Ph.D. thesis

Formulation of the Atiyah-Patodi-Singer index in lattice gauge theory

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Abstract

Lattice gauge theory is a non-perturbative and gauge-invariant formulation of gauge theory defined on a discrete spacetime. With the overlap fermion which satisfies the Ginsparg-Wilson relation, the Atiyah-Singer (AS) index theorem, in which the chiral symmetry plays a central role, can be formulated even with a finite lattice spacing. However, the Atiyah-Patodi-Singer (APS) index theorem which is an extension of the AS index theorem to a manifold with boundaries was not formulated in lattice gauge theory. The difficulty lies in the nontrivial boundary condition of the APS, which is incompatible with the Ginsparg-Wilson relation.

In this thesis, we propose a non-perturbative formulation of the APS index in lattice gauge theory in four dimensions, discretizing a massive reformulation of the index recently proposed in continuum theory. The formulation is given by the so-called eta invariant of the domain-wall fermion Dirac operator, to which we do not impose any nonlocal boundary condition. Our proposal does not require the chiral symmetry via the Ginsparg-Wilson relation, either. To verify this proposal, we show perturbatively in the classical continuum limit that the eta invariant of the lattice domain-wall Dirac operator coincides with the APS index formula. We find in the continuum limit that the standard curvature term in the APS index appears as the contribution from the massive bulk extended modes, while the boundary eta invariant comes entirely from the massless edge-localized modes. Since the eta invariant of the lattice domain-wall fermion is guaranteed to be an integer by its definition, it can rigorously describe the anomaly inflow mechanism in the lattice gauge theory.

Contents

1 Introduction

Lattice gauge theory [1] is a non-perturbative and gauge-invariant formulation of gauge theory defined on a discrete spacetime. However, chiral symmetry and its associated topological charge have been a difficult challenge due to the doubling problem [2,3] of the fermion action. On a periodic lattice, this issue was positively solved by the overlap fermion Dirac operator [4,5], which guarantees a modified chiral symmetry [6] on the lattice through the Ginsparg-Wilson relation [7]. It was found in [8] that the Atiyah-Singer (AS) index theorem [9–13] can be formulated even with a finite lattice spacing. However, the topological properties of the lattice gauge theory in the presence of a boundary have not been studied so far.

Recently, physical systems with boundaries have been actively studied. One of such systems is the symmetry-protected topological (SPT) phases of matter [14] in condensed matter physics. In topological insulators, for example, the so-called bulk-edge correspondence is known, which relates the properties of the conducting electrons at the surface (edge) and those inside the bulk.

In [15], it was pointed out that the anomaly inflow mechanism [16] is a key to understanding the bulk-edge correspondence. The anomaly inflow indicates that the anomaly in the edge fermion partition function must be canceled by that in bulk for protecting the symmetry. As the anomaly arises only for massless fermions, in general, the inflow assures the existence of the edge-localized massless modes on the surface.

For a system with even-dimensional bulk and odd-dimensional edge, the parity anomaly or time-reversal (T) anomaly is described by the Atiyah-Patodi-Singer (APS) index theorem [17–19], which is an extension of the AS index theorem to a manifold with boundaries. On a four-dimensional flat manifold X with a flat boundary Y, the APS index theorem is given by

$$n_+ - n_- = \frac{1}{32\pi^2}\int_X d^4x \epsilon^{\mu\nu\rho\sigma}\mathrm{tr_c}F_{\mu\nu}F_{\rho\sigma} - \frac{1}{2}\eta(iD_Y), \tag{1}$$

where $\eta(iD_Y)$ is the eta invariant of the boundary Dirac operator iD_Y.

The first term of the right-hand side (RHS) is an integral of the instanton number density and is the effective action of the massive bulk fermion, which appears in the phase of the partition function. Unlike closed manifolds, it is not an integer on a manifold with boundaries. Since the instanton number density is odd under parity or T, the bulk fermion alone is not invariant under the symmetry transformation. The second term of the RHS is the contribution from the three-dimensional massless fermion theory at the boundary, which also appears in the phase of the partition function. The boundary eta invariant is also odd under parity or T symmetry, and the boundary theory alone is anomalous under this transformation. The APS index theorem guarantees that the sum of the two terms is an integer, which implies that the parity or T symmetry of the partition function of the entire system of the bulk and the boundary is preserved. Thus, the APS index describes the anomaly inflow mechanism, where the edge anomaly is canceled by the contribution from the bulk.

The left-hand side (LHS) of the APS index theorem is, however, somewhat puzzling. It is defined by the zero modes of a massless Dirac operator on a whole system, while our physics target described by the RHS of the theorem is a gapped or massive fermion. In fact, in order to preserve the chirality operator, we must impose a non-local condition known as the APS boundary condition by hand, which is unlikely to be realized in nature.

A unified reformulation of the index theorems was proposed in the continuum theory in [20–22]. They considered a domain-wall fermion on a closed manifold X, where the positive and negative mass regions are separated by a thin co-dimension one domain-wall. Then they found that the eta invariant of the domain-wall fermion Dirac operator on a closed manifold X coincides with the APS index defined in the negative mass region of X. When the positive mass region is absent, it corresponds to the AS index on X. The new formulation does not require chiral symmetry at all. Moreover, a local and physically sensible boundary condition is automatically imposed on the fermions. The eta invariant can be easily separated into the bulk and edge contributions so that their anomaly inflow is manifest.

Interestingly, the reformulation of the AS index by the eta invariant of the massive Dirac operator matches with the index theorem on a lattice. The AS index on the lattice is formulated using the overlap fermion, where we have a sign function of the massive Wilson Dirac operator. When we substitute the definition of the overlap Dirac operator into the index formula, we obtain the η invariant of the massive Wilson Dirac operator. This fact is encouraging in that the index can be defined without the Ginsparg-Wilson relation, and it is natural to assume that the formula should be valid even when we have a domain-wall structure in the mass term.

In this thesis, we give a non-perturbative formulation of the Atiyah-Patodi-Singer index in the lattice gauge theory in four dimensions. We actually show that the eta invariant of the domain-wall fermion Dirac operator on the lattice coincides with the APS index formula in the classical continuum limit. In a similar way to the continuum study [20–22], we can naturally separate the bulk and edge contributions and manifestly show the anomaly inflow of them. Using the eigenmode set of the square of the free domain-wall fermion, We find in the continuum limit that the standard curvature term in the APS index appears as the contribution from the massive bulk extended modes, while the boundary eta invariant comes entirely from the massless edge-localized modes. Since the eta invariant of the domain-wall fermion at a finite lattice spacing is guaranteed to be integers by its definition, the APS index on the lattice can rigorously describe the anomaly inflow mechanism in the lattice gauge theory.

This thesis is organized as follows.
In section 2, we introduce a basic review of lattice fermions. We start with a naive discretization of the fermion action and review some formulations of the lattice fermions. We also present a realization of chiral symmetry as well as the AS index theorem on a lattice.
In section 3, we present the APS index theorem in continuum theory and its physicist-friendly reformulation. We discuss the difficulties of the non-local boundary condition introduced in the original setup and then present the new formulation of the APS index using the domain-wall fermion.
In section 4, we introduce a unified view of the AS and APS index theorems.
In section 5, we formulate the Atiyah-Patodi-Singer index non-perturbatively in the framework of the lattice gauge theory in four dimensions.
Conclusions and outlooks are given in section 6.

This thesis is based on the following papers:

- H. Fukaya, N. Kawai, Y. Matsuki, M. Mori, K. Nakayama, T. Onogi and S. Yamaguchi, "The Atiyah–Patodi–Singer index on a lattice," PTEP **2020**, no.4, 043B04 (2020) doi:10.1093/ptep/ptaa031 [arXiv:1910.09675 [hep-lat]] [23].

- H. Fukaya, N. Kawai, Y. Matsuki, M. Mori, K. Nakayama, T. Onogi and S. Yamaguchi, "A lattice formulation of the Atiyah-Patodi-Singer index," PoS **LATTICE2019**, 149 (2019) doi:10.22323/1.363.0149 [arXiv:2001.03319 [hep-lat]] [24].

2 Fermions and Chiral symmetry on a lattice

This section will review the formulations of the lattice fermions and their chiral symmetry to understand how the index theorem on the four-dimensional torus was established in the previous works.

Starting from the naive fermion and its doubling problem, we will discuss the Wilson fermion. Then we review how the chiral symmetry is realized in the domain-wall fermion and the overlap fermion. We will see that the Atiyah-Singer index theorem can be formulated even when the lattice spacing is finite.

2.1 Naive discretization and fermion doubling problem

First of all, we review how to construct fermion fields on a lattice and its difficulty. To see the problem of the naive discretization, let us consider the Dirac fermion for one flavor in the 4-dimensional Euclidean spacetime and treat the gauge field A_μ as a background field,

$$S_F = \int d^4x \bar{\psi}(x) \left(D - m\right) \psi(x), \tag{2}$$

where $D = \gamma^\mu(\partial_\mu + iA_\mu)$ and γ^μ matrices are the one given in Appendix.A. The lattice regularization of the theory is made by replacing derivatives with differences and integrals with sums. We discretize the four-dimensional Euclidean spacetime $\mathbb{R}^4$ to

$$\mathbb{L}^4 \equiv \left\{x_\mu = an_\mu | n_\mu \in \mathbb{Z}^4\right\}, \tag{3}$$

where a is the lattice spacing. Also, we place the fermion field $\psi(x)$ on the site x and treat the gauge field as a link variable $U_\mu(x)$ that lives on the link $\{x, \mu\}$.

Let us discretize the action (2) in a naive way:

$$\begin{aligned} S &= a^4 \sum_x \bar{\psi}(x) \left[\sum_\mu \frac{1}{2a}\gamma^\mu \Big(U_\mu(x)\psi(x+a\hat{\mu}) - U_\mu^\dagger(x-a\hat{\mu})\psi(x-a\hat{\mu})\Big) - m\psi(x)\right] \\ &= a^4 \sum_x \bar{\psi}(x) \left[\gamma^\mu D_\mu(U) - m\right] \psi(x), \end{aligned} \tag{4}$$

where $\hat{\mu}$ is the unit vector in the μ direction and $U_\mu(x)$ is the link variable. $D_\mu(U)$ is the lattice Dirac operator defined by

$$D_\mu(U) \equiv \frac{1}{2}\left[\nabla_\mu(U) + \nabla_\mu^*(U)\right], \tag{5}$$

where $\nabla_\mu(U)$ and $\nabla_\mu^*(U)$ are the covariant forward and backward difference operators respectively.

To see the problem with a naive discretization of the Dirac fermion, we consider the free case for simplicity. (In other words, we put ${}^\forall U_\mu(x) = 1$.)

$$S = a^4 \sum_x \bar{\psi}(x) \left[\gamma^\mu \frac{\psi(x+a\hat{\mu}) - \psi(x-a\hat{\mu})}{2a} - m\psi(x)\right]. \tag{6}$$

With the Fourier transformation,

$$\psi(x) = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^4p}{(2\pi)^2} e^{ipx} \tilde{\psi}(x), \tag{7}$$

we obtain

$$S = \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{d^4p}{(2\pi)^2} \tilde{\bar{\psi}}(p) \left[\frac{i}{a} \gamma^\mu \sin p_\mu a - m \right] \tilde{\psi}(p). \tag{8}$$

Then the propagator of the free field is given by

$$G(p) = \frac{1}{i\gamma_\mu s_\mu(p)} = \frac{-i\gamma_\mu s_\mu - m}{s^2(p) + m^2}, \tag{9}$$

where $s_\mu(p) = \frac{1}{a} \sin p_\mu a$.

The particle propagation is described by its poles, whose dispersion relation is

$$s^2(p) + m^2 = 0. \tag{10}$$

Near $p = (0,0,0,0)$, the dispersion relation becomes

$$p_\mu^2 + m^2 + \mathcal{O}(a) = 0. \tag{11}$$

On the other hand, if we consider the case that some momentum components are π/a (e.g. $\bar{p} = (\pi/a, 0, 0, 0)$) and the expansion around it as $p_\mu = \bar{p} + \tilde{p}_\mu$, then the dispersion relation becomes

$$\tilde{p}_\mu^2 + m^2 + \mathcal{O}(a) = 0. \tag{12}$$

This implies that in the continuum limit, not only the small momenta $p \sim 0$ but also those at the cut-off scale $p \sim 1/a$ contribute. The extra degrees of freedom are called doublers. In four dimensions, we have unphysical 15 doubler modes.

Nielsen and Ninomiya proved that doublers could not be avoided if the lattice Dirac operator satisfies the following five conditions [2,3]:

1. translational invariance on the lattice,
2. chiral symmetry,
3. Hermiticity,
4. bilinear form,
5. locality

This theorem is called the Nielsen-Ninomiya theorem. Therefore, to get away from the doubling problem, we must give up at least one of them.

2.2 Wilson fermion

Wilson introduced an $O(a)$ term to the action, which does not affect the physical pole in the continuum limit but eliminate the doublers [25],

$$\begin{aligned} S' &= \frac{ar}{2}\int d^4x\bar{\psi}(x)D^2\psi(x) \\ &\to \frac{r}{2}a^4\sum_{x,\mu}\bar{\psi}(x)\frac{1}{a}\Big[U_\mu(x)\psi(x+a\hat{\mu})+U_\mu^\dagger(x-a\hat{\mu})\psi(x-a\hat{\mu})-2\psi(x)\Big]. \end{aligned} \tag{13}$$

This term is called the Wilson term, and a parameter r is called the Wilson parameter. From now on, we set $r=1$ unless stated. After adding Wilson term, the lattice fermion action is

$$\begin{aligned} S_W &= a^4\sum_x\bar{\psi}(x)\left[\sum_\mu\frac{1}{2a}\gamma^\mu\Big[U_\mu(x)\psi(x+a\hat{\mu})-U_\mu^\dagger(x-a\hat{\mu})\psi(x-a\hat{\mu})\Big]-m\psi(x)\right] \\ &+a^4\sum_{x,\mu}\bar{\psi}(x)\frac{1}{2a}\Big[U_\mu(x)\psi(x+a\hat{\mu})+U_\mu^\dagger(x-a\hat{\mu})\psi(x-a\hat{\mu})-2\psi(x)\Big] \\ &= a^4\sum_x\bar{\psi}(x)\left[D_{\mathrm{W}}-m\right]\psi(x), \end{aligned} \tag{14}$$

where D_{W} is so-called the Wilson-Dirac operator defined by

$$D_{\mathrm{W}}=\frac{1}{2}\gamma^\mu\Big(\nabla_\mu(U)+\nabla_\mu^\dagger(U)\Big)-\frac{a}{2}\sum_{\mu=1}^{4}\nabla_\mu^\dagger(U)\nabla_\mu(U), \tag{15}$$

and this fermion is called as the Wilson fermion.

The free fermion action in momentum space is

$$S_W=\int\frac{d^4p}{(2\pi)^4}\tilde{\bar{\psi}}(p)\left[\sum_\mu\frac{i}{a}\gamma^\mu\sin p_\mu a-\left\{m+\frac{1}{a}\sum_\mu\left(1-\cos p_\mu a\right)\right\}\right]\tilde{\psi}(p). \tag{16}$$

The fermion propagator with the Wilson term is written by

$$G_0(p)=\frac{-i\sum_\mu\gamma^\mu s_\mu(p)-M(p)}{s(p)^2+M(p)^2}, \tag{17}$$

where、$M(p)\equiv m+\frac{1}{a}\sum_\mu\left(1-\cos p_\mu a\right)$, and the dispersion relation becomes

$$s(p)^2+M(p)^2=0. \tag{18}$$

In the continuum limit, we have

$$M(p)=m \quad \text{for} \quad p_\mu\approx(0,0,0,0) \tag{19}$$

$$M(p)=m+\mathcal{O}(1/a) \quad \text{for} \quad {}^{\exists}p_\mu\approx\pi/a, \tag{20}$$

The Wilson fermion makes the doublers very massive and decoupled from the theory.

Finally, we comment on the Hermiticity of the Wilson-Dirac operator. The Wilson-Dirac operator satisfies

$$\gamma_5 D_{\mathrm{W}}\gamma_5=D_{\mathrm{W}}^\dagger, \tag{21}$$

and this is called the γ_5-Hermiticity.

2.3 Domain-wall fermion

In this section, we review the domain-wall fermion [16, 26] which plays a central role in this thesis. The domain-wall fermion is introduced by Kaplan [27] to formulate a lattice chiral fermion. The domain-wall fermion is a five-dimensional massive fermion whose mass term flips its sign on a four-dimensional surface, which is called domain-wall. It was found that a massless Weyl fermion is exponentially localized at the domain-wall.

2.3.1 Domain-wall fermion in the continuum theory

Here, we introduce the domain-wall fermion and review how the chiral fermion is localized around the kink in continuum five-dimensional space. Here we denote x as the four-dimensional space coordinates and s as the fifth coordinate. The action of the free domain-wall fermion is written by

$$S = \int d^4x ds \bar{\psi}(x,s) \left[\sum_{\mu=1}^{5} \gamma^\mu \partial_\mu - m(s) \right] \psi(x,s) \tag{22}$$

$$= \int d^4x ds \bar{\psi}(x,s) \left[\sum_{\mu=1}^{4} \gamma^\mu \partial_\mu + \gamma^s \partial_s - m(s) \right] \psi(x,s), \tag{23}$$

where $m(s)$ is a s-dependent mass term,

$$m(s) = m\epsilon(s) \quad (m > 0) \tag{24}$$

$$= \begin{cases} +m & s > 0 \\ 0 & s = 0 \\ -m & s < 0. \end{cases} \tag{25}$$

The Dirac equation is given by

$$\left[\sum_{\mu=1}^{4} \gamma^\mu \partial_\mu + \gamma^s \partial_s - m(s) \right] \psi(x,s) = 0. \tag{26}$$

To solve this equation, we assume a separable form $\psi(x,s) = \eta_\pm(x) f_\pm(s)$, where $f_\pm(s)$ is a scalar function depending only on s and $\eta_\pm(x)$ is a four-component spinor. We note that γ^s represents the chirality operator in the four-dimensional subspace. The subscript of $\eta_\pm$ represents the eigenvalue of the four-dimensional chirality operator. The separated equations are the massless Dirac equation on the $s = 0$ surface,

$$\sum_{\mu=1}^{4} \gamma^\mu \partial_\mu \eta_\pm(x) = 0, \tag{27}$$

and

$$\begin{cases} \gamma^s \eta_\pm(x) = \pm \eta_\pm(x), \\ \pm \partial_s f_\pm(s) - m(s) f_\pm(s) = 0. \end{cases} \tag{28}$$

Note that only $f_-(s)$ has a normalizable solution

$$\psi(x,s) = \eta_-(x)\exp\left[-\int_0^s ds' m(s')\right], \tag{29}$$

$$\sum_{\mu=1}^{4}\gamma^\mu\partial_\mu\eta_-(x) = 0, \quad \gamma^s\eta_-(x) = -\eta_-(x), \tag{30}$$

The factor $\exp[-\int_0^s ds' m(s')]$ decays exponentially as $|s|$ increases. Therefore, we have a massless left-handed fermion localized at the kink $s = 0$. The right-handed fermion can be put by changing the sign of the mass.

The surface mode or edge mode of the domain-wall fermion is stable even when introducing gauge field connections. However, a single Weyl fermion should have a gauge anomaly, which makes the theory inconsistent. The gauge symmetry is protected in the total five-dimensional massive fermion theory. This means that the massive bulk modes precisely cancel the anomaly of the edge modes, which is called the anomaly inflow mechanism [16].

2.3.2 Domain-wall fermion on a lattice

Next, we construct the domain-wall fermion on a lattice. Naively, all we have to do is to discretize (22), eliminating fermion doublers. Since the formulation on a lattice is done in a finite volume, it is necessary to impose some boundary conditions. The boundary conditions are also required in the fifth dimension, and usually periodic boundary conditions are taken. Let the period be L_5 and the periodic boundary condition for the mass $m(s)$ is taken to be $m(s + 2L_5) = m(s)$. For $m > 0$, we set

$$m(s) = \begin{cases} +m & (0 < s < L_5), \\ -m & (L_5 < s < 2L_5), \end{cases} \tag{31}$$

then there exists the kink at $s = 0$ and the anti-kink at $s = L_5$. ψ_L is localized at $s = 0$ and ψ_R is localized at $s = L_5$. Note that the chiral symmetry is not exact until the $L_5 = \infty$ limit is taken.

The action for the domain-wall fermion on the lattice is given by,

$$\begin{aligned} S_{\mathrm{DW}} &= a^5 \sum_x \bar\psi(x)\left[D_{\mathrm{W}}^{5\mathrm{D}} - m\epsilon(s)\right]\psi(x) && (32)\\ &= a^5 \sum_x \bar\psi(x) D_{\mathrm{DW}}^{5\mathrm{D}}(x), && (33)\end{aligned}$$

where the domain-wall Dirac operator is given by

$$\begin{aligned} D_{\mathrm{DW}}^{5\mathrm{D}}(x) = &\frac{1}{2}\gamma^\mu\left(\nabla_\mu(U) + \nabla_\mu^\dagger(U)\right) - \frac{a}{2}\sum_{\mu=1}^{4}\nabla_\mu^\dagger(U)\nabla_\mu(U) \\ &+ \frac{1}{2}\gamma^s\left(\nabla_s(\mathbf{1}) + \nabla_s^\dagger(\mathbf{1})\right) - \frac{a}{2}\nabla_s^\dagger(\mathbf{1})\nabla_s(\mathbf{1}) - m\epsilon(s). \end{aligned} \tag{34}$$

Note here that the link variables in the 5-th direction are taken to be unity and those in the other directions $U_\mu(x)$ are independent of s.

2.3.3 Shamir-type domain-wall fermion

Shamir [28] (see also [29]) pointed out that to localize chiral fermion in domain-wall fermion formulation, it is not necessarily for the mass term to have a kink structure. If we impose Dirichlet boundary conditions on both ends of a finite fifth-dimensional direction and keep the mass term constant, chiral fermions are localized at both ends.

The action of Shamir-type domain-wall fermion is given by

$$
\begin{aligned}
S = &\frac{1}{2}a^5\sum_{x,s}\bar{\psi}(x,s)\left[\sum_\mu \gamma^\mu \frac{1}{a}(U_\mu(x)\psi(x+a\hat{\mu},s) - U_\mu^\dagger(x-a\hat{\mu})\psi(x-a\hat{\mu},s))\right.\\
&\left.+\gamma_5\frac{1}{a}(\psi(x,s+a)-\psi(x,s-a)\right] - a^5\sum_{x,s} m\bar{\psi}(x,s)\psi(x,s)\\
&-\frac{1}{2}a^5\sum_{x,s}\bar{\psi}(x,s)\left[\sum_\mu \frac{1}{a}\Big(U_\mu(x)\psi(x+a\hat{\mu},s)+U_\mu^\dagger(x-a\hat{\mu})\psi(x-a\hat{\mu},s)-2\psi(x,s)\Big)\right.\\
&\left.+\frac{1}{a}\left(\psi(x,s+a)+\psi(x,s-a)-2\psi(x,s)\right)\right].
\end{aligned}
\tag{35}
$$

x denotes the four-dimensional coordinate with periodic boundary condition and $s \in \{1, 2, \cdots, N_s\}$ denotes the fifth dimensional coordinate with dirichlet boundary condition,

$$
\psi(x, s=0) = 0, \quad \psi(x, s=N_s+1) = 0. \tag{36}
$$

In this formalism, the fifth coordinate s does not describe physical degrees of freedom (d.o.f), and then the fifth dimension can be treated as an internal flavor space. The action is rewritten by

$$
\begin{aligned}
S = &a^5\sum_{n,\mu,s}\frac{1}{2}\bar{\psi}_s(x)\gamma^\mu\frac{1}{a}\Big(U_\mu(x)\psi_s(x+a\hat{\mu})-U_\mu^\dagger(x-a\hat{\mu})\psi_s(x-a\hat{\mu})\Big)\\
&+\sum_{x,y,s,t}\bar{\psi}_s(x)\Big[MP_L+M^\dagger P_R\Big]_{s,t}^{x,y}\psi_t(y),
\end{aligned}
\tag{37}
$$

where $P_R = (1+\gamma_5)/2$ and $P_L = (1-\gamma_5)/2$, and the matrix M is the mass term for mixing flavor s which is given by

$$
\begin{aligned}
(M)_{s,t}^{x,y}\psi_t(y) &= -\frac{1}{2a}\sum_\mu\Big(U_\mu(x)\psi_s(x+a\hat{\mu})+U_\mu^\dagger(x-a\hat{\mu})\psi_s(x-a\hat{\mu})-2\psi_s(x)\Big)\\
&\quad -\frac{1}{a}\left(\psi_{s+1}(x)-\psi_s(x)\right)-m\psi_s(x)\\
&= -(\Delta\psi)_s(x)-\frac{1}{a}\left(\psi_{s+1}(x)-\psi_s(x)\right)-m\psi_s(x),
\end{aligned}
\tag{38}
$$

$$
(M^\dagger)_{s,t}^{x,y}\psi_t(y) = -(\Delta\psi)_s(x)-\frac{1}{a}\left(\psi_{s-1}(x)-\psi_s(x)\right)-m\psi_s(x). \tag{39}
$$

Concretely, we write down the matrix M,

$$
M = \begin{pmatrix} W(U) & -1/a & 0 & \cdots \\ 0 & W(U) & -1/a & \\ 0 & 0 & W(U) & \\ \vdots & & & \ddots \end{pmatrix}, \tag{40}
$$

$$M^\dagger = \begin{pmatrix} W(U) & 0 & 0 & \cdots \\ -1/a & W(U) & 0 & \\ 0 & -1/a & W(U) & \\ \vdots & & & \ddots \end{pmatrix}, \tag{41}$$

where $W(U) = -\Delta + 1/a - m$.

Let us consider the free case ($U_\mu(x) = 1$). After the Fourier transformation on the four-dimensional physical space, the action is written by

$$S = a \sum_{s,t} \int \frac{d^4p}{(2\pi)^4} \bar{\psi}_s(-p) \left[i\hat{p} + (MP_L + M^\dagger P_R) \right]_{s,t} \psi_t(p), \tag{42}$$

where $\hat{p} = \sum_\mu \gamma_\mu \hat{p}_\mu$, $\hat{p}_\mu = \frac{1}{a} \sin p_\mu a$ and the mass matrix M is given by (40) with $W(U = \mathbf{1}) = 1/a - m + \sum_\mu (1 - \cos p_\mu a)/a$. If matrices M or $M^\dagger$ have zero eigenvalues, i.e. there exist left- and right-handed zero modes solutions u_L and u_R such that

$$\sum_t M_{s,t} u_L(t,p) = 0, \quad \sum_t M^\dagger_{s,t} u_R(t,p) = 0, \tag{43}$$

and we set ψ as

$$\psi_s(p) = P_L u_L(s,p) + P_R u_R(s,p), \tag{44}$$

then ψ represents massless Dirac fermion.

We discuss the condition for having a zero mode solution.

$$\sum_t M_{s,t} \phi_t = W\phi_s - \frac{1}{a}\phi_{s+1} = 0, \tag{45}$$

then the solution of this equation is given by

$$\phi_s = (aW)^{s-1} \phi_1. \tag{46}$$

Due to the Dirichlet boundary condition $\phi_{N_s+1} = 0$, this solution implies

$$\phi_{N_s+1} = (aW)^{N_s} \phi_1 = 0. \tag{47}$$

Therefore when sW satisfies $|aW| < 1$, there exists a non-zero solution ϕ_1 for infinitely large N_s. In the same way, non-zero solution can exist only when $|aW| < 1$ and infinitely large N_s for another equation $\sum_s M^\dagger_{s,t} \phi_s = 0$.

Let us take a closer look at the condition for aW, $|aW| < 1$. We write this condition concretely:

$$\begin{aligned} -1 < 1 - ma + \sum_\mu (1 - \cos p_\mu a) < +1 \\ \Leftrightarrow \quad 0 < ma - \sum_\mu (1 - \cos p_\mu a) < 2. \end{aligned} \tag{48}$$

This relation leads to Table 1. This table implies that for physical mode $p_\mu = (0,0,0,0)$ there exists zero mode solution only when $0 < ma < 2$, and for $p_\mu = (\pi/a, 0, 0, 0)$ only when $2 < ma < 4$, and so on. In other words, if we take $0 < ma < 2$ only physical mode has zero mode solution, and fermion doublers are avoided.

(p_μ)	Condition for ma	# of poles
$(0,0,0,0)$	$0 < ma < 2$	1
$(\pi/a,0,0,0)\cdots$	$2 < ma < 4$	4
$(\pi/a,\pi/a,0,0)\cdots$	$4 < ma < 6$	6
$(\pi/a,\pi/a,\pi/a,0)\cdots$	$6 < ma < 8$	4
$(\pi/a,\pi/a,\pi/a,\pi/a)$	$8 < ma < 10$	1

Table 1: Condition for ma with several momenta

2.4 Chiral symmetry on the lattice

As mentioned above, the Nielsen-Ninomiya theorem claims that the construction of lattice fermion without fermion doubler is difficult. In particular, the construction of the lattice fermions described above, e.g., Wilson fermion, gave up the chiral symmetry to avoid doublers.

In 1982, Ginsparg and Wilson suggested avoiding doublers and preserving the consequences of chiral symmetry. They allow small violations of the symmetry relation, which preserve chiral symmetry relation under the block spin transformation. Due to their work, the chiral fermion can be defined on the lattice, which approaches the chiral fermion in the continuum theory under the continuum limit.

First, we will discuss the chiral symmetry in the continuum theory, and then we will discuss the chiral symmetry on the lattice introduced by Ginsparg and Wilson. Finally, we will mention the spectral properties of the lattice action with chiral symmetry.

2.4.1 Chiral symmetry in continuum theory

First, we discuss chiral symmetry for the simple case in the continuum theory. The action for massless fermion is

$$\begin{aligned} S &= \int d^4x \bar{\psi}(x)\gamma_\mu D_\mu \psi(x) \\ &= \int d^4x \bar{\psi}(x) D \psi(x). \end{aligned} \tag{49}$$

This action is invariant under

$$\psi(x) \to \psi'(x) = e^{i\alpha\gamma_5}\psi(x), \quad \bar{\psi}(x) \to \bar{\psi}'(x) = \bar{\psi}(x)e^{i\alpha\gamma_5} \tag{50}$$

where α is a real parameter. This global symmetry is chiral symmetry. If a mass term is introduced, this symmetry is broken since it transforms as

$$m\bar{\psi}\psi \to m\bar{\psi}'\psi' = e^{2i\alpha\gamma_5}\bar{\psi}\psi. \tag{51}$$

The essential property of this symmetry is the fact that the massless Dirac operator D anti-commutes with the chirality operator γ_5:

$$D\gamma_5 + \gamma_5 D = 0. \tag{52}$$

In other words, the action with the Dirac operator satisfying this relation has chiral symmetry.

2.4.2 Ginsparg-Wilson relation and chiral symmetry on a lattice

Based on a renormalization group analysis, Ginsparg and Wilson [7] insisted that the chiral symmetric Dirac operator on the lattice should satisfy

$$D\gamma_5 + \gamma_5 D = aD\gamma_5 D. \tag{53}$$

This relation is called Ginsparg-Wilson relaiton. In order to discuss the effect of the extra term for the propagator, multiplying (53) with D^{-1} from both sides we obtain

$$\gamma_5 D^{-1}_{x,y} + D^{-1}_{x,y}\gamma_5 = a\gamma_5\delta_{x,y}. \tag{54}$$

The chiral symmetry breaking for the propagator D^{-1} is a local $\mathcal{O}(a)$ effect. Therefore the breaking effect does not contribute to the long-range physics and vanishes in the continuum limit.

The action with Dirac operator satisfying Ginsparg-Wilson relation

$$S = a^4 \sum_x \bar{\psi}(x) D\psi(x), \tag{55}$$

has the exact chiral symmetry [6]: it is invariant under

$$\begin{aligned}\psi(x) &\to \exp\left[i\alpha\gamma_5\left(1-\frac{1}{2}aD\right)\right]\psi(x),\\ \bar{\psi}(x) &\to \bar{\psi}(x)\exp\left[i\alpha\left(1-\frac{1}{2}aD\right)\gamma_5\right].\end{aligned} \tag{56}$$

Next, we discuss the eigenvalue spectrum of the Dirac operator on a finite lattice. Let $|\lambda\rangle$ be an eigenstate of D with an eigenvalue λ,

$$D|\lambda\rangle = \lambda|\lambda\rangle, \quad \lambda \in \mathbb{C}. \tag{57}$$

Note that D is not a Hermitian operator and its conjugate is

$$\langle\lambda| D^\dagger = \langle\lambda|\lambda^*, \tag{58}$$

where λ^* represents a complex conjugate of λ. From the Ginsparg-Wilson relation, we have $D + D^\dagger = aD^\dagger D$, which implies

$$\lambda + \lambda^* = a\lambda^*\lambda. \tag{59}$$

Writing the eigenvalue as $\lambda = x + iy$, this relation turns into

$$\left(x - \frac{1}{a}\right)^2 + y^2 = \left(\frac{1}{a}\right)^2. \tag{60}$$

Therefore, the eigenvalue spectrum forms a circle in the complex plane with the center at $(1/a, 0)$ and radius $1/a$. The eigenvalues near the origin are the physical modes, while those near 2/a are the doubler modes.

Let us introduce $H \equiv \gamma_5 D$ and a new chiralilty operator on the lattice as

$$\Gamma_5 = \gamma_5 \left(1 - \frac{a}{2}D\right). \tag{61}$$

Due to the Ginsparg-Wilson relation, H anti-commutes with Γ_5. This relation suggests that if

$$H \left|\lambda_H\right\rangle = \lambda_H \left|\lambda_H\right\rangle, \quad \left\langle\lambda_H|\lambda_H\right\rangle = 1, \tag{62}$$

then

$$H(\Gamma_5 \left|\lambda_H\right\rangle) = -\lambda_H(\Gamma_5 \left|\lambda_H\right\rangle). \tag{63}$$

The eigenvalues of H are always paired $(\lambda_H, -\lambda_H)$ except in the cases of $\lambda_H = 0$ and $((\left\langle\lambda_H\right| \Gamma_5)(\Gamma_5 \left|\lambda_H\right\rangle) = 0$. In the latter case we obtain

$$\left\langle\lambda_H\right| \Gamma_5\Gamma_5 \left|\lambda_H\right\rangle = \left\langle\lambda_H\right| \left(1 - \frac{a^2}{4}H^2\right) \left|\lambda_H\right\rangle = 1 - \frac{a^2}{4}\lambda_H^2 = 0, \tag{64}$$

then $\lambda_H = \pm\frac{2}{a}$.

Finally we summarise the spectral properties of the Ginsparg-Wilson Dirac operator.

1. Zero-modes $\lambda_H = 0$
   The eigenstates of H is chiral modes:
   $$H \left|\lambda_H\right\rangle = 0 \tag{65}$$
   $$\gamma_5 \left|\lambda_H\right\rangle = \pm \left|\lambda_H\right\rangle \tag{66}$$

2. $0 < |\lambda_H| < \frac{2}{a}$
   $$H \left|\lambda_H\right\rangle = \lambda_H \left|\lambda_H\right\rangle, \tag{67}$$
   $$H \left(\Gamma_5 \left|\lambda_H\right\rangle\right) = -\lambda_H \left(\Gamma_5 \left|\lambda_H\right\rangle\right). \tag{68}$$

3. $\lambda_H = \pm\frac{2}{a}$
   In this case
   $$\Gamma_5 \left|\lambda_H\right\rangle = 0, \tag{69}$$
   then,
   $$H \left|\lambda_H\right\rangle = +\frac{2}{a} \left|\lambda_H\right\rangle, \quad \gamma_5 \left|\lambda_H\right\rangle = + \left|\lambda_H\right\rangle, \tag{70}$$
   $$H \left|\lambda_H\right\rangle = -\frac{2}{a} \left|\lambda_H\right\rangle, \quad \gamma_5 \left|\lambda_H\right\rangle = - \left|\lambda_H\right\rangle, \tag{71}$$
   positive and negative eigenvalues of H correspond to positive and negative eigenvalues of γ_5.

Using these spectral properties of H, we can prove the Atiyah-Singer index theorem, as discussed later.

2.5 Overlap fermion

An example of the lattice Dirac operator satisfying the GW relation is the overlap Dirac operator [4, 5] defined by

$$D_{\rm ov} = \frac{1}{a}\left(1 + X\frac{1}{\sqrt{X^\dagger X}}\right) \tag{72}$$

$$X = D_{\rm W} - m, \tag{73}$$

where $D_{\rm W}$ is the Wilson-Dirac operator and m is the cutoff scale mass ($\sim 1/a$).

Next, we discuss how doubler modes are decoupled in the overlap Dirac operator. In the free case, the Wilson-Dirac operator in the momentum space is given by

$$X = \frac{1}{a}\sum_\mu \gamma_\mu \sin ap_\mu + \frac{1}{a}\sum_\mu (1-\cos ap_\mu) - m, \tag{74}$$

then we obtain

$$X^\dagger X = \frac{1}{a^2}s^2 + M(p)^2, \tag{75}$$

where $s = \sin ap_\mu$ and $M(p) = \sum_\mu (1-\cos ap_\mu) - m$. For $m = \mathcal{O}(1)$ and $a \ll 1$, $M(p)$ is expanded as

$$M(p) = \begin{cases} -m + \mathcal{O}(a^2) & {}^\forall p_\mu \simeq 0, \\ -m + 2n\frac{1}{a} + \mathcal{O}(a^2) & {}^\exists p_\mu \simeq \pi/a,\ n = \#\text{ of }\pi'\text{s}. \end{cases} \tag{76}$$

For physical modes (${}^\forall p_\mu \simeq 0$), the overlap Dirac operator becomes

$$D_{\rm ov} = \frac{1}{a}\left[1 + \frac{i\gamma_\mu p_\mu - m}{m}\right] = \frac{1}{ma} i\gamma_\mu p_\mu. \tag{77}$$

In this way, the overlap Dirac operator describes massless fermion. On the other hand, for doubler modes, if we assume $0 < ma < 2$, the overlap Dirac operator becomes

$$D_{\rm ov} = \frac{1}{a}\left[1 + \frac{i\gamma_\mu \pi - m + 2n/a}{2n/a - m}\right] = \frac{1}{2n - ma}\left[i\gamma_\mu p_\mu + \frac{2}{a}(2n - ma)\right]. \tag{78}$$

Thus, doubler modes have cut-off scale mass and do not contribute to low energy physics.

2.6 Atiyah-Singer index theorem on the lattice

Finally, we discuss the Atiyah-Singer (AS) index theorem [9–13]. In continuum theory, the AS index theorem states that for an elliptic differential operator D on a manifold without boundary, the analytical index related to the zero eigenvalues of D is equal to the topological index on the manifold. The elliptic operator of our interest is the Dirac operator.

On a four-dimensional closed Euclidean manifold X with flat metric, the Atiyah-Singer index theorem for the Dirac operator D asserts

$$\text{index}(D) = Q_{\rm top}. \tag{79}$$

Here $Q_{\rm top}$ is the topological charge of the gauge field:

$$Q_{\rm top} = \frac{1}{32\pi^2}\int_X d^4x \epsilon_{\mu\nu\rho\sigma} {\rm tr_c} F^{\mu\nu}F^{\rho\sigma} \tag{80}$$

where $F_{\mu\nu}$ is the field strength of $SU(N)$ or $U(1)$ gauge fields and this quantity is called the instanton number. Often it is useful to define a quantity called the topological charge density $q_{\rm top}(x) = \frac{1}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}{\rm tr_c}F^{\mu\nu}F^{\rho\sigma}$. The instanton number is topological invariant under continuous deformation of the gauge field. The analytical index index(D) counts the mismatch of the left-handed modes and right-handed modes of fermions. It concretely holds index$(D) = n_+ - n_-$ and $n_\pm$ denotes the number of $\pm$ chiral zero modes of the Dirac operator D.

The AS index theorem is closely related to physical phenomena and is well understood in terms of physics, especially quantum field theory language. The topological charge density is nothing but the axial $U(1)$ anomaly [30, 31]. The anomaly can be interpreted as arising from the Jacobian of the path integral measure under the symmetry transformation, and the method to derive the anomaly under this interpretation is called Fujikawa's method [32]. The index theorem can be easily derived by using Fujikawa's method.

In the following, we will derive the AS index theorem from Fujikawa's method for chiral $U(1)$ transformations for both continuum and lattice theories.

2.6.1 Atiyah-Singer index theorem in continuum theory

To derive the AS index theorem, we consider the Jacobian of the fermionic path integral measure with respect to the chiral symmetry (52),

$$\mathcal{D}\bar{\psi}'\mathcal{D}\psi' = J\mathcal{D}\bar{\psi}\mathcal{D}\psi, \tag{81}$$

where the Jacobian factor is given by

$$J \equiv \exp[-2i\alpha \lim_{N\to\infty}\sum_{n=1}^{N}\int d^4\phi_n^\dagger(x)\gamma_5\phi_n(x)]. \tag{82}$$

This factor is divergent in general but can be calculated using a regularization that does not break gauge symmetry, such as the heat kernel regularization. After a lengthy calculation, the Jacobian becomes

$$J = \exp\left[-2i\alpha\int d^4x \frac{1}{32\pi^2}\epsilon^{\mu\nu\rho\sigma}{\rm tr_c}F_{\mu\nu}F_{\rho\sigma}\right]. \tag{83}$$

Using $D\gamma_5 + \gamma_5 D = 0$, it turns out that $\gamma_5\phi_n(x)$ is also the eigenfunction of iD with opposite eigenvalue $-\lambda_n$

$$iD\gamma_5\phi_n(x) = -\lambda_n\gamma_5\phi_n(x). \tag{84}$$

Due to the Hermiticity of iD, the inner product becomes

$$\begin{aligned}(\phi_n, iD\gamma_5\phi_n) &= \int d^4x\phi_n^\dagger(x)iD\gamma_5\phi_n(x) = -\lambda_n\int d^4x\phi^\dagger(x)\gamma_5\phi_n(x)\\ &= -\lambda_n(\phi_n,\gamma_5\phi_n),\end{aligned} \tag{85}$$

$$
\begin{aligned}
(\phi_n, iD\gamma_5\phi_n) &= \int d^4x (iD)^\dagger \phi_n^\dagger(x)\gamma_5\phi_n(x) = \lambda_n \int d^4x \phi^\dagger(x)\gamma_5\phi_n(x) \\
&= \lambda_n(\phi_n, \gamma_5\phi_n),
\end{aligned} \tag{86}
$$

it implies that

$$
(\phi_n, \gamma_5\phi_n) = \int d^4x \phi_n^\dagger(x)\gamma_5\phi_n(x) = 0, \qquad \text{for } \lambda_n \neq 0. \tag{87}
$$

For zero modes ($\lambda_n = 0$), the eigenfunctions satisfy

$$
iD\phi_n^0(x) = 0, \quad iD\gamma_5\phi_n^0(x) = 0, \tag{88}
$$

then it can also be treated as eigenfunction of chirality operator:

$$
iD\phi_{n\pm}^0 = \frac{1}{2} iD(1 \pm \gamma_5)\phi_n^0(x) = 0, \tag{89}
$$

$$
\gamma_5\phi_{n+}^0 = +\phi_{n+}^0, \quad \gamma_5\phi_{n-}^0 = -\phi_{n-}^0. \tag{90}
$$

Then the Jacobian factor can be written as

$$
\begin{aligned}
\sum_n \int d^4\phi_n^\dagger(x)\gamma_5\phi_n(x) &= \int d^4x \sum_n \phi_n^{0\dagger}(x)\gamma_5\phi_n^0(x) \\
&= \int d^4x \sum_n \phi_{n=+}^{0\dagger}(x)\phi_{n+}^0(x) - \int d^4x \sum_n \phi_{n-}^{0\dagger}(x)\phi_{n-}^0(x) \\
&= n_+ - n_-,
\end{aligned} \tag{91}
$$

where $n_\pm$ is the number of zero modes with chirality $\pm$.

Therefore, we obtain the Jacobian factor

$$
\begin{aligned}
J &= \exp\left[-2i\alpha \int d^4x \frac{1}{32\pi^2} \epsilon^{\mu\nu\rho\sigma} \mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}\right] \\
&= \exp[-2i\alpha(n_+ - n_-)].
\end{aligned} \tag{92}
$$

This leads to the AS index theorem

$$
n_+ - n_- = \frac{1}{32\pi^2} \int d^4x \epsilon^{\mu\nu\rho\sigma} \mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}. \tag{93}
$$

We could derive the AS index theorem *physically* through Fujikawa's method.

According to the above discussion, the index of the Dirac operator is given by well-regularized trace of the chirality operator γ_5, such as the heat kernel regularization:

$$
\begin{aligned}
\mathrm{index}(D) &= \mathrm{Tr}_{\mathrm{reg.}}\gamma_5, \\
&= \lim_{M\to\infty} \mathrm{Tr}\gamma_5 e^{-D^2/M^2}.
\end{aligned} \tag{94}
$$

2.6.2 Atiyah-Singer index theorem on the lattice

In the framework of the lattice field theory, the AS index theorem was established by the seminal work by Hasenfratz *et al.* [8][1].

As in the continuum theory, the fermionic path integral measure is not invariant with respect to the lattice chiral symmetry (56).

$$\mathcal{D}\psi\mathcal{D}\bar{\psi} \to J\mathcal{D}\psi\mathcal{D}\bar{\psi}, \tag{95}$$

where the Jacobian factor is given by

$$\begin{aligned} J &= \exp\left[-2i\alpha \mathrm{Tr}\gamma_5\left(1-\frac{a}{2}D\right)\right] \\ &= \exp\left[-2i\alpha a^4\sum_x \mathrm{tr}\gamma_5\left(1-\frac{a}{2}D(x)\right)\right] = \exp\left[-2i\alpha\mathrm{Tr}\Gamma_5\right]. \end{aligned} \tag{96}$$

Note that D satisfies the Ginsparg-Wilson relation. Recalling the discussion in continuum theory, we can see that the proof of the AS index theorem on the lattice is completed by showing that the content of the Jacobian factor is equal to $n_+ - n_-$ and the topological charge.

First, using the spectral properties of the Ginsparg-Wilson-Dirac operator, we can prove that the trace of the lattice chirality operator Γ_5 coincides with $n_+ - n_-$:

$$\mathrm{Tr}\Gamma_5 = n_+ - n_-. \tag{97}$$

The proof is straightforward,

$$\begin{aligned} \mathrm{Tr}\Gamma_5 &= \mathrm{Tr}\gamma_5\left(1-\frac{a}{2}D\right) = \sum_{\lambda_H}\langle\lambda_H|\,\Gamma_5\,|\lambda_H\rangle\,, \\ &= \sum_{\lambda_H=0}\langle\lambda_H|\,\Gamma_5\,|\lambda_H\rangle + \sum_{0<|\lambda_H|<2/a}\langle\lambda_H|\,\Gamma_5\,|\lambda_H\rangle + \sum_{\lambda_H=\pm 2/a}\langle\lambda_H|\,\Gamma_5\,|\lambda_H\rangle\,, \\ &= \sum_{\lambda_H=0}\langle\lambda_H|\,\Gamma_5\,|\lambda_H\rangle\,, \\ &= n_+ - n_-, \end{aligned} \tag{98}$$

where in the second step, we use the spectral properties of the Ginsparg-Wilson Dirac operator.

Next, we will show that the trace of the lattice chirality operator coincides with the topological charge in the continuum limit [33–37][2]. Using $\mathrm{Tr}\gamma_5 = 0$ on a finite lattice[3], we can show that $-\frac{a}{2}\mathrm{tr}\gamma_5 D$ converges to the topological charge density $q^{\mathrm{lat}}_{\mathrm{top}}(x)$,

$$q^{\mathrm{lat}}_{\mathrm{top}} = I(m,r)\frac{1}{32\pi^2}\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}(x) + \mathcal{O}(a). \tag{99}$$

[1] First, the index theorem was established using so-called Fixed Point action also satisfying the Ginsparg-Wilson relation, introduced by Hasenfratz.

[2] Since this explicit computation is important in later discussion, we review the evaluation by [36] in the Appendix C.

[3] The physical implications of $\mathrm{Tr}\gamma_5 = 0$ is analysed in [38, 39].

	$0 < ma < 2$	$2 < ma < 4$	$4 < ma < 6$	$6 < ma < 8$	$ma \notin [0, 8]$
$I(m, 1) =$	1	-3	3	-1	0

Table 2: The dependence on m in $I(m, r)$

where $I(m, r)$ is given by

$$I(m, r) = \theta(am/r) - 4\theta(am/r - 2) + 6\theta(am/r - 4) - 4\theta(am/r - 6) + \theta(am/r - 8), \quad (100)$$

where $\theta(x)$ is a step function satisfying

$$\theta(x) = \begin{cases} 1 & (x > 0) \\ 0 & (x < 0). \end{cases} \quad (101)$$

3 Atiyah-Patodi-Singer index and domain-wall fermion

In the previous section, we discussed lattice discretization of fermions and showed that the chiral symmetry as well as the Atiyah-Singer index theorem can be formulated even with a finite lattice spacing. Now let us extend the discussion to a space-time with a boundary, where it is known that the Atiyah-Patodi-Singer (APS) index theorem [17–19] holds. The original formulation of APS index is, however, not very physicist-friendly in that a non-local boundary condition is imposed. The non-locality is unacceptable in physics and an obstacle for the lattice formulation as well. In this section, we review the APS index theorem in continuum and its unphysical properties. Then we introduce a physicist-friendly reformulation of the APS index recently proposed in [20, 21] using the domain-wall fermion Dirac operator.

3.1 Atiyah-Patodi-Singer index theorem

Let us consider a flat four-dimensional closed Euclidean manifold X with boundary $Y = \partial X$. The manifold X extends only in the region $x_4 > 0$ for the x_4-direction. The boundary Y at $x_4 = 0$ is a three-dimensional manifold with a flat metric Y. Atiyah, Patodi, and Singer showed that the index for the Dirac operator D with imposing a nontrivial boundary condition (APS boundary condition) is given by

$$\mathrm{Ind}_{\mathrm{APS}}(D) = \frac{1}{32\pi^2} \int_{x_4 > 0} d^4x \epsilon^{\mu\nu\rho\sigma} \mathrm{tr}_c F_{\mu\nu} F_{\rho\sigma} - \frac{1}{2}\eta\left(iD^{\mathrm{3D}}\right), \quad (102)$$

where iD^{3D} is the Dirac operator on the three-dimensional manifold Y and $\eta(H)$ is the so-called APS eta invariant or simply eta invariant which is defined by the summation of sign of the eigenvalues of the Hermitian operator H. The concrete formula, for example, using ζ-function regularization is given by

$$\eta(H) = \lim_{s \to 0} \sum_{\lambda \neq 0} \frac{\lambda}{|\lambda|^{1+s}} + h, \quad (103)$$

where λ is the nonzero eigenvalues of H, and h denotes the number of zero modes of H. In general, $\eta\left(iD^{3\mathrm{D}}\right)$ does not take an integer value and $\eta\left(iD^{3\mathrm{D}}\right)$ is equal to the Chern-Simons term.

$$\frac{1}{2}\eta\left(iD^{3\mathrm{D}}\right) = \frac{CS}{2\pi} \quad \text{mod integer}, \tag{104}$$

$$CS \equiv \frac{1}{4\pi}\int_Y d^3x \mathrm{tr}\left[\epsilon^{\nu\rho\sigma}\left(A_\nu\partial_\rho A_\sigma + \frac{2i}{3}A_\nu A_\rho A_\sigma\right)\right]. \tag{105}$$

(105) is canceled out by the surface term of the first term in (102). Therefore, the total contribution of the APS index is guaranteed to be an integer.

3.1.1 APS boundary condition

The massless Dirac operator for $x_4 > 0$ with the $A_4 = 0$ gauge is given by

$$D = \gamma_4\left(\partial_4 + B\right), \tag{106}$$

where $B = \gamma_4\sum_{i=1}^{3}\gamma^i D_i$ is the three-dimensional operator on Y. Then we impose the following conditions

$$(B + |B|)\psi|_{x_4=0} = 0, \quad (B + |B|)D\psi|_{x_4=0} = 0, \tag{107}$$

which is called the APS boundary condition. For simplicity, we assume that the operator B has no zero eigenvalues. Since the APS boundary condition keeps the anti-Hermiticity of the Dirac operator and chirality, the index can be defined by the chiral zero modes

$$\mathrm{index}_{\mathrm{APS}}(D) = \lim_{M\to\infty}\mathrm{Tr}\gamma_5 e^{(iD)^2/M^2}|_{\mathrm{APS\ b.c.}}. \tag{108}$$

as is explicitly shown below.

To perform the computation, we first need a complete set satisfying the APS boundary condition when B has no x_4-dependence (this corresponds to the leading order contribution in adiabatic approximation, which assumes a slow x_4-dependence.).

Using the chiral representation of the γ-matrices, three-dimensional boundary operator B can be written as

$$B = \gamma_4\sum_{1=1}^{3}\gamma^i D_i = \sum_{i=1}^{3}\begin{pmatrix}-i\sigma_i & 0\\ 0 & i\sigma_i\end{pmatrix}D_i = \begin{pmatrix}iD^{3\mathrm{D}} & 0\\ 0 & -iD^{3\mathrm{D}}\end{pmatrix} = \tau_3\otimes iD^{3\mathrm{D}}, \tag{109}$$

where $D^{3\mathrm{D}} = -\sigma_i D_i$ is a three-dimensional massless Dirac operator. We use the eigenfunction of $(iD)^2$ with eigenvalue Λ^2,

$$(iD)^2\phi(\boldsymbol{x}, x_4) = \Lambda^2\phi(\boldsymbol{x}, x_4), \tag{110}$$

and we can take the eigenfunction the following form

$$\phi(\boldsymbol{x}, x_4) = \phi_\pm^\omega(x_4)\otimes\phi_\lambda(\boldsymbol{x}), \tag{111}$$

where the subscript $\pm$ denotes the chirality: $\tau_3\phi^\omega_\pm(x_4) = \pm\phi^\omega_\pm(x_4)$, ω is the momentum in the x_4-direction, and $\phi_\lambda(\boldsymbol{x})$ is the eigenfunction of the three-dimensional Dirac operator $iD^{\rm 3D}$ with the eigenvalue λ: $iD^{\rm 3D}\phi_\lambda(\boldsymbol{x}) = \lambda\phi_\lambda(\boldsymbol{x})$. In this case, the APS boundary condition corresponds to

$$\phi^\omega_+(x_4)|x_4 = 0 = 0, \quad (\partial_4 - \lambda)\phi^\omega_-(x_4)|_{x_4=0} = 0, \quad \text{for } \lambda > 0, \tag{112}$$

$$\phi^\omega_-(x_4)|x_4 = 0 = 0, \quad (\partial_4 + \lambda)\phi^\omega_+(x_4)|_{x_4=0} = 0, \quad \text{for } \lambda < 0. \tag{113}$$

The eigenfunction of $(iD)^2$ with above condition is given by, for $\lambda > 0$ case

$$\phi^\omega_+(x_4) = \frac{e^{i\omega x_4} - e^{-i\omega x_4}}{\sqrt{2\pi}}, \quad \phi^\omega_-(x_4) = \frac{(i\omega+\lambda)e^{i\omega x_4} + (i\omega-\lambda)e^{-i\omega x_4}}{\sqrt{2\pi(\omega^2+\lambda^2)}}, \tag{114}$$

and for $\lambda < 0$ case

$$\phi^\omega_-(x_4) = \frac{e^{i\omega x_4} - e^{-i\omega x_4}}{\sqrt{2\pi}}, \quad \phi^\omega_+(x_4) = \frac{(i\omega-\lambda)e^{i\omega x_4} + (i\omega+\lambda)e^{-i\omega x_4}}{\sqrt{2\pi(\omega^2+\lambda^2)}}. \tag{115}$$

Note that there is no edge-localized mode.

We compute the index with the APS boundary condition using the above complete set. At the leading order (LO) of the adiabatic approximation, we obtain

$$\begin{aligned}
&\lim_{M\to\infty} {\rm Tr}\gamma_5 e^{(iD)^2/M^2}|_{\rm LO} \\
&\quad = \lim_{M\to\infty}\sum_\lambda \int_{x_4\geq 0} d^4x\,{\rm sgn}(\lambda)e^{-\lambda^2/M^2}\int\frac{d\omega}{2\pi}\left(-1+\frac{2i|\lambda|}{\omega+i|\lambda|}e^{-\omega^2/M^2+2i\omega x_4}\right) \\
&\quad = -\frac{1}{2}\sum_\lambda {\rm sgn}(\lambda)\lim_{M\to\infty}{\rm erfc}(|\lambda|/M) \\
&\quad = -\frac{1}{2}\eta\left(iD^{\rm 3D}\right),
\end{aligned} \tag{116}$$

where ${\rm erfc}(x)$ is the error function defined by

$$ {\rm erfc}(x) = \frac{2}{\sqrt{\pi}}\int_x^\infty d\xi e^{-\xi^2}, \quad {\rm erfc}(0) = 0, \quad {\rm erfc}(\infty) = 0. \tag{117}$$

From the next-to-leading order (NLO), we obtain, see [40] for detail derivation,

$$\lim_{M\to\infty} {\rm Tr}\gamma_5 e^{(iD)^2/M^2}|_{\rm NLO} = \frac{1}{32\pi^2}\int_x d^4x e^{\mu\nu\rho\sigma}{\rm tr}_c F_{\mu\nu}F_{\rho\sigma}. \tag{118}$$

3.1.2 Difficulties of APS boundary conditon

Here, we discuss the necessity of the APS boundary condition and its difficulties in application to physical systems.

When a manifold has a boundary, the Dirac operator in general loses anti-Hermiticity:

$$\begin{aligned}
(\phi_1, D\phi_2) &\equiv \int_X d^4x\phi_1^\dagger(x)D\phi_2(x) \\
&= \int_Y d^3x\phi_1^\dagger(x)\gamma_4\phi_2(x)|_{x_4=0} - (D\phi_1,\phi_2),
\end{aligned} \tag{119}$$

unless we impose a boundary condition which satisfies

$$\int_Y d^3x \phi_1^\dagger(x)\gamma_4\phi_2(x)|_{x_4=0} = 0. \tag{120}$$

The APS boundary condition is one of such conditions, since $\gamma_4\phi_2$ has a support only from eigenfunction of B with opposite sign of eigenvalues to that of ϕ_1 due to $\{\gamma_4, B\} = 0$.

The APS boundary condition also keeps the chirality of the fermion field since B commutes with γ_5. Then it keeps the bulk fermion massless [41], and the index can be written by the chiral zero modes, as usual: $n_+ - n_-$.

However, the APS boundary condition cannot be directly imposed on the physical systems for the following reasons. First, it requires non-local information of the eigenfunctions extended in the entire Y. Suppose that the eigenvalues of $iD^{\rm 3D}$ cross zero due to a change in the local gauge field. This information must be immediately reflected in the whole region of the boundary through the APS boundary condition. The desired boundary conditions for physics are local and not given by hand.

Second, the APS boundary condition does not allow any edge-localized modes to exist. For simplicity, we suppose that B has no x_4-dependence. In this case, the zero mode localized at the boundary can be written as

$$\phi(x) = \phi_\lambda e^{-\lambda x_4}, \quad D\phi = 0, \tag{121}$$

where ϕ_λ is an eigenfunction of B with the eigenvalue λ. This solution is normalizable only when $\lambda > 0$ but it is prohibited by the APS boundary condition. As shown in Eq.(116), the eta invariant of the boundary Dirac operator $\eta(iD^{\rm 3D})$ originates from the bulk extended modes with a non-trivial singularity in the ω integral.

Recently it was pointed out that the APS index theorem is a key to understand the bulk-edge correspondence in symmetry-protected topological insulators [15, 42]. Each term of the APS index theorem corresponds to each phase of the edge and bulk fermion determinants, representing the anomaly inflow of the time reversal (T) symmetry. The APS index gives a mathematical guarantee that the total system is protected from the T-anomaly. However, the original setup of the APS boundary condition discussed above is very different from that of topological materials. With the APS boundary condition, the bulk Dirac operator is kept massless and there is no edge-localized mode to produce the eta invariant.

Moreover, a manifold with boundaries is unnatural in physics. It is as if the world ends beyond the boundary, but there is an outside of the boundary in actual physical systems. For example, we can think of the outside of a topological insulator as being covered by a standard insulator (vacuum). Therefore the desired set-up should be one that can also describe the outside of the boundary.

In summary, the desired set-up is one in which there is a massive fermion as a bulk fermion, a localized mode at the edge, naturally chosen boundary conditions, and a closed system including the outside of the boundary. The domain-wall fermion discussed in 2.3 perfectly matches this set-up.

3.2 APS index theorem from domain-wall Dirac operator

Now we discuss the physicist-friendly reformulation of the APS index theorem proposed in [20, 21], using the domain-wall fermion[4].

The domain-wall fermion provides a natural set up for physical systems with boundaries. The hermitian domain-wall Dirac operator is given by

$$H_{\mathrm{DW}} = \gamma_5[D - M\epsilon(x_4)], \quad \epsilon(x_4) = \mathrm{sign}(x_4), \tag{122}$$

where the mass is positive $M > 0$. Unlike considering a manifold with boundary using the APS boundary condition, x_4 is defined on $-\infty < x_4 < \infty$, so no boundary condition by hand is needed. We will introduce the Pauli-Villars field to cancel out the contributions from the bulk at $x_4 < 0$. This domain-wall fermion gives a model for a fermion system where a topological insulator is put in the region $x_4 > 0$, while the outside or $x_4 < 0$ part is a normal insulator. The edge mode appears at $x_4 = 0$, which plays an essential role in defining the index.

New index $\mathcal{I}$ is formally defined by a regularized eta invariant of (122):

$$\mathcal{I} \equiv -\frac{1}{2}\eta\left(H_{\mathrm{DW}}^{\mathrm{reg.}}\right) = -\frac{1}{2}\eta\left(H_{\mathrm{DW}}\right) + \frac{1}{2}\eta\left(H_{\mathrm{PV}}\right), \tag{123}$$

where the hermitian Pauli-Villars operator is $H_{\mathrm{PV}} = \gamma_5[D + M]$. As shown next, we can verify that this new index definition coincides with the APS index formula:

$$-\frac{1}{2}\eta\left(H_{\mathrm{DW}}^{\mathrm{reg.}}\right) = \frac{1}{32\pi^2}\int_{x_4>0} d^4x\,\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma} - \frac{1}{2}\eta\left(iD^{\mathrm{3D}}\right). \tag{124}$$

Here we slightly generalize the domain-wall fermion Dirac operator to have different absolute masses in each domain:

$$H_{\mathrm{ADW}} = \gamma_5[D - M_1\epsilon(x_4) + M_2], \tag{125}$$

where D is the four-dimensional Dirac operator, and we take both M_1 and M_2 positive. To evaluate the eta invariant of (125) we choose the eigenfunction set of the free domain-wall Dirac operator squared $(H_{\mathrm{ADW}}^{\mathrm{free}})^2$. The solution to

$$\left(-\partial_\mu^2 + M_1^2 + M_2^2 + 2M_1\gamma_4\delta(x_4) - 2M_1M_2\epsilon(x_4)\right)\phi = \Lambda^2\phi \tag{126}$$

has the form $\varphi_\pm^{\omega/\mathrm{edge}}(x_4)\otimes e^{i\boldsymbol{p}\cdot\boldsymbol{x}}$, where the subscript $\pm$ denotes the eigenvalue of γ_4. Depending on the eigenvalue Λ, we have three types of solutions. For $|\Lambda| < |M_1 - M_2|$, we have edge-localized solutions

$$\varphi_-^{\mathrm{edge}}(x_4) = \begin{cases} u_-\sqrt{\frac{M_1^2-M_2^2}{M_1}}e^{-(M_1-M_2)x_4} & (x_4 \geq 0), \\ u_-\sqrt{\frac{M_1^2-M_2^2}{M_1}}e^{(M_1+M_2)x_4} & (x_4 < 0) \end{cases} \tag{127}$$

where the eigenvalue is $\Lambda^2 = \boldsymbol{p}^2$ and $u_\pm$ represent the spinor components $\gamma_4 u_\pm = \pm u_\pm$. The edge mode appears only in the $\gamma_4 = -1$ sector. For $|M_1 - M_2| \leq \Lambda \leq |M_1 + M_2|$, we have

[4]The study of the index theorem with domain-wall structure has been done in [43, 44].

extended bulk modes only in the region $x_4 \geq 0$:

$$\varphi^{\omega}_{\pm}(x_4) = \begin{cases} \frac{u_\pm}{\sqrt{2\pi(\omega^2+\mu_\pm^2)}} \left[(i\omega + \mu_\pm)e^{i\omega x_4} + (i\omega - \mu_\pm)e^{-i\omega x_4}\right] & (x_4 \geq 0), \\ u_\pm \frac{2i\omega}{\sqrt{2\pi(\omega^2+\mu_\pm^2)}} e^{\Omega x_4} & (x_4 < 0) \end{cases} \tag{128}$$

where $\omega = \sqrt{\Lambda^2 - \boldsymbol{p}^2 - (M_1 - M_2)^2}$, $\Omega = \sqrt{-\Lambda^2 + \boldsymbol{p}^2 + (M_1 + M_2)^2}$ and $\mu_\pm = \Omega \pm 2M_1$. For $|M_1 + M_2| \leq \Lambda$, we have plane wave solutions in the whole region:

$$\varphi^{\omega}_{\pm}(x_4) = \begin{cases} u_\pm(Ae^{i\omega_1 x_4} + Be^{-i\omega_1 x_4}) & (x_4 \geq 0), \\ u_\pm(Ce^{i\omega_2 x_4} + De^{-i\omega_2 x_4} & (x_4 < 0), \end{cases} \tag{129}$$

where $\omega_1 = \sqrt{\Lambda^2 - \boldsymbol{p}^2 - (M_1 - M_2)^2}$ and $\omega_2 = \sqrt{\Lambda^2 - \boldsymbol{p}^2 - (M_1 + M_2)^2}$, and the coefficients satisfy $A + B = C + D$ and $-i\omega_1(A - B) + i\omega_2(C - D) \pm 2M_1(A + B) = 0$.

These solutions satisfy a nontrivial boundary condition,

$$-\lim_{\epsilon\to 0}\left(\partial_4\varphi^{\omega/\mathrm{edge}}_{\pm}(+\epsilon) - \partial_4\varphi^{\omega/\mathrm{edge}}_{\pm}(-\epsilon)\right) \pm 2M_1\varphi^{\omega/\mathrm{edge}}_{\pm}(0) = 0. \tag{130}$$

This condition respects $SO(3)$ rotational symmetry on the surface.

When $M_1 > M_2$, the appropriate Pauli-Villars operator is given by

$$H_{\mathrm{PV}} = \gamma_5[D + M_1 - M_2\epsilon(x_4)]. \tag{131}$$

The total mass $M_1 - M_2\epsilon(x_4)$ does not change its sign when x_4 is changed, and therefore, the edge localized mode does not appear.

The additional mass M_2 does not break the γ_5-hermiticity of the domain-wall Dirac operator and the Pauli-Villars Dirac operator. Then the index can be defined as

$$\mathrm{index}_{\mathrm{APS}}(D) = -\frac{1}{2}\eta(H_{\mathrm{ADW}}) + \frac{1}{2}\eta(H_{\mathrm{PV}}). \tag{132}$$

In Ref. [20, 21] it was shown that this index is independent of the additional mass M_2.

$$\frac{d\mathrm{index}_{\mathrm{APS}}(D)}{dM_2} = 0. \tag{133}$$

Therefore, let us consider an extremal case, where the mass in the $x_4 < 0$ region is infinitely large so that all the wave functions are constrained to the $x_4 \geq 0$ region, which corresponds to the Shamir-type domain-wall fermion discussed in 2.3.3.

Such a situation is made by the limit of $M_1 + M_2 = \infty$, while $M_1 - M_2 = M$ is fixed. In this limit, the asymmetric domain-wall Dirac operator and the Pauli-Villars operator become

$$H_{\mathrm{ADW}} \to H_{\mathrm{SDW}} = \gamma_5(D - M), \tag{134}$$

$$H_{\mathrm{PV}} \to H_{\mathrm{SPV}} = \gamma_5(D + M). \tag{135}$$

The boundary condition is locally given by

$$\varphi_+|_{x_4=0} = 0, \quad (\partial_4 + M)\varphi_-|_{x_4=0} = 0. \tag{136}$$

In this case, only the eigenfunctions of type (i) and (ii) survive to form a complete set. The edge mode becomes

$$\varphi_-^{\mathrm{edge}}(x_4) = u_+\sqrt{2M}e^{-Mx_4} \tag{137}$$

where $\Lambda^2 = \boldsymbol{p}^2$. The bulk mode becomes

$$\varphi_-^{\omega}(x_4) = \frac{u_+}{\sqrt{2\pi(\omega^2+M^2)}}\left[(i\omega - M)e^{i\omega x_4} + (i\omega + M)e^{-i\omega x_4}\right], \tag{138}$$

and

$$\varphi_+^{\omega}(x_4) = \frac{u_-}{\sqrt{2\pi}}[e^{i\omega x_4} - e^{-i\omega x_4}], \tag{139}$$

where $\Lambda^2 = \boldsymbol{p}^2 + \omega^2 + M^2$. These wave functions are defined only in $x_4 \geq 0$ and zero in $x_4 < 0$.

After a perturbative calculation, the result are summarized as

$$\eta(H_{\mathrm{SDW}}) = -\frac{1}{32\pi^2}\int_{x_4>0} d^4x\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma} + \eta(iD^{\mathrm{3D}}), \tag{140}$$

$$\eta(H_{\mathrm{SPV}}) = \frac{1}{32\pi^2}\int_{x_4>0} d^4x\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}, \tag{141}$$

which confirms that Eq.(132) coincides with the APS index.

4 Index theorem from massive fermion

The original AS and APS indices require the exact chiral symmetry to define the chiral zero modes in the continuum theory. However, in the previous section, we gave up the bulk chiral symmetry and used the massive fermion to formulate the APS index theorem in the physically natural set-up using the domain-wall fermion. In this section, we introduce a unified perspective using massive fermions to fill the gap between the standard formulation and the new formulation, which gives a hint for the lattice formulation of the APS index.

The original AS index theorem in the continuum is formulated for the massless Dirac operator, and the analytical index is written by the chiral zero modes. The lattice AS index by Hasenfratz *et al.* is formulated by the Dirac operator satisfying the Ginsparg-Wilson relation, which realizes the lattice chiral symmetry. For the original APS index theorem, the bulk chiral symmetry induced by the APS boundary condition plays an important role.

However, how to formulate the lattice version of the APS index has not been known. In the lattice gauge theory, it is difficult to impose the APS boundary condition. The APS boundary condition is imposed by separating the normal and tangent parts of the Dirac operator to the boundary. For the overlap Dirac operator D_{ov}, there is no simple way to separate the boundary part of the operator. Moreover, even we managed to impose a physically sensible boundary condition, it would be incompatible with the Ginsparg-Wilson relation [45]. Therefore, we have to give up the lattice chiral symmetry in the formulation of the APS index. An important hint is found in the lattice AS index and the continuum APS index using the domain-wall fermion Dirac operator, which was discussed in the previous sections.

	continuum	lattice
AS	$\mathrm{Tr}\gamma_5 e^{(iD)^2/M^2}$	$\mathrm{Tr}\gamma_5(1-aD_{\mathrm{ov}}/2)$
APS	$\mathrm{Tr}\gamma_5 e^{(iD)^2/M^2}$ w/ APS b.c	not known.

Table 3: The standard formulation of the index with massless Dirac operator

	continuum	lattice
AS	$-\frac{1}{2}\eta(\gamma_5(D-M))^{\mathrm{reg.}}$	$-\frac{1}{2}\eta(\gamma_5(D_{\mathrm{W}}-M))$
APS	$-\frac{1}{2}\eta(\gamma_5(D-M\epsilon(x_4)))^{\mathrm{reg.}}$	$-\frac{1}{2}\eta(\gamma_5(D_{\mathrm{W}}-M\epsilon(x_4)))$

Table 4: The η-invariant of massive Dirac operator

First, let us go back to the AS index theorem on the four-dimensional periodic lattice. It is given by

$$\mathrm{index}_{\mathrm{AS}}(D_{\mathrm{ov}}) = \mathrm{Tr}\gamma_5\left(1-\frac{a}{2}D_{\mathrm{ov}}\right) = -\frac{1}{2}\mathrm{Tr}\gamma_5 a D_{\mathrm{ov}}, \tag{142}$$

where we use $\mathrm{Tr}\gamma_5 = 0$ which is justified by finite lattice, and D_{ov} is the overlap Dirac operator

$$D_{\mathrm{ov}} = \frac{1}{a}\left(1+X\frac{1}{\sqrt{X^\dagger X}}\right) = \frac{1}{a}\left(1+\gamma_5\frac{H_{\mathrm{W}}}{\sqrt{(H_{\mathrm{W}})^2}}\right), \tag{143}$$

where $H_{\mathrm{W}} = \gamma_5(D_{\mathrm{W}}-m)$ is a Hermitian Wilson-Dirac operator. When we substitute this formula to the index formula,

$$\begin{aligned}\mathrm{index}(D_{\mathrm{ov}}) &= -\frac{1}{2}\mathrm{Tr}\gamma_5 a D_{\mathrm{ov}} = -\frac{1}{2}\mathrm{Tr}\gamma_5\left(1+\gamma_5\frac{H_{\mathrm{W}}}{\sqrt{(H_{\mathrm{W}})^2}}\right)\\ &= -\frac{1}{2}\mathrm{Tr}\frac{H_{\mathrm{W}}}{\sqrt{(H_{\mathrm{W}})^2}} \equiv -\frac{1}{2}\eta(H_{\mathrm{W}}),\end{aligned} \tag{144}$$

we see that the index of the overlap Dirac operator is equivalent to the eta invariant of the massive Wilson-Dirac operator. It is interesting to note that the structure of the eta invariant is naturally embedded in the index theorem with the overlap Dirac operator. This fact suggests that the index may be defined by the massive fermion that has no chiral symmetry or Ginsparg-Wilson relations at all. In fact, this possibility was known in [37,46]. However, it has rarely been discussed that the eta invariant of the massive Dirac operator without chiral symmetry is as important as the original index.

As a byproduct of the reformulation of the APS index in continuum theory, it has been proposed that the AS index in the continuum can be formulated using the eta invariant of the massive Dirac operator. The nonperturbative or mathematical proof that the new definition of the AS index equals the original one is given in [22].

In Tab. 3 and 4, we summarize the massless and massive formulations of the indices. In the massless formulation, we need special care to maintain the chiral symmetry. For the APS index in continuum, we need a non-local boundary condition. For the lattice AS index, we need a special type of Dirac operator satisfying the Ginsparg-Wilson relation.

The eta invariant of the massive Dirac operator on a closed manifold gives a unified view of the index theorems. In the continuum, the APS index theorem is given by just adding a kink structure to the mass in the AS formula. For the lattice version of the AS index, we only need the Wilson-Dirac operator. Therefore it is natural to assume that the eta invariant of the Wilson Dirac operator with sign flipping mass, or namely, domain-wall fermion in four-dimension should be the lattice version of the APS index:

$$\mathrm{index}_{\mathrm{APS}}(D) = -\frac{1}{2}\eta(\gamma_5(D_{\mathrm{W}} - M\epsilon(x_4))). \tag{145}$$

In the next section, we will prove this perturbatively.

5 Atiyah-Patodi-Singer index theorem on a lattice

In this section, we propose a non-perturbative formulation of the Atiyah-Patodi-Singer index in four-dimensional lattice gauge theory [23, 24]. We will show that the eta invariant of the domain-wall fermion Dirac operator on a four-dimensional periodic lattice coincides with the APS index in the negative mass region. In the computation of the eta invariant, we can separate the bulk and edge contributions.

5.1 Main argument

Here, we assume a periodic boundary condition identifying $x_4 = L_4$ and $x_4 = -L_4$, setting L_4/a an integer. In this system, two domain walls are located at $x_4 = -a/2$ and $x_4 = L_4 - a/2$. Note that we put the kink structure on the link, not on the site [5]. We use the periodic boundary condition with the same periodicity L for the other three directions.

The domain-wall Dirac operator is given by

$$H_{\mathrm{DW}} = \gamma_5 \left[D_{\mathrm{W}} - M_1 \epsilon \left(x_4 + \frac{a}{2} \right) \epsilon \left(L_4 - \frac{a}{2} - x_4 \right) + M_2 \right]. \tag{146}$$

This four-dimensional operator should not be confused with the standard domain-wall fermion in five dimensions that is used for numerical simulation of QCD. We assume $M_1 > M_2 > 0$. Our goal is to show that the eta invariant of the domain-wall Dirac operator gives a non-perturbative formulation of the APS index theorem on a lattice. Namely, we will show

$$-\frac{1}{2}\eta(H_{\mathrm{DW}}) = \frac{1}{32\pi^2} \int_{0<x_4<L_4} d^4x \epsilon^{\mu\nu\rho\sigma} \mathrm{tr}_c F_{\mu\nu} F_{\rho\sigma} - \frac{1}{2}\eta(iD^{3\mathrm{D}})|_{x_4=0} + \frac{1}{2}\eta(iD^{3\mathrm{D}})|_{x_4=L_4} \tag{147}$$

in the continuum limit.

$\eta(H_{\mathrm{DW}})$ is guaranteed to be an integer by definition, since H_{DW} is a Hermitian operator on a finite-dimensional vector space. Moreover, its variation is always zero,

$$\begin{aligned} \delta\eta(H_{\mathrm{DW}}) &= \mathrm{Tr} \left[\delta H_{\mathrm{DW}} (H_{\mathrm{DW}})^{-\frac{1}{2}} - \frac{1}{2} H_{\mathrm{DW}} (H_{\mathrm{DW}})^{-\frac{3}{2}} (\delta H_{\mathrm{DW}} H_{\mathrm{DW}} + H_{\mathrm{DW}} \delta H_{\mathrm{DW}}) \right] \\ &= 0. \end{aligned} \tag{148}$$

under the condition that no eigenvalues of H_{DW} crosses zero.

[5] In the lattice gauge theory, we have two choices for the location of the kink mass: on the sites or between the sites. We find that putting the domain-wall between the sites (at the links) is convenient for solving the difference equation.

Then we take a hierarchical scaling limit $|\lambda_{\rm edge}| \ll M \ll 1/a$, where $\lambda_{\rm edge}$ denotes a typical eigenvalue of low-lying edge-localized modes. The bulk modes have large energy in this limit, and their correlations exponentially decay in every direction. Therefore, the density of the eta invariant near $x_4 = 0$ can be locally evaluated using a complete set of semi-infinite space-time in $x_4 \geq 0$, and simply interpolated to the result obtained near $x_4 = L_4$. We also treat the momenta in other directions as continuous for the same reason.

5.2 Free domain-wall fermion complete set

First let us consider the eigenproblem of $a^2 H_{\rm DW}^2$ for the free fermion, taking the $L_4 = \infty$ limit. The free domain-wall Dirac operator is given by

$$H_{\rm DW}^0 = \gamma_5 \left[D_{\rm W}^0 - M_1 \epsilon \left(x_4 + \frac{a}{2} \right) + M_2 \right], \tag{149}$$

where the free Wilson-Dirac operator $D_{\rm W}^0$ is written by

$$\begin{aligned} D_{\rm W}^0 &= \gamma^\mu \partial_\mu + R^0 \\ &= \frac{1}{2} \gamma^\mu \left[\nabla_\mu(\mathbf{1}) + \nabla_\mu^*(\mathbf{1}) \right] - \frac{a}{2} \sum\nolimits_\mu \nabla_\mu^*(\mathbf{1}) \nabla_\mu(\mathbf{1}). \end{aligned} \tag{150}$$

We can assume a tensor-product form of the solutions,

$$\phi(\boldsymbol{x}, x_4) = \varphi(x_4) \otimes \psi_{\boldsymbol{p}}^{\rm 3D}(\boldsymbol{x}), \tag{151}$$

where $\psi_{\boldsymbol{p}}^{\rm 3D}(\boldsymbol{x}) = e^{i\boldsymbol{p}\cdot\boldsymbol{x}}/\sqrt{(2\pi)^3}$ denotes the plane wave in the horizontal directions $(x_{i=1,2,3})$ with momentum $\boldsymbol{p} = (p_1, p_2, p_3)$, having two-spinor components, and $\varphi(x_4)$ that in the x_4 direction.

The squared free domain-wall Dirac operator is expressed by

$$\begin{aligned} (aH_{\rm DW}^0)^2 = &-(a\partial_i)^2 + \left[aR_i^0 - aM\epsilon \left(x_4 + \frac{a}{2} \right) + aM_2 \right]^2 \\ &- \left[1 + a \left(R_i^0 - M\epsilon \left(x_4 + \frac{a}{2} \right) + M_2 a \right) \right] a^2 \nabla_4^*(\mathbf{1}) \nabla_4(\mathbf{1}) \\ &+ 2M_1 a \left[P_+ \delta_{x_4,-a} S_4^+ - P_- \delta_{x_4,0} S_4^- \right], \end{aligned} \tag{152}$$

where $P_\pm$ is a projection operator defined as $P_\pm = (1 + \gamma_4)/2$, and $S_\mu^\pm$ is a shift operator by the unit lattice vector $a\hat{\mu}$: $S_\mu^\pm f(x) = f(x \pm a\hat{\mu})$. The shift operator comes from the violation of the Leibniz rule of the difference operators,

$$\nabla_\mu(\mathbf{1})(f(x)g(x)) = (\nabla_\mu(\mathbf{1})f(x)) S_\mu^+ g(x) + f(x)(\nabla_\mu(\mathbf{1})g(x)), \tag{153}$$

$$\nabla_\mu^*(\mathbf{1})(f(x)g(x)) = (\nabla_\mu^*(\mathbf{1})f(x)) S_\mu^- g(x) + f(x)(\nabla_\mu^*(\mathbf{1})g(x)). \tag{154}$$

We also use the following facts for the sign function $\epsilon(x + a/2)$,

$$a\nabla_4(\mathbf{1}) \epsilon \left(x_4 + \frac{a}{2} \right) = 2\delta_{x_4,-a}, \tag{155}$$

$$a\nabla_4^*(\mathbf{1}) \epsilon \left(x_4 + \frac{a}{2} \right) = 2\delta_{x_4,0}. \tag{156}$$

These terms correspond to the δ-function-like potentials in the classical continuum limit.

After applying the wave function in the $x_{i=1,2,3}$ directions , $(aH^0_{\rm DW})^2$ is expressed as

$$\begin{aligned}(aH^0_{\rm DW})^2 &= s_i^2+\theta(x_4+a/2)\{M_+^2-(1+M_+)(a^2\nabla_4^*(\mathbf{1})\nabla_4(\mathbf{1}))\}\\ &\quad+\theta(-x_4-a/2)\{M_-^2-(1+M_-)(a^2\nabla_4^*(\mathbf{1})\nabla_4(\mathbf{1}))\}\\ &\quad+2M_1a\left[P_+\delta_{x_4,-a}S_4^+-P_-\delta_{x_4,0}S_4^-\right], \qquad (157)\\ M_\pm &= \sum_{i=1,2,3}(1-c_i)\mp M_1a+M_2a, \qquad (158)\end{aligned}$$

where $\theta(x)=(\epsilon(x)+1)/2$ is the step function, and we denote $s_i=\sin(p_ia)$ and $c_i=\cos(p_ia)$.

Let us find the solution $\varphi(x_4)$ for the equation

$$(aH^0_{\rm DW})^2\varphi(x_4)\otimes\psi_p^{3D}(\boldsymbol{x})=\Lambda^2\varphi(x_4)\otimes\psi_p^{3D}(\boldsymbol{x}). \qquad (159)$$

We will have three types of eigenfunctions in the x_4 direction: (i) edge-localized modes at $x_4=0$, (ii)extended modes but only for $x_4\geq 0$, (iii) extended modes at any x_4.

To simplify the computation, we consider the $M_1+M_2\to\infty$ limit with $M_1-M_2=M$ fixed as in Sec:3.2. In this limit, the domain-wall Dirac operator becomes

$$\begin{aligned}H_{\rm DW} &= \gamma_5\left[D_{\rm W}-M_1\epsilon(x+a/2)+M_2\right],\\ &\to\gamma_5\left[D_{\rm W}-M\right]\equiv H_{\rm SDW}, \qquad (160)\end{aligned}$$

and $M_\pm$ become

$$M_+=\sum_{i=1,2,3}(1-c_i)-(M_1a-M_2a)\to\sum_{i=1,2,3}(1-c_i)-Ma \qquad (161)$$

$$M_-=\sum_{i=1,2,3}(1-c_i)+(M_1a+M_2a)\to\infty. \qquad (162)$$

The mass gap in the $x_4<0$ region M_- is infinitely large, and all wave functions are constrained to the $x_4\geq 0$ region. This is nothing but the Shamir-type domain-wall fermion discussed in 2.3.3. In the continuum theory, it is shown that the index with usual domain-wall set-up is equivalent to the index with Shamir-type domain-wall set-up [21].

Under this limit, we can safely neglect the type (iii) of the eigensolutions. Only the eigenmodes of types (i) and (ii) survive, forming a complete set. They coincide with those for the Shamir domain-wall fermion on which the simple Dirichlet boundary condition $\phi(x_4)=0$ for $x_4<0$ is imposed. We have

(i) edge localized mode

$$\begin{aligned}\phi_-^{\rm edge}(x_4) &= \sqrt{-M_+(2+M_+)/a}\,e^{-Kx_4}, \qquad (163)\\ e^{-Ka} &= 1+M_+. \qquad (164)\end{aligned}$$

(ii) bulk modes

$$\phi_+^\omega(x_4) = \frac{1}{\sqrt{2\pi}}\left[e^{i\omega(x_4+a)} - e^{-i\omega(x_4+a)}\right], \tag{165}$$

$$\phi_-^\omega(x_4) = \frac{1}{\sqrt{2\pi}}\left[C_\omega e^{i\omega x_4} - C_\omega^* e^{-i\omega x_4}\right], \tag{166}$$

$$C_\omega = \frac{(1+M_+)e^{i\omega a}-1}{|(1+M_+)e^{i\omega a}-1|}. \tag{167}$$

in the region $x_4 \leq 0$, where the subscript $\pm$ denotes the eigenvalue of $\gamma_4 = \pm$. For the normalizability of the edge localized mode, we obtain the condition: $|1+M_+| < 1$. Here we choose the fermion mass in the range $0 < Ma < 2$. This choice is consistent with the normalizability condition and eliminates the contribution from the doubler modes, which have $|\boldsymbol{p}| \sim \pi/a$. The edge mode can only exist $\gamma_4 = -1$ sector.

The eigenvalue of $(aH^0_{\mathrm{SDW}})^2$ is

$$\Lambda^2 = \begin{cases} s_i^2 & \text{(edge)}, \\ (s_i^2 + M_+^2 - 2(1+M_+)(\cos\omega a - 1)) & \text{(bulk)}. \end{cases} \tag{168}$$

With these eigenfunctions, we can separately evaluate the contributions from the bulk and edge modes.

We can confirm that the above eigenfunctions form a complete set. The eigenmode set satisfies the orthonormal condition,

$$a\sum_{x_4=0}^{\infty}\left[\phi_-^{\mathrm{edge}}(x_4)\right]^\dagger \phi_-^{\mathrm{edge}}(x_4) = 1, \tag{169}$$

$$a\sum_{x_4=0}^{\infty}\left[\phi_\pm^{\omega'}(x_4)\right]^\dagger \phi_\pm^{\omega}(x_4) = \delta(\omega-\omega'), \tag{170}$$

where the summation over x_4 is taken for integer multiples of a. The orthonormality of the bulk modes can be shown using the relations[6]

$$a\sum_{x=0}^{\infty} e^{i\omega x} = \pi\delta(\omega) + a\mathcal{P}\left(\frac{1}{1-e^{i\omega a}}\right), \tag{171}$$

where $\mathcal{P}$ denotes the principal value. The eigenfunction set satisfies the completeness

$$\sum_{g=\pm}\int_0^{\pi/a} d\omega u_g \phi_g^\omega(x_4)\phi_g^\omega(x_4')^\dagger u_g^\dagger + u_-\phi_-^{\mathrm{edge}}(x_4)\phi_-^{\mathrm{edge}}(x_4')^\dagger u_-^\dagger = \frac{1}{a}\delta_{x_4,x_4'} I_{2\times 2}, \tag{172}$$

where $u_\pm$ and $I_{2\times2}$ are the eigenvectors and the 2×2 identity matrix in the eigenvector space of γ_4, respectively.

[6]This relation is a discretized version of the relation

$$\int_0^\infty dx e^{i\omega x} = \pi\delta(\omega) + i\mathcal{P}\frac{1}{\omega},$$

and (171) can be easily shown using Sato's hyperfunction formula of the delta function

$$2\pi\delta(\omega) = \lim_{\epsilon\to 0}\left[\frac{i}{\omega+i\epsilon} - \frac{i}{\omega - i\epsilon}\right].$$

5.3 Evaluation of eta invariant of the domain-wall operator

In this subsection, we perturbatively evaluate the eta invariant of the domain-wall Dirac operator and show that it agrees with the APS index in the classical continuum limit. Since the complete set derived in the previous section can be separated into bulk and edge parts, we can completely decompose the eta invariant into bulk and edge contributions.

$$
\begin{aligned}
\eta(H_{\mathrm{SDW}}) &= \sum_{\boldsymbol{x},x_4\geq 0} \mathrm{tr}\frac{H_{\mathrm{SDW}}}{\sqrt{H_{\mathrm{SDW}}^2}}(x)\delta_{x,x'}|_{x=x'} \\
&= a^4 \sum_{\boldsymbol{x},x_4\geq 0}\sum_{s=\uparrow,\downarrow}\sum_{g=\pm}\int_0^{\pi/a} d\omega \int_{-\pi/a}^{\pi/a} d^3p \\
&\quad\times \mathrm{tr}\left[\frac{H_{\mathrm{SDW}}}{\sqrt{H_{\mathrm{SDW}}^2}}(u_g\otimes v_s)\left[\phi_g^{\omega}(x_4)\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x})\right]\left[\phi_g^{\omega}(x_4')\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x}')\right]^{\dagger}(u_g\otimes v_s)^{\dagger}\right]_{x=x'} \\
&\quad + a^4 \sum_{\boldsymbol{x},x_4\geq 0}\sum_{s=\uparrow,\downarrow}\int_{-\pi/a}^{\pi/a} d^3p \\
&\quad\times \mathrm{tr}\left[\frac{H_{\mathrm{SDW}}}{\sqrt{H_{\mathrm{SDW}}^2}}(u_-\otimes v_s)\left[\phi_-^{\mathrm{edge}}\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x})\right]\left[\phi_-^{\mathrm{edge}}(x_4')\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x}')\right]^{\dagger}(u_-\otimes v_s)^{\dagger}\right]_{x=x'} \\
&= a^4 \sum_{\boldsymbol{x},x_4\geq 0}\mathrm{tr}\frac{H_{\mathrm{SDW}}}{\sqrt{H_{\mathrm{SDW}}^2}}(x)^{\mathrm{bulk}} + a^4 \sum_{\boldsymbol{x},x_4\geq 0}\mathrm{tr}\frac{H_{\mathrm{SDW}}}{\sqrt{H_{\mathrm{SDW}}^2}}(x)^{\mathrm{edge}}, \qquad (173)
\end{aligned}
$$

where we insert the completeness condition,

$$
\begin{aligned}
&\sum_{s=\uparrow,\downarrow}\sum_{g=\pm}\int_0^{\pi/a} d\omega \int_{-\pi/a}^{\pi/a} d^3p\,(u_g\otimes v_s)\left[\phi_g^{\omega}(x_4)\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x})\right]\left[\phi_g^{\omega}(x_4')\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x}')\right]^{\dagger}(u_g\otimes v_s)^{\dagger} \\
&+ \sum_{s=\uparrow,\downarrow}\int_{-\pi/a}^{\pi/a} d^3p\,(u_-\otimes v_s)\left[\phi_-^{\mathrm{edge}}\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x})\right]\left[\phi_-^{\mathrm{edge}}(x_4')\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x}')\right]^{\dagger}(u_-\otimes v_s)^{\dagger} \\
&\quad = \frac{1}{a^4}\delta_{x_4,x_4'}\delta_{\boldsymbol{x},\boldsymbol{x}'}I_{4\times 4}, \qquad (174)
\end{aligned}
$$

where $I_{4\times 4}$ is the 4×4 identity matrix in the spinor space. In the rest of this subsection, we evaluate each contribution. The bulk part is evaluated by expanding it in a lattice spacing a, in a similar way on a periodic lattice studied in [36]. On the other hand, the edge part is evaluated by an adiabatic approximation.

5.3.1 Bulk part contribution

For the bulk contribution, we consider the density of the eta invariant rather than its integral form. Since every bulk mode has a larger energy than M_+^2, the density is expressed as a local function. The analysis is similar to that of the AS index theorem for the periodic lattice studied in [36]. First we rewrite the density of the eta invariant as

$$
\begin{aligned}
& -\frac{1}{2}\mathrm{tr}\frac{H_{\mathrm{SDW}}}{\sqrt{H_{\mathrm{SDW}}^2}}(x)^{\mathrm{bulk}} \\
&= -\frac{1}{2}\sum_{s=\uparrow,\downarrow}\sum_{g=\pm}\int_0^{\pi/a} d\omega \int_{-\pi/a}^{\pi/a} d^3p \\
&\quad \left[\phi_g^{\omega}(x_4)\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x})\right]^{\dagger}(u_g\otimes v_s)^{\dagger}\,\mathrm{tr}_c\frac{H_{\mathrm{SDW}}}{\sqrt{H_{\mathrm{SDW}}^2}}(u_g\otimes v_s)\left[\phi_g^{\omega}(x_4)\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x})\right] \\
&= -\frac{1}{2}\sum_{g=\pm}\int_0^{\pi/a} d\omega \int_{-\pi/a}^{\pi/a} d^3p\left[\phi_g^{\omega}(x_4)\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x})\right]^{\dagger}\mathrm{tr}\left[P_g\frac{H_{\mathrm{SDW}}}{\sqrt{H_{\mathrm{SDW}}^2}}P_g\right]\left[\phi_g^{\omega}(x_4)\psi_{\boldsymbol{p}}^{\mathrm{3D}}(\boldsymbol{x})\right] \quad (175)
\end{aligned}
$$

using the spinor properties [7]. Here, the trace tr is taken over color and spinor indices and tr_c is taken over color index only.

Substituting the explicit forms of the domain-wall fermion complete set, the density of the eta invariant becomes

$$
\begin{aligned}
& -\frac{1}{2}\int_0^{\pi/a} d\omega \int_{-\pi/a}^{\pi/a} d^3p\left[\phi_+^{\omega}(x_4)\psi_p^{\mathrm{3D}}(x)\right]^{\dagger}\mathrm{tr}\left[P_+\frac{aH_{\mathrm{SDW}}}{\sqrt{(aH_{\mathrm{SDW}})^2}}P_+\right]\left[\phi_+^{\omega}(x_4)\psi_p^{\mathrm{3D}}(x)\right] \\
&= -\frac{1}{2}\int_{-\pi/a}^{\pi/a}\frac{d^3p\,d\omega}{(2\pi)^4}[1-e^{2i\omega(x_4+a)}]\mathrm{tr}\left[P_+\frac{a\tilde{H}_{\mathrm{SDW}}}{\sqrt{(a\tilde{H}_{\mathrm{SDW}})^2}}P_+\right], \quad (176)
\end{aligned}
$$

and the $\gamma_4 = -1$ sector

$$
\begin{aligned}
& -\frac{1}{2}\int_0^{\pi/a} d\omega \int_{-\pi/a}^{\pi/a} d^3p\left[\phi_-^{\omega}(x_4)\psi_p^{\mathrm{3D}}(x)\right]^{\dagger}\mathrm{tr}\left[P_-\frac{aH_{\mathrm{SDW}}}{\sqrt{(aH_{\mathrm{SDW}})^2}}P_-\right]\left[\phi_-^{\omega}(x_4)\psi_p^{\mathrm{3D}}(x)\right] \\
&= -\frac{1}{2}\int_{-\pi/a}^{\pi/a}\frac{d^3p\,d\omega}{(2\pi)^4}[1-C_\omega^2 e^{2i\omega x_4}]\mathrm{tr}\left[P_-\frac{a\tilde{H}_{\mathrm{SDW}}}{\sqrt{(a\tilde{H}_{\mathrm{SDW}})^2}}P_-\right]. \quad (177)
\end{aligned}
$$

The dependence on the gauge link variables is perturbatively treated as

$$
(a\tilde{H}_{\mathrm{SDW}})^2 = (a\tilde{H}^0_{\mathrm{SDW}})^2 + \Delta(aH_{\mathrm{SDW}})^2 \quad (178)
$$

[7] Spinor property

$$
\begin{aligned}
& \sum_{g=\pm}\sum_{s=\uparrow,\downarrow}(u_g\otimes v_s)^{\dagger}\,\Gamma\,(u_g\otimes v_s) = \sum_{s=\uparrow,\downarrow}\begin{pmatrix} v_s^{\dagger} & 0\end{pmatrix}\Gamma\begin{pmatrix} v_s \\ 0\end{pmatrix} + \sum_{s=\uparrow,\downarrow}\begin{pmatrix} 0 & v_s^{\dagger}\end{pmatrix}\Gamma\begin{pmatrix} 0 \\ v_s\end{pmatrix} \\
&= \sum_{s=\uparrow,\downarrow}\begin{pmatrix} v_s^{\dagger} & 0\end{pmatrix}P_+\Gamma P_+\begin{pmatrix} v_s \\ 0\end{pmatrix} + \sum_{s=\uparrow,\downarrow}\begin{pmatrix} 0 & v_s^{\dagger}\end{pmatrix}P_+\Gamma P_+\begin{pmatrix} 0 \\ v_s\end{pmatrix} \\
&\quad + \sum_{s=\uparrow,\downarrow}\begin{pmatrix} v_s^{\dagger} & 0\end{pmatrix}P_-\Gamma P_-\begin{pmatrix} v_s \\ 0\end{pmatrix} + \sum_{s=\uparrow,\downarrow}\begin{pmatrix} 0 & v_s^{\dagger}\end{pmatrix}P_-\Gamma P_-\begin{pmatrix} 0 \\ v_s\end{pmatrix} \\
&= \mathrm{tr}_s\left[P_+\Gamma P_+\right] + \mathrm{tr}_s\left[P_-\Gamma P_-\right],
\end{aligned}
$$

where Γ has arbitrary spinor structure and tr_s is taken over spinor index.

$$\Delta(aH_{\mathrm{SDW}})^2 = -\frac{a^2}{2}\sum_{\mu,\nu}\gamma^\mu\gamma^\nu\left[\tilde{D}_\mu,\tilde{D}_\nu\right] - a^2\gamma^\mu\left[\tilde{D}_\mu,\tilde{R}\right] + \cdots, \tag{179}$$

where $\cdots$ part includes no γ^μ's, which do not contribute to the index. We can express

$$\tilde{D}_\mu = \frac{1}{2a}\left[e^{ip_\mu a}\left(U_\mu(x)S_\mu^+ - 1\right) - e^{-ip_\mu a}\left(S_\mu^- U_\mu^\dagger(x) - 1\right)\right], \tag{180}$$

$$\tilde{R} = -\frac{1}{2a}\sum_{\mu=1}^{4}\left[e^{ip_\mu a}\left(U_\mu(x)S_\mu^+ - 1\right) + e^{-ip_\mu a}\left(S_\mu^- U_\mu^\dagger(x) - 1\right)\right]. \tag{181}$$

We denote the four-momentum by $p_\mu = (p_1, p_2, p_3, \omega)$. Inside the bulk, $(a\tilde{H}^0_{\mathrm{SDW}})^2$ can be expressed as

$$\begin{aligned}(a\tilde{H}^0_{\mathrm{SDW}})^2 &= s_\mu^2 + \left\{Ma - \sum\nolimits_\mu(1-c_\mu)\right\}^2 \\ &= s_i^2 + M_+^2 - 2(1+M_+)(c_4 - 1) = \Lambda^2,\end{aligned} \tag{182}$$

then we can expand $1/\sqrt{(aH_{\mathrm{SDW}})^2}$ as if the operators were all commuting [8]. Noting the existence of γ_4 in the projection operator $P_\pm$, and that of γ_5 and γ^μ in the numerator, those terms having three of four gamma matrices can survive the spinor trace (230). After some lengthy but straightforward computations we find that only the first two terms in the following expression are relevant [9].

$$\begin{aligned}&\mathrm{tr}\left[P_\pm\frac{a\tilde{H}_{\mathrm{SDW}}}{\sqrt{(a\tilde{H}_{\mathrm{SDW}})^2}}P_\pm\right] \\ &= \frac{3a^4}{8}\sum_{\mu,\nu,\rho,\sigma}\mathrm{tr}\left[\gamma_5 M'_+\frac{\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma}{4}\left[\tilde{D}_\mu,\tilde{D}_\nu\right]\left[\tilde{D}_\rho,\tilde{D}_\sigma\right](x)\right](\Lambda^2)^{-5/2} \\ &\quad+\frac{3a^4}{8}\sum_{\mu,\nu,\rho,\sigma}\mathrm{tr}\left[\gamma_5 i\gamma^\sigma s_\sigma(\gamma^\mu\gamma^\nu\gamma^\rho + \gamma^\rho\gamma^\mu\gamma^\nu)\left[\tilde{D}_\mu,\tilde{D}_\nu\right]\left[\tilde{D}_\rho,\tilde{R}\right](x)\right](\Lambda^2)^{-5/2} \\ &\quad+\cdots,\end{aligned} \tag{183}$$

where $M'_+ = M_+ + (1 - c_4)$.

Substituting the explicit forms of the domain-wall fermion complete set, and using the standard expansion $U_\mu(x) = \exp(iaA_\mu(x))$,

$$\left[\tilde{D}_\mu,\tilde{D}_\nu\right] = ic_\mu c_\nu F_{\mu\nu} + \mathcal{O}(a), \tag{184}$$

$$\left[\tilde{D}_\mu,\tilde{R}\right] = c_\mu\sum_\nu s_\nu F_{\mu\nu} + \mathcal{O}(a), \tag{185}$$

[8] Note that near the boundary $(a\tilde{H}^0_{\mathrm{SDW}})^2$ and $\Delta(a\tilde{H}_{\mathrm{SDW}})^2$ do not commute essentially due to the boundary effect. However, their commutator increases the order of a (by the derivatives), then the expansion is also valid near the boundary.

[9] We can easily show that the first and second terms in the expansion vanish, due to the spinor trace, odd function in the integral, and the Bianchi identity $\mathrm{tr}_c\epsilon^{\mu\nu\rho}\left[\tilde{D}_\mu[\tilde{D}_\nu,\tilde{D}_\rho]\right] = 0$

where we use the abbreviations $s_\mu = \sin(p_\mu a)$ and $c_\mu = \cos(p_\mu a)$, we obtain

$$-\frac{1}{2}\mathrm{tr}\frac{H_{\rm DW}}{\sqrt{H_{\rm DW}^2}}(x)^{\rm bulk} = \left(I(M) + I^{\rm DW}(M,x_4)\right)\frac{1}{32\pi^2}\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}, \tag{186}$$

up to $\mathcal{O}(a)$ corrections. The factors $I(M)$ and $I^{\rm DW}(M,x_4)$ are

$$I(M) = \frac{3a^4}{8\pi^2}\int_{-\pi/a}^{\pi/a} d\omega d^3p \prod_\mu c_\mu \frac{-M'_+ + \sum_\nu s_\nu^2/c_\nu}{\Lambda^{5/2}}, \tag{187}$$

and

$$I^{\rm DW}(M,x_4) = \frac{3a^4}{8\pi^2}\int_{-\pi/a}^{\pi/a} d\omega d^3p \prod_\mu c_\mu \frac{-M'_+ + \sum_\nu s_\nu^2/c_\nu}{\Lambda^{5/2}}\left(-\frac{C_\omega^2 + e^{2i\omega a}}{2}e^{2i\omega x_4}\right). \tag{188}$$

· Contribution from $I(M)$

The factor $I(M)$ is explicitly evaluated in [36] (see Appendix. C), and we have

$$I(M) = \theta(Ma) - 4\theta(Ma-2) + 6\theta(Ma-4) - 4\theta(Ma-6) + \theta(Ma-8). \tag{189}$$

For our choice of the fermion mass $0 < Ma < 2$, we obtain $I(M) = 1$ in the continuum limit.

· Contribution from $I^{DW}(M,x_4)$

First we note the phase factor $e^{2i\omega x_4}$ (188), to which the singularity due to doublers gives a contribution suppressed as $e^{-x_4/a}$. Therefore, we can take a naive continuum limit only taking the physical poles into account, approximating $s_\mu \sim p_\mu a$ and $c_\mu \sim 1$. In this limit, $I^{DW}(M,x_4)$ becomes

$$\begin{aligned} I^{\rm DW}(M,x_4) &= 3M\int_0^\infty dpp^2\int_{-\infty}^\infty \frac{d\omega}{2\pi}\frac{1}{(p^2+M^2+\omega^2)^{5/2}}\left[\frac{iM}{\omega - iM}e^{2i\omega x_4}\right] \\ &= 2M\int_0^\infty dt\sqrt{t}\frac{\partial^2}{\partial t^2}J(t,M,x_4), \end{aligned} \tag{190}$$

where we define

$$J(t,M,x_4) = \int_{-\infty}^\infty \frac{d\omega}{2\pi}\frac{1}{(t+M^2+\omega^2)^{1/2}}\left[\frac{iM}{\omega-iM}e^{2i\omega x_4}\right]. \tag{191}$$

We can formally integrate $J(t,M,x_4)$, which consists of two terms:

$$\begin{aligned} J(t,M,x_4) &= J_1(t,M,x_4) + J_2(t,M,x_4), \\ J_1(t,M,x_4) &= -\frac{2M}{\pi}e^{-2Mx_4}\left[\frac{1}{2\sqrt{t}}\arccos\left(\frac{M}{\sqrt{M^2+t}}\right)\right], \end{aligned} \tag{192}$$

$$J_2(t,M,x_4) = -\frac{2M}{\pi}e^{-2Mx_4}\left[\int_0^{x_4} dx'_4 e^{2Mx'_4}K_0\left(2\sqrt{M^2+t}x'_4\right)\right], \tag{193}$$

where $K_\nu(x)$ denotes the modified Bessel function of the second kind. For $J_1(t, M, x_4)$, it is not difficult to compute

$$2M \int_0^\infty dt\sqrt{t}\frac{\partial^2}{\partial t^2} J_1(t, M, x_4) = -\frac{1}{4}e^{-2Mx_4}. \tag{194}$$

For $J_2(t, M, x_4)$, we take a partial integration

$$\begin{aligned} 2M \int_0^\infty & dt\sqrt{t}\frac{\partial^2}{\partial t^2} J_2(t, M, x_4) \\ &= -\frac{4M^2}{\pi}\left[\sqrt{t}\frac{\partial}{\partial t}\left\{e^{-2Mx_4}\int_0^{x_4} dx_4' e^{2Mx_4'} K_0\left(2\sqrt{M^2+t}x_4'\right)\right\}\right]_0^\infty \\ &\quad - M\int_0^\infty dt \frac{1}{\sqrt{t}}\frac{\partial}{\partial t} J_2(t, M, x_4). \end{aligned} \tag{195}$$

The first term is zero since $\sqrt{t}$ goes to zero faster than the t derivative of $K_0\left(2\sqrt{M^2+t}x_4'\right)$ and $K_0\left(2\sqrt{M^2+t}x_4'\right)$ is exponentially small at $t=\infty$. We can also evaluate the second term as

$$-M\int_0^\infty dt\frac{1}{\sqrt{t}}\frac{\partial}{\partial t}J_2(t, M, x_4) = -\frac{2M^2 e^{-2Mx_4}}{\pi}\left[\int_0^{x_4} dx_4' x_4' e^{2Mx_4'}\int_0^\infty dt \frac{K_1\left(2\sqrt{M^2+t}x_4'\right)}{\sqrt{t}\sqrt{M^2+t}}\right]. \tag{196}$$

Combining these results, we obtain

$$I^{\mathrm{DW}}(M, x_4) = -e^{-2Mx_4}\left[\frac{1}{4} + \frac{2M^2}{\pi}\int_0^{x_4} dx_4' x_4' e^{2Mx_4'}\int_0^\infty dt\frac{K_1\left(2\sqrt{M^2+t}x_4'\right)}{\sqrt{t}\sqrt{M^2+t}}\right]. \tag{197}$$

Noting the fact that $I^{\mathrm{DW}}(M, x_4)$ is negative at any x_4, we have an inequality

$$\left|\int d^4x I^{\mathrm{DW}}(M, x_4)\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}(x)\right| < \left|\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}\right|^{\max}(\boldsymbol{x})\int_0^\infty dx_4\left|I^{\mathrm{DW}}(M, x_4)\right|, \tag{198}$$

where $|O|^{\max}(\boldsymbol{x})$ is the absolute maximum of the function $O(x)$ along the string at $\boldsymbol{x} = (x_1, x_2, x_3)$ extending in the x_4 direction. The x_4 integral is analytically computable as follows:

$$\begin{aligned} \int_0^\infty dx_4\left|I^{\mathrm{DW}}(M, x_4)\right| &= \frac{1}{8M} + \frac{M}{\pi}\int_0^\infty dx_4' x_4' \int_0^\infty dt\frac{K_1(2\sqrt{M^2+t}x_4')}{\sqrt{t}\sqrt{M^2+t}} \\ &= \frac{1}{8M} + \frac{M}{\pi}\int_0^\infty dt \frac{1}{\sqrt{t}\sqrt{M^2+t}}\frac{\pi}{8(M^2+t)} \\ &= \frac{3}{8M}. \end{aligned} \tag{199}$$

We have performed the integration in the order of x_4, x_4', and t, and have used the following relations

$$\int_0^\infty dx x^{\mu-1} K_\nu(ax) = 2^{\mu-2} a^{-\mu} \Gamma\left(\frac{\mu-\nu}{2}\right)\Gamma\left(\frac{\mu+\nu}{2}\right) \quad (\mathrm{Re}\mu > |\mathrm{Re}\nu|, a > 0)\,, \tag{200}$$

$$\int_0^\infty dx \frac{x^{\alpha-1}}{(ax+b)^{\alpha+1}} = \frac{1}{\alpha a^\alpha b} \quad (\alpha, a, b > 0). \tag{201}$$

Therefore, we can conclude that $I(M) + I^{\mathrm{DW}}(M, x_4) = 1 + \mathcal{O}(1/M)$ and the bulk contribution is the standard curvature term:

$$-\frac{1}{2}\mathrm{tr}\frac{H_{\mathrm{SDW}}}{\sqrt{H_{\mathrm{SDW}}^2}}(x)^{\mathrm{bulk}} = \frac{1}{32\pi^2}\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}(x) + \mathcal{O}(a, 1/M). \tag{202}$$

5.3.2 Edge part contribution

Next, let us evaluate the contribution from the edge-localized mode. To this end, we reconsider the eigenproblem for the edge modes with nontrivial gauge link variables, assuming its mild x_4 dependence compared to $1/M$. Namely, we assume that the x_4 dependence of the gauge field is less steep than that of the edge wave function. This assumption is always valid since no matter how violent the change in the gauge field is, it can be realized by decreasing the lattice spacing (keeping Ma fixed).

$$H_{\mathrm{DW}}\phi(x) = \Lambda\phi(x). \tag{203}$$

More explicitly, we have, in the $U_4 = \mathbf{1}$ gauge,

$$\begin{aligned} H_{\mathrm{DW}} &= \gamma_5\left[\gamma^i D_i(x_4) + \gamma^4\partial_4 + R(x) - M\right] \\ &= \gamma_5\left[-P_4\nabla_4(\mathbf{1}) + P_4\nabla_4^*(\mathbf{1}) + \gamma^i D_i(x_4) + M_+(x)/a\right], \end{aligned} \tag{204}$$

where $D_i(x_4)$ is the symmetrized spatial covariant difference operator at a slice x_4,

$$D_i(x_4) = \frac{1}{2}\left[\nabla_i(U) + \nabla_i^*(U)\right], \tag{205}$$

and $M_+(x_4)/a$ is

$$M_+(x)/a = -\frac{1}{2a}\sum_{i=1,2,3}\left[(U_i(x)S_i^+ - 1) + (S_i^- U_i^\dagger(x) - 1)\right] - M. \tag{206}$$

Note that $D_i(x_4)$ depends on x_4 through the link variables. $M_+(x)$ is also x_μ dependent through the link variables. In the following, we assume that the eigenvalue Λ is low compared to M and the mass of the doublers modes, where we can approximate $M_+(x)/a = -M + \mathcal{O}(a)$ and ignore the position dependence. Under this assumption, the domain-wall Dirac operator is written by

$$H_{\mathrm{DW}} = \gamma_5[-P_-\nabla_4(\mathbf{1}) + P_+\nabla_4^*(\mathbf{1}) + \gamma^i D_i(x_4) - M + \mathcal{O}(a)]. \tag{207}$$

Since three-dimensional Dirac operator $D_i(x_4)$ has still x_4-dependence, the eigenvalues $\lambda(x_4)$ of $\gamma^i D_i(x_4)$ depend also on x_4.

At the leading order of the adiabatic approximation, where x_4-dependence is mild, we have a solution of the form

$$\phi(x) = \phi^{\mathrm{3D}}_{\lambda(0)}(\boldsymbol{x}) \otimes \phi^{\mathrm{edge}}(x_4), \tag{208}$$

where $\phi^{\mathrm{3D}}_{\lambda(0)}(\boldsymbol{x})$ is an eigenstate of $i\sigma^i D_i(x_4 = 0)$ with eigenvalue $\lambda(0)$. Recalling the complete set of the free domain-wall Dirac operator square, the edge localized mode only appears in the $\gamma_4 = -1$ sector: $\phi^{\mathrm{edge}}(x_4) = P_-\phi^{\mathrm{edge}}_-(x_4)$. Then the edge mode satisfies

$$(-P_-\nabla_4(\mathbf{1}) + P_+\nabla^*_4(\mathbf{1}))P_-\phi^{\mathrm{edge}}_-(x_4) = (M + \mathcal{O}(a))P_-\phi^{\mathrm{edge}}_-(x_4). \tag{209}$$

$\phi^{\mathrm{edge}}_-(x_4)$ has the form

$$\phi^{\mathrm{edge}}_-(x_4) = \sqrt{M(2 - Ma)}e^{-Kx_4}, \tag{210}$$

where $e^{-Ka} = (1 - Ma)$[10].

Employing the Dirac representation (228), for the edge modes, the domain-wall Dirac operator acts as

$$\begin{aligned}
&H_{\mathrm{DW}}\phi^{\mathrm{3D}}_{\lambda(0)}(\boldsymbol{x}) \otimes \phi^{\mathrm{edge}}_-(x_4)\\
&\quad= (\gamma_5\gamma^i P_-)D_i(x_4)\phi^{\mathrm{3D}}_{\lambda(0)}(\boldsymbol{x}) \otimes \phi^{\mathrm{edge}}_-(x_4)\\
&\quad= \begin{pmatrix} 0 & i\mathbf{1}_{2\times 2} \\ -i\mathbf{1}_{2\times 2} & 0 \end{pmatrix}\begin{pmatrix} 0 & \sigma_i D_i(x_4) \\ \sigma_i D_i(x_4) & 0 \end{pmatrix}\begin{pmatrix} 0 & 0 \\ 0 & \mathbf{1}_{2\times 2} \end{pmatrix}\phi^{\mathrm{3D}}_{\lambda(0)}(\boldsymbol{x}) \otimes \phi^{\mathrm{edge}}_-(x_4)\\
&\quad= \begin{pmatrix} 0 & 0 \\ 0 & iD^{\mathrm{3D}} \end{pmatrix}\phi^{\mathrm{3D}}_{\lambda(0)}(\boldsymbol{x}) \otimes \phi^{\mathrm{edge}}_-(x_4),
\end{aligned} \tag{211}$$

where $iD^{\mathrm{3D}} = -i\sigma_i D_i(x_4)$. Therefore, the eigenvalue Λ essentially equals to $\lambda(0)$.

In this evaluation, we use different eigenfunction set in the evaluations of the bulk and edge modes. Therefore, the orthogonality is generally lost. Since $K = M + \mathcal{O}(a)$, the orthogonality with the bulk modes which was given in terms of the free domain-wall fermion is guaranteed in the continuum limit.

Let us consider the free bulk fermion mode $\phi^{\omega}_-(x_4)$ and the edge mode $\phi^{\mathrm{edge}}_-(x_4)$. Since the nontrivial link-variable-dependent part is neglected, the edge mode wave function is slightly

---

[10]

$$\begin{aligned}
&(-P_-\nabla_4(\mathbf{1}) + P_+\nabla^*_4(\mathbf{1}))P_-\phi^{\mathrm{edge}}_-(x_4) = (M + \mathcal{O}(a))P_-\phi^{\mathrm{edge}}_-(x_4)\\
&\Leftrightarrow -\nabla_4(\mathbf{1})\phi^{\mathrm{edge}}_-(x_4) = (M + \mathcal{O}(a))\phi^{\mathrm{edge}}_-(x_4)
\end{aligned}$$

Suppose $\phi^{\mathrm{edge}}_-(x_4) = Ae^{-Kx_4}$, then

$$\begin{aligned}
&-\frac{1}{a}[Ae^{-K(x_4+a)} - Ae^{-Kx_4}] = [M + \mathcal{O}(a)]Ae^{-Kx_4}\\
&\Leftrightarrow -[e^{-Ka} - 1] = Ma + \mathcal{O}(a^2)\\
&\Leftrightarrow e^{-Ka} = (1 - Ma)
\end{aligned}$$

From the normalization condition, A is written as $A = \sqrt{M(2 - Ma)}$.

different from the free case. The inner product is evaluated as

$$
\begin{aligned}
&a\sum_{x_4=0}^{\infty}\left(\phi_-^{\text{edge}}(x_4)\right)^\dagger\phi_-^{\omega}(x_4)\\
&\quad=a\sqrt{\frac{M(1-Ma)}{2\pi}}\sum_{x_4=0}^{\infty}\left[C_\omega e^{-(K-i\omega)x_4}-C_\omega^* e^{-(K+i\omega)x_4}\right]\\
&\quad=a\sqrt{\frac{M(1-Ma)}{2\pi}}\left[C_\omega\frac{1}{1-(1-Ma)e^{i\omega a}}-C_\omega^*\frac{1}{1-(1-Ma)e^{-i\omega a}}\right].
\end{aligned}
\tag{212}
$$

Note that C_ω is proportional to $(1+M_+)e^{i\omega}-1$ and $1+M_+=1-Ma+\Delta a^2$, where Δ expresses the contribution from the Wilson term near the physical pole. Then

$$
\begin{aligned}
&=a\sqrt{\frac{M(1-Ma)}{2\pi}}\frac{1}{|(1+M_+)e^{i\omega}-1|}\left[\frac{(1-Ma+\Delta a^2)e^{i\omega a}-1}{1-(1-Ma)e^{i\omega a}}-\frac{(1-Ma+\Delta a^2)e^{-\omega a}-1}{1-(1-Ma)e^{-i\omega a}}\right]\\
&=a\sqrt{\frac{M(1-Ma)}{2\pi}}\frac{1}{|(1+M_+)e^{i\omega}-1|}\left[\frac{\Delta a^2 e^{i\omega a}}{1-(1-Ma)e^{i\omega a}}-\frac{\Delta a^2 e^{-\omega a}}{1-(1-Ma)e^{-i\omega a}}\right]
\end{aligned}
\tag{213}
$$

which vanishes in the $a\to 0$ limit.

In fact, the leading-order solution is enough to evaluate the edge mode part, as the exponential dumping of the eigenfunctions allows us to expand the operator in x_4, and its dependence is suppressed as

$$
\sum_{x_4}\left(\phi_-^{\text{edge}}(x_4)\right)^\dagger x_4^n\phi_-^{\text{edge}}(x_4)\sim\sum_{x_4}x_4^n e^{-2Kx_4}=\frac{1}{(-2)^n}\frac{d^n}{dK^n}\frac{1}{1-e^{-2Ka}}\sim 1/M^{n+1}. \tag{214}
$$

For example, in the x_4 expansion of $\gamma^i D_i(x_4)$ in H_{DW}, the linear contribution in x_4 to the eta invariant $\mathrm{Tr}_{\text{edge}}\frac{H_{\text{DW}}}{\sqrt{(H_{\text{DW}})^2}}$ is suppressed by

$$
\begin{aligned}
&a\sum_{x_4=0}^{\infty}\left(\phi_-^{\text{edge}}(x_4)\right)^\dagger\frac{x_4\partial_{x_4}\gamma_5\gamma^i D_i(x_4=0)}{\sqrt{\lambda(0)^2}}\phi_-^{\text{edge}}(x_4)\\
&\quad=\frac{a\lambda'(0)}{\sqrt{\lambda(0)^2}}M(2-Ma)\sum_{x_4=0}^{\infty}x_4e^{-2Kx_4}=\frac{a\lambda'(0)}{\sqrt{\lambda(0)^2}}M(2-Ma)\frac{1}{(-2)}\frac{d}{dK}\sum_{x_4=0}^{\infty}e^{-2Kx_4}\\
&\quad=\frac{a\lambda'(0)}{\sqrt{\lambda(0)^2}}\frac{1-2Ma+(Ma)^2}{2Ma-(Ma)^2}=-\frac{a\lambda'(0)}{\sqrt{\lambda(0)^2}}+\frac{a\lambda'(0)}{\sqrt{\lambda(0)^2}}\frac{1}{2Ma-(Ma)^2}\\
&\quad\sim\frac{a\lambda'(0)}{\sqrt{\lambda(0)^2}}\frac{1}{2M}
\end{aligned}
\tag{215}
$$

where we have taken the $a\to 0$ limit in the last step, and $\lambda'(0)$ is the x_4 derivative of the eigenvalue at $x_4=0$ in the adiabatic evaluation. Therefore, if we take M to be big enough compared to the derivative of the gauge fields, the leading adiabatic evaluation is valid.

The leading order of the edge mode's contribution to the η-invariant is

$$\begin{aligned}-\frac{1}{2}\eta(H_{\mathrm{DW}})^{\mathrm{edge}}|_{x_4\sim 0} &= -\frac{1}{2}\mathrm{Tr}_{\mathrm{edge}}\frac{H_{\mathrm{DW}}}{\sqrt{(H_{\mathrm{DW}})^2}} \\ &= -\frac{1}{2}\sum_{\lambda(0)} a^4 \sum_{\boldsymbol{x},x_4}\left[\phi^{\mathrm{3D}}_{\lambda(0)}(\boldsymbol{x})\otimes\phi^{\mathrm{edge}}_{-}(x_4)\right]^{\dagger}\frac{\lambda(0)}{\sqrt{(\lambda(0))^2}}\left[\phi^{\mathrm{3D}}_{\lambda(0)}(\boldsymbol{x})\otimes\phi^{\mathrm{edge}}_{-}(x_4)\right] \\ &= -\frac{1}{2}\sum_{\lambda(0)}\mathrm{sgn}\lambda(0) = -\frac{1}{2}\eta(iD^{\mathrm{3D}})|_{x_4=0}, \end{aligned} \tag{216}$$

where we use $iD^{\mathrm{3D}}\phi^{\mathrm{3D}}_{\lambda(0)}(\boldsymbol{x}) = \lambda(0)\phi^{\mathrm{3D}}_{\lambda(0)}(\boldsymbol{x})$. Note, however, that the above approximation does not hold for higher energy $\lambda(0)\sim M$ where the bulk and edge modes mix. Therefore, the edge mode part alone is not an integer, and it is difficult to separate the edge and bulk contributions in such an energy region.

5.3.3 Main result and discussion

Let us consider the anti-domain-wall at $x_4 = L_4 - a/2$. In the discussion so far, we have calculated under the fourth direction $L_4 = \infty$ and neglected the finiteness of x_4-direction. Since the effect of the anti-domain-wall in bulk is suppressed by e^{-ML_4}, in the $\lambda_{\mathrm{edge}} \ll M \ll 1/a$ scaling limit, we can safely interpolate our result to that with the anti-domain-wall. Our final result is

$$\begin{aligned}&-\frac{1}{2}\eta(H_{\mathrm{DW}}) \\ &=\frac{1}{32\pi^2}\int_{0<x_4<L_4} d^4x\epsilon^{\mu\nu\rho\sigma}\mathrm{tr_c}F_{\mu\nu}F_{\rho\sigma}(x) - \frac{1}{2}\eta(iD^{\mathrm{3D}})|_{x_4=0} + -\frac{1}{2}\eta(iD^{\mathrm{3D}})|_{x_4=L_4} + \mathcal{O}(a,1/M).\end{aligned} \tag{217}$$

Let us take the variation with respect to the link variables. From (148), we have the explicit "bulk-edge correspondence"

$$-\frac{1}{2}\delta\mathrm{Tr}_{\mathrm{edge}}\frac{H_{\mathrm{DW}}}{\sqrt{H^2_{\mathrm{DW}}}} = \frac{1}{2}\delta\mathrm{Tr}_{\mathrm{bulk}}\frac{H_{\mathrm{DW}}}{\sqrt{H^2_{\mathrm{DW}}}}, \tag{218}$$

where $\mathrm{Tr}_{\mathrm{bulk/edge}}$ is the trace taken over the bulk/edge modes only. Thanks to the locality of the gapped bulk modes, the right-hand side is much easier to perturbatively compute, leading to

$$= -\frac{1}{16\pi^2}\int d^3x\delta\mathrm{tr}_c\left[\epsilon_{0\nu\rho\sigma}\left(A^{\nu}\partial^{\rho}A^{\sigma} + \frac{2i}{3}A^{\nu}A^{\rho}A^{\sigma}\right)\right]. \tag{219}$$

Namely, the non-integer part of the edge-localized contribution is the Chern-Simons action, except for some extra gauge-invariant and constant contributions. Thus, we can clearly see in (218) the cancellation of the parity or T anomaly between the bulk and edge states.

6 Conclusions and Outlooks

6.1 Conclusions

In this thesis, we have proposed a non-perturbative definition of the Atiyah-Patodi-Singer index in the lattice gauge theory. We have shown that the eta invariant of the domain-wall Dirac operator converges to the APS index formula in the classical continuum limit. To evaluate the eta invariant, we have derived the eigenmode set of the square of the free domain-wall fermion. Then we have evaluated the eta invariant in the extreme situation of the Shamir type domain-wall using the eigenmode set. We have found in the continuum limit that the standard curvature term in the APS index appears as the contribution from the massive bulk extended modes, while the boundary eta invariant comes entirely from the massless edge-localized modes. Since the eta invariant of the domain-wall fermion at a finite lattice spacing is guaranteed to be integers by its definition, the APS index on the lattice can rigorously describe the anomaly inflow mechanism in the lattice gauge theory. We have achieved a non-perturbative formulation of the APS index theorem on the lattice.

Our result can be easily generalized to any $2n$-dimensional lattice:

$$-\frac{1}{2}\eta(H_{\mathrm{DW}}^{2n}) = \int_{X_{2n}} \mathrm{ch}(F) - \frac{1}{2}\eta(iD^{(2n-1)\mathrm{D}})|_{x_{2n}=0} + \frac{1}{2}\eta(iD^{(2n-1)\mathrm{D}})|_{x_{2n}=L_{2n}}, \tag{220}$$

where X_{2n} is the $2n$-dimensional flat manifold with boundary at $x_{2n}=0$ and $x_{2n}=L_{2n}$, and $\mathrm{ch}(F)$ is the Chern character

$$\mathrm{ch}(F) = \frac{1}{n!}\left(\frac{i}{2\pi}\right)^n \mathrm{tr}F^n, \tag{221}$$

and $iD^{(2n-1)\mathrm{D}}$ is the Diarc operator on the boundary.

We also comment on the admissibility condition on the link variables [47].

$$||1 - P_{\mu\nu}(x)|| \leq \epsilon \quad \text{for all } x, \mu, \nu, \tag{222}$$

where $||O||$ denotes the norm of operator O and $P_{\mu\nu}(x)$ is the plaquette

$$P_{\mu\nu}(x) = U_\mu(x)U_\nu(x+a\hat{\mu})U_\mu^\dagger(x+a\hat{\nu})U_\nu^\dagger(x). \tag{223}$$

This condition divides the space of lattice gauge fields into topological sectors. This condition requires a certain smoothness of the gauge field on the lattice, which prevents the appearance of a vortex and other phenomena that do not exist in continuum theories. Thanks to this condition, space-time can be treated geometrically, even on the lattice [34]. The AS index theorem is well-defined even on the lattice if this condition is imposed. This condition also guarantees the locality of the overlap Dirac operator (see Appendix B.2).

Let us consider whether the admissibility condition on the link variables is necessary in the case of the APS index theorem on the lattice. Recalling the proof of locality of the overlap Dirac operator, this condition is necessary for the Wilson-Dirac operator to have no zero eigenvalues. In the case of the APS index theorem, where the domain-wall fermion Dirac operator is used, the Dirac operator has the same form as the AS index theorem, so the same admissibility condition is needed for the APS index to be topological. In general, however, the APS index is not a topological invariant because it can change its value through the eta invariant at the boundary. As shown in (148), when the eigenvalues of H_{DW} does not cross zero, the APS index is invariant under the infinitesimal deformation of the gauge field. Then it seems sufficient to impose the same admissibility condition as for the AS index.

6.2 Outlooks

Finally, we show some perspectives of this work.

Anomaly descent equation

The APS index theorem is an integral representation of a part of the anomaly descent equations [48–52]. The anomaly descent equations describe the relationship between anomalies from $2n+2$ to $2n$ dimensions. The APS index theorem describes that the parity anomaly or T anomaly in $2n+1$ dimensions appears at the surface term of the axial $U(1)$ anomaly in $2n+2$ dimensions. It indicates that massless edge-localized modes, having parity anomaly, must appear to cancel the parity violation induced by the U(1) anomaly of bulk fermions.

It is interesting to extend our work to the $2n$-dimensional chiral fermion system, which appears as the edge-localized state of the $2n+1$-dimensional gapped bulk fermions. As already investigated in the literature [53–55], the gauge anomaly should be canceled by the surface contribution from the bulk eta invariant. It is known that the APS index theorem between odd-dimensional bulk and even dimensional edge does not exist mathematically. However, we consider that our formulation using the domain-wall fermions can be applied in general dimensions. Furthermore, since the correspondence with lattice theory is obvious, we expect our formulation to provide a non-perturbative formulation of the anomaly descent equations relating odd-dimensional bulks to even-dimensional edges, which has not been known before.

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A Notations

Through this thesis, we use the Euclidean signature $g^{\mu\nu} = \delta^{\mu\nu}$ and the space-time indices μ, ν run from 1 to 4.

A.1 Gamma matrices

The γ-matrices are all chosen to be hermitian as

$$\{\gamma^\mu, \gamma^\nu\} = 2\delta^{\mu\nu}, \quad (\gamma^\mu)^\dagger = \gamma^\mu. \tag{224}$$

The chirality operator is defined as

$$\gamma_5 = -\gamma_1\gamma_2\gamma_3\gamma_4, \quad (\gamma_5)^\dagger = \gamma_5. \tag{225}$$

Chiral representation

$$\gamma^i = \begin{pmatrix} 0 & i\sigma_i \\ -i\sigma_i & 0 \end{pmatrix} = -\tau_2 \otimes \sigma_i, \quad \gamma_4 = \begin{pmatrix} 0 & \mathbf{1}_{2\times 2} \\ \mathbf{1}_{2\times 2} & 0 \end{pmatrix} = \tau_1 \otimes \mathbf{1}_{2\times 2}, \tag{226}$$

$$\gamma_5 = -\gamma_1\gamma_2\gamma_3\gamma_4 = \begin{pmatrix} \mathbf{1}_{2\times 2} & 0 \\ 0 & -\mathbf{1}_{2\times 2} \end{pmatrix} = \tau_3 \otimes \mathbf{1}_{2\times 2}, \tag{227}$$

Dirac representation

$$\gamma^i = \begin{pmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{pmatrix} = \tau_1 \otimes \sigma_i, \quad \gamma_4 = \begin{pmatrix} \mathbf{1}_{2\times 2} & 0 \\ 0 & -\mathbf{1}_{2\times 2} \end{pmatrix} = \tau_3 \otimes \mathbf{1}_{2\times 2}, \tag{228}$$

$$\gamma_5 = -\gamma_1\gamma_2\gamma_3\gamma_4 = \begin{pmatrix} 0 & i\mathbf{1}_{2\times 2} \\ -i\mathbf{1}_{2\times 2} & 0 \end{pmatrix} = -\tau_2 \otimes \mathbf{1}_{2\times 2}, \tag{229}$$

τ_i and σ_i denote the Pauli matrices. The spinor trace properties of the gamma matrices

$$\begin{aligned} &\mathrm{tr}\gamma_5 = \mathrm{tr}\gamma_5\gamma^\mu\gamma^\nu = 0 \\ &\mathrm{tr}\gamma_5[\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma] = -4\epsilon^{\mu\nu\rho\sigma} \\ &\mathrm{tr}(\text{any odd \# of } \gamma'\text{s}) = 0. \end{aligned} \tag{230}$$

A.2 Lattice difference operator

$\nabla_\mu(U)$ and $\nabla^\dagger_\mu(U)$ are the forward and backward covariant difference operator acting as

$$\nabla_\mu(U)\psi(x) = \frac{1}{a}[U_\mu(x)\psi(x+a\hat{\mu}) - \psi(x)], \tag{231}$$

$$\nabla^\dagger_\mu(U)\psi(x) = \frac{1}{a}[\psi(x) - U^\dagger_\mu(x-a\hat{\mu})\psi(x-a\hat{\mu})]. \tag{232}$$

For the free case, the difference operator act as

$$\nabla_\mu(\mathbf{1})\psi(x) = \frac{1}{a}[\psi(x+a\hat{\mu}) - \psi(x)], \tag{233}$$

$$\nabla^\dagger_\mu(\mathbf{1})\psi(x) = \frac{1}{a}[\psi(x) - \psi(x-a\hat{\mu})]. \tag{234}$$

B Some properties of the overlap fermion

B.1 Proof of the overlap operator satisfies the Ginsparg-Wilson relation

We write the overlap Dirac operator as

$$D_{\text{ov}} = \frac{1}{a}\left(1+V\right), \quad V \equiv \frac{X}{\sqrt{X^\dagger X}}. \tag{235}$$

Then V has the γ_5-hermiticity and is unitary,

$$\gamma_5 V \gamma_5 = V^\dagger, \tag{236}$$
$$VV^\dagger = 1, \tag{237}$$

because

$$\begin{aligned}\gamma_5 V\gamma_5 &= \gamma_5 X(X^\dagger X)^{-1/2}\gamma_5 = \gamma_5 X\gamma_5\gamma_5(X^\dagger X)^{-1/2}\gamma_5 = X^\dagger(XX^\dagger)^{-1/2} \\ &= \sum_n a_n X^\dagger(XX^\dagger)^n = \sum_n a_n (X^\dagger X)^n X^\dagger = (X^\dagger X)^{-1/2}X^\dagger = V^\dagger,\end{aligned} \tag{238}$$

and

$$VV^\dagger = X(X^\dagger X)^{-1/2}(X^\dagger X)^{-1/2}X^\dagger = X(X^\dagger X)^{-1}X^\dagger = 1. \tag{239}$$

We also have

$$\gamma_5\frac{1}{1+V}\gamma_5 = \frac{1}{1+\gamma_5 V\gamma_5} = \frac{1}{1+V^\dagger} = \frac{V}{1+V} = 1-\frac{1}{1+V}. \tag{240}$$

This means

$$\begin{aligned}&\gamma_5 D_{\text{ov}}^{-1}\gamma_5 = a - D_{\text{ov}}^{-1} \\ \Leftrightarrow&\gamma_5 D_{\text{ov}}^{-1} + D_{\text{ov}}^{-1}\gamma_5 = a\gamma_5,\end{aligned} \tag{241}$$

the Ginsparg-Wilson relation, therefore the overlap Dirac operator satisfies the GW relation.

B.2 Locality of the overlap operator

From the definition of the overlap operator(72), D_{ov} is manifestly gauge covariant, however, it is not clear that the overlap operator is local due to the inverse square root of $X^\dagger X$. Here we prove that D_{ov} is local if the gauge field is sufficiently smooth at the scale of the cutoff, according to [56]. In this discussion, the detail form of $X^\dagger X$ does not matter. $(X^\dagger X)^{-1/2}$ can be expanded in a series of Legendre polynomials and to ensure the convergence we assume that the bounds on the spectrum of $(aX)^\dagger(aX)$,

$$u \le (aX)^\dagger(aX) \le v, \tag{242}$$

for positive constants $u < v$. From now on, we denote aX as $\tilde{X}$. The Legendre polynomials $P_k(z)$ is defined through the generating function,

$$(1-2tz+t^2)^{-1/2} = \sum_{k=0}^{\infty} t^k P_k(z). \tag{243}$$

z is taken to be

$$z = (v + u - 2\tilde{X}^\dagger \tilde{X})/(v - u), \tag{244}$$

using the bounds we can show that $||z|| \le 1$. Due to the properties of the Legendre polynomials, it implies

$$||P_k(z)|| \le 1. \tag{245}$$

Then the expansion is convergent for $|t| < 1$. Now we introduce a parameter θ as

$$\cosh\theta = (v + u)/(v - u), \qquad \theta > 0, \tag{246}$$

and set $t = e^{-\theta}$. Using these parameters, the Legendre polynomial has the form

$$(\tilde{X}^\dagger \tilde{X})^{-1/2} = \kappa \sum_{k=0}^{\infty} t^k P_k(z), \qquad \kappa = \left(\frac{4t}{v-u}\right)^{1/2}. \tag{247}$$

We define the kernel $G(x, y)$ for $(\tilde{X}^\dagger \tilde{X})^{-1/2}$,

$$(\tilde{X}^\dagger \tilde{X})^{-1/2}\psi(x) = a^4 \sum_y G(x, y)\psi(y), \tag{248}$$

where $\psi(x)$ is an arbitrary fermion field. If we define the kernels $G_k(x, y)$ like $P_k(z)$, we have

$$G(x, y) = \kappa \sum_{k=0}^{\infty} t^k G_k(x, y). \tag{249}$$

The norm convergence of the Legendre expansion implies that the absolute convergence of this series for all point x and y. From the norm of $P_k(z)$, we obtain

$$a^4 ||G_k(x, y)|| \le 1 \quad \text{for all } k, x, y, \tag{250}$$

where the norm for $G_k(x, y)$ is the matrix norm for 12×12 matrix $G_k(z, y)$ in color and spinor indices. If we define the taxi driver distance

$$||x - y||_1 = \sum_\mu |x_\mu - y_\mu|, \tag{251}$$

we can obtain the bound for the kernel

$$a^4 ||G(x, y)|| \le \frac{\kappa}{1 - t} \exp\{-\theta ||x - y||_1/2a\}. \tag{252}$$

It implies that $G(x, y)$ is exponentially decaying depending on the distances between x and y and in the continuum limit $G(x, y)$ becomes zero except for the distance

$$||x - y||_1 = \mathcal{O}(a). \tag{253}$$

Therefore, $(\tilde{X}^\dagger \tilde{X})^{-1/2}$ is exponentially decaying for finite lattice spacing and strictly local in the continuum limit only if the bounds (242) are satisfied.

Finally we will show the validity of the bounds (242) for any gauge fields. The Wilson-Dirac operator can be written as

$$aX = -ma + \sum_{\mu} \left\{ \frac{1}{2}(1-\gamma_\mu)a\nabla_\mu - \frac{1}{2}(1+\gamma_\mu)a\nabla_\mu^* \right\}, \quad 0 < ma < 2. \tag{254}$$

Using the triangle inequality and the property of unitary matrices $||U_\mu(x)|| \leq 1$, it follows that

$$||aX|| = ||aX^\dagger|| \leq 8 \Longrightarrow ||a^2 X^\dagger X|| \leq ||aX^\dagger|| \cdot ||aX|| \leq 64, \tag{255}$$

hence $X^\dagger X$ is uniformly bounded from above.

To obtain the lower bound, we expand $X^\dagger X$ as

$$a^2 X^\dagger X = 1 + \frac{1}{2}\sum_{\mu \neq \nu}[B_{\mu\nu} + C_{\mu\nu} + D_{\mu\nu}], \tag{256}$$

where we set $ma = 1$ and

$$\begin{aligned} B_{\mu\nu} &= a^4 \nabla_\mu^* \nabla_\mu \nabla_\nu^* \nabla_\nu, \\ C_{\mu\nu} &= -\frac{a^2}{4}[\gamma_\mu, \gamma_\nu][\nabla_\mu^* + \nabla_\mu, \nabla_\nu^* + \nabla_\nu], \\ D_{\mu\nu} &= -a^2 \gamma_\mu [\nabla_\mu^* + \nabla_\mu, \nabla_\nu^* - \nabla_\nu]. \end{aligned} \tag{257}$$

The commutator of the covariant derivative is

$$\begin{aligned} a^2[\nabla_\mu, \nabla_\nu]\psi(x) &= \{U_\mu(x)U_\nu(x+\hat{\mu}a) - U_\nu(x)U_\mu(x+\hat{\nu}a)\}\psi(x+\hat{\mu}a+\hat{\nu}a), \\ &= U_\mu(x)U_\nu(x+\hat{\mu}a)\left(1 - P_{\mu\nu}^\dagger(x)\right)\psi(x+\hat{\mu}a+\hat{\nu}a). \end{aligned} \tag{258}$$

If we suppose a condition for the link variables

$$||1 - P_{\mu\nu}(x)|| \leq \epsilon \quad \text{for all } x, \mu, \nu, \tag{259}$$

so-called the admissibility condition [47], the bracket of the covariant derivative satisfies

$$||a^2[\nabla_\mu, \nabla_\nu]|| \leqq \epsilon, \tag{260}$$

and the same inequality also holds for $[\nabla_\mu^*, \nabla_\nu]$ and $[\nabla_\mu^*, \nabla_\nu^*]$. In this way it is easy to show that

$$||C_{\mu\nu}|| \leq 2\epsilon, \quad ||D_{\mu\nu}|| \leq 4\epsilon. \tag{261}$$

For $B_{\mu\nu}$, we rewrite it in the form

$$B_{\mu\nu} = a^4 \nabla_\mu^* \nabla_\nu^* \nabla_\mu \nabla_\nu - a^3 \nabla_\mu^* [\nabla_\mu, \nabla_\nu - \nabla_\nu^*]. \tag{262}$$

The first term has strictly positive eigenvalues and the second term becomes

$$||a^3 \nabla_\mu^* [\nabla_\mu, \nabla_\nu - \nabla_\nu^*]|| \leq 2\epsilon ||\nabla_\mu^*|| \leq 4\epsilon. \tag{263}$$

Hence the lower bound for $X^\dagger X$ is given by

$$a^2 X^\dagger X \geq 1 - 30\epsilon. \tag{264}$$

Therefore the locality of the overlap operator is guaranteed if $\epsilon < 1/30$ and the admissibility condition is satisfied.

C Explicit evaluation of the topological charge density

C.1 Evaluation of the topological charge density in continuum theory

In this appendix, we give an explicit evaluation for a Jacobian factor of the fermionic path integral with respect to the chiral symmetry using Fujikawa's method. We start with the QCD-type Euclidean action with $SU(N)$ background gauge fields

$$S = \int d^4x \bar{\psi}(x)(D - m)\psi(x) \tag{265}$$

where $D = \gamma^\mu(\partial_\mu + iA_\mu)$. To analyse the chiral Jacobian we expand the fermion fields:

$$\psi(x) = \sum_n a_n \phi_n(x) = \sum_n a_n \langle x|n\rangle \,, \tag{266}$$

$$\bar{\psi}(x) = \sum_n \bar{b}_n \phi_n^\dagger(x) = \sum_n \bar{b}_n \langle n|x\rangle \,, \tag{267}$$

where $\phi(x)$ is the eigenfunction of hermitian operator iD satisfying,

$$iD\phi_n(x) = \lambda_n \phi_n(x), \tag{268}$$

$$\int d^4x \phi_n^\dagger(x)\phi_m(x) = \delta_{nm} \tag{269}$$

and $a_n,\ \bar{b}_n$ are the Grassmann number. Then the fermionic path integral measure is written as

$$\begin{aligned} \mathcal{D}\bar{\psi}\mathcal{D}\psi &= [\det \phi_n^\dagger(x)]^{-1}[\det \phi_n(x)]^{-1} \lim_{N\to\infty} \prod_{n=1}^{N} d\bar{b}_n da_n, \\ &= \lim_{N\to\infty} \prod_{n=1}^{N} d\bar{b}_n da_n. \end{aligned} \tag{270}$$

Under $U(1)$ chiral transformation, the fermion fields transfrom as

$$\begin{aligned} \psi(x) \to \psi'(x) = e^{i\alpha\gamma_5}\psi(x) &= \psi(x) + i\alpha\gamma_5\psi(x), \\ &= \sum_n a_n\phi(x) + i\alpha\gamma_5 \sum_n a_n\phi_n(x), \end{aligned} \tag{271}$$

$$\begin{aligned} \bar{\psi}(x) \to \bar{\psi}'(x) = \bar{\psi}(x)e^{i\alpha\gamma_5} &= \bar{\psi}(x) + \bar{\psi}(x)i\alpha\gamma_5, \\ &= \sum_n \bar{b}_n\phi_n^\dagger(x) + \sum_n \bar{b}_n\phi_n^\dagger(x)i\alpha\gamma_5, \end{aligned} \tag{272}$$

then using the orthogonality of $\phi_n(x)$, we obtain

$$a_n' = a_n + \sum_m i\alpha \int d^4x \phi_n^\dagger(x)\gamma_5\phi_m(x)a_m. \tag{273}$$

In the same way,

$$\bar{b}_n' = \bar{b}_n + \sum_m i\alpha\bar{b}_m \int d^4x \phi_m^\dagger(x)\gamma_5\phi_n(x). \tag{274}$$

Then, the transformation of the fermionic path integral measure is given by

$$\begin{aligned}\prod_{n=1}^{N} d\bar{b}'_n da'_n &= \det[\delta_{nm} + i\alpha \int d^4x \phi_n^\dagger(x)\gamma_5\phi_m(x)]^{-1} \prod_{n=1}^{N} d\bar{b}_n \\ &\quad \times \det[\delta_{nm} + i\alpha \int d^4x \phi_n^\dagger(x)\gamma_5\phi_m(x)]^{-1} \prod_{n=1}^{N} da_n \\ &= \det[\delta_{nm} + i\alpha \int d^4x \phi_n^\dagger(x)\gamma_5\phi_m(x)]^{-2} \prod_{n=1}^{N} d\bar{b}_n da_n, \end{aligned} \tag{275}$$

Thus the Jacobian of the path integral measure is expressed as,

$$\begin{aligned}\det[\delta_{nm} + i\alpha \int d^4x \phi_n^\dagger(x)\gamma_5\phi_m(x)]^{-2} &= \exp\left[-2\mathrm{tr}\ln\left\{\delta_{nm} + i\alpha \int d^4x \phi_n^\dagger(x)\gamma_5\phi_m(x)\right\}\right] \\ &= \exp\left[-2i\alpha \sum_n \int d^4\phi_n^\dagger(x)\gamma_5\phi_n(x)\right], \end{aligned} \tag{276}$$

using $\det C = \exp[\mathrm{tr}\ln C]$ and $\ln[1+C] = C + \mathcal{O}(C^2)$. We obtain the Jacobian factor:

$$\mathcal{D}\bar{\psi}'\mathcal{D}\psi' = J\mathcal{D}\bar{\psi}\mathcal{D}\psi, \tag{277}$$

$$J \equiv \exp[-2i\alpha \lim_{N\to\infty} \sum_{n=1}^{N} \int d^4\phi_n^\dagger(x)\gamma_5\phi_n(x)]. \tag{278}$$

Since this summation is divergent in general, so we use the mode cut-off $\lim_{N\to\infty}\sum_{n=1}^{N}$, however, this regularization breaks the gauge symmetry. Therefore, we need to change the regularization in a way that does not break the gauge symmetry. One example of such a regularization is the heat kernel regularization, which is regularized by a smooth cut as shown below.

$$\begin{aligned}\lim_{N\to\infty}\sum_{n=1}^{N}\int d^4\phi_n^\dagger(x)\gamma_5\phi_n(x) &= \lim_{M\to\infty}\sum_{n=1}^{\infty}\int d^4x\phi_n^\dagger(x)\gamma_5 f((\lambda_n)^2/M^2)\phi_n(x) \\ &= \lim_{M\to\infty}\sum_{n=1}^{\infty}\phi_n^\dagger(x)\gamma_5 f((i\not{D})^2/M^2)\phi_n(x) \qquad (279) \\ &= \lim_{M\to\infty}\mathrm{Tr}\gamma_5 f((i\not{D})^2/M^2), \qquad (280)\end{aligned}$$

where $f(x)$ is an arbitrary function which satisfies,

$$f(0) = 1, \quad f(\infty) = 0, \quad xf'(x)|_{x=0} = xf'(x)|_{x=\infty} = 0, \tag{281}$$

and Tr is taken over space-time coordinates, spinor and color indices. Now we can expand in the plane wave basis for each x,

$$\lim_{M\to\infty}\mathrm{tr}\gamma_5 f((iD)^2/M^2) = \mathrm{tr}[\int \frac{d^4k}{(2\pi)^4} e^{-ikx}\gamma_5 f((iD)^2/M^2)e^{ikx}]. \tag{282}$$

The covariant derivative can be decomposed into two parts,

$$\begin{aligned} D^2 = \gamma^\mu \gamma^\nu D_\mu D_\nu &= D_\mu D^\mu + \frac{1}{4}[\gamma^\mu, \gamma^\nu][D_\mu, D_\nu] \\ &= D_\mu D^\mu + \frac{i}{4}[\gamma^\mu, \gamma^\nu] F_{\mu\nu}. \end{aligned} \tag{283}$$

Then the regularization function is evaluated as:

$$\begin{aligned} &\int \frac{d^4k}{(2\pi)^4} e^{-ikx} f((iD)^2/M^2) e^{ikx} \\ &\quad = \int \frac{d^4k}{(2\pi)^4} e^{-ikx} f(-(D_\mu D^\mu + \frac{i}{4}[\gamma^\mu, \gamma^\nu] F_{\mu\nu})/M^2) e^{ikx} \\ &\quad = \int \frac{d^4k}{(2\pi)^4} f\left(-\frac{1}{M^2}(D_\mu + ik_\mu)(D^\mu + ik^\mu) - \frac{i}{4M^2}[\gamma^\mu, \gamma^\nu] F_{\mu\nu}\right) \\ &\quad = \int \frac{d^4k}{(2\pi)^4} M^4 f\left(k_\mu k^\mu - \frac{2ik_\mu D^\mu}{M} - \frac{D_\mu D^\mu}{M^2} - \frac{i}{4M^2}[\gamma^\mu, \gamma^\nu] F_{\mu\nu}\right), \end{aligned} \tag{284}$$

in the third step, we rescale $k_\mu \to M k_\mu$. We expand $f(x)$ around $x_0 = k^2$ as,

$$\begin{aligned} &f\left(k_\mu k^\mu - \frac{2ik_\mu D^\mu}{M} - \frac{D_\mu D^\mu}{M^2} - \frac{i}{4M^2}[\gamma^\mu, \gamma^\nu] F_{\mu\nu}\right) \\ &\quad = f(k_\mu k^\mu) + f^{(1)}(k_\mu k^\mu)\left(-\frac{2ik_\mu D^\mu}{M} - \frac{D_\mu D^\mu}{M^2} - \frac{i}{4M^2}[\gamma^\mu, \gamma^\nu] F_{\mu\nu}\right) \\ &\qquad + \frac{1}{2!} f^{(2)}(k_\mu k^\mu)\left(-\frac{2ik_\mu D^\mu}{M} - \frac{D_\mu D^\mu}{M^2} - \frac{i}{4M^2}[\gamma^\mu, \gamma^\nu] F_{\mu\nu}\right)^2 + \cdots. \end{aligned} \tag{285}$$

Using the trace properties of γ matrices,

$$\mathrm{tr}\gamma_5 = 0, \quad \mathrm{tr}\gamma_5[\gamma^\mu, \gamma^\nu] = 0, \quad \mathrm{tr}\gamma_5[\gamma^\mu, \gamma^\nu][\gamma^\rho, \gamma^\sigma] = -16\epsilon^{\mu\nu\rho\sigma}, \tag{286}$$

then

$$\begin{aligned} &\lim_{M\to\infty} \int \frac{d^4k}{(2\pi)^4} M^4 \mathrm{tr}\left[\gamma_5 f\left(k_\mu k^\mu - \frac{2ik_\mu D^\mu}{M} - \frac{D_\mu D^\mu}{M^2} - \frac{i}{4M^2}[\gamma^\mu, \gamma^\nu] F_{\mu\nu}\right)\right] \\ &\quad = \lim_{M\to\infty} \int \frac{d^4k}{(2\pi)^4} M^4 \mathrm{tr}\left[\gamma_5 \frac{1}{2!}\left(-\frac{i}{4M^2}[\gamma^\mu, \gamma^\nu] F_{\mu\nu}\right)^2 f^{(2)}(k^2) + \mathcal{O}(1/M^5)\right] \\ &\quad = \mathrm{tr}\left[\gamma_5 \frac{1}{2!}\left(-\frac{i}{4}[\gamma^\mu, \gamma^\nu] F_{\mu\nu}\right)^2\right] \int \frac{d^4k}{(2\pi)^4} f^{(2)}(k^2). \end{aligned} \tag{287}$$

The integral in the final line can be calculated by using the property of regularization function $f(x)$,

$$\begin{aligned} \int \frac{d^4k}{(2\pi)^4} f^{(2)}(k^2) &= \frac{1}{16\pi^2} \int_0^\infty dx f^{(2)}(x) \\ &= \left[\frac{1}{16\pi^2} x f^{(1)}(x)\right]_0^\infty - \frac{1}{16\pi^2} \int_0^\infty dx f^{(1)}(x) \\ &= \frac{1}{16\pi^2}. \end{aligned} \tag{288}$$

Finally we obtain following expression,

$$\lim_{M\to\infty} \mathrm{tr}\gamma_5 f((iD)^2/M^2) = \frac{1}{32\pi^2}\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}. \tag{289}$$

Therefore the Jacobian of the fermionic path integral measure becomes

$$J = \exp\left[-2i\alpha\int d^4x \frac{1}{32\pi^2}\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}\right]. \tag{290}$$

C.2 Evaluation of the topological charge density using Overlap fermion

In this subsection, we explicitly show that the lattice topological charge density $-\frac{a}{2}\mathrm{tr}\gamma_5 D_{\rm ov}(x)$ converges to the topological charge density $q^{\rm lat}_{\rm top}(x)$,

$$q^{\rm lat}_{\rm top} = I(m,r)\frac{1}{32\pi^2}\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma} + \mathcal{O}(a). \tag{291}$$

without using the gauge coupling expansion.

Let us review the situation. $D_{\rm ov}$ is the overlap Dirac operator (72) and $X(x)$ is the Wilson Dirac operator (73). The lattice Dirac operator $D_\mu(x)$ and the Wilson term $R(x)$ is given by

$$D_\mu(x) = \frac{1}{2a}\left[U_\mu(x)e^{a\partial_\mu} - e^{-a\partial_\mu}U^\dagger_\mu(x)\right], \tag{292}$$

$$R(x) = \frac{r}{2a}\sum_\mu\left[2 - U_\mu(x)e^{a\partial_\mu} - e^{-a\partial_\mu}U^\dagger_\mu(x)\right] \tag{293}$$

where $U_\mu(x)$ is the link variable. In this subsection, the Wilson parameter r is not fixed to one.

First,

$$\begin{aligned}
&-\frac{1}{2}\mathrm{tr}\gamma_5 a D_{\rm ov}(x)\delta(x,y)|_{y=x}\\
&\quad= -\frac{1}{2}\mathrm{tr}\gamma_5\left[1 + X(x)\frac{1}{\sqrt{X^\dagger(x)X(x)}}\right]\delta(x,y)|_{y=x},\\
&\quad= -\frac{1}{2}\mathrm{tr}\gamma_5(D(x)-m+R(x))\left[(D(x)-m+R(x))^\dagger(D(x)-m+R(x))\right]^{-\frac{1}{2}}\delta(x,y)|_{y=x}.
\end{aligned}$$

The denominator of above is

$$\begin{aligned}
&(D-m+R)^\dagger(D-m+R) = \gamma_5(D-m+R)\gamma_5(D-m+R)\\
&= -\sum_\mu D_\mu D^\mu - \frac{1}{4}\sum_{\mu,\nu}[\gamma^\mu,\gamma^\nu][D_\mu,D_\nu] - [\gamma^\mu D_\mu, R] + (m-R)^2.
\end{aligned} \tag{294}$$

Therefore

$$
\begin{aligned}
&-\frac{1}{2}\mathrm{tr}\gamma_5 aD_{\mathrm{ov}}(x)\delta(x,y)|_{y=x} \\
&\quad= -\frac{1}{2}\mathrm{tr}\gamma_5(D-m+R) \\
&\quad\quad\times\left[-\sum_\mu D_\mu D^\mu - \frac{1}{4}\sum_{\mu,\nu}\left[\gamma^\mu,\gamma^\nu\right]\left[D_\mu,D_\nu\right] - \left[\gamma^\mu D_\mu, R\right] + (m-R)^2\right]^{-\frac{1}{2}}\delta(x,y)|_{y=x}. \\
&\quad= -\frac{1}{2}\int_{-\frac{\pi}{a}}^{\frac{\pi}{a}}\frac{d^4k}{(2\pi)^4}\mathrm{tr}\gamma_5 e^{-ikx}(D-m+R) \\
&\quad\quad\times\left[-\sum_\mu D_\mu D^\mu - \frac{1}{4}\sum_{\mu,\nu}\left[\gamma^\mu,\gamma^\nu\right]\left[D_\mu,D_\nu\right] - \left[\gamma^\mu D_\mu, R\right] + (m-R)^2\right]^{-\frac{1}{2}} e^{ikx}.
\end{aligned}
$$

substituting the relation $\delta(x,y) = \int_{-\pi/a}^{\pi/a} d^4k e^{ik(x-y)}/\left(2\pi\right)^4$. And we use the relation,

$$
e^{-ikx}D_\mu e^{ikx} = \frac{i}{a}s_\mu + \tilde{D}_\mu, \tag{295}
$$

$$
e^{-ikx}Re^{ikx} = \frac{r}{a}\sum_\mu\left(1-c_\mu\right) + \tilde{R}, \tag{296}
$$

where $s_\mu = \sin ak_\mu$ and $c_\mu = \cos ak_\mu$ and

$$
\tilde{D}_\mu = \frac{1}{2a}\left[e^{iak_\mu}\left(U_\mu e^{a\partial_\mu}-1\right) - e^{-ik_\mu}\left(e^{-a\partial_\mu}U_\mu^\dagger - 1\right)\right] \tag{297}
$$

$$
\tilde{R} = -\frac{r}{2a}\sum_\mu\left[e^{iak_\mu}\left(U_\mu e^{a\partial_\mu}-1\right) - e^{-iak_\mu}\left(e^{-a\partial_\mu}U_\mu^\dagger - 1\right)\right] \tag{298}
$$

Then

$$
\begin{aligned}
&-\frac{1}{2}\mathrm{tr}\gamma_5 aD_{\mathrm{ov}}(x)\delta(x,y)|_{y=x} \\
&= -\frac{1}{2}\mathrm{tr}\gamma_5\int_{-\pi/a}^{\pi/a}\frac{d^4k}{(2\pi)^4}\left[i\gamma^\mu s_\mu - ma + r\sum\nolimits_\mu(1-c_\mu) + a\gamma^\mu\tilde{D}_\mu + a\tilde{R}\right] \\
&\quad\times\Big\{-\sum\nolimits_\nu(is_\nu + a\tilde{D}_\nu)^2 + \left[ma - r\sum\nolimits_\nu(1-c_\nu) - a\tilde{R}\right] \\
&\quad\quad -\frac{a^2}{2}\sum\nolimits_{\nu\rho}\gamma^\nu\gamma^\rho\left[\tilde{D}_\nu,\tilde{D}_\rho\right] - a^2\left[\gamma^\nu\tilde{D}_\nu,\tilde{R}\right]\Big\}^{-\frac{1}{2}}.
\end{aligned} \tag{299}
$$

According to the trace properties of gamma matrices, γ_5 requires at least four gamma matrices. By parameterizing the link variables as $U_\mu(x) = \exp[iaA_\mu(x)]$, we have

$$
\tilde{D}_\mu = c_\mu D_\mu^c + \mathcal{O}(a), \qquad \tilde{R} = -ir\sum_\mu s_\mu D_\mu^c + \mathcal{O}(a), \tag{300}
$$

where $D_\mu^a \equiv \partial_\mu + iA_\mu$ is the covariant derivative of the continuum. Therefore the commutators of $\tilde{D}_\mu$ and R become

$$
\left[\tilde{D}_\mu,\tilde{D}_\nu\right] = c_\mu c_\nu F_{\mu\nu} + \mathcal{O}(a) \qquad \left[\tilde{D}_\mu,\tilde{R}\right] = -grc_\mu\sum_\nu s_\nu F_{\mu\nu} + \mathcal{O}(a). \tag{301}
$$

We find

$$
\begin{aligned}
&-\frac{1}{2}\mathrm{tr}\gamma_5 aD_{\mathrm{ov}}(x)\delta(x,y)|_{y=x} \\
&= -\frac{1}{2}\mathrm{tr}\gamma_5 \int_{-\pi/a}^{\pi/a}\frac{d^4k}{(2\pi)^4}\left[i\gamma^\mu s_\mu - ma + r\sum\nolimits_\mu (1-c_\mu) + a\gamma^\mu \tilde{D}_\mu + a\tilde{R}\right] \\
&\quad\times\left\{-\sum\nolimits_\nu (is_\nu + a\tilde{D}_\nu)^2 + \left[ma - r\sum\nolimits_\nu (1-c_\nu) - a\tilde{R}\right]\right. \\
&\qquad\left. -\frac{a^2}{2}\sum\nolimits_{\nu\rho}\gamma^\nu\gamma^\rho\left[\tilde{D}_\nu,\tilde{D}_\rho\right] - a^2\left[\gamma^\nu\tilde{D}_\nu,\tilde{R}\right]\right\}^{-\frac{1}{2}}
\end{aligned}
$$

The denominator is

$$
\begin{aligned}
&\left[-\sum\nolimits_\nu (is_\nu + a\tilde{D}_\nu)^2 + \left[ma - r\sum\nolimits_\nu (1-c_\nu) - a\tilde{R}\right]\right. \\
&\quad\left. -\frac{a^2}{2}\sum\nolimits_{\nu\rho}\gamma^\nu\gamma^\rho\left[\tilde{D}_\nu,\tilde{D}_\rho\right] - a^2\left[\gamma^\nu\tilde{D}_\nu,\tilde{R}\right]\right]^{-\frac{1}{2}} \\
&= \left[s^2 + \left(ma - r\sum\nolimits_\nu (1-c_\nu)\right)^2\right. \\
&\qquad\left. -\frac{ia^2}{2}\sum\nolimits_{\nu,\rho}\gamma^\nu\gamma^\rho c_\nu c_\rho F_{\nu\rho} - a^2 r\sum\nolimits_{\nu\rho} c_\nu s_\rho \gamma^\nu F_{\nu\rho} + \mathcal{O}(a)\right]^{-\frac{1}{2}}.
\end{aligned}
\tag{302}
$$

(The terms in $\mathcal{O}(a)$ contain gamma matrices, but only in terms above $\mathcal{O}(a)$. There are only at most two gamma matrices in $\mathcal{O}(a)$.) If we define

$$
\begin{aligned}
(\tilde{H}_{\mathrm{W}}^0)^2 &= s^2 + \left(ma - \sum\nolimits_\nu (1-c_\nu)\right)^2, \\
\Delta\tilde{H}_{\mathrm{W}}^2 &= -\frac{ia^2}{2}\sum\nolimits_{\nu,\rho}\gamma^\nu\gamma^\rho c_\nu c_\rho F_{\nu\rho} - a^2 r\sum\nolimits_{\nu\rho} c_\nu s_\rho\gamma^\nu F_{\nu\rho} + \mathcal{O}(a),
\end{aligned}
$$

$(\tilde{H}_{\mathrm{W}}^0)^2$ and $\Delta\tilde{H}_{\mathrm{W}}^2$ are commute $[(\tilde{H}_{\mathrm{W}}^0)^2, \Delta\tilde{H}_{\mathrm{W}}^2] = 0$, then we have

$$
\begin{aligned}
&\left[\left\{s^2 + \left(ma - r\sum\nolimits_\nu (1-c_\nu)\right)^2\right\} - \frac{ia^2}{2}\sum\nolimits_{\nu,\rho}\gamma^\nu\gamma^\rho c_\nu c_\rho F_{\nu\rho} - a^2 r\sum\nolimits_{\nu\rho} c_\nu s_\rho\gamma^\nu F_{\nu\rho} + \mathcal{O}(a)\right]^{-\frac{1}{2}} \\
&= \left[s^2 + \left(ma - r\sum\nolimits_\nu (1-c_\nu)\right)^2\right]^{-\frac{1}{2}} \\
&\times\left[1 + \frac{a^2}{2}\left(\frac{i}{2}\sum\nolimits_{\nu,\rho}\gamma^\nu\gamma^\rho c_\nu c_\rho F_{\nu\rho} + r\sum\nolimits_{\nu\rho} c_\nu s_\rho\gamma^\nu F_{\nu\rho}\right)\left[s^2 + \left(ma - r\sum\nolimits_\nu (1-c_\nu)\right)^2\right]^{-1}\right. \\
&\left. + \frac{3a^4}{8}\left(\frac{i}{2}\sum\nolimits_{\nu,\rho}\gamma^\nu\gamma^\rho c_\nu c_\rho F_{\nu\rho} + r\sum\nolimits_{\nu\rho} c_\nu s_\rho\gamma^\nu F_{\nu\rho}\right)^2\left[s^2 + \left(ma - r\sum\nolimits_\nu (1-c_\nu)\right)^2\right]^{-2} + \cdots\right]
\end{aligned}
\tag{303}
$$

The denominator is expanded in terms of a, and considering the spinor structure and the order of a, the third term only survives. The third term becomes

$$
\begin{aligned}
&\left(\frac{i}{2}\sum_{\mu,\nu}\gamma^\mu\gamma^\nu c_\mu c_\nu F_{\mu\nu} + r\sum_{\mu\nu} c_\mu s_\nu \gamma^\mu F_{\mu\nu}\right)\left(\frac{i}{2}\sum_{\rho,\sigma}\gamma^\rho\gamma^\sigma c_\rho c_\sigma F_{\rho\sigma} + r\sum_{\rho\sigma} c_\rho s_\sigma \gamma^\rho F_{\rho\sigma}\right) \\
&= -\frac{1}{4}\sum_{\mu,\nu,\rho,\sigma}\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma c_\mu c_\nu c_\rho c_\sigma F_{\mu\nu}F_{\rho\sigma} + r^2\sum_{\mu,\nu,\rho,\sigma} c_\mu s_\nu c_\rho s_\sigma \gamma^\mu\gamma^\rho F_{\mu\nu}F_{\rho\sigma} \\
&\quad + \frac{ir}{2}\sum_{\mu,\nu,\rho}(\gamma^\mu\gamma^\nu\gamma^\rho + \gamma^\rho\gamma^\mu\gamma^\nu)c_\mu c_\nu c_\rho \sum_\sigma s_\sigma F_{\mu\nu}F_{\rho\sigma}
\end{aligned} \tag{304}
$$

For simplicity, we denote

$$
\mathcal{M} = s^2 + \left\{ma - r\sum_\nu (1-c_\nu)\right\}^2. \tag{305}
$$

$$
\begin{aligned}
&-\frac{1}{2}\mathrm{tr}\gamma_5 a D_{\mathrm{ov}}(x)\delta(x,y)|_{y=x} \\
&= -\frac{1}{2}\int_{-\pi/a}^{\pi/a}\frac{d^4k}{(2\pi)^4}\mathrm{tr}\gamma_5\left[i\gamma^\mu s_\mu - ma + r\sum_\mu(1-c_\mu) + a\gamma^\mu D^c_\mu - iar\sum_\mu s_\mu D^c_\mu + \mathcal{O}(a^2)\right] \\
&\quad\times\left[\mathcal{M}^{-\frac{1}{2}} + \frac{a^2}{2}\left(\frac{i}{2}\sum_{\mu,\nu}\gamma^\mu\gamma^\nu c_\mu c_\nu F_{\mu\nu} + r\sum_{\mu,\nu} c_\mu s_\nu\gamma^\mu F_{\mu\nu}\right)\mathcal{M}^{-\frac{3}{2}}\right. \\
&\qquad + \frac{3a^4}{8}\left\{-\frac{1}{4}\sum_{\mu,\nu,\rho,\sigma}\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma c_\mu c_\nu c_\rho c_\sigma F_{\mu\nu}F_{\rho\sigma} + r^2\sum_{\mu,\nu,\rho,\sigma} c_\mu s_\nu c_\rho s_\sigma\gamma^\mu\gamma^\rho F_{\mu\nu}F_{\rho\sigma}\right. \\
&\qquad\left.\left. + \frac{ir}{2}\sum_{\mu,\nu,\rho}(\gamma^\mu\gamma^\nu\gamma^\rho + \gamma^\rho\gamma^\mu\gamma^\nu)c_\mu c_\nu c_\rho\sum_\sigma s_\sigma F_{\mu\nu}F_{\rho\sigma}\right\}\mathcal{M}^{-\frac{5}{2}} + \cdots\right]
\end{aligned} \tag{306}
$$

Considering the spinor structure and the order of a

$$
\begin{aligned}
&-\frac{1}{2}\int_{-\pi/a}^{\pi/a}\frac{d^4k}{(2\pi)^4}\mathrm{tr}\gamma_5\left[i\gamma^\mu s_\mu - ma + r\sum_\mu(1-c_\mu)\right]\mathcal{M}^{-\frac{5}{2}} \\
&\times\frac{3a^4}{8}\left[-\frac{1}{4}\sum_{\mu,\nu,\rho,\sigma}\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma c_\mu c_\nu c_\rho c_\sigma F_{\mu\nu}F_{\rho\sigma} + \frac{ir}{2}\sum_{\mu,\nu,\rho,\sigma}(\gamma^\mu\gamma^\nu\gamma^\rho + \gamma^\rho\gamma^\mu\gamma^\nu)c_\mu c_\nu c_\rho s_\sigma F_{\mu\nu}F_{\rho\sigma}\right]
\end{aligned} \tag{307}
$$

For the first term

$$
\begin{aligned}
&\frac{3a^4}{64}\int_{-\pi/a}^{\pi/a}\frac{d^4k}{(2\pi)^4}\left[-ma + r\sum_\mu(1-c_\mu)\right]\sum_{\mu,\nu,\rho,\sigma}\mathrm{tr}\gamma_5[\gamma^\mu\gamma^\nu\gamma^\rho\gamma^\sigma]c_\mu c_\nu c_\rho c_\sigma \mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}\mathcal{M}^{-\frac{5}{2}} \\
&= \frac{3a^4}{16}\epsilon^{\mu\nu\rho\sigma}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}\int_{-\pi/a}^{\pi/a}\frac{d^4k}{(2\pi)^4}\prod_\mu c_\mu\left[ma + r\sum_\mu(c_\mu - 1)\right]\mathcal{M}^{-\frac{5}{2}}.
\end{aligned} \tag{308}
$$

For the second term

$$
\begin{aligned}
&-\frac{3a^4 ir}{32}\int_{-\pi/a}^{\pi/a}\frac{d^4k}{(2\pi)^4}\mathrm{tr}\gamma_5\left[i\sum_\alpha\gamma^\alpha s_\alpha\right]\sum_{\mu,\nu,\rho,\sigma}(\gamma^\mu\gamma^\nu\gamma^\rho + \gamma^\rho\gamma^\mu\gamma^\nu)c_\mu c_\nu c_\rho s_\sigma F_{\mu\nu}F_{\rho\sigma}\mathcal{M}^{-\frac{5}{2}} \\
&= \frac{3a^4 r}{4}\int_{-\pi/a}^{\pi/a}\frac{d^4k}{(2\pi)^4}\sum_{\alpha,\mu,\nu,\rho,\sigma}s_\alpha c_\mu c_\nu c_\rho s_\sigma\epsilon^{\mu\nu\rho\alpha}\mathrm{tr}_c F_{\mu\nu}F_{\rho\sigma}\mathcal{M}^{-\frac{5}{2}}
\end{aligned}
$$

Since s_μ is an function, only $\sigma = \alpha$ remains

$$
\begin{aligned}
&= \frac{3a^4 r}{4} \int_{-\pi/a}^{\pi/a} \frac{d^4k}{(2\pi)^4} \sum_{\mu,\nu,\rho,\sigma} c_\mu c_\nu c_\rho s_\sigma^2 \epsilon^{\mu\nu\rho\sigma} \mathrm{tr}_c F_{\mu\nu} F_{\rho\sigma} \mathcal{M}^{-\frac{5}{2}} \\
&= \frac{3a^4 r}{16} \epsilon^{\mu\nu\rho\sigma} \mathrm{tr}_c F_{\mu\nu} F_{\rho\sigma} \int_{-\pi/a}^{\pi/a} \frac{d^4k}{(2\pi)^4} \prod_\mu c_\mu \left(\sum_\nu \frac{s_\nu^2}{c_\nu} \right) \mathcal{M}^{-\frac{5}{2}}.
\end{aligned} \tag{309}
$$

As a result, we obtain

$$
\begin{aligned}
&-\frac{1}{2} \mathrm{tr} \gamma_5 a D_{\mathrm{ov}}(x) \delta(x,y)|_{x=y} \\
&\quad = \frac{3a^4}{16} \epsilon^{\mu\nu\rho\sigma} \mathrm{tr}_c F_{\mu\nu} F_{\rho\sigma} \int_{-\pi/a}^{\pi/a} \frac{d^4k}{(2\pi)^4} \prod_\mu c_\mu \left[ma + r \textstyle\sum_\mu (c_\mu - 1) \right] \mathcal{M}^{-\frac{5}{2}} \\
&\qquad + \frac{3a^4 r}{16} \epsilon^{\mu\nu\rho\sigma} \mathrm{tr}_c F_{\mu\nu} F_{\rho\sigma} \int_{-\pi/a}^{\pi/a} \frac{d^4k}{(2\pi)^4} \prod_\mu c_\mu \left(\sum_\nu \frac{s_\nu^2}{c_\nu} \right) \mathcal{M}^{-\frac{5}{2}} \\
&\quad = \frac{1}{32\pi^2} I(ma,r) \epsilon^{\mu\nu\rho\sigma} \mathrm{tr}_c F_{\mu\nu} F_{\rho\sigma}
\end{aligned} \tag{310}
$$

where

$$
I(ma,r) = \frac{3}{8\pi^2} \int_{-\pi}^{\pi} d^4k \prod_\mu c_\mu \left[ma + +r \sum_\mu (c_\mu - 1) + r \sum_\nu \frac{s_\nu^2}{c_\nu} \right] \mathcal{M}^{-\frac{5}{2}} \tag{311}
$$

In the following, we evaluate the factor $I(ma,r)$. First, we change the integration variable from k_μ to $\sin k_\mu$ by splitting the integration region into $-\pi/2 \le k_\mu < \pi/2$ and $\pi/2 \le k_\mu < 3\pi/2$ in each direction. The original integration region has been split int $2^4 = 16$ blocks, then we have

$$
\begin{aligned}
&\int_{-\frac{\pi}{2}}^{\frac{3\pi}{2}} d^4k \prod_\mu c_\mu \\
&= \left[\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} + \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} dk_1 c_1 \right] \left[\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} + \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} dk_2 c_2 \right] \left[\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} + \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} dk_3 c_3 \right] \left[\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} + \int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} dk_4 c_4 \right] \\
&= \sum_{\epsilon_\mu = \pm 1} \int_{-1}^{1} ds_1 \epsilon_1 \cdot \int_{-1}^{1} ds_2 \epsilon_2 \cdot \int_{-1}^{1} ds_3 \epsilon_3 \cdot \int_{-1}^{1} ds_4 \epsilon_4 \\
&= \sum_{\epsilon_\mu = \pm 1} \left(\prod_\mu \epsilon_\mu \right) \int_{-1}^{1} d^4 s.
\end{aligned} \tag{312}
$$

$\epsilon_\mu = (\pm 1, \pm 1, \pm 1, \pm 1)$ specifies the individual block. Note that $\cos k_\mu$ is expressed as $c_\mu =$

$\epsilon_\mu(1-s_\mu^2)^{1/2}$. Therefore we rewrite $I(ma,r)$ as

$$
\begin{aligned}
& I(ma,r) \\
&= \frac{3}{8\pi^2}\int_{-\pi}^{\pi} d^4k \prod_\mu c_\mu \left[ma + +r\sum_\nu (c_\nu - 1) + r\sum_\nu \frac{s_\nu^2}{c_\nu}\right]\left[s^2 + \left\{ma - r\sum\nolimits_\rho (1-c_\rho)\right\}^2\right]^{-\frac{5}{2}} \\
&= \frac{3}{8\pi^2}\sum_{\epsilon_\mu=\pm 1}\left(\prod_\mu \epsilon_\mu\right)\int_{-1}^{1} d^4s \\
&\quad \times \left[ma + +r\sum_\nu \{\epsilon_\nu(1-s_\nu^2)^{1/2} - 1\} + r\sum_\nu s_\nu^2\epsilon_\nu(1-s_\nu^2)^{-1/2}\right] B(s)^{-5/2}, \qquad (313)
\end{aligned}
$$

where

$$
B(s) \equiv \sum\nolimits_\mu s_\mu^2 + \left\{ma + r\sum\nolimits_\mu (\epsilon_\mu(1-s_\mu^2)^{1/2} - 1)\right\}^2. \qquad (314)
$$

To reproduce the correct coefficient of the chiral anomaly for a single fermion, one would expect $I(ma,r) = 1$ at least in some parameter region. In fact, the factor $I(ma,r)$ is topological. It does not vary under an infinitesimal variation of the parameters ma and r. We note the identity

$$
\begin{aligned}
&\left[ma + r\sum_\mu \left\{\epsilon_\mu(1-s_\mu^2)^{1/2} - 1\right\} + r\sum_\mu s_\mu^2\epsilon_\mu(1-s_\mu^2)^{-1/2}\right]\left[ma + r\sum_\nu \left\{\epsilon_\nu(1-s_\nu^2)^{1/2} - 1\right\}\right] \\
&\qquad = B(s) + \frac{1}{5}B(s)^{7/2}\sum_\mu \frac{\partial}{\partial s_\mu} B(s)^{-5/2}. \qquad (315)
\end{aligned}
$$

This identity is easily shown, for the right-hand-side of it

$$
\begin{aligned}
&\frac{1}{5}B(s)^{7/2}\sum\nolimits_\mu \frac{\partial}{\partial s_\mu}B(s)^{-5/2} \\
&= -\sum\nolimits_\mu \left[s_\mu^2 - s_\mu^2\left(ma + r\sum\nolimits_\nu \left[\epsilon_\nu(1-s_\nu^2)^{1/2} - 1\right]\right)\cdot\left(r\sum\nolimits_\rho \epsilon_\rho(1-s_\rho^2)^{-1/2}\right)\right]. \qquad (316)
\end{aligned}
$$

Then we have

$$
\begin{aligned}
&B(s) + \frac{1}{5}B(s)^{7/2}\sum\nolimits_\mu \frac{\partial}{\partial s_\mu}B(s)^{-5/2} \\
&= \sum\nolimits_\mu s_\mu^2 + \left\{ma + r\sum\nolimits_\mu (\epsilon_\mu(1-s_\mu^2)^{1/2} - 1)\right\}^2 \\
&\quad - \sum\nolimits_\mu s_\mu^2 + \sum\nolimits_\mu \left[s_\mu^2\left(ma + r\sum\nolimits_\nu \left[\epsilon_\nu(1-s_\nu^2)^{1/2} - 1\right]\right)\cdot\left(r\sum\nolimits_\rho \frac{1}{2}\epsilon_\rho(1-s_\rho^2)^{-1/2}\right)\right] \\
&= \left[ma + r\sum_\mu \left\{\epsilon_\mu(1-s_\mu^2)^{1/2} - 1\right\} + r\sum_\mu s_\mu^2\epsilon_\mu(1-s_\mu^2)^{-1/2}\right]\left[ma + r\sum_\nu \left\{\epsilon_\nu(1-s_\nu^2)^{1/2} - 1\right\}\right] \\
&\qquad (317)
\end{aligned}
$$

Using above identity, we obtain

$$
\frac{\partial}{\partial ma}I(m,r) = -\frac{3}{8\pi^2}\sum_{\epsilon_\mu=\pm 1}\left(\prod_\mu \epsilon_\mu\right)\int_{-1}^{1} d^4s\left[4 + \sum_\nu s_\nu\frac{\partial}{\partial s_\nu}\right]B(s)^{-5/2}. \qquad (318)
$$

And similarly,

$$\frac{\partial}{\partial r}I(m,r) = -\frac{3}{8\pi^2}\sum_{\epsilon_\mu=\pm 1}\left(\prod_\mu \epsilon_\mu\right)\int_{-1}^{1} d^4s \left(4+\sum_\nu s_\nu \frac{\partial}{\partial s_\nu}\right)\left[\epsilon_\rho(1-s_\rho^2)^{\frac{1}{2}}-1\right]B(s)^{-5/2} \tag{319}$$

When $ma \neq 0, 2r, 4r, 6r, 8r,\ B(s)^{-\frac{5}{2}}$ is regular in $-1 \leqq s_\mu \leqq 1$, then we can perform the partial integration. We can show that $\partial I(m,r)/\partial ma = \partial I(m,r)/\partial r = 0$.

$$\begin{aligned}\frac{\partial}{\partial ma}I(m,r) &= \frac{3}{8\pi^2}\sum_{\epsilon_\mu=\pm 1}\left(\prod_\mu \epsilon_\mu\right)\int_{-1}^{1} d^4s \left[\frac{\partial}{\partial s_1}\left(s_1 B(s)^{-5/2}\right)+\frac{\partial}{\partial s_2}\left(s_2 B(s)^{-5/2}\right)\right.\\ &\qquad\left.+\frac{\partial}{\partial s_3}\left(s_3 B(s)^{-5/2}\right)+\frac{\partial}{\partial s_4}\left(s_4 B(s)^{-5/2}\right)\right]\\ &= 0\end{aligned} \tag{320}$$

$\partial I(m,r)/\partial(ma)$ is zero since each term is an odd function with respect to s_μ.

$$\begin{aligned}\frac{\partial}{\partial r}I(m,r) &= -\frac{3}{8\pi^2}\sum_{\epsilon_\mu=\pm 1}\left(\prod_\mu \epsilon_\mu\right)\int_{-1}^{1} d^4sa\left(4-\sum_\nu\right)\left[\epsilon_\rho(1-s_\rho^2)^{\frac{1}{2}}-1\right]B(s)^{-5/2}\\ &\quad+\frac{3}{8\pi^2}\sum_{\epsilon_\mu=\pm 1}\left(\prod_\mu \epsilon_\mu\right)\int_{-1}^{1} d^4s\sum_\nu\frac{\partial}{\partial s_\nu}\left(s_\nu\left[\epsilon_\rho(1-s_\rho^2)^{\frac{1}{2}}-1\right]B(s)^{-5/2}\right) \qquad (321)\\ &= 0 \qquad (322)\end{aligned}$$

As in the case of $\partial I(m,r)/\partial(ma)$, each term is an odd function with respect to each s_μ, so the integral is 0. Therefore, it is confirmed that the coefficients of $I(ma,r)$ are stable and topological for the mass m and the Wilson parameter r.

$I(m,r)$ can be regarded as a function of the ratio of two parameters $\alpha = ma/r$ and the Wilson parameter r. When we fix α, for $\alpha \neq 0,2,4,6,8$, $I(m,r)$ is independent of the value of r. Therefore, we evaluate it with a certain value of r and consider the limit $r \to 0$. We change the integration variable in $I(\alpha r, r)$ as $s_\mu \to r s_\mu$,

$$\begin{aligned}&I(m,r)\\ &= \frac{3}{8\pi^2}\sum_{\epsilon_\mu=\pm 1}\left(\prod_\mu \epsilon_\mu\right)\int_{-1/r}^{1/r} d^4s\left\{\alpha+\sum_\nu\left\{\epsilon_\nu(1-r^2s_\nu^2)^{1/2}-1\right\}+\sum_\nu r^2 s_\nu^2\epsilon_\nu(1-r^2s_\nu^2)^{-1/2}\right\}\\ &\qquad\times\left[\sum_\rho s_\rho^2+\left\{\alpha+\sum_\rho\epsilon_\rho(1-r^2s_\rho^2)^{-1/2}-1\right\}^2\right]^{-5/2},\end{aligned} \tag{323}$$

where the third term in the numerator is $\mathcal{O}(r^2)$ is not necessary for the evaluation at $r \to 0$, so we neglect it. Therefore we have

$$I(\alpha r, r) = \frac{3}{8\pi^2} \sum_{\epsilon_\mu=\pm 1} \left(\prod_\mu \epsilon_\mu\right) \int_{-1/r}^{1/r} d^4 s \\ \times \frac{\alpha + \sum_\nu \left\{\epsilon_\nu (1 - r^2 s_\nu^2)^{1/2} - 1\right\}}{\left(\sum_\rho s_\rho^2 + \left\{\alpha + \sum_\rho \epsilon_\rho (1 - r^2 s_\rho^2)^{-1/2} - 1\right\}^2\right)^{5/2}}. \tag{324}$$

To consider the limit $r \to 0$, we divide the integration region $[-1/r, 1/r]^4$ of $I(\alpha r, r)$ into a four-dimensional cylinder $C(L) \equiv S^3 \times [-L, L]$ and the rest $R(L) \equiv [-1/r, 1/r]^4 - C(L)$. The radius of S^3 is L ($L < 1/r$), and the direction of the cylinder is taken along the ν-direction in the numerator. For the latter integral $I(\alpha r, r)_{R(L)}$, we can show that the limit of $r \to 0$ of the integral vanishes as $L \to \infty$. Therefore the integral becomes

$$\begin{aligned} &\lim_{r\to 0} I(\alpha r, r) \\ &= \frac{3}{8\pi^2} \sum_{\epsilon_\mu=\pm 1} \left(\prod_\mu \epsilon_\mu\right) \lim_{L\to\infty} \lim_{r\to 0} \int_{-L}^{L} d^4 s \frac{\alpha + \sum_\nu \left\{\epsilon_\nu (1 - r^2 s_\nu^2)^{1/2} - 1\right\}}{\left(\sum_\rho s_\rho^2 + \left\{\alpha + \sum_\rho \epsilon_\rho (1 - r^2 s_\rho^2)^{-1/2} - 1\right\}^2\right)^{5/2}} \\ &= \frac{1}{2} \sum_{\epsilon_\mu=\pm 1} \left(\prod_\mu \epsilon_\mu\right) \frac{\alpha + \sum_\nu (\epsilon_\nu - 1)}{\left|\alpha + \sum_\rho (\epsilon_\rho - 1)\right|}. \end{aligned} \tag{325}$$

$\frac{1}{2}\frac{\alpha+\sum_\nu(\epsilon_\nu-1)}{|\alpha+\sum_\rho(\epsilon_\rho-1)|}$ is a step function and performing the summation about ϵ_μ, we obtain

$(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4)$	$\prod_\mu \epsilon_\mu$	$\alpha + \sum_\nu(\epsilon_\nu - 1)$	# of (ϵ_μ)	$\frac{1}{2}\frac{\alpha+\sum_\nu(\epsilon_\nu-1)}{\lvert\alpha+\sum_\rho(\epsilon_\rho-1)\rvert}$
$(+1, +1, +1, +1)$	$+1$	α	1	$\theta(am/r)$
$(+1, +1, +1, -1)\cdots$	-1	$\alpha - 2$	4	$-4\theta(am/r - 2)$
$(+1, +1, -1, -1)\cdots$	$+1$	$\alpha - 4$	6	$+6\theta(am/r - 4)$
$(+1, -1, -1, -1)\cdots$	-1	$\alpha - 6$	4	$-4\theta(am/r - 6)$
$(-1, -1, -1, -1)$	$+1$	$\alpha - 8$	1	$\theta(am/r - 8)$

Therefore, the factor $I(ma, r)$ is given by

$$\begin{aligned} I(ma, r) &= \lim_{r\to 0} I(\alpha r, r) \\ &= \theta(am/r) - 4\theta(am/r - 2) + 6\theta(am/r - 4) - 4\theta(am/r - 6) + \theta(am/r - 8), \end{aligned} \tag{326}$$

where $\theta(x)$ is the step function.

D Asymmetric domain-wall fermion on a lattice

In this Appendix, we summarize the eigenfunction set of the squared of the asymmetric domain-wall Dirac operator. There are three types of eigenfunctions in the x_4 direction: (i) edge-localized modes at $x_4 = 0$, (ii)extended modes but only for $x_4 \geq 0$, (iii) extended modes at any x_4.

(i) Edge-localized modes at $x_4 = 0$

$$\phi_-^{\mathrm{edge}}(x_4) = \sqrt{\frac{M_+ M_-(2+M_+)(2+M_-)}{a(M_+ - M_-)(2+M_+ + M_-)}} \times \begin{cases} e^{-\kappa_+ x_4} & (x_4 \geqq 0) \\ e^{\kappa_- x_4} & (x_4 \leqq -a) \end{cases} \tag{327}$$

$$e^{-\kappa_+ a} = 1 + M_+,\ e^{\kappa_- a} = 1 + M_-.$$

(ii) Extended modes but only for $x_4 \geq 0$

$$\phi_{1,+}^{\omega}(x_4) = \begin{cases} \frac{1}{\sqrt{2\pi}|I_+|}\left[I_+ e^{i\omega(x_4+a)} - I_+^* e^{-i\omega(x_4+a)}\right] & (x_4 \geqq 0), \\ \frac{\tilde{I}_+}{\sqrt{2\pi}|I_+|} e^{k(x_4+a)} & (x_4 \leqq -a). \end{cases} \tag{328}$$

$$I_+ = \frac{1+M_-}{1+M_+} e^{ka} - e^{-i\omega a}, \quad \tilde{I}_+ = e^{i\omega a} - e^{-i\omega a}$$

$$\phi_{1,-}^{\omega}(x_4) = \begin{cases} D_- \left[I_- e^{i\omega(x_4+a)} - I_-^* e^{-i\omega(x_4+a)}\right] & (x_4 \geqq 0), \\ D_- \tilde{I}_- e^{k(x_4+a)} & (x_4 \leqq -a). \end{cases} \tag{329}$$

$$D_- = \frac{1}{\sqrt{2\pi}|I_-|}, \quad I_- = \frac{1+M_+}{1+M_-} e^{ka} - e^{-i\omega a}, \quad \tilde{I}_- = \frac{1+M_+}{1+M_-}\left[e^{i\omega a} - e^{-i\omega a}\right]$$

(iii) Extended modes at any x_4

$$\phi_{2,+}^{\omega(1)}(x_4) = \begin{cases} \frac{1}{\sqrt{2\pi}} T_{+,1} e^{i\omega_+(x_4+a)} & (x_4 \geqq 0), \\ \frac{1}{\sqrt{2\pi}}\left[e^{i\omega_-(x_4+a)} + R_{+,1} e^{-i\omega_-(x_4+a)}\right] & (x_4 \leqq -a). \end{cases} \tag{330}$$

$$R_{+,1} \equiv -\frac{(1+M_+) - (1+M_-)e^{-i(\omega_+ - \omega_-)a}}{(1+M_+) - (1+M_-)e^{-i(\omega_+ + \omega_-)a}} \quad T_{+,1} \equiv \frac{(1+M_-)e^{-i\omega_+ a} 2i \sin\omega_- a}{(1+M_+) - (1+M_-)e^{-i(\omega_+ + \omega_-)a}}$$

$$\phi_{2,+}^{\omega(2)}(x_4) = \begin{cases} \frac{1}{\sqrt{2\pi}}\left[e^{-i\omega_+(x_4+a)} + R_{+,2} e^{i\omega_+(x_4+a)}\right] & (x_4 \geqq 0), \\ \frac{1}{\sqrt{2\pi}} T_{+,2} e^{-i\omega_-(x_4+a)} & (x_4 \leqq -a). \end{cases} \tag{331}$$

$$R_{+,2} \equiv -\frac{(1+M_-) - (1+M_+)e^{-i(\omega_+ - \omega_-)a}}{(1+M_-) - (1+M_+)e^{i(\omega_+ + \omega_-)a}} \quad T_{+,2} \equiv \frac{-(1+M_+)e^{i\omega_- a} 2i \sin\omega_+ a}{(1+M_-) - (1+M_+)e^{i(\omega_+ + \omega_-)a}}$$

$$\phi_{2,-}^{\omega(1)}(x_4) = \begin{cases} \frac{1}{\sqrt{2\pi}} T_{-,1} e^{i\omega_+(x_4+a)} & (x_4 \geqq 0), \\ \frac{1}{\sqrt{2\pi}}\left[e^{i\omega_-(x_4+a)} + R_{-,1} e^{-i\omega_-(x_4+a)}\right] & (x_4 \leqq -a). \end{cases} \tag{332}$$

$$R_{-,1} \equiv -\frac{(1+M_-)e^{i\omega_+ a} - (1+M_+)e^{i\omega_- a}}{(1+M_-)e^{i\omega_+ a} - (1+M_+)e^{-i\omega_- a}} \quad T_{-,1} \equiv \frac{(1+M_-) 2i \sin\omega_- a}{(1+M_-)e^{i\omega_+ a} - (1+M_+)e^{-i\omega_- a}}$$

$$\phi_{2,-}^{\omega(2)}(x_4) = \begin{cases} \frac{1}{\sqrt{2\pi}}\left[e^{-i\omega_+(x_4+a)} + R_{-,2} e^{i\omega_+(x_4+a)}\right] & (x_4 \geqq 0), \\ \frac{1}{\sqrt{2\pi}} T_{-,2} e^{-i\omega_-(x_4+a)} & (x_4 \leqq -a). \end{cases} \tag{333}$$

$$R_{-,2} \equiv -\frac{(1+M_+)e^{-i\omega_- a} - (1+M_-)e^{-i\omega_+ a}}{(1+M_+)e^{-i\omega_- a} - (1+M_-)e^{i\omega_+ a}} \quad T_{-,2} \equiv \frac{-(1+M_+) 2i \sin\omega_+ a}{(1+M_+)e^{-i\omega_- a} - (1+M_-)e^{i\omega_+ a}}$$

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