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Schrödinger functional formalism with domain-wall fermion

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Abstract: Finite volume renormalization scheme is one of the most fascinating scheme for non-perturbative renormalization on lattice. By using the step scaling function one can follow running of renormalized quantities with reasonable cost. It has been established the Schrödinger functional is very convenient to define a field theory in a finite volume for this purpose. The Schrödinger functional, which is characterized by a Dirichlet boundary condition in temporal direction, is well defined and works well for the Yang-Mills theory and QCD. Furthermore it matches well with lattice regularization. However one easily runs into difficulties if one sets the same sort of the Dirichlet boundary condition for the overlap Dirac operator or the domain-wall fermion on lattice. In this paper we propose an orbifolding projection procedure to impose the Schrödinger functional Dirichlet boundary condition on the domain-wall fermion.

1. Introduction

Perturbative renormalization factor is a source of systematic errors in numerical investigation of lattice QCD. There has been progress in numerical simulation with dynamical fermions nowadays and sources of systematic error is decreasing. Evaluation of renormalization factors in non-perturbative method is required. Finite volume renormalization scheme is one of the most fascinating procedure to define non-perturbative renormalization scheme on lattice. By using the step scaling function one can follow running of renormalized quantities from low energy region to perturbative region with reasonable cost for recent computers. It has been established that the Schrödinger functional is very convenient to define a field theory in a finite volume for renormalization scheme.

The Schrödinger functional (SF) is defined as a transition amplitude between two boundary states with finite time separation [1, 2, 3, 4]

$$Z = \left\langle C'; x_0 = T | C; x_0 = 0 \right\rangle = \int \mathcal{D}\Phi e^{-S[\Phi]} \tag{1.1}$$

and is written in a path integral representation of the field theory with some boundary condition. The renormalization scale can be introduced by a finite volume $T \times L^3 \sim L^4$ of the system in this formulation defined through the SF. One of motivation to adopt the SF is that it matches with the lattice regularization very well, although the SF is independent of a regularization. The formulation is already accomplished for the non-linear σ-model [5], the non-Abelian gauge theory [6] and the QCD [7, 8] including $\mathcal{O}(a)$ improvement procedure for the Wilson fermion [9, 10]. (See Ref. [11] for review.)

Several renormalization quantities like running gauge coupling [12, 13, 14, 15, 16, 17, 18], Z-factors and $\mathcal{O}(a)$ improvement factors [19, 20, 21, 22, 23, 24] are extracted conveniently by using a Dirichlet boundary conditions for spatial component of the gauge field

$$A_k(x)|_{x_0=0} = C_k(\vec{x}), \quad A_k(x)|_{x_0=T} = C'_k(\vec{x}) \tag{1.2}$$

and for the quark fields

$$P_+\psi(x)|_{x_0=0} = \rho(\vec{x}), \quad P_-\psi(x)|_{x_0=T} = \rho'(\vec{x}), \tag{1.3}$$

$$\overline{\psi}(x)P_-|_{x_0=0} = \overline{\rho}(\vec{x}), \quad \overline{\psi}(x)P_+|_{x_0=T} = \overline{\rho}'(\vec{x}), \tag{1.4}$$

$$P_\pm = \frac{1 \pm \gamma_0}{2}. \tag{1.5}$$

One of advantage of this Dirichlet boundary condition is that the system acquire a mass gap proportional to $1/T$ and there is no infra-red divergence. The finite volume plays a role of an infra-red cut-off. Field theory with Dirichlet boundary condition is shown to be renormalizable for the pure gauge theory [6] and QCD at one loop order [8].

Although it is essential to adopt Dirichlet boundary condition for a mass gap and renormalizability, it has a potential problem of zero mode in fermion system. For instance starting from a free Lagrangian

$$\mathcal{L} = \overline{\psi}\left(\gamma_\mu \partial_\mu + m\right)\psi \tag{1.6}$$

with positive constant mass $m > 0$ and the Dirichlet boundary condition

$$P_-\psi|_{x_0=0} = 0, \quad P_+\psi|_{x_0=T} = 0 \tag{1.7}$$

the zero eigenvalue equation $(\gamma_0\partial_0 + m)\,\psi = 0$ in temporal direction allows a solution

$$\psi = P_+e^{-mx_0} + P_-e^{-m(T-x_0)} \tag{1.8}$$

in $T \to \infty$ limit and a similar solution remains even for finite T with an exponentially small eigenvalue $\propto e^{-mT}$. * In the SF formalism this solution is forbidden by adopting an "opposite" Dirichlet boundary condition (1.3) and the system has a finite gap even for $m = 0$ [7].

For the Wilson fermion [7] on lattice the Dirichlet boundary condition is automatically chosen among

$$P_\pm\psi|_{x_0=0} = 0, \quad P_\mp\psi|_{x_0=T} = 0 \tag{1.9}$$

depending on signature of the Wilson term. For example if we adopt a typical signature of the Wilson parameter $r = 1$

$$D_W = \gamma_\mu\frac{1}{2}\left(\nabla^*_\mu + \nabla_\mu\right) - \frac{a}{2}\nabla^*_\mu\nabla_\mu + M \tag{1.10}$$

the allowed Dirichlet boundary condition is the same as (1.3). In this case the zero mode solution is forbidden by choosing a proper signature for the mass term; the mass should be kept positive $M \geq 0$ to eliminate the zero mode [7, 17] †.

However as was discussed in the previous paper [25, 26] this zero mode problem may become fatal in the overlap Dirac operator [27, 28] and the domain-wall fermion [29, 30, 31]. Both the overlap Dirac operator and the domain-wall fermion is defined through the four dimensional Wilson Dirac operator (1.10) but with a relatively opposite signature for the Wilson fermion mass parameter M (domain-wall height) to the Wilson parameter r. An opposite signature is necessary to impose heavy masses on the doublers and a single massless mode to survive. A requirement to the four dimensional Wilson Dirac operator is that D_W should have a gap from zero. If this is not the case the chiral Ward-Takahashi identity is broken dynamically for the domain-wall fermion that the explicit breaking term does not vanish [31]. For the overlap Dirac operator closing of the gap may cause to break locality of the Dirac operator [32].

If the Dirichlet boundary condition (1.3) (1.4) is imposed to all fermion fields of the overlap Dirac operator or the domain-wall fermion exponentially small eigenvalues are allowed in the kernel D_W because of a relatively opposite signature of the Wilson parameter and the domain-wall height. Since these small eigenvalues are continuous in spatial momentum a gap closes in D_W, which may become a lethal problem in large T limit to break essential properties of the chiral Dirac operator.

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*If we keep the mass in the range $0 < m < 1/T$ we have a finite eigenvalue [7].

†This condition for mass M is valid at tree level. The Wilson fermion mass receives additive quantum correction δM with interaction and the condition becomes $M + \delta M \geq 0$.

One may wonder that the small eigenvalues are boundary effect and should be localized near the temporal boundary. If one considers physics apart from the boundary there should be no harm. However this is not the case for our purpose to define renormalization scheme. In finite volume scheme the renormalization scale is given by a size of the box, which is realized by considering a correlation function of operators to be separated by an order of box size. At least one of operators cannot be away from the boundary. Furthermore it is convenient for the SF scheme to set one of the operator at the boundary.

In order to solve this problem an orbifolding projection procedure was proposed for the overlap Dirac operator in Ref. [25]. [‡] In this formulation we start from a theory on $S^1 \times R^3$ and impose orbifolding projection S^1/Z_2 on temporal direction. Since we have set anti-periodic boundary condition in temporal direction S^1 before projection we have a mass gap proportional to $1/T$, which is not broken by the orbifolding. Because of this mass gap we can avoid the zero mode problem of Dirichlet boundary condition.

In this paper the orbifolding formulation of the SF boundary condition is applied to the domain-wall fermion. In section 2 the domain-wall fermion on $S^1 \times T^3$ is introduced. Formulation of domain-wall fermion in finite volume with the SF boundary condition is discussed in section 3. Application of orbifolding procedure to fermionic part is almost straightforward as was discussed in Ref. [26]. We can use the same kind of symmetry argument as in the previous paper [25]. Difficulty is in a treatment of the Pauli-Villars field. We adopted effective Dirac operator for this purpose. The proper Dirichlet boundary condition (1.3) (1.4) may not be the unique choice to define a finite volume renormalization scheme. In section 4 a chirally twisted boundary condition is discussed to define a finite volume field theory keeping a good property of the SF boundary condition. Section 5 is devoted for conclusion.

2. Domain-wall fermion action

The purpose of this paper is to introduce the domain-wall fermion system, with which we can define a finite volume renormalization scheme (Schrödinger functional scheme). The formulation for the pure Yang-Mills theory has been established in Ref. [6] by using a transition amplitude between two boundary states (Schrödinger functional). In this formulation the gauge field (link variable) lives in a finite box $N_T \times N_L^3$ with a periodic boundary condition in spatial direction and the SF Dirichlet boundary condition at the temporal boundary

$$U_k(\vec{x}, 0) = W_k(\vec{x}), \quad U_k(\vec{x}, N_T) = W'_k(\vec{x}). \tag{2.1}$$

We shall adopt this procedure for the gauge part and treat the gauge field as an external field in this paper.

The transition amplitude of the fermion field has been introduced for the Wilson fermion using the transfer matrix in Ref. [7]. The fermion field resides in the same finite

[‡]After finishing this paper a new paper appeared to propose a method to define chiral symmetric theory with the SF Dirichlet boundary condition [33].

box for the path integral formalism with periodic or twisted boundary condition [9] in spatial direction and the SF Dirichlet boundary condition (1.3) and (1.4) in temporal direction. This fermion system is renormalizable including a shift in the boundary field ρ and $\overline{\rho}$ [8]. Another specific property is that this system has a mass gap proportional to the temporal length $1/T$ and the finite box serves as an infra-red regulator.

We shall construct the domain-wall fermion system in a finite box keeping the same sort of properties as the Wilson fermion; (i) the theory has a mass gap proportional to $1/T$, (ii) there are boundary fields ρ and $\overline{\rho}$ in temporal direction and the theory is renormalizable including a shift in these fields. If one naively impose the boundary condition (1.3) and (1.4) to all the fifth dimensional field $\psi(x,s)$ then the chiral symmetry is broken "dynamically" as explained in the introduction. In order to avoid this problem we adopt an orbifolding procedure, where we start from doubled time length $2N_T$ and fermion fields in the finite box of length N_T with the Dirichlet boundary condition is realized by an orbifolding projection. For this purpose we copy gauge configuration with the SF boundary condition (2.1) into negative region and produce a time reflection symmetric configuration, which satisfies

$$U_k(\vec{x},x_0)=U_k(\vec{x},-x_0),\quad U_0(\vec{x},x_0)=U_0^\dagger(\vec{x},-x_0-1) \tag{2.2}$$

as in the previous formulation of overlap Dirac operator [25]. The periodic boundary condition is set with length $2N_T$

$$U_\mu(\vec{x},x_0+2N_T)=U_\mu(\vec{x},x_0). \tag{2.3}$$

In this paper we adopt the Shamir's domain-wall fermion [30, 31] on a lattice $2N_T\times N_L^3\times N_5$

$$S=a^4\sum_{\vec{x},\vec{y}}\sum_{x_0,y_0=-N_T+1}^{N_T}\sum_{s,t=1}^{N_5}\overline{\psi}(x,s)D_{\rm dwf}(x,y;s,t)\psi(y,t). \tag{2.4}$$

x_0 and y_0 represent the temporal coordinate which runs $-N_T+1\le x_0\le N_T$. s and t are used for the fifth dimensional coordinate which runs $1\le s\le N_5$. Summation over repeated temporal and fifth dimensional indices is taken implicitly in the following unless otherwise stated. For later use of orbifolding we set the anti-periodic boundary condition in temporal direction

$$\psi(\vec{x},x_0+2N_T,s)=-\psi(\vec{x},x_0,s),\quad \overline{\psi}(\vec{x},x_0+2N_T,s)=-\overline{\psi}(\vec{x},x_0,s). \tag{2.5}$$

The Dirac operator is given as a five dimensional Wilson's one with conventional Wilson parameter $r=1$ and negative mass parameter (domain-wall height) $-M$ with $0<M<2$

$$\begin{aligned}
aD_{\rm dwf}(x,y;s,t) &= \gamma_M D_M-\frac{1}{2}D^2-M\\
&= \left(\frac{-1+\gamma_0}{2}U_0(x)W^+_{x_0,y_0}+\frac{-1-\gamma_0}{2}U_0^\dagger(y)W^-_{x_0,y_0}\right)\delta_{x_i,y_i}\delta_{s,t}\\
&\quad+\left(\frac{-1+\gamma_i}{2}U_i(x)\delta_{y_i,x_i+1}+\frac{-1-\gamma_i}{2}U_i^\dagger(y)\delta_{y_i,x_i-1}\right)\delta_{x_0,y_0}\delta_{s,t}\\
&\quad+\left(\frac{-1+\gamma_5}{2}\Omega^+(m_f)_{s,t}+\frac{-1-\gamma_5}{2}\Omega^-(m_f)_{s,t}\right)\delta_{x,y}\\
&\quad+(5-M)\delta_{x,y}\delta_{s,t},
\end{aligned} \tag{2.6}$$

where $W^{\pm}$ are hopping operator in temporal direction with anti-periodic boundary condition, whose explicit form for $2N_T = 6$ is written as

$$W^{+}_{x_0,y_0} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad W^{-} = \left(W^{+}\right)^{\dagger}. \tag{2.7}$$

$\Omega^{\pm}$ are hopping operator in fifth direction with Dirichlet boundary condition (for massless case), whose matrix form for $N_5 = 6$ is given by

$$\Omega^{+}(m_f)_{s,t} = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ -m_f & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad \Omega^{-}(m_f) = \left(\Omega^{+}(m_f)\right)^{\dagger}. \tag{2.8}$$

Here m_f is a physical quark mass.

The physical quark field is defined by the fifth dimensional boundary field with chiral projection

$$q(x) = \left(P_L\delta_{s,1} + P_R\delta_{s,N_5}\right)\psi(x,s), \tag{2.9}$$

$$\overline{q}(x) = \overline{\psi}(x,s)\left(\delta_{s,N_5}P_L + \delta_{s,1}P_R\right), \tag{2.10}$$

$$P_{R/L} = \frac{1 \pm \gamma_5}{2}. \tag{2.11}$$

The physical quark mass term is given as an ordinary form $\mathcal{L}_{\text{mass}} = m_f\overline{q}q$ with this quark field.

3. Schrödinger functional with conventional boundary condition

In this section we shall construct the domain-wall fermion system in finite box, in which the conventional SF Dirichlet boundary condition (1.3) and (1.4) is satisfied by the physical quark field. This formulation will be done by making use of an orbifolding in temporal direction.

3.1 Orbifolding construction of SF boundary condition

Since we adopted anti-periodic boundary condition in temporal direction with period $2N_T$ fermion field is living on S^1. The orbifolding S^1/Z_2 is to identify the negative time coordinate with the positive one $x_0 = -x_0$. Identification of fields on S^1 is performed according to the symmetry of the theory including the time reflection. A homogeneous Dirichlet boundary condition will appear at fixed points.

The time reversal symmetry of the domain-wall fermion is given by

$$\psi(\vec{x}, x_0, s) \to \overline{\Sigma}_{x_0,y_0;s,t}\psi(\vec{x}, y_0, t), \quad \overline{\psi}(\vec{x}, x_0, s) \to \overline{\psi}(\vec{x}, y_0, t)\overline{\Sigma}_{y_0,x_0;t,s}, \tag{3.1}$$

$$\overline{\Sigma}_{x_0,y_0;s,t} = i\gamma_5\gamma_0 R_{x_0,y_0} P_{s,t}, \tag{3.2}$$

where P is a parity transformation in fifth direction $P_{s,t}\psi(\vec{x}, x_0, t) = \psi(\vec{x}, x_0, N_5 - s + 1)$, whose matrix representation is

$$P_{s,t} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (N_5 = 6) \tag{3.3}$$

and R is a time reflection operator acting on the temporal direction $R_{x_0,y_0}\psi(\vec{x}, y_0, s) = \psi(\vec{x}, -x_0, s)$, whose matrix form is given by

$$R_{x_0,y_0} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \quad (2N_T = 6) \tag{3.4}$$

to satisfy anti-periodicity in $2N_T$. We notice that R has a symmetric fixed point $x_0 = 0$ and an anti-symmetric fixed point $x_0 = N_T$

$$R\psi(\vec{x}, 0, s) = \psi(\vec{x}, 0, s), \quad R\psi(\vec{x}, N_T, s) = -\psi(\vec{x}, N_T, s). \tag{3.5}$$

The domain-wall fermion Dirac operator is invariant under the time reflection

$$\left[\overline{\Sigma}, D_{\rm dwf}\right] = 0 \tag{3.6}$$

since the reflection invariant gauge configuration (2.2) is adopted .

In order to realize the SF boundary condition at the fixed points we need to combine the chiral transformation with the time reflection [25]. The chiral transformation is given by a vector like rotation of fermion field but with a different charge for two boundaries in fifth direction [31]

$$\psi(x, s) \to iQ_{s,t}\psi(x, t), \quad \overline{\psi}(x, s) \to -\overline{\psi}(x, t)iQ_{t,s}, \tag{3.7}$$

where Q is the vector charge matrix which flips sign in the middle of the fifth direction [§]

$$Q_{s,t} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \quad (N_5 = 6). \tag{3.8}$$

We consider massless $m_f = 0$ theory in this sub-section.

Here we should notice that this chiral rotation is not an exact symmetry of the domain-wall fermion Dirac operator but we have an explicit breaking term

$$Q D_{\rm dwf} Q - D_{\rm dwf} = 2X, \tag{3.9}$$

where X is a contribution from the middle layer, which picks up a charge difference there

$$aX = \left(P_L \delta_{s,\frac{N_5}{2}} \delta_{t,\frac{N_5}{2}+1} + P_R \delta_{s,\frac{N_5}{2}+1} \delta_{t,\frac{N_5}{2}} \right) \delta_{x,y}. \tag{3.10}$$

However it was discussed in Ref. [31] that if we consider correlation functions between the bilinear $\overline{\psi} X \psi$ and the physical quark operators contribution is suppressed exponentially in N_5 under the condition that the transfer matrix in fifth direction has a gap from unity. Furthermore the domain-wall fermion Dirac operator with explicit time reflection invariance (3.6) does not have index [25], since the contribution to the index [34]

$$\lim_{N_5\to\infty} a^4 \sum_x \left\langle \overline{\psi}(x,s) \gamma_5 X_{s,t} \psi(x,t) \right\rangle = - \lim_{N_5\to\infty} \mathrm{tr} \left(\gamma_5 X \frac{1}{D_{\rm dwf}} \right) \tag{3.11}$$

can be shown to vanish by using anti-commutativity $\left\{ \gamma_5 X, \overline{\Sigma} \right\} = 0$. We expect that X has no effect on anomaly. We shall ignore this term in the following by constraining that we treat the physical quark Green's functions only.

Another way to avoid the explicit breaking term is to include it into the Dirac operator. By using an anti-commutative nature $\{Q, X\} = 0$ we can define a chiral symmetric Dirac operator by

$$D_{\rm dwf}^{\rm sym} = D_{\rm dwf} + X, \tag{3.12}$$

which commutes with Q exactly even at finite N_5. The orbifolding projection in the following can be defined in an exact sense. A compensation of the exact chiral symmetry at finite N_5 is a non-locality in the effective Dirac operator, which however is suppressed exponentially in N_5. Detailed property of this Dirac operator is deferred in appendix A.

[§]We notice that definition of Q is rather ambiguous. A requirement is that a total distance from a kink (where signature of the vector charge changes) to both the boundary is $\mathcal{O}(N_5)$. In this sense one can set the kink anywhere. Although definition of the explicit breaking term X changes, the same proof of the chiral WT identity in Ref. [31] is applicable. One can define Q appropriately for odd N_5.

Combining the time reversal transformation (3.1) and the chiral transformation (3.7) we define the orbifolding transformation

$$\psi(\vec{x}, x_0, s) \to A_{x_0,y_0;s,t}\psi(\vec{x}, y_0, t), \quad \overline{\psi}(\vec{x}, x_0, s) \to \overline{\psi}(\vec{x}, y_0, t)A_{y_0,x_0;t,s}, \tag{3.13}$$

$$A_{x_0,y_0;s,t} = \gamma_0\gamma_5(PQ)_{s,t}R_{x_0,y_0}. \tag{3.14}$$

The domain-wall fermion Dirac operator has time reversal symmetry (3.6) and we assume that the chiral transformation is an exact symmetry of the Dirac operator

$$[Q, D_{\rm dwf}] = 0 \tag{3.15}$$

by ignoring effect of the explicit breaking term X or by adopting the symmetric Dirac operator ¶. The orbifolding transformation becomes symmetry of the Dirac operator

$$[A, D_{\rm dwf}] = 0. \tag{3.16}$$

In order to show this we may use a relation $\{P, Q\} = 0$.

The operator A satisfies a property $A^2 = 1$ and can be used to define a projection operator. The orbifolding identification of the fermion field is given by projecting out the following symmetric sub-space

$$\overline{\Pi}_-\psi(x, s) = 0, \quad \left(\overline{\psi}\,\overline{\Pi}_-\right)(x, s) = 0, \quad \overline{\Pi}_\pm = \frac{1 \pm A}{2}. \tag{3.17}$$

This projection relates fields in negative region to those in the positive $\psi(\vec{x}, -x_0, s) = \gamma_0\gamma_5 PQ\psi(\vec{x}, x_0, s)$, which means fields in the negative is not independent. As will be discussed in appendix C if we consider non-negative region $0 \le x_0 \le N_T$, fields in the bulk $0 < x_0 < N_T$ is not constrained. Only the boundary fields obey a projection condition

$$\overline{P}_-\psi(\vec{x}, 0, s) = 0, \quad \overline{P}_+\psi(\vec{x}, N_T, s) = 0, \tag{3.18}$$

$$\left(\overline{\psi}\,\overline{P}_-\right)(\vec{x}, 0, s) = 0, \quad \left(\overline{\psi}\,\overline{P}_+\right)(\vec{x}, N_T, s) = 0 \tag{3.19}$$

with projection operator

$$\overline{P}_\pm = \frac{1 \pm \overline{\Gamma}}{2}, \quad \overline{\Gamma} = \gamma_0\gamma_5 PQ. \tag{3.20}$$

The orbifolding projection for the physical quark field is given by picking up the boundary components from the projected fermion field

$$(P_L\delta_{s,1} + P_R\delta_{s,N_5})\left(\overline{\Pi}_-\right)_{s,t}\psi(x, t) = \Pi_+ q(x) = 0, \tag{3.21}$$

$$\overline{\psi}(x, t)\left(\overline{\Pi}_-\right)_{t,s}(\delta_{s,N_5}P_L + \delta_{s,1}P_R) = \overline{q}(x)\Pi_- = 0, \tag{3.22}$$

$$\Pi_\pm = \frac{1 \pm \Gamma}{2}, \quad \Gamma = \gamma_0 R, \tag{3.23}$$

¶Effect of the explicit breaking term X at finite N_5 is discussed in appendix B.

which turns out to be the same condition for the continuum theory in Ref. [25]. The proper homogeneous SF Dirichlet boundary condition is provided at fixed points $x_0 = 0, N_T$ for the physical quark fields

$$P_+ q(x)|_{x_0=0} = 0, \quad P_- q(x)|_{x_0=N_T} = 0, \tag{3.24}$$

$$\overline{q}(x) P_-|_{x_0=0} = 0, \quad \overline{q}(x) P_+|_{x_0=N_T} = 0. \tag{3.25}$$

The massless orbifolded action is given by projection

$$S_{\rm SF} = a^4 \sum \frac{1}{2} \overline{\psi} D_{\rm dwf}^{\rm SF} \psi, \quad D_{\rm dwf}^{\rm SF} = \overline{\Pi}_+ D_{\rm dwf} \overline{\Pi}_+. \tag{3.26}$$

We notice the massless SF Dirac operator $D_{\rm dwf}^{\rm SF}$ breaks "chiral symmetry" (3.7) explicitly by the projection $\overline{\Pi}_+$. However the symmetry breaking effect comes from the projection (3.18) (3.19) at the boundary. Ordinary chiral Ward-Takahashi identity [31] is satisfied in the bulk $0 < x_0 < N_T$ where fields are not constrained.

Our original theory on S^1 has a gap because of the anti-periodic boundary condition. This gap is kept intact after orbifolding, which can be confirmed at tree level. We have a Hermiticity relation for the SF Dirac operator

$$\left(D_{\rm dwf}^{\rm SF}\right)^\dagger = \gamma_5 P D_{\rm dwf}^{\rm SF} \gamma_5 P \tag{3.27}$$

and this Dirac operator connects the same Hilbert sub-space

$$D_{\rm dwf}^{\rm SF} : \overline{\mathcal{H}}_- \to \overline{\mathcal{H}}_-, \quad \overline{\mathcal{H}}_- = \left\{ \psi \left| \overline{\Pi}_- \psi = 0 \right. \right\}. \tag{3.28}$$

It is straightforward to solve the eigenvalue problem numerically at tree level. Here we omit the detail but we can easily see that the lowest eigenvalue (a gap) converge to $\pi/2T$ in the continuum limit, which agrees with that of continuum massless theory [7].

We have a comment on mass term. We dropped quark mass term since it breaks the chiral symmetry. However as was discussed in Ref. [25] it is possible to introduce a mass term which is consistent with the orbifolding symmetry (3.13). One of candidates is

$$S_{\rm mass} = \sum_x m_f \overline{q}(x) \eta(x_0) q(x), \tag{3.29}$$

where η is an anti-symmetric step function

$$\begin{aligned} &\eta(-x_0) = -\eta(x_0), \quad \eta(x_0 + 2T) = \eta(x_0), \\ &\eta(x_0) = 1 \quad \text{for} \quad 0 < x_0 < N_T. \end{aligned} \tag{3.30}$$

As will be discussed in appendix C the bulk part of this projected Dirac operator is exactly the same as that of the ordinary domain-wall fermion. The physical quark fields satisfies the proper boundary condition. Together with existence of the mass gap this orbifolded system is a strong candidate of QCD with the SF boundary condition to define a finite volume scheme.

3.2 Free propagator

In order to check that the orbifolded domain-wall fermion system describes the QCD with the SF boundary condition properly we consider the physical quark propagator at tree level. The massless fermion propagator is given as an inverse of the projected Dirac operator

$$a^3 G^{\mathrm{SF}}_{\mathrm{dwf}}(x,y;s,t) = 2\left(aD^{\mathrm{SF}}_{\mathrm{dwf}}\right)^{-1}_{x,y;s,t} = 2\left(\overline{\Pi}_+ \frac{1}{aD_{\mathrm{dwf}}}\overline{\Pi}_+\right)_{x,y;s,t}. \tag{3.31}$$

where inverse is defined in the sub-space $\overline{\mathcal{H}}_-$

$$D^{\mathrm{SF}}_{\mathrm{dwf}}\left(D^{\mathrm{SF}}_{\mathrm{dwf}}\right)^{-1} = \left(D^{\mathrm{SF}}_{\mathrm{dwf}}\right)^{-1} D^{\mathrm{SF}}_{\mathrm{dwf}} = \overline{\Pi}_+. \tag{3.32}$$

At tree level this propagator can be written in a simple form as

$$a^3 G^{\mathrm{SF}}_{\mathrm{dwf}}(x,y;s,t) = \frac{1}{N_L^3}\sum_{\vec{p}} e^{i\vec{p}(\vec{x}-\vec{y})} G^{\mathrm{SF}}_{\mathrm{dwf}}(\vec{p};x_0,y_0;s,t), \tag{3.33}$$

$$\begin{aligned} G^{\mathrm{SF}}_{\mathrm{dwf}}(\vec{p};x_0,y_0;s,t) = \frac{1}{2aN_T}\sum_{n=-N_T+1}^{N_T}\left(\frac{1}{D_{\mathrm{dwf}}(p)}\right)_{s,t'} &\left\{\left(e^{ip_0(x_0-y_0)} + e^{ip_0(x_0+y_0)}\right)\left(\overline{P}_+\right)_{t',t}\right. \\ &\left. + \left(e^{ip_0(x_0-y_0)} - e^{ip_0(x_0+y_0)}\right)\left(\overline{P}_-\right)_{t',t}\right\}, \end{aligned} \tag{3.34}$$

where the projection operator $\overline{P}_\pm$ is defined in (3.20). The momentum p_μ is multiplied by lattice spacing implicitly and is dimensionless. The temporal momentum p_0 satisfies the quantization condition

$$p_0 = \frac{2n-1}{2N_T}\pi, \quad -N_T+1 \le n \le N_T \tag{3.35}$$

for anti-periodicity in $2N_T$. $D_{\mathrm{dwf}}(p)$ is the domain-wall fermion Dirac operator in momentum space without orbifolding projection

$$aD_{\mathrm{dwf}}(p) = i\gamma_\mu \sin p_\mu + W(p) - P_L\Omega^+ - P_R\Omega^-, \tag{3.36}$$

$$W(p) = 1 - M + \sum_\mu\left(1-\cos p_\mu\right). \tag{3.37}$$

The explicit form of its inverse can be derived according to Ref. [30], which we defer to appendix D.

The physical quark propagator is given by selecting the contribution from the boundary fields in fifth direction

$$\begin{aligned} G^{\mathrm{SF}}_{\mathrm{quark}}(x,y) &= \left(P_L\delta_{s,1} + P_R\delta_{s,N_5}\right) G^{\mathrm{SF}}_{\mathrm{dwf}}(x,y;s,t)\left(\delta_{t,N_5}P_L + \delta_{t,1}P_R\right) \\ &= 2\left(\Pi_- G_{\mathrm{quark}}\Pi_+\right)_{x,y}, \end{aligned} \tag{3.38}$$

where

$$a^3 G_{\mathrm{quark}}(x,y) = \left(P_L\delta_{s,1} + P_R\delta_{s,N_5}\right)\left(\frac{1}{aD_{\mathrm{dwf}}}\right)_{x,y;s,t}\left(\delta_{t,N_5}P_L + \delta_{t,1}P_R\right) \tag{3.39}$$

is the physical quark propagator in $2N_T \times N_L^3$ space-time without any projection. The proper Dirichlet boundary conditions [10]

$$P_+ G^{\rm SF}_{\rm quark}(x,y)|_{x_0=0} = 0, \quad P_- G^{\rm SF}_{\rm quark}(x,y)|_{x_0=N_T} = 0, \tag{3.40}$$
$$G^{\rm SF}_{\rm quark}(x,y)|_{y_0=0} P_- = 0, \quad G^{\rm SF}_{\rm quark}(x,y)|_{y_0=N_T} P_+ = 0 \tag{3.41}$$

are satisfied for this quark propagator because of the projection $\Pi_\pm$. By ignoring sub-leading terms in e^{-N_5} the propagator takes the following form at tree level

$$a^3 \sum_{\vec{x}} e^{-i\vec{p}(\vec{x}-\vec{y})} G^{\rm SF}_{\rm quark}(x,y) = \frac{1}{2N_T} \sum_{n=-N_T+1}^{N_T} \left(\frac{i\gamma_\mu \sin p_\mu}{1-e^\alpha W(p)} \right) e^{ip_0 x_0}$$
$$\times \left\{ \left(e^{-ip_0 y_0} + e^{ip_0 y_0}\right) P_+ + \left(e^{-ip_0 y_0} - e^{ip_0 y_0}\right) P_- \right\}, \tag{3.42}$$

which can be shown to approach to the continuum SF propagator of Ref. [10] without any $\mathcal{O}(a)$ term. This system has no extra zero mode we encountered in naive formulation and we conclude that this is equivalent to the QCD with SF boundary condition.

3.3 Renormalizability

In this sub-section we discuss renormalizability of the theory from a symmetry point of view. As ordinary QCD the domain-wall fermion system has a symmetry under parity

$$\psi(x,s) \to \gamma_0 P_{st} \psi(-\vec{x}, x_0, t), \quad \overline{\psi}(x,s) \to \overline{\psi}(-\vec{x}, x_0, t)\gamma_0 P_{ts}, \tag{3.43}$$

and charge conjugation transformation

$$\psi(x,s) \to C P_{st} \overline{\psi}^T(x,t), \quad \overline{\psi}(x,s) \to \psi^T(x,t) P_{ts} \left(-C^{-1}\right), \quad C = \gamma_2\gamma_0, \tag{3.44}$$

where we need fifth dimensional parity transformation matrix P to compensate a variation in extra degrees of freedom. The system also has a flavour symmetry and a chiral symmetry (3.7) for massless case in the bulk $0 < x_0 < N_T$, where chiral Ward-Takahashi identity of Ref. [31] is satisfied.

Almost all the candidates for extra counter term, which are not included in the tree level system, are ruled out by these symmetries. Here we should notice that this statement is valid if we restrict ourselves to Green's functions with the physical quark fields only. If we consider a whole system including unphysical bulk fields it is shown that an extra term appears in the effective action at one loop order [35]. However this is not a crucial problem because a detailed form of the five dimensional action is not important. A point is that the four dimensional QCD is defined by the physical quark field at fifth dimensional boundary. When we treat Green's functions with the physical quark field it was shown that quantum correction is renormalized into the quark field, the quark mass and the physical operators at one loop level [36, 37]. In this sense we consider counter terms which is written in terms of the physical quark field only to survive in the physical Green's function.

Now a candidate for an extra counter term is a mass like term $\overline{q}q$ and $\overline{q}\gamma_0 q$ at the boundary, which is not forbidden by the chiral symmetry. However since the action (3.26) is given by projecting onto a symmetric sub-space we have a symmetry under a "chiral" orbifolding transformation

$$\delta\left(\overline{\Pi}_+\psi\right)(x,s)=\alpha\left(\overline{\Pi}_+\psi\right)(x,s), \tag{3.45}$$
$$\delta\left(\overline{\psi}\,\overline{\Pi}_+\right)(x,s)=-\alpha\left(\overline{\psi}\,\overline{\Pi}_+\right)(x,s), \tag{3.46}$$

where opposite degrees of freedom $\overline{\Pi}_-\psi$ and $\overline{\psi}\,\overline{\Pi}_-$ are kept intact. Using the orbifolding projection (3.17) it is easy to show that this transformation is a "chiral" transformation only at the boundary

$$\delta\left(\overline{P}_+\psi\right)(\vec{x},0,s)=\alpha\left(\overline{P}_+\psi\right)(\vec{x},0,s), \tag{3.47}$$
$$\delta\left(\overline{\psi}\,\overline{P}_+\right)(\vec{x},0,s)=-\alpha\left(\overline{\psi}\,\overline{P}_+\right)(\vec{x},0,s), \tag{3.48}$$
$$\delta\left(\overline{P}_-\psi\right)(\vec{x},N_T,s)=\alpha\left(\overline{P}_-\psi\right)(\vec{x},N_T,s), \tag{3.49}$$
$$\delta\left(\overline{\psi}\,\overline{P}_-\right)(\vec{x},N_T,s)=-\alpha\left(\overline{\psi}\,\overline{P}_-\right)(\vec{x},N_T,s) \tag{3.50}$$

and is a vector $U(1)$ transformation in the bulk $0<x_0<N_T$

$$\delta\psi(\vec{x},x_0,s)=\alpha\psi(\vec{x},x_0,s),\quad \delta\overline{\psi}(\vec{x},x_0,s)=-\alpha\overline{\psi}(\vec{x},x_0,s). \tag{3.51}$$

In terms of the physical quark field the chiral orbifolding transformation is given by

$$\delta\left(P_-q(\vec{x},0)\right)=\alpha P_-q(\vec{x},0),\quad \delta\left(\overline{q}(\vec{x},0)P_+\right)=-\alpha\overline{q}(\vec{x},0)P_+, \tag{3.52}$$
$$\delta\left(P_+q(\vec{x},N_T)\right)=\alpha P_+q(\vec{x},N_T),\quad \delta\left(\overline{q}(\vec{x},N_T)P_-\right)=-\alpha\overline{q}(\vec{x},N_T)P_-. \tag{3.53}$$

A mass like term $\overline{q}q$ and $\overline{q}\gamma_0 q$ is forbidden at the boundary by this chiral orbifolding symmetry.

According to a similar discussion to that for chiral index (3.11) we can easily show that orbifolding matrix A does not have an index and the orbifolding symmetry is not broken by anomaly. No extra counter term is needed to renormalize the orbifolded theory with homogeneous boundary condition. Orbifolding symmetry under (3.45) (3.46) keeps renormalizability. Boundary source fields are introduced to break orbifolding symmetry in the next sub-section and renormalizability will be discussed again.

3.4 Surface term

In the orbifolding construction of the SF formalism only the homogeneous boundary condition (3.24) (3.25) can be introduced. However in general SF formalism the Dirichlet boundary condition is inhomogeneous as (1.3) and (1.4). The boundary values $\rho,\cdots,\overline{\rho}'$ are regarded as external source fields coupled to the dynamical fields and the correlation functions involving the boundary fields

$$\zeta(\vec{x})=\frac{\delta}{\delta\overline{\rho}(\vec{x})},\quad \overline{\zeta}(\vec{x})=-\frac{\delta}{\delta\rho(\vec{x})}, \tag{3.54}$$
$$\zeta'(\vec{x})=\frac{\delta}{\delta\overline{\rho}'(\vec{x})},\quad \overline{\zeta}'(\vec{x})=-\frac{\delta}{\delta\rho'(\vec{x})} \tag{3.55}$$

are used conveniently to extract the renormalization factors.

Couplings between the boundary source fields and the dynamical fields are not introduced automatically in our formulation since the boundary value vanishes by projection. The boundary source fields are elements of projected degrees of freedom $\overline{\Pi}_-\psi$ and $\overline{\psi}\,\overline{\Pi}_-$. The surface term is given to connect the boundary source fields and the dynamical fields $\overline{\Pi}_+\psi$, $\overline{\psi}\,\overline{\Pi}_+$ and it is not consistent with the orbifolding symmetry (3.45) (3.46).

In this paper we define a surface term as an orbifolding symmetry breaking term, which is consistent with other symmetries of the orbifolded domain-wall fermion; parity, charge conjugation, flavor and chiral symmetry in the bulk. We notice that the orbifolding symmetry becomes ordinary vector like $U(1)$ symmetry (3.51) in the bulk, which should not be broken. A reasonable way is to break it at the boundary, where the symmetry becomes "chiral". One of candidates is a physical quark mass term $m_f\overline{q}q$, which keeps the bulk vector like $U(1)$ symmetry. But this is forbidden by the chiral Ward-Takahashi identity in the bulk. The symmetry should be broken only at the boundary.

We introduce boundary source fields as a component of projected out degrees of freedom in (3.18) and (3.19)

$$\lambda(\vec{x},s)=\overline{P}_-\psi(\vec{x},0,s),\quad \lambda'(\vec{x},s)=\overline{P}_+\psi(\vec{x},N_T,s), \tag{3.56}$$

$$\overline{\lambda}(\vec{x},s)=\left(\overline{\psi}\,\overline{P}_-\right)(\vec{x},0,s),\quad \overline{\lambda}'(\vec{x},s)=\left(\overline{\psi}\,\overline{P}_+\right)(\vec{x},N_T,s) \tag{3.57}$$

The orbifolding symmetry breaking term takes the form

$$\begin{aligned} S_{\text{breaking}} = {} & \overline{\lambda}(\vec{x},s)\hat{O}_{st}\overline{P}_+\psi(\vec{x},0,t)+\left(\overline{\psi}\,\overline{P}_+\right)(\vec{x},0,s)\hat{O}_{st}\lambda(\vec{x},t) \\ & +\overline{\lambda}'(\vec{x},s)\hat{O}_{st}\overline{P}_-\psi(\vec{x},N_T,t)+\left(\overline{\psi}\,\overline{P}_-\right)(\vec{x},N_T,s)\hat{O}_{st}\lambda'(\vec{x},t), \end{aligned} \tag{3.58}$$

where $\hat{O}$ is a local operator which anti-commute with $\overline{\Gamma}=\gamma_0\gamma_5 PQ$. Candidates of $\hat{O}$ are γ_0, γ_5, Q, P and

$$K(u)_{st}=\left(P_L\delta_{s,N_5+1-u}+P_R\delta_{s,u}\right)\left(P_L\delta_{t,u}+P_R\delta_{t,N_5+1-u}\right), \tag{3.59}$$

$$\widetilde{K}(u)_{st}=\left(P_R\delta_{s,N_5+1-u}+P_L\delta_{s,u}\right)\left(P_R\delta_{t,u}+P_L\delta_{t,N_5+1-u}\right), \tag{3.60}$$

where summation over u is not taken. Among these candidates γ_5 and Q are forbidden by the parity symmetry. γ_0 is not consistent with the charge conjugation. P, $K(u)$ and $\widetilde{K}(u)$ break chiral symmetry, which however is not a problem at the boundary. Since P, $K(u)$ and $\widetilde{K}(u)$ are consistent with parity and charge conjugation they are proper candidates of orbifolding symmetry breaking term.

Here we remember a requirement for symmetry breaking term in the domain-wall fermion. A whole five dimensional symmetry needs not to be broken since our ultimate interest is a four dimensional chiral symmetric effective theory defined at the fifth dimensional boundary. Only a four dimensional symmetry of the effective theory should be broken. An example is the physical quark mass term. It is not the unique term which breaks the chiral symmetry (3.7). Other terms like $\overline{\psi}P\psi$, $\overline{\psi}K(u)\psi$ and $\overline{\psi}\widetilde{K}(u)\psi$ also break the chiral symmetry and are consistent with the parity and the charge conjugation. However we adopt only the physical quark mass term $m_f\overline{q}q$ as the chiral symmetry breaking term. This is because we are not interested in detailed form of the five dimensional action and in terms of the effective theory the quark mass term is the only candidate to break four dimensional chiral symmetry. ‖

In this paper we restrict ourselves to physical quark operator for symmetry breaking term. Now our task is to find dimension three physical quark operator which is consistent with the parity and charge conjugation and breaks the orbifolding symmetry (3.52) (3.53). The only candidate is the mass term $\overline{q}q$ and charge conjugation odd term $\overline{q}\gamma_0 q$. We notice that $K(1)$ produces a physical quark mass term $\overline{\psi}K(1)\psi = \overline{q}q$ and the surface term is given by

$$\begin{aligned} S_{\rm surface} &= -a^3 \sum_{\vec{x}} \Big(\overline{\lambda}(\vec{x},s) K(1)_{st} \overline{P}_{+} \psi(\vec{x},0,t) + \left(\overline{\psi}\ \overline{P}_{+}\right)(\vec{x},0,s) K(1)_{st} \lambda(\vec{x},t) \\ &\quad + \overline{\lambda}'(\vec{x},s) K(1)_{st} \overline{P}_{-} \psi(\vec{x},N_T,t) + \left(\overline{\psi}\ \overline{P}_{-}\right)(\vec{x},N_T,s) K(1)_{st} \lambda'(\vec{x},t) \Big) \\ &= a^3 \sum_{\vec{x}} \Big(- \overline{\rho}(\vec{x}) P_{-} q(x)\big|_{x_0=0} - \overline{q}(x) P_{+} \rho(\vec{x})\big|_{x_0=0} \\ &\quad - \overline{\rho}'(\vec{x}) P_{+} q(x)\big|_{x_0=N_T} - \overline{q}(x) P_{-} \rho'(\vec{x})\big|_{x_0=N_T} \Big), \end{aligned} \tag{3.61}$$

where q and $\overline{q}$ are active dynamical fields at the temporal boundary. ρ and $\overline{\rho}$ are boundary source fields for the physical quark fields

$$P_{+} q(x)|_{x_0=0} = \rho(\vec{x}), \quad P_{-} q(x)|_{x_0=N_T} = \rho'(\vec{x}), \tag{3.62}$$

$$\overline{q}(x) P_{-}|_{x_0=0} = \overline{\rho}(\vec{x}), \quad \overline{q}(x) P_{+}|_{x_0=N_T} = \overline{\rho}'(\vec{x}). \tag{3.63}$$

This surface term converge to that of the continuum theory in $a \to 0$ limit.

Since this surface term is not a general orbifolding symmetry breaking term of domain-wall fermion, general anticipation is that all sort of breaking terms will appear by quantum corrections in five dimensional theory. However our main concern is the four dimensional effective theory defined through the physical quark fields and renormalizability should be discussed in terms of the effective theory. According to our experience for the physical quark mass term we may not need all the breaking terms to renormalize the physical effective theory. This is because our surface term (3.61) is a general form of the orbifolding symmetry breaking in the effective theory. The effective theory is realized by considering Green functions constructed with physical quark operators only. We may expect that quantum correction which appear in these Green functions is proportional to the original surface term and can be renormalized into a shift of physical operators and physical quark source fields ρ, $\overline{\rho}$, ρ' and $\overline{\rho}'$. Explicit calculation is necessary to confirm this expectation.

We check validity of this surface term at tree level. According to Ref. [10] we introduce the generating functional

$$Z_F \left[\overline{\rho}', \rho'; \overline{\rho}, \rho; \overline{\eta}, \eta; U\right] = \int D\psi D\overline{\psi} \exp\Big\{ -S_F \left[U, \overline{\psi}, \psi; \overline{\rho}', \rho', \overline{\rho}, \rho\right]$$

‖As was mentioned in the previous sub-section if we introduce the physical quark mass, other breaking terms like $\overline{\psi}P\psi$ appear in five dimensional action by quantum correction. However if we consider Green's functions constructed with the physical quark operators we can show that quantum corrections are renormalized into the quark field, quark mass and the physical operators at one loop level [36].

$$+a^4\sum_{x,s}\left(\overline{\psi}(x,s)\eta(x,s)+\overline{\eta}(x,s)\psi(x,s)\right)\Big\}, \tag{3.64}$$

where $\eta(x)$ and $\overline{\eta}(x)$ are source fields for the fermion and the total action S_F is given as a sum of the bulk action (3.26) and the surface term (3.61). We notice that the fermion fields ψ and $\overline{\psi}$ obey the orbifolding condition (3.17). The correlation functions between the boundary fields are derived with the same procedure as Ref. [10].

$$\left\langle\psi(x,s)\overline{\psi}(y,t)\right\rangle = G^{\rm SF}_{\rm dwf}(x,y;s,t), \tag{3.65}$$
$$\langle q(x)\overline{q}(y)\rangle = G^{\rm SF}_{\rm quark}(x,y), \tag{3.66}$$
$$\left\langle q(x)\overline{\zeta}(\vec{y})\right\rangle = G^{\rm SF}_{\rm quark}(x,y)P_+\big|_{y_0=0} \tag{3.67}$$
$$\left\langle q(x)\overline{\zeta}'(\vec{y})\right\rangle = G^{\rm SF}_{\rm quark}(x,y)P_-\big|_{y_0=N_T}, \tag{3.68}$$
$$\langle\zeta(\vec{x})\overline{q}(y)\rangle = P_-\ G^{\rm SF}_{\rm quark}(x,y)\big|_{x_0=0}, \tag{3.69}$$
$$\left\langle\zeta'(\vec{x})\overline{q}(y)\right\rangle = P_+\ G^{\rm SF}_{\rm quark}(x,y)\big|_{x_0=N_T}, \tag{3.70}$$
$$\left\langle\zeta(\vec{x})\overline{\zeta}(\vec{y})\right\rangle = P_-\ G^{\rm SF}_{\rm quark}(x,y)P_+\big|_{x_0=0,y_0=0}, \tag{3.71}$$
$$\left\langle\zeta(\vec{x})\overline{\zeta}'(\vec{y})\right\rangle = P_-\ G^{\rm SF}_{\rm quark}(x,y)P_-\big|_{x_0=0,y_0=N_T}, \tag{3.72}$$
$$\left\langle\zeta'(\vec{x})\overline{\zeta}(\vec{y})\right\rangle = P_+\ G^{\rm SF}_{\rm quark}(x,y)P_+\big|_{x_0=N_T,y_0=0}, \tag{3.73}$$
$$\left\langle\zeta'(\vec{x})\overline{\zeta}'(\vec{y})\right\rangle = P_+\ G^{\rm SF}_{\rm quark}(x,y)P_-\big|_{x_0=N_T,y_0=N_T}. \tag{3.74}$$

The propagator $G^{\rm SF}_{\rm dwf}$ and $G^{\rm SF}_{\rm quark}$ are given in (3.31) and (3.38). We notice that the above propagators between the boundary fields and physical quark fields approach to the continuum SF boundary propagator without any $\mathcal{O}(a)$ term at tree level.

3.5 Effective action of the domain-wall fermion

In order to perform numerical simulation with dynamical fermion we need to introduce the Pauli-Villars field to cancel bulk contribution in fifth direction. The Pauli-Villars field is a four component complex scalar and its action is given by

$$S_{\rm PV} = a^4\sum_{\vec{x},\vec{y}}\sum_{x_0,y_0=-N_T+1}^{N_T}\sum_{s,t=1}^{N_5}\overline{\phi}(x,s)D_{\rm PV}(x,y;s,t)\phi(y,t), \tag{3.75}$$

where Dirac operator for the Pauli-Villars field is given in the same form as the domain-wall fermion Dirac operator (2.6) with $m_f=1$

$$D_{\rm PV} = D_{\rm dwf}(m_f=1). \tag{3.76}$$

This Dirac operator does not commute with the orbifolding operator $A=\gamma_0\gamma_5 PQR$ because of the mass term. It is not straightforward to introduce the Pauli-Villars field by orbifolding. In this paper we propose to implement it by the effective Dirac operator [34, 38].

The effective Dirac operator appears in an effective action of the physical quark field (2.9) (2.10) and "physical" Pauli-Villars field

$$Q(x) = (P_L\delta_{s,1}+P_R\delta_{s,N_5})\,\phi(x,s), \tag{3.77}$$
$$\overline{Q}(x) = \overline{\phi}(x,s)\,(\delta_{s,N_5}P_L+\delta_{s,1}P_R). \tag{3.78}$$

The effective action is given by integrating out all the bulk fields other than physical fields at the fifth dimensional boundary [34]

$$S_{\text{eff}} = a^4 \sum \left[\overline{q}(x) \left(D_{\text{eff}}\right)_{xy} q(y) + \overline{Q}(x) \left(D_{\text{eff}} + \frac{1}{a} \right)_{xy} Q(y) \right]. \tag{3.79}$$

In its derivation the effective Dirac operator D_{eff} is given as an inverse of the full physical quark propagator

$$aD_{\text{eff}} = \frac{1}{a^3 \langle q\overline{q} \rangle}, \tag{3.80}$$

whose explicit form is

$$aD_{\text{eff}} = \frac{1+\gamma_5 S}{1-\gamma_5 S}, \quad S = \frac{1-T^{N_5}}{1+T^{N_5}}, \quad T = \frac{1-H'}{1+H'}, \quad H' = \gamma_5 D_W \frac{1}{2+D_W}. \tag{3.81}$$

Here D_W is a four dimensional Wilson Dirac operator with negative mass $-2 < -M < 0$. In $N_5 \to \infty$ limit the Dirac operator becomes

$$aD_{\text{eff}} = \frac{1+\gamma_5 \epsilon\left(\widetilde{H}\right)}{1-\gamma_5 \epsilon\left(\widetilde{H}\right)}, \quad T = e^{-\widetilde{H}}, \tag{3.82}$$

where $\epsilon(x)$ is a sign function

$$\epsilon(x) = \frac{x}{\sqrt{x^2}}. \tag{3.83}$$

We can easily check that this Dirac operator is exactly chiral symmetric

$$\{\gamma_5, D_{\text{eff}}\} = 0 \tag{3.84}$$

in $N_5 \to \infty$ limit and should be non-local to satisfy the Nielsen-Ninomiya's no-go theorem.

The effective Dirac operator is related to the original domain-wall fermion and the Pauli-Villars field Dirac operator through determinant

$$\det \frac{1}{D_{\text{PV}}} D_{\text{dwf}} = \det \frac{aD_{\text{eff}}}{aD_{\text{eff}}+1} = \det aD_{N_5}, \tag{3.85}$$

where D_{N_5} is a truncated overlap Dirac operator [34, 38]. Hereafter we take $N_5 \to \infty$ limit implicitly and write $D_{N_5 \to \infty} = D_{\text{OD}}$. In terms of the domain-wall fermion the overlap Dirac operator is defined as

$$D_{\text{OD}} = \frac{D_{\text{eff}}}{aD_{\text{eff}}+1}. \tag{3.86}$$

D_{OD} satisfies the Ginsparg-Wilson relation [39] **

$$\{\gamma_5, D_{\text{OD}}\} = 2aD_{\text{OD}}\gamma_5 D_{\text{OD}}. \tag{3.87}$$

**The Ginsparg-Wilson relation derived from a standard notation of the domain-wall fermion has a factor two. This corresponds to $\overline{a} = 2a$ for the GW relation adopted in Ref. [25].

If we introduce physical quark mass term we have a massive overlap Dirac operator through determinant

$$D_{\mathrm{OD}}(m_f) = \frac{D_{\mathrm{eff}} + m_f}{aD_{\mathrm{eff}} + 1} = D_{\mathrm{OD}} + m_f\left(1 - aD_{\mathrm{OD}}\right). \tag{3.88}$$

The effective Dirac operator of the orbifolded domain-wall fermion system is defined in a similar way. Since the four dimensional Wilson Dirac operator D_W commute with the four dimensional time reflection operator $\Sigma = i\gamma_5\gamma_0 R$ we have following anti-commutation relations

$$\left\{\Sigma, H'\right\} = 0, \quad \left\{\Sigma, \widetilde{H}\right\} = 0. \tag{3.89}$$

By using these relations we can easily show that the effective Dirac operator (3.82) anti-commute with the four dimensional orbifolding operator Γ defined in (3.23)

$$\{\Gamma, D_{\mathrm{eff}}\} = 0. \tag{3.90}$$

The massless overlap Dirac operator (3.86) satisfy “Ginsparg-Wilson relation” for the orbifolding transformation [25]

$$\{\Gamma, D_{\mathrm{OD}}\} = 2aD_{\mathrm{OD}}\Gamma D_{\mathrm{OD}}. \tag{3.91}$$

We define the Schrödinger functional effective Dirac operator as an inverse of the orbifolded full quark propagator (3.38)

$$aD_{\mathrm{eff}}^{\mathrm{SF}} = \Pi_+ \frac{1}{a^3\left\langle q\overline{q}\right\rangle}\Pi_- = \Pi_+ aD_{\mathrm{eff}}\Pi_-, \tag{3.92}$$

where inverse means that in a sub-space

$$a^4 D_{\mathrm{eff}}^{\mathrm{SF}} G_{\mathrm{quark}}^{\mathrm{SF}} = 2\Pi_+, \quad a^4 G_{\mathrm{quark}}^{\mathrm{SF}} D_{\mathrm{eff}}^{\mathrm{SF}} = 2\Pi_-. \tag{3.93}$$

Contribution from the Pauli-Villars field is introduced to reproduce the Schrödinger functional overlap Dirac operator defined in Ref. [25] ††

$$D_{\mathrm{OD}}^{\mathrm{SF}} = \Pi_+ D_{\mathrm{eff}}\Pi_- \frac{1}{aD_{\mathrm{eff}} + 1} = \Pi_+ D_{\mathrm{OD}}\widehat{\Pi}_-, \tag{3.94}$$

where

$$\widehat{\Pi}_\pm = \frac{1 \pm \widehat{\Gamma}}{2}, \quad \widehat{\Gamma} = \Gamma\left(1 - 2aD_{\mathrm{OD}}\right). \tag{3.95}$$

This is not a unique definition of the SF overlap Dirac operator but we can define another Dirac operator as

$$\overline{D}_{\mathrm{OD}}^{\mathrm{SF}} = \frac{1}{aD_{\mathrm{eff}} + 1}\Pi_+ D_{\mathrm{eff}}\Pi_-. \tag{3.96}$$

††The Ginsparg-Wilson relation (3.91) in this paper corresponds to $\overline{a} = 2a$ in Ref. [25] and so is the definition of $\widehat{\Gamma}$.

These two Dirac operators are related by unitary operators

$$u = \frac{1+\Sigma}{2}\left(1-2aD_{\mathrm{OD}}\right) + \frac{1-\Sigma}{2}, \quad u' = \gamma_5 u \gamma_5 \tag{3.97}$$

as

$$u D_{\mathrm{OD}}^{\mathrm{SF}} u^{\dagger} = \overline{D}_{\mathrm{OD}}^{\mathrm{SF}}, \quad u'^{\dagger} D_{\mathrm{OD}}^{\mathrm{SF}} u' = \overline{D}_{\mathrm{OD}}^{\mathrm{SF}}. \tag{3.98}$$

Here we used a fact that the effective and the overlap Dirac operators commute with the four dimensional time reflection operator Σ.

As was discussed in Ref. [25] the SF overlap Dirac operator does not have γ_5 Hermiticity relation. Instead we have

$$\left(D_{\mathrm{OD}}^{\mathrm{SF}}\right)^{\dagger} = \gamma_5 \overline{D}_{\mathrm{OD}}^{\mathrm{SF}} \gamma_5. \tag{3.99}$$

In order to define real fermion determinant we may need even numbers of flavours and different Dirac operators for each flavours. An example for two flavours case is

$$D_{\mathrm{SF}}^{(2)} = \begin{pmatrix} D_{\mathrm{OD}}^{\mathrm{SF}} & \\ & \overline{D}_{\mathrm{OD}}^{\mathrm{SF}} \end{pmatrix}. \tag{3.100}$$

We notice that $U(2)$ vector flavour symmetry is broken to $U(1) \times U(1)$. Determinant of this Dirac operator is

$$\det aD_{\mathrm{SF}}^{(2)} = \det aD_{\mathrm{SF}}^{(2)}\gamma_5 = \det_{\mathcal{H}_-}\left(\Pi_+ aD_{\mathrm{eff}} \frac{1}{aD_{\mathrm{eff}}+1} \frac{1}{aD_{\mathrm{eff}}^{\dagger}+1} aD_{\mathrm{eff}}^{\dagger}\Pi_+\right), \tag{3.101}$$

which is re-written in terms of pseudo-fermion field χ

$$\det aD_{\mathrm{SF}}^{(2)} = \int \mathcal{D}\left(\Pi_+\chi^{\dagger}\right)\mathcal{D}\left(\Pi_+\chi\right)\exp\left(-\chi^{\dagger}\Pi_+\left(\frac{1}{aD_{\mathrm{eff}}^{\dagger}}+1\right)\left(\frac{1}{aD_{\mathrm{eff}}}+1\right)\Pi_+\chi\right). \tag{3.102}$$

The determinant is defined in a sub-space $\mathcal{H}_- = \{\psi | \Pi_-\psi = 0\}$ of eigenfunctions. In evaluation of the fermion force we need to calculate

$$\left(\frac{1}{aD_{\mathrm{eff}}}+1\right)^{-1} = \left(a^3\langle q\overline{q}\rangle + 1\right)^{-1}, \tag{3.103}$$

which corresponds to inverse of the overlap Dirac operator.

The orbifolded effective Dirac operator is modified as follows when we introduce the mass term (3.29)

$$D_{\mathrm{eff}}^{\mathrm{SF}}(m_f) = \frac{1}{2}\Pi_+\left(D_{\mathrm{eff}} + m_f\eta\right)\Pi_-. \tag{3.104}$$

Taking into account a contribution from the Pauli-Villars Dirac operator the massive SF overlap Dirac operator is defined as

$$D_{\mathrm{OD}}^{\mathrm{SF}}(m_f) = \frac{1}{2}\Pi_+\left(D_{\mathrm{eff}} + m_f\eta\right)\Pi_-\frac{1}{aD_{\mathrm{eff}}+1} = \frac{1}{2}\Pi_+\left(D_{\mathrm{OD}} + m_f\eta\left(1-aD_{\mathrm{OD}}\right)\right)\widehat{\Pi}_-, \tag{3.105}$$

$$\overline{D}_{\mathrm{OD}}^{\mathrm{SF}}(m_f) = \frac{1}{2}\frac{1}{aD_{\mathrm{eff}}+1}\Pi_+\left(D_{\mathrm{eff}} + m_f\eta\right)\Pi_-. \tag{3.106}$$

Although we do not have a unitary transformation to relate $D_{\mathrm{OD}}^{\mathrm{SF}}(m_f)$ and $\overline{D}_{\mathrm{OD}}^{\mathrm{SF}}(m_f)$ we have a Hermiticity relation

$$\left(D_{\mathrm{OD}}^{\mathrm{SF}}(m_f)\right)^\dagger = \gamma_5 \overline{D}_{\mathrm{OD}}^{\mathrm{SF}}(m_f)\gamma_5. \tag{3.107}$$

We also need even numbers of flavours to define a real fermion determinant.

4. Schrödinger functional with twisted boundary condition

In the previous section we presented an orbifolding formulation of domain-wall fermion in finite box, in which the homogeneous proper boundary condition (3.24) (3.25) is satisfied. This is a solution of our purpose to define a finite volume renormalization scheme. However this may not be the unique solution of our requirement that the theory has a mass gap and is kept to be renormalizable in a finite box. In this section we propose another orbifolding formulation to adopt chirally twisted boundary condition [25, 40]. As was discussed in Ref. [25] the chirally twisted boundary condition has advantages that the fermion determinant becomes real and the mass term is introduced easier. For domain-wall fermion the Pauli-Villars field can be treated in a straightforward way by orbifolding.

4.1 Orbifolding construction of chirally twisted boundary condition

In this section we adopt two flavours case for instance since the fermion determinant becomes real for even numbers of flavours as will be discussed later. We start from the massless orbifolded action (3.26) and introduce the twisted orbifolding by chirally rotating the fermion field

$$\psi = e^{i\frac{\pi}{4}Q\tau^3}\psi', \quad \overline{\psi} = \overline{\psi}' e^{-i\frac{\pi}{4}Q\tau^3}, \tag{4.1}$$

where τ^3 is the Pauli matrix to act on flavour space and Q is the vector charge (3.8) for chiral transformation. In terms of the rotated field the orbifolded action is given by

$$S_{\mathrm{SF}} = a^4 \sum \frac{1}{2}\overline{\psi}' \widetilde{D}_{\mathrm{dwf}}^{\mathrm{SF}} \psi', \quad \widetilde{D}_{\mathrm{dwf}}^{\mathrm{SF}} = \overline{\overline{\Pi}}_- D_{\mathrm{dwf}} \overline{\overline{\Pi}}_-, \tag{4.2}$$

where

$$\overline{\overline{\Pi}}_\pm = \frac{1 \pm \overline{\Sigma}\tau^3}{2} \tag{4.3}$$

is a twisted orbifolding projection with time reflection operator $\overline{\Sigma}$ defined in (3.1).

As was discussed in sub-section 3.1 the Dirac operator has no index and the chiral transformation is not anomalous even for Abelian case. This formulation with twisted orbifolding projection is equivalent to the original one for massless theory. Hereafter we regard that a new orbifolded theory is defined by a projection (4.3) and drop prime from the chirally rotated fermion field for simplicity. We notice that the twisted orbifolding operator $\overline{\Sigma}\tau^3$ commute with the massive domain-wall fermion Dirac operator

$$\left[\overline{\Sigma}\tau^3, D_{\mathrm{dwf}}(m_f)\right] = 0 \tag{4.4}$$

since we adopted time reflection invariant gauge configuration. We can extend this twisted formulation to massive theory

$$S_{\rm dwf}^{\rm twist}=a^4\sum\frac{1}{2}\overline{\psi}\widetilde{D}_{\rm dwf}^{\rm SF}(m_f)\psi,\quad \widetilde{D}_{\rm dwf}^{\rm SF}=\overline{\overline{\widetilde{\Pi}}}_-D_{\rm dwf}(m_f)\overline{\overline{\widetilde{\Pi}}}_-. \tag{4.5}$$

It is straightforward to introduce the Pauli-Villars field through orbifolding

$$S_{\rm PV}^{\rm twist}=a^4\sum\frac{1}{2}\overline{\phi}\widetilde{D}_{\rm PV}^{\rm SF}\phi,\quad \widetilde{D}_{\rm PV}^{\rm SF}=\overline{\overline{\widetilde{\Pi}}}_-D_{\rm PV}\overline{\overline{\widetilde{\Pi}}}_- \tag{4.6}$$

since $D_{\rm PV}=D_{\rm dwf}(m_f=1)$ and is commutable with the orbifolding operator.

The fermion fields satisfy the twisted orbifolding projection condition in this action

$$\overline{\overline{\widetilde{\Pi}}}_+\psi=0,\quad \overline{\psi}\overline{\overline{\widetilde{\Pi}}}_+=0, \tag{4.7}$$

which brings the following boundary conditions

$$\overline{\overline{\widetilde{P}}}_+\psi(\vec{x},0,s)=0,\quad \overline{\overline{\widetilde{P}}}_-\psi(\vec{x},N_T,s)=0, \tag{4.8}$$

$$\left(\overline{\psi}\,\overline{\overline{\widetilde{P}}}_+\right)(\vec{x},0,s)=0,\quad \left(\overline{\psi}\,\overline{\overline{\widetilde{P}}}_-\right)(\vec{x},N_T,s)=0 \tag{4.9}$$

with projection operator

$$\overline{\overline{\widetilde{P}}}_\pm=\frac{1\pm i\gamma_5\gamma_0P\tau^3}{2}. \tag{4.10}$$

In terms of the physical quark field the projection condition becomes

$$(P_L\delta_{s,1}+P_R\delta_{s,N_5})\left(\overline{\overline{\widetilde{\Pi}}}_+\right)_{s,t}\psi(x,t)=\widetilde{\Pi}_+q(x)=0, \tag{4.11}$$

$$\overline{\psi}(x,t)\left(\overline{\overline{\widetilde{\Pi}}}_+\right)_{t,s}(\delta_{s,N_5}P_L+\delta_{s,1}P_R)=\overline{q}(x)\widetilde{\Pi}_+=0, \tag{4.12}$$

$$\widetilde{\Pi}_\pm=\frac{1\pm\Sigma\tau^3}{2},\quad \Sigma=i\gamma_5\gamma_0R, \tag{4.13}$$

where Σ is the time reflection operator in four dimensions. The boundary condition for the physical quark field is

$$\widetilde{P}_+q(x)|_{x_0=0}=0,\quad \widetilde{P}_-q(x)|_{x_0=N_T}=0, \tag{4.14}$$

$$\overline{q}(x)\widetilde{P}_+|_{x_0=0}=0,\quad \overline{q}(x)\widetilde{P}_-|_{x_0=N_T}=0, \tag{4.15}$$

$$\widetilde{P}_\pm=\frac{1\pm i\gamma_5\gamma_0\tau^3}{2}. \tag{4.16}$$

We have two comments. The orbifolded Dirac operator with twisted projection has a following Hermiticity relation

$$\widetilde{D}_{\rm SF}(m)^\dagger=\gamma_5\tau^{1,2}\widetilde{D}_{\rm SF}(m)\gamma_5\tau^{1,2}, \tag{4.17}$$

which is also the same for the orbifolded Pauli-Villars Dirac operator. The $U(2)$ flavour symmetry is broken to $U(1)_V\times U(1)_3$ as in the chirally twisted mass QCD.

4.2 Free propagator

The original theory before orbifolding has a mass gap proportional to $1/T$ because of anti-periodicity in temporal direction. This property is robust against orbifolding process and survive in the twisted orbifolding formulation. We will check this property at tree level by using propagator.

The fermion propagator is defined as an inverse of the orbifolded Dirac operator in a sub-space

$$a^3\widetilde{G}^{\rm SF}_{\rm dwf}(x,y;s,t) = 2\left(a\widetilde{D}^{\rm SF}_{\rm dwf}\right)^{-1}_{x,y;s,t} = 2\left(\overline{\overline{\Pi}}_{-}\frac{1}{aD_{\rm dwf}}\overline{\overline{\Pi}}_{-}\right)_{x,y;s,t}, \tag{4.18}$$

$$\widetilde{D}^{\rm SF}_{\rm dwf}\left(\widetilde{D}^{\rm SF}_{\rm dwf}\right)^{-1} = \left(\widetilde{D}^{\rm SF}_{\rm dwf}\right)^{-1}\widetilde{D}^{\rm SF}_{\rm dwf} = \overline{\overline{\Pi}}_{-}. \tag{4.19}$$

At tree level this propagator can be written in a simple form as

$$a^3\widetilde{G}^{\rm SF}_{\rm dwf}(x,y;s,t) = \frac{1}{N_L^3}\sum_{\vec{p}} e^{i\vec{p}(\vec{x}-\vec{y})}\widetilde{G}^{\rm SF}_{\rm dwf}(\vec{p};x_0,y_0;s,t), \tag{4.20}$$

$$\begin{aligned}\widetilde{G}^{\rm SF}_{\rm dwf}(\vec{p};x_0,y_0;s,t) = \frac{1}{2aN_T}\sum_{n=-N_T+1}^{N_T}\left(\frac{1}{D_{\rm dwf}(p)}\right)_{s,t'}\Bigg\{&\left(e^{ip_0(x_0-y_0)}-e^{ip_0(x_0+y_0)}\right)\left(\overline{\widetilde{P}}_{+}\right)_{t',t}\\ &+\left(e^{ip_0(x_0-y_0)}+e^{ip_0(x_0+y_0)}\right)\left(\overline{\widetilde{P}}_{-}\right)_{t',t}\Bigg\}.\end{aligned} \tag{4.21}$$

$D_{\rm dwf}(p)$ is the domain-wall fermion Dirac operator in momentum space without orbifolding projection, whose inverse is given in appendix D. We notice that the temporal momentum p_0 satisfies the quantization condition (3.35) and there is no extra fermion zero mode.

The physical quark propagator is given by selecting the contribution from the boundary fields in fifth direction

$$\begin{aligned}\widetilde{G}^{\rm SF}_{\rm quark}(x,y) &= \left(P_L\delta_{s,1}+P_R\delta_{s,N_5}\right)\widetilde{G}^{\rm SF}_{\rm dwf}(x,y;s,t)\left(\delta_{t,N_5}P_L+\delta_{t,1}P_R\right)\\ &= 2\left(\widetilde{\Pi}_{-}G_{\rm quark}\widetilde{\Pi}_{-}\right)_{x,y},\end{aligned} \tag{4.22}$$

where $G_{\rm quark}(x,y)$ is the physical quark propagator in $2N_T\times N_L^3$ space-time without any projection. Following Dirichlet boundary conditions

$$\widetilde{P}_{+}G^{\rm SF}_{\rm quark}(x,y)|_{x_0=0}=0,\quad \widetilde{P}_{-}G^{\rm SF}_{\rm quark}(x,y)|_{x_0=N_T}=0, \tag{4.23}$$

$$G^{\rm SF}_{\rm quark}(x,y)|_{y_0=0}\widetilde{P}_{+}=0,\quad G^{\rm SF}_{\rm quark}(x,y)|_{y_0=N_T}\widetilde{P}_{-}=0 \tag{4.24}$$

are satisfied for this quark propagator. By ignoring sub-leading terms in e^{-N_5} the propagator takes the following form at tree level

$$\begin{aligned}a^3\sum_{\vec{x}}e^{-i\vec{p}(\vec{x}-\vec{y})}G^{\rm SF}_{\rm quark}(x,y) &= \frac{1}{2N_T}\sum_{n=-N_T+1}^{N_T}\left(\frac{i\gamma_\mu\sin p_\mu}{1-e^{\alpha}W(p)}\right)e^{ip_0x_0}\\ &\times\left\{\left(e^{-ip_0y_0}-e^{ip_0y_0}\right)\widetilde{P}_{+}+\left(e^{-ip_0y_0}+e^{ip_0y_0}\right)\widetilde{P}_{-}\right\}\end{aligned} \tag{4.25}$$

We emphasize that the physical quark has a gap (3.35) proportional to $1/T$ because of the anti-periodicity. This formulation satisfies one of the requirement.

4.3 Surface term

In this subsection we consider a twisted orbifolding symmetry and introduce a coupling to the boundary source field (surface term) as a symmetry breaking term. The orbifolded action (4.5) is invariant under the following twisted orbifolding transformation

$$\delta\left(\overline{\overline{\Pi}}_{-}\psi\right)(x,s)=\alpha\left(\overline{\overline{\Pi}}_{-}\psi\right)(x,s),\quad \delta\left(\overline{\psi}\overline{\overline{\Pi}}_{-}\right)(x,s)=-\alpha\left(\overline{\psi}\overline{\overline{\Pi}}_{-}\right)(x,s),\tag{4.26}$$

where remaining degrees of freedom $\overline{\overline{\Pi}}_{+}\psi$ and $\overline{\psi}\overline{\overline{\Pi}}_{+}$ are kept intact. The boundary source fields are elements of $\overline{\overline{\Pi}}_{+}\psi$ and $\overline{\psi}\overline{\overline{\Pi}}_{+}$.

We define a surface term as an orbifolding symmetry breaking term, which is consistent with parity

$$\psi(x,s)\to\gamma_0 P_{st}\tau^{1,2}\psi(-\vec{x},x_0,t),\quad \overline{\psi}(x,s)\to\overline{\psi}(-\vec{x},x_0,t)\gamma_0 P_{ts}\tau^{1,2},\tag{4.27}$$

charge conjugation

$$\psi(x,s)\to CP_{st}\tau^{1,2}\overline{\psi}^{T}(x,t),\quad \overline{\psi}(x,s)\to\psi^{T}(x,t)\left(-C^{-1}\right)P_{ts}\tau^{1,2},\quad C=\gamma_2\gamma_0\tag{4.28}$$

and

$$\psi(x,s)\to C(PQ)_{st}\overline{\psi}^{T}(x,t),\quad \overline{\psi}(x,s)\to\psi^{T}(x,t)\left(-C^{-1}\right)(PQ)_{ts},\quad C=\gamma_2\gamma_0\tag{4.29}$$

and vector $U(1)_3$ symmetry

$$\delta\psi(x,s)=\beta\tau^3\psi(x,s),\quad \delta\overline{\psi}(x,s)=-\beta\overline{\psi}(x,s)\tau^3.\tag{4.30}$$

of the orbifolded domain-wall fermion. Here we modified the parity and the charge conjugation transformation to be consistent with the twisted orbifolding projection.

Using the orbifolding projection (4.7) the orbifolding transformation (4.26) is shown to be a "chiral" transformation at the boundary in which a half of degrees is rotated

$$\delta\left(\overline{\overline{P}}_{-}\psi\right)(\vec{x},0,s)=\alpha\left(\overline{\overline{P}}_{-}\psi\right)(\vec{x},0,s),\tag{4.31}$$

$$\delta\left(\overline{\psi}\overline{\overline{P}}_{-}\right)(\vec{x},0,s)=-\alpha\left(\overline{\psi}\overline{\overline{P}}_{-}\right)(\vec{x},0,s),\tag{4.32}$$

$$\delta\left(\overline{\overline{P}}_{+}\psi\right)(\vec{x},N_T,s)=\alpha\left(\overline{\overline{P}}_{+}\psi\right)(\vec{x},N_T,s),\tag{4.33}$$

$$\delta\left(\overline{\psi}\overline{\overline{P}}_{+}\right)(\vec{x},N_T,s)=-\alpha\left(\overline{\psi}\overline{\overline{P}}_{+}\right)(\vec{x},N_T,s)\tag{4.34}$$

and is a vector $U(1)$ transformation in the bulk $0<x_0<N_T$

$$\delta\psi(\vec{x},x_0,s)=\alpha\psi(\vec{x},x_0,s),\quad \delta\overline{\psi}(\vec{x},x_0,s)=-\alpha\overline{\psi}(\vec{x},x_0,s).\tag{4.35}$$

The symmetry should be broken only at the boundary.

We introduce boundary source fields as a component of projected out degrees of freedom

$$\lambda(\vec{x},s)=\overline{\overline{P}}_{+}\psi(\vec{x},0,s),\quad \lambda'(\vec{x},s)=\overline{\overline{P}}_{-}\psi(\vec{x},N_T,s),\tag{4.36}$$

$$\overline{\lambda}(\vec{x},s)=\left(\overline{\psi}\,\overline{\overline{P}}_{+}\right)(\vec{x},0,s),\quad \overline{\lambda}'(\vec{x},s)=\left(\overline{\psi}\,\overline{\overline{P}}_{-}\right)(\vec{x},N_T,s).\tag{4.37}$$

The orbifolding symmetry breaking term takes the form

$$S_{\text{breaking}} = \overline{\lambda}(\vec{x},s)\widetilde{O}_{st}\overline{\overline{P}}_{-}\psi(\vec{x},0,t) + \left(\overline{\psi}\,\overline{\overline{P}}_{-}\right)(\vec{x},0,s)\widetilde{O}_{st}\lambda(\vec{x},t)$$
$$+\overline{\lambda}'(\vec{x},s)\widetilde{O}_{st}\overline{\overline{P}}_{+}\psi(\vec{x},N_T,t) + \left(\overline{\psi}\,\overline{\overline{P}}_{+}\right)(\vec{x},N_T,s)\widetilde{O}_{st}\lambda'(\vec{x},t), \tag{4.38}$$

where $\widetilde{O}$ is a local operator which anti-commute with $i\gamma_5\gamma_0 P\tau^3$. Candidates of $\widetilde{O}$ which is consistent with the parity, charge conjugation and $U(1)_3$ symmetries are $PQ\tau^3$, $K(u)Q\tau^3$ and $\widetilde{K}(u)Q\tau^3$, where K and $\widetilde{K}$ are defined in (3.59) (3.60).

As in the previous section we restrict ourselves to the physical quark field for symmetry breaking term and adopt $K(1)Q$ for the surface term

$$\begin{aligned}S_{\text{surface}} &= -a^3\sum_{\vec{x}}\Big(\overline{\lambda}(\vec{x},s)(K(1)Q)_{st}\tau^3\overline{\overline{P}}_{-}\psi(\vec{x},0,t) + \left(\overline{\psi}\,\overline{\overline{P}}_{-}\right)(\vec{x},0,s)(K(1)Q)_{st}\tau^3\lambda(\vec{x},t)\\ &\quad +\overline{\lambda}'(\vec{x},s)(K(1)Q)_{st}\tau^3\overline{\overline{P}}_{+}\psi(\vec{x},N_T,t) + \left(\overline{\psi}\,\overline{\overline{P}}_{+}\right)(\vec{x},N_T,s)(K(1)Q)_{st}\tau^3\lambda'(\vec{x},t)\Big)\\ &= a^3\sum_{\vec{x}}\Big(-\overline{\rho}(\vec{x})\gamma_5\tau^3\widetilde{P}_{-}q(x)\Big|_{x_0=0} - \overline{q}(x)\widetilde{P}_{-}\gamma_5\tau^3\rho(\vec{x})\Big|_{x_0=0}\\ &\quad -\overline{\rho}'(\vec{x})\gamma_5\tau^3\widetilde{P}_{+}q(x)\Big|_{x_0=N_T} - \overline{q}(x)\widetilde{P}_{+}\gamma_5\tau^3\rho'(\vec{x})\Big|_{x_0=N_T}\Big).\end{aligned} \tag{4.39}$$

ρ and $\overline{\rho}$ are boundary source fields for the physical quark fields

$$\widetilde{P}_{+}q(x)|_{x_0=0} = \rho(\vec{x}), \quad \widetilde{P}_{-}q(x)|_{x_0=N_T} = \rho'(\vec{x}), \tag{4.40}$$
$$\overline{q}(x)\widetilde{P}_{+}|_{x_0=0} = \overline{\rho}(\vec{x}), \quad \overline{q}(x)\widetilde{P}_{-}|_{x_0=N_T} = \overline{\rho}'(\vec{x}). \tag{4.41}$$

Although this surface term is not a general symmetry breaking term, we also expect that quantum corrections can be renormalized into a shift of physical operators and physical quark source fields ρ, $\overline{\rho}$, ρ' and $\overline{\rho}'$ if we consider Green functions constructed with physical quark operators only.

4.4 Effective action of the domain-wall fermion

For the twisted orbifolding formulation of finite volume field theory the Pauli-Villars field is introduced directly as in (4.6). Total contributions from fermion and Pauli-Villars field is

$$\det_{\overline{\overline{\mathcal{H}}}_{+}}\overline{\overline{\Pi}}_{-}\frac{1}{D_{\text{PV}}}D_{\text{dwf}}(m_f)\overline{\overline{\Pi}}_{-}, \tag{4.42}$$

where the determinant is defined in a sub-space $\overline{\overline{\mathcal{H}}}_{+} = \left\{\psi|\overline{\overline{\Pi}}_{+}\psi = 0\right\}$ of eigenfunctions. In this sub-section we will show that this determinant is equivalent to that of the overlap Dirac operator with twisted orbifolding [25]

$$\det_{\overline{\overline{\mathcal{H}}}_{+}}\overline{\overline{\Pi}}_{-}\frac{1}{D_{\text{PV}}}D_{\text{dwf}}(m_f)\overline{\overline{\Pi}}_{-} = \det_{\widetilde{\mathcal{H}}_{+}}\widetilde{\Pi}_{-}aD_{\text{OD}}(m_f)\widetilde{\Pi}_{-}. \tag{4.43}$$

For this purpose we adopt the Schur decomposition procedure for the effective Dirac operator [41, 42]. Statement of the Schur decomposition is that the overlap Dirac operator is given as a Schur complement of the domain-wall fermion Dirac operator divided by the Pauli-Villars Dirac operator

$$\frac{1}{D_{\mathrm{PV}}}D_{\mathrm{dwf}}(m_f)=\mathcal{P}U^{-1}(1)D_{\mathrm{OD}}^{(5)}(m_f)U(am_f)\mathcal{P}^{\dagger}. \tag{4.44}$$

Here $\mathcal{P}$, $U(am_f)$ and $D_{\mathrm{OD}}^{(5)}(m_f)$ are matrices in fifth dimension and their explicit forms for $N_5=6$ case are given by

$$\mathcal{P}=\begin{pmatrix} P_R & & & & & P_L \\ P_L & P_R & & & & \\ & P_L & P_R & & & \\ & & P_L & P_R & & \\ & & & P_L & P_R & \\ & & & & P_L & P_R \end{pmatrix}=P_R+\Omega^{-}(-1)P_L, \tag{4.45}$$

$$U(am_f)=\begin{pmatrix} 1 & & & & & -T\left(P_L-am_fP_R\right) \\ & 1 & & & & -T^2\left(P_L-am_fP_R\right) \\ & & 1 & & & -T^3\left(P_L-am_fP_R\right) \\ & & & 1 & & -T^4\left(P_L-am_fP_R\right) \\ & & & & 1 & -T^5\left(P_L-am_fP_R\right) \\ & & & & & 1 \end{pmatrix}, \tag{4.46}$$

$$D_{\mathrm{OD}}^{(5)}(m_f)=\begin{pmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & 1 & \\ & & & & & aD_{\mathrm{OD}}(m_f) \end{pmatrix}, \tag{4.47}$$

where $D_{\mathrm{OD}}(m_f)$ is a truncated four dimensional massive overlap Dirac operator

$$aD_{\mathrm{OD}}(m_f)=\frac{1}{2}\left(1+\gamma_5S\right)+am_f\left(1-\frac{1}{2}\left(1+\gamma_5S\right)\right) \tag{4.48}$$

with the same definition for S in (3.81). The truncated Dirac operator turns out to be the ordinary overlap Dirac operator (3.88) in $N_5\to\infty$ limit. $\Omega^{-}(m_f)$ is a hopping operator in fifth direction (2.8). So we have

$$\det\frac{1}{D_{\mathrm{PV}}}D_{\mathrm{dwf}}(m_f)=\det aD_{\mathrm{OD}}(m_f) \tag{4.49}$$

for ordinary domain-wall fermion system.

We start from the orbifolded domain-wall fermion Dirac operator divided by the Pauli-Villars Dirac operator

$$D_{\mathrm{SF}}^{(5)}=\overline{\overline{\Pi}}_{-}\frac{1}{D_{\mathrm{PV}}}D_{\mathrm{dwf}}(m_f)\overline{\overline{\Pi}}_{-}=\overline{\overline{\Pi}}_{-}\mathcal{P}U^{-1}(1)D_{\mathrm{OD}}^{(5)}(m_f)U(m_f)\mathcal{P}^{\dagger}\overline{\overline{\Pi}}_{-}. \tag{4.50}$$

We consider multiplication of the projection operator on unitary matrix $\mathcal{P}$ and we have

$$\overline{\overline{\Pi}}_{-}\mathcal{P}=\overline{\overline{\Pi}}_{-}\mathcal{P}\widehat{\widehat{\Pi}}_{-},\quad \widehat{\widehat{\Pi}}_{\pm}=\frac{1\pm P\Omega^{-}(-1)\Sigma\tau^3}{2}. \tag{4.51}$$

We notice that a matrix in the projection $\widehat{\widetilde{\widetilde{\Pi}}}_{\pm}$ has a following form

$$P\Omega^{-}(-1) = \Omega^{+}(-1)P = \begin{pmatrix} P_{(N_5-1)} & 0 \\ 0 & 1 \end{pmatrix}, \tag{4.52}$$

where $P_{(N_5-1)}$ is a $(N_5-1)\times(N_5-1)$ matrix of the form

$$P_{(N_5-1)} = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad (N_5 = 6). \tag{4.53}$$

The projection operator $\widehat{\widetilde{\widetilde{\Pi}}}_{\pm}$ is written as a direct sum of two projections

$$\widehat{\widetilde{\widetilde{\Pi}}}_{\pm} = \begin{pmatrix} \widetilde{\widetilde{\Pi}}_{\pm}^{(N_5-1)} & \\ & \widetilde{\Pi}_{\pm} \end{pmatrix}, \tag{4.54}$$

where

$$\widetilde{\widetilde{\Pi}}_{\pm}^{(N_5-1)} = \frac{1 \pm P_{(N_5-1)}\Sigma\tau^3}{2} \tag{4.55}$$

is a projection operator in N_5-1 sub-space.

Taking into account the explicit form of the matrix $U(m_f)$ its determinant multiplied by the projection becomes

$$\det_{(+\text{subspace})} U(m)\widehat{\widetilde{\widetilde{\Pi}}}_{-} = \det_{(+\text{subspace})} \widehat{\widetilde{\widetilde{\Pi}}}_{-}U(m)\widehat{\widetilde{\widetilde{\Pi}}}_{-} = \det_{(+\text{subspace})} \begin{pmatrix} \widetilde{\widetilde{\Pi}}_{-}^{(N_5-1)} & \\ & \widetilde{\Pi}_{-} \end{pmatrix} = 1, \tag{4.56}$$

$$\det_{(+\text{subspace})} \widehat{\widetilde{\widetilde{\Pi}}}_{-}U^{-1}(m) = \det_{(+\text{subspace})} \widehat{\widetilde{\widetilde{\Pi}}}_{-}U^{-1}(m)\widehat{\widetilde{\widetilde{\Pi}}}_{-} = \det_{(+\text{subspace})} \begin{pmatrix} \widetilde{\widetilde{\Pi}}_{-}^{(N_5-1)} & \\ & \widetilde{\Pi}_{-} \end{pmatrix} = 1. \tag{4.57}$$

Substituting this relation determinant of the total Dirac operator is equivalent to that of the orbifolded overlap Dirac operator

$$\begin{aligned} \det_{\widetilde{\mathcal{H}}_{+}} D_{\text{SF}}^{(5)} &= \det_{\widetilde{\mathcal{H}}_{+}} \widetilde{\widetilde{\Pi}}_{-}\mathcal{P}\widehat{\widetilde{\widetilde{\Pi}}}_{-}U^{-1}(1)\widehat{\widetilde{\widetilde{\Pi}}}_{-}D_{\text{OD}}^{(5)}(m_f)\widehat{\widetilde{\widetilde{\Pi}}}_{-}U(m_f)\widehat{\widetilde{\widetilde{\Pi}}}_{-}\mathcal{P}^{\dagger}\widetilde{\widetilde{\Pi}}_{-} \\ &= \det_{(+\text{subspace})} \left(\widehat{\widetilde{\widetilde{\Pi}}}_{-}D_{\text{OD}}^{(5)}(m_f)\widehat{\widetilde{\widetilde{\Pi}}}_{-}\right) \\ &= \det_{(+\text{subspace})} \begin{pmatrix} \widetilde{\widetilde{\Pi}}_{-}^{(N_5-1)} & \\ & \widetilde{\Pi}_{-} \end{pmatrix} \begin{pmatrix} 1_{(N_5-1)} & \\ & aD_{\text{OD}}(m_f) \end{pmatrix} \begin{pmatrix} \widetilde{\widetilde{\Pi}}_{-}^{(N_5-1)} & \\ & \widetilde{\Pi}_{-} \end{pmatrix} \\ &= \det_{\widetilde{\mathcal{H}}_{+}} \widetilde{\Pi}_{-}aD_{\text{OD}}(m_f)\widetilde{\Pi}_{-} \end{aligned} \tag{4.58}$$

and we get expected result.

At last we have a comment on Hermiticity. The five dimensional total Dirac operator $D_{\mathrm{SF}}^{(5)}$ has a following Hermiticity relation

$$D_{\mathrm{SF}}^{(5)\dagger} = \gamma_5 \tau^{1,2} D_{\mathrm{SF}}^{(5)} \gamma_5 \tau^{1,2} \tag{4.59}$$

and its determinant is real. Since our domain-wall fermion Dirac operator does not have index the chiral rotation (4.1) is well defined even for single flavour case and we can define a single flavour orbifolded Dirac operator as

$$D_{\mathrm{SF}}^{\mathrm{single}} = \frac{1-\overline{\Sigma}}{2} \frac{1}{D_{\mathrm{PV}}} D_{\mathrm{dwf}}(m_f) \frac{1-\overline{\Sigma}}{2}. \tag{4.60}$$

However we do not have a Hermiticity relation for this Dirac operator and the determinant is not shown to be real. We may need even numbers of flavours to avoid this problem.

5. Conclusion

In this paper the orbifolding formulation of the finite volume field theory is applied to the domain-wall fermion. In order to reproduce the proper SF Dirichlet boundary condition we need both the time reflection and the chiral symmetries. Application of this procedure to fermionic part is straightforward because of good chiral symmetry of the domain-wall fermion. Since there is no chiral symmetry for the Pauli-Villars field it is introduced by using the effective Dirac operator to reproduce the SF overlap Dirac operator. The surface term is given as an external source field to break the orbifolding symmetry.

The SF Dirichlet boundary condition may not be the unique choice to define a finite volume field theory suitable for renormalization scheme. A finite volume field theory with chirally twisted boundary condition is also proposed. Time reflection symmetry is enough to reproduce the twisted boundary condition by orbifolding. We can treat the fermionic part and the Pauli-Villars field in an equal footing. We have a γ_5 Hermiticity relation for the orbifolded Dirac operator and the total determinant is real. This formulation is applicable to two flavours dynamical simulation.

A. Effective action of chiral symmetric Dirac operator

In this appendix we derive the effective Dirac operator of the physical quark field for an action with the chiral symmetric Dirac operator (3.12). Four dimensional part of the symmetric Dirac operator is the same as the ordinary Dirac operator (2.6). Hopping term of this Dirac operator into the fifth direction takes the form

$$P_L \Omega^+(m_f=0) + P_R \Omega^-(m_f=0) = \begin{pmatrix} 0 & P_L & 0 & 0 & 0 & 0 \\ P_R & 0 & P_L & 0 & 0 & 0 \\ 0 & P_R & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & P_L & 0 \\ 0 & 0 & 0 & P_R & 0 & P_L \\ 0 & 0 & 0 & 0 & P_R & 0 \end{pmatrix} \tag{A.1}$$

for massless case. If there were no quark mass this Dirac operator is equivalent to two independent domain-wall fermion with half fifth dimensional size of $N_5/2$. It is easily shown that there are two extra zero mode (doublers) at the middle boundary $s = \frac{N_5}{2}$ and $s = \frac{N_5}{2} + 1$ related to the exact chiral symmetry at finite N_5.

The physical quark fields may be defined in the same manner as (2.9) and (2.10). We can integrate out the bulk field other than q and $\overline{q}$ according to Ref. [34, 38, 41]. We start by writing the fermion field as a vector in fifth direction and chirality. For $N_5 = 6$ we have

$$\Psi^T = (\, \psi_{1R} \quad \psi_{1L} \quad \psi_{2R} \quad \psi_{2L} \quad \psi_{3R} \quad \psi_{3L} \quad \psi_{4R} \quad \psi_{4L} \quad \psi_{5R} \quad \psi_{5L} \quad \psi_{6R} \quad \psi_{6L} \,),$$
$$\overline{\Psi} = (\, \overline{\psi}_{1L} \quad \overline{\psi}_{1R} \quad \overline{\psi}_{2L} \quad \overline{\psi}_{2R} \quad \overline{\psi}_{3L} \quad \overline{\psi}_{3R} \quad \overline{\psi}_{4L} \quad \overline{\psi}_{4R} \quad \overline{\psi}_{5L} \quad \overline{\psi}_{5R} \quad \overline{\psi}_{6L} \quad \overline{\psi}_{6R} \,),$$

where

$$\psi_{R/L} = P_{R/L}\psi, \quad \overline{\psi}_{R/L} = \overline{\psi} P_{L/R}. \tag{A.2}$$

Then we change variable as

$$\Psi'^T = (\, \psi_{1L} \quad \psi_{1R} \quad \psi_{2L} \quad \psi_{2R} \quad \psi_{3L} \quad \psi_{3R} \quad \psi_{4L} \quad \psi_{4R} \quad \psi_{5L} \quad \psi_{5R} \quad \psi_{6L} \quad \psi_{6R} \,),$$
$$\overline{\Psi}' = (\, \overline{\psi}_{1R} \quad \overline{\psi}_{2L} \quad \overline{\psi}_{2R} \quad \overline{\psi}_{3L} \quad \overline{\psi}_{3R} \quad \overline{\psi}_{1L} \quad \overline{\psi}_{4R} \quad \overline{\psi}_{5L} \quad \overline{\psi}_{5R} \quad \overline{\psi}_{6L} \quad \overline{\psi}_{6R} \quad \overline{\psi}_{4L} \,).$$

The Dirac operator is written as follows in terms of the primed field

$$aD_{\mathrm{dwf}} = \begin{pmatrix} \alpha & \beta & & & & \\ & \alpha & \beta & & & \\ \beta_0 & & \alpha_0 & & & \\ & & & \alpha & \beta & \\ & & & & \alpha & \beta \\ & & & \beta_0 & & \alpha_0 \end{pmatrix}, \tag{A.3}$$

where

$$\alpha = \begin{pmatrix} B & -C^\dagger \\ & -1 \end{pmatrix}, \quad \alpha_0 = P_R \alpha, \tag{A.4}$$

$$\beta = \begin{pmatrix} -1 & \\ C & B \end{pmatrix}, \quad \beta_0 = P_L \beta, \tag{A.5}$$

$$C_{xy} = \sigma_\mu \frac{1}{2} \left(\delta_{x+\mu,y} U_\mu(x) - \delta_{x-\mu,y} U_\mu^\dagger(y) \right), \tag{A.6}$$

$$B_{xy} = (1-M)\delta_{xy} - \frac{1}{2} \left(\delta_{x+\mu,y} U_\mu(x) + \delta_{x-\mu,y} U_\mu^\dagger(y) - 2\delta_{xy} \right), \tag{A.7}$$

$$\gamma_\mu = \begin{pmatrix} & \sigma_\mu \\ \sigma_\mu^\dagger & \end{pmatrix}. \tag{A.8}$$

We integrate out all the fields except for the physical quark field

$$q(x) = P_L \psi(x,1) + P_R \psi(x,N_5) = P_L \gamma_0 \psi'(x,1) + P_R \gamma_0 \psi'(x,N_5), \tag{A.9}$$

$$\overline{q}(x) = \overline{\psi}(x,1) P_R + \overline{\psi}(x,N_5) P_L = \overline{\psi}'(x, \frac{N_5}{2}) \gamma_0 P_R + \overline{\psi}'(x,N_5) \gamma_0 P_L \tag{A.10}$$

according to Ref. [34]. Result is given as a full quark propagator

$$a^3 \langle q\overline{q} \rangle = \frac{1}{2}\left(\frac{1}{aD_{\text{eff}}} - \gamma_5 \frac{1}{aD_{\text{eff}}}\gamma_5\right) = \frac{1}{aD_{\text{eff}}^{\text{sym}}}. \tag{A.11}$$

Here D_{eff} is the truncated effective Dirac operator (3.81) with half size of fifth dimensional length

$$aD_{\text{eff}} = \frac{1+\gamma_5 S}{1-\gamma_5 S}, \quad S = \frac{1-T^{\frac{N_5}{2}}}{1+T^{\frac{N_5}{2}}}. \tag{A.12}$$

Transfer matrix is given by

$$T = \gamma_5\gamma_0\left(-\alpha\beta^{-1}\right)\gamma_0\gamma_5 = \frac{1-H'}{1+H'} \tag{A.13}$$

with H' defined in (3.81). The full quark propagator anti-commutes with γ_5 even at finite N_5. In $N_5 \to \infty$ limit the effective Dirac operator D_{eff} anti-commutes with γ_5 exactly and the effective Dirac operator $D_{\text{eff}}^{\text{sym}}$ with symmetric construction becomes the same as that of the ordinary domain-wall fermion D_{eff}.

We introduce the Pauli-Villars field in the same manner with the Dirac operator

$$D_{\text{PV}}^{\text{sym}} = D_{\text{dwf}}(m_f = 1) + X. \tag{A.14}$$

The effective action of the physical quark field q, $\overline{q}$ and the physical Pauli-Villars field Q, $\overline{Q}$ is given by

$$S_{\text{eff}} = a^4 \sum \left[\overline{q} D_{\text{eff}}^{\text{sym}} q + \overline{Q}\left(D_{\text{eff}}^{\text{sym}} + \frac{1}{a}\right) Q\right]. \tag{A.15}$$

The overlap Dirac operator is given to reproduce the same determinant as the effective action

$$D_{\text{OD}}^{\text{sym}} = \frac{D_{\text{eff}}^{\text{sym}}}{aD_{\text{eff}}^{\text{sym}} + 1}. \tag{A.16}$$

Because of exact chiral symmetry of $D_{\text{eff}}^{\text{sym}}$ the overlap Dirac operator $D_{\text{OD}}^{\text{sym}}$ satisfies the Ginsparg-Wilson relation even at finite N_5.

Compensation of the exact chirality at finite N_5 is a non-locality in the overlap Dirac operator, which comes from the extra zero mode in the middle of fifth direction. However we can show that the non-locality is exponentially small in N_5 and disappears in $N_5 \to \infty$ limit. In order to extract the non-locality we define explicit breaking term of the chiral symmetry of the ordinary effective Dirac operator (3.81) or the truncated overlap Dirac operator at finite N_5

$$\delta_{N_5} = \gamma_5 \frac{1}{D_{\text{eff}}(N_5)} + \frac{1}{D_{\text{eff}}(N_5)}\gamma_5 = \gamma_5 \frac{1}{D_{\text{OD}}(N_5)} + \frac{1}{D_{\text{OD}}(N_5)}\gamma_5 - 2a\gamma_5. \tag{A.17}$$

The chiral symmetric effective Dirac operator is re-written as

$$\frac{1}{D_{\text{eff}}^{\text{sym}}} = \frac{1}{D_{\text{eff}}} - \frac{1}{2}\gamma_5 \delta_{\frac{N_5}{2}}, \tag{A.18}$$

where we used a fact that the breaking term commutes with γ_5

$$[\delta_{N_5}, \gamma_5] = 0. \tag{A.19}$$

The chiral symmetric overlap Dirac operator is given in a following form

$$D_{\mathrm{OD}}^{\mathrm{sym}} = \frac{1}{1 - \frac{1}{2} D_{\mathrm{OD}} \gamma_5 \delta_{\frac{N_5}{2}}} D_{\mathrm{OD}}. \tag{A.20}$$

D_{OD} in denominator may bring a non-local factor into the overlap Dirac operator. However as was shown in Ref. [34] δ_{N_5} is exponentially small in N_5. The physical part of the chiral symmetric Dirac operator $D_{\mathrm{dwf}}^{\mathrm{sym}}$ coincides with that of the ordinary Dirac operator in $N_5 \to \infty$ limit.

B. Effect of explicit breaking term at finite N_5

An effect of the explicit chiral symmetry breaking on the orbifolding procedure at finite N_5 will be discussed in this appendix. The chiral symmetry breaking in the domain-wall fermion is given as a non-invariant part of the Dirac operator (3.9). The same sort of breaking term appears for the orbifolding symmetry since it includes the chiral transformation

$$[A, D_{\mathrm{dwf}}] = -2AX. \tag{B.1}$$

The projection operator $\overline{\Pi}_{\pm}$ plays an essential role in the orbifolding construction of the SF. A key property $A^2 = 1$ remains intact at finite N_5 and $\overline{\Pi}_{\pm}$ keeps a projection property. An orbifolding symmetry breaking effect appears as a mixing between two different Hilbert sub-spaces $\overline{\mathcal{H}}_{\pm}$

$$\overline{\Pi}_{+} D_{\mathrm{dwf}} \overline{\Pi}_{-} = -\overline{\Pi}_{+} X \overline{\Pi}_{-}, \tag{B.2}$$

$$\overline{\Pi}_{-} D_{\mathrm{dwf}} \overline{\Pi}_{+} = -\overline{\Pi}_{-} X \overline{\Pi}_{+}. \tag{B.3}$$

We can define the same theory (3.26) projecting out the sub-space $\overline{\mathcal{H}}_{+}$ by (3.17). But a discussion of renormalizability in sub-section 3.3 is not valid anymore. A field belonging to $\overline{\mathcal{H}}_{+}$ will be introduced by quantum correction through the mixing. We may need additive counter term to keep the projection condition (3.17) and the action (3.26).

However as was shown in Ref. [31] an effect of the chiral symmetry breaking term is suppressed exponentially in a Green's function with physical quark operator

$$\left\langle \left(\overline{\psi} X \psi\right) \mathcal{O}(q, \overline{q}) \right\rangle < e^{-CN_5}, \tag{B.4}$$

where C is a constant related to a gap of the four dimensional Wilson Dirac operator D_W. Since the orbifolding symmetry breaking term is proportional to X a quantum correction from the mixing term is also suppressed exponentially in a physical Green's function and would be no harm in large N_5 limit.

An inverse of the orbifolded Dirac operator should be modified if we take into account an effect of the explicit breaking term X. We define an inverse of the orbifolded Dirac operator $D_{\rm dwf}^{\rm SF}$ in the sub-space (3.32). By making use of the relation (B.1) one can show that the inverse in exact sense is given by

$$\left(D_{\rm dwf}^{\rm SF}\right)^{-1} = \overline{\Pi}_{+}\frac{1}{D_{\rm dwf}+X}\overline{\Pi}_{+}. \tag{B.5}$$

The Dirac operator $D_{\rm dwf}+X$ is nothing but the chiral symmetric Dirac operator (3.12) and is equivalent to two independent domain-wall fermion with half fifth dimensional size for massless case. Its inverse is given as a direct sum of two independent domain-wall fermion Dirac operator of half size

$$\left(\frac{1}{D_{\rm dwf}+X}\right)_{st} = \begin{pmatrix} \left(D_{\rm dwf}^{-1}(\frac{N_5}{2})\right) & 0 \\ 0 & \left(D_{\rm dwf}^{-1}(\frac{N_5}{2})\right) \end{pmatrix} \tag{B.6}$$

where upper row corresponds to $1 \le s,t \le \frac{N_5}{2}$ and lower row to $\frac{N_5}{2}+1 \le s,t \le N_5$. Tree level propagator is given by replacing $N_5 \to N_5/2$ in appendix D for each row. The physical quark propagator is given in the same manner

$$\langle q(p)\overline{q}(-p)\rangle = \left(P_L\delta_{s,1}+P_R\delta_{s,N_5}\right)\left(\frac{1}{D_{\rm dwf}(p)+X}\right)_{s,t}\left(\delta_{t,N_5}P_L+\delta_{t,1}P_R\right). \tag{B.7}$$

A difference from the ordinary quark propagator (D.12) is $\mathcal{O}(e^{-\alpha N_5})$ at tree level. The orbifolded propagator is given by replacing $D_{\rm dwf} \to D_{\rm dwf}+X$ in sub-section 3.2.

C. Folding of temporal direction

In our formulation with the orbifolding (3.17) fermion fields in negative time $-N_T < x_0 < 0$ can be written in term of those in the positive region

$$\psi(\vec{x},-x_0,s) = \left(\overline{\Gamma}\right)_{s,t}\psi(\vec{x},x_0,t), \quad \overline{\Gamma} = \gamma_0\gamma_5 PQ. \tag{C.1}$$

Half of the field degrees of freedom can be eliminated explicitly by folding the temporal axis into the non-negative range $0 \le x_0 \le N_T$ together with the boundary condition (3.18) (3.19).

For this purpose we introduce four projection operators in temporal direction

$$\begin{array}{lll} T_- & \text{for} & -N_T+1 \le x_0 \le -1, \\ T_0 & \text{for} & x_0 = 0, \\ T_+ & \text{for} & 1 \le x_0 \le N_T-1, \\ T_T & \text{for} & x_0 = N_T, \end{array}$$

which pick up the fermion fields on the corresponding region. For instance

$$\left(T_+\right)_{x_0,y_0}\psi(y_0) = \begin{cases} \psi(x_0) \text{ for } 1 \le x_0 \le N_T-1 \\ 0 \qquad\quad \text{otherwise} \end{cases}. \tag{C.2}$$

Summing up four projection operators we have a unity

$$1 = T_- + T_0 + T_+ + T_T \tag{C.3}$$

and T_α's have a projection property

$$T_\alpha T_\beta = T_\alpha \delta_{\alpha,\beta}, \tag{C.4}$$

where summation is not taken over α. These projection operators satisfy the following relation with the time reflection operator R

$$RT_+ = T_- R, \quad RT_- = T_+ R, \quad RT_0 = T_0 R = T_0, \quad RT_T = T_T R = -T_T. \tag{C.5}$$

By using these properties we have an identity relation

$$\begin{aligned}\overline{\Pi}_+ &= \overline{\Pi}_+ \left(T_+ + T_- + T_0 + T_T\right) \\ &= \overline{\Pi}_+ \left(T_+ + T_0 + T_T\right)\left(2T_+ + T_0 + T_T\right)\overline{\Pi}_+ \end{aligned} \tag{C.6}$$

and the orbifolded action (3.26) can be re-written in terms of the fermion fields depending on the non-negative region only

$$S = a^4 \sum_{\vec{x},\vec{y}} \sum_{x_0,y_0=0}^{N_T} \sum_{s,t} \overline{\psi}''(x,s) D_{\rm dwf}^{\rm folded}(x,y;s,t)\psi''(y,t), \tag{C.7}$$

where ψ'' and $\overline{\psi}''$ are defined as

$$\psi''(\vec{x},x_0,s) = \left(\left(T_+ + T_0 + T_T\right)\overline{\Pi}_+\right)_{x_0,y_0;s,t}\psi(\vec{x},y_0,t), \tag{C.8}$$

$$\overline{\psi}''(\vec{x},x_0,s) = \overline{\psi}(\vec{x},y_0,t)\left(\overline{\Pi}_+\left(T_+ + T_0 + T_T\right)\right)_{y_0,x_0;t,s}, \tag{C.9}$$

which have no dependence on negative time. These fields can further be written as

$$\psi''(\vec{x},x_0,s) = \left(T_+ + T_0\overline{P}_+ + T_T\overline{P}_-\right)_{x_0,y_0;s,t}\psi(\vec{x},y_0,t), \tag{C.10}$$

$$\overline{\psi}''(\vec{x},x_0,s) = \overline{\psi}(\vec{x},y_0,t)\left(T_+ + \overline{P}_+ T_0 + \overline{P}_- T_T\right)_{y_0,x_0;t,s} \tag{C.11}$$

by using (C.5) and identification (C.1). There is no constraint on positive bulk fields.

The folded Dirac operator $D_{\rm dwf}^{\rm folded}$ is given formally as

$$D_{\rm dwf}^{\rm folded} = \frac{1}{2}\left(2T_+ + T_0 + T_T\right)\overline{\Pi}_+ D_{\rm dwf}\overline{\Pi}_+\left(2T_+ + T_0 + T_T\right). \tag{C.12}$$

This Dirac operator can be written in more explicit form by using the orbifolding symmetry (3.16) and the ultra local property of the domain-wall fermion Dirac operator, with which we eliminate the term like $T_+ D_{\rm dwf} A T_+ = T_+ D_{\rm dwf} T_- A$

$$\begin{aligned} aD_{\rm dwf}^{\rm folded} &= \frac{1}{2}T_0\overline{P}_+ aD_{\rm dwf}\overline{P}_+ T_0 + T_0\overline{P}_+ aD_{\rm dwf}T_+ + T_+ aD_{\rm dwf}\overline{P}_+ T_0 + T_+ aD_{\rm dwf}T_+ \\ &\quad + T_T\overline{P}_- aD_{\rm dwf}T_+ + T_+ aD_{\rm dwf}\overline{P}_- T_T + \frac{1}{2}T_T\overline{P}_- aD_{\rm dwf}\overline{P}_- T_T \end{aligned} \tag{C.13}$$

$$= \begin{pmatrix} \overline{P}_+\frac{D^{(3+1)}}{2}\overline{P}_+ & -\overline{P}_+ P_- U_0(0) & & & \\ -P_+\overline{P}_+ U_0^\dagger(0) & D^{(3+1)} & -P_- U_0(1) & & \\ & -P_+ U_0^\dagger(1) & D^{(3+1)} & -P_- U_0(2) & \\ & & -P_+ U_0^\dagger(2) & D^{(3+1)} & -P_-\overline{P}_- U_0(3) \\ & & & -\overline{P}_- P_+ U_0^\dagger(3) & \overline{P}_-\frac{D^{(3+1)}}{2}\overline{P}_- \end{pmatrix} \tag{C.14}$$

where the matrix represents the Dirac operator in temporal direction for $N_T = 4$. $D^{(3+1)}$ is the Dirac operator in spatial direction and the fifth direction

$$D^{(3+1)}(x, y; s, t) = \left(\frac{-1 + \gamma_i}{2} U_i(x) \delta_{y_i, x_i+1} + \frac{-1 - \gamma_i}{2} U_i^\dagger(y) \delta_{y_i, x_i-1} \right) \delta_{x_0, y_0} \delta_{s,t}$$
$$+ \left(\frac{-1 + \gamma_5}{2} \Omega^+_{s,t} + \frac{-1 - \gamma_5}{2} \Omega^-_{s,t} \right) \delta_{x,y} + (5 - M) \delta_{x,y} \delta_{s,t}. \quad \text{(C.15)}$$

There is no constraint for the bulk region $1 < x_0, y_0 < N_T - 1$, which is nothing but ordinary domain-wall fermion Dirac operator.

We notice that the projection operator $\overline{P}_\pm$ at the boundary does not commute with the γ_0 chiral projection $P_\pm$. If we consider an eigenvalue equation of this Dirac operator a zero mode dumping solution

$$\psi = P_-(1 - M)^{x_0} + P_+(1 - M)^{(N_T - x_0)} \quad \text{(C.16)}$$

in temporal direction, which have broken the chiral symmetry "dynamically" in a naive formulation, is forbidden by this boundary term.

The fermion propagator is given as an inverse of the folded Dirac operator

$$a^3 G^{\text{folded}}_{\text{dwf}} = 2\left(T_+ + T_0 + T_T\right) \overline{\Pi}_+ \left(aD_{\text{dwf}}\right)^{-1} \overline{\Pi}_+ \left(T_+ + T_0 + T_T\right), \quad \text{(C.17)}$$

where the inverse is defined in the ordinary meaning for the positive bulk region $0 < x_0 < N_T$ and in terms of the projected sub-space at the boundary

$$a^4 D^{\text{folded}}_{\text{dwf}} G^{\text{folded}}_{\text{dwf}} = T_+ + \overline{P}_+ T_0 + \overline{P}_- T_T. \quad \text{(C.18)}$$

D. Free fermion propagator

Inverse of the massless domain-wall fermion Dirac operator in momentum space is derived according to the procedure of Ref. [30]. In this appendix we omit derivation and give the result:

$$\frac{1}{aD_{\text{dwf}}(p)} = \left(-i\gamma_\mu \sin p_\mu + W - \Omega^-\right) G_R P_L + \left(-i\gamma_\mu \sin p_\mu + W - \Omega^+\right) G_L P_R, \quad \text{(D.1)}$$

where Ω and W are defined in (2.8) and (3.37). G_R and G_L are defined as

$$G_{\text{R}}(s, t) = G^0(s - t) + A_{++} e^{\alpha(s+t)} + A_{+-} e^{\alpha(s-t)} + A_{-+} e^{\alpha(-s+t)} + A_{--} e^{\alpha(-s-t)} \quad \text{(D.2)}$$
$$G_{\text{L}}(s, t) = G^0(s - t) + B_{++} e^{\alpha(s+t)} + B_{+-} e^{\alpha(s-t)} + B_{-+} e^{\alpha(-s+t)} + B_{--} e^{\alpha(-s-t)}, \quad \text{(D.3)}$$
$$G^0(s - t) = C \left(e^{\alpha(N_5 - |s-t|)} + e^{-\alpha(N_5 - |s-t|)} \right) \quad \text{(D.4)}$$

with exponent and coefficients given by

$$\cosh \alpha = \frac{1 + W^2 + \sin^2 p_\mu}{2|W|}, \quad \text{(D.5)}$$
$$C = \frac{1}{4W \sinh \alpha \sinh(\alpha N_5)}, \quad \text{(D.6)}$$

$$A_{++} = F(1 - We^{-\alpha})(e^{-2\alpha N_5} - 1), \quad A_{--} = F(1 - We^{\alpha})(1 - e^{2\alpha N_5}), \tag{D.7}$$
$$B_{++} = e^{-2\alpha(N_5+1)} A_{--}, \quad B_{--} = e^{2\alpha(N_5+1)} A_{++}, \tag{D.8}$$
$$A_{-+} = A_{+-} = B_{-+} = B_{+-} = FW(e^{\alpha} - e^{-\alpha}), \tag{D.9}$$
$$F = \frac{C}{e^{\alpha N_5}(1 - We^{\alpha}) - e^{-\alpha N_5}(1 - We^{-\alpha})}. \tag{D.10}$$

This notation is valid for positive W and for negative case we define

$$e^{\pm\alpha} = \cosh\alpha \pm \sqrt{\cosh^2\alpha - 1} \tag{D.11}$$

and flip their sign $e^{\pm\alpha} \to -e^{\pm\alpha}$ according to $\mathrm{sgn}(W)$.

The physical quark propagator in momentum space is defined by picking up the boundary components

$$\begin{aligned} a^3 \langle q(p)\overline{q}(-p)\rangle &= (P_L\delta_{s,1} + P_R\delta_{s,N_5}) \left(\frac{1}{aD_{\mathrm{dwf}}(p)}\right)_{s,t} (\delta_{t,N_5}P_L + \delta_{t,1}P_R) \\ &= -i\gamma_\mu \sin p_\mu G_R(N_5, N_5) + WG_R(1, N_5). \end{aligned} \tag{D.12}$$

Ignoring the next to leading term in N_5 the quark propagator has a simple form

$$a^3 \langle q(p)\overline{q}(-p)\rangle = \frac{i\gamma_\mu \sin p_\mu}{1 - We^{\alpha}}. \tag{D.13}$$

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