A formulation of domain wall fermions in the Schrodinger functional

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We present a formulation of domain wall fermions in the Schrodinger functional by following the universality argument given by Lüscher. To check whether the formulation works, we examine the lowest eigenmode of the free domain wall fermion operator. We confirm that the theory belongs to a correct universality class and that the eigenvector is localized near the boundaries of the fifth dimension. We also investigate the chiral symmetry breaking structure of the four dimensional effective operator. We observe that the bulk chiral symmetry breaking disappears for a large fifth dimensional size, while the breaking originated by the boundary effects persists and exponentially decays away from the time boundaries.

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1. Introduction

In the study of CP violation by CKM unitary triangle analysis, hadron matrix elements of four-fermion operators, such as $B_K$, play a vital role. Accurate calculations of this quantity from first principles are an important task for the lattice QCD community. In such calculations, having chiral symmetry is crucial to avoid an operator mixing problem which causes uncontrollable systematic errors. Therefore, the RBC/UKQCD collaboration [1] is currently using lattice chiral fermions, such as, domain wall fermions (DWF), to compute $B_K$. In the course of the computation, there are many sources of systematic errors which one has to control. Among them, the non-perturbative renormalization (NPR) could be a serious source. At the moment, the collaboration has been using conventional schemes, namely, the RI/MOM scheme and its variant [2, 3]. However, this scheme could be subtle depending on the target quantity. To avoid such difficulties, a new scheme was invented, known as the Schrodinger functional (SF) scheme [4]. This scheme provides a reliable way of estimating errors in the NPR. If one wants to use this scheme for the renormalization of $B_K$ given by the RBC collaboration, first of all, one has to formulate DWF in the SF setup. This is a purpose of this paper.

In the SF setup, a formulation of lattice chiral fermions is in fact a non-trivial task. This can be seen as follows. First, let us consider the continuum theory with the SF boundary conditions,

$$P_+ \psi(x)|_{x_0=0} = P_- \psi(x)|_{x_0=T} = 0,$$

$$\bar{\psi}(x) P_- |_{x_0=0} = \bar{\psi}(x) P_+ |_{x_0=T} = 0,$$

with $P_{\pm} = (1 \pm \gamma_0)/2$. These boundary conditions break chiral symmetry explicitly. This fact indicates that the fermion propagator in such a theory does not anti-commute with $\gamma_5$ and breaking term [5] is given by

$$\gamma_5 D^{-1} + D^{-1} \gamma_5 = \Delta.$$

The breaking term $\Delta$ is supported at the time boundaries, whereas the anti-commutation relation holds in a bulk. This is a situation of the continuum theory. On the other hand, if one naively defines lattice chiral fermions by using the SF Wilson kernel operator, such a chiral operator automatically satisfies the Ginsparg-Wilson (GW) relation [6] and its inverse cannot reproduce the continuum results in eq.(1.3). This shows a difficulty of formulating the chiral fermions on the SF.

To overcome such a situation, Taniguchi [7] made the first attempt of formulating overlap fermions in the SF by using an orbifolding technique. Furthermore, he extended his idea to DWF [8] and then he and his collaborators obtained the renormalized $B_K$ in the quenched QCD [9]. However, in dynamical simulations, his approach for overlap fermions has a sign problem for odd flavors. Although this problem can be removed for even flavors, the flavor symmetry is broken explicitly as an expense. Sint [10] proposed a solution for even numbers of flavors which preserves the flavor symmetry exactly. However, this formulation can only be applied for the even number of flavors. This conflicts with the current trend toward large scale dynamical $2+1$ flavor simulations. To overcome such a circumstance, Lüscher [5] proposed a completely different approach following the universality and symmetry considerations. In that paper, he gave a formulation for overlap fermions. However, DWF from this approach has not been discussed so far, therefore we address this issue in this paper.
In the following, after introducing Lüscher’s argument, we give a formulation of DWF in the SF setup. And then we show some investigations to check how it really works. To enhance readability, in the following, the lattice spacing is suppressed unless necessary.

2. Universality argument

The argument in the continuum theory given in the previous section suggests that on the lattice, the GW relation has to be modified to correctly reproduce the continuum results. To this end, a chiral fermion operator also has to be modified compared with that of the usual infinite lattice. It is not so hard to break the GW relation itself and one can easily imagine that such a modification would be local and related with the boundary conditions. However, it is not clear how the SF boundary conditions come out? Lüscher gave an answer to the question [5], which uses a symmetry consideration and an order counting. What he concludes is that the SF boundary conditions are natural and more stable than other boundary conditions in the continuum limit, because the dimension of the Dirichlet type boundary conditions is lower than that of the Neumann type boundary conditions. Bottom line is that it is guaranteed that the SF boundary conditions are automatically reproduced in the continuum limit without fine tuning if the lattice fermion operator is modified such that the GW relation is broken near the time boundaries.

Before going into the concrete discussion of DWF, let us summarize a general instruction to formulate chiral fermions in the SF from the Lüscher’s argument. Firstly, including additional terms, which break the GW relation, to a lattice fermion operator such that the GW breaking is supported near the time boundaries. Secondly, keeping other symmetries, like C, P, T and flavor symmetries etc., which we do not want to lose. This instruction does not dictate a unique form of the operator, and actually there are an infinite number of possibilities. The important thing here is that the details of the operator actually do not matter as long as it fulfills these conditions. When these conditions hold, the corresponding lattice fermions are automatically guaranteed to follow the SF boundary condition in the continuum limit thanks to the order counting argument. By following this instruction, we define DWF in the SF in the next section.

3. Universality formulation of DWF

A possible form of the massless DWF operator in the SF is given by

\[
D_{\text{DWF}} = \begin{bmatrix}
D_w + 1 & -P_L & -P_R & -cB & cB \\
-P_R & D_w + 1 & -P_L & cB & -P_L + cB \\
-P_R & D_w + 1 & -P_L & cB & -P_L \\
-cB & -P_R & D_w + 1 & -P_L & -P_R \\
-cB & -P_R & D_w + 1 & -P_L & -P_R \\
\end{bmatrix}
\]  \(3.1\)

This is a five dimensional block form and the block elements are four dimensional operator. \(D_w(m_5)\) is the Wilson fermion operator in the SF [1] with the parameter \(m_5\) and is supported in a range of the time \(1 \leq x_0 \leq T - 1\). Here, the size for the fifth direction\(^1\) is taken as \(L_5 = 6\) as

\(^1\)We assume that \(L_5\) is an even number.
an example. The additional terms which are proportional to the coefficient $c$ are distributed along the cross diagonal elements. This is something like a generalized mass term and breaks the chiral symmetry explicitly. The block element $B$ is now supported only near time boundary,

$$B(x,y) = \delta_{x,y} \delta_{\delta x_0, \delta y_0} \gamma_5 (\delta_{\delta x_0, 1} P_- + \delta_{\delta x_0, T-1} P_+).$$

(3.2)

This time dependence comes from a motivation that we do want to maintain the chiral symmetry in a bulk in time. We will check that the breaking of the GW relation is really supported near the time boundaries exponentially (see Section 4.2). In this way, such fifth dimensional coordinate and time dependences are determined. Next, how about the spinor structure? Actually, this structure may be fixed to some extent by requiring the C, P, T symmetries and the $\Gamma_5$-Hermiticity. These requirements are not so strong to determine the spinor structure completely and there is some freedom. The structure given in eq.(3.2) is one of many solutions. Actually, we examined several choices of the spinor structure in the boundary term and confirmed the universal results in the continuum limit for the lowest eigenvalue.

The coefficient $^2 c \neq 0$ is a parameter which can be used to achieve the O($a$) improvement. The physical mass term can be added in the same way as the infinite lattice case.

4. Check of formulation

The next step is to check how it works. We investigate several things as follows. First, we study the lowest eigenmode for the free operator to see the importance of the presence of the boundary term. Second, we address the breaking of the GW relation for the four dimensional effective operator. This is to see what the chiral breaking term looks like. We also checked scaling properties of the free spectrum of the lowest ten eigenvalues and carried out the one-loop calculation and obtained sensible results. However we do not show them here due to limited space. In the near future, we will show them in a full paper.

4.1 The lowest eigenmode for free massless operator

Let us see the lowest eigenmode of the free massless operator $D_{\text{DWF}}^\dagger D_{\text{DWF}}$

$$D_{\text{DWF}}^\dagger D_{\text{DWF}} \psi = \lambda_{\text{min}} \psi.$$  

(4.1)

To show the importance of the boundary term, we consider two cases with $c = 1$ and $c = 0$. In the free case, the Fourier transformation can be performed for the spatial directions and we project onto the zero momentum configuration.

For $c = 1$, we obtained the minimum eigenvalue, $T^2 \lambda_{\text{min}} = 2.59...$ This value is rather close to the continuum one $\pi^2/4 = 2.47...$ in Ref.[12]. The difference is considered to be a lattice artifact. The eigenfunction in Figure [1] (left panel) shows the expected behavior, namely, being localized in the fifth direction while propagating in the time direction. This is apparently a physical mode. On the other hand, when switching off the boundary term $c = 0$, the eigenvalue $0.61...$ is quite far from the continuum value. Actually, a scaling study with larger lattice sizes shows that the theory

\[ c = 0 \] is not allowed as we will see in Section 4.1.
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Figure 1: \( |\psi(x_0, s)|_{\text{spin}} \) with the zero spatial momentum with the parameters \( T = L_s = 40, \theta = 0 \) and \( m_5 = 1 \). The norm for the eigenvector is taken for the spinor space. The left (right) panel is for \( c = 1 \) (\( c = 0 \)).

does not belong to the correct universality class. Furthermore, the eigenfunction in the right panel of Figure 1 appears to propagate in the fifth direction. This is not a physical mode anymore.

This result shows that the presence of the boundary term is essential to correctly produce the continuum results. In other words, this term is essential to be in a correct universality class.

4.2 Chiral symmetry breaking by boundary effect

Next, let us check that DWF in the SF has an expected chiral symmetry breaking structure. To this end, for the effective four dimensional operator \([13, 14]\),

\[
\det[D^{(L_s)}_{\text{eff}}] = \det[D_{\text{DWF}}/D_{\text{PV}}],
\]

let us consider the breaking of the GW relation

\[
\Delta^{(L_s)} = \gamma_5 D^{(L_s)}_{\text{eff}} + D^{(L_s)}_{\text{eff}} \gamma_5 - 2 D^{(L_s)}_{\text{eff}} \gamma_5 D^{(L_s)}_{\text{eff}}.
\]

For finite \( L_s \), there are two sources of chiral symmetry breaking, namely, a bulk source and a boundary source. The former can be removed by taking \( L_s \) to infinity. After this limit, the remaining chiral symmetry breaking must be due to the boundary source only. Actually, it is known that the corresponding breaking for overlap fermions exponentially decays away from the time boundaries \([5]\). We want to check this kind of phenomena for DWF in a free case numerically.

Figure 2 shows the magnitude of the chiral symmetry breaking \( \Delta^{(L_s)} \) in eq.(4.3) with the zero spatial momentum configuration. The norm in \( ||\Delta||_{\text{spin}} \) is taken for the spinor index. For \( L_s = 4 \), we can see large chiral symmetry breaking in diagonal elements not only near boundaries but also in a bulk. However, at increased \( L_s \), the bulk breaking gets smaller and then finally it disappears for \( L_s = 24 \). In the end, the remaining breaking is exponentially localized near boundaries and we observe the expected behavior mentioned above.
5. Concluding remarks and outlook

By following the universality argument, we constructed DWF in the SF setup. And then we checked some fundamental properties of the theory, namely, that the lowest eigenmode is localized around the fifth dimensional boundaries and the GW relation breaking for the effective four dimensional operator has the expected structure. Although we do not show it in this paper, we also checked the universality at the one-loop level. In total, our formulation works very well.

We are now ready to study NPR of $B_K$ for any flavors with DWF by using the SF scheme. Finally, we comment that by using our formulation, one can carry out a search for a conformal window. Since chiral fermions have benefits such as requiring no mass tuning to realize the mass independent renormalization scheme and no constraint on the number of flavors, our formulation can play a crucial role for solid quantitative studies.

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