Effect of low-lying fermion modes in the $\epsilon$-regime of QCD

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Abstract

We investigate the effects of low-lying fermion eigenmodes on the QCD partition function in the $\epsilon$-regime. The fermion determinant is approximated by a truncated product of low-lying eigenvalues of the overlap-Dirac operator. With two flavors of dynamical quarks, we observe that the lattice results for the lowest eigenvalue distribution, eigenvalue sum rules and partition function reproduce the analytic predictions made by Leutwyler and Smilga, which strongly depend on the topological charge of the background gauge configuration. The value of chiral condensate extracted from these measurements are consistent with each other. For one dynamical quark flavor, on the other hand, we find an apparent disagreement among different determinations of the chiral condensate, which may suggest the failure of the $\epsilon$-expansion in the absence of massless Nambu-Goldstone boson.
§1. Introduction

Chiral perturbation theory (ChPT) is an effective field theory to describe the dynamics of Quantum Chromodynamics (QCD) at low energies ($\ll \Lambda \sim 1$ GeV), where the Nambu-Goldstone pion excitations dominate the dynamics while other particles are too heavy to be excited. In the infinite volume, ChPT provides a method to express low energy amplitudes of pion as an expansion in terms of pion mass squared $m_\pi^2$ and its momentum squared $p^2$. Thus it enables us to calculate low energy pion amplitudes in a systematic manner. When the system is put in a finite volume, for which the pion Compton wavelength ($\sim 2\pi/m_\pi$) is much larger than the linear extent $L$ of the space-time, *i.e.* $m_\pi L \ll 1$, while $L$ is kept large enough compared to the QCD scale $1/\Lambda_{QCD}$, the low energy effective theory can still be constructed as an expansion in terms of small $\epsilon^2 \sim m_\pi/\Lambda \sim p^2/\Lambda^2$, which is known as the $\epsilon$-expansion.\(^1\) In this setup, the so-called $\epsilon$-regime of ChPT, the chiral symmetry is not spontaneously broken and one must explicitly integrate over different vacua in the path integral, which leads to characteristic behavior of the partition function and other physical quantities. In particular, they strongly depend on the gauge field topology (or the existence of fermion zero modes).\(^2\)

Lattice QCD simulation is well suited to the study of finite volume physics. Since the chiral symmetry plays an essential role in the $\epsilon$-regime, one should use lattice fermion formulations that respect chiral symmetry. Such fermion formulation has become available relatively recently, *i.e.* the overlap fermion\(^3\),\(^4\) and the domain-wall fermion.\(^5\),\(^6\) These fermion formulations satisfy the Ginsparg-Wilson relation,\(^7\) with which the fermion action can be shown to have exact chiral symmetry at finite lattice spacings.\(^8\) Quenched lattice simulations have so far been done in the $\epsilon$-regime to calculate the chiral condensate\(^9\) and other low energy constants.\(^10\)–\(^13\) It has also been shown that the distribution of low-lying eigenvalues of the lattice overlap Dirac operator agrees well with expectations from the chiral Random Matrix Theory (RMT)\(^14\)–\(^16\) (for a review of RMT, see\(^17\)), which is equivalent to the chiral Lagrangian at the leading order of the $\epsilon$-expansion.

In this work we extend these previous lattice studies to the case of non-zero dynamical fermion flavors. In particular we calculate the topological susceptibility and partition function with one and two flavors of dynamical quarks, and investigate their dependence on the quark mass. The predictions from ChPT in the $\epsilon$-regime are available from the work by Leutwyler and Smilga.\(^2\) Due to the presence of fermion zero-modes the partition function is drastically different for different topological sectors of background gauge field. We therefore calculate them for each topological sector identified by the number of fermion zero-modes. We also investigate the sum rules of Dirac operator eigenvalues (the so-called Leutwyler-
Smilga sum rules\footnote{2} derived from the quark mass dependence of the partition function. For these quantities we found that the lattice data with one or two fermion flavors are well described by the known analytic formulas.

We also extend the comparison of low-lying eigenvalue distributions with the RMT results to the case of non-zero number of flavors. In RMT there is an universality among the number of flavor $N_f$ and topological charge $\nu$. Namely the prediction depends only on the combination $N_f + |\nu|$, which should be observed in the lattice data.

In order to investigate the effect of dynamical fermions, we employ an approximation for the fermion determinant. Namely, we approximate the fermion determinant by a product of low-lying eigenvalues of the overlap Dirac operator. The effects of higher fermion modes are neglected, which we call the truncated determinant approximation. Since the eigenvalues much higher than the quark mass and the QCD scale $\Lambda_{\text{QCD}}$ should be irrelevant to low energy physics, this approximation is expected to be effective for the study of the $\epsilon$-regime. The higher eigenmodes are sensitive to lattice artifacts and their main effect for low energy physics appears through the renormalization of parameters in the theory, \textit{i.e.} in this case the gauge coupling constant and quark masses. As we neglect such effects, we effectively choose a different renormalization scheme. To what extent this approximation works can be tested by varying the cutoff for the Dirac operator eigenvalues.

This paper is organized as follows. First, in Section 2 we briefly review the analytic expectations from ChPT following the seminal paper by Leutwyler and Smilga.\footnote{2} We then explain our calculation methods and describe the truncated determinant approximation in some detail in Sections 3 and 4, respectively. Numerical results are presented in Section 5. An earlier presentation of this work is found in.\footnote{18}

\S 2. Leutwyler-Smilga’s analytic predictions

In this section we briefly review the analytic predictions made by Leutwyler and Smilga\footnote{2} using the chiral Lagrangian in the $\epsilon$-regime.

At the leading order in the $\epsilon$-expansion the kinetic term in the chiral Lagrangian is suppressed, because the momentum excitation energy is large in a small volume even for the unit momentum $2\pi/L$. The partition function is then given by

$$Z = \exp \left[ \Sigma V \text{Re}(me^{i\theta}) \right]$$

(2.1)

for $N_f = 1$ and

$$Z = \int_{\text{SU}(N_f)} d\mu(U_0) \exp \left[ \Sigma V \text{Re}[me^{i\theta/N_f} \text{Tr}(U_0^\dagger U_0)] \right]$$

(2.2)
for $N_f \geq 2$. Here, $\Sigma$ represents the chiral condensate and $V$ is the space-time volume. They appear in the combination $m\Sigma V$ together with the quark mass $m$. The integral in (2.2) runs over compact SU($N_f$) elements $U_0$ corresponding to the zero momentum mode wave function, and $d\mu(U_0)$ is its Haar measure. This integral is necessary because the chiral symmetry is not spontaneously broken in the finite volume. For $N_f = 1$ (Eq. (2.1)), on the other hand, this degree of freedom does not remain due to the U(1) chiral anomaly. The parameter $\theta$ is the CP angle of the QCD vacuum.

The partition function in each topological sector labeled by the topological charge $\nu$ is obtained by Fourier transforming (2.1) and (2.2). They are

\begin{align}
Z_\nu &= I_\nu(x) \quad \text{for } N_f = 1, \\
Z_\nu &= I_{\nu}^2(x) - I_{\nu+1}(x)I_{\nu-1}(x) \quad \text{for } N_f = 2.
\end{align}

$I_\nu(x)$ is the modified Bessel function and its argument $x$ is $x \equiv m\Sigma V$. Near the massless limit it behaves as $(x/2)^{|\nu|}/|\nu|!$.

The probability to find a configuration with a given topological charge $\nu$ is given by $Z_\nu/Z$, where $Z = \sum_\nu Z_\nu$ is $e^x$ and $I_1(2x)/x$ for $N_f = 1$ and 2, respectively. The topological susceptibility $\langle \nu^2 \rangle / V$ is then obtained through the definition $\langle \nu^2 \rangle = \sum_\nu \nu^2 Z_\nu / Z$ as

\begin{align}
\langle \nu^2 \rangle / V &= m\Sigma \quad \text{for } N_f = 1, \\
\langle \nu^2 \rangle / V &= \frac{m\Sigma I_2(m\Sigma V)}{2I_1(m\Sigma V)} \quad \text{for } N_f = 2.
\end{align}

Asymptotically, it behaves as $\langle \nu^2 \rangle / V \propto m^{N_f}$ for $x \ll 1$ and $\langle \nu^2 \rangle / V = m\Sigma/N_f$ for $x \gg 1$.

The above results for the partition function should agree with the partition function of the underlying theory, QCD, in the appropriate limit. The QCD partition function for a given topological charge $\nu$ is written as

\begin{equation}
Z_\nu = m^{N_f|\nu|} \int [dG] e^{-S_G} \prod_n \left( |\lambda_n|^2 + m^2 \right)^{N_f}.
\end{equation}

The path integral over the gauge field configuration is done for a fixed topology $\nu$ with a weight given by the gauge action $S_G$. The fermion determinant is written in the form of a product of the eigenvalues $\lambda_n$ of the Dirac operator. Non-zero eigenvalues appear with their complex conjugate and the index $n$ in (2.7) runs over eigenvalues with positive imaginary part only. The prime on the product indicates that it excludes the zero modes, which are factored out as $m^{N_f|\nu|}$. Defining the expectation value in the massless limit as $\langle \langle \cdots \rangle \rangle_\nu$, the above expression is rewritten as

\begin{equation}
\lim_{m \to 0} \frac{m^{-N_f|\nu|} Z_\nu(m)}{m^{-N_f|\nu|} Z_\nu(m)} = \left\langle \prod_n \left( 1 + \frac{m^2}{|\lambda_n|^2} \right)^{N_f} \right\rangle_\nu.
\end{equation}
In the effective theory the same quantity is given by
\[
|\nu|! \left( \frac{2}{x} \right)^{|\nu|} I_\nu(x) \quad \text{for } N_f = 1, \tag{2.9}
\]
\[
\left[ \left( \frac{1}{|\nu|} \right)^2 - \frac{1}{(|\nu| + 1)!|\nu - 1|!} \right]^{-1} \left( \frac{2}{x} \right)^{2|\nu|} Z_\nu(x) \quad \text{for } N_f = 2. \tag{2.10}
\]

By taking a derivative with respect to \( m^2 \) for both QCD and the effective theory and equating them at \( m = 0 \), we arrive at the so-called Leutwyler-Smilga sum rules. From the first derivative we obtain
\[
\left\langle \left\langle \sum_n \frac{1}{(|\lambda_n|\Sigma^2)^2} \right\rangle \right\rangle_{\nu} = \frac{1}{4(N_f + |\nu|)}, \tag{2.11}
\]
which we call the sum rule I in this paper. The prime on the sum implies that it does not include the zero modes. For non-degenerate flavors with masses \( m_i \) and \( m_j \) we can extract two sum rules from second derivatives corresponding to \( m_i^2 m_j^2 \) and \( m_i^4 \)

\[
\left\langle \left\langle \left[ \sum_n \frac{1}{(|\lambda_n|\Sigma^2)^2} \right]^2 \right\rangle \right\rangle_{\nu} = \frac{1}{16((N_f + |\nu|)^2 - 1)}, \tag{2.12}
\]
\[
\left\langle \left\langle \left[ \sum_n \frac{1}{(|\lambda_n|\Sigma^2)^2} \right]^2 - \sum_n \frac{1}{(|\lambda_n|\Sigma^4)^4} \right\rangle \right\rangle_{\nu} = \frac{1}{16(N_f + |\nu| + 1)(N_f + |\nu| + 2)} \tag{2.13}
\]
which we call the sum rules IIa and IIb, respectively. Their difference gives
\[
\left\langle \left\langle \sum_n \frac{1}{(|\lambda_n|\Sigma^2)^4} \right\rangle \right\rangle_{\nu} = \frac{1}{16(N_f + |\nu|)((N_f + |\nu|)^2 - 1)}, \tag{2.14}
\]
(sum rule IIc). Note that there is a universality among the number of flavors and topological charge, i.e. they appear only in the combination \( N_f + |\nu| \).

These sum rules (2.11)-(2.14) do not make sense as they stand, because the left hand side is ultraviolet divergent while the right hand side is a definite number. In fact, since the eigenvalue density \( \rho(\lambda) = \frac{1}{V} \left\langle \sum_n \delta(\lambda_n - \lambda) \right\rangle \) increases as \( \sim V\lambda^3 \) for large \( \lambda \), the sum rule I is quadratically divergent. The sum rules IIa and IIb have quartic divergences, which cancel in the rule IIc and only a logarithmic divergence remains. In spite of these divergences, the sum rules (2.11)-(2.14) are consistent, because they only affect the corrections of order 1/V or higher, and thus can be removed by first taking a limit \( V \to \infty \). In the following numerical work we do not perform this extrapolation, which is very expensive, but consider differences between different topological sectors. Since the eigenvalue density becomes independent of topology for large \( \lambda \), the ultraviolet divergence cancels in such differences.
Table I. The number of quenched gauge configurations for each topological sector.

| Topological charge | $|\nu|$ | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
|--------------------|-------|---|---|---|---|---|---|---|
| #config            |       | 169 | 290 | 149 | 68 | 20 | 4 | 3 |

§3. Lattice details

The chiral symmetry is essential for the lattice study in the $\epsilon$-regime. We use the Neu-berger (or the so-called overlap) Dirac operator\(^3,^4\) which respects the Ginsparg-Wilson relation, and thus the chiral symmetry is preserved at finite lattice spacing.

The overlap Dirac operator $D$ is defined as

$$D = \frac{1}{\bar{a}} [1 + \gamma_5 \text{sgn}(aH_W)], \quad (3.1)$$

with

$$H_W = \gamma_5 \left[D_W - \frac{1}{\bar{a}}\right], \quad (3.2)$$

$$D_W = \frac{1}{2} \sum_\mu \{\gamma_\mu (\nabla^*_\mu + \nabla_\mu) - a\nabla^*_\mu \nabla_\mu\}, \quad (3.3)$$

and $\bar{a} = a/(1 + s)$. Here $D_W$ is the conventional Wilson-Dirac operator and $\nabla$ ($\nabla^*$) denotes a forward (backward) gauge-covariant differential operator on the lattice. The parameter $s$ is introduced to optimize the negative mass term given in the kernel $H_W$. In this work we choose $s = 0.6$ at $\beta = 5.85$. The sign function in (3.1) is approximated using the Chebyshev polynomial after subtracting out several lowest eigenmodes of $H_W$. The order of polynomial is optimized for each gauge configuration to ensure the accuracy of $10^{-11}$ for the sign function, and it is typically around 100–200 when we subtract 14 lowest-lying eigenvalues of $H_W$.

We work on quenched gauge configurations generated with the plaquette gauge action at $\beta = 5.85$ on a $10^4$ lattice. The lattice spacing determined through the Sommer scale $r_0$ is 0.123 fm. The topological charge for these gauge configurations is determined by the number of zero modes of the overlap-Dirac operator (3.1). The number of gauge configuration for each topological sector is given in Table I.

For the overlap-Dirac operator (3.1) we calculate 50 lowest eigenvalues and their eigenvectors for each gauge configuration. We utilize the numerical package ARPACK,\(^{19}\) which implements the implicitly restarted Arnoldi method to compute the eigenvalues. Instead of treating the operator $D$ as it is, we consider a chirally projected operator $D^\pm \equiv P_\pm DP_\pm$, where $P_\pm \equiv (1 \pm \gamma_5)/2$. The size of the matrix is then a factor of 2 smaller and the numerical calculation becomes about 2 times faster. The eigenvalues of $D$ can be obtained from the
eigenvalues of $P_{\pm}DP_{\pm}$, using the property that the chirally projected operator gives a real part of the eigenvalues of the original operator. Since the eigenvalues of $D$ lie on a circle satisfying $|1-\lambda|^2 = 1$, we can construct a pair of eigenvalues of $D$, namely $\lambda$ and $\lambda^*$. The corresponding eigenvectors $u$ of $D$ can also be reconstructed from the eigenvectors $u^\pm = P_{\pm}u$ of the chirally projected operator $D^\pm$ using a formula

$$u = \frac{D - \lambda^*}{\text{Im}\lambda} u^+ = \frac{D - \lambda^*}{\text{Im}\lambda} u^-.$$  

(3.4)

In order to identify the number of left-handed and right-handed zero modes, we have to compute the eigenvalues of both $P_{\pm}DP_{\pm}$ and $P_{-}DP_{-}$. We carry out such calculation until we achieve enough precision to identify pairing non-zero eigenvalues of both operators.\textsuperscript{20} The number of zero modes is then determined unambiguously, and we continue the calculation of the rest of the eigenvalues on the operator for which we do not find the zero modes.

\textbf{§4. Truncated determinant approximation}

In our calculation the effects of dynamical fermions are incorporated in the partition function by including a product of eigenvalues of Dirac operator in the pure gauge path integral.

$$Z_\nu = m^{N_f|\nu|} \int [dU]_\nu e^{-S_G} \prod_n (\bar{\lambda}_n^2 + m^2)^{N_f} = m^{N_f|\nu|} \left\langle \prod_n (\bar{\lambda}_n^2 + m^2)^{N_f} \right\rangle^Q$$

(4.1)

where $\bar{\lambda}_n = |\lambda_n|\sqrt{1 - (\bar{a}m)^2/4}$. The eigenvalues of the overlap-Dirac operator appear in complex conjugate pairs ($\lambda, \lambda^*$) except for the zero-modes as in the continuum case. The notation $\langle \cdots \rangle^Q_\nu$ denotes an expectation value evaluated on quenched gauge configurations with a fixed topological charge $\nu$. Namely, we generate the gauge configurations with a weight determined by the pure gauge action and reweight them with the product of eigenvalues.

This method requires a calculation of all eigenvalues of the overlap-Dirac operator for each configuration, but it is not feasible unless the lattice size is extremely small ($\sim 4^4$). Instead, we approximate the fermion determinant by a truncated product of eigenvalues in (4.1). The upper limit of the eigenvalue plays a role of an ultraviolet cutoff for the fermionic degrees of freedom. Qualitatively, this procedure is justified, since the physical effects of the fermion determinant are expected to come from the low-lying eigenmodes, while the higher eigenmodes should be irrelevant for low energy physics. As in the usual renormalization program, cutoff dependence of physical quantity can be absorbed in the coupling constants and anomalous dimensions up to lattice artifacts. In our case the bulk of the effects of higher fermion modes is neglected, and thus the relation between the lattice bare coupling and the lattice spacing is mostly the same as in the quenched approximation.
The role of the cutoff in the fermion determinant can be rephrased by defining a new Dirac operator $D_{LM}$ (LM stands for low-lying modes) as

$$D_{LM} = \gamma_5 f(H, \lambda_{\text{cutoff}})$$  \hspace{1cm} (4.2)

with $H = \gamma_5 D$ and a function $f(x, \lambda_{\text{cutoff}})$ satisfying a condition

$$f(x, \lambda_{\text{cutoff}}) = \begin{cases} x & (|x| \ll \lambda_{\text{cutoff}}), \\ \lambda_{\text{cutoff}} & (|x| \gg \lambda_{\text{cutoff}}). \end{cases} \hspace{1cm} (4.3)$$

The truncation corresponds to a non-smooth function, which transfers from $x$ to a constant $\lambda_{\text{cutoff}}$ at $\lambda_{\text{cutoff}}$. One can also interpolate the two regions smoothly using an analytic function, e.g. $f(x, \lambda_{\text{cutoff}}) = \lambda_{\text{cutoff}} \tanh(x/\lambda_{\text{cutoff}})$. For such analytic functions the locality and unitarity of the new Dirac operator $D_{LM}$ can be proved.\textsuperscript{21} Furthermore, the operator $D_{LM}$ satisfies a modified Ginsparg-Wilson relation

$$\gamma_5 D_{LM} + D_{LM} \gamma_5 = \bar{a} D \gamma_5 D_{LM} = \bar{a} D_{LM} \gamma_5 D,$$  \hspace{1cm} (4.4)

as far as $f(x, \lambda_{\text{cutoff}})$ is written in terms of a polynomial. It implies that the fermion action constructed with the truncated operator $D_{LM}$ is invariant under the chiral transformation $\delta \psi = \gamma_5 (1 - \bar{a} D/2) \psi$ and $\delta \bar{\psi} = \bar{\psi} (1 - \bar{a} D/2) \gamma_5$, just like the original overlap-Dirac operator. The truncated operator $D_{LM}$ may, therefore, be used as an alternative definition of the Dirac operator with exact chiral symmetry. It should be noted, however, that our choice for the function $f(x, \lambda_{\text{cutoff}})$ (hard cutoff) has to be understood as an approximation as it is not a smooth analytic function.

On a $10^4$ lattice at $\beta = 5.85$, we calculated 50 smallest eigenvalues of the chirally projected overlap-Dirac operator. Among them, the maximum eigenvalue corresponds to the physical scale $\sim 1200$ MeV, which is large enough as a cutoff for the study of the low energy physics of interest. We define the truncated determinant as

$$\det(D + m) \equiv \prod_{n=1}^{N_{\text{cut}}} (\lambda_n^2 + m^2)$$  \hspace{1cm} (4.5)

with a fixed number $N_{\text{cut}}$ of eigenvalues. Figure 11 shows a correlation between the truncated determinant with $N_{\text{cut}} = 10$ and that with $N_{\text{cut}} = 50$ for topological sectors $\nu = 0, 1,$ and $2$. The quark mass is set to zero, and the zero-modes are factored out for non-trivial topological sectors. We observe that they are strongly correlated up to an order of magnitude variations, while the truncated determinant itself varies as much as 8 orders of magnitude when measured on quenched gauge configurations. It suggests that the truncated determinant provides a good approximation of the full determinant already at $N_{\text{cut}} = 10$. 

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Fig. 1. Correlation between the truncated determinant with $N_{\text{cut}} = 10$ (horizontal axis) and that with $N_{\text{cut}} = 50$ (vertical). Each point corresponds to a gauge configuration with topological charge 0 (pluses), 1 (crosses), and 2 (stars). The quark mass is set equal to zero. Zero-modes for nontrivial topological sectors are not included in the product.

Fig. 2. Relative weight due to the truncated determinant for the massless overlap-Dirac operator as a function of $N_{\text{cut}}$ for five representative gauge configurations with $\nu = 0$.

One may also see how much the relative size of the truncated determinant depends on the value of cutoff $N_{\text{cut}}$. In Figure 2 we plot the truncated determinant for the massless overlap-Dirac operator as a function of $N_{\text{cut}}$ for five representative gauge configurations, for which we calculated 300 smallest eigenvalues. The value is normalized by an average over these five configurations at a given value of $N_{\text{cut}}$, and thus the plot shows a relative size of the weight factor due to the approximate determinant. We find that the relative weight
varies rapidly for small $N_{\text{cut}} \sim 10$, while it becomes roughly constant above $N_{\text{cut}} \gtrsim 50$. It supports our expectation that the truncated determinant is a good approximation of the full determinant for $N_{\text{cut}} \simeq 50$. In the following studies we also test how much our results depend on the parameter $N_{\text{cut}}$ for each quantity we measure.

The number of necessary eigenvalues to be included in the truncated determinant is expected to be unchanged even at smaller lattice spacings as long as the physical volume is kept fixed. This is because the the eigenvalue density $\rho(\lambda)$ depends on the physical parameters $\Sigma$ and $V$ but not on the lattice cutoff $1/a$ (up to lattice artifacts). It depends on the physical volume linearly, and therefore the number of eigenvalues to be calculated would become prohibitively large, e.g. about 14 times larger on a (2 fm)$^3 \times$ (4 fm) lattice, which is a typical lattice size used for hadron spectrum calculations.

The truncated determinant was previously introduced by Duncan, Eichten and Thacker to develop an efficient algorithm for light dynamical quarks with the Wilson fermion. They also proposed a method to include the higher fermion modes to make the algorithm exact using the multiboson technique of Lüschner. A similar method can also be applied in our case, but the effective bosonic action becomes non-local with the overlap-Dirac operator and the simple heat-bath updation would be impractical.

An immediate problem of the reweighting with the approximate determinant is that the overlap of the unquenched vacuum with the quenched vacuum could be tiny and thus the Monte Carlo sampling becomes inefficient especially for small quark masses we are interested in. If this happens, only a few configurations give a dominant contribution to the Monte Carlo average and others are suppressed by the reweighting factor representing the approximate determinant. We may quantify this effect by considering an effective number of statistics $N_{\text{eff}}$ as

$$N_{\text{eff}} = \frac{\sum_{i=1}^{N} \frac{\det D^{(i)}}{\max_j(\det D^{(j)})}}{N}.$$  \hspace{1cm} (4.6)

Here, $i$ and $j$ label gauge configurations and $N$ is the number of the configurations. $\det D^{(i)}$ denotes the truncated determinant for the $i$-th gauge configuration, and $\max_j(\det D^{(j)})$ is its maximum value in the gauge ensemble. Figure 3 shows the effective number of statistics (normalized by the quenched statistics) as a function of quark mass. The effective number of statistics decreases for smaller quark masses as expected. For a given topological sector, it goes down to $\sim 0.05$ ($0.02$) for $N_f = 1$ (2), when the quark mass is decreased to $\bar{a}m \sim 0.01$, which corresponds to $m \sim 26$ MeV. If we combine all topological charges, we loose another factor of $\sim 5$, because only the configurations with zero topological charge contribute for small quark masses. Therefore, the number of configurations we are using (Table 1) are not
Fig. 3. Effective number of statistics $N_{\text{eff}}$ normalized by the quenched statistics $N$ for $N_f = 1$ (top panel) and $N_f = 2$ (bottom panel). It is calculated for each topological sector (squares, crosses and bursts for $|\nu| = 0, 1, \text{ and } 2,$ respectively) and for all topological sectors (pluses).

large enough for precision study of unquenched lattices.

§5. Numerical results

In this section we present our numerical results for the eigenvalues of the overlap-Dirac operator. An eigenvalue $\lambda$ of the overlap-Dirac operator lies on a circle defined by $|1 - a\lambda| = 1$. In the continuum limit $a \to 0$ they become pure imaginary, corresponding to the eigenvalues of the continuum Dirac operator. At the finite lattice spacings, on the other hand, there is a freedom to define the eigenvalue projected onto the imaginary axis. We simply take an absolute value of the eigenvalue of the overlap-Dirac operator. The ambiguity in the choice
Fig. 4. Eigenvalue distribution $\rho(\lambda)/\Sigma$ of the overlap-Dirac operator as a function of $\lambda \Sigma V$. Distributions are shown for topological sectors $|\nu| = 0$ (solid), 1 (dashed) and 2 (dotted). The asymptotic behavior $\sim \lambda^3$ in the bulk region is shown by a solid curve, while the fits with RMT are drawn by dashed curves.

of the projection leads to a systematic uncertainty of order $(a\lambda)^2$. In the following discussion we misuse $\lambda$ for the meaning of $|\lambda|$. $N_{\text{cut}}$ is 50 unless otherwise stated.

5.1. Eigenvalue distribution

First of all, we show the distribution of the low-lying eigenvalues in Figure 4. The plot shows the eigenvalue density $\rho(\lambda) = \left\langle \frac{1}{V} \sum_n \delta(\bar{\lambda}_n - \lambda) \right\rangle$ normalized by the chiral condensate $\Sigma$. This normalization is determined for each topological sector by comparing an average of the lowest eigenvalue with its RMT expectation, as discussed below.

As expected from the dimensional analysis, the spectral density behaves as $\sim \lambda^3$ in the large $\lambda \Sigma V$ region. This behavior is independent of the gauge field topology, and a fit with $c_0 + c_3 (\lambda \Sigma V)^3$ for the entire gauge field ensemble is shown by a solid curve ($c_0 = 0.55$, $c_3 = 1.15 \times 10^{-4}$). Below $\lambda \Sigma V \simeq 10$, on the other hand, one can see a difference among different topological sectors. The curves show a fit with the expected functional form from the chiral RMT.

In Figure 5 we compare the distribution of the lowest non-zero eigenvalue with the prediction from RMT. Unlike the previous works, we also obtain the distributions for non-zero number of flavors, $N_f = 1$ and 2. For the quenched case, our results confirm the previous works that found an agreement with the RMT predictions.

The unquenched distributions are obtained by the reweighting with the truncated determinant. The lowest eigenvalue distribution is probably one of the most difficult quantities
Fig. 5. Lowest non-zero eigenvalue distribution on gauge configurations with a topological charge $\nu = 0$ (left), 1 (middle) and 2 (right). The results are shown for $N_f = 0$ (top), 1 (middle), and 2 (bottom). The horizontal axis is normalized such that the average agrees with the RMT expectation.

to be measured using the reweighting method. For instance, for $\nu = 0$ almost all eigenvalues lie in the region $\lambda \Sigma V \lesssim 5$ on the quenched lattice, while only about a half of eigenvalues are expected to fall in that region for $N_f = 2$ as shown in the plot by a dotted curve. The other half in the region $\lambda \Sigma V \gtrsim 5$ is not sampled well with the reweighting.

In Table II we summarize the average of the lowest non-zero eigenvalue $\lambda_1$ predicted by RMT and our results. For the RMT an expectation value of $\lambda_1 \Sigma V$ is listed, while the lattice data are bare values $\bar{a} \lambda_1$. From these results we can extract the value of chiral condensate $\Sigma$ for each $|\nu|$ and $N_f$. For the lattice spacing we use the quenched value $a = 0.123$ fm even for unquenched data, assuming that the heavy quark potential is not much affected by the truncated determinant. The chiral condensate $\Sigma$ obtained in this work corresponds to the
Table II. Expectation value of the lowest non-zero eigenvalue predicted by RMT \( \lambda_1 \Sigma V \) and the lattice results \( \bar{a} \lambda_1 \). The chiral condensate \( \Sigma \) is obtained with an input for lattice spacing \( a = 0.123 \) fm at \( \beta = 5.85 \).

| \( N_f \) | \( |\nu| \) | RMT (\( \lambda_1 \Sigma V \)) | Lattice (\( \bar{a} \lambda_1 \)) | \( \Sigma^{1/3} \) [MeV] |
|---|---|---|---|---|
| 0 | 0 | 1.77 | 0.0289(13) | 250(4) |
| | 1 | 3.11 | 0.0486(12) | 254(2) |
| | 2 | 4.34 | 0.0701(20) | 251(2) |
| 1 | 0 | 3.11 | 0.0569(59) | 241(8) |
| | 1 | 4.34 | 0.0833(34) | 238(3) |
| | 2 | 5.53 | 0.100(6) | 242(5) |
| 2 | 0 | 4.34 | 0.067(12) | 254(15) |
| | 1 | 5.53 | 0.0939(42) | 247(04) |
| | 2 | 6.69 | 0.112(14) | 248(10) |

The agreement of \( \Sigma \) given in Table II among different topological sectors is encouraging. The values with non-zero flavors are also in reasonable agreement, though they are not necessarily agree since the underlying theory is different.

5.2. Partition function

Employing the truncated determinant approximation, we calculate the unquenched partition function at a fixed topology \( Z_\nu \) \( (2.7) \) as a function of the quark mass.

The number of eigenvalues included in the truncated determinant has to be equal for different topological charges in order to make the mass dimension consistent for different topological sectors. This is relevant for the partition function, because we consider \( Z_\nu / Z \), and \( Z \) in the denominator is a sum over all topological charges. Therefore, we slightly modify the truncated determinant as \( m^{[\nu]} \prod_{n=1}^{N_{\text{cut}} - |\nu|/2} (\lambda_n^2 + m^2) \) when \( |\nu| \) is even, or as \( m^{[\nu]} \prod_{n=1}^{N_{\text{cut}} - (|\nu|+1)/2} (\lambda_n^2 + m^2) \times \sqrt{\lambda_{N_{\text{cut}} - (|\nu|-1)/2}^2 + m^2} \) when \( |\nu| \) is odd.

In Figure 6 we plot \( Z_\nu / Z \) as a function of \( m \Sigma V \) for \( N_f = 1 \) (top panel) and 2 (bottom panel). We find a good agreement with the expectation from the chiral Lagrangian in the small quark mass region \( (2.3) \) and \( (2.4) \). A fit in the range \( \bar{a} m \leq 0.03 \) with a free parameter \( \Sigma \) yields \( \Sigma^{1/3} = 214(6) \) MeV and 248(6) MeV for \( N_f = 1 \) and 2, respectively. These results are quite insensitive to the value of \( N_{\text{cut}} \). They vary from 212(4) MeV to 214(6) MeV by changing \( N_{\text{cut}} \) from 10 to 50 for \( N_f = 1 \). The variation is from 234(7) MeV to 248(6) MeV for \( N_f = 2 \).
5.3. Eigenvalue sum rules

Here we investigate the sum rules (2.11)-(2.14) of the Dirac operator eigenvalues.

As discussed in Section 2, the sums $\sum'_n 1/\lambda_n^2$ and $\sum'_n 1/\lambda_n^4$ are divergent in the ultraviolet regime. This behavior is explicitly shown in Figure 7 for $N_f = 1$. The left panels are divergent sums as a function of $\lambda_{\text{cut}} \Sigma V$ with $\lambda_{\text{cut}}$ the largest eigenvalue included in the sum. The sum rule I (top left) does not seem to show the expected quadratic divergence but looks more like a linear divergence. But, it is in fact consistent with the integral $\int^{\lambda_{\text{cut}}} \lambda \rho(\lambda)/\lambda^2$ with the form $\rho(\lambda) = \rho_{(0)}(\lambda) + \rho_{(3)}(\lambda)^3$ suggested in Section 5.1. Here, $\rho_{(3)}(\lambda)^3$ represents the bulk distribution of eigenvalues, which is independent of the gauge field topology, while the
Fig. 7. Sum rules I (2.11) and IIb (2.13) for $N_f = 1$. The ultraviolet divergence is shown on the left panels as a function of $\lambda_{\text{cut}} \Sigma V$ with $\lambda_{\text{cut}}$ the largest eigenvalue included in the sum. The right panels show a saturation for the difference between different topological sectors.

$\rho^{(0)}_\nu(\lambda)$ term shows the oscillating behavior depending on the topological charge. For large $\lambda \Sigma V$, $\rho^{(0)}_\nu(\lambda)$ approaches to a constant $\rho^{(0)}$, which is independent of the topology. In the integral $\int^{\lambda_{\text{cut}}} \frac{d\lambda \rho(\lambda)}{\lambda^2}$, we observe that the curvature of $-\rho^{(0)}/\lambda_{\text{cut}}$ cancels that of $\rho^{(3)} \lambda^2_{\text{cut}}$ in the region plotted in Figure 7.

Similar plots are shown for $N_f = 2$ in Figure 8. The first order (sum rule I) and the second order (sum rules IIa, IIb and IIc) are plotted. The sum rule I is quadratically divergent as in the $N_f = 1$ case; the divergence of the sum rule IIc (2.14) is mild as it is only logarithmic. For the other second order sum rules (IIa and IIb), the divergence is quartic, since it has the form $(\int^{\lambda_{\text{cut}}} d\lambda \rho(\lambda)/\lambda^2)^2$.

In order to subtract these ultraviolet divergences, we consider the differences of the eigenvalue sum rules among different topological sectors. This is motivated by an expectation that the bulk distribution $\rho^{(3)} \lambda^3$ is independent of the gauge field topology as we can see in Figure 4. On the other hand, the term $\rho^{(0)}_\nu$ carries the information of the topology and shows the oscillating behavior expected from RMT. For the sum rule I (2.11), to be explicit, the divergent piece are common for all topological sectors and cancel in the differences. In fact, the lattice data for the differences $(\nu = 0) - (\nu = 1)$, $(\nu = 0) - (\nu = 2)$ and $(\nu = 1) - (\nu = 2)$ are almost independent of the cutoff $\lambda_{\text{cut}}$ as shown in Figure 7 (top right panel). The same
Fig. 8. Sum rules I (2.11), IIa (2.12), IIb (2.13) and IIc (2.14) for $N_f = 2$. The ultraviolet divergence is shown on the left panels as a function of $\lambda_{\text{cut}} \Sigma V$ with $\lambda_{\text{cut}}$ the largest eigenvalue included in the sum. The right panels show a saturation for the difference between different topological sectors.
is true for the sum rule IIc as shown in Figure 8 (4th row, right).

The cancellation of the ultraviolet divergence is not expected for the sum rules IIa (2.12) and IIb (2.13). This is because they include a square of the integral \( \int \rho(\lambda) d\lambda \rho(\lambda)/\lambda^2 \) and it contains a cross term \( \rho^{(0)}(\lambda) \times \rho^{(3)}(\lambda \lambda_{cut}^2) \), which is divergent but still topology-dependent through \( \rho^{(0)}(\lambda) \). The lattice data support this expectation as shown in Figure 7 (bottom right panel) and in Figure 8 (2nd and 3rd rows, right).

We use the sum rules I and IIc to extract \( \Sigma \) from the comparison of lattice data with the analytic formulae. For \( N_f = 1 \), only the sum rule I can be used, and we obtain \( \Sigma^{1/3} \) as 239(9), 238(7) and 233(9) MeV for the differences \( \nu = 0 \)–\( \nu = 1 \), \( \nu = 0 \)–\( \nu = 2 \) and \( \nu = 1 \)–\( \nu = 2 \), respectively. Similarly, for \( N_f = 2 \) we obtain 268(17), 260(13) and 241(17) MeV from the sum rule I, and 257(12), 254(11) and 237(10) MeV from the sum rule IIc.

5.4. Topological susceptibility

The mass dependence of the topological susceptibility \( \langle \nu^2 \rangle/V \) in the \( \epsilon \)-regime is analytically known as (2.5) and (2.6). Lattice calculation of this quantity is straight-forward from the partition function discussed in Section 5.2. In Figure 9 we plot \( \langle \nu^2 \rangle \) as a function of \( m\Sigma V \). The value of \( \Sigma \) extracted by fitting in the region \( \bar{a}m \leq 0.03 \) is \( \Sigma^{1/3} = 216(9) \) MeV for \( N_f = 1 \), and 257(18) MeV for \( N_f = 2 \). These results are quite stable under the change of \( N_{cut} \). The variation for \( N_{cut} = 10–50 \) is 215(7)–216(9) MeV for \( N_f = 1 \) and 246(27)–257(18) MeV for \( N_f = 2 \).
The clear mass dependence of the topological susceptibility as observed in Figure 9 has not been obtained before in the dynamical fermion simulations, except an exploratory work by Kovács, which utilized the same reweighting technique as employed in our work. The reason is partly that the quark mass is not small enough to realize the \( \epsilon \)-regime. A recent work with slightly smaller quark masses shows an indication of the suppression of the topological susceptibility. Also, the (improved) Wilson fermion formulation employed in the previous dynamical simulations does not respect the chiral symmetry, and it is questionable if the expected quark mass dependence is obtained at finite lattice spacings. For the improved staggered dynamical quarks, with which one can reach the small quark mass region, there is an indication that the expected quark mass dependence is reproduced in the continuum limit

5.5. Comparison

In Table III, we summarize the values of chiral condensate \( \Sigma \) extracted from our numerical data. We set \( a = 0.123 \text{ fm} \) from the Sommer scale \( r_0 \) at \( \beta = 5.85 \).

First of all, the quenched (\( N_f = 0 \)) results obtained from the lowest eigenvalue distribution are consistent among different topological sectors, and in perfect agreement with a previous work by Bietenholz et al., who used the same lattice parameters, \( i.e. \beta = 5.85 \) and \( 10^4 \) lattice, and extracted \( \Sigma \) from the lowest eigenvalue distribution as \( \Sigma^{1/3} \simeq 253 \text{ MeV} \). In we investigated the meson correlators in the \( \epsilon \)-regime at the same \( \beta \) value but on a larger lattice \( 10^3 \times 20 \). The quenched chiral condensate is extracted from the scalar and pseudo-scalar meson correlators as \( \Sigma^{1/3} \simeq 257(14) \text{ MeV} \), which is also consistent with the present work.

For \( N_f = 1 \), we find an agreement between the results from the lowest eigenvalue distribution and those from the sum rule I. The results are around \( \Sigma^{1/3} \simeq 240 \text{ MeV} \), which is in the same ballpark with the quenched results. On the other hand, the fits for the partition function and the topological susceptibility yield substantially lower values, 214(6) MeV and 216(9) MeV, respectively. At first sight, this disagreement seems puzzling, because the eigenvalue sum rules are derived through the derivatives of the partition function with respect to \( m^2 \). The main difference is that the partition function and the topological susceptibility involve the relative weight among different topological sectors. Namely, the leading mass dependence of the partition function \( Z_\nu \propto m^{\nu |} \), which is most relevant to the relative weight, is factored out before the sum rules are derived. The eigenvalue sum rules represent the non-leading mass dependence. Therefore, the disagreement implies that the relative weight among different topological sectors is not well described by \( \epsilon(23) \).

In contrast to the \( N_f = 1 \) case, the results for \( \Sigma \) from several different methods nicely
Table III. Summary of the results for chiral condensate $\Sigma^{1/3}$. Results from the lowest eigenvalue distribution, eigenvalue sum rules I and IIc, partition function, and topological susceptibility are listed for $N_f = 0$, 1, and 2. The second column indicates the topological charge of the gauge configuration used for the measurement.

agree with each other for $N_f = 2$. Probably, the extraction from the lowest eigenvalue distribution contains substantial systematic error due to the sampling problem, as discussed in Section 5.1. The sum rules are less problematic, because they involve the inverse of the low-lying eigenvalues and its most important contribution comes from lower side of the distribution, which is well sampled with the reweighting method.
§6. Conclusions

The effect of the fermion determinant to the QCD vacuum is substantial for small enough quark masses. In the language of chiral perturbation theory, the constant modes dominate the low energy dynamics, when the system is confined in a finite volume. The quark mass dependence of the partition function can be analytically derived using the $\epsilon$-expansion in the chiral perturbation theory. The analytic formulae by Leutwyler and Smilga show strong dependence on the topological charge and the number of dynamical quark flavors. In this numerical work we explicitly tested these analytic expectations using lattice QCD simulations.

The fermion determinant is approximated by a truncated product of low-lying eigenvalues of the overlap-Dirac operator. The eigenvalues are truncated at around 1200 MeV. Intuitively, this approximation should be effective as far as the low energy dynamics is concerned, and in fact the relative weight among gauge configurations is roughly unchanged when we further increase the cutoff for the eigenvalue.

From our lattice calculations of (i) lowest-lying eigenvalue distribution, (ii) eigenvalue sum rules, (iii) quark mass dependence of the partition function, and (iv) topological susceptibility, we found good agreement with the analytic predictions. For these quantities, the only free parameter in the chiral perturbation theory (at the leading order) is the chiral condensate $\Sigma$, which we can extract from the lattice data. The extraction of $\Sigma$ from the methods (i)–(iv) provides a highly non-trivial cross-check of the theory (or the lattice calculation), and our results at $N_f = 2$ are all consistent with each other. A problem remains at $N_f = 1$, for which the extraction with a fixed topological charge ((i) and (ii)) and the fits to all topological charges ((iii) and (iv)) are mutually inconsistent. It may signal a breakdown of the $\epsilon$-expansion at $N_f = 1$, for which no Nambu-Goldstone massless pion exists and therefore the finite momentum excitation is not large compared to the ground state energy.

Although the reweighting method with the truncated determinant provides a good qualitative approximation, its limitation is also apparent. First of all, the systematic uncertainty due to the truncation is hardly estimated. For the quantities (i)–(iv) we explicitly checked that the results are unchanged by varying the number of eigenvalues from 10 to 50, but it does not guarantee that they remain unchanged until the limit of the exact determinant is reached. This problem could be solved either by defining an effective Dirac operator which includes the low-lying eigenvalues only or by incorporating the effects of the rest of the eigenmodes using stochastic methods. Second, the Monte Carlo sampling with the pure gauge action becomes ineffective when quark mass becomes small. Near the massless limit, we loose nearly 95% (98%) of the statistics for $N_f = 1$ (2) by the suppression factor due to the
fermion determinant. This problem can only be cured by including the fermion determinant into the Boltzmann weight when the gauge configuration is generated.

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References

1) J. Gasser and H. Leutwyler, Phys. Lett. B 188, 477 (1987).
2) H. Leutwyler and A. Smilga, Phys. Rev. D 46, 5607 (1992).
3) H. Neuberger, Phys. Lett. B 417, 141 (1998) [arXiv:hep-lat/9707022].
4) H. Neuberger, Phys. Lett. B 427, 353 (1998) [arXiv:hep-lat/9801031].
5) D. B. Kaplan, Phys. Lett. B 288, 342 (1992) [arXiv:hep-lat/9206013].
6) Y. Shamir, Nucl. Phys. B 406, 90 (1993) [arXiv:hep-lat/9303005].
7) P. H. Ginsparg and K. G. Wilson, Phys. Rev. D 25, 2649 (1982).
8) M. Luscher, Phys. Lett. B 428, 342 (1998) [arXiv:hep-lat/9802011].
9) P. Hernandez, K. Jansen and L. Lellouch, Phys. Lett. B 469, 198 (1999) [arXiv:hep-lat/9907022].
10) W. Bietenholz, T. Chiarappa, K. Jansen, K. I. Nagai and S. Shcheredin, JHEP 0402, 023 (2004) [arXiv:hep-lat/0311012].
11) L. Giusti, P. Hernandez, M. Laine, P. Weisz and H. Wittig, JHEP 0401, 003 (2004) [arXiv:hep-lat/0312012].
12) L. Giusti, P. Hernandez, M. Laine, P. Weisz and H. Wittig, JHEP 0404, 013 (2004) [arXiv:hep-lat/0402002].
13) H. Fukaya, S. Hashimoto and K. Ogawa, arXiv:hep-lat/0504018.
14) R. G. Edwards, U. M. Heller, J. E. Kiskis and R. Narayanan, Phys. Rev. Lett. 82, 4188 (1999) [arXiv:hep-th/9902117].
15) W. Bietenholz, K. Jansen and S. Shcheredin, JHEP 0307, 033 (2003) [arXiv:hep-lat/0306022].
16) L. Giusti, M. Luscher, P. Weisz and H. Wittig, JHEP 0311, 023 (2003) [arXiv:hep-lat/0309189].
17) J. J. M. Verbaarschot and T. Wettig, Ann. Rev. Nucl. Part. Sci. 50, 343 (2000) [arXiv:hep-ph/0003017].
18) K. Ogawa and S. Hashimoto, arXiv:hep-lat/0409103.
19) ARPACK, available from http://www.caam.rice.edu/software/ARPACK/
20) L. Giusti, C. Hoebling, M. Luscher and H. Wittig, Comput. Phys. Commun. 153,
31 (2003) [arXiv:hep-lat/0212012].
21) A. Borici [UKQCD collaboration], Phys. Rev. D 67, 114501 (2003) [arXiv:hep-lat/0205011].
22) A. Duncan, E. Eichten and H. Thacker, Phys. Rev. D 59, 014505 (1999) [arXiv:hep-lat/9806020].
23) M. Luscher, Nucl. Phys. B 418, 637 (1994) [arXiv:hep-lat/9311007].
24) S. M. Nishigaki, P. H. Damgaard and T. Wettig, Phys. Rev. D 58, 087704 (1998) [arXiv:hep-th/9803007].
25) S. Durr, Nucl. Phys. B 611, 281 (2001) [arXiv:hep-lat/0103011].
26) T. G. Kovacs, arXiv:hep-lat/0111021.
27) C. R. Allton et al. [UKQCD Collaboration], Phys. Rev. D 70, 014501 (2004) [arXiv:hep-lat/0403007].
28) C. Bernard et al., Phys. Rev. D 68, 114501 (2003) [arXiv:hep-lat/0308019].