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Automatic O(a) improvement for twisted-mass QCD

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We present a condition for automatic O(a) improvement in twisted mass lattice QCD, using symmetries of the Symanzik effective theory. If the continuum part of the Symanzik effective theory is invariant under a particular transformation, named T_1 in this report, scaling violations of all quantities invariant under T_1 transformation are even in the lattice spacing a. On the other hand, quantities non-invariant under T_1 vanish in the continuum limit with odd powers in a. We prove this statement even for the massive case without using the equation of motion. We also consider a few different criteria for the T_1 invariant condition in lattice theories and discuss ambiguities of the lattice condition for O(a) improvement.

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1. Introduction

It becomes more and more apparent that twisted mass Lattice QCD (tmLQCD) [1, 2] is a promising formulation to approach the chiral limit of QCD, despite the fact that the flavor symmetry is explicitly broken. A twisted mass protects the Wilson-Dirac operator against small eigenvalues and therefore solves the problem of exceptional configurations [3, 4], thus making numerical simulations with small quark masses feasible [5]. This numerical advantage of tmLQCD is supplemented by the property of automatic O(a) improvement [6]. For a recent review of these and some more results in twisted mass LQCD see Ref. [7].

The so-called "maximal twist" condition, required for the proof of automatic O(a) improvement [6], however, causes some confusions. For example, it has been suggested [6] that maximal twist can be achieved by setting the bare untwisted mass to the critical quark mass of the Wilson fermion where the pion mass vanishes (we call this choice "the pion mass definition" in the following). However, it has been pointed out [8] that this choice does not lead to automatic O(a) improvement. Indeed, terms linear in a and with fractional powers of a are predicted by Wilson Chiral Perturbation Theory (WChPT) for very small twisted quark masses. On the other hand, automatic O(a) improvement is expected to hold if the critical mass is defined through the partially conserved axial vector Ward identity quark mass (PCAC mass definition).

In this report we present an explicit condition based on symmetries of the Symanzik theory, required for automatic O(a) improvement, and prove that scaling violations of all quantities which have non-zero values in the continuum limit are even in a (O(a) improvement). The detailed proof of this statement has already been published in Ref. [9]. Therefore, in this report we try to avoid unnecessary rigorousness in our proof and stress the mechanism which leads to O(a) improvement in twisted mass QCD.

2. Condition and proof for automatic O(a) improvement

We first give our statement, which will be proven in this report. Twisted mass QCD with a certain condition leads to automatic O(a) improvement, which means that operators as well as the action are automatically $O(a)$ improved without any improvement coefficients. This holds true even in the massive case and without the explicit use of the equations of motion. More explicitly, all scaling violations of non-zero physical quantities are even in a, while quantities which vanish in the continuum limit have only odd powers in a.

2.1 Main idea of the proof

The twisted mass lattice QCD action for the 2-flavor theory is given by $S_{\rm tm} = S_G + S_F$, where S_G is the gauge action and

$$S_F = \sum_{x,\mu} \bar\psi_L(x)\frac{1}{2}\left[\gamma_\mu(\nabla_\mu^+ + \nabla_\mu^-)\psi_L - ar\nabla_\mu^+\nabla_\mu^-\psi_L\right](x) + \sum_x \bar\psi_L(x) M_0 e^{i\theta_0\gamma_5\tau^3}\psi_L(x) \qquad (2.1)$$

is the 2-flavor Wilson fermion action with a twisted mass term, where M_0 and θ_0 denote the bare mass and bare twist angle. It is also customary to write $M_0 e^{i\theta_0\gamma_5\tau^3} = m_0 + i\mu_0\gamma_5\tau^3$, using the bare untwisted mass m_0 and the bare twisted mass μ_0.

This action is invariant under the following global transformations: (1) U(1)⊗U(1) vector symmetry, $\psi_L \to e^{i(\alpha_0+\alpha_3\tau^3)}\psi_L,\ \bar\psi_L \to \bar\psi_L e^{-i(\alpha_0+\alpha_3\tau^3)}$. This transformation is part of the U(2) flavor symmetry of the untwisted theory. (2) Extended parity symmetry $P_F^{1,2}:\ \psi_L(x) \to \tau^{1,2}\gamma_4\psi_L(Px)$, $\bar\psi_L(x) \to \bar\psi_L(Px)\gamma_4\tau^{1,2}$ where P is the parity transformation. Alternatively, one can also augment P with a sign change of the twisted mass term μ_0, $\tilde P = P\times[\mu_0 \to -\mu_0]$, which is also a symmetry of the action. (3) Standard charge conjugation symmetry, as in the untwisted theory.

The lattice theory can be described by an effective continuum theory (the Symanzik theory), whose effective action is restricted by locality and the symmetries of the underlying lattice theory. Taking into account the symmetries listed above one finds $S_{\rm eff} = S_0 + aS_1 + a^2S_2 + \cdots$, where the first two terms are given as

$$S_0 = S_{0,\rm gauge} + \int d^4x\, \bar\psi(x)\left[\gamma_\mu D_\mu + M_R e^{i\theta\gamma_5\tau^3}\right]\psi(x), \tag{2.2}$$

$$S_1 = C_1 \int d^4x\, \bar\psi(x)\sigma_{\mu\nu}F_{\mu\nu}(x)\psi(x). \tag{2.3}$$

$S_{0,\rm gauge}$ denotes the standard continuum gauge field action in terms of the gauge field tensor $F_{\mu\nu}$. The second term in S_0 is the continuum twisted mass fermion action. It is worth mentioning that there is no "twisted" Pauli term $\bar\psi\gamma_5\tau^3\sigma_{\mu\nu}F_{\mu\nu}\psi$ present in S_1, since such a term violates the symmetry $\tilde P$.

In addition to the effective action we have to specify the direction of the chiral condensate, since chiral symmetry is spontaneously broken. From the fact that the direction of the chiral condensate is completely controlled by the direction of the symmetry breaking external field (i.e. the quark mass) in the continuum theory, we can take

$$\langle \bar\psi^i_\alpha \psi^j_\beta\rangle_{S_0} = \frac{v(M_R)}{8}\left[e^{-i\theta\gamma_5\tau^3}\right]^{ji}_{\beta\alpha}, \tag{2.4}$$

where $\lim_{M_R\to 0}\lim_{V\to\infty} v(M_R) \neq 0$. Here the vacuum expectation value (VEV) is defined with respect to the continuum action S_0. To say it differently, the VEV (2.4) defines the twist angle θ in the Symanzik theory.

We now want to argue that the choice $\theta = \pi/2$ (or $-\pi/2$) corresponds to "maximal twist". In terms of the mass parameters this is equivalent to $M_R = \mu_R$ and $m_R = 0$. In this case the action and the VEVs become

$$S_0 = S_{0,\rm gauge} + \int d^4x\ \bar\psi(x)\left[\gamma_\mu D_\mu + iM_R\gamma_5\tau^3\right]\psi(x), \tag{2.5}$$

$\langle\bar\psi\psi\rangle_{S_0} = 0,\ \langle\bar\psi i\gamma_5\tau^3\psi\rangle_{S_0} = v(M_R)$. It is easy to check that S_0, the continuum part of the effective action is invariant under $\psi \to e^{iw\gamma_5\tau^{1,2}}\psi,\ \bar\psi \to \bar\psi e^{iw\gamma_5\tau^{1,2}}$, and therefore also under the Z_2 subgroup T_1 of this continuous transformation, defined by $T_1\psi = i\gamma_5\tau^1\psi,\ T_1\bar\psi = \bar\psi i\gamma_5\tau^1$. Since $T_1^2 = 1$ in the space of fermion number conserving operators, which contain equal numbers of ψ and $\bar\psi$, the eigenvalues of T_1 are 1 (T_1-even) or -1 (T_1-odd). The crucial observation is that the VEVs $\langle\bar\psi\psi\rangle$ and $\langle\bar\psi i\gamma_5\tau^3\psi\rangle$ are also invariant under this transformation. The T_1 symmetry is *not* spontaneously broken, hence it is an exact symmetry of the continuum theory. The O(a) term $aS_1 = aC_1\int d^4x\ \bar\psi(x)\sigma_{\mu\nu}F_{\mu\nu}(x)\psi(x)$, on the other hand, is odd under T_1. Therefore, non-vanishing physical observables, which must be even under T_1, can not have an O(a) contribution, since the O(a) term is odd under T_1 and therefore must vanish identically. This is automatic O(a) improvement at "maximal twist". Note that non-invariant, i.e. T_1-odd quantities, which vanish in the continuum limit, can have O(a) contributions.

The above argument gives just the main idea of our proof for automatic O(a) improvement, and we will give a detailed proof in the next subsection. However, one of the most important points of our analysis is that the condition for automatic O(a) improvement is the invariance of theory under T_1 transformation, or more generally its continuous version, which corresponds to a part of the exact vector symmetry in continuum QCD at "maximal twist". One might even say that the T_1 invariance is more fundamental for automatic $O(a)$ improvement than the notion of "maximal twist", which is one of the consequences of T_1 invariance.

2.2 General proof

Let us consider an arbitrary multi-local lattice operator $O_{\rm lat}^{tp,d}(\{x\})$, where $\{x\}$ represents $x_1, x_2, \cdots, x_n$, d is the canonical dimension of the operator, $t = 0,1$ and $p = 0,1$ denote the transformation properties under T_1 and P:

$$T_1:\ O_{\rm lat}^{tp,d}(\{x\}) \ \rightarrow\ (-1)^t O_{\rm lat}^{tp,d}(\{x\}), \quad P:\ O_{\rm lat}^{tp,d}(\{\vec{x},t\}) \rightarrow (-1)^p O_{\rm lat}^{tp,d}(\{-\vec{x},t\}). \tag{2.6}$$

Here we do not include the dimension coming from powers of the quark mass in the canonical dimension d of the operators.

The lattice operator $O_{\rm lat}^{tp,d}$ corresponds to a sum of continuum operators $O^{t_n p_n,n}$ (n: non-negative integer) in the Symanzik theory as

$$O_{\rm lat}^{tp,d} \ =\ \sum_{n=d}^{\infty} a^{n-d} \sum_{t_n,p_n} c_{t_n p_n,n}^{tp,d} O^{t_n p_n,n}, \tag{2.7}$$

where n is the canonical dimension of the continuum operator $O^{t_n p_n,n}$ which consists of $\bar\psi$, ψ, A_μ and D_μ only without any mass parameters, and

$$T_1:\ O^{t_n p_n,n}(\{x\}) \ \rightarrow\ (-1)^{t_n} O^{t_n p_n,n}(\{x\}), \quad P:\ O^{t_n p_n,n}(\{\vec{x},t\}) \rightarrow (-1)^{p_n} O^{t_n p_n,n}(\{-\vec{x},t\}), \tag{2.8}$$

with $t_n, p_n = 0,1$. To have a total dimension d in the expansion in Eq. (2.7), the coefficients $c_{t_n p_n,n}^{tp,d}$ must be dimensionless. Here, to make an argument simpler, we consider the lattice operator, whose power divergences can be subtracted without spoiling our proof[9].

The following selection rules among these operators are crucial for our proof of automatic O(a) improvement:

$$t+p+d \ =\ t_n + p_n + n \quad \mathrm{mod}(2), \quad p + \#\mu_0 = p_n + (\#\mu_0)_n \quad \mathrm{mod}(2), \tag{2.9}$$

where $\#\mu_0$ and $(\#\mu_0)_n$ denote the numbers of μ_0's in $O_{\rm lat}^{tp,d}$ and $c_{t_n p_n,n}^{tp,d}$, respectively. The second equality can be easily proven by the invariance of the lattice action (2.1) under the $\tilde P = P \times [\mu_0 \rightarrow -\mu_0]$ transformation. To prove the first equality, we introduce the following transformation:

$$\mathscr{D}_d^1:\ \left\{ \begin{array}{lcl} U_\mu(x) & \rightarrow & U_\mu^\dagger(-x-a\mu) \\ \Big(A_\mu(x) & \rightarrow & -A_\mu(-x)\Big) \\ \psi(x) & \rightarrow & \left(e^{i\pi\tau_1}\right)^{3/2}\psi(-x) \\ \bar\psi(x) & \rightarrow & \bar\psi(-x)\left(e^{i\pi\tau_1}\right)^{3/2} \end{array} \right., \tag{2.10}$$

which is a modified version of the transformation $\mathscr{D}_d$ introduced in Ref. [6]. Since it is easy to show that the lattice action (2.1) is invariant under $T_1 \times \mathscr{D}_d^1$, in addition to the invariance under P_F^1, the lattice action is invariant under $T_1 \times \mathscr{D}_d^1 \times P_F^1$. On the other hand, we can easily see that $\mathscr{D}_d^1 \times P_F^1$ counts the canonical dimension times the parity of the operator as

$$\mathscr{D}_d^1 \times P_F^1 :\ O_{\rm lat}^{tp,d}(\{\vec{x},t\}) \to (-1)^{d+p} O_{\rm lat}^{tp,d}(\{\vec{x},-t\}), \tag{2.11}$$

$$\mathscr{D}_d^1 \times P_F^1 :\ O^{t_n p_n,n}(\{\vec{x},t\}) \to (-1)^{n+p_n} O^{t_n p_n,n}(\{\vec{x},-t\}). \tag{2.12}$$

Therefore, the invariance of the action under $T_1 \times \mathscr{D}_d^1 \times P_F^1$ implies the first selection rule.

Let us show how these selection rules are used to determine the structure of operators in the Symanzik theory. We first consider the Symanzik expansion of the lattice action $S_{\rm tm}$:

$$S_{\rm tm} = \sum_{n=0}^{\infty} \left[a^{2n}(S^{00,2n} + \mu_0 a S^{11,2n}) + a^{2n-1}(\mu_0 a S^{01,2n-1} + S^{10,2n-1}) \right] \tag{2.13}$$

$$= S_0^0 + mS_{-1}^1 + \sum_{n=1}^{\infty} \left[a^{2n} S_{2n}^0 + a^{2n-1} S_{2n-1}^1 \right], \tag{2.14}$$

where $S^{t_n p_n,n}$ denotes the action in the Symanzik theory whose canonical dimension and transformation properties under T_1 and P are (d_n, t_n, n). Here we pull out the μa factor from terms which have odd powers in $\mu_0 a$. Therefore remaining factors always have even powers in $\mu_0 a$. To derive the first equality we use the selection rules such that $0 = n + t_n + p_n \bmod (2)$ $0 = p_n + (\#\mu_0)_n \bmod (2)$ since the lattice action satisfies $d + t + p = 0$ and $p + \#\mu_0 = 0$. In the second equality we define

$$S_{2n}^0 = S^{00,2n} + \mu_0 S^{01,2n-1}, \quad mS_{-1}^1 = S^{10,-1}/a,\ S_{2n-1}^1 = S^{10,2n-1} + \mu_0 S^{11,2n-2} (n \geq 1), \tag{2.15}$$

and the superscript 0 or 1 denotes the transformation property under T_1 as evident from the above definition. Similarly we have

$$O_{{\rm lat},d}^0 = O_d^0 + \sum_{n=1}^{\infty} \left[a^{2n} O_{d+2n}^0 + + a^{2n-1} O_{d+2n-1}^1 \right], \tag{2.16}$$

$$O_{{\rm lat},d}^1 = O_d^1 + \sum_{n=1}^{\infty} \left[a^{2n} O_{d+2n}^1 + + a^{2n-1} O_{d+2n-1}^0 \right], \tag{2.17}$$

for the multi-local operator with the canonical dimension d, where again the superscript 0 or 1 denotes the transformation property under T_1.

Now we can specify the condition for automatic $O(a)$ improvement: It is stated that the continuum part of the action (2.14) is invariant under T_1. This condition leads to $m = 0$, so that the continuum part of the action is given solely by S_0^0. We will consider the scaling behaviour of the vacuum expectation value of an arbitrary multi-local operator, $\langle O_{{\rm lat},d}^t(\{x\}) \rangle$. For this purpose we define

$$e^{S_{\rm tm}} = e^{S_0^0} \exp\left\{ \sum_{n=1}^{\infty} \left[a^{2n} S_{2n}^0 + a^{2n-1} S_{2n-1}^1 \right] \right\} \equiv e^{S_0^0} \sum_{n=0}^{\infty} a^n S^{(n)}, \tag{2.18}$$

where we define $a^n S^{(n)}$ to be the sum of the a^n terms in eq. (2.18). For example, the first few terms are given as $S^{(0)} = 1$, $S^{(1)} = S_1^1$, and $S^{(2)} = S_2^0 + (S_1^1)^2/2!$. Under the T_1 transformation, they behave as $T_1 :\ S^{(n)} \to (-1)^n S^{(n)}$. By expanding both action and operator, we have

$$\langle O_{\rm lat}^t(\{x\}) \rangle = \sum_{n=0}^{\infty} a^n \langle O_n^{t_n}(\{x\}) \rangle_{S_{\rm tm}} = \sum_{n=l=0}^{\infty} a^{n+l} \langle O_n^{t_n}(\{x\}) S^{(l)} \rangle_{S_0^0} \tag{2.19}$$

where $t_n = n+t$ mod (2). In the second line the T_1 invariance tells us that $\langle O_n^{t_n}(\{x\})S^{(l)}\rangle_{S_0^0} = 0$ unless $t_n + l = t+n+l = 0$ mod (2). Therefore we have

$$\langle O^t_{\rm lat}(\{x\})\rangle = \sum_{s=0}^{\infty} a^{2s+t} \sum_{n=0}^{2s+t} \langle O_n^{t_n}(\{x\})S^{(2s+t-n)}\rangle_{S_0^0}, \tag{2.20}$$

from which we derive

$$\langle O^0_{\rm lat}(\{x\})\rangle = \langle O_0^0(\{x\})\rangle_{S_0^0} + O(a^2) + O(a^4) + \cdots \tag{2.21}$$

$$\langle O^1_{\rm lat}(\{x\})\rangle = O(a) + O(a^3) + O(a^5) + \cdots . \tag{2.22}$$

This proves our statement that the scaling violation of all T_1 invariant operators, which have non-zero VEV in the continuum limit, are even in a, while that of T_1 non-invariant operators, whose VEV vanish in the continuum limit, are odd in a. This is true for non-zero μ_0 and does not require the use of the equation of motion.

2.3 Condition for O(a) improvement in the lattice theory

In the Symanzik theory, the condition for O(a) improvement is uniquely defined by the condition that an arbitrary T_1 non-invariant operator $O^{t=1\,p,d}$ has a vanishing expectation value. Provided this condition is fulfilled, the expectation values of all T_1 non-invariant operators vanish. Hence the particular choice for $O^{1p,d}$ is irrelevant, and in that sense the condition is unique. In the lattice theory, however, the condition defined by $\langle O^{1p,d}_{\rm lat}\rangle = 0$ depends on the choice of the operator $O^{1p,d}_{\rm lat}$, and is therefore not unique. In terms of the Symanzik theory, for this condition to be satisfied, an equation

$$aF_0(a^2, ma, \mu_0) + mF_1(a^2, ma, \mu_0) = 0,$$

where $F_{0,1}$ are some functions of a^2, ma and μ_0, must be fulfilled by tuning the untwisted mass m. Since this equation is invariant under $(m,a) \to (-m,-a)$, the solution has the form that $m = af(a^2,\mu_0)$ under the assumption that the solution to the equation is unique. If one takes a different lattice operator to define the T_1 invariant condition, the solution is given by $m' = af'(a^2,\mu)$. Therefore the difference between two definitions is O(a): $m - m' = a(f-f')$. Note that a solution m in general depends on μ_0, inherited from the μ_0 dependence of $F_{0,1}$.

Let us consider some examples for the condition in the lattice theory. A simple one is given by $\langle(\bar\psi\psi)_{\rm lat}\rangle = 0$. Unfortunately, this definition is not very useful in practice, since the subtraction of power divergences necessary for $\langle\bar\psi\psi\rangle$ prevents a reliable determination of this VEV in the lattice theory. Instead one may take $O_{\rm lat}(x,y) = A^a_\mu(x)P^a(y)$ or $O_{\rm lat}(x,y) = \partial_\mu A^a_\mu(x)P^a(y)$ $(a=1,2)$, as was done in Refs. [10, 11, 12]:

$$\langle A^a_\mu(x)P^a(y)\rangle = 0 \quad \text{or} \quad \langle\partial_\mu A^a_\mu(x)P^a(y)\rangle = 0, \tag{2.23}$$

where A^a_μ and P^a denote the axial vector current and pseudo scalar density, respectively. Yet another choice is [13]

$$\langle A^3_\mu(x)P^3(y)\rangle = 0.$$

Depending on the choice for the axial vector current, either the local or the conserved one, the conditions (2.23) lead to a different definition for maximal twist. However, the difference will be again of O(a).

We close this section with a final comment. Any condition for $\mathrm{O}(a)$ improvement in the lattice theory determines a value for the bare untwisted mass m_0 as a function of the bare twisted mass μ_0. It has been suggested to tune the untwisted mass to its critical value $m_0 = m_{\mathrm{cr}}$ where the pion mass vanishes in the untwisted theory. However, this condition is not related to T_1 invariance. For example, contributions from excited states violate eq. (2.23) even at $m_\pi = 0$. Consequently, the pion mass definition does not correspond to automatic $\mathrm{O}(a)$ improvement according to the T_1 invariance condition.

3. Conclusion

In this paper we gave a comprehensive proof for automatic $\mathrm{O}(a)$ improvement in twisted mass lattice QCD. The most important observation is that a precise definition for $\mathrm{O}(a)$ improvement is described by the symmetry in the continuum theory. If the continuum part of the Symanzik theory is invariant under T_1 transformation, scaling violations for all quantities are shown to be even powers in a, as long as they are invariant under the T_1 transformation. Non-invariant quantities, on the other hand, vanish as odd powers in a.

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