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CP breaking in lattice chiral gauge theories

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Abstract: The CP symmetry is not manifestly implemented for the local and doubler-free Ginsparg-Wilson operator in lattice chiral gauge theory. We precisely identify where the effects of this CP breaking appear. We show that they appear in: (I) Overall constant phase of the fermion generating functional. (II) Overall constant coefficient of the fermion generating functional. (III) Fermion propagator appearing in external fermion lines and the propagator connected to Yukawa vertices. The first effect appears from the transformation of the path integral measure and it is absorbed into a suitable definition of the constant phase factor for each topological sector; in this sense there appears no "CP anomaly". The second constant arises from the explicit breaking in the action and it is absorbed by the suitable weights with which topological sectors are summed. The last one in the propagator is inherent to this formulation and cannot be avoided by a mere modification of the projection operator, for example, in the framework of the Ginsparg-Wilson operator. This breaking emerges as an (almost) contact term in the propagator when the Higgs field, which is treated perturbatively, has no vacuum expectation value. In the presence of the vacuum expectation value, however, a completely new situation arises and the breaking becomes intrinsically non-local, though this breaking may still be removed in a suitable continuum limit. This non-local CP breaking is expected to persist for a non-perturbative treatment of the Higgs coupling.

Keywords: Renormalization, Regularization and Renormalons, Lattice Gauge Field Theories, Gauge Symmetry, Anomalies in Field and String Theories.

Contents

1. Introduction

Discovery of gauge covariant local lattice Dirac operators [1, 2], which satisfy the Ginsparg-Wilson relation [3], paved a way to a manifestly local and gauge invariant lattice formulation of anomaly-free chiral gauge theories [4]–[10].[1] See also related early works in refs. [13, 14], and refs. [15]–[19] for reviews.

It has been however pointed out that the CP symmetry, the fundamental discrete symmetry in chiral gauge theories, is not manifestly implemented in this formulation. The basic observation related to this effect is as follows [20]: in the formulation, the chirality is imposed through [21, 15]

$$P_{-}\psi = \psi \,, \qquad \overline{\psi P}_{+} = \overline{\psi} \,, \tag{1.1}$$

[1] The locality of the overlap Dirac operator [2] was shown in refs. [11, 12].

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where $\overline{P}_{\pm} = (1 \pm \gamma_5)/2$ and $P_{\pm} = (1 \pm \hat{\gamma}_5)/2$ with $\hat{\gamma}_5 = \gamma_5(1 - 2aD)$, and D is the Dirac operator. The Ginsparg-Wilson relation then guarantees that the kinetic term is consistently decomposed, $\overline{\psi} \overline{P}_+ D\psi = \overline{\psi} D P_- \psi$. However, since the above condition is not symmetric in the fermion and anti-fermion and since CP exchanges these two, CP symmetry is explicitly broken. In fact, the fermion action in the case of pure chiral gauge theory without Higgs couplings changes under CP as[2]

$$S_{\rm F} = a^4 \sum_x \overline{\psi}(x) \overline{P}_+ D P_- \psi(x) \to S_{\rm F} = a^4 \sum_x \overline{\psi}(x) \gamma_5 P_+ \gamma_5 D \overline{P}_- \psi(x) \,, \tag{1.2}$$

and this causes the change in the propagator

$$\begin{aligned} \frac{\langle \psi(x) \overline{\psi}(y) \rangle_{\rm F}}{\langle 1 \rangle_{\rm F}} &= P_- \frac{1}{D} \overline{P}_+(x,y) \,, \\ \to \frac{\langle \psi(x) \overline{\psi}(y) \rangle_{\rm F}}{\langle 1 \rangle_{\rm F}} &= \overline{P}_- \frac{1}{D} \gamma_5 P_+ \gamma_5(x,y) = P_- \frac{1}{D} \overline{P}_+(x,y) - a\gamma_5 a^{-4} \delta_{x,y} \,. \end{aligned} \tag{1.3}$$

One might think that a suitable modification of the chiral projectors would remedy this CP breaking. That this is impossible with the standard CP transformation law has been shown [22] under rather mild assumptions for a general class of Ginsparg-Wilson operators, as long as they are local and free of species doublers. The above CP breaking is thus regarded as an inherent feature of this formulation. Also, the chirality constraint (1.1) is very fundamental and it influences the construction of the fermion integration measure, one might then worry that the CP breaking emerges in many other places and an analysis of CP violation (in the conventional sense) with this formulation would be greatly hampered. It is thus important to precisely identify where the effects of the above CP breaking inherent in this formulation appear.

The purpose of this paper is to clarify the above issue. Following the formulation of refs. [4, 6], we show that the effects of CP violation emerge only at: (I) Overall constant phase of the fermion generating functional. (II) Overall constant coefficient of the fermion generating functional. (III) Fermion propagator appearing in external fermion lines and the propagator connected to Yukawa vertices. Our result is summarized in eq. (4.21) for pure chiral gauge theory and, when there is a Yukawa coupling, in eq. (6.8). The first two constants above depend only on the topological sectors concerned and the problem is reduced to the choice of weights with which various topological sectors are summed. This problem, which is not particular to this formulation, is thus fixed by a suitable choice of weight factors. The last effect in the fermion propagator, on the other hand, is inherent to this formulation. When the Higgs field has no expectation value, as we have seen above, it emerges as an (almost) contact term. However, in the presence of the Higgs expectation value, this breaking becomes intrinsically non-local.

[2]For our conventions, see appendix A. Note that the action of vector-like gauge theories is manifestly invariant under this CP transformation.

2. Formulation

2.1 General Ginsparg-Wilson relation

In our analysis, we assume that the Dirac operator satisfies a general form of the Ginsparg-Wilson relation. In terms of the hermitean operator H

$$H = a\gamma_5 D = aD^\dagger\gamma_5 = H^\dagger\,, \tag{2.1}$$

the relation we adopt is written as

$$\gamma_5 H + H\gamma_5 = 2H^2 f(H^2)\,, \tag{2.2}$$

where $f(H^2)$ is a regular function of H^2 and $f(H^2)^\dagger = f(H^2)$. For simplicity, we assume that $f(x)$ is monotonous and non-decreasing for $x \geq 0$. The simplest choice $f(H^2) = 1$ corresponds to the conventional Ginsparg-Wilson relation [3]. The explicit form of H has been analyzed for $f(H^2) = H^{2k}$ with a positive integer k [23]. The following formal analyses are valid for general $f(H^2)$, and one can recover the standard overlap operator by setting $f(H^2) = 1$ at any stage of our analyses. As an important consequence of eq. (2.2), one has

$$\gamma_5 H^2 = (\gamma_5 H + H\gamma_5)H - H(\gamma_5 H + H\gamma_5) + H^2\gamma_5 = H^2\gamma_5\,. \tag{2.3}$$

With this general Ginsparg-Wilson relation, one may introduce a one-parameter family of lattice analogue of γ_5:

$$\gamma_5^{(t)} = \frac{\gamma_5 - tHf(H^2)}{\sqrt{1 + t(t-2)H^2 f^2(H^2)}}\,. \tag{2.4}$$

Note that $\gamma_5^{(0)} = \gamma_5$ and, when $f(H^2) = 1$, $\gamma_5^{(2)} = \hat\gamma_5$ corresponds to the conventional modified chiral matrix [15]. Also the combination

$$\Gamma_5 = \gamma_5 - Hf(H^2)\,, \tag{2.5}$$

has a special role due to the property

$$\Gamma_5 H + H\Gamma_5 = 0\,. \tag{2.6}$$

Note that $\gamma_5^{(1)} = \Gamma_5/\sqrt{\Gamma_5^2}$. The "conjugate" of $\gamma_5^{(t)}$ is defined by

$$\overline{\gamma}_5^{(t)} = \gamma_5\gamma_5^{(2-t)}\gamma_5\,, \tag{2.7}$$

and they satisfy the following relations:

$$\gamma_5^{(t)\dagger} = \gamma_5^{(t)}\,, \qquad \overline{\gamma}_5^{(t)\dagger} = \overline{\gamma}_5^{(t)}\,, \qquad (\gamma_5^{(t)})^2 = (\overline{\gamma}_5^{(t)})^2 = 1\,, \qquad \overline{\gamma}_5^{(t)} D + D\gamma_5^{(t)} = 0\,. \tag{2.8}$$

In view of the last relation, we introduce the chiral projection operators by

$$P_\pm^{(t)} = \frac{1}{2}\left(1 \pm \gamma_5^{(t)}\right)\,, \qquad \overline{P}_\pm^{(t)} = \frac{1}{2}\left(1 \pm \overline{\gamma}_5^{(t)}\right)\,, \tag{2.9}$$

so that

$$\overline{P}_\pm^{(t)} D = DP_\mp^{(t)}\,. \tag{2.10}$$

Then the chirality may be defined by[3]

$$P_-^{(t)}\psi = \psi\,, \qquad \overline{\psi P_+^{(t)}} = \overline{\psi}\,. \tag{2.11}$$

The kinetic term is then consistently decomposed according to the chirality.

[3]For definiteness, we consider the left-handed Weyl fermion.

2.2 Generating functional and the measure term

In the formulation of refs. [4, 6], the expectation value of an operator $\mathcal{O}$ is given by

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \sum_M \int_M \mathrm{D}[U]\, e^{-S_G} \mathcal{N}_M e^{i\vartheta_M} \langle \mathcal{O} \rangle_{\mathrm{F}}^M \,, \tag{2.12}$$

where M denotes the topological sector specified by the admissibility,[4]

$$\|1 - R[U(x,\mu,\nu)]\| < \epsilon \,, \qquad \text{for all plaquettes } (x,\mu,\nu)\,, \tag{2.13}$$

which guarantees the locality[5] and the smoothness of the Dirac operator [11, 12]. The "topological weight", $\mathcal{N}_M e^{i\vartheta_M}$, with which the topological sectors are summed, is not fixed within this formulation. In each topological sector M, the average with respect to the fermion fields $\langle \mathcal{O} \rangle_{\mathrm{F}}^M$ is defined by the generating functional of fermion Green's functions

$$Z_{\mathrm{F}}[U,\eta,\overline{\eta};t] = \int \mathrm{D}[\psi]\mathrm{D}[\overline{\psi}]\, e^{-S_{\mathrm{F}}} \,, \tag{2.14}$$

where we have written the dependence on the parameter t in eq. (2.4) explicitly and

$$S_{\mathrm{F}} = a^4 \sum_x \left[\overline{\psi}(x) D\psi(x) - \overline{\psi}(x)\eta(x) - \overline{\eta}(x)\psi(x) \right] . \tag{2.15}$$

The fermion integration variables are subject to the chirality constraint (2.11).[6]

To define the fermion integration measure, we thus introduce certain orthonormal vectors in the constrained space,

$$P_-^{(t)} v_j(x) = v_j(x), \qquad \overline{v}_k \overline{P}_+^{(t)}(x) = \overline{v}_k(x)\,, \tag{2.16}$$

and expand the fields as

$$\psi(x) = \sum_j v_j(x) c_j, \qquad \overline{\psi}(x) = \sum_k \overline{c}_k \overline{v}_k(x)\,. \tag{2.17}$$

Then the (ideal) integration measure is defined by

$$\mathrm{D}[\psi]\mathrm{D}[\overline{\psi}] = \prod_j \mathrm{d}c_j \prod_k \mathrm{d}\overline{c}_k\,. \tag{2.18}$$

The condition (2.16) shows that the basis vectors may depend on the gauge field because the chiral projectors depend on it. However, the condition (2.16) alone does not specify

[4]Throughout this paper, we assume that the representation of the gauge group, R, is unitary.

[5]The locality of the operator in eq. (2.2) for general $f(H^2)$ is not known. The locality of free H for $f(H^2) = H^{2k}$ with a positive integer k has been established, and the topological properties of H for $f(H^2) = H^{2k}$ with a positive integer k are known to be identical to those of the standard overlap operator [23].

[6]We first analyze the case of pure chiral gauge theory without Higgs couplings, and we shall later analyze the case with Higgs couplings in section 6.

the fermion measure uniquely and there is an ambiguity of the phase. For two different choices of basis, $\{v, \overline{v}\}$ and $\{w, \overline{w}\}$, we have

$$Z_{\mathrm{F}}^{\{v,\overline{v}\}}[U,\eta,\overline{\eta};t] = e^{i\theta[U;t]} Z_{\mathrm{F}}^{\{w,\overline{w}\}}[U,\eta,\overline{\eta};t] \,, \tag{2.19}$$

where the phase is given by the jacobian for the change of basis

$$\begin{aligned} e^{i\theta[U;t]} &= \det \mathcal{Q} \det \overline{\mathcal{Q}} \\ &= \exp(\mathrm{Tr} \ln \mathcal{Q} + \mathrm{Tr} \ln \overline{\mathcal{Q}}) \,, \end{aligned} \tag{2.20}$$

where $\mathcal{Q}_{jk} = (w_j, v_k)$ and $\overline{\mathcal{Q}}_{jk} = (\overline{v}_j^\dagger, \overline{w}_k^\dagger)$. Note that the phase depends only on the gauge field. Under an infinitesimal variation of the gauge field,

$$\delta_\eta U(x,\mu) = a\eta_\mu(x) U(x,\mu) \,, \tag{2.21}$$

the variation of the phase is given by[7]

$$\delta_\eta \theta[U;t] = -\mathfrak{L}_\eta^{\{v,\overline{v}\}}[U;t] + \mathfrak{L}_\eta^{\{w,\overline{w}\}}[U;t] \,, \tag{2.23}$$

where the "measure term" is defined by

$$\mathfrak{L}_\eta^{\{v,\overline{v}\}}[U;t] = i \sum_j (v_j, \delta_\eta v_j) + i \sum_k (\delta_\eta \overline{v}_k^\dagger, \overline{v}_k^\dagger) \,. \tag{2.24}$$

To see the physical meaning of the measure term, let us temporarily assume that there is no zero-modes of the Dirac operator. Then the effective action without fermion sources is given by

$$\langle 1 \rangle_{\mathrm{F}} = \det M, \qquad M_{kj} = a^4 \sum_x \overline{v}_k(x) D v_j(x) \,, \tag{2.25}$$

and its variation under eq. (2.21) is given by[8]

$$\delta_\eta \ln \det M = \mathrm{Tr}(\delta_\eta D P_-^{(t)} D^{-1} \overline{P}_+^{(t)}) - i\mathfrak{L}_\eta^{\{v,\overline{v}\}} \,. \tag{2.26}$$

[7]This is derived from

$$\begin{aligned} i\theta[U;t] + i\delta_\eta\theta[U;t] &= \mathrm{Tr} \ln(w_j + \delta_\eta w_j, v_k + \delta_\eta v_k) + \mathrm{Tr} \ln(\overline{v}_j^\dagger + \delta_\eta \overline{v}_j^\dagger, \overline{w}_k^\dagger + \delta_\eta \overline{w}_k^\dagger) \\ &= i\theta[U;t] - i\mathfrak{L}_\eta^{\{v,\overline{v}\}}[U;t] + i\mathfrak{L}_\eta^{\{w,\overline{w}\}}[U;t] \,. \end{aligned} \tag{2.22}$$

[8]We note that how the basis vectors v_j and $\overline{v}_k$ change when the gauge field is varied cannot be determined by the constraint (2.16) alone. We first note the identity $\delta_\eta v_j = P_-^{(t)} \delta_\eta v_j + (1 - P_-^{(t)}) \delta_\eta v_j$, and then note that the constraint (2.16) implies $(1 - P_-^{(t)}) \delta_\eta v_j = \delta_\eta P_-^{(t)} v_j$ and $\delta_\eta P_-^{(t)}$ is given by the construction of $P_-^{(t)}$. Consequently, the second term of the variation $\delta_\eta v_j$, $(1 - P_-^{(t)}) \delta_\eta v_j$, is fixed uniquely. However, the component of $\delta_\eta v_j$ residing in the constrained space, $P_-^{(t)} \delta_\eta v_j$, is not determined by the constraint (2.16). If one assumes that v_j and $\overline{v}_k$ change gauge covariantly under an infinitesimal gauge transformation, $\delta_\eta v_j(x) = R(\omega(x)) v_j(x)$ and $\delta_\eta \overline{v}_k(x) = -\overline{v}_k(x) R(\omega(x))$, then the effective action (2.25) becomes invariant under the gauge transformation. This assumption of the specific gauge variation of (ideal) basis vectors, however, modifies the physical contents of the theory in general, because it does not reproduce the gauge anomaly. We will see such an example of basis vectors in section 3.

Since the measure term $-i\mathfrak{L}_\eta$ is pure imaginary, as its definition (2.20) implies, it contributes only to the imaginary part of eq. (2.26):

$$\begin{aligned}\frac{1}{2}\left[\mathrm{Tr}(\delta_\eta D P_-^{(t)} D^{-1}\overline{P}_+^{(t)}) - \mathrm{Tr}(\delta_\eta D P_-^{(t)} D^{-1}\overline{P}_+^{(t)})^*\right] &=\\ &= \frac{1}{2}\left[\mathrm{Tr}(\delta_\eta D P_-^{(t)} D^{-1}) - \mathrm{Tr}(\delta_\eta D P_+^{(2-t)} D^{-1})\right]\\ &= -\frac{1}{4}\,\mathrm{Tr}\,\delta_\eta D(\gamma_5^{(t)} + \gamma_5^{(2-t)})D^{-1}\,, \end{aligned} \tag{2.27}$$

where we have used $D^\dagger = \gamma_5 D \gamma_5$ and eq. (2.7). The measure term is then chosen to improve the imaginary part of the effective action (see, for example, ref. [5]).

The above general setup, which is closely related to the overlap formulation in refs. [13, 14], does not specify the formulation uniquely, leaving the phase unspecified. The crucial next task is to find an ideal basis in eq. (2.18) or the associated measure term for which the gauge invariance (assuming the fermion multiplet is anomaly-free) and the locality are ensured for finite lattice spacings. For U(1) theories, such a measure was constructed by Lüscher [4]. For general non-abelian theories, the measure has been constructed only in perturbation theory [9, 7] but the existence of such an ideal fermion measure in non-perturbative level has not been established (except the case of electroweak $\mathrm{SU}(2)\times\mathrm{U}(1)$ on the infinite volume lattice [8]). In this paper, we discuss the effect of CP breaking in this formulation by simply assuming the existence of such an ideal measure.[9]

Our strategy to analyze the CP breaking is as follows: we first determine the general structure of the fermion generating functional by using a convenient auxiliary basis. Then using an argument of the change of basis and a property of the measure term, we find the CP transformation law of the generating functional.

3. General structure of the generating functional

3.1 Generating functional with an auxiliary basis

The relation (2.19) shows that we may use any basis $\{w,\overline{w}\}$ as an intermediate tool in analyzing $Z_{\mathrm{F}}^{\{v,\overline{v}\}}$, if $e^{i\theta[U;t]}$ and $Z_{\mathrm{F}}^{\{w,\overline{w}\}}$ are properly treated. A particularly convenient basis is provided by the eigenfunctions of the hermitean operator $D^\dagger D = H^2/a^2$:

$$D^\dagger D u_j(x) = \frac{1}{a^2} H^2 u_j(x) = \frac{\lambda_j^2}{a^2} u_j(x)\,, \qquad \lambda_j \geq 0\,, \tag{3.1}$$

and their appropriate projection

$$w_j(x) = P_-^{(t)} u_j(x)\,, \qquad (w_j, w_k) = \delta_{jk}\,. \tag{3.2}$$

Note that $D^\dagger D$ and $P_-^{(t)}$ commute. From appendix B, where the properties of these eigenfunctions are summarized, we see that the following vectors have an appropriate chiral-

[9] Note however that our analysis is relevant for a manifestly gauge invariant perturbation theory [9] based on this formulation.

ity as w_j:

$$\begin{aligned}
&\varphi_0^-(x)\,, && \lambda_j=0\,,\\
&\varphi_j^-(x)\,, && \lambda_j>0\,,\quad \lambda_j\neq\Lambda\,,\\
&\begin{cases}\Psi_+(x)\,, & \text{for } t>1\,,\\ \Psi_-(x)\,, & \text{for } t<1\,,\end{cases} && \lambda_j=\Lambda\,,
\end{aligned}\tag{3.3}$$

where the number Λ is a solution of $\Lambda f(\Lambda^2)=1$.

As for the vectors $\overline{w}_k$, we may adopt the left eigenfunctions of the hermitean operator $DD^\dagger$.[10] For non-zero eigenvalues, as is well-known, there is a one-to-one correspondence between the eigenfunctions of $D^\dagger D$ and $DD^\dagger$:

$$\overline{w}_j(x)=\frac{a}{\lambda_j}w_j^\dagger D^\dagger(x)\,.\tag{3.4}$$

This has the proper chirality as $\overline{w}_k$, $\overline{w}_k\overline{P}_+^{(t)}=\overline{w}_k$. The zero-modes of $DD^\dagger$ cannot be expressed in this way and we may use instead

$$\varphi_0^{+\dagger}(x)\,.\tag{3.5}$$

Then eqs. (3.4) and (3.5) span a complete set in the constrained space $\overline{w}_k\overline{P}_+^{(t)}=\overline{w}_k$.

Once having specified basis vectors $\{w,\overline{w}\}$, it is straightforward to perform the integration in $Z_{\rm F}^{\{w,\overline{w}\}}$. After some calculation, we have

$$\begin{aligned}
Z_{\rm F}^{\{w,\overline{w}\}}[U,\eta,\overline{\eta};t]={}&\left(\frac{\Lambda}{a}\right)^N\prod^{n_-}\left[a^4\sum_x\overline{\eta}(x)\varphi_0^-(x)\right]\prod^{n_+}\left[a^4\sum_x\varphi_0^{+\dagger}(x)\eta(x)\right]\prod_{\substack{\lambda_j>0\\ \lambda_j\neq\Lambda}}\left(\frac{\lambda_j}{a}\right)\times\\
&\times\exp\left[a^8\sum_{x,y}\overline{\eta}(x)G^{(t)}(x,y)\eta(y)\right],
\end{aligned}\tag{3.6}$$

up to the over-all sign ±1 which depends on the ordering in the measure $\prod_j {\rm d}c_j\prod_k {\rm d}\overline{c}_k$.[11] In this expression, the Green's function has been defined by

$$DG^{(t)}(x,y)=\overline{P}_+^{(t)}(x,y)-\sum^{n_+}\varphi_0^+(x)\varphi_0^{+\dagger}(y)\,,\tag{3.7}$$

or more explicitly,

$$G^{(t)}(x,y)=\sum_{\lambda_j>0}\frac{a^2}{\lambda_j^2}\,\varphi_j^-(x)\varphi_j^{-\dagger}D^\dagger(y)\,.\tag{3.8}$$

The number of zero-modes φ_0^- (φ_0^+) has been denoted by n_- (n_+) and

$$N=\begin{cases}N_+\,, & \text{for } t>1\,,\\ N_-\,, & \text{for } t<1\,,\end{cases}\tag{3.9}$$

where N_+ and N_- stand for the numbers of eigenfunctions Ψ_+ and Ψ_-, respectively (see appendix B). Since eigenvalues λ_j are gauge invariant and eigenfunctions φ_j can be chosen to be gauge covariant, the above $Z_{\rm F}^{\{w,\overline{w}\}}$ is manifestly gauge invariant for gauge covariant

[10] Incidentally, the Ginsparg-Wilson relation implies that $DD^\dagger=\gamma_5H^2\gamma_5/a^2=H^2/a^2=D^\dagger D$.

[11] This sign factor can be absorbed into the phase $\theta[U;t]$ without loss of generality.

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external sources. However, this $Z_{\mathrm{F}}^{\{w,\overline{w}\}}$ as it stands cannot be interpreted as the generating functional for the Weyl fermion, as we will explain shortly (rather it is regarded as representing a half of the Dirac fermion).

3.2 Measure term for the auxiliary basis

Let us consider the measure term (2.24) for the auxiliary basis. Namely,

$$\mathfrak{L}_\eta^{\{w,\overline{w}\}}[U;t] = i\sum_j (w_j, \delta_\eta w_j) + i\sum_k \left(\delta_\eta \overline{w}_k^\dagger, \overline{w}_k^\dagger\right). \tag{3.10}$$

Noting $H^2 w_j = \lambda_j^2 w_j$ and thus

$$\delta_\eta \lambda_j^2 = \left(w_j, \delta_\eta H^2 w_j\right), \tag{3.11}$$

we have from eq. (3.4),

$$\left(\delta_\eta \overline{w}_j^\dagger, \overline{w}_j^\dagger\right) = -\frac{1}{2\lambda_j^2}\left(w_j, [H, \delta_\eta H] w_j\right) + \left(\delta_\eta w_j, w_j\right). \tag{3.12}$$

Taking the contribution of zero-modes into account, we thus have

$$\mathfrak{L}_\eta^{\{w,\overline{w}\}}[U;t] = i\sum^{n_-}\left(\varphi_0^-, \delta_\eta \varphi_0^-\right) + i\sum^{n_+}\left(\delta_\eta \varphi_0^+, \varphi_0^+\right) - \frac{i}{2}\sum_{\lambda_j>0}\left(\varphi_j^-, [H^{-1}, \delta_\eta H]\varphi_j^-\right). \tag{3.13}$$

The last term may be written in a basis independent way

$$\begin{aligned} -\frac{i}{2}\,\mathrm{Tr}'\left[H^{-1}, \delta_\eta H\right] P_-^{(t)} &= \frac{i}{4}\,\mathrm{Tr}'\left(H^{-1}\delta_\eta H \gamma_5^{(t)} - \delta_\eta H H^{-1}\gamma_5^{(t)}\right) \\ &= \frac{i}{4}\,\mathrm{Tr}'\,\delta_\eta H\left(\gamma_5^{(t)} + \gamma_5^{(2-t)}\right) H^{-1}, \end{aligned} \tag{3.14}$$

where Tr' denotes the trace over the subspace of non-zero modes of the hermitean operator H.[12] In deriving the last line, we have used the relation $H^{-1}\gamma_5^{(t)} = -\gamma_5^{(2-t)}H^{-1}$ being valid in this subspace. Noting $H^{-1}\gamma_5\gamma_5\delta_\eta H = D^{-1}\delta_\eta D$, we have

$$\mathfrak{L}_\eta^{\{w,\overline{w}\}}[U;t] = i\sum^{n_-}\left(\varphi_0^-, \delta_\eta \varphi_0^-\right) + i\sum^{n_+}\left(\delta_\eta \varphi_0^+, \varphi_0^+\right) + \frac{i}{4}\,\mathrm{Tr}'\,\delta_\eta D\left(\gamma_5^{(t)} + \gamma_5^{(2-t)}\right) D^{-1}. \tag{3.15}$$

This expression shows that the auxiliary basis w_j and $\overline{w}_k$ cannot be a physically sensible one (namely, we cannot take $\{v,\overline{v}\} = \{w,\overline{w}\}$) because the measure term is non-local, containing the propagator D^{-1}. In fact, we see that $i\mathfrak{L}_\eta^{\{w,\overline{w}\}}$ is identical to (a variation of) the main part of the imaginary part of the fermion effective action (2.27), when there is no zero-modes. Consequently, this basis when identified as $\{v,\overline{v}\} = \{w,\overline{w}\}$ modifies the physical contents of the theory, eliminating the imaginary part. This explains why the generating functional with this basis is gauge invariant, even if the fermion multiplet is not anomaly-free. Nevertheless, this basis is convenient as an intermediate tool as one can work out all the quantities.

[12] One thus has to be careful whether the operator concerned preserves this subspace when using the cyclic property of the trace.

3.3 $Z_{\mathrm{F}}^{\{v,\overline{v}\}}$

From eqs. (2.19) and (3.6), the general structure of the fermion generating functional is given by (omitting the superscript $\{v,\overline{v}\}$)

$$Z_{\mathrm{F}}[U,\eta,\overline{\eta};t] = e^{i\theta[U;t]}\left(\frac{\Lambda}{a}\right)^{N}\prod^{n_-}\left[a^4\sum_x \overline{\eta}(x)\varphi_0^-(x)\right]\prod^{n_+}\left[a^4\sum_x \varphi_0^{+\dagger}(x)\eta(x)\right]\prod_{\substack{\lambda_j>0\\ \lambda_j\neq\Lambda}}\left(\frac{\lambda_j}{a}\right)\times$$
$$\times\exp\left[a^8\sum_{x,y}\overline{\eta}(x)G^{(t)}(x,y)\eta(y)\right], \tag{3.16}$$

where the variation of the phase $\theta[U;t]$ is given by eq. (2.23) and the measure term for the auxiliary basis is given by eq. (3.15). We see that the vital characterization as the *chiral* theory is contained in the phase $\theta[U;t]$ which may be computed, only after finding the ideal basis $\{v,\overline{v}\}$ (or the associated measure). For our discussion of CP breaking, however, only a certain property of the measure term $\mathfrak{L}_\eta^{\{v,\overline{v}\}}[U;t]$ will turn out to be sufficient.

4. CP transformed generating functional

4.1 Generating functional and CP transformation

We first note

$$\begin{aligned}\left\|1-R\left[U^{\mathrm{CP}}(x,i,j)\right]\right\| &= \left\|1-R\left[U(\bar{x}-a\hat{i}-a\hat{j},i,j)\right]\right\|,\\ \left\|1-R\left[U^{\mathrm{CP}}(x,i,4)\right]\right\| &= \left\|1-R\left[U(\bar{x}-a\hat{i},i,4)\right]\right\|,\end{aligned} \tag{4.1}$$

according to the CP transformation law of the plaquette variables in appendix A. Thus, if U is an admissible configuration, so is U^{CP}; CP preserves the admissibility. Note however that U and U^{CP} may belong to different topological sectors in general. In fact, the index $n_+ - n_-$ [24] is opposite for U and for U^{CP} (see appendix B):

$$\operatorname{Tr}\Gamma_5(U) = n_+ - n_- = -\operatorname{Tr}\Gamma_5\left(U^{\mathrm{CP}}\right), \tag{4.2}$$

from $\Gamma_5\left(U^{\mathrm{CP}}\right) = -W^{-1}\left(\gamma_5\Gamma_5(U)\gamma_5\right)^T W$.[13]

[13] We have

$$H\left(U^{\mathrm{CP}}\right) = -W^{-1}(\gamma_5 H(U)\gamma_5)^T W, \tag{4.3}$$

and

$$\begin{aligned}\gamma_5^{(t)}\left(U^{\mathrm{CP}}\right) &= -W^{-1}\overline{\gamma}_5^{(2-t)}(U)^T W, & \overline{\gamma}_5^{(t)}\left(U^{\mathrm{CP}}\right) &= -W^{-1}\gamma_5^{(2-t)}(U)^T W,\\ P_\pm^{(t)}\left(U^{\mathrm{CP}}\right) &= W^{-1}\overline{P}_\mp^{(2-t)}(U)^T W, & \overline{P}_\pm^{(t)}\left(U^{\mathrm{CP}}\right) &= W^{-1}P_\mp^{(2-t)}(U)^T W,\end{aligned} \tag{4.4}$$

from the CP transformation law in appendix A. Throughout this paper, the transpose operation and the complex conjugation of an operator are defined with respect to the corresponding kernel in position space. Strictly speaking, the coordinates x in these expressions are replaced by $\bar{x} = (-x_i, x_4)$ under CP. We can forgo writing this explicitly, because our final expressions always involve an integration over x and $\sum_x = \sum_{\bar{x}}$.

Now, let us consider the CP transformed generating functional[14]

$$Z_{\mathrm{F}}\left[U^{\mathrm{CP}}, -W^{-1}\overline{\eta}^{T}, \eta^{T}W; t\right] = \int \mathrm{D}\left[\psi\right] \mathrm{D}\left[\overline{\psi}\right]\, e^{-S_{\mathrm{F}}}\,, \tag{4.6}$$

where

$$S_{\mathrm{F}} = a^4 \sum_x \left[\overline{\psi}(x) D\left(U^{\mathrm{CP}}\right)\psi(x) + \overline{\psi}(x) W^{-1}\overline{\eta}^{T}(x) - \eta^{T}(x) W \psi(x)\right]\,, \tag{4.7}$$

and $\mathrm{D}[\psi]\mathrm{D}[\overline{\psi}] = \prod_j \mathrm{d}c_j \prod_k \mathrm{d}\bar{c}_k$. Here the ideal basis vectors in $\psi(x) = \sum_j v_j(x) c_j$ and $\overline{\psi}(x) = \sum_k \bar{c}_k \overline{v}_k(x)$ are defined through the constraints:

$$P_-^{(t)}\left(U^{\mathrm{CP}}\right) v_j(x) = v_j(x)\,, \qquad \overline{v}_k(x) \overline{P}_+^{(t)}\left(U^{\mathrm{CP}}\right) = \overline{v}_k(x)\,. \tag{4.8}$$

The generating functional (4.6) can then be written as

$$\begin{aligned} &Z_{\mathrm{F}}\left[U^{\mathrm{CP}}, -W^{-1}\overline{\eta}^{T}, \eta^{T}W; t\right] = \\ &= \int \prod_j \mathrm{d}c_j \prod_k \mathrm{d}\bar{c}_k \, \exp\left\{-a^4 \sum_x \left[\overline{\psi}'(x) D(U)\psi'(x) - \overline{\eta}(x)\psi'(x) - \overline{\psi}'(x)\eta(x)\right]\right\}, \end{aligned} \tag{4.9}$$

where

$$\begin{aligned} \psi'(x) &= \left[\overline{\psi}(\bar{x}) W^{-1}\right]^T = \sum_k \bar{c}_k \left[\overline{v}_k(\bar{x}) W^{-1}\right]^T, \\ \overline{\psi}'(x) &= \left[-W\psi(\bar{x})\right]^T = \sum_j \left[-W v_j(\bar{x})\right]^T c_j\,. \end{aligned} \tag{4.10}$$

Since the basis vectors in eq. (4.10),

$$v'_k = \left(\overline{v}_k W^{-1}\right)^T\,, \qquad \overline{v}'_j = \left(-W v_j\right)^T\,, \tag{4.11}$$

satisfy the constraints

$$P_-^{(2-t)}(U) v'_k = v'_k\,, \qquad \overline{v}'_j \overline{P}_+^{(2-t)}(U) = \overline{v}'_j\,, \tag{4.12}$$

a comparison of eq. (4.9) with the original generating functional (2.14) shows

$$Z_{\mathrm{F}}\left[U^{\mathrm{CP}}, -W^{-1}\overline{\eta}^{T}, \eta^{T}W; t\right] = Z_{\mathrm{F}}[U, \eta, \overline{\eta}; 2-t]\,. \tag{4.13}$$

Thus the sole effect of the CP transformation is given by the change of the parameter, $t \to 2-t$. Instead of repeating the calculation in section 3 for U^{CP}, it is thus enough to examine the effect of $t \to 2-t$ in eq. (3.16).[15]

[14] It is possible to write this formula as

$$\begin{aligned} &Z_{\mathrm{F}}\left[U^{\mathrm{CP}}, -W^{-1}\overline{\eta}^{T}, \eta^{T}W; t\right] = \\ &= \int \mathrm{D}\left[\psi^{\mathrm{CP}}\right] \mathrm{D}\left[\overline{\psi}^{\mathrm{CP}}\right] \exp\left\{-a^4 \sum_x \left[\overline{\psi}^{\mathrm{CP}}(x) D\left(U^{\mathrm{CP}}\right)\psi^{\mathrm{CP}}(x) + \overline{\psi}^{\mathrm{CP}}(x) W^{-1}\overline{\eta}^{T}(x) - \eta^{T}(x) W \psi^{\mathrm{CP}}(x)\right]\right\}. \end{aligned} \tag{4.5}$$

One thus sees that there are two possible sources of CP violation: an explicit breaking in the action and an anomalous breaking in the path integral measure.

[15] The dimensionality of fermionic spaces before and after CP transformation is however different,

$$\mathrm{Tr}\left[\overline{P}_+^{(2-t)}(U) + P_-^{(2-t)}(U)\right] - \mathrm{Tr}\left[\overline{P}_+^{(t)}(U) + P_-^{(t)}(U)\right] = 2\frac{t-1}{|t-1|}(n_+ - n_-)\,, \tag{4.14}$$

namely, the dimensionality jumps at $t = 1$ in the presence of topologically non-trivial gauge field.

In eq. (3.16), we note that the zero-modes φ_0^-, φ_0^+ and the eigenvalues λ_j are independent of t (see appendix B). The change $t \to 2-t$, however, causes the exchange of Ψ_+ and Ψ_- as shown in eq. (3.3) and thus $N \to \overline{N}$, where

$$\overline{N} = \begin{cases} N_- & \text{for } t > 1\,, \\ N_+ & \text{for } t < 1\,. \end{cases} \tag{4.15}$$

Thus, we immediately have

$$\begin{aligned} Z_{\mathrm{F}}\left[U^{\mathrm{CP}}, -W^{-1}\overline{\eta}^T, \eta^T W; t\right] &= \\ = e^{i\theta[U;2-t]}\left(\frac{\Lambda}{a}\right)^{\overline{N}} &\prod^{n_-}\left[a^4\sum_x \overline{\eta}(x)\varphi_0^-(x)\right]\prod^{n_+}\left[a^4\sum_x \varphi_0^{+\dagger}(x)\eta(x)\right]\prod_{\substack{\lambda_j>0\\ \lambda_j\neq\Lambda}}\left(\frac{\lambda_j}{a}\right)\times \\ \times \exp&\left[a^8\sum_{x,y}\overline{\eta}(x)G^{(2-t)}(x,y)\eta(y)\right], \end{aligned} \tag{4.16}$$

for the generating functional.

As for the phase factor $e^{i\theta[U;t]}$, its variation is given by eq. (2.23). The measure terms for the auxiliary basis $\mathfrak{L}_\eta^{\{w,\overline{w}\}}$ is invariant under $t \to 2-t$:

$$\mathfrak{L}_\eta^{\{w,\overline{w}\}}[U; 2-t] = \mathfrak{L}_\eta^{\{w,\overline{w}\}}[U; t]\,, \tag{4.17}$$

as can readily be seen from eq. (3.15). Moreover, in the next section, we will show that it is always possible to choose the ideal basis vectors such that

$$\mathfrak{L}_\eta^{\{v,\overline{v}\}}[U; 2-t] = \mathfrak{L}_\eta^{\{v,\overline{v}\}}[U; t]\,. \tag{4.18}$$

As a result, we have

$$\delta_\eta\left(\theta[U;2-t] - \theta[U;t]\right) = 0\,, \tag{4.19}$$

and the difference, $\theta[U;2-t] - \theta[U;t]$, if it exists, is a *constant*:

$$\theta[U;2-t] = \theta[U;t] + \theta_M\,, \tag{4.20}$$

where the constant θ_M is assigned for each topological sector M, $U \in M$.

From the above analysis, we have

$$\begin{aligned} Z_{\mathrm{F}}[U^{\mathrm{CP}}, -W^{-1}\overline{\eta}^T, \eta^T W; t] &= \\ = e^{i\theta_M}\left(\frac{\Lambda}{a}\right)^{\overline{N}-N} &\frac{\exp\left[a^8\sum_{x,y}\overline{\eta}(x)G^{(2-t)}(x,y)\eta(y)\right]}{\exp\left[a^8\sum_{x,y}\overline{\eta}(x)G^{(t)}(x,y)\eta(y)\right]} Z_{\mathrm{F}}[U,\eta,\overline{\eta};t]\,. \end{aligned} \tag{4.21}$$

In particular, in the vacuum sector which contains the trivial configuration $U_0(x,\mu) = 1$, $U_0^{\mathrm{CP}} = U_0$ and thus one has $\theta_M = 0$ (recall that the phase depends only on the gauge field).

From eq. (4.21), we see that the CP breaking in this formulation appears in three places: (I) Difference in the overall constant phase θ_M. (II) Difference in the overall coefficient $(\Lambda/a)^{\overline{N}-N}$ (III) Difference in the propagator, $G^{(t)}$ and $G^{(2-t)}$. We discuss their implications in this order:

(I) The *constant* phase θ_M may be absorbed into a redefinition of the phase factor ϑ_M in eq. (2.12) as

$$\vartheta_M \to \vartheta_M + \frac{1}{2}\theta_M , \qquad \vartheta_{M^{\rm CP}} \to \vartheta_{M^{\rm CP}} - \frac{1}{2}\theta_M . \tag{4.22}$$

Then the overall phases in $Z_{\rm F}[U]$ and $Z_{\rm F}[U^{\rm CP}]$ become identical (no "CP anomaly" from the path integral measure) and the discussion of CP violation is reduced to how one should choose the "topological phase" ϑ_M; this is a problem analogous to the strong CP problem.

(II) The breaking $(\Lambda/a)^{\overline{N}-N}$ can also be absorbed into the topological weight $\mathcal{N}_M$ in eq. (2.12). Namely, we may redefine

$$\mathcal{N}_M \to \mathcal{N}_M \left(\frac{\Lambda}{a}\right)^{(-N+\overline{N})/2} , \qquad \mathcal{N}_{M^{\rm CP}} \to \mathcal{N}_{M^{\rm CP}} \left(\frac{\Lambda}{a}\right)^{(N-\overline{N})/2} . \tag{4.23}$$

This redefinition is consistent because the roles of N and $\overline{N}$ are exchanged under $U \leftrightarrow U^{\rm CP}$. Note that

$$-N + \overline{N} = \begin{cases} n_+ - n_- , & \text{for } t > 1 , \\ n_- - n_+ , & \text{for } t < 1 , \end{cases} \tag{4.24}$$

due to the chirality sum rule [25, 26]. (The index $n_+ - n_-$ does not depend on $f(H^2)$, see appendix B.) The simplest CP invariant choice is then $\mathcal{N}_M = 1$ for all topological sectors. However, whether this simplest choice is consistent with other physical requirements, such as the cluster decomposition, is another question which we do not discuss in this paper. Interestingly, this simplest CP invariant choice is also suggested [27] by a matching with the "Majorana formulation".

(III) It seems impossible to remedy the breaking $G^{(2-t)} \neq G^{(t)}$ in the propagator. Note that the propagator is independent of the choice of the basis vectors or the path integral measure. For the symmetric choice $t = 1$, $\gamma_5^{(1)} = \Gamma_5/\sqrt{\Gamma_5^2}$ is plagued with the singularity due to zero-modes of Γ_5, whose inevitable presence is proven under rather mild assumptions [22]. However, observe that the CP breaking for $t \neq 1$ is quite modest. For example, when there are no zero-modes,

$$G^{(2-t)} = P_-^{(2-t)} \frac{1}{D} \overline{P}_+^{(2-t)} = G^{(t)} + \frac{a(1-t)f(H^2)}{\sqrt{1 + t(t-2)H^2 f^2(H^2)}} \gamma_5 , \tag{4.25}$$

thus the breaking term is local. In particular, for the conventional choice, $t = 2$ and $f(H^2) = 1$,

$$G^{(2-t)}(x,y) = G^{(t)}(x,y) - a\gamma_5 \frac{1}{a^4} \delta_{x,y} , \tag{4.26}$$

and the breaking appears as an (ultra-local) contact term, as we have noted in Introduction. It is thus expected that this breaking is safely removed in a suitable continuum limit in the case of pure chiral gauge theory. However, there appear additional complications when the Yukawa coupling is included and the Higgs field acquires the expectation value; this issue will be discussed in section 6.

In summary, the inherent CP violation in this framework emerges only in the fermion propagator which is connected to external sources. This implies that diagrams with external fermion lines or with a fermion composite operator would behave differently from the naively expected one under CP, but the vacuum polarization, for example, respects CP. As for other possible sources of CP violation in relative topological weight factors, the same problem appears in continuum theory also and it is not particular to the present formulation of lattice chiral gauge theory.

5. Property of the ideal measure term

5.1 Reconstruction theorem[16]

In our formulation, the basis vectors $\overline{v}_k(x)$ for $\overline{\psi}(x)$ may also depend on the gauge field. Thus, to accommodate this case, we need to slightly generalize the reconstruction theorem [4, 6] which represents precise conditions for the "ideal" measure term.

The measure term $\mathfrak{L}_\eta$ can be interpreted as the U(1) connection associated to a fiber bundle defined over the space of admissible configurations [28, 4]. The U(1) connection is characterized by its "curvature"[17]

$$\begin{aligned}\delta_\eta\mathfrak{L}_\zeta-\delta_\zeta\mathfrak{L}_\eta+a\mathfrak{L}_{[\eta,\zeta]}&=i\,\mathrm{Tr}\,P_-^{(t)}\left[\delta_\eta P_-^{(t)},\delta_\zeta P_-^{(t)}\right]+i\,\mathrm{Tr}\,\overline{P}_+^{(t)}\left[\delta_\zeta\overline{P}_+^{(t)},\delta_\eta\overline{P}_+^{(t)}\right]\\&=-\frac{i}{8}\,\mathrm{Tr}\,\gamma_5^{(t)}\left[\delta_\eta\gamma_5^{(t)},\delta_\zeta\gamma_5^{(t)}\right]-\frac{i}{8}\,\mathrm{Tr}\,\gamma_5^{(2-t)}\left[\delta_\eta\gamma_5^{(2-t)},\delta_\zeta\gamma_5^{(2-t)}\right],\end{aligned}\tag{5.1}$$

and, by the "Wilson line" along a curve $U_\tau(x,\mu)$ $(0\leq\tau\leq1)$,

$$W=\exp\left(i\int_0^1\mathrm{d}\tau\,\mathfrak{L}_\eta\right),\qquad a\eta_\mu(x)=\partial_\tau U_\tau(x,\mu)U_\tau(x,\mu)^{-1}.\tag{5.2}$$

Assuming that the fermion measure is smoothly defined over the space of admissible configurations, the Wilson line along a *loop*, for which $U_1=U_0$, is given by (see ref. [6])

$$\begin{aligned}W&=\det\left(1-P_0^{(t)}+P_0^{(t)}Q_1^{(t)}\right)\det{}^{-1}\left(1-\overline{P}_0^{(t)}+\overline{P}_0^{(t)}\gamma_5Q_1^{(2-t)}\gamma_5\right)\\&=\det\left(1-P_0^{(t)}+P_0^{(t)}Q_1^{(t)}\right)\det\left(1-P_0^{(2-t)}+P_0^{(2-t)}Q_1^{(2-t)}\right),\end{aligned}\tag{5.3}$$

where $P_\tau^{(t)}=P_-^{(t)}|_{U=U_\tau}$ and $\overline{P}_\tau^{(t)}=\overline{P}_+^{(t)}|_{U=U_\tau}$. The unitary operator $Q_\tau^{(t)}$ in this expression is defined by

$$\partial_\tau Q_\tau^{(t)}=\frac{1}{4}\left[\partial_\tau\gamma_\tau^{(t)},\gamma_\tau^{(t)}\right]Q_\tau^{(t)},\qquad Q_0^{(t)}=1,\tag{5.4}$$

where $\gamma_\tau^{(t)}=\gamma_5^{(t)}|_{U=U_\tau}$. From this, we have $\gamma_\tau^{(t)}=Q_\tau^{(t)}\gamma_0^{(t)}Q_\tau^{(t)\dagger}$ and thus

$$P_\tau^{(t)}=Q_\tau^{(t)}P_0^{(t)}Q_\tau^{(t)\dagger},\qquad\overline{P}_\tau^{(t)}=\gamma_5Q_\tau^{(2-t)}\gamma_5\overline{P}_0^{(t)}\left(\gamma_5Q_\tau^{(2-t)}\gamma_5\right)^\dagger.\tag{5.5}$$

These relations have been used in deriving the first line of eq. (5.3). From the first line to the second line in eq. (5.3), we have noted $\det Q_\tau^{(t)}=1$.

[16] This sub-section gives a brief sketch of the result of extensive analyses. Those who are interested in further details are asked to refer to refs. [4, 6]. For our analysis of CP symmetry, the relation in eq. (5.10) or eq. (5.15) is essential.

[17] Here the variations η and ζ are assumed to be independent of the gauge field.

The gauge variation of the expectation value, on the other hand, is given by

$$
\begin{aligned}
\delta_\eta \langle \mathcal{O} \rangle_{\mathrm{F}} &= \langle \delta_\eta \mathcal{O} \rangle_{\mathrm{F}} + i a^4 \sum_x \omega^a(x) \left[\mathcal{A}^a(x) - (\nabla_\mu^* j_\mu)^a(x) \right] \langle \mathcal{O} \rangle_{\mathrm{F}} \,, \\
\mathcal{A}^a(x) &= -\frac{i}{2} \operatorname{tr} R(T^a) \left(\gamma_5^{(t)} + \gamma_5^{(2-t)} \right)(x,x) \,,
\end{aligned} \tag{5.6}
$$

by setting $\eta_\mu(x) = -\nabla_\mu \omega(x)$ and $\mathfrak{L}_\eta = a^4 \sum_x \eta_\mu^a(x) j_\mu^a(x)$.[18] So, for the gauge invariant measure, the measure term should satisfy the "anomalous conservation law":

$$
(\nabla_\mu^* j_\mu)^a(x) = \mathcal{A}^a(x) \,. \tag{5.8}
$$

Now, we have observed that for a smooth gauge invariant fermion measure, the associated measure term satisfies the conditions, eqs. (5.3) and (5.8) [eq. (5.1) can be derived from eq. (5.3)]. Conversely, these two conditions are in fact sufficient. Namely, if one has a certain current $j_\mu^a(x)$ such that eq. (5.8) is fulfilled and the combination $\mathfrak{L}_\eta = a^4 \sum_x \eta_\mu^a(x) j_\mu^a(x)$ satisfies eq. (5.3) for any loop, then there exists a smooth gauge invariant fermion measure. This is the reconstruction theorem and the proof is given by an explicit construction: we may set the fermionic basis vectors for the gauge field U as

$$
v_j = \begin{cases} Q_1^{(t)} u_1 W^{-1} \,, & \text{for } j = 1 \,, \\ Q_1^{(t)} u_j \,, & \text{otherwise} \,, \end{cases} \qquad \overline{v}_k = \overline{u}_k \left(\gamma_5 Q_1^{(2-t)} \gamma_5 \right)^\dagger \,, \tag{5.9}
$$

where u_j and $\overline{u}_k$ are fixed bases defined for the reference configuration U_0. The vectors are then transported by the operators $Q_\tau^{(t)}$ and $Q_\tau^{(2-t)}$ along a certain curve connecting U_0 and $U = U_1$. The Wilson line W is also defined along this curve. The above basis depends on the curve chosen, but the associated measure does not, because of eq. (5.3). Thus the measure is smooth. The measure term for the basis (5.9) is given by $\mathfrak{L}_\eta$. Thus the anomalous conservation law is also fulfilled.

5.2 Invariance under $t \to 2-t$ and the CP property of the measure term

In the last subsection, we have observed that the requirements for the ideal measure term are given by eqs. (5.3) and (5.8).[19] The remarkable fact is that these conditions are invariant under $t \to 2-t$. Thus, if we have an ideal measure term $\mathfrak{L}_\eta[U;t]$ which works for U with respect to $\gamma_5^{(t)}$, then we may use the *same* measure term for U with respect to $\gamma_5^{(2-t)}$. Therefore, we may set without loss of generality

$$
\mathfrak{L}_\eta[U; 2-t] = \mathfrak{L}_\eta[U;t] \,. \tag{5.10}
$$

This is the equality (4.18) we have used in the previous section.

[18] Covariant derivatives in these expressions are defined by

$$
\begin{aligned}
\nabla_\mu \omega(x) &= \frac{1}{a} \left[U(x,\mu) \omega(x + a\hat{\mu}) U(x,\mu)^{-1} - \omega(x) \right] \,, \\
\nabla_\mu^* j_\mu(x) &= \frac{1}{a} \left[j_\mu(x) - U(x - a\hat{\mu}, \mu)^{-1} j_\mu(x - a\hat{\mu}) U(x - a\hat{\mu}, \mu) \right] \,.
\end{aligned} \tag{5.7}
$$

[19] Another important requirement is that the measure term must be local, to be consistent with the locality of the theory.

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This equality can be interpreted in a more physically transparent language; this is equivalent to the CP invariance of the measure term. To see this, let us recall that basis vectors for U^{CP} with respect to $\gamma_5^{(t)}$ [which is specified by eq. (4.8)] and basis vectors for U with respect to $\gamma_5^{(2-t)}$ [which is specified by eq. (4.12)] can be related as eq. (4.11). This particular choice of bases, which may always be made, leads to

$$\mathfrak{L}_\eta\left[U^{\mathrm{CP}};t\right] = \mathfrak{L}_\eta[U;2-t]\,, \tag{5.11}$$

and thus eq. (5.10) implies

$$\mathfrak{L}_\eta\left[U^{\mathrm{CP}};t\right] = \mathfrak{L}_\eta[U;t]\,. \tag{5.12}$$

In fact, it is physically natural to take basis vectors such that the relation (5.12) holds. In the continuum theory, the action of the Weyl fermion is CP invariant and the imaginary part of the effective action is too (it is independent of the regularization chosen and is given by the so-called η-invariant [29]). This property is shared with our lattice transcription (2.27), as one can verify from CP transformation law of various operators.[20] If the measure term is not invariant under CP, it then produces another unphysical source of CP breaking as eq. (2.26) shows. In other words, the requirement (5.12) eliminates an unnecessary CP violation which may result from a wrong choice of the fermion measure (which might be called “fake CP anomaly”). Fortunately, it is always possible to construct the CP invariant ideal measure term by the average over CP [4, 9]:

$$\begin{aligned}\mathfrak{L}_\eta^{\{v,\bar{v}\}}[U;t] &= a^4\sum_x \eta_\mu^a(x) j_\mu^a(x)[U;t]\\ &\to \frac{1}{2}\left[a^4\sum_x \eta_\mu^a(x) j_\mu^a(x)[U;t] + a^4\sum_x \eta_\mu^{\mathrm{CP}a}(x) j_\mu^a(x)[U^{\mathrm{CP}};t]\right].\end{aligned} \tag{5.15}$$

This average is possible even if U and U^{CP} belong to different topological sectors M and M^{CP}, because the CP operation defines a differentiable one-to-one onto-mapping from M to M^{CP}. Then CP invariance of the measure term is ensured and this is equivalent to eq. (5.10), and vice versa.

6. Yukawa couplings

It is straightforward to add the Yukawa coupling to the present formulation.[21] By intro-

[20] One should however be careful about the meaning of the variation δ_η. Under $U(x,\mu) \to U(x,\mu) + \delta_\eta U(x,\mu)$, the CP transformed configuration changes as $U^{\mathrm{CP}}(x,\mu) \to U^{\mathrm{CP}}(x,\mu) + \delta_\eta U^{\mathrm{CP}}(x,\mu)$. With this understanding, defining

$$\delta_\eta U^{\mathrm{CP}}(x,\mu) = a\eta_\mu^{\mathrm{CP}}(x) U^{\mathrm{CP}}(x,\mu)\,, \tag{5.13}$$

one has

$$\eta_\mu^{\mathrm{CP}}(x) = \begin{cases} -U^{\mathrm{CP}}(x,i)\eta_i(\bar{x}-a\hat{i})^* U^{\mathrm{CP}}(x,i)^{-1}\,, & \text{for } \mu = i\,,\\ \eta_4(\bar{x})^*\,, & \text{for } \mu = 4\,. \end{cases} \tag{5.14}$$

Note that $(\eta_\mu^{\mathrm{CP}})^{\mathrm{CP}}(x) = \eta_\mu(x)$ corresponding to $(U^{\mathrm{CP}})^{\mathrm{CP}}(x,\mu) = U(x,\mu)$. This definition of the variation implies, in particular, $\delta_\eta D(U^{\mathrm{CP}}) = W\delta_\eta D(U)^T W^{-1}$.

[21] It has been pointed out that a conflict with the Majorana reduction in the presence of the Yukawa coupling and CP symmetry are closely related to each other [22, 30].

ducing the right-handed Weyl fermion and the Higgs field, we set

$$S_{\mathrm{F}} = a^4 \sum_x \Big[\overline{\psi}_L(x) D\psi_L(x) + \overline{\psi}_R(x) D'\psi_R(x) + \overline{\psi}_L(x)\phi(x)\psi_R(x) + \overline{\psi}_R(x)\phi^\dagger(x)\psi_L(x) - \\ - \overline{\psi}_L(x)\eta_L(x) - \overline{\eta}_L(x)\psi_L(x) - \overline{\psi}_R(x)\eta_R(x) - \overline{\eta}_R(x)\psi_R(x)\Big], \tag{6.1}$$

where

$$\begin{aligned} P_-^{(t)}\psi_L &= \psi_L\,, & \overline{\psi}_L\overline{P}_+^{(t)} &= \overline{\psi}_L\,, \\ P_+^{\prime(t)}\psi_R &= \psi_R\,, & \overline{\psi}_R\overline{P}_-^{\prime(t)} &= \overline{\psi}_R\,. \end{aligned} \tag{6.2}$$

We assume that the left-handed fermion $\psi_L(x)$ belongs to the representation R_L of the gauge group and the right-handed fermion $\psi_R(x)$ belongs to R_R (the Higgs field $\phi(x)$ transforms as $R_L \otimes (R_R)^*$). The gauge couplings in the Dirac operator D (D'), and correspondingly in $P_-^{(t)}$ and $\overline{P}_+^{(t)}$ ($P_+^{\prime(t)}$ and $\overline{P}_-^{\prime(t)}$), are thus defined with respect to the representation R_L (R_R).

We first note the relation[22]

$$Z_{\mathrm{F}}[U,\phi,\eta_L,\overline{\eta}_L,\eta_R,\overline{\eta}_R;t] = \int \mathrm{D}[\psi]\mathrm{D}[\overline{\psi}]\, e^{-S_{\mathrm{F}}} = \\ = \exp\left\{a^{-4}\sum_x \left[\frac{\partial}{\partial\eta_L(x)}\overline{P}_+^{(t)}\phi(x)P_+^{\prime(t)}\frac{\partial}{\partial\overline{\eta}_R(x)} + \frac{\partial}{\partial\eta_R(x)}\overline{P}_-^{\prime(t)}\phi^\dagger(x)P_-^{(t)}\frac{\partial}{\partial\overline{\eta}_L(x)}\right]\right\} \times \\ \times Z_{\mathrm{F}}[U,0,\eta_L,\overline{\eta}_L,\eta_R,\overline{\eta}_R;t]\,, \tag{6.3}$$

because the fermion integration measure refers to neither source fields nor the Higgs field. The generating functional without the Yukawa coupling can be analyzed as before, and we have[23]

$$Z_{\mathrm{F}}[U,0,\eta_L,\overline{\eta}_L,\eta_R,\overline{\eta}_R;t] = \\ = e^{i\theta[U;t]}\left(\frac{\Lambda}{a}\right)^N \prod^{n_-}\left[a^4\sum_x \overline{\eta}_L(x)\varphi_0^-(x)\right]\prod^{n_+}\left[a^4\sum_x \varphi_0^{+\dagger}(x)\eta_L(x)\right]\prod_{\substack{\lambda_j>0\\ \lambda_j\neq\Lambda}}\left(\frac{\lambda_j}{a}\right)\times \\ \times \exp\left[a^8\sum_{x,y}\overline{\eta}_L(x)G^{(t)}(x,y)\eta_L(y)\right]\times \\ \times \left(\frac{\Lambda}{a}\right)^{\overline{N}'}\prod^{n'_+}\left[a^4\sum_x \overline{\eta}_R(x)\varphi_0^{\prime+}(x)\right]\prod^{n'_-}\left[a^4\sum_x \varphi_0^{\prime-\dagger}(x)\eta_R(x)\right]\prod_{\substack{\lambda'_j>0\\ \lambda'_j\neq\Lambda}}\left(\frac{\lambda'_j}{a}\right)\times \\ \times \exp\left[a^8\sum_{x,y}\overline{\eta}_R(x)G^{\prime(t)}(x,y)\eta_R(y)\right], \tag{6.4}$$

[22]This formula assumes a perturbative treatment of the Higgs coupling.

[23]It is interesting to note that topologically non-trivial (i.e., $n_+ - n_- \neq 0$, $n'_+ - n'_- \neq 0$) sectors also contribute to fermion number *non*-violating processes in the presence of the Yukawa coupling. H.S. would like to thank Yoshio Kikukawa for a discussion on this issue.

as a product of left-handed and right-handed contributions. In this expression, all quantities with the prime ($'$) are defined with respect to $H' = a\gamma_5 D'$ and

$$D'G'^{(t)}(x,y) = \overline{P}'^{(t)}_{-}(x,y) - \sum^{n'_-} \varphi'^{-}_0(x)\varphi'^{-\dagger}_0(y)\,. \tag{6.5}$$

By repeating the same arguments as before[24] for $Z_{\rm F}[U,0,\eta_L,\overline{\eta}_L,\eta_R,\overline{\eta}_R;t]$ we finally have, corresponding to eq. (4.21),

$$\begin{aligned}
&Z_{\rm F}\left[U^{\rm CP},\phi^\dagger,-W^{-1}\overline{\eta}_L^T,\eta_L^T W,-W^{-1}\overline{\eta}_R^T,\eta_R^T W;t\right] = \\
&= e^{i\theta_M}\left(\frac{\Lambda}{a}\right)^{\overline{N}-N-\overline{N}'+N'} \times \\
&\times \exp\left\{a^{-4}\sum_x\left[\frac{\partial}{\partial\eta_L(x)}\overline{P}^{(2-t)}_{+}\phi(x)P'^{(2-t)}_{+}\frac{\partial}{\partial\overline{\eta}_R(x)}+\frac{\partial}{\partial\eta_R(x)}\overline{P}'^{(2-t)}_{-}\phi^\dagger(x)P^{(2-t)}_{-}\frac{\partial}{\partial\overline{\eta}_L(x)}\right]\right\}\times \\
&\times\frac{\exp\left\{a^8\sum_{x,y}\left[\overline{\eta}_L(x)G^{(2-t)}(x,y)\eta_L(y)+\overline{\eta}_R(x)G'^{(2-t)}(x,y)\eta_R(y)\right]\right\}}{\exp\left\{a^8\sum_{x,y}\left[\overline{\eta}_L(x)G^{(t)}(x,y)\eta_L(y)+\overline{\eta}_R(x)G'^{(t)}(x,y)\eta_R(y)\right]\right\}}\times \\
&\times Z_{\rm F}[U,0,\eta_L,\overline{\eta}_L,\eta_R,\overline{\eta}_R;t]\,.
\end{aligned} \tag{6.8}$$

Thus we see that the effect of the CP breaking appears precisely in the same places as before, except for the terms consisting of Yukawa couplings connected by the propagators.[25] However, when the Higgs field acquires the expectation value, a completely new situation arises. Setting $\phi(x) = v$, the fermion propagators read

$$\begin{aligned}
\frac{\langle\psi_L(x)\overline{\psi}_L(y)\rangle_{\rm F}}{\langle 1\rangle_{\rm F}} &= P^{(t)}_{-}\frac{1}{D-v_+D'^{-1}v_-}\overline{P}^{(t)}_{+}(x,y)\,,\\
\frac{\langle\psi_L(x)\overline{\psi}_R(y)\rangle_{\rm F}}{\langle 1\rangle_{\rm F}} &= P^{(t)}_{-}\frac{1}{v_- - D'v_+^{-1}D}\overline{P}'^{(t)}_{-}(x,y)\,,\\
\frac{\langle\psi_R(x)\overline{\psi}_R(y)\rangle_{\rm F}}{\langle 1\rangle_{\rm F}} &= P'^{(t)}_{+}\frac{1}{D'-v_-D^{-1}v_+}\overline{P}'^{(t)}_{-}(x,y)\,,\\
\frac{\langle\psi_R(x)\overline{\psi}_L(y)\rangle_{\rm F}}{\langle 1\rangle_{\rm F}} &= P'^{(t)}_{+}\frac{1}{v_+ - Dv_-^{-1}D'}\overline{P}^{(t)}_{+}(x,y)\,,
\end{aligned} \tag{6.9}$$

---

[24] Since the charge conjugation flips the chirality as

$$\overline{\psi}_R D'\psi_R = (\psi_R^T C)D'_{R_R\to(R_R)^*}\left(-C^{-1}\overline{\psi}_R^T\right), \tag{6.6}$$

and

$$\left(\psi_R^T C\right)\overline{P}^{(2-t)}_{+,R_R\to(R_R)^*} = \left(\psi_R^T C\right), \qquad P^{(2-t)}_{-,R_R\to(R_R)^*}\left(-C^{-1}\overline{\psi}_R^T\right) = \left(-C^{-1}\overline{\psi}_R^T\right), \tag{6.7}$$

the right-handed fermion may be treated as the left-handed one, belonging to the conjugate representation $(R_R)^*$ (with the change $t\to 2-t$). In particular, the reconstruction theorem is applied with trivial modifications.

[25] Note that the same projection operator, $P'^{(2-t)}_{+}$ for example, appears in the Yukawa vertex in the combination $\phi(x)P'^{(2-t)}_{+}$ and in the propagator of the Weyl fermion in the combination $P'^{(2-t)}_{+}/D'$. Consequently, it does not matter if one says that CP is broken either by the propagator or by the Yukawa vertex. When $R_L = R_R$, however, it is natural to combine ψ_L and ψ_R into a Dirac fermion ψ. In this case, the propagator of ψ is manifestly CP invariant and the (chirally symmetric) Yukawa vertex breaks CP.

where we have defined $v_+ = \overline{P}_+^{(t)} v P_+'^{(t)}$ and $v_- = \overline{P}_-'^{(t)} v^\dagger P_-^{(t)}$. One thus sees that this time the change $t \to 2-t$ produces *non-local* differences in the propagator. For example, in $\langle \psi_L(x)\overline{\psi}_R(y)\rangle_{\rm F}/\langle 1\rangle_{\rm F}$, the difference $\overline{P}_-'^{(2-t)} - \overline{P}_-'^{(t)} \propto a(t-1)D'\gamma_5 f(H'^2)$ cannot cancel the denominator $v_- - D'v_+^{-1}D$, leaving a non-local difference.[26] Though we expect that this breaking, even if it is non-local, will eventually be removed in a suitable continuum limit, a more careful study is required to confirm this expectation.[27] (If one forms the free Dirac-type propagator, the CP breaking does not appear in the propagator. This means that the coupling of chiral gauge fields induces CP breaking.)

7. Conclusion and discussion

In this paper we have analyzed the possible implications of CP breaking in lattice chiral gauge theory, which is a result of the very definition of chirality (1.1) for the Ginsparg-Wilson operator [20]. This CP breaking is known to be directly related to the basic notions of locality and the absence of species doubling in the Ginsparg-Wilson operator [22]. Although the non-perturbative construction of the ideal path integral measure for non-abelian chiral gauge theories has not been established yet, we analyzed the CP transformation properties of the path integral measure on the basis of a working ansatz. Our conclusion is that there exists no "CP anomaly" arising from the path integral measure. The breaking of CP is thus limited to the explicit breaking in the action of chiral gauge theory, and it basically appears in the fermion propagator. When the Higgs field has no vacuum expectation value or in pure chiral gauge theory without the Higgs field, it emerges as as an (almost) contact term. In the presence of the Higgs expectation value, however, the breaking becomes intrinsically non-local. We expect that these breakings in the propagator, either local or non-local, do not survive in a suitable continuum limit, but a more careful analysis is required to make a definite conclusion of this issue.

In this paper, we identified where the effect of CP breaking in the present lattice formulation appears for generic chiral gauge theories. When more general composite operators are considered, further complications associated to this effect could arise. As an example, we comment on the computation of the kaon B parameter, B_K (see, for example, refs. [31, 32]). The following matrix element of the effective weak hamiltonian is then relevant:

$$\langle \overline{K}^0 |\, \overline{s}\gamma_5\Gamma_5\gamma_\mu \frac{1-\gamma_5}{2}\gamma_5\Gamma_5 d\; \overline{s}\gamma_5\Gamma_5\gamma_\mu \frac{1-\gamma_5}{2}\gamma_5\Gamma_5 d\,| K^0\rangle\,, \tag{7.1}$$

where we have adopted the $O(a)$ improved operator [33]. Since the gauge action and the Ginsparg-Wilson action in QCD are invariant under CP, eq. (6.1) is equal to its CP transformation

$$\langle K^0 |\, \overline{d}\gamma_5\Gamma_5\gamma_\mu \frac{1-\gamma_5}{2}\gamma_5\Gamma_5 s\; \overline{d}\gamma_5\Gamma_5\gamma_\mu \frac{1-\gamma_5}{2}\gamma_5\Gamma_5 s\,| \overline{K}^0\rangle\,. \tag{7.2}$$

[26] Although the kernel $1/(v_- - D'v_+^{-1}D)(x,y)$ decays exponentially as $|x-y| \to \infty$, this cannot be regarded as local; the decaying rate in the lattice unit is $\sim 1/(\sqrt{vv^\dagger}a) \to \infty$ in the continuum limit $a \to 0$, because $vv^\dagger$ is kept fixed in this limit (i.e., $vv^\dagger$ has the physical mass scale).

[27] This non-local CP breaking will persist for a non-perturbative treatment of the Higgs coupling, though a detailed analysis remains to be performed.

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which coincides with the lattice transcription of the *naive* CP transformation of eq. (7.1). This shows that the $O(a)$ improvement in ref. [33], which eliminates $O(a)$ chiral symmetry breakings (in the sense of continuum theory), maintains the desired behavior of the amplitude (7.1) under CP.

From a view point of the present analysis of CP symmetry, however, the above $O(a)$ improved expression of the effective hamiltonian, if applied to off-shell amplitudes, is not completely satisfactory.[28] For example, one can confirm that the right-handed component of the $\overline{s}(1-\gamma_5)/2$ quark[29] contributes to the above *weak* effective hamiltonian in eq. (7.1), if applied to off-shell Green's functions. Although this is the order $O(a)$ effect, this breaks $\mathrm{SU}(2)_L$ gauge symmetry of electroweak interactions. This illustrates that great care need to be exercised in the analysis of lattice chiral symmetry and CP invariance.

A. C, P and CP

We adopt the following convention of γ-matrices:

$$\begin{aligned} \{\gamma_\mu,\gamma_\nu\} &= 2\delta_{\mu\nu}\,, \qquad \gamma_\mu^\dagger = \gamma_\mu\,, \qquad \gamma_5 = -\gamma_1\gamma_2\gamma_3\gamma_4 = \gamma_5^\dagger\,, \\ \gamma_1^T &= -\gamma_1\,, \qquad \gamma_2^T = \gamma_2\,, \qquad \gamma_3^T = -\gamma_3\,, \qquad \gamma_4^T = \gamma_4, \qquad \gamma_5^T = \gamma_5\,. \end{aligned} \tag{A.1}$$

The charge conjugation is defined by

$$\psi(x) \to -C^{-1}\overline{\psi}^T(x)\,, \qquad \overline{\psi}(x) \to \psi^T(x)C\,, \qquad U(x,\mu) \to U^{\mathrm{C}}(x,\mu) = U(x,\mu)^*\,, \tag{A.2}$$

where the charge conjugation matrix $C = \gamma_2\gamma_4$ satisfies

$$C^\dagger C = 1\,, \qquad C^T = -C\,, \qquad C\gamma_\mu C^{-1} = -\gamma_\mu^T\,, \qquad C\gamma_5 C^{-1} = \gamma_5^T\,. \tag{A.3}$$

Under this transformation, the kernel of Dirac operator transforms as[30]

$$D\left(U^{\mathrm{C}}\right)(x,y) = C^{-1}D(U)(x,y)^T C\,, \tag{A.4}$$

where the transpose operation T acts not only on the matrices involved but also on the arguments as $(x,y) \to (y,x)$.

The parity transformation is defined by

$$\begin{aligned} \psi(x) &\to \gamma_4\psi(\bar{x}), \qquad \overline{\psi}(x) \to \overline{\psi}(\bar{x})\gamma_4\,, \\ U(x,\mu) &\to U^{\mathrm{P}}(x,\mu) = \begin{cases} U(\bar{x}-a\hat{i},i)^{-1}\,, & \text{for } \mu = i\,, \\ U(\bar{x},4)\,, & \text{for } \mu = 4\,, \end{cases} \end{aligned} \tag{A.5}$$

where

$$\bar{x} = (-x_i, x_4)\,, \tag{A.6}$$

[28] For on-shell amplitudes such as in eq. (7.1), the amplitude is reduced to the one in continuum $V-A$ theory if the equations of motion for quarks are used. In this sense, eq. (7.1) and other schemes are consistent. We thank Martin Lüscher for bringing this fact to our attention.

[29] The right-handed component of an anti-quark does not couple to the W boson either in continuum theory or in the standard lattice formulation with the overlap operator.

[30] We assume that the basic building block of the Dirac operator is the Wilson-Dirac operator.

for $x = (x_i, x_4)$ $(i = 1,\, 2,\, 3)$. Under this,

$$D\left(U^{\mathrm{P}}\right)(x,y) = \gamma_4 D(U)(\bar{x},\bar{y})\gamma_4\,. \tag{A.7}$$

Finally, we define the CP transformation as

$$\begin{aligned} \psi(x) &\to -W^{-1}\overline{\psi}^T(\bar{x})\,, \qquad \overline{\psi}(x) \to \psi^T(\bar{x})W \\ U(x,\mu) &\to U^{\mathrm{CP}}(x,\mu) = \begin{cases} U(\bar{x}-a\hat{i},i)^{-1*}\,, & \text{for } \mu = i\,, \\ U(\bar{x},4)^*\,, & \text{for } \mu = 4\,, \end{cases} \end{aligned} \tag{A.8}$$

where

$$\begin{aligned} W &= \gamma_2\,, \qquad W^\dagger W = 1\,, \\ W\gamma_\mu W^{-1} &= \begin{cases} \gamma_i^T\,, & \text{for } \mu = i\,, \\ -\gamma_4^T\,, & \text{for } \mu = 4\,, \end{cases} \qquad W\gamma_5 W^{-1} = -\gamma_5^T\,, \end{aligned} \tag{A.9}$$

and thus CP acts on the plaquette variables $U(x,\mu,\nu)$ as $(\varphi(\bar{x}-a\hat{i}-a\hat{j},i,j) = U(\bar{x}-a\hat{i}-a\hat{j},j)^*U(\bar{x}-a\hat{i},i)^*)$

$$\begin{aligned} U(x,i,j) &\to U^{\mathrm{CP}}(x,i,j) = \varphi\Big(\bar{x}-a\hat{i}-a\hat{j},i,j\Big)^{-1} U\Big(\bar{x}-a\hat{i}-a\hat{j},i,j\Big)^{*} \varphi\Big(\bar{x}-a\hat{i}-a\hat{j},i,j\Big), \\ U(x,i,4) &\to U^{\mathrm{CP}}(x,i,4) = U\left(\bar{x}-a\hat{i},i\right)^{*-1} U\left(\bar{x}-a\hat{i},i,4\right)^{-1*} U\left(\bar{x}-a\hat{i},i\right)^{*}. \end{aligned} \tag{A.10}$$

Under this transformation, we have

$$D\left(U^{\mathrm{CP}}\right)(x,y) = W^{-1}D(U)(\bar{x},\bar{y})^T W\,. \tag{A.11}$$

B. Eigenvalue problem of H^2

To consider the eigenvalue problem of H^2 (3.1), it is better to consider first

$$H\varphi_n(x) = \lambda_n\varphi_n(x)\,, \qquad (\varphi_n,\varphi_m) = \delta_{nm}\,. \tag{B.1}$$

We note

$$H\Gamma_5\varphi_n(x) = -\Gamma_5 H\varphi_n(x) = -\lambda_n\Gamma_5\varphi_n(x)\,, \tag{B.2}$$

and

$$(\Gamma_5\varphi_n,\Gamma_5\varphi_m) = \left[1-\lambda_n^2 f^2(\lambda_n^2)\right]\delta_{nm}\,. \tag{B.3}$$

These relations show that eigenfunctions with $\lambda_n \neq 0$ (when $\lambda_n = 0$, $\varphi_0(x)$ and $\Gamma_5\varphi_0(x)$ are not necessarily linear-independent) and $\lambda_n f(\lambda_n^2) \neq \pm 1$ come in pairs as λ_n and $-\lambda_n$.

We can thus classify eigenfunctions in eq. (B.1) as follows:

(i) $\lambda_n = 0$ $(H\varphi_0(x) = 0)$. For this

$$H\frac{1\pm\gamma_5}{2}\varphi_0(x) = H\frac{1\pm\Gamma_5}{2}\varphi_0(x) = \frac{1\mp\Gamma_5}{2}H\varphi_0(x) = 0\,, \tag{B.4}$$

so we may impose the chirality on $\varphi_0(x)$ as

$$\gamma_5\varphi_0^\pm(x) = \Gamma_5\varphi_0^\pm(x) = \pm\varphi_0^\pm(x)\,. \tag{B.5}$$

We denote the number of $\varphi_0^+(x)$ $(\varphi_0^-(x))$ as n_+ (n_-).

(ii) $\lambda_n \neq 0$ and $\lambda_n f(\lambda_n^2) \neq \pm 1$. As shown above,

$$H\varphi_n(x) = \lambda_n \varphi_n(x)\,, \qquad H\widetilde{\varphi}_n(x) = -\lambda_n \widetilde{\varphi}_n(x)\,, \tag{B.6}$$

where

$$\widetilde{\varphi}_n(x) = \frac{1}{\sqrt{1-\lambda_n^2 f^2(\lambda_n^2)}}\Gamma_5 \varphi_n(x)\,. \tag{B.7}$$

We have

$$\Gamma_5\varphi_n(x) = \sqrt{1-\lambda_n^2 f^2(\lambda_n^2)}\,\widetilde{\varphi}_n(x)\,, \qquad \Gamma_5\widetilde{\varphi}_n(x) = \sqrt{1-\lambda_n^2 f^2(\lambda_n^2)}\,\varphi_n(x)\,, \tag{B.8}$$

and

$$\gamma_5 \begin{pmatrix} \varphi_n \\ \widetilde{\varphi}_n \end{pmatrix} = \begin{pmatrix} \lambda_n f(\lambda_n^2) & \sqrt{1-\lambda_n^2 f^2(\lambda_n^2)} \\ \sqrt{1-\lambda_n^2 f^2(\lambda_n^2)} & -\lambda_n f(\lambda_n^2) \end{pmatrix} \begin{pmatrix} \varphi_n \\ \widetilde{\varphi}_n \end{pmatrix}. \tag{B.9}$$

(iii) $\lambda_n f(\lambda_n^2) = \pm 1$, or

$$H\Psi_\pm(x) = \pm\Lambda\Psi_\pm(x)\,, \qquad \Lambda f(\Lambda^2) = 1\,. \tag{B.10}$$

We see

$$\Gamma_5 \Psi_\pm(x) = 0\,, \tag{B.11}$$

and

$$\gamma_5 \Psi_\pm(x) = \pm\Lambda f(\Lambda^2)\Psi_\pm(x) = \pm\Psi_\pm(x)\,. \tag{B.12}$$

We denote the number of $\Psi_+(x)$ ($\Psi_-(x)$) as N_+ (N_-).

As the application of the above relations, we can establish the index theorem [24]. Noting $(\varphi_n, \Gamma_5\varphi_n) = (\widetilde{\varphi}_n, \Gamma_5\widetilde{\varphi}_n) = 0$ for modes with $\lambda_n \neq 0$, we see

$$\mathrm{Tr}\,\Gamma_5 = n_+ - n_-\,. \tag{B.13}$$

Since Γ_5 depends smoothly on the gauge field within the space of admissible configurations (2.13), the integer $n_+ - n_-$ is a constant in a connected component of the space of admissible configurations; $n_+ - n_-$ thus provides a topological characterization of the gauge field configuration, i.e., the index.

Next, using above relations, we have

$$\mathrm{Tr}\,\gamma_5 = n_+ - n_- + N_+ - N_-\,. \tag{B.14}$$

If we further note $\mathrm{Tr}\,\gamma_5 = 0$ on the lattice, we have the chirality sum rule [25, 26]

$$n_+ - n_- + N_+ - N_- = 0\,. \tag{B.15}$$

Going back to our original problem (3.1), it is obvious that eigenfunctions are given by the above eigenfunctions of H, by identifying $\varphi_j \leftrightarrow \varphi_n$ and $\lambda_j \leftrightarrow |\lambda_n|$ (so λ_j is doubly degenerated). To find appropriate components for eq. (3.2), we have to know the action of chiral projectors on these eigenfunctions φ_n. From above, we have

(i) For zero modes, we simply have

$$\gamma_5^{(t)}\varphi_0^{\pm} = \gamma_5\varphi_0^{\pm} = \pm\varphi_0^{\pm}\,, \tag{B.16}$$

and thus

$$P_{\pm}^{(t)}\varphi_0^{\pm} = \pm\varphi_0^{\pm}\,. \tag{B.17}$$

(ii) For modes with $\lambda_n \neq 0$ and $\lambda_n \neq \pm\Lambda$,

$$\gamma_5^{(t)}\begin{pmatrix}\varphi_n\\ \widetilde{\varphi}_n\end{pmatrix} = \frac{1}{\sqrt{1+t(t-2)\lambda_n^2 f^2(\lambda_n^2)}}\begin{pmatrix}(1-t)\lambda_n f(\lambda_n^2) & \sqrt{1-\lambda_n^2 f^2(\lambda_n^2)}\\ \sqrt{1-\lambda_n^2 f^2(\lambda_n^2)} & -(1-t)\lambda_n f(\lambda_n^2)\end{pmatrix}\begin{pmatrix}\varphi_n\\ \widetilde{\varphi}_n\end{pmatrix}. \tag{B.18}$$

Since this is a traceless matrix whose determinant is -1, the eigenvalues of $\gamma_5^{(t)}$ in this subspace are $+1$ and -1. This shows that one linear combination of φ_n and $\widetilde{\varphi}_n$ is annihilated by $P_+^{(t)}$ and the orthogonal combination is annihilated by $P_-^{(t)}$. Therefore we can take suitable linear combinations of φ_n and $\widetilde{\varphi}_n$ such that

$$P_{\pm}^{(t)}\varphi_n^{\pm}(x) = \varphi_n^{\pm}(x)\,, \qquad (\varphi_n^{\pm},\varphi_m^{\pm}) = \delta_{nm}\,. \tag{B.19}$$

(iii) For the modes with $\lambda_n = \pm\Lambda$, we have

$$\gamma_5^{(t)}\Psi_{\pm}(x) = \begin{cases}\mp\Psi_{\pm}(x)\,, & \text{for } t>1\,,\\ \pm\Psi_{\pm}(x)\,, & \text{for } t<1\,.\end{cases} \tag{B.20}$$

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