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Determination of the Chiral Condensate from (2 + 1)-Flavor Lattice QCD

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We perform a precise calculation of the chiral condensate in QCD using lattice QCD with 2 + 1 flavors of dynamical overlap quarks. Up and down quark masses cover a range between 3 and 100 MeV on a $16^3 \times 48$ lattice at a lattice spacing $\sim 0.11$ fm. At the lightest sea quark mass, the finite volume system on the lattice is in the $\epsilon$ regime. By matching the low-lying eigenvalue spectrum of the Dirac operator with the prediction of chiral perturbation theory at the next-to-leading order, we determine the chiral condensate in (2 + 1)-flavor QCD with strange quark mass fixed at its physical value as $\Sigma^{\overline{MS}}(2 \text{ GeV}) = [242(04)(-18)]$ MeV where the errors are statistical and systematic, respectively.

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Spontaneous breaking of chiral symmetry is one of the most fundamental properties of quantum chromodynamics (QCD), as it produces the bulk of the hadron masses. The symmetry breaking is indicated by a nonzero value of the chiral condensate $\Sigma$, which is an expectation value of the scalar density operator $\bar{q}q$. Despite its importance, calculation of $\Sigma$ remains a significant challenge, even using the numerical simulation of QCD on the lattice, due to both ultraviolet and infrared problems.

On the ultraviolet side, an additive renormalization of the scalar operator diverges as $\sim 1/a^2$ as the lattice spacing $a$ decreases, when the chiral symmetry is violated. Even with exact chiral symmetry, there exists a quadratic divergence proportional to the quark mass. On the infrared side, since spontaneous symmetry breaking does not occur at finite volume, the infinite volume limit has to be taken before going to the massless limit. Therefore, careful study of the scaling in the chiral and infinite volume limits is crucial to determine $\Sigma$.

Our previous work [1,2] opened a new possibility to overcome these difficulties by performing a lattice QCD employing the overlap fermion formulation [3,4], which preserves exact chiral symmetry at finite lattice spacings. The ultraviolet problem is avoided by using the spectrum of low-lying fermion modes. According to the Banks-Casher relation [5], the spectral density $\rho(\lambda)$ of the Dirac operator at $\lambda = 0$ is related to the chiral condensate as $\Sigma = \pi \rho(0)$. At a large but finite volume $V$, chiral perturbation theory (ChPT) can be used to predict the volume scaling of the near-zero modes, which is also equivalently described by the chiral random matrix theory [6–9]. By matching the theoretical prediction with the lattice data, the chiral condensate $\Sigma$ was determined at the leading order (LO) in the $\epsilon$ expansion (see also [10]).

This Letter extends the previous work in several directions. (i) Based on a new ChPT calculation by Damgaard and Fukaya [11], which is valid in the conventional $\rho$ regime as well as in the $\epsilon$ regime, we use the lattice data at several values of sea quark masses. (ii) The new formula consistently treats the next-to-leading order (NLO) effects in the $\rho$ expansion and thus, the result of $\Sigma$ has the NLO accuracy (A similar NLO analysis of the lattice data taken with the Wilson fermion in the $\rho$ regime has been done recently [12]). (iii) The lattice data are newly generated including the effect of strange quark, so that the result corresponds QCD in nature. (iv) The finite volume scaling is confirmed using two volumes $16^3 \times 48$ and $24^3 \times 48$. With these new developments, the determination of $\Sigma$ is made more precise and reliable.

The spectral density at a given topological charge $Q$ is calculated within ChPT at NLO as [11]

$$
\rho_Q(\lambda) = \Sigma_{\text{eff}} \hat{\rho}_Q(\lambda \Sigma_{\text{eff}} V, \{m_{\text{sea}} \Sigma_{\text{eff}} V\}) + \rho_{Q}(\lambda, \{m_{\text{sea}}\}),
$$

for an eigenvalue $\lambda$ of the Dirac operator. Assuming the analyticity, $\rho_Q(\lambda)$ is obtained through the real part of the $\Sigma$ matrix

$$
\langle J_Q^{+} \rangle = \frac{1}{2} \sum_{\mathcal{A}} \frac{\det \hat{B}}{\det \mathcal{A}} \frac{1}{\det \mathcal{A}}.
$$

with $N_f \times N_f$ matrix $\mathcal{A}$ and $(N_f + 2)(N_f + 2)$ matrix $\hat{B}$ defined by $\mathcal{A}_{ij} = \mu_{j}^{-1} I_{Q+j-1}(\mu_i)$ and $\hat{B}_{ij} = \xi^{-1} \hat{B}_{Q+j-1}(\xi, \xi^{-1} I_{Q+j-1}(\xi)) = (-\mu_{j-2})^{-1} I_{Q+j-1}(\mu_{j-2})$ $(i \neq 1, 2)$, respectively ($J_Q^{+}$'s

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and \( I_1 \)'s denote the (modified) Bessel functions). The phase factor \( C_2 \) is 1 for \( N_f = 2 \) or 3.

The second term in (1) is the NLO correction seen in the ordinary \( p \)-expansion [13]. With the meson mass \( M_{ij}^2 = (m_i + m_j) \Sigma / F^2 \), which is made of either sea quark (\( f \)) or valence quark (\( v \)), it is expressed as

\[
\rho^p(\lambda, \{m_{\text{sea}}\}) = - \sum_i \pi F^2 \text{Re} \left[ \sum_j N_f \left( \tilde{\Delta}(M_{ij}^2) - \tilde{\Delta}(M_{ff}^2)/2 \right) \right]

- \left( \tilde{G}(M_{ff}^2) - \tilde{G}(0) \right)_{\text{eff}} \text{condensate} (\lambda, \{m_{\text{sea}}\}).
\]

(3)

The function \( \tilde{\Delta}(M^2) \) contains the chiral logarithm, \( \tilde{\Delta}(M^2) = \frac{M}{16\pi^2} \ln \frac{m_{\text{sub}}^2}{\mu_{\text{sub}}^2} + \tilde{g}_1(M^2) \), with \( \tilde{g}_1(M^2) \) representing the finite volume effect [14]. The subtraction scale \( \mu_{\text{sub}} \) is set at 770 MeV in this work. The other function \( \tilde{G}(M^2) \) has a double-pole contribution due to the partial quenching. The explicit forms of \( \tilde{g}_1(M^2) \) and \( \tilde{G}(M^2) \) are given in [11] [In this Letter, we use a simplified notation. \( \tilde{G}(M^2) \) corresponds to \( \tilde{G}(0, M^2, M^2) \) in [11]]. The effective chiral condensate \( \Sigma_{\text{eff}} \) in (1) is given by

\[
\Sigma_{\text{eff}} = \left[ 1 - \frac{1}{F^2} \left( \sum_j \left( \Delta(M_{ff}^2) - \tilde{G}(0) \right) - 16L_6' \sum_j M_{ff}^2 \right) \right],
\]

(4)

where \( L_6' \) (renormalized at \( \mu_{\text{sub}} \)) is one of the low-energy constants at NLO [15].

Numerical simulations of lattice QCD are performed using the Iwasaki gauge action at \( \beta = 2.3 \) including 2 + 1 flavors of dynamical overlap quarks on a \( 16^3 \times 48 \) lattice. The lattice spacing \( a = 0.1075(7) \) fm is determined from the heavy quark potential with an input \( \tau_0 = 0.49 \) fm. For the strange quark mass, we choose two different values \( m_s = 0.080 \) and 0.100 in the lattice unit. For the former, six values of up and down quark masses \( m_{ud} = 0.002, 0.015, 0.025, 0.035, 0.050, \) and 0.080 are taken. For the latter, five values \( m_{ud} = 0.015, 0.025, 0.035, 0.050, \) and 0.100 are used. The smallest value \( m_{ud} = 0.002 \) roughly corresponds to 3 MeV in the physical unit, with which pions are in the \( \epsilon \) regime. In order to investigate the finite volume scaling, we also simulate on a \( 24^3 \times 48 \) lattice with one choice of the sea quark masses \( m_{ud} = 0.025 \) and \( m_s = 0.080 \).

In the hybrid Monte Carlo (HMC) updates, the global topological charge \( Q \) of the gauge field is fixed to its initial value by introducing extra (unphysical) Wilson fermions, which have a mass of cutoff order [16]. In our main runs, we set \( Q = 0 \). We also simulate another sector of topological charge \( Q = 1 \) at \( m_{ud} = 0.015 \) and \( m_s = 0.080 \).

We accumulate 2500 HMC trajectories for the main runs in the \( p \) regime, 4750 (but the trajectory length is 0.5) for the \( \epsilon \) regime lattice, 1800 for the \( Q = 1 \) run, and 1900 on the \( 24^3 \times 48 \) lattice. Eighty pairs of low-lying eigenvalues of the massless overlap operator \( D \) are computed at every 5 (or 10 in the \( Q = 1 \) and \( L = 24 \) runs) trajectories. For the comparison with ChPT, every complex eigenvalue \( \lambda^{ov} \) is projected onto the imaginary axis as \( \lambda = \text{Im} \lambda^{ov} / (1 - \text{Re} \Delta^{ov} / (2m_0)) \). Here \( m_0 = 1.6 \) is a parameter to define the overlap-Dirac operator. In the analysis, we consider positive \( \lambda \) only. The integrated autocorrelation time of the lowest \( \lambda \) is measured as 6–24 trajectories depending on the simulation parameters. The statistical error is estimated by the jackknife method after binning data in every 100 trajectories. Details of the numerical simulation will be reported elsewhere.

At each set of sea quark masses, the formula (1) is described by two unknown quantities \( \Sigma_{\text{eff}} \) and \( F \). Note that \( \Sigma \) in (3) can be replaced by \( \Sigma_{\text{eff}} \) neglecting higher order effects. We first determine these parameters from the lattice data of \( \rho_Q(\lambda) \). Roughly speaking, the height of \( \rho_Q(\lambda) \) near \( \lambda = 0 \) determines \( \Sigma_{\text{eff}} \) according to the Banks-Casher relation, while the shape in the bulk region is controlled by \( F \), as far as \( \lambda \) is in the region of convergence of the chiral expansion.

Figure 1 shows the spectral density \( \rho_Q(\lambda) \) multiplied by \( \sigma \) (left panel) and the mode number below \( \lambda \), \( N_Q(\lambda) \equiv V \int_0^\lambda d\lambda' \rho_Q(\lambda') \) (right), calculated at \( m_{ud} = 0.015 \) and

![FIG. 1 (color online). Spectral density \( \rho_Q(\lambda) \) (left) and mode number \( N_Q(\lambda) \) (right) of the Dirac operator at \( m_{ud} = 0.015 \), \( m_s = 0.080 \) and \( Q = 0 \). The lattice result (given by histogram (left) or solid symbols (right)) is compared with the ChPT formula (1) drawn by solid curves. For comparison, the prediction at the leading order of \( \epsilon \)-expansion (dashed curves) is also shown.](https://example.com/figure1.png)

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The lattice data well in the region below $C_2$ under the leading contribution in an expansion in important for the consistency between QCD and ChPT. The numerical results of $\Sigma_{\text{eff}}$ and $F$ are, in fact, insensitive to the choice of $N_f$ in the formula, except for $F$ in the heavy mass region. We also note that there is no significant difference of $\Sigma_{\text{eff}}$ between $m_s = 0.080$ and 0.100, which confirms decoupling of the strange quark from the low-energy dynamics.

From the data in the nontrivial topological sector $Q = 1$, we observe that the topological charge $Q$ largely affects the spectral density near $\lambda = 0$, but the values of $\Sigma_{\text{eff}} = 0.00354(48)$ and $F = 0.0521(25)$ are consistent with those at $Q = 0$. The data at $L = 24$ also show the expected scaling behavior from (1). Since the definition of $\Sigma_{\text{eff}}$ explicitly contains the lattice volume, the results from different volumes cannot be compared directly. After converting the $L = 24$ lattice result $\Sigma_{\text{eff}} = 0.003 06(7)$ to that of $L = 16$, we obtain $0.003 41(18)$, which is consistent with $0.003 33(18)$ obtained on the $L = 16$ lattice.

Next, we analyze the sea quark mass dependence of $\Sigma_{\text{eff}}$ from which $\Sigma$, $F$, and $L_q$ can be determined. To see the convergence of the chiral expansion, we carry out fits using four, five and six lightest data points as a function of $m_{ud}$ with $m_s$ fixed at 0.080. The data points and fit curves of the $N_f = 2 + 1$ formula are shown in Fig. 3. The curvature due to the chiral logarithm in (4) is manifest. The fit result for $\Sigma_{\text{phys}}$, which is $\Sigma_{\text{eff}}$ in the limit of $V = \infty$ and $m_{ud} = 0$ while keeping $m_s$ fixed at 0.08, is stable under change of the fitting range. Since we observe no sizable $m_s$ dependence (see Table I), $\Sigma_{\text{phys}}$ can be considered as the one at the physical strange quark mass. From the five points fit, we obtain $\Sigma_{\text{phys}} = 0.011 86(10)$, $F = 0.0406(5)$, and $L_q^N = -0.000 11(25)$ in the lattice unit, with $\chi^2/\text{dof} = 0.7$.

Since $F$ appears starting at the NLO correction in the formula, $m_{ud}$ dependence of the data given in Table I reflects the NNLO effects, which is beyond the scope of this work. A naive linear extrapolation to the chiral limit yields $F = 0.0410(46)$, which roughly agrees with the value from the fit of $\Sigma_{\text{eff}}$.

Our final result for the chiral condensate $\Sigma_{\text{phys}}$, in the limit of $m_{ud} = 0$ and $m_s$ fixed at its physical value, is

$$\Sigma_{\text{MS}}(2 \text{ GeV}) = \left[ 242(04)(^{+19}_{-18}) \text{ MeV} \right]^3,$$

where the errors are statistical and systematic, respectively. The lattice scale $a = 0.1075(7)$ fm is determined from the heavy quark potential $r_0 = 0.49$ fm. We use the nonperturbatively calculated renormalization factor $1/Z_{\text{c}}(2 \text{ GeV}) = 0.806(12)(^{+24}_{-26})$ [18] to convert the result to the $\overline{\text{MS}}$ scheme at 2 GeV.

Possible systematic errors are listed in Table II. The error from chiral fit is estimated by taking variations of the fitting range and the choice of $N_f$ in the ChPT formula. Finite volume effect is estimated by taking the difference terms of the large strange quark mass. $\Sigma$ and $F$ in this framework depend on the strange quark mass. The curves in Figs. 1 and 2 are drawn using the $N_f = 2 + 1$ formula, but the difference from $N_f = 2$ is hardly visible in the range $\lambda < 0.03$. The numerical results of $\Sigma_{\text{eff}}$ and $F$ are, in fact, insensitive to the choice of $N_f$ in the formula, except for $F$ in the heavy mass region. We also note that there is no significant difference of $\Sigma_{\text{eff}}$ between $m_s = 0.080$ and 0.100, which confirms decoupling of the strange quark from the low-energy dynamics.

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Possible systematic errors are listed in Table II. The error from chiral fit is estimated by taking variations of the fitting range and the choice of $N_f$ in the ChPT formula. Finite volume effect is estimated by taking the difference

![FIG. 2 (color online). Same as the left panel of Fig. 1, but calculated on the $e$ regime lattice, at $m_{ud} = 0.002$ and $m_s = 0.080$.](image-url)
between the data on $16^3 \times 48$ and $24^3 \times 48$ lattices. The discretization effect is hard to estimate within the calculation done at a single lattice spacing, but partly reflected in the mismatch of the lattice spacing obtained from different inputs: 0.100(5) fm from the pion decay constant [19] and 0.109(2) fm from the $\Omega$ baryon mass [20]. To be conservative, the maximum deviation from the central value ($\sim 7.4\%$) is added in both positive and negative directions in Table II.

The chiral condensate obtained in this work (5) is consistent with other determinations from the pseudoscalar meson mass, $\Sigma_{\text{MS}}^{\text{NNLO}}(2 \text{ GeV}) = [257(14) \text{ MeV}]^3$ [19] and from the topological susceptibility, $\Sigma_{\text{MS}}^{\text{NNLO}}(2 \text{ GeV}) = [249(4) \text{ MeV}]^3$ [21,22]. The former is obtained with the NNLO ChPT formula, while the latter only uses the LO relation (and the errors do not contain the systematic effects). Our result is also consistent with two-flavor results in the previous works [1,2,12,17,23,24]. Namely, there is no significant effect of the strange sea quark.

We also obtain $F = 74(1)(8) \text{ MeV}$ and $\Lambda_\rho(770 \text{ MeV}) = -0.00011(25)(11)$. Their systematic errors are estimated in a similar manner.

By the use of the eigenvalue density of the Dirac operator calculated on the lattice, the chiral condensate is determined without suffering from large subtraction of ultraviolet divergences. The dependence on the volume, topological charge and quark masses is well described by the ultraviolet divergences. The dependence on the volume, determined without suffering from large subtraction of the calculation done on the lattice, the chiral condensate is determined, without suffering from large subtraction of the calculation done on the lattice, the chiral condensate is determined.

### Table II

<table>
<thead>
<tr>
<th>Source of Error</th>
<th>Contribution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Renormalization</td>
<td>$+1.2%$</td>
</tr>
<tr>
<td>Chiral fit</td>
<td>$+1.4%$</td>
</tr>
<tr>
<td>Finite volume</td>
<td>$+0.7%$</td>
</tr>
<tr>
<td>Finite $a$</td>
<td>$+1.2%$</td>
</tr>
<tr>
<td>Total</td>
<td>$+7.9%$</td>
</tr>
</tbody>
</table>

The total error is obtained by adding each estimate by quadrature.

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