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A perturbative study of the chirally rotated Schrödinger Functional in QCD

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The chirally rotated Schrödinger functional (χSF) renders the mechanism of automatic $O(a)$ improvement compatible with the Schrödinger functional (SF) formulation. Here we report on the determination to 1-loop order in perturbation theory of the renormalization coefficients necessary to achieve automatic $O(a)$ improvement and the boundary improvement coefficients needed to eliminate the extra boundary $O(a)$ effects present in any SF formulation. After this is done, we perform a set of tests of automatic $O(a)$ improvement and of the universality between standard and chirally rotated SF formulations.

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1. Introduction

Schrödinger functional schemes [1] have been successfully used in several renormalization problems in lattice field theory. In this formulation, however, the presence of temporal boundaries together with local boundary conditions for the fields are a source of extra cutoff effects. A theory regulated with Wilson fermions is hence affected by lattice artefacts coming from the bulk and also by those originating at the boundaries. These can be removed following Symanzik's improvement program by adding a set of counterterms to the action in the bulk and at the boundaries. An appealing alternative to the standard formulation of Wilson fermions in the SF is the recently proposed chirally rotated Schrödinger functional (χSF), which implements the mechanism of (bulk) automatic $O(a)$ improvement [2]. In the continuum (and chiral) limit it is directly related to the standard SF formulation via a chiral rotation of the fermion fields. The chirally rotated fields satisfy modified boundary conditions which respect a version of chiral symmetry augmented with a flavour structure. In this situation, the argument for automatic $O(a)$ improvement can be invoked in terms of a rotated version of parity. Physical observables are then only affected by $O(a^2)$ discretization effects (provided that the effects from the boundaries have been removed) without the need of introducing new operators in the bulk.

Here we report on a perturbative 1-loop calculation of the coefficients necessary for the renormalization and the improvement of the theory in the χSF set-up. After this is done, we perform a set of tests (also within perturbation theory) confirming the universality between the standard and chirally rotated set-ups, as well as the mechanism of automatic $O(a)$ improvement.

2. The χSF set-up

For a flavour doublet chirally rotated boundary conditions take the form [2]

$$\widetilde{Q}_+ \psi(x)\Big|_{x_0=0} = \widetilde{Q}_- \psi(x)\Big|_{x_0=T} = 0, \qquad \overline{\psi}(x)\widetilde{Q}_+\Big|_{x_0=0} = \overline{\psi}(x)\widetilde{Q}_-\Big|_{x_0=T}, \tag{2.1}$$

with the projectors $\widetilde{Q}_\pm = \frac{1}{2}(1 \pm i\gamma_0\gamma_5\tau^3)$ and where τ^i are the Pauli matrices.

The projectors commute with $i\gamma_0\gamma_5\tau^3$. A rotated version of parity P_5 can hence be used to distinguish between even and odd observables in the χSF[1]. On the lattice P_5-even correlations are automatically $O(a)$ improved and all $O(a)$ effects fall into P_5-odd observables.

The boundary conditions Eq.(2.1) can be derived from the standard SF boundary conditions by applying a non-anomalous chiral rotation to the flavour doublet

$$\psi \to R(\alpha)\psi, \quad \overline{\psi} \to \overline{\psi}R(\alpha), \quad R(\alpha) = \exp(i\alpha\gamma_5\tau^3/2). \tag{2.2}$$

The rotated fields satisfy Eq.(2.1) for $\alpha = \pi/2$ (standard SF boundary conditions are recovered for $\alpha = 0$). Since the rotation $R(\alpha)$ is a symmetry of the massless continuum action, the two set-ups are equivalent, with correlation functions related through

$$\langle \mathscr{O}[\psi,\overline{\psi}]\rangle_{\chi\mathrm{SF}} = \langle \mathscr{O}[R(-\pi/2)\psi, \overline{\psi}R(-\pi/2)]\rangle_{\mathrm{SF}}. \tag{2.3}$$

[1] $P_5 : \psi(x) \to i\gamma_0\gamma - 5\tau^3\psi(\tilde{x}), \quad P_5 : \overline{\psi}(x) \to -\overline{\psi}(\tilde{x})i\gamma_0\gamma_5\tau^3, \quad \tilde{x} = (x_0, -\mathbf{x}).$

When the theory is implemented on the lattice with Wilson quarks, these relations are expected to hold between renormalized correlation functions once the continuum limit is taken. Implementing χSF boundary conditions on the lattice is non-trivial. Here we consider the lattice set-up form [2] in which the fermionic action reads

$$S_f = a^4 \sum_{x_0=0}^{T} \sum_{\mathbf{x}} \overline{\psi}(x)\left(\mathscr{D}_W + \delta\mathscr{D}_W + m_0\right)\psi(x). \tag{2.4}$$

The Wilson-Dirac operator, which includes the clover term[2], reads

$$a\mathscr{D}_{\mathrm{W}}\psi(x) = \begin{cases} -U_0(x)P_-\psi(x+a\hat{0}) + (K + i\gamma_5\tau^3 P_-)\psi(x), & x_0 = 0, \\ -U_0(x)P_-\psi(x+a\hat{0}) + K\psi(x) - U_0(x-a\hat{0})^\dagger P_+\psi(x-a\hat{0}), & 0 < x_0 < T, \\ (K + i\gamma_5\tau^3 P_+)\psi(x) - U_0(x-a\hat{0})^\dagger P_+\psi(x-a\hat{0}), & x_0 = T, \end{cases} \tag{2.5}$$

with the diagonal part K given by

$$K\psi(x) = \left(1 + \frac{1}{2}\sum_{k=1}^{3}\left\{a\left(\nabla_k + \nabla_k^*\right)\gamma_k - a^2\nabla_k^*\nabla_k\right\}\right)\psi(x) + c_{\mathrm{sw}}\frac{i}{4}a\sum_{\mu,\nu=0}^{3}\sigma_{\mu\nu}\hat{F}_{\mu\nu}(x)\psi(x). \tag{2.6}$$

The boundary counterterms read

$$\delta\mathscr{D}_W\psi(x) = \left(\delta_{x_0,0} + \delta_{x_0,T}\right)\left[(z_f - 1) + (d_s - 1)a\mathbf{D}_s\right]\psi(x), \tag{2.7}$$

with the operator

$$a\mathbf{D}_s = \frac{a}{2}\sum_k\left(\nabla_k + \nabla_k^*\right)\gamma_k - \frac{a^2}{2}\sum_k \nabla_k^*\nabla_k. \tag{2.8}$$

Here z_f is the coefficient of a dimension 3 boundary counterterm necessary to restore the P_5 symmetry which is broken by the lattice regulator. The coefficient d_s multiplies a dim 4 counterterm at the boundaries and can be tuned to remove $O(a)$ effects from the boundaries. While d_s can be understood as the χSF counterpart of the $\widetilde{c}_t$ coefficient in the SF, z_f is special from this set-up [2]. In perturbation theory these coefficients read

$$z_f = z_f^{(0)} + g_0^2 z_f^{(1)} + O(g_0^4), \qquad d_s = d_s^{(0)} + g_0^2 d_s^{(1)} + O(g_0^4), \tag{2.9}$$

where $z_f^{(0)} = 1$ and $d_s^{(0)} = 1/2$. One of the central goals of this work is to determine $z_f^{(1)}$ and $d_s^{(1)}$. Although knowing d_s to 1-loop is enough in practise, in a non-perturbative calculation z_f must be known also non-perturbatively in order to ensure that the correct symmetries are recovered in the continuum limit [3]. The knowledge of $z_f^{(1)}$ can help to guide the non-perturbtive tuning and it is moreover required in further perturbative calculations.

3. Correlation functions in the SF and the χSF

Correlation functions in the χSF set-up are defined in a similar way as in the standard SF. Writing explicitly the flavour assignments, boundary to bulk correlation functions are given by

$$g_X^{f_1 f_2}(x_0) = -\frac{1}{2}\langle X^{f_1 f_2}(x_0)\mathscr{Q}_5^{f_2 f_1}\rangle, \qquad \text{and} \qquad l_Y^{f_1 f_2}(x_0) = -\frac{1}{6}\sum_{k=1}^{3}\langle Y_k^{f_1 f_2}(x_0)\mathscr{Q}_k^{f_2 f_1}\rangle, \tag{3.1}$$

[2] Although the clover term is not needed for automatic $O(a)$ improvement, including it removes some $O(a)$ effects from P_5-odd quantities.

with the fermion bilinears being $X = A_0, V_0, S, P$, and $Y_k = A_k, V_k, T_{k0}, \widetilde{T}_{k0}$. Boundary to boundary correlation functions read

$$g_1^{f_1 f_2} = -\frac{1}{2}\langle \mathcal{Q}_5^{f_1 f_2} \mathcal{Q}'^{f_2 f_1}_5 \rangle, \qquad \text{and} \qquad l_1^{f_1 f_2} = -\frac{1}{6}\sum_{k=1}^{3}\langle \mathcal{Q}_k^{f_1 f_2} \mathcal{Q}'^{f_2 f_1}_k \rangle. \tag{3.2}$$

The boundary operators $\mathcal{Q}_5^{f_1 f_2}, \ldots$, are constructed by applying the rotation Eq.(2.2) to the standard SF boundary operators such that Eq.(2.3) holds. For avoiding the computation of disconnected diagrams occurring in correlation functions with repeated flavour assignments we consider a partially quenched set-up with 2 types of up quarks (u and u') and 2 types of down quarks (d and d') [4].

For the standard SF we use correlation functions following conventions from the literature. Following Eq.(2.3) we can write a dictionary relating correlation functions in the 2 set-ups similar to that relating standard and twisted mass QCD. Some relations with the P_5-even correlations are

$$f_A = g_A^{uu'} = -ig_V^{ud}, \qquad f_P = ig_S^{uu'} = g_P^{ud}, \qquad k_V = l_V^{uu'} = -il_A^{ud}, \qquad k_T = il_{\widetilde{T}}^{uu'} = l_T^{ud}, \tag{3.3}$$

and with P_5-odd correlation functions

$$f_V = g_V^{uu'} = -ig_A^{ud}, \qquad f_S = ig_P^{uu'} = g_S^{ud}, \qquad k_A = l_A^{uu'} = -il_V^{ud}, \qquad k_{\widetilde{T}} = il_T^{uu'} = l_{\widetilde{T}}^{ud}. \tag{3.4}$$

The tuning of z_f and m_c accounts for the restoration of P_5 and chiral symmetries and must be done simultaneously. A typical condition for fixing $m_0 = m_c$ is to demand the PCAC mass to be zero at the middle of the lattice. For determining z_f one can require any P_5-odd quantity to vanish. In this study we consider 4 renormalization conditions for z_f, i.e.

$$i)\ g_P^{uu'} = 0, \qquad ii)\ g_A^{ud} = 0, \qquad iii)\ g_V^{uu'} = 0, \qquad \text{and} \qquad iv)\ g_S^{ud} = 0. \tag{3.5}$$

Different renormalization conditions for z_f lead to differences Δz_f which vanish linearly in a/L.

4. Perturbation theory

In perturbation theory, the correlation functions of the previous subsection are expanded to 1-loop order as

$$g_X(x_0) = g_X^{(0)}(x_0) + g_X^{(1)}(x_0) g_0^2 + O(g_0^4), \qquad g_1 = g_1^{(0)} + g_1^{(1)} g_0^2 + O(g_0^4), \tag{4.1}$$

and similarly with all the other correlation functions. The gauge fixing procedure is the same as in [5], and so is the gluon propagator. The calculation of $g_X^{(1)}$ and $g_1^{(1)}$ requires de evaluation of the same set of diagrams as those shown in [5, 6], together with the contribution due to the χSF boundary counterterms Eq.(2.7). Explicit expressions for the vertices and quark propagator derived from Eq.(2.5) will be given elsewhere [7].

We have produced a program for the fast evaluation of a large set of correlation functions of fermion bilinears to 1-loop in perturbation theory for both the standard and chirally rotated set-ups. We calculate correlation functions for $L/a \in [6, 48]$ from which it is possible to extract the different terms of the asymptotic expansion of the 1-loop coefficients.

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4.1 Determination of $m_c^{(1)}$ and $z_f^{(1)}$

The 1-loop coefficients $m_c^{(1)}$ and $z_f^{(1)}$ are obtained by expanding the renormalization conditions in section 3 and solving them up to 1-loop order for a range of lattice spacings. After taking the continuum extrapolation $a/L \to 0$ we obtain

$$\begin{cases} m_c^{(1)}(c_{\rm sw}=1) = -0.2025565(1)\times C_2(R), \\ m_c^{(1)}(c_{\rm sw}=0) = -0.325721(7)\times C_2(R), \end{cases} \qquad \begin{cases} z_f^{(1)}(c_{\rm sw}=1) = 0.167572(2)\times C_2(R), \\ z_f^{(1)}(c_{\rm sw}=0) = 0.33023(6)\times C_2(R). \end{cases} \tag{4.2}$$

where $C_2(R)$ is the quadratic casimir operator in the representation[3] R.

The coefficient $m_c^{(1)}$ reproduces the known values of the critical mass for $c_{\rm sw}=1$ and 0, as expected. The coefficient $z_f^{(1)}$ has been calculated here for the first time. It is worth noting that the determination of m_c is quite independent from z_f, which has also been observed in quenched calculations [4, 8] and in dynamical studies [3].

Next we calculate the differences $\Delta z_f^{(X)} = z_f^{(1)}\Big|_X - z_f^{(1)}\Big|_{iv}$ in determining z_f using the different renormalization conditions in Eq.(3.5). In figure 1 it can be seen that $\Delta z_f^{(X)}$ vanish linearly as $a/L \to 0$ for $c_{\rm sw}=0$, while for $c_{\rm sw}=1$ the convergence is much faster.

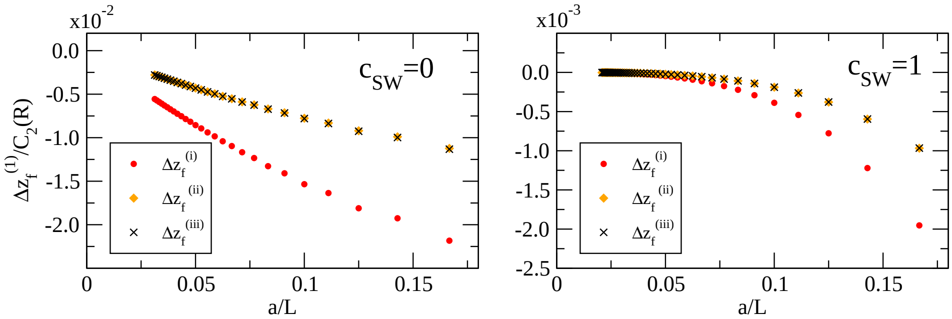

Figure 1: Differences in the 1-loop value $z_f^{(1)}$ at finite lattice spacing for the different tuning conditions.

4.2 Determination of $d_s^{(1)}$

The determination of the 1-loop boundary improvement coefficient $d_s^{(1)}$ can be done by requiring the absence of $O(a)$ terms at 1-loop in some P_5-even quantity. We consider an even quantity evaluated to 1-loop order and at several values of the fermion boundary angle θ, i.e.

$$\frac{\left[g_P^{ud}(x_0,\theta,a/L)\right]_R}{\left[g_P^{ud}(x_0,0,a/L)\right]_R}\Bigg|_{x_0=T/2}, \qquad d_s^{(1)} = -0.0009(3)\times C_2(R). \tag{4.3}$$

For $\theta = 0.1$, 0.5 and 1.0 we consistently find the value of $d_s^{(1)}$ given in Eq.(4.3).

4.3 Test of automatic $O(a)$ improvement

Once the determination of the improvement and renormalization coefficients has been done we would like to test whether the mechanism of automatic $O(a)$ improvement works.

[3] $C_2(F) = (N^2-1)/2N$ for the fundamental representation.

First of all we check that the boundary conditions Eq.(2.1) are correctly realised. After z_f is tuned to its critical value eq.(2.1) should hold up to cutoff effects. To test this we evaluate a set of even correlation functions for which the projectors at the boundary operators have been reverted[4] $Q_\pm \to Q_\mp$. Such correlations should vanish provided that boundary conditions are correctly implemented. In figure 2 it can be seen that correlation functions with reverted projectors are very small and vanish as the continuum limit is approached.

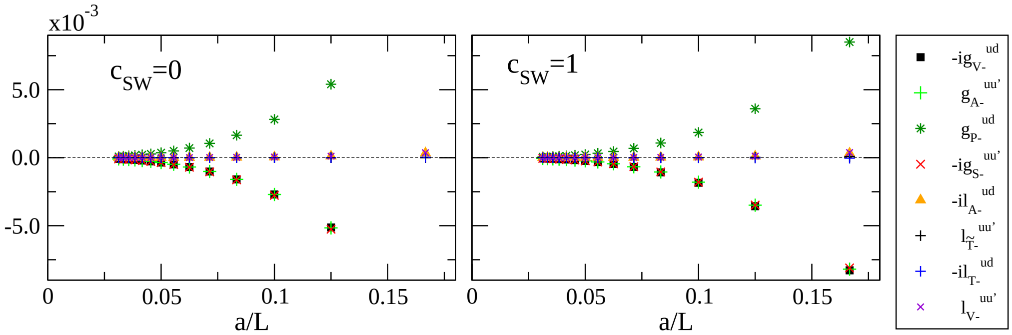

Figure 2: Vanishing correlation functions with reversed projectors in the boundary operators.

Secondly, we study the continuum limit of P_5-odd correlation functions and verify that these, being pure cutoff effects, vanish with the expected rate in a/L (see figure 3).

4.4 Universality

Once the coefficients z_f and m_c are known, the equalities in Eqs.(3.3) and (3.4) are expected to hold between ratios of renormalized correlation functions. For instance, the ratios

$$R_A = \left[\frac{g_A^{uu'}(T/2)}{\sqrt{g_1^{uu'}}}\right] \times \left[\frac{f_A(T/2)}{\sqrt{f_1}}\right]^{-1}, \qquad \text{and} \qquad R_P = \left[\frac{g_P^{ud}(T/2)}{\sqrt{g_1^{ud}}}\right] \times \left[\frac{f_P(T/2)}{\sqrt{f_1}}\right]^{-1}, \tag{4.4}$$

should approach 1 as $a/L \to 0$. In perturbation theory, the ratios are expanded as

$$R_X = R_X^{(0)} + g_0^2 R_X^{(1)} + O(g_0^4). \tag{4.5}$$

Universality implies that $R_X^{(0)} \to 1$ and $R_X^{(1)} \to 0$ as $a/L \to 0$. As can be seen from figure 4, we confirm the expected convergence of the universality relations as the continuum limit is approached.

5. Conclusions

Here we have calculated for the first time to 1-loop order in perturbation theory the renormalization and $O(a)$ improvement coefficients $z_f^{(1)}$ and $d_s^{(1)}$ for the χSF set-up. With the knowledge of these coefficients we have confirmed, always in the framework of perturbation theory, that automatic $O(a)$ improvement is at work. Also, the universality between standard and chirally rotated frameworks is confirmed. The χSF opens new possibilities for determining finite renormalization constants and $O(a)$ improvement coefficients for theories with Wilson type fermions [3]. Further perturbative calculations are essential to determine them in a way in which cutoff effects are minimal.

[4]These correlations are labelled with a "$-$"sign, i.e. $g_{X,-}^{f_1 f_2}$.

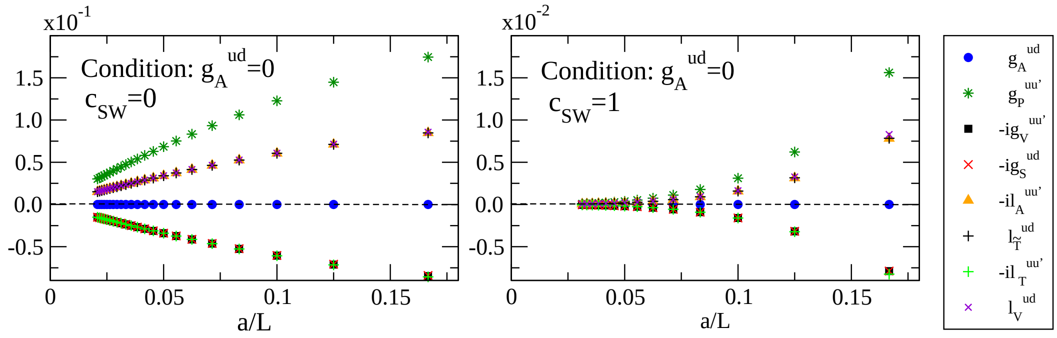

Figure 3: Vanishing P_5-odd correlation functions at 1-loop calculated for $c_{\rm SW} = 0$ and 1, with z_f fixed using the renormalization condition $g_A^{ud} = 0$.

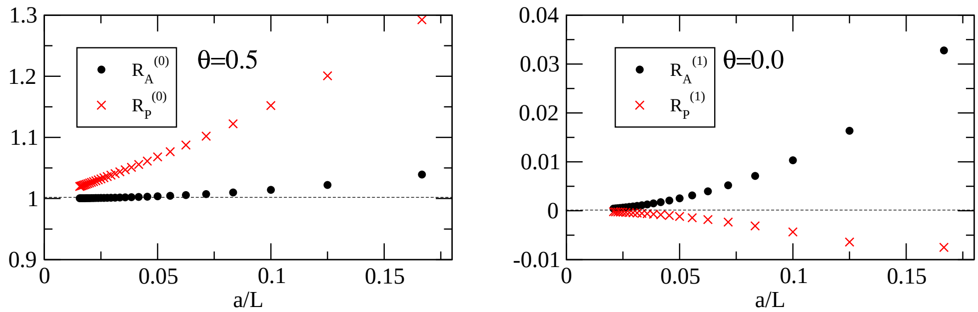

Figure 4: Ratios R_A and R_P at tree level (left panel) and 1-loop (right panel). For the tree level ratios, the fermion boundary angle is chosen to be $\theta \neq 0$. Otherwise, for the choice $\theta = 0$ cutoff effects are absent from tree-level correlation functions and the ratio is exactly 1.

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