{\cos(\alpha), \sin(\alpha)}(x), \quad (3.4)$$

$$a\text{-}\eta' : \quad i\bar{\lambda}_x \gamma_5 e^{i\alpha\gamma_5} \lambda_x = O_{-\sin(\alpha), \cos(\alpha)}(x). \quad (3.5)$$

Then, we can calculate the (general) expectation values

$$\begin{aligned} M_{a,b}(x, x') \equiv \langle O_{a,b}(x) O_{a,b}^\dagger(x') \rangle_F &= a^2 \langle \bar{\lambda}_x \lambda_x \bar{\lambda}_{x'} \lambda_{x'} \rangle_F - b^2 \langle \bar{\lambda}_x \gamma_5 \lambda_x \bar{\lambda}_{x'} \gamma_5 \lambda_{x'} \rangle_F \\ &\quad + abi \langle \bar{\lambda}_x \lambda_x \bar{\lambda}_{x'} \gamma_5 \lambda_{x'} \rangle_F + abi \langle \bar{\lambda}_x \gamma_5 \lambda_x \bar{\lambda}_{x'} \lambda_{x'} \rangle_F. \end{aligned} \quad (3.6)$$

The two terms in the last row have negative parity and thus must vanish. This can be seen explicitly, because the Green's function with parity transformed gauge field configuration $\mathcal{U}^P$ is related to the Green's function with the original configuration $\mathcal{U}$ as follows

$$G(\mathcal{U}^P; t, \vec{x}; t', \vec{x}') = \gamma_0 G(\mathcal{U}; t, -\vec{x}; t', -\vec{x}') \gamma_0. \quad (3.7)$$

For our parity-invariant theory,¹⁰ $\mathcal{U}$ and $\mathcal{U}^P$ have equal weight, such that indeed

$$\begin{aligned} C_{a\text{-}f_0, a\text{-}\eta'}(t) &= \frac{1}{|\Lambda_3|} \sum_{\vec{x}} \langle \bar{\lambda}(t, \vec{x}) \lambda(t, \vec{x}) \bar{\lambda}(0, \vec{0}) \gamma_5 \lambda(0, \vec{0}) \rangle \\ &= \frac{1}{|\Lambda_3|} \sum_{\vec{x}} \left\langle \text{tr}(G(t, \vec{x}; t, \vec{x})) \text{tr}(\gamma_5 G(0, \vec{0}; 0, \vec{0})) - 2 \text{tr}(G(t, \vec{x}; 0, \vec{0}) \gamma_5 G(0, \vec{0}; t, \vec{x})) \right\rangle_{\mathcal{U}} \\ &= -C_{a\text{-}f_0, a\text{-}\eta'}(t), \end{aligned} \quad (3.8)$$

i.e. $C_{a\text{-}f_0, a\text{-}\eta'}(t)$ vanishes. Thus, we get the expectation values

$$\begin{aligned} \langle O_{a\text{-}f_0}(x) O_{a\text{-}f_0}^\dagger(x') \rangle(\alpha) &= \langle M_{\cos(\alpha), \sin(\alpha)}(x, x') \rangle_{\mathcal{U}}, \\ \langle O_{a\text{-}\eta'}(x) O_{a\text{-}\eta'}^\dagger(x') \rangle(\alpha) &= \langle M_{-\sin(\alpha), \cos(\alpha)}(x, x') \rangle_{\mathcal{U}} \end{aligned} \quad (3.9)$$

and we see immediately that for the angle $\alpha = 45^\circ$,

$$\langle O_{a\text{-}f_0}(x) O_{a\text{-}f_0}^\dagger(x') \rangle(45^\circ) = \langle O_{a\text{-}\eta'}(x) O_{a\text{-}\eta'}^\dagger(x') \rangle(45^\circ). \quad (3.10)$$

The two mesons in the supermultiplet have identical correlators and thus the same mass.

In section 4.3 this mass-degeneracy on the lattice is verified, although at finite lattice spacing supersymmetry and chiral symmetry are broken. Actually, in the simulations we

¹⁰At the moment, the twist is only on the level of the observable and the action consists of the parity-invariant Wilson Dirac fermion action and for example the Wilson gauge action.

did not chirally rotate the fermion field in the observables (as we did in our analytic analysis) but instead used the Wilson Dirac operator with twisted mass term (2.8). We have argued that (up to a twist of the irrelevant Wilson term) this is equivalent to twisting the field in the observables.

Finally, let us see how the third particle in the VY-supermultiplet is affected by a chiral rotation (2.14). The starting point is the interpolating operator (2.23) for the fermionic gluino-gluon state with a twist,

$$[O_{\tilde{g}g}(x)]_\mu = [\Sigma_{ij}]_{\mu\nu} \text{tr} \left(F^{ij}(x) [e^{i\alpha\gamma_5/2} \lambda(x)]^\nu \right).$$

The corresponding correlator has the form

$$\langle \Gamma^{\mu\delta} [O_{\tilde{g}g}(x)]_\mu [\bar{O}_{\tilde{g}g}(y)]_\delta \rangle = - \left\langle \text{tr} \Gamma^T F^{ij}(x) \Sigma_{ij} e^{i\alpha\gamma_5/2} G_{x,y} e^{i\alpha\gamma_5/2} F^{lm}(y) \Sigma_{lm} \right\rangle_{\mathcal{U}}. \quad (3.11)$$

With the cyclicity of the trace one easily sees that for the antisymmetric correlator with $\Gamma = \mathbb{1}_4$ a chiral phase factor $e^{i\alpha\gamma_5}$ arises and for the symmetric correlator with $\Gamma = \gamma_4$ the chiral twists cancel.

3.2 Supersymmetry transformations of the lattice operators

When the gluino is twisted as in eq. (2.14), then no additional terms arise in the supersymmetry transformations. The only modification is an additional chiral phase factor multiplying the spinor field λ , and this is carried through the whole calculation. It follows that every supermultiplet stays intact. Without twists the off-shell supersymmetry transformations of the continuum theory have the simple form

$$\begin{aligned} \delta_\epsilon \lambda(x) &= \frac{1}{4} \Sigma_{\mu\nu} F^{\mu\nu}(x) \epsilon + i\mathcal{G}(x) \gamma_5 \epsilon, & \delta_\epsilon A_\mu(x) &= i\bar{\epsilon} \gamma_\mu \lambda(x), \\ \delta_\epsilon \bar{\lambda}(x) &= -\frac{1}{4} \bar{\epsilon} \Sigma_{\mu\nu} F^{\mu\nu}(x) + i\bar{\epsilon} \mathcal{G}(x) \gamma_5, & \delta_\epsilon \mathcal{G}(x) &= \bar{\epsilon} \gamma_5 \not{D} \lambda(x). \end{aligned} \quad (3.12)$$

Therein, ϵ is a constant Majorana-valued anticommuting parameter and $\mathcal{G}$ is an auxiliary field. To determine the transformation of the gluino-gluon state one needs the transformation of the field strength tensor,

$$\delta_\epsilon F_{\mu\nu}(x) = i\bar{\epsilon} (\gamma_\nu D_\mu - \gamma_\mu D_\nu) \lambda(x). \quad (3.13)$$

The supersymmetry transformations of the composite operators generating the VY-supermultiplet are obtained with help of Fierz identities [53, 54], derived from the general identity

$$4\psi\bar{\chi} = -(\bar{\chi}\psi) - \gamma_\mu(\bar{\chi}\gamma^\mu\psi) + \frac{1}{2}\gamma_{\mu\nu}(\bar{\chi}\gamma^{\mu\nu}\psi) + \gamma_5\gamma_\mu(\bar{\chi}\gamma_5\gamma^\mu\psi) - \gamma_5(\bar{\chi}\gamma_5\psi). \quad (3.14)$$

One finds the transformations

$$\delta_\epsilon O_{a-f_0}(x) = -\frac{1}{2} \bar{\epsilon} O_{\tilde{g}g}(x) + 2i\bar{\epsilon} \mathcal{G}(x) \gamma_5 \lambda(x), \quad (3.15)$$

$$\delta_\epsilon O_{a-\eta'}(x) = -\frac{1}{2} \bar{\epsilon} \gamma_5 O_{\tilde{g}g}(x) + 2i\bar{\epsilon} \mathcal{G}(x) \lambda(x), \quad (3.16)$$

$$\delta_\epsilon (O_{\tilde{g}g}(x) - 4i\mathcal{G}(x) \gamma_5 \lambda(x)) = 2i\not{D} O_{a-f_0}(x) \epsilon + 2i\gamma_5 \not{D} O_{a-\eta'}(x) \epsilon + \dots \quad (3.17)$$

The terms linear in the auxiliary field $\mathcal{G}$ as well as further terms indicated with the dots in eq. (3.17) vanish on-shell and thus the VY-supermultiplet defines a chiral supermultiplet.

After a Wick-rotation to Euclidean spacetime, the on-shell supersymmetry transformation in eq. (3.12) read [55–57]

$$\delta_\epsilon A_\mu(x) = i\bar{\epsilon}\gamma_\mu\lambda(x), \quad \delta_\epsilon\lambda(x) = \frac{1}{4i}\Sigma_{\mu\nu}F^{\mu\nu}(x)\epsilon, \quad \delta_\epsilon\bar{\lambda}(x) = -\frac{1}{4i}\bar{\epsilon}\Sigma_{\mu\nu}F^{\mu\nu}(x). \quad (3.18)$$

Although Majorana spinors in 4-dimensional Euclidean spacetime cannot be defined consistently, we instead may use the consistent condition $\bar{\lambda} = \lambda^T \mathcal{C}$ [58]. This way the same symmetries for the bilinears $\bar{\psi}\gamma^{\mu_1\cdots\mu_n}\chi$ hold as in Minkowski spacetime. The corresponding transformations of the composite fields $O_{a-f_0}(x)$, $O_{a-\eta'}(x)$ and $O_{\tilde{g}g}(x)$ in Euclidean spacetime are just the Wick-rotations of the transformations (3.15), (3.16) and (3.17). This can be shown explicitly by observing that the Fierz identities used to derive these transformations exist in Minkowski and Euclidean spacetime.

At finite lattice spacing supersymmetry is broken and this will lead to additional terms in the transformation laws. The lattice susy transformation can be formulated as [56, 59]

$$\delta_\theta \mathcal{U}_\mu(x) = -\frac{ig}{2}(\bar{\theta}(x)\gamma_\mu \mathcal{U}_\mu(x)\lambda(x) + \bar{\theta}(x+\hat{\mu})\gamma_\mu\lambda(x+\hat{\mu})\mathcal{U}_\mu(x)) \quad (3.19)$$

$$\delta_\theta \mathcal{U}_\mu^\dagger(x) = \frac{ig}{2}(\bar{\theta}(x)\gamma_\mu\lambda(x)\mathcal{U}_\mu^\dagger(x) + \bar{\theta}(x+\hat{\mu})\gamma_\mu\mathcal{U}_\mu^\dagger(x)\lambda(x+\hat{\mu})) \quad (3.20)$$

$$\delta_\theta\lambda(x) = \frac{1}{4i}\Sigma_{\mu\nu}P^{\mu\nu}(x)\theta(x) \quad (3.21)$$

$$\delta_\theta\bar{\lambda}(x) = -\frac{1}{4i}\bar{\theta}(x)\Sigma_{\mu\nu}P^{\mu\nu}(x) \quad (3.22)$$

with clover plaquette $P^{\mu\nu}(x)$ and infinitesimal Majorana parameters $\bar{\theta}$ and θ . In the continuum limit the corresponding transformations (3.18) are recovered.

3.3 Eigenvalues of the free Wilson Dirac operator

For particular twists of the free lattice Dirac operator in lower-dimensional Wess-Zumino models an improvement up to order $\mathcal{O}(a^4)$ can be achieved [7, 60]. In order to see whether an improvement is also possible for the double-twisted lattice Dirac operator in supersymmetric gauge theory we determine the eigenvalues of the operator D_W^{dtw} (see eq. (2.12)) for free fermions, that is for trivial link variables $\mathcal{V}_\mu = \mathbb{1}$. Thus we calculate the eigenvalues and expand them in powers of the lattice spacing a to study the discretization errors. Then, the dependence on the twist angles α, φ is analyzed to check if $\mathcal{O}(a)$ improvement is possible for particular choices.¹¹ We decompose the double-twisted lattice Dirac operator for free fermions,

$$D_W^{\text{dtw}} = \gamma^\mu \hat{\partial}_\mu + M e^{i\alpha\gamma_5} - \frac{aR}{2} e^{i\varphi\gamma_5} \hat{\Delta} = \gamma^\mu \hat{\partial}_\mu + X + i\gamma_5 Y, \quad (3.23)$$

which contains the naive antisymmetric lattice derivative $\hat{\partial}_\mu$ and the symmetric lattice Laplacian $\hat{\Delta}$ (we use the notation of [61]). The real operators X, Y in the last decomposition are

$$X = M \cos \alpha - \frac{aR}{2} \hat{\Delta} \cos \varphi, \quad Y = M \sin \alpha - \frac{aR}{2} \hat{\Delta} \sin \varphi. \quad (3.24)$$

¹¹In our simulations, $(r, r_5) = (1, 0)$ resp. $R = \sqrt{r^2 + r_5^2} = 1$ and $\varphi = 0$ is chosen if no other value is stated.

The periodic eigenfunctions are constant spinors times plane waves on a $L^3 \times T$ lattice:

$$\psi_p(x) = u_p e^{ip_\mu x^\mu}, \quad p_0 = \frac{2\pi}{aN_t} \left(n_0 + \frac{1}{2} \right), \quad p_i = \frac{2\pi}{aN} n_i. \quad (3.25)$$

Plane waves are eigenfunctions of the derivative operators and the Laplacian,

$$\hat{\partial}_\mu \mapsto i\hat{p}_\mu, \quad \hat{p}_\mu = \frac{1}{a} \sin(ap_\mu), \quad \hat{\Delta} \mapsto -\hat{p}_\mu \hat{p}^\mu, \quad \hat{p}_\mu = \frac{2}{a} \sin\left(\frac{ap_\mu}{2}\right). \quad (3.26)$$

In a sector with fixed momentum the operator X is a constant X_p which just shifts the eigenvalues of D_W^{dtw} in eq. (3.23). Hence it suffices to determine the imaginary eigenvalues of the 4-dimensional anti-Hermitian matrix $\mathcal{A}$ in $D_W^{\text{dtw}} = \mathcal{A} + X$ for fixed momentum,

$$\mathcal{A}_p u_p = (i\gamma^\mu \hat{p}_\mu + i\gamma_5 Y_p) u_p = i\mu_p u_p, \quad \mu_p \text{ real}. \quad (3.27)$$

Since $\mathcal{A}_p \mathcal{A}_p^\dagger = \hat{p}^2 + Y_p^2$ is a multiple of the identity matrix we conclude that $\mu_p^2 = \hat{p}^2 + Y_p^2$. In Euclidean spacetime there exists an antisymmetric charge conjugation matrix $\mathcal{C}_+$ with

$$\mathcal{C}_+ \gamma_\mu^T \mathcal{C}_+^{-1} = \gamma_\mu, \quad \mathcal{C}_+ \gamma_5^T \mathcal{C}_+^{-1} = \gamma_5. \quad (3.28)$$

Taking the complex conjugate of the eigenvalue equation (3.27) and acting with $\mathcal{C}_+$ on this equation (and also using that γ^μ and γ_5 are Hermitian) we see that the charge conjugated constant spinor $\mathcal{C}_+ u_p^*$ is a second eigenvector with the same eigenvalue $i\mu_p$. Finally, since $\text{tr}(\mathcal{A}_p) = 0$ we deduce, that $\mathcal{A}_p$ has two eigenvalues $i\mu_p$ and two eigenvalues $-i\mu_p$. We conclude that for fixed p_μ the twisted Dirac operator $D_W^{\text{dtw}} = \mathcal{A} + X$ has the double degenerate eigenvalues

$$\lambda_p = X_p + i\mu_p \quad \text{and} \quad \lambda_p^* = X_p - i\mu_p, \quad \mu_p = \sqrt{\hat{p}^2 + Y_p^2}. \quad (3.29)$$

Up to a possible sign the Pfaffian of the Dirac operator is the square root of its determinant and hence given by the product of all $|\lambda_p|^2$, where

$$|\lambda_p|^2 = \hat{p}^2 + X_p^2 + Y_p^2 = \hat{p}^2 + M^2 + \frac{(aR)^2}{4} \hat{p}^2 \hat{p}^2 + (aR) M \hat{p}^2 \cos(\alpha - \varphi). \quad (3.30)$$

Inserting the small- a expansions of $\hat{p}_\mu$ and $\hat{p}^\mu$ in eq. (3.26) gives rise to

$$|\lambda_p|^2 = p^2 + M^2 + (aR) M p^2 \cos(\alpha - \varphi) + \frac{a^2}{12} \left(3R^2 (p_\mu p^\mu)^2 - 4 \sum_\mu p_\mu^4 \right) + \mathcal{O}(a^3). \quad (3.31)$$

Here we see explicitly that setting $\alpha - \varphi = 90^\circ$ leads to an $\mathcal{O}(a)$ improvement in the fermionic sector — at least for free fermions.

Table 4 summarizes the values for $|\lambda_p|^2$ and their small- a expansions for various lattice Dirac operators considered in the present work. Starting from the Wilson Dirac operator D_1 with $\mathcal{O}(a)$ discretization errors, we can remove the leading discretization effects by choosing a 90° -twist like in D_2 (as in fully twisted lattice QCD [40]) or by modifying the Wilson term like in D_3 . In general, for free fermions $\mathcal{O}(a)$ improvement can be achieved when the mass term and Wilson term are orthogonal to each other, i.e. $\alpha - \varphi = 90^\circ \pmod{180^\circ}$ in D_4 .

The mass difference of the superpartners $a\text{-}f_0$ and $a\text{-}\eta'$ is minimal for $\alpha - \varphi = 45^\circ$, see figure 7. Since in the present work our main focus is on the restoration of supersymmetry and chirality we choose $\alpha - \varphi = \alpha = 45^\circ$ in our simulations. Then there is a reduction of the leading order discretization errors by a factor of $\cos(45^\circ) = 1/\sqrt{2}$.

lattice Dirac operator	eigenvalues $ \lambda_p ^2$
$D_1 = \gamma^\mu \hat{\partial}_\mu + M - \frac{aR}{2} \hat{\Delta}$	$p^2 + M^2 + aMRp^2 + \mathcal{O}(a^2)$
$D_2 = \gamma^\mu \hat{\partial}_\mu + M - \frac{iaR}{2} \gamma_5 \hat{\Delta}$	$p^2 + M^2 + \kappa a^2 + \mathcal{O}(a^4)$
$D_3 = \gamma^\mu \hat{\partial}_\mu + M e^{i\alpha\gamma_5} - \frac{aR}{2} \hat{\Delta}$	$p^2 + M^2 + aMRp^2 \cos(\alpha) + \mathcal{O}(a^2)$
$D_4 = \gamma^\mu \hat{\partial}_\mu + M e^{i\alpha\gamma_5} - \frac{aR}{2} e^{i\varphi\gamma_5} \hat{\Delta}$	$p^2 + M^2 + aMRp^2 \cos(\alpha - \varphi) + \kappa a^2 + \mathcal{O}(a^3)$

Table 4. Eigenvalues $|\lambda_p|^2$ of several lattice Dirac operators D_i , expanded in powers of the lattice spacing a . We defined $\kappa \equiv -\frac{1}{3} \sum_\mu p_\mu^4 + \frac{R^2}{4} (p_\mu p^\mu)^2$.

4 Numerical investigations

In this section we present, compare and discuss our lattice results for $\mathcal{N} = 1$ SYM theory with and without twisted mass term. As demonstrated below, finite size effects are clearly visible in the data, while lattice spacing artifacts are more or less absent. That means it will be beneficial to choose a slightly larger gauge coupling in future simulations. However, as we shall see in this section, for the optimal twist angle $\alpha = 45^\circ$ finite size effects are less severe. Table 6 in appendix B lists the lattice couplings, lattice sizes, mass parameters and Wilson parameters used in the simulations.

4.1 Scale-setting

To set the scale, the Sommer parameter and QCD units are used, i.e., $r_0 = 0.5 \text{ fm}$ [62]. In the given context this is somewhat arbitrary but it allows for a direct comparison with results in the literature.

For our estimates of a/r_0 , we calculate rectangular Wilson loops of different size and extract the static potential $V(R)$ for a range of spatial separations R . In temporal direction all loops are sufficiently large such that $V(R)$ remains stable. Furthermore, different levels of stout smearing are applied to the gauge fields (with staple weight $\rho = 0.1$ [63]) and the Wilson fermion mass term is varied to allow for a safe extrapolation to the critical point, $m \rightarrow m_{\text{crit}}$. For the different levels of smearing and Wilson term mass values, the results for $V(R)$ are separately fitted to

$$V(R) = V_0 + \sigma R - \frac{\alpha}{R}. \quad (4.1)$$

From the fit parameters and setting

$$\frac{r_0}{a} \equiv \sqrt{\frac{1.65 - \alpha}{\sigma a^2}} \quad (4.2)$$

we obtain the lattice spacing and can extrapolate to the critical point.

As an example, the lattice spacing for ensemble (II) is shown in figure 2 for different steps of stout smearing, and for $m \rightarrow m_{\text{crit}}$. We find that for a large number of stout smearing steps, the static potential changes its shape, but for a moderate number, as shown in figure 2, the lattice spacing values are all comparable. Combining the data in a linear fit

Figure 2. Dimensionless lattice spacing a/r_0 vs. gauge smearing steps. The values include an extrapolation to the critical point at m_{crit} . To this end the parameter set (II) is fitted to $V(R)$ for different m , see table 6 in section B. As long as only a few gauge smearing steps are applied, all values are comparable.

Figure 3. Left/Center: $a\text{-}\pi$ resp. $a\text{-}a$ correlator at $\beta = 5.4$ and $(m, m_5) = (-0.8950, 0.0)$ with 2-cosh-fits. The gray data points are excluded from the fit to reduce contributions from higher states and to stabilize the fit. Error bars are smaller than the symbol size. Right: the dominant mass contribution d from fits with different cuts $t_{\text{cut}} = (t_1, t_2)$. The gray vertical lines separate regions with different values of t_2 .

leads to the lattice spacing $a = (0.040 \pm 0.002)$ fm for ensemble (II). This translates into a spatial lattice $aL = (0.64 \pm 0.03)$ fm for this ensemble. In comparison to other lattice studies, e.g. [64], a box length $aL < 1$ fm appears small and finite size effects need to be carefully analyzed. This is provided in the following section.

4.2 Finite size analysis

We continue with ensemble (V) and show data for the $a\text{-}\pi$ and $a\text{-}a$ correlators for $(m, m_5) = (-0.8950, 0.0)$ in figure 3. Looking at the left and middle panel of this figure, one clearly

Figure 4. Dominant mass contribution of $a\text{-}\pi$ and $a\text{-}a$ for different lattice sizes $L^3 \times 2L$ with $L \in \{4, 8, 12, 16, 20, 24\}$. The bare gluino mass is $(m, m_5) = (-1.0506, 0.0)$ and the lattice coupling $\beta = 5.0$. Points are slightly displaced for better visibility.

sees both correlators would not fit a simple cosh-like t -dependence. Up to $t = 5$ (and $T - t = 5$), contributions from higher states are significant, and the interval where a single exponential behavior dominates is rather short. To fit the t -dependence we therefore choose a 2-cosh ansatz

$$C(t) = c_1 \cosh(d_1(t - T/2)) + c_2 \cosh(d_2(t - T/2)) \quad (4.3)$$

and vary the fit ranges $t \in [t_1, T/2 - t_2]$ and $t \in [T/2 + t_2, T - t_1]$. Furthermore, we will refer to $d = \min(d_1, d_2)$ as the *dominant mass contribution*. It corresponds to the ground state mass on sufficiently large lattices.

As an example, the 2-cosh fits for $t_1 = 2$ and $t_2 = 4$ are included in figure 3. Colored symbols refer to points inside the fit range, while gray symbols to points outside. Although cutting the inner time slices is not necessary, as we will see, it turns out to be useful nonetheless: near the critical point, the correlators of the connected part of the mesonic states are flat while those of the disconnected part are dominated by statistical noise. Applying cuts on both sides of the fit ranges stabilizes the fits and reduces the contributions of excited states.

Results for $d_{a\text{-}\pi}$ and $d_{a\text{-}a}$, and for different combinations of t_1 and t_2 , are shown in the right panel of figure 3. There, the upper t_2 -axis divides the panel (vertical lines) into four domains and each domain shows d versus t_1 at constant t_2 . We see that a variation of t_2 has a minor effect on the value for d , whereas there is a clear linear dependence on t_1 . In particular for $a\text{-}a$ this dependence is significant.

Using the same ansatz as before we can analyze d as a function of L . For $\beta = 5.0$ and $(m, m_5) = (-1.0506, 0.0)$ we did simulations for $L = 4, \dots, 24$ and the results for the adjoint states are shown in figure 4 (for $(t_1, t_2) = (2, 0)$). For the adjoint pion, d forms a plateau at approximately $d = 0.2$ for $L \geq 16$, while for $a\text{-}a$ the situation is not as clear. A

similar behavior is seen for $\beta = 4.5$. The volume effects for $a\text{-}\pi$ are mild, while for $a\text{-}a$ an unambiguous mass extraction is more difficult despite a good signal-to-noise ratio.

Volume effects are also apparent in the effective mass plots. Such plots, and the corresponding $a\text{-}\pi$ and $a\text{-}a$ correlators, are shown in figure 5, again for $\beta = 5.0$, $(m, m_5) = (-1.0506, 0.0)$ and $L = 8, 16, 24$. The first three columns compare the effective mass and the correlators for $a\text{-}\pi$ and $a\text{-}a$ for a fixed lattice size, while the panels in column 4 and 5 show them separately for $a\text{-}\pi$ and $a\text{-}a$ for different volumes and versus t/T . Looking at the first three upper panels in figure 5 we notice an intersection of the effective mass values at a certain t . The effective mass of $a\text{-}a$ falls off faster with t than that of $a\text{-}\pi$ and approaches a lower value. Furthermore, the deviations seem to increase with increasing volume. This is in contrast to common expectations, because $a\text{-}\pi$ should be the lighter state. Most likely it is the small volume ($aL < 1$ fm) which causes $a\text{-}a$ appearing lighter than $a\text{-}\pi$.

Indications for this are also provided by the last two upper panels of figure 5 showing the same data sets as the first three panels but as function of the rescaled variable t/T such that finite size effects are better visible. We see the effective mass curves of $a\text{-}\pi$ settle on the same value on all lattices and only the length of the plateau increases with lattice size. But for the $a\text{-}a$ state the effective mass seems not to approach a single plateau, if at all, rather m_{eff} gets smaller when increasing the lattice size which indicates an enhanced correlation length. This is in line with the correlator plots in the lower panels of figure 5. There, the $a\text{-}a$ correlator on the largest lattice ($24^3 \times 48$) decays visibly faster than the $a\text{-}\pi$ correlator for $0 < t \lesssim 15$. For the smaller lattices this effect is less pronounced. Again we see that finite size effects are small for $a\text{-}\pi$, while they are more pronounced for $a\text{-}a$. This supports our interpretation of the results in figure 4.

In summary, especially the $a\text{-}a$ state is problematic in small volumes, where a flat region appears in its correlator and the extracted dominant mass contribution is underestimated. In some distance to the critical point this lattice artifact is less pronounced and the mass hierarchy is as expected, $m_{a\text{-}a} > m_{a\text{-}\pi}$. But with D^{mtw} and optimal twist angle, the correlators of $a\text{-}\pi$ and $a\text{-}a$ have identical shapes and no observable finite volume artifacts remain.

Let us recall at this point that the connected mesonic states are not part of the physical spectrum of the $\mathcal{N} = 1$ SYM theory. But these auxiliary states are very useful, mainly because the signal-to-noise-ratio of the related correlators are much better compared to those of the physical mesonic states with disconnected contributions. Therefore we use the connected mesons for ensembles with low statistics, like in this section or the parameter scan in the next section. In addition, the connected diagrams contribute to the correlators of the physical states, see eq. (2.20) and (2.21). Hence, the connected mesonic states partly determine the behavior of the full physical states.

4.3 Parameter scan

After discussing finite size effects for the untwisted system, we now analyze the effect of a twisted mass term for Wilson fermions. To this end, we calculate the dominant mass contribution of the $a\text{-}\pi$ and $a\text{-}a$ correlators in the (m, m_5) parameter space by performing a parameter scan. For this scan we fix the lattice coupling and size to $\beta = 5.4$ and $8^3 \times 16$ and

Figure 5. Top/Bottom: effective masses/correlators of the adjoint pion and the adjoint a at fixed bare gluino mass $m = -1.0506$ and lattice coupling $\beta = 5.0$, without mass twist. From left to right the first three columns show results for a - π and a - a from a $8^3 \times 16$, $16^3 \times 32$ and $24^3 \times 48$ lattice. The last two compare a - π and a - a for different lattice sizes. Most error bars are smaller than the symbol size. In the last two columns, data points are connected by lines and symbols and error bars are omitted for better visibility.

vary the mass parameter $m \in [-1.4, -0.6]$ and the twist parameter $m_5 \in [-0.4, 0.4]$ around the critical point, $(m, m_5) = (-0.967, 0.0)$. Due to the $(m_5 \leftrightarrow -m_5)$ -symmetry, fine parameter steps are necessary only in the upper half-plane of the parameter space; see left and middle plot of figure 6. Every gauge ensemble consists of approximately 200 thermalized configurations which is sufficient for a good signal-to-noise-ratio for the correlators. To determine their dominant mass contribution d , all correlators are fitted to the ansatz (4.3) as in the previous section. On a rather small $8^3 \times 16$ lattice, the quantity d is only a rough estimate for the ground state mass and the results for the latter are more qualitative than quantitative. However, the simulation results on a larger $16^3 \times 32$ lattice support our findings.

Note that we treat the twist as a deformation of the lattice action and do *not* rotate observables back, as is done in twisted mass QCD. In the limit $(m \rightarrow m_{\text{crit}}, m_5 \rightarrow 0)$ the twisted Wilson Dirac operator D_W^{mtw} (2.8) is equivalent to the Wilson Dirac operator D_W (2.11) such that both operators correspond to the same continuum theory. But along certain paths ending at the critical parameters (belonging to the continuum theory) the breaking of chiral symmetry and of supersymmetry maybe suppressed.

Figure 6 shows the dominant mass contributions. The left and center panel show $d_{a-\pi}$ and d_{a-a} , respectively, while in the right panel the subtracted ratio $d_{a-\pi}/d_{a-a} - 1$ near the critical point is shown. Three interesting choices for the twist angle α are highlighted in these panels:

- The data points for the untwisted case with $\alpha = 0^\circ$ and $m_5 = 0$ along the gray line indicate that $d_{a-\pi}$ is greater than d_{a-a} .

Figure 6. Parameter scan in m and m_5 on a $8^3 \times 16$ lattice. In the left and middle plot the dominant mass contribution d of the a - π (connected part of the a - η') resp. a - a (connected part of the a - f_0) are shown. The right plot combines those results in the subtracted ratio $d_{a-\pi}/d_{a-a} - 1$. Note the different axis ranges. The colored lines (gray, magenta and yellow) are discussed in the text.

- For $\alpha = 45^\circ$ along the diagonal magenta line, the dominant mass contributions of the chiral partners a - π and a - a seem to match.
- At maximal twist, i.e., $\alpha = 90^\circ$, where the bare gluino mass is kept fixed at its critical value, $m = m_{\text{crit}} = -0.967$, and only the twisted mass parameter m_5 is varied, d_{a-a} is greater than $d_{a-\pi}$, see vertical yellow line.

The results clearly favor a twist angle $\alpha = 45^\circ$ with improved chiral properties at finite lattice spacing. This interpretation is supported by the results shown in figure 7, where the dominant mass contributions d_{a-a} and $d_{a-\pi}$ are shown versus the renormalized gluino mass $m^R \propto m_{a-\pi}^2$. At $\alpha = 45^\circ$ the two chiral partners have equal mass within errors. In contrast, for $\alpha = 0^\circ$ and $\alpha = 90^\circ$ we clearly see a split of the two masses.¹²

To substantiate this observation on the small $8^3 \times 16$ lattice, we double the lattice in each direction and repeat our calculation for the gauge couplings $\beta \in \{4.5, 5.0, 5.4\}$ along the three aforementioned directions in parameter space. For the fit we choose $t_{\text{cut}} = (2, 4)$. The results are summarized in figure 8. We see that without twist the dominant a - a contribution is greater than the a - π contribution, at $\alpha = 45^\circ$ both contributions are equal, and at maximal twist $\alpha = 90^\circ$ the a - a contribution is smaller than that of a - π . Compared to the small volume results in figure 7, the mass hierarchies for $\alpha = 0^\circ$ and $\alpha = 90^\circ$ are inverted, which is a finite size effect, but our findings for $\alpha = 45^\circ$ remain and are barely affected by the size of the lattice.

In subsequent sections, we will therefore focus on the twist angle $\alpha = 45^\circ$ with improved chiral and supersymmetry properties at finite lattice spacing. Furthermore from section 3.3 we know this special twist comes with an $\mathcal{O}(a)$ improvement at tree level which may at least reduce lattice spacing artifacts also at the non-perturbative level. Performing continuum extrapolations along the $\alpha = 45^\circ$ direction may thus be beneficial.

What remains is a cross-check of our findings for other observables. The chiral condensate $\Sigma \sim \langle \bar{\lambda}(x)\lambda(x) \rangle$ and the parity condensate $\Sigma^P \sim \langle i\bar{\lambda}(x)\gamma_5\lambda(x) \rangle$ are good candidates built from the gluino field, see eqs. (2.27) and (2.28). A parameter scan of those conden-

¹²See appendix A for a discussion of the expected mass hierarchy and also compare with figure 8.

Figure 7. The three plots correspond to twist angles $\alpha \in \{0^\circ, 45^\circ, 90^\circ\}$ marked in figure 6 with lines in gray, magenta and yellow. The same data of the $8^3 \times 16$ lattice is used and three clearly different mass hierarchies of the dominant contribution d are revealed. Some error bars are smaller than the symbol size. The gray solid lines visualize the dependence of the adjoint pion on the renormalized gluino mass, see eq. (2.5).

sates along the three “directions”, i.e., $\alpha \in \{0^\circ, 45^\circ, 90^\circ\}$, is shown in figure 9. In the left panel we notice that the chiral condensate is maximal for $m_5 = 0$ and falls off as soon as $m_5 \neq 0$. Again we see a mirror symmetry in $m_5 \leftrightarrow -m_5$ as for the dominant mass contribution $d_{a-\pi}$ of the adjoint pion. The chiral condensate can be fitted well with a polynomial of second order while for the parity condensate a first order polynomial is sufficient. The parity condensate is shown in the right panel of figure 9. Along $m_5 = 0$ it is zero, but if m_5 increases the condensate decreases linearly and vice versa.

Altogether we learn from figure 9, for the condensates $\alpha = 45^\circ$ is not a distinguished direction in the (m, m_5) parameter plane. Only on-axis directions, that is 0° and 90° , are special. However, we will see below that for a double-twisted Dirac operator, $\alpha = \varphi = 45^\circ$ is special also for the condensates, because then the condensates are equal (see figure 15 and eq. (4.5) in section 4.8).

4.4 Physical mesonic states

Up to now, only the connected contribution to the mesonic states $a-\eta'$ and $a-f_0$ has been analyzed. For a determination of their mass in the VY-supermultiplet, additional lattice calculations of the correlator’s disconnected diagram is required, see eqs. (2.20) and (2.21). Compared to the connected contribution, the numerical effort for the disconnected part is rather large. Its magnitude is small and it comes with a large statistical uncertainty. Furthermore, there are two contributions: $\langle \text{tr}(\Gamma G_{xx}) \text{tr}(\Gamma G_{yy}) \rangle_{\mathcal{U}}$ and $\langle \text{tr}(\Gamma G_{xx}) \rangle \langle \text{tr}(\Gamma G_{yy}) \rangle_{\mathcal{U}}$, whose difference enters the correlator. High statistics is thus a prerequisite for a reasonable mass estimate not only for those two VY-supermultiplet partners.

For the twist angle $\alpha = 45^\circ$, we have performed high-statistics calculations of both the connected and disconnected contribution for a fixed lattice coupling ($\beta = 5.0$) and a

Figure 8. Connected mesons on the $16^3 \times 32$ lattice. From left to right the twist angle $\alpha \in \{0^\circ, 45^\circ, 90^\circ\}$ rises. From top to bottom the lattice coupling $\beta \in \{4, 5.5, 5.4\}$ increases. Some error bars are smaller than the symbol size and some data points for $\alpha = 45^\circ$ lie on top of each other. The gray solid lines visualize eq. (2.5).

single lattice size ($16^3 \times 32$). Thereby the mass and twisted-mass parameters were varied to extrapolate them afterwards towards their critical values (see table 7(b)).

Results for the dominant mass contribution (i.e., for the approximate ground state mass) for $a\text{-}\eta'$ and $a\text{-}f_0$ are shown in figure 10 versus the renormalized gluino mass. They are obtained from fits of the lattice two-point correlators to the same 2-cosh ansatz as used above. For $a\text{-}f_0$, additional results from a 1-cosh fit are shown. For $a\text{-}\eta'$ there are also results for the next higher state, d^* , in figure 10.

While for $d_{a\text{-}f_0}$ the statistical fluctuations are large, both for the 2-cosh and 1-cosh fit, the results for $a\text{-}\eta'$ are much preciser such that a trend can be seen. For $a\text{-}\eta'$, d and d^* clearly decrease with m^R and approach finite values at $m^R = 0$. One would expect, the ground state mass of $a\text{-}\eta'$ near the critical point is approximately 0.2 in lattice units, while the mass of the next higher state tends towards a value above 1. For $d_{a\text{-}f_0}$, the lowest mass

Figure 9. Left: the (unrenormalized) chiral condensate Σ and fit to polynomial of second order. Right: the parity condensate Σ^P and fit to a plane. The squares, triangles and circles correspond to $\alpha = 0^\circ, 45^\circ$ and 90° .

contribution is below 0.4 within errors.

Within statistical fluctuations we can hardly distinguish the correlation functions of the physical mesons $a\text{-}\eta'$, $a\text{-}f_0$ and from those of their partially quenched approximations $a\text{-}\pi$ and $a\text{-}a$. Since the ground state masses of $a\text{-}\pi$ and $a\text{-}a$ vanish in the chiral limit this would also be true for the physical meson masses. However in section 4.7, we will revisit the chiral extrapolations of the would-be Goldstone bosons and physical mesons and argue that the physical masses remain massive in the chiral limit. In addition we include further states beside the two mesonic states considered here.

Although the $a\text{-}f_0$ correlator is noisy, in particular at the inner time slices, we try to get an approximate value for its first excited state at small t where the signal-to-noise-ratio is better. Without knowing the exact ground state mass, we assume $d_{a\text{-}f_0} = d_{a\text{-}\eta'}$ and fit $C(t) - c_1 e^{-dt} \approx c_2 e^{-d^*t}$. Repeating the same analysis with $d_{a\text{-}f_0} = 0.9 \cdot d_{a\text{-}\eta'}$ and $d_{a\text{-}f_0} = 1.1 \cdot d_{a\text{-}\eta'}$, to account for a ground state mass error, we finally get $d_{a\text{-}f_0}^* \approx 1.02 \pm 0.02$ at the bare mass parameter $m = -1.0105$. This value is significantly lower than $d_{a\text{-}\eta'}^* \approx 1.73$ at the same parameters but still in the ballpark of allowed values, given all the other uncertainties and systematic errors (in particular due to the finite box size).

4.5 Gluino-gluon

We continue with the third particle of the VY-supermultiplet, the gluino-gluon $\tilde{g}g$. Figure 11 shows its dominant mass contribution for different numbers of stout smearing steps, specifically for $n_s = 4, 8, 16$ and 32 . Gauge-link smearing smoothes the t -dependence of the correlators and suppresses contributions from excited states, if a sufficiently (but not too) large number of smearing steps are applied to the gauge links. Figure 11 suggests that $n_s = 8, \dots, 16$ smearing steps are optimal for our simulation parameters. For both cases the lowest mass contribution of the gluino-gluon near the critical point is between 0.2 and

Figure 10. Masses for $a\text{-}f_0$ and $a\text{-}\eta'$ from a $16^3 \times 32$ lattice at $\beta = 5.0$ and for a twist angle $\alpha = 45^\circ$. Results are shown as a function of the renormalized gluino mass m^R . Left: lowest d and next higher mass contribution d^* of $a\text{-}\eta'$ extracted by a 2-cosh-fit. Center/Right: lowest contribution d of $a\text{-}f_0$ extracted by a 1-cosh-fit/2-cosh-fit. Two resp. four time slices are excluded in the correlator fit at the boundary resp. around the inner time slice, i.e., $t_{\text{cut}} = (2, 4)$.

0.4 in lattice units, and between 0.7 and 0.9 for the next higher state. In comparison, fits to correlators for only $n_s = 4$ smearing steps lead to higher uncertainties, while for $n_s = 32$ some fits even fail.

In figure 12, we compare (the absolute value of) the symmetric and antisymmetric correlators of the gluino-gluon. Clearly, most data points lie on top of each other, but the noise of the antisymmetric correlator is increased at the inner time slices, where the sinh-shaped correlator crosses zero. Hence, no additional insight from the antisymmetric gluino-gluon can be expected. Focusing on the cosh-shaped symmetric gluino-gluon should be sufficient.

4.6 Glueballs

Before continuing with a chiral extrapolation of the VY-supermultiplet states in the next section, let us present some results for the FGS-supermultiplet. This multiplet contains two glueballs and a further gluino-glueball, see table 2. A lattice determination is thus numerically demanding. Enhanced gauge link fluctuations in the glueball interpolator fields require large ensemble sizes. A reasonable mass determination would exceed our computing time budget. Hence all results presented here are exploratory and preliminary.

Figure 13 shows the dominant mass contributions for the glueballs with quantum numbers 0^{++} and 0^{-+} . Within errors, d does not depend on the renormalized gluino mass m^R . Similar holds for the next higher state of the scalar glueball. Extrapolated to the critical point, the scalar glueball is somewhat lighter than the pseudoscalar glueball, cf. top and bottom rows of figure 13. The extrapolated values at critical gluino mass is somewhere between 0.2 and 0.3 in lattice units. The mass of the next higher state of the scalar glueball extrapolates to a value somewhere between 0.6 and 1.3.

Figure 11. Symmetric gluino-gluon from a $16^3 \times 32$ lattice and for twist angle $\alpha = 45^\circ$ versus the gluino mass m^R . The different panels show data for $n_s = 4, 8, 16$ and 32 stout smearing steps. For the fits, two time-slices have been excluded at both ends, $t_{\text{cut}} = (2, 2)$.

Figure 12. Comparison of time-symmetric (S) and time-antisymmetric (A) gluino-gluon correlator at $m = -1.0105$, and for $n_s = 8$ stout smearing steps. Absolute values are shown for a better comparison of the cosh- and sinh-shaped correlators.

Comparing the three columns in figure 13 we see that the number of stout smearing steps clearly affects d . Extrapolations to the critical mass are consistent with a horizontal line in all panels, that is a m^R dependency is not resolvable, but the offset of each line depends on the number of smearing steps. For the chiral extrapolation of all multiplet

Figure 13. Top/Bottom: scalar/pseudoscalar glueball on the $16^3 \times 32$ lattice with twist angle $\alpha = 45^\circ$ as a function of the gluino mass m^R . Data points are slightly displaced for better visibility. In the different panels, $n_s = \{4, 8, 16\}$ steps of stout smearing are applied to smooth the data. Both 1-cosh-fit and 2-cosh-fit results are shown for comparison. Two resp. four time slices are ignored in the correlator fit at the lattice boundary resp. in the center. For better clarity some (over-estimated) error bars are not shown.

states in the next section we will choose the results for $n_s = 8$ stout smearing steps. Only for the lowest mass contribution of 0^{++} , the results for $n_s = 4$ are chosen, because the mass hierarchy is better seen (see top row of figure 13).

Fitting the dominant mass contribution of the 0^{-+} , and that of the next higher state, is difficult, even with a 2-cosh-fit ansatz (see bottom row of figure 13). The small lattice volume does not allow for a reasonable determination of the ground state mass. Therefore, only one (excited) contribution has been determined with a value between 0.7 and 1.5 in lattice units, depending on the number of stout smearing steps. In [17, 24] it was reported that the lowest state of the pseudoscalar glueball is comparable with the first excited states of mesonic states and the gluino-gluon. This agrees with our observations.

4.7 Chiral limit

To connect lattice results with the supersymmetric continuum theory, first an extrapolation to the critical point and then to the continuum limit should be performed. In what follows, all previously discussed results (see sections 4.4, 4.5 and 4.6) will be extrapolated to the critical point where the renormalized gluino mass vanishes at fixed lattice spacing. In the

Figure 14. Left/Right: chiral extrapolation of the VY/FGS-supermultiplet. Each particle is depicted with a different color. Solid/Dashed lines are linear fits to the lowest/next higher mass contribution. The amount of smearing steps is indicated in the indices, e.g. $\tilde{g}g_{88}$ stands for 8 levels of stout smearing. For the gluino-gluon the symmetric operator is considered as discussed in section 4.5. Two resp. four time slices are ignored in all correlator fits at the lattice boundary resp. in the center. All fits are 2-cosh except 0_{88}^{++} and 0_{88}^{-+} , which are fitted to a single cosh.

previous sections this extrapolation has been discussed for the individual states already. The focus here is on a comparison of the extrapolated values for all supersymmetric partners of a multiplet, in particular if they coincide within errors.

The leading order of chiral perturbation theory suggests that the residual gluino mass m^{R} is given by squared mass of the would-be Goldstone bosons, i.e. $m^{\text{R}} \propto m_{\text{a-}\pi}^2$. In [65–68] it has been argued that the leading correction to non-zero meson and baryon masses in the chiral limit is also proportional to $m_{\text{a-}\pi}^2$ such that we assume a linear m^{R} dependency in the extrapolation to the chiral point. Hence we will obtain non-zero masses for the physical mesons — in contrast to the partially quenched approximations in the chiral limit — although at our finite values of m^{R} the masses are hardly distinguishable.

For the VY-supermultiplet, the linear extrapolations are depicted in the left panel of figure 14, and the corresponding values are given in table 5. We see that the lowest mass contributions of $a\text{-}\eta'$, $a\text{-}f_0$ and $\tilde{g}g_{S8}$ (this index indicates the usage of 8 stout smearing steps) are degenerated within errors. For the next higher state of the VY-supermultiplet, the situation is less clear. Nonetheless, a tendency for a mass degeneracy is seen which may be manifest in the continuum limit. Possibly the relatively small lattice size causes the second excited state to superpose with the first, resulting in larger contributions to $d_{a\text{-}\eta'}^*$ which we cannot resolve. Conversely, smearing the gluino-gluon operator may have overly dampened the first excited state $d_{\tilde{g}g}^*$ such that its mass is underestimated.

The right panel of figure 14 shows the extrapolation of the FGS-supermultiplet states. Looking at the ground state, the scalar glueball 0^{++} shows a clear mass degeneracy with the gluino-gluon. It is as heavy as the $a-f_0$ of the VY-supermultiplet, but slightly heavier than

state	d	s	d^*	s^*
$a\text{-}\eta'$	0.14 ± 0.01	1.60 ± 0.04	1.09 ± 0.02	1.48 ± 0.23
$a\text{-}f_0$	0.19 ± 0.12	1.23 ± 1.49	—	—
$\tilde{g}g_{S8}$	0.21 ± 0.12	1.09 ± 0.40	0.89 ± 0.09	0.55 ± 0.43
0_{S8}^{++}	0.20 ± 0.05	0.73 ± 0.32	0.83 ± 0.05	0.14 ± 0.02
0_{S8}^{-+}	—	—	1.14 ± 0.06	-0.19 ± 0.25

Table 5. Results of the linear fits. The lowest mass contribution d , the next higher mass contribution d^* , the corresponding slopes s resp. s^* and their fit errors are rounded to 2 digits.

the $a\text{-}\eta'$ state. A prediction which of the two multiplets is the lightest in the continuum limit is not possible with the present data. In the excited spectrum, 0_{S8}^{++} , $\tilde{g}g_{S8}$ and 0_{S8}^{-+} lie in the interval $[0.8, 1.2]$. If those states all belong to the first excitation, or if this excitation in fact is a superposition of all higher states, cannot be resolved. Simulations in larger volumes are required to address this in a reasonable manner.

We identified the lowest contribution of the 0^{-+} glueball as its first excited state. This is in accordance to [16], where $m_{0^{++}}^1 \approx m_{0^{-+}}^0$ was found. In another study [17], results from a lattice calculation using the variational method are discussed. The authors found that the $a\text{-}\eta'$ and 0^{-+} operators do not mix in the variational basis, even though both lead to the same masses for the excited states when analyzed individually. In [24], in which $SU(3)$ $\mathcal{N} = 1$ SYM theory has been addressed, the scalar glueball and $a\text{-}f_0$ interpolation operators were combined into a variational basis. Both operators showed a good overlap with the lowest state and mixing occurs. In the pseudoscalar channel, the lowest state was dominated by the $a\text{-}\eta'$ operator while the signal for the 0^{-+} operator was comparably small.

To conclude, our spectroscopic results of the VY- and FGS-supermultiplet with the twisted Wilson Dirac operator demonstrate that a mass degeneracy of the ground states can be observed. In future studies, the first excited states should be refined and with a continuum extrapolation the question, which of the supermultiplets is the lightest, should be addressed.

4.8 Chiral anomaly and relevance of Wilson term

Disregarding a potential anomaly due to a non-invariance of the measure a twist of both the mass term and Wilson term with the same angle can be undone by a chiral rotation (2.14) which rotates the interpolating operators. So far we have investigated mesonic correlators of the type $\langle \bar{\lambda}_x \Gamma^1 \lambda_x \bar{\lambda}_{x'} \Gamma^2 \lambda_{x'} \rangle$. Above we have compared connected and disconnected contributions to these correlators. Thereby one should keep in mind that the latter depend via the condensates very sensitive on external conditions. To quantify a possible anomaly and at the same time study the quality of the 45° -twist, we now consider the chiral and parity condensate, i.e. condensates of type $\sum_x \langle \bar{\lambda}_x \Gamma \lambda_x \rangle$ with $\Gamma = 1, \gamma_5$. Under a chiral transformation (2.14), the doublet of bilinears is rotated, see (2.15), and so are the condensates (2.27)

and (2.28):

$$\begin{aligned}\Sigma(\alpha) &= \cos(\alpha)\Sigma + \sin(\alpha)\Sigma^P, \\ \Sigma^P(\alpha) &= \cos(\alpha)\Sigma^P - \sin(\alpha)\Sigma.\end{aligned}\tag{4.4}$$

Hence the sum $|\Sigma(\alpha)|^2 + |\Sigma^P(\alpha)|^2 = |\Sigma|^2 + |\Sigma^P|^2$ is independent of α and the difference

$$|\Sigma(\alpha)|^2 - |\Sigma^P(\alpha)|^2 = |\Sigma|^2(\cos^2(\alpha) - \sin^2(\alpha)) - |\Sigma^P|^2(\cos^2(\alpha) - \sin^2(\alpha))\tag{4.5}$$

should be zero at $\alpha = \pm 45^\circ$. For $\varphi = 0^\circ$ eq. (4.5) measures both the breaking of chirality by the measure and by the irrelevant Wilson term. If instead the difference is measured for the double-twist $\alpha = \varphi = 45^\circ$ then the difference is only due to a potential non-invariance of the measure. This way we can disentangle the breaking of chirality by the Wilson term and the measure. The right panel of figure 15 is compatible with the chiral invariance of the latter. On the $8^3 \times 16$ lattice the deviation of $|\Sigma|^2 - |\Sigma^P|^2$ from zero is smaller than 10^{-4} and on the $16^3 \times 32$ lattice even below 10^{-5} . A possible deviation is so small that we see no symmetry breaking induced by a non-invariant measure. In subsequent studies a perturbative lattice calculation should support this finding.

The similarity of the condensates for a double-twist $\alpha = \varphi = 45^\circ$ can be used to our advantage when we analyze the physical mesonic states. Their disconnected contributions depend on the chiral condensate resp. the parity condensate. In section 3.1 we argued that $a\text{-}\eta'$ and $a\text{-}f_0$ are identical when the spinors are rotated with 45° . Without twisting the Wilson term, that is for $\varphi = 0^\circ$, the numerical data presented in section 4.3 show that the connected part of $a\text{-}\eta'$ and $a\text{-}f_0$ agree. At the same time, the chiral condensate Σ is much bigger than the parity condensate $\Sigma^P \ll 1$, see left part of figure 15. It follows that in the $a\text{-}f_0$ correlator large numbers of the order $\langle \text{tr}(\Gamma G_{xx}) \rangle \langle \text{tr}(\Gamma G_{yy}) \rangle \sim |\Lambda| \cdot \Sigma^2$ must be subtracted unlike for the $a\text{-}\eta'$. This explains the unequal noise in those two correlators at $\alpha = 45^\circ$ — even though we would expect them to be equal according to section 3.1.

Now, with a rotation of the mass term and the Wilson term, i.e. $\alpha = \varphi = 45^\circ$, also the disconnected contributions of those two mesonic states match. This implies an even better degeneracy of the $a\text{-}\eta'$ and $a\text{-}f_0$. A compromise would be the choice $\alpha = 45^\circ = -\varphi$, where the difference of the condensates is significantly lower than in the scenario with $\varphi = 0^\circ$, see left panel of figure 15. Additionally this difference shrinks linearly towards the critical point and for $\alpha - \varphi = 90^\circ$ discretization improvements of $\mathcal{O}(a)$ are possible as discussed in section 3.3.

Altogether, there are several interesting setups (α, φ) for future investigations compared to the untwisted Wilson Dirac operator, which all lead to an improved mass degeneracy of the chiral partners:

1. $(45^\circ, 0^\circ)$: equal connected contributions to $a\text{-}\eta'$ and $a\text{-}f_0$, $\mathcal{O}(a)$ errors reduced.
2. $(45^\circ, 45^\circ)$: equal connected and disconnected contributions to $a\text{-}\eta'$ and $a\text{-}f_0$. Note that this choice amounts to a redefinition of the observables.
3. $(45^\circ, -45^\circ)$: equal connected contributions to $a\text{-}\eta'$ and $a\text{-}f_0$, disconnected contributions become equal as the critical point is approached, $\mathcal{O}(a)$ improvement.

Figure 15. Difference of the absolute values squared of the chiral condensate Σ and the parity condensate Σ^p . For $\varphi = 0^\circ$ the chiral condensate dominates this value while for $\varphi = 45^\circ$ the contributions of the chiral condensate and the parity condensate are approximately the same. Left: different twist angles (α, φ) on the $16^3 \times 32$ lattice. Right: different lattice sizes for $\alpha = \varphi = 45^\circ$.

4.9 Sign of the Pfaffian

In order to have a positive Boltzmann weight in the path integral, the Pfaffian must be positive. Otherwise our lattice calculations may suffer a sign problem. In the continuum, the Pfaffian of $\mathcal{N} = 1$ SYM theory is real, but our twisted lattice Dirac operator may have a complex Pfaffian. To check the severeness of that problem additional lattice calculations of the Pfaffian on lattices up to a size of $7^3 \times 14$ have been performed. Since the computational costs scale as $\mathcal{O}(N^3)$ and the memory requirement as $\mathcal{O}(N^2)$ with the size N of the Dirac matrix, the explicit calculation of the Pfaffian with the optimized serial algorithm [69] was only performed for lattice sizes from $2^3 \times 4$ to $7^3 \times 14$.

The left panel of figure 16 shows the phase ω of $\text{Pf}(CD_W^{\text{mtw}}) = |CD_W^{\text{mtw}}| \cdot e^{i\omega}$ for different lattice sizes and simulation parameters: $\beta = 5.4$ and $(m, m_5) = (-0.85, 0.1)$, where $d_{a-\pi} \approx 0.60$. Extrapolated to the typical lattice size of our calculations, $16^3 \times 32$, we find the phase remains small: $1 - \cos(\omega) < 0.035$. That is, we expect no significant sign problem for our calculations. Furthermore we find that the phase becomes smaller towards the critical point, see right plot of figure 16.

4.10 Multigrid acceleration

When calculating correlator functions, a large amount of computation time is spent in the inversion of the Wilson Dirac operator. In lattice QCD, the implementation of multigrid methods has led to a significant speed-up. Their strength is the separate treatment of high and low modes by an alternating application of a domain decomposition smoother and a coarse-grid correction. We adjusted the adaptive aggregation-based domain decomposition multigrid (DDαAMG) library [70, 71] to the adjoint representation of $\mathcal{N} = 1$ SYM theory and used the DDαAMG inverter when calculating correlators or condensates. This turned out as a valuable investment, because it has allowed us to significantly reduce the statistical noise for all results presented in the sections 4.4 to 4.7 by using a large number of stochastic estimators and point sources. This would have been impossible with the commonly used conjugate gradient (CG) algorithm, in particular given our limited CPU time budget.

Figure 16. Left: phase of the Pfaffian for different lattice sizes ranging from $2^3 \times 4$ to $7^3 \times 14$. The green line is an exponential fit to extrapolate the results to the lattice size $16^3 \times 32$. Right: phase of the Pfaffian for different values of $m_5 \in [0, 0.15]$. When approaching the critical point at $m_5 = 0$, the phase of the Pfaffian decreases. Error bars are mostly smaller than the symbol size.

To illustrate the performance boost by the DD α AMG inverter, we perform a benchmark study with the following setup: inversion precision 10^{-12} , two multigrid levels, block size 2^4 , mixed precision and the solver combination FGMRES with red-black Schwarz.

Figure 17 shows the timings for inversions of the Wilson Dirac operator for the CG and the DD α AMG inverter. The left panel is for the Wilson Dirac operator in the fundamental representation, the right for the adjoint representation of SU(3). In both cases up to 100 stochastic estimators and 5 point sources are considered. For comparison, the timings for two different lattice sizes, $8^3 \times 16$ and $16^3 \times 32$, are shown. We see that on the $16^3 \times 32$ lattice the DD α AMG solver is always faster than the CG algorithm. Only for the fundamental representation with a single right-hand side the CG solver is slightly faster. This is because of the time needed for the DD α AMG setup. However, if many different right-hand sides are calculated this setup time becomes negligible. Especially, on large lattices and for the adjoint representation the DD α AMG algorithm yields a significant performance gain and is much faster than the CG. For this case our benchmark study reveals a speed-up factor of 20. Additionally, the DD α AMG can reduce the critical slowing down near the critical point.

5 Summary and outlook

In this work we have introduced, analyzed and applied a new type of Wilson Dirac operator for lattice calculations of $\mathcal{N} = 1$ supersymmetric SU(3) Yang-Mills theory. Inspired by twisted-mass lattice QCD and simulations of lower-dimensional supersymmetric theories we have added a twisted mass term to the fermionic lattice action and interpreted it as a deformation whose parameter requires tuning. With analytical arguments we showed that at 45° twist the correlators of the chiral partners in the Veneziano-Yankielowicz supermultiplet are identical and additionally the discretization artifacts are reduced at tree level. With the help of lattice simulations we have demonstrated that this particular twist angle leads to an improvement of the mass degeneracy of the mesonic chiral partners at finite

Figure 17. Left/Right: measured time in seconds to invert the Wilson Dirac operator for different numbers of right-hand sides in the fundamental/adjoint representation of $SU(3)$. The different colors correspond to the lattice sizes $8^3 \times 16$ resp. $16^3 \times 32$. Solid (dotted) lines are for the DD α AMG (CG) inverter. Note the double-logarithmic scale.

lattice spacing. Consequently, chiral symmetry as well as supersymmetry are improved reducing the distance to the supersymmetric continuum limit.

In the exploratory simulations presented in this work the lattice parameters were not optimally chosen such that some lattice results are afflicted with non-negligible volume artifacts. Nonetheless, on a qualitative level our findings presumably will not change and we leave it to forthcoming lattice studies to verify them on larger volumes. Those studies should start at smaller (inverse) gauge couplings β to increase the physical box size. Depending on the available computer time, a larger lattice size may be helpful to reduce the statistical noise. Furthermore, a combination of ensembles with different couplings should enable us to better extrapolate to the continuum limit and to determine the physical masses of the Veneziano-Yankielowicz and Farrar-Gabadadze-Schwetz supermultiplets.

After twisting the mass term only, we also analyzed the double-twist scenario with a twist angle α for the mass term and another angle φ for the Wilson term. Preliminary results of the two condensates suggest that no anomaly occurs at $\alpha = \varphi = 45^\circ$. We observed that a double-twist can reduce the numerical difference of the disconnected contributions between the chiral partners $a\text{-}\eta'$ and $a\text{-}f_0$. Optimally chosen twist angles reduce lattice artifacts such that the double-twist approach provides a promising improvement of lattice Super-Yang-Mills theory and could be used in future lattice simulations.

Much improvement has been achieved with an adapted DD α AMG multigrid algorithm for fermions in the adjoint representation. In a benchmark study, a speed-up factor of 20 has been achieved. This way, we could reduce our computation cost considerably and at the same time increase the number of stochastic estimators and point sources.

Ultimately, dynamical supersymmetric quarks (squarks) should be added to perform lattice studies for Supersymmetric Quantum Chromodynamics (aka. Super-QCD). First steps in that direction are presented in [72–74]. One-flavor Super-QCD with Wilson fermions has nine relevant operators, but as demonstrated in [73], certain properties of the one-loop potential of the squark field may help to fine-tune these parameters. With

respect to the R -symmetry of Super-QCD, the twisted formulation provides a variety of options. One possibility is to twist only the gluinos or to twist gluinos and squarks in the same resp. the opposite direction. Upcoming numerical studies may clarify the influence of the Yukawa-type interaction between the two fermionic fields on the masses of bound states.

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A Why the pion is the lightest mesonic state

For the benefit of the reader we elaborate on an argument put forward by Weingarten [75] which makes clear that the pion is the lightest mesonic state on the lattice (see the texts [76, 77]). Clearly, if two (connected) correlators obey for large enough x (where excited states do not contribute) the inequality

$$|C_1(0, x)| > |C_2(0, x)|, \quad x \gg 1, \quad (\text{A.1})$$

then the exponential decay of C_2 is faster and thus the ground state mass of the corresponding particle is heavier. Starting from a generic mesonic creation and annihilation operator with mass-degenerated fermions ψ_1 and ψ_2 , the mesonic correlator is

$$\begin{aligned} C(0, x) &= \langle \bar{\psi}_1(0) \Gamma \psi_2(0) \bar{\psi}_2(x) \tilde{\Gamma} \psi_1(x) \rangle = \langle \text{tr}(G(0, x) \Gamma G(x, 0) \tilde{\Gamma}) \rangle_{\mathcal{U}} \\ &= \langle \text{tr}(G(0, x) \Gamma \gamma_5 G^\dagger(0, x) \gamma_5 \tilde{\Gamma}) \rangle_{\mathcal{U}}, \end{aligned} \quad (\text{A.2})$$

where the subscript $\mathcal{U}$ indicates the average with respect to gluonic degrees of freedom and the trace is in color and spinor space. In the last step we used the γ_5 -hermiticity (which holds for untwisted fermions) and that the Green function can be written as

$$G(x, y) = \gamma_5 \langle x | \gamma_5 \frac{1}{D} \gamma_5 | y \rangle \gamma_5 = \gamma_5 \langle x | \frac{1}{D^\dagger} | y \rangle \gamma_5 = \gamma_5 G^\dagger(y, x) \gamma_5,$$

where the adjoint is in spinor and color space only. In the following x is fixed and we are dealing with a matrix problem in color and spinor space only. We recall the Frobenius scalar product of two matrices and the Frobenius norm of a matrix,

$$(A, B) = \text{tr}(A^\dagger B) \quad \text{with} \quad \|A\| = \sqrt{(A, A)}.$$

They fulfill all properties of a scalar product, in particular

$$|(A, B)| \leq \|A\| \|B\|.$$

Figure 18. Correlators for our four mass parameters at $\beta = 5.0$ from untwisted simulations on the $16^3 \times 32$ lattice without normalization, see top four rows of table 7(b). Solid/dotted lines with filled/open markers connect the data points of a- π resp. a- a to guide the eye. The labels indicate the distance $|m - m_{\text{crit}}|$ to the critical point. Errors are mostly smaller than the marker size.

Since the Hermitean γ_5 squares to $\mathbb{1}$ we have (we set $G(0, x) = G_x$)

$$|C(0, x)| = |(G_x, \gamma_5 \tilde{\Gamma} G_x \Gamma \gamma_5)| \leq \|G_x\| \|\gamma_5 \tilde{\Gamma} G_x \Gamma \gamma_5\| = \|G_x\| \|\tilde{\Gamma} G_x \Gamma\|. \quad (\text{A.3})$$

The inequality turns into an equality if and only if the two arguments of the scalar product are linearly dependent,

$$\gamma_5 \tilde{\Gamma} G_x \Gamma \gamma_5 = \lambda G_x. \quad (\text{A.4})$$

For the a- a with $\Gamma = \tilde{\Gamma} = \mathbb{1}_4$ the condition (A.4) is not fulfilled and we obtain

$$|C_{a-a}(0, x)| < \|G_x\|^2. \quad (\text{A.5})$$

For the a- π with $\Gamma = \tilde{\Gamma} = \gamma_5$ the condition (A.4) is fulfilled and we obtain

$$|C_{a-\pi}(0, x)| = \|G_x\|^2. \quad (\text{A.6})$$

The two last relations imply the inequality

$$|C_{a-a}(0, x)| < |C_{a-\pi}(0, x)|. \quad (\text{A.7})$$

In conclusion, the a- a (and all other mesonic states) are heavier than the a- π . Note that this proof is only correct without twist when the Dirac operator is γ_5 -hermitean. We also used that the expectation values $\langle \dots \rangle_{\mathcal{U}}$ are calculated with a positive measure which we do not have in case there is a sign problem. Finally, the conclusion about the mass-hierarchy only holds for infinite volume, when all connected correlators approach zero. In a finite volume the correlators are cosh-shaped and (A.7) would not necessarily imply $m_{a-\pi} < m_{a-a}$.

To see whether the results in section 4.3 are in line with above inequality, we have a closer look at the correlators of a- π and a- a . This way we can check whether the unexpected mass-hierarchy originates from problems with fitting the correlators correctly. Figure 18

ID	β	$L^3 \times T$	m_{crit}	m	m_5	r	r_5
(I)	4.5	$16^3 \times 32$	-1.22428	$[-1.1443, -1.22428]$	$[0.0000, 0.0800]$	1.0000	0.0000
(II)	5.0	$16^3 \times 32$	-1.0706	$[-0.9856, -1.0706]$	$[0.0000, 0.0850]$	1.0000	0.0000
(III)	5.0	$16^3 \times 32$	-0.7570	$[-0.6156, -0.8277]$	$[-0.6156, -0.8277]$	0.7071	0.7071
(IV)	5.4	$8^3 \times 16$	-0.967	$[-1.4000, -0.6000]$	$[-0.4000, 0.4000]$	1.0000	0.0000
(V)	5.4	$16^3 \times 32$	-0.9750	$[-0.8450, -0.9750]$	$[0.0000, 0.1300]$	1.0000	0.0000

Table 6. Overview of the parameter sets. Three different lattice couplings β , two different lattice volumes $V = L^3 \times T$ and two different combinations of (r, r_5) are used within this paper. For each setting, the mass parameter m_{crit} of the critical point as well as the ranges of m and m_5 are listed.

m	m_5	#	m	m_5	#	m	m_5	#
-1.2143	0.0000	100	-1.0606	0.0000	200	-0.9650	0.0000	100
-1.2043	0.0000	100	-1.0506	0.0000	200	-0.9500	0.0000	100
-1.1743	0.0000	100	-1.0206	0.0000	200	-0.8950	0.0000	100
-1.1443	0.0000	100	-0.9856	0.0000	200	-0.8450	0.0000	100
-1.2172	0.0071	100	-1.0635	0.0071	2110	-0.9679	0.0071	100
-1.2101	0.0141	100	-1.0565	0.0141	2370	-0.9573	0.0177	100
-1.1889	0.0354	100	-1.0352	0.0354	2705	-0.9184	0.0566	100
-1.1677	0.0566	100	-1.0105	0.0601	3100	-0.8831	0.0919	100
-1.22428	0.0100	50	-1.0706	0.0100	50	-0.9750	0.0100	100
-1.22428	0.0200	50	-1.0706	0.0200	100	-0.9750	0.0250	100
-1.22428	0.0500	50	-1.0706	0.0500	50	-0.9750	0.0800	100
-1.22428	0.0800	50	-1.0706	0.0850	50	-0.9750	0.1300	100

(a) $\beta = 4.5$
(b) $\beta = 5.0$
(c) $\beta = 5.4$

Table 7. Ensemble sizes on the $16^3 \times 32$ lattice.

depicts the correlators of both connected mesonic states without normalization. In full agreement with (A.7) we see that the correlator of the a - π is always above that of a - a such that the adjoint pion should be lighter. In the range $t \in [2, 12]$ the a - a correlator falls off faster than the a - π correlator and thus $m_{a-a} > m_{a-\pi}$, as expected. With an appropriate fit range, the influence of excited states at small t and the lattice artifacts around $t = T/2$ can be reduced. See section 4.1 for a further discussion of the mass extraction and section 4.2 for the finite size effects. Similar observations hold for the other lattice gauge couplings $\beta \in \{4.5, 5.4\}$.

B Overview of numerical data

In table 6, we summarize the parameters of our simulations. For the parameter scan on the $8^3 \times 16$ lattice at $\beta = 5.4$, all ensembles have around 200 configurations. Table 7 contains the values of the bare mass m , the twisted mass m_5 as well as the number of configurations for the various gauge couplings β on the $16^3 \times 32$ lattice.

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