Analytical formulae of the Polyakov and Wilson loops with Dirac eigenmodes in lattice QCD

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We derive an analytical gauge-invariant formula between the Polyakov loop \(L_P\) and the Dirac eigenvalues \(\lambda_n\) in QCD, i.e., \(L_P \propto \sum_n \lambda_n^{N_t-1} \langle n|\hat{U}_4|n\rangle\), in ordinary periodic square lattice QCD with odd-number temporal size \(N_t\). Here, \(|n\rangle\) denotes the Dirac eigenstate, and \(\hat{U}_4\) the temporal link-variable operator. This formula is a Dirac spectral representation of the Polyakov loop in terms of Dirac eigenmodes \(|n\rangle\). Because of the factor \(\lambda_n^{N_t-1}\) in the Dirac spectral sum, this formula indicates a negligibly small contribution of low-lying Dirac modes to the Polyakov loop in both confinement and deconfinement phases, while these modes are essential for chiral symmetry breaking. Next, we find a similar formula between the Wilson loop and Dirac modes on arbitrary square lattices, without restriction of odd-number size. This formula suggests a small contribution of low-lying Dirac modes to the string tension \(\sigma\), or the confining force. These findings support no crucial role of low-lying Dirac modes for confinement, i.e., no direct one-to-one correspondence between confinement and chiral symmetry breaking in QCD, which seems to be natural because heavy quarks are also confined even without light quarks or the chiral symmetry.

Subject Index B01, B02, B03, B64

1. Introduction

Since quantum chromodynamics (QCD) was established as the fundamental theory of strong interaction [1–3], it has been an important problem in theoretical physics to clarify color confinement and spontaneous chiral symmetry breaking [4,5]. However, in spite of many and various studies, these two nonperturbative phenomena have not been well understood directly from QCD.

Dynamical chiral symmetry breaking in QCD is categorized as well-known spontaneous symmetry breaking, which widely appears in various phenomena in physics. The standard order parameter of chiral symmetry breaking is the quark condensate \(\langle \bar{q}q \rangle\), and it is directly related to low-lying Dirac modes, as the Banks–Casher relation indicates [6]. Here, Dirac modes are eigenmodes of the Dirac operator \(\hat{D}\), which directly appears in the QCD Lagrangian.

In contrast to chiral symmetry breaking, color confinement is a quite unique phenomenon peculiar to QCD, and the quark confinement is characterized by the area law of the Wilson loop, i.e., non-zero string tension, or the zero Polyakov loop, i.e., infinite single-quark free energy.

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The Polyakov loop $L_P$ is one of the typical order parameters, and it relates to the single-quark free energy $E_q$ as $\langle L_P \rangle \propto e^{-E_q/T}$ at temperature $T$. The Polyakov loop is also an order parameter of spontaneous breaking of the $Z_{N_c}$ center symmetry in QCD [7,8].

In addition to the study of each nonperturbative phenomenon, to clarify the relation between confinement and chiral symmetry breaking is one of the challenging important subjects in theoretical physics [9–29], and their relation is not yet clarified directly from QCD.

A strong correlation between confinement and chiral symmetry breaking has been suggested by the near coincidence of deconfinement and chiral restoration temperatures [7,30], although slight difference of about 25 MeV between them is pointed out in recent lattice QCD studies [31,32]. Their correlation has also been suggested in terms of QCD-monopoles [9–12], which topologically appear in QCD in the maximally Abelian gauge. By removing the monopoles from the QCD vacuum, confinement and chiral symmetry breaking are simultaneously lost [9–12], which indicates an important role of QCD-monopoles to both phenomena, and thus these two phenomena seem to be related via the monopole.

As another type of pioneering study, Gattringer, Bruckmann, and Hagen showed that the Polyakov loop can be analytically expressed with the Dirac eigenvalues under the temporally twisted boundary condition for temporal link variables [13,14]. Although a temporal (nontwisted) periodic boundary condition is physically required for link variables in real QCD at finite temperature, such an analytical formula would be useful to consider the relation between confinement and chiral symmetry breaking.

In our recent series of studies [16–22], we have numerically investigated the Wilson loop and the Polyakov loop in terms of the “Dirac mode expansion,” and have found that quark confinement properties are almost kept even in the absence of low-lying Dirac modes. (Also, “hadrons” appear without low-lying Dirac modes [33,34], suggesting survival of confinement.) Note that the Dirac mode expansion is just a mathematical expansion by eigenmodes $|n\rangle$ of the Dirac operator $D = \gamma_\mu D_\mu$, using the completeness of $\sum_n |n\rangle\langle n| = 1$. In general, instead of $D$, one can consider any (anti-)Hermitian operator, e.g., $D^2 = D_\mu D_\mu$, and the expansion in terms of its eigenmodes [35,36]. To investigate chiral symmetry breaking, however, it is appropriate to consider $D$ and the expansion by its eigenmodes.

In this paper, we derive analytical formulae of the Polyakov and Wilson loops with the Dirac modes in the lattice QCD formalism [23–29], and discuss the relation between confinement and chiral symmetry breaking.

The organization of this paper is as follows. In Sect. 2, we briefly review the lattice QCD formalism for the Dirac operator, Dirac eigenvalues, and Dirac modes. In Sect. 3, we derive an analytical formula between the Polyakov loop and the Dirac modes in lattice QCD where the temporal size is an odd number. In Sect. 4, we investigate the properties of the formula obtained, and discuss the contribution from the low-lying Dirac modes to the Polyakov loop. In Sect. 5, we consider the relation between the Wilson loop and Dirac modes on arbitrary square lattices, without the restriction of odd-number size. Section 6 will be devoted to the summary.

### 2. Lattice QCD formalism

To begin with, we state the setup condition of lattice QCD formalism adopted in this study. We use an ordinary square lattice with spacing $a$ and size $N_s^3 \times N_t$. The normal nontwisted periodic boundary condition is used for the link variable $U_\mu(s) = e^{iaA_\mu(s)}$ in the temporal direction, with the gluon field $A_\mu(s)$, the gauge coupling $g$, and the site $s$. This temporal periodicity is physically required at
finite temperature. In this paper, we take SU($N_c$) with $N_c$ being the color number as the gauge group of the theory. However, an arbitrary gauge group $G$ can be taken for most arguments in the following.

2.1. Lattice QCD formalism and anatomy of gauge ensemble

In the Euclidean lattice formalism, the QCD generating functional is expressed with the QCD action $S_{QCD}$ as

$$Z_{QCD} = \int D\bar{q} Dq D[U] e^{-S_{QCD} + \bar{q} K[U] q}$$

where $S_{gauge}[U]$ denotes the lattice gauge action and $K[U]$ a fermionic kernel. In this study, one can freely choose any type of lattice fermions such as the Wilson fermion, the Kogut–Susskind fermion, the overlap fermion, and so on [7,8]. As importance sampling for the generating function $Z_{QCD}$, one can generate gauge configurations $\{U_k\}_{k=1,2,3,...,N}$ using Monte Carlo simulations. The expectation value of any operator $O[U]$ is given by the gauge ensemble average as

$$\langle O[U] \rangle = \frac{1}{Z_{QCD}} \int DU e^{-S_{gauge}[U] \det K[U]} \cdot O[U] = \lim_{N \to \infty} \frac{1}{N} \sum_{k=1}^{N} O[U_k].$$

In this study, we consider some analytical relations between Dirac modes and confinement properties for the gauge configurations $\{U_k\}_{k=1,2,3,...,N}$, generated in full QCD or quenched QCD with setting $\det K[U] = 1$.

In this paper, we perform “anatomy” for the nonperturbative QCD vacuum, i.e., the gauge ensemble which is in principle generated for the QCD generating functional $Z_{QCD}$. In our approach, we do not change the QCD action $S_{QCD}$ or $Z_{QCD}$, but analyze the QCD vacuum for $Z_{QCD}$ in terms of the Dirac modes. This approach is similar to our previous work [16–22] and that of Lang et al. [33,34], where low-lying Dirac modes are removed from the lattice QCD configurations, after their numerical generation in standard Monte Carlo simulations for $Z_{QCD}$. In these studies, $Z_{QCD}$ is not changed at all. Our approach is also similar to that of Abelian dominance [37,38] and monopole dominance [39] for the argument of quark confinement in the maximally Abelian (MA) gauge. After generating the QCD configuration in the MA gauge, off-diagonal gluons or monopoles are removed from the QCD vacuum, and confinement properties are investigated in the processed QCD vacuum. In these studies, $Z_{QCD}$ is also unchanged. (If off-diagonal gluons are removed from $Z_{QCD}$ at the action level, the system becomes QED, which is no longer meaningful for the study of QCD.) In fact, the main interest is the QCD vacuum, and it has been investigated from the viewpoint of some relevant modes, such as low-lying Dirac modes, monopoles, and so on. In this work, we analyze the lattice gauge ensemble, generated for $Z_{QCD}$, in terms of the Dirac modes.

2.2. Dirac operator, Dirac eigenvalues, and Dirac modes in lattice QCD

Here, we mathematically define the Dirac operator $\not{D}$, Dirac eigenvalues $\lambda_n$, and Dirac eigenmodes $|n\rangle$ in lattice QCD.

In lattice QCD, the Dirac operator $\not{D} = \gamma_\mu D_\mu$ is expressed with $U_\mu(s) = e^{i a g A_\mu(s)}$. In our study, we take the lattice Dirac operator of

$$\not{D}_{s,s'} = \frac{1}{2a} \sum_{\mu=1}^{4} \gamma_\mu \left[ U_\mu(s) \delta_{s+s'+\mu,0} - U_{-\mu}(s) \delta_{s-s',\mu} \right].$$

$$3/15$$
where \( \hat{\mu} \) is the unit vector in the \( \mu \)-direction in the lattice unit, and \( U_{-\mu}(s) \equiv U^\dagger_\mu(s - \hat{\mu}) \). Adopting Hermitian \( \gamma \)-matrices as \( \gamma^\dagger_\mu = \gamma_\mu \), the Dirac operator \( \slashed{D} \) is anti-Hermitian and satisfies \( \slashed{D}^\dagger \equiv -\slashed{D} \). (Note that the Dirac operator \( \slashed{D}_{s,s'} \) defined here is not identical with the fermionic kernel \( K_{s,s'}[U] \) in Sect. 2.1. The relation between \( \slashed{D} \) and \( K[U] \) will be discussed in Sect. 2.4.)

We introduce the normalized Dirac eigenstate \( |n\rangle \) as

\[
\slashed{D}|n\rangle = i\lambda_n |n\rangle, \quad \langle m|n\rangle = \delta_{mn},
\]

with the Dirac eigenvalue \( i\lambda_n (\lambda_n \in \mathbb{R}) \). Because of \( \{\gamma_5, \slashed{D}\} = 0 \), the state \( \gamma_5|n\rangle \) is also an eigenstate of \( \slashed{D} \) with the eigenvalue \(-i\lambda_n \). Here, the Dirac eigenstate \( |n\rangle \) satisfies the completeness of

\[
\sum_n |n\rangle \langle n| = 1.
\]

For the Dirac eigenfunction \( \psi_n(s) \equiv \langle s|n\rangle \), the Dirac eigenvalue equation \( \slashed{D}\psi_n(s) = i\lambda_n \psi_n(s) \) is expressed by

\[
\sum_{s'} \slashed{D}_{s,s'}\psi_n(s') = i\lambda_n \psi_n(s)
\]

in lattice QCD, and its explicit form is written by

\[
\frac{1}{2d} \sum_{\mu=1}^{4} \gamma_\mu \left[ U_\mu(s)\psi_n(s + \hat{\mu}) - U_{-\mu}(s)\psi_n(s - \hat{\mu}) \right] = i\lambda_n \psi_n(s).
\]

The Dirac eigenfunction \( \psi_n(s) \) can be numerically obtained in lattice QCD, apart from a phase factor. By the gauge transformation of \( U_\mu(s) \rightarrow V(s)U_\mu(s)V^\dagger(s + \hat{\mu}) \), \( \psi_n(s) \) is gauge-transformed as

\[
\psi_n(s) \rightarrow V(s)\psi_n(s),
\]

which is the same as that of the quark field, although, to be strict, there can appear an irrelevant \( n \)-dependent global phase factor \( e^{i\phi_n[V]} \), according to the arbitrariness of the phase in the basis \( |n\rangle \) [19].

Note that the spectral density \( \rho(\lambda) \) of the Dirac operator \( \slashed{D} \) relates to chiral symmetry breaking in continuum QCD. For example, from the Banks–Casher relation [6], the zero-eigenvalue density \( \rho(0) \) leads to \( \langle \bar{q}q \rangle \) as

\[
\langle \bar{q}q \rangle = -\lim_{m \to 0} \lim_{V_{\text{phys}} \to \infty} \pi \rho(0),
\]

with space-time volume \( V_{\text{phys}} \). (In lattice QCD, the use of the Dirac operator \( \slashed{D} \) in Eq. (3) accompanies an overall degeneracy factor \( 2^4 \), which will be discussed in Sect. 2.4.) In any case, the low-lying Dirac modes can be regarded as the essential modes responsible for spontaneous chiral symmetry breaking in QCD.
2.3. Operator formalism in lattice QCD

Now, we present the operator formalism in lattice QCD [16–29]. To begin with, we introduce the link variable operator \( \hat{U}_\mu (\mu = \pm 1, \ldots, \pm 4) \) defined by the matrix element of the fermionic kernel

\[
\langle s \mid \hat{U}_{\pm \mu} \mid s' \rangle = U_{\pm \mu}(s) \delta_{s \pm \mu, s'}.
\] (11)

Because of \( U_{-\mu}(s) = U_{\mu}^\dagger(s - \hat{\mu}) \), \( \hat{U}_{\pm \mu} \) are Hermite conjugate with each other and satisfy

\[
\hat{U}_{-\mu} = \hat{U}_\mu^\dagger.
\] (12)

With the link variable operator \( \hat{U}_{\pm \mu} \), the covariant derivative is written as

\[
\hat{D}_\mu = \frac{1}{2a} (\hat{U}_\mu - \hat{U}_{-\mu}),
\] (13)

and the Dirac operator defined by Eq. (3) is simply expressed as

\[
\hat{D} = \frac{1}{2a} \sum_{\mu=1}^{4} \gamma_\mu (\hat{U}_\mu - \hat{U}_{-\mu}).
\] (14)

Both \( \hat{D} \) and \( \hat{D}_\mu \) are anti-Hermite operators. The Dirac mode matrix element of the link variable operator \( \hat{U}_\mu (\mu = \pm 1, \ldots, \pm 4) \) can be expressed with \( \psi_n(s) \):

\[
\langle m \mid \hat{U}_\mu \mid n \rangle = \sum_s \langle m \mid s \rangle \langle s \mid \hat{U}_\mu \mid s + \hat{\mu} \rangle \langle s + \hat{\mu} \mid n \rangle = \sum_s \psi_m^\dagger(s) U_{\mu}(s) \psi_n(s + \hat{\mu}).
\] (15)

Note that the matrix element is gauge invariant, apart from an irrelevant phase factor. Actually, using the gauge transformation (8), we find the gauge transformation of the matrix element to be [19]

\[
\langle m \mid \hat{U}_\mu \mid n \rangle = \sum_s \psi_m^\dagger(s) U_{\mu}(s) \psi_n(s + \hat{\mu})
\]

\[
\rightarrow \sum_s \psi_m^\dagger(s) V^\dagger(s) \cdot V(s) U_{\mu}(s) V^\dagger(s + \hat{\mu}) \cdot V(s + \hat{\mu}) \psi_n(s + \hat{\mu})
\]

\[
= \sum_s \psi_m^\dagger(s) U_{\mu}(s) \psi_n(s + \hat{\mu}) = \langle m \mid \hat{U}_\mu \mid n \rangle.
\] (16)

To be strict, there appears an \( n \)-dependent global phase factor, corresponding to the arbitrariness of the phase in the basis \( \{ n \} \). However, this phase factor cancels as \( e^{i\psi_m} e^{-i\psi_n} = 1 \) between \( \{ n \} \) and \( \langle n \rangle \), and does not appear for physical quantities such as the Wilson loop and the Polyakov loop [19].

2.4. Relation between Dirac operator \( \mathcal{D} \) and fermionic kernel \( K \)

In this subsection, we discuss the relation between the Dirac operator \( \mathcal{D} \) defined in Eq. (3) or (14) and the fermionic kernel \( K(U) \) in lattice QCD in Eq. (1).

In lattice QCD, the simple Dirac operator \( \mathcal{D} \) has \( 2^D \) degeneracy, with \( D = 4 \) being the number of the space-time dimension [7,8]. In the fermionic kernel \( K(U) \), the doubler contribution is effectively removed in some way. For a typical example of the Wilson fermion, a large extra energy of \( O(1/a) \) is added only for doublers, which makes the doublers inactive in the low-energy region. Then, 16 degenerate low-lying Dirac modes of \( \mathcal{D} \) correspond to one low-lying mode and 15 doubler modes in terms of the fermionic kernel \( K(U) \).

In fact, each low-lying mode of \( K(U) \) is expected to have a large overlap with an eigenmode of \( \mathcal{D} \), but the chiral property is largely different between \( \mathcal{D} \) and \( K(U) \). Actually, if \( \mathcal{D} \) is misleadingly...
used instead of $K[U]$ in Eq. (1), the theoretical structure may be largely changed due to many flavors of 16 species [40,41]. In addition, the axial anomaly is totally different, since it is not broken in the Dirac operator $\hat{D}$ due to the cancellation from the doublers [7,8].

Here, we denote by $|\nu\rangle_K$ the normalized mode of the fermionic kernel $K[U]$, to distinguish it from the Dirac mode $|n\rangle$. Because of $\sum_n |n\rangle\langle n| = 1$, one finds the identity

$$|\nu\rangle_K = \sum_n |n\rangle\langle n|\nu\rangle_K.$$  \hspace{1cm} (17)

In this paper, we assume that each low-lying mode of the fermionic kernel $K[U]$ is mainly expressed with the low-lying Dirac modes of $\hat{D}$. This assumption does not mean one-to-one correspondence between a low-lying Dirac mode and a low-lying mode of $K[U]$, but saturation of each low-lying mode of $K[U]$ by low-lying Dirac modes of some range. In fact, for each low-lying mode $|\nu\rangle_K$, we assume

$$|\nu\rangle_K \simeq \sum_{\text{low-lying } n} |n\rangle\langle n|\nu\rangle_K,$$  \hspace{1cm} (18)

which means

$$\sum_{\text{low-lying } n} |\langle n|\nu\rangle_K|^2 \simeq 1.$$  \hspace{1cm} (19)

Here, $\sum_{\text{low-lying } n}$ denotes the sum over low-lying Dirac modes. This assumption would be natural, although it is desired to examine (19) quantitatively in lattice QCD. From this assumption, if the low-lying Dirac modes of $\hat{D}$ are removed, the low-lying modes $|\nu\rangle_K$ of the fermionic kernel $K[U]$ are also removed approximately. In fact, this assumption links the Dirac mode expansion to the low-lying modes of $K[U]$, which is more directly connected to chiral symmetry breaking.

2.5. Dirac operator and Polyakov loop in finite-temperature QCD

In this subsection, we investigate the Dirac operator and the Polyakov loop in finite-temperature QCD. In the imaginary-time formalism, the finite-temperature system requires periodicity for bosons and anti-periodicity for fermions in the Euclidean temporal direction [7]. Here, we consider such a temporally (anti-)periodic lattice with the temporal size $N_t$, which corresponds to the temperature $T = 1/(N_ta)$. In this thermal system, any fermion field $\psi(s)$ obeys

$$\psi(s + N_t\hat{t}) = -\psi(s),$$  \hspace{1cm} (20)

with $\hat{t} = \hat{4}$, and the temporal anti-periodicity of quarks also reflects in the Dirac operator $\hat{D}$. In fact, the temporal structure of the matrix $\hat{D}_4$ which acts on quarks is expressed as [42]

$$\hat{D}_4 = \frac{1}{2a} \begin{pmatrix}
  0 & U_4(1) & 0 & \cdots & 0 & U_4^\dagger(N_t) \\
  -U_4^\dagger(1) & 0 & U_4(2) & \cdots & 0 & 0 \\
  0 & -U_4^\dagger(2) & 0 & \cdots & 0 & 0 \\
  \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
  0 & 0 & 0 & \cdots & 0 & U_4(N_t - 1) \\
  -U_4(N_t) & 0 & 0 & \cdots & -U_4^\dagger(N_t - 1) & 0
\end{pmatrix}.$$  \hspace{1cm} (21)
where $U_4(t) \equiv U_4(s, t)$ $(t = 1, 2, \ldots, N_t)$ is an abbreviation of the temporal link variable. The additional minus sign in front of $U_4(N_t)$ and $U_4^+(N_t)$ reflects the anti-periodicity of quarks in the temporal direction.

For the thermal system, the link variable operator $\hat{U}_{\pm \mu}$ is basically defined by the matrix element (11). However, taking account of the temporal anti-periodicity in $\hat{D}_4$ acting on quarks, it is convenient to add a minus sign to the matrix element of the temporal link variable operator $\hat{U}_{\pm 4}$ at the temporal boundary of $t = N_t (= 0)$:

$$\begin{align*}
\{s, N_t|\hat{U}_4(s, N_t)\} = -U_4(s, N_t), & \quad \{s, 1|\hat{U}_{-4}|s, N_t\} = -U_{-4}(s, 1) = -U_4^+(s, N_t). \tag{22}
\end{align*}$$

Here, $\hat{U}_{-\mu} = \hat{U}_\mu^+$ is satisfied. For thermal QCD, by using this definition of the link variable operator $\hat{U}_{\pm \mu}$, the Dirac operator and the covariant derivative are also simply expressed as

$$\hat{D} = \frac{1}{2a} \sum_{\mu=1}^4 \gamma_\mu (\hat{U}_\mu - \hat{U}_{-\mu}), \quad \hat{D}_\mu = \frac{1}{2a} (\hat{U}_\mu - \hat{U}_{-\mu}), \tag{23}$$

which are consistent with Eq. (21).

The Polyakov loop $L_P$ is also simply written as the functional trace of $\hat{U}_4^{N_t}$,

$$L_P = -\frac{1}{N_c V} \text{Tr}_c \left\{ \hat{U}_4^{N_t} \right\} = \frac{1}{N_c V} \sum_s \text{tr}_c \left\{ \prod_{n=0}^{N_t-1} U_4(s + n\tau) \right\}, \tag{24}$$

with the four-dimensional lattice volume $V \equiv N_s^4 \times N_t$. Here, “$\text{Tr}_c$” denotes the functional trace of $\text{Tr}_c \equiv \sum_s \text{tr}_c$ with the trace $\text{tr}_c$ over the color index. The minus sign stems from the additional minus on $U_4(s, N_t)$ in Eq. (22).

### 3. Analytical formula between Polyakov loop and Dirac modes in lattice QCD with odd temporal size

Now, we consider lattice QCD with odd-number temporal lattice size $N_t$, as shown in Fig. 1. Here, we use an ordinary square lattice with the normal nontwisted periodic boundary condition for the link variable in the temporal direction. (Of course, this temporal periodicity is physically required at finite temperature.) The spatial lattice size $N_s$ is taken to be larger than $N_t$, i.e., $N_s > N_t$. Note that, in the continuum limit of $a \to 0$ and $N_t \to \infty$, any number of large $N_t$ gives the same physical result. Then, in principle, it is no problem to use the odd-number lattice.

In general, only gauge-invariant quantities such as closed loops and the Polyakov loop survive in QCD, according to the Elitzur theorem [7]. All the non-closed lines are gauge variant and their expectation values are zero. Note here that any closed loop, except for the Polyakov loop, needs even-number link variables on the square lattice, as shown in Fig. 1.

Note also that, from the definition of the link variable operator $\hat{U}_\mu$ $(\mu \in \{\pm 1, \ldots, \pm 4\})$ in Eq. (11), the functional trace of the product of $\hat{U}_{\mu k}$ along any non-closed trajectory is zero, i.e.,

$$\text{Tr}_c \left( \hat{U}_{\mu_1} \hat{U}_{\mu_2} \cdots \hat{U}_{\mu_N} \right) = \text{tr}_c \left\{ \sum_s \{ \hat{U}_{\mu_1} \hat{U}_{\mu_2} \cdots \hat{U}_{\mu_N} \} | s \} \right. \right.$$

$$\left. \quad = \text{tr}_c \sum_s U_{\mu_1}(s) U_{\mu_2}(s + \hat{\mu}_1) \cdots U_{\mu_N}(s + \sum_{k=1}^{N-1} \hat{\mu}_k) \left( \sum_{k=1}^N \hat{\mu}_k \right) | s \} = 0 \tag{25}$$

for the non-closed trajectory with $\sum_{k=1}^N \hat{\mu}_k \neq 0$. (Here, $\hat{\mu}_k$ can take positive or negative direction as $\hat{\mu}_k \in \{ \pm \hat{1}, \ldots, \pm 4 \}$, and any closed loop satisfies $\sum_{k=1}^N \hat{\mu}_k = 0$.)
In lattice QCD with odd-number temporal size $N_t$, we consider the functional trace of

$$I \equiv \text{Tr}_{c,y} \left( \hat{U}_4 \hat{D}^{N_t-1} \right),$$

where $\text{Tr}_{c,y} \equiv \sum_s \text{tr}_c \text{tr}_y$ includes $\text{tr}_c$ and the trace $\text{tr}_y$ over spinor index. Its expectation value

$$\langle I \rangle = \left\langle \text{Tr}_{c,y} \left( \hat{U}_4 \hat{D}^{N_t-1} \right) \right\rangle$$

is obtained as the gauge-configuration average in lattice QCD. In the case of a large enough volume $V$, one can expect $\langle O \rangle \simeq \text{Tr} \ O / \text{Tr} \ 1$ for any operator $O$ at each gauge configuration.

From Eq. (14), $\hat{U}_4 \hat{D}^{N_t-1}$ is expressed as a sum of products of $N_t$ link variable operators, since the Dirac operator $\hat{D}$ includes one link variable operator in each direction of $\pm \mu$. Then, $\hat{U}_4 \hat{D}^{N_t-1}$ includes many trajectories with the total length $N_t$ in the lattice unit on the square lattice, as shown in Fig. 2. Note that all the trajectories with the odd-number length $N_t$ cannot form a closed loop on the square lattice, and thus give a gauge-variant contribution, except for the Polyakov loop.

Therefore, among the trajectories stemming from $\text{Tr}_{c,y} \left( \hat{U}_4 \hat{D}^{N_t-1} \right)$, all the non-loop trajectories are gauge variant and give no contribution, according to the Elitzur theorem [7]. The only exception is the Polyakov loop (see Figs. 2 and 3). For each trajectory in $\hat{U}_4 \hat{D}^{N_t-1}$, the first step is the positive temporal direction corresponding to $\hat{U}_4$, and hence $\text{Tr}_{c,y} \left( \hat{U}_4 \hat{D}^{N_t-1} \right)$ cannot include the
Among the trajectories stemming from $\text{Tr}_{c,y} \left( \hat{U}_4 \hat{D}^{N_t - 1}_4 \right)$, only the Polyakov-loop ingredient can survive as a gauge-invariant quantity. Here, $\text{Tr}_{c,y} \left( \hat{U}_4 \hat{D}^{N_t - 1}_4 \right)$ does not include $L^\dagger_\eta$, because of the first factor $\hat{U}_4$.

anti-Polyakov loop $L^\dagger_\eta$. Thus, in the functional trace $I = \text{Tr}_{c,y} \left( \hat{U}_4 \hat{D}^{N_t - 1}_4 \right)$, only the Polyakov-loop ingredient can survive as the gauge-invariant quantity, and $I$ is proportional to the Polyakov loop $L_P$.

Actually, we can mathematically derive the following relation:

$$ I = \text{Tr}_{c,y} \left( \hat{U}_4 \hat{D}^{N_t - 1}_4 \right) = 4 \text{Tr}_c \left\{ \hat{U}_4 \left( \gamma_4 \hat{D} \right)^{N_t - 1}_4 \right\} = -4 N_c V \frac{2a}{(2a)^{N_t - 1}} L_P. \quad (28) $$

Here, a minus appears from Eq. (24), which reflects the temporal anti-periodicity of $\hat{D}$. We thus obtain the relation between $I = \text{Tr}_{c,y} \left( \hat{U}_4 \hat{D}^{N_t - 1}_4 \right)$ and the Polyakov loop $L_P$,

$$ I = -4 N_c V \frac{2a}{(2a)^{N_t - 1}} L_P. \quad (29) $$

On the other hand, we calculate the functional trace in Eq. (27) using the complete set of the Dirac mode basis $|n\rangle$ satisfying $\sum_n |n\rangle\langle n| = 1$, and find the Dirac mode representation of

$$ I = \sum_n \langle n | \hat{U}_4 \hat{D}^{N_t - 1}_4 | n \rangle = i^{N_t - 1} \sum_n \lambda^{N_t - 1}_n \langle n | \hat{U}_4 | n \rangle. \quad (30) $$

Combing Eqs. (29) and (30), we obtain the analytical formula between the Polyakov loop $L_P$ and the Dirac eigenvalues $i\lambda_n$:

$$ L_P = -\frac{(2ai)^{N_t - 1}}{4N_c V} \sum_n \lambda^{N_t - 1}_n \langle n | \hat{U}_4 | n \rangle \quad (31) $$

for each gauge configuration. Taking the gauge-configuration average, we obtain

$$ \langle L_P \rangle = -\frac{(2ai)^{N_t - 1}}{4N_c V} \left\langle \sum_n \lambda^{N_t - 1}_n \langle n | \hat{U}_4 | n \rangle \right\rangle_{\text{gauge avg}}. \quad (32) $$

This is a direct relation between the Polyakov loop $\langle L_P \rangle$ and the Dirac modes in QCD, and is mathematically valid in lattice QCD with odd-number temporal size in both confinement and deconfinement phases. The formula (31) is a Dirac spectral representation of the Polyakov loop, and we can investigate each Dirac mode contribution to the Polyakov loop individually, based on Eq. (31). (For example, each contribution specified by $n$ is numerically calculable in lattice QCD [27–29].)
As a remarkable fact, because of the factor $\lambda_n^{N_t-1}$, the contribution from low-lying Dirac modes with $|\lambda_n| \simeq 0$ is negligibly small in the Dirac spectral sum of the right-hand side of Eq. (31), in comparison with the other Dirac mode contribution. In fact, the low-lying Dirac modes have a fairly small contribution to the Polyakov loop in Eq. (31), regardless of confinement or deconfinement phase.

This is consistent with the previous numerical lattice QCD result that confinement properties are almost unchanged by removing low-lying Dirac modes from the QCD vacuum [16–22].

4. Discussions on the Dirac spectral representation of the Polyakov loop

In this section, we consider the Dirac spectral representation of the Polyakov loop, i.e., the formula (31) between the Polyakov loop and Dirac modes, and discuss its physical meaning. In particular, we consider the contribution from low-lying Dirac modes to the Polyakov loop.

4.1. Properties of the formula between the Polyakov loop and Dirac modes

First, we note that Eq. (31) is a manifestly gauge-invariant formula. Actually, the matrix element $\langle n | \hat{U}_4 | n \rangle$ can be expressed with the Dirac eigenfunction $\psi_n(s)$ and the temporal link variable $U_4(s)$ as

$$
\langle n | \hat{U}_4 | n \rangle = \sum_s \langle n | s \rangle \langle s | \hat{U}_4 | s + \hat{t} \rangle \langle s + \hat{t} | n \rangle = \sum_s \psi_n^\dagger(s) U_4(s) \psi_n(s + \hat{t}).
$$

and each term $\psi_n^\dagger(s) U_4(s) \psi_n(s + \hat{t})$ is manifestly gauge invariant, because of the gauge transformation property (8). Here, the irrelevant global phase factors also cancel exactly as $e^{-i\phi_n} e^{i\phi_n} = 1$ between $|n\rangle$ and $|n\rangle$ [16–22].

Second, we note the chiral property and nontriviality of Eq. (31). In the right-hand side of Eq. (31), there is no cancellation between chiral-pair Dirac eigenstates, $|n\rangle$ and $\gamma_5 | n \rangle$, because $(N_t - 1)$ is even, i.e., $(-\lambda_n)^{N_t-1} = \lambda_n^{N_t-1}$, and $\langle n | \gamma_5 \hat{U}_4 \gamma_5 | n \rangle = \langle n | \hat{U}_4 | n \rangle$.

Third, Eq. (31) is correct for any odd number $N_t (>1)$ and is applicable to both confinement and deconfinement phases. Then, Eq. (31) obtained on the odd-number lattice is expected to hold in the continuum limit of $a \to 0$ and $N_t \to \infty$, since any number of large $N_t$ gives the same physical result.

Finally, we comment on the generality and wide applicability of Eq. (31). In the argument to derive Eq. (31), we only use a few setup conditions:

i) square lattice (including anisotropic cases)

ii) odd-number temporal size $N_t(<N_s)$

iii) temporal periodicity for link variables.

Accordingly, Eq. (31) is widely correct in the case of an arbitrary gauge group for the theory. For example, Eq. (31) is applicable in the SU($N_c$) gauge theory for the arbitrary color number $N_c$. In addition, regardless of the presence or absence of dynamical quarks, Eq. (31) is formally correct as the Dirac mode expansion. In fact, Eq. (31) can also be derived for the gauge configuration after integrating out quark degrees of freedom. Of course, the dynamical quark effect appears in the Polyakov loop $L_P$, the Dirac eigenvalue distribution $\rho(\lambda)$, and $\langle n | \hat{U}_4 | n \rangle$. However, the formula (31) holds even in the presence of dynamical quarks. Therefore, the formula (31) is applicable at finite density and finite temperature.

4.2. On the small contribution from low-lying Dirac modes to the Polyakov loop

In this subsection, we consider the contribution from low-lying Dirac modes to the Polyakov loop based on Eq. (31). Due to the factor $\lambda_n^{N_t-1}$, the contribution from low-lying Dirac modes with
$|\lambda_n|\simeq 0$ is negligibly small in the right-hand side in Eq. (31), compared with the other Dirac mode contribution, so that the low-lying Dirac modes have a small contribution to the Polyakov loop in both confinement and deconfinement phases.

If the right-hand side of Eq. (31) were not a sum but a product, low-lying Dirac modes, or the small $|\lambda_n|$ region, should have given an important contribution to the Polyakov loop as a crucial reduction factor of $\lambda_n^{N_t-1}$. In the sum, however, the contribution ($\propto \lambda_n^{N_t-1}$) from the small $|\lambda_n|$ region is negligible.

Even if $\langle n\mid \hat{U}_4\mid n \rangle$ behaves as the \(\delta\) function $\delta(\lambda)$, the factor $\lambda_n^{N_t-1}$ is still crucial in the right-hand side of Eq. (31), because of $\lambda \delta(\lambda) = 0$. In fact, without the appearance of the extra counter factor $\lambda_n^{-(N_t-1)}$ from $\langle n\mid \hat{U}_4\mid n \rangle$, the crucial factor $\lambda_n^{N_t-1}$ inevitably leads to a small contribution for low-lying Dirac modes. Note here that the explicit $N_t$ dependence appears as the factor $\lambda_n^{N_t-1}$ in the right-hand side of Eq. (31), and the matrix element $\langle n\mid \hat{U}_4\mid n \rangle$ does not include $N_t$ dependence in an explicit manner. Then, it seems rather difficult to consider the appearance of the counter factor $\lambda_n^{-(N_t-1)}$ from the matrix element $\langle n\mid \hat{U}_4\mid n \rangle$.

One may suspect the necessity of renormalization for the Polyakov loop, although the Polyakov loop is at present one of the typical order parameters of confinement, and most arguments on the QCD phase transition have been done in terms of the simple Polyakov loop. Even in the presence of a possible multiplicative renormalization factor for the Polyakov loop like $Z_P L_P$, the contribution from the low-lying Dirac modes, or the small $|\lambda_n|$ region, is relatively negligible compared with other Dirac mode contributions in the sum of the right-hand side of Eq. (31).

### 4.3. Numerical confirmation with lattice QCD

It is notable that all the above arguments can be numerically confirmed by lattice QCD calculations. In this subsection, we briefly mention the numerical confirmation with lattice QCD Monte Carlo calculations [27–29].

Using actual lattice QCD calculations at the quenched level, we numerically confirm the analytical formula (31), the non-zero finiteness of $\langle n\mid \hat{U}_4\mid n \rangle$ for each Dirac mode, and the negligibly small contribution of low-lying Dirac modes to the Polyakov loop, i.e., the Polyakov loop is almost unchanged even by removing low-lying Dirac mode contributions from the QCD vacuum generated by lattice QCD simulations, in both confinement and deconfinement phases [27–29].

As for the matrix element $\langle n\mid \hat{U}_4\mid n \rangle$, its behavior is different between confinement and deconfinement phases. In the confinement phase, we find a “positive/negative symmetry” in the distribution of the matrix element $\langle n\mid \hat{U}_4\mid n \rangle$ [27–29], i.e., its actual value seems to appear as “pair-wise” plus and minus, and this symmetry is one of the reasons for the zero value of the Polyakov loop $L_P$. In fact, due to this symmetry of $\langle n\mid \hat{U}_4\mid n \rangle$ in the confinement phase, the contribution from partial Dirac modes in an arbitrary region $a \leq \lambda_n \leq b$ leads to $L_P = 0$. In particular, the high-lying Dirac modes do not contribute to the Polyakov loop $L_P$, in spite of the large factor $\lambda_n^{N_t-1}$. This behavior is consistent with our previous lattice QCD results [16–22], which indicate that the “seed” of confinement is distributed in a wider region of the Dirac eigenmodes, unlike chiral symmetry breaking. In the deconfinement phase, there is no such symmetry in the distribution of $\langle n\mid \hat{U}_4\mid n \rangle$, and this asymmetry leads to a non-zero value of the Polyakov loop [27–29].

In any case, regardless of the behavior of $\langle n\mid \hat{U}_4\mid n \rangle$, we numerically confirm that the contribution from low-lying Dirac modes to the Polyakov loop is negligibly small [27–29] in both confinement and deconfinement phases, owing to the factor $\lambda_n^{N_t-1}$ in Eq. (31).
Fig. 4. The left figure shows the Wilson loop $W$ defined on an $R \times T$ rectangle. The right figure shows the factorization of the Wilson-loop operator as a product of $\hat{U}_{\text{staple}} \equiv \hat{U}^R_1 \hat{U}^T_{-1} \hat{U}^R_4$ and $\hat{U}^T_4$. Here, $T$, $R$, and the lattice size are arbitrary.

From the analytical formula (31) and the numerical confirmation, low-lying Dirac modes have a small contribution to the Polyakov loop, and are not essential for confinement, while these modes are essential for chiral symmetry breaking.

5. A similar formula for the Wilson loop on arbitrary square lattices

In this section, we attempt a similar consideration of the Wilson loop and the string tension on arbitrary square lattices (including anisotropic cases) with any number of $N_t$, i.e., without the restriction of an odd-number size. We consider the ordinary Wilson loop on an $R \times T$ rectangle, where $T$ and $R$ are arbitrary positive integers. The Wilson loop is expressed by the functional trace \[ W \equiv \text{Tr}_c \hat{U}^R_1 \hat{U}^T_{-1} \hat{U}^R_4 = \text{Tr}_c \hat{U}_{\text{staple}} \hat{U}^T_4, \] (34)

where we introduce the “staple operator” $\hat{U}_{\text{staple}}$ as
\[ \hat{U}_{\text{staple}} \equiv \hat{U}^R_1 \hat{U}^T_{-1} \hat{U}^R_4. \] (35)

Here, the Wilson-loop operator is factorized as a product of $\hat{U}_{\text{staple}}$ and $\hat{U}^T_4$, as shown in Fig. 4. We note that $W \propto \langle W \rangle_{\text{gauge avg}}$ for a lattice of large enough volume [16–19].

In the case of an even number $T$, let us consider the functional trace of $J \equiv \text{Tr}_c,\gamma \hat{U}_{\text{staple}} \hat{D}^T_4$. (36)

From similar arguments to Sect. 3, we obtain
\[ J = \text{Tr}_c,\gamma \hat{U}_{\text{staple}} \hat{D}^T_4 = \text{Tr}_c,\gamma \hat{U}_{\text{staple}} (\gamma_4 \hat{D}_4)^T = 4 \text{Tr}_c \hat{U}_{\text{staple}} \hat{D}^T_4 = \frac{4}{(2a)^T} \text{Tr}_c \hat{U}_{\text{staple}} \hat{U}^T_4 = \frac{4}{(2a)^T} W, \] (37)

and
\[ J = \sum_n \langle n | \hat{U}_{\text{staple}} \hat{D}^T_4 | n \rangle = (-)^T \sum_n \lambda_n^T \langle n | \hat{U}_{\text{staple}} | n \rangle. \] (38)

Therefore, we obtain for even $T$ the simple formula
\[ W = \frac{(-)^T (2a)^T}{4} \sum_n \lambda_n^T \langle n | \hat{U}_{\text{staple}} | n \rangle. \] (39)
Again, because of the factor $\lambda_T^n$, the contribution from low-lying Dirac modes is expected to be small also for the Wilson loop, although the matrix element $|n\rangle \langle \hat{U}_{\text{staple}} n\rangle$ includes explicit $T$ dependence and its behavior is not so clear, unlike the formula (31) for the Polyakov loop.

In the case of odd $T$, similar results can be obtained by considering

$$K = \text{Tr}_{c,y} \hat{U}_{\text{staple}} \hat{D}^{T-1}$$

instead of $J$. Actually, one finds

$$K = \text{Tr}_{c,y} \hat{U}_{\text{staple}} \hat{D}^{T-1} = \text{Tr}_{c,y} \hat{U}_{\text{staple}} (\gamma_4 \hat{D}_4)^T = 4 \text{Tr}_{c} \hat{U}_{\text{staple}} \hat{D}_4^{T-1}$$

$$= \frac{4}{(2a)^T-1} \text{Tr}_c \hat{U}_{\text{staple}} (\hat{U}_4 - \hat{U}_{-4})^{T-1} = \frac{4}{(2a)^T-1} \text{Tr}_c \hat{U}_{\text{staple}} \hat{U}_4^{T-1} = \frac{4}{(2a)^T-1} \text{W},$$

and

$$K = \sum_n \langle n | \hat{U}_{\text{staple}} \hat{D}^{T-1} | n \rangle = (-)^{T-1} \sum_n \lambda_n^{T-1} \langle n | \hat{U}_{\text{staple}} \hat{U}_4 | n \rangle,$$

so that one finds for odd $T$ the similar formula of

$$W = \left(\frac{-(-)^{T-1}}{4} \frac{(2a)^T-1}{4} \sum_n \lambda_n^{T-1} \langle n | \hat{U}_{\text{staple}} \hat{U}_4 | n \rangle. \right)$$

Finally, for the even $T$ case, we show the inter-quark potential $V(R)$ and the string tension $\sigma$. From the expression (39) for the Wilson loop $W$, we obtain the inter-quark potential $V(R)$ and the string tension $\sigma$:

$$V(R) = - \lim_{T \to \infty} \frac{1}{T} \ln W = - \lim_{T \to \infty} \frac{1}{T} \ln \left| \sum_n (2a\lambda_n)^T \langle n | \hat{U}_{\text{staple}} | n \rangle \right|,$$

$$\sigma = - \lim_{R,T \to \infty} \frac{1}{RT} \ln W = - \lim_{R,T \to \infty} \frac{1}{RT} \ln \left| \sum_n (2a\lambda_n)^T \langle n | \hat{U}_{\text{staple}} | n \rangle \right|. \right)$$

Because of the factor $\lambda_n^{-T}$ in the sum, the low-lying Dirac mode contribution is to be small for the Wilson loop $W$, the inter-quark potential $V(R)$, and the string tension $\sigma$, unless the extra counter factor $\lambda_n^{-T}$ appears from $\langle n | \hat{U}_{\text{staple}} | n \rangle$. Also for the odd $T$ case, similar arguments can be made with Eq. (43).

In this way, the string tension $\sigma$, or the confining force, is expected to be unchanged by the removal of the low-lying Dirac mode contribution, which is consistent with our previous numerical work for lattice QCD [16–19].

Taking the assumption (19) in Sect. 2.4, the removal of low-lying Dirac modes of $D$ leads to an approximate removal of low-lying modes of the fermionic kernel $K[U]$, which largely reduces the chiral condensate. Then, the insensitivity of confinement to low-lying Dirac modes suggested above indicates no direct one-to-one correspondence between confinement and chiral symmetry breaking in QCD.

6. Summary and concluding remarks

We have derived an analytical gauge-invariant formula between the Polyakov loop $L_P$ and the Dirac eigenvalues $\lambda_n$ as $L_p \sim \sum_n \lambda_n^{N_t-1} \langle n | \hat{U}_4 | n \rangle$ in lattice QCD with odd-number temporal size $N_t$, by considering $\text{Tr} \left( \hat{U}_4 \hat{D}^{N_t-1} \right)$ on the ordinary square lattice with the normal (nontwisted) temporally
periodic boundary condition for link variables. Here, $|n\rangle$ denotes the Dirac eigenstate, and $\hat{U}_4$ the temporal link variable operator.

This formula is a Dirac spectral representation of the Polyakov loop in terms of Dirac eigenmodes $|n\rangle$, and expresses each contribution of the Dirac eigenmode to the Polyakov loop. Because of the factor $\lambda N_t^{-1} n$ in the Dirac spectral sum, this formula indicates a fairly small contribution of low-lying Dirac modes to the Polyakov loop in both confinement and deconfinement phases, while these modes are essential for chiral symmetry breaking.

Next, we have found a similar formula between the Wilson loop and Dirac modes on arbitrary lattices, without restriction of odd-number size. This formula suggests a small contribution of low-lying Dirac modes to the string tension $\sigma$, or the confining force.

Thus, it is likely that low-lying Dirac modes have fairly small contributions to the Polyakov loop and the string tension, and are not essential modes for confinement, while these modes are essential for chiral symmetry breaking. This suggests no direct one-to-one correspondence between confinement and chiral symmetry breaking in QCD. Note here that the independence of confinement and chiral symmetry breaking would be natural, because heavy quarks are also confined even without light quarks or chiral symmetry.

Also, for thermal QCD, we have investigated the relation between confinement and chiral symmetry breaking using the ratio of the susceptibility of the Polyakov loop $[43,44]$, the importance of which for the deconfinement transition has been pointed out $[45,46]$.

Finally, we state some cautions and future works in this framework in order.

In Sect. 2.4, for the strict connection to chiral symmetry breaking, we have assumed that each low-lying mode of the fermionic kernel $K[U]$ is mainly expressed with the low-lying Dirac modes of $\tilde{D}$. We are now investigating this assumption (19) quantitatively in lattice QCD.

In this paper, we have derived the Dirac mode expansion Eq. (31), which is mathematically correct. In this expansion, each Dirac mode contribution is explicitly expressed, and we have focused on this explicit contribution. This treatment would be appropriate in quenched QCD. For a more definite argument in full QCD, however, we have to clarify an implicit contribution of the Dirac modes in the fermionic determinant, which can actually alter the properties of the QCD vacuum $[40,41]$.

It is important to take the continuum limit of the mathematical formulae obtained on the lattice, although it seems a difficult problem. It is also interesting to compare with other lattice QCD results on the important role of infrared gluons (below about 1 GeV) for confinement in the Landau gauge $[47,48]$, in contrast to the insensitivity of confinement against low-lying Dirac modes.

This work suggests some possible independence between confinement and chiral symmetry breaking in QCD, and this may lead to a richer phase structure of QCD in various environments. In fact, there is an interesting possibility that QCD phase transition points can be generally different between deconfinement and chiral symmetry restoration, e.g., in the presence of strong electromagnetic fields, because of their nontrivial effect on the chiral symmetry $[49,50]$.

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