Chiral condensate of lattice QCD with massless quarks from the probability distribution function method

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We apply the probability distribution function method to the study of chiral properties of QCD with quarks in the exact massless limit. A relation among the chiral condensate, the zeros of the Bessel function, and the eigenvalue of the Dirac operator is also given. The chiral condensate in this limit can be measured with a small number of eigenvalues of the massless Dirac operator and without any ambiguous mass extrapolation. The results for SU(3) gauge theory with quenched Kogut-Susskind quarks on the 10^4 lattice are shown.

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I. INTRODUCTION

One cannot completely understand the physics of hadrons without understanding the QCD vacuum, the main properties of which are confinement and spontaneous chiral-symmetry breaking, characterized by the nonvanishing chiral condensate in the massless (chiral) limit. Suppose the quarks are degenerate. The chiral condensate per flavor is

$$\langle \bar{\psi}\psi \rangle = \frac{1}{N_c V} \langle \mathrm{Tr}\, \Delta^{-1} \rangle, \tag{1}$$

where $N_c = 3$ is the number of colors, V is the number of lattice sites, and Δ is the fermionic matrix. The trace is taken in the color, spin, and position space.

On a finite lattice, however, the direct computation of the chiral condensate from a chiral symmetric action leads to $\langle \bar{\psi}\psi \rangle|_{m=0} = 0$, even though there would be spontaneous chiral-symmetry breaking in the infinite volume limit. In standard lattice simulations, one has to add a mass term $\Sigma_x m \bar{\psi}\psi$ to the action and calculate $\langle \bar{\psi}\psi \rangle$ at some set of nonzero bare fermion mass m, and then extrapolate $\langle \bar{\psi}\psi \rangle$ to the massless limit by means of some modeled fitting functions (e.g., linear function, polynomial, or logarithmic corrections). Unfortunately, such a process might not be well justified, and sometimes it gives very different results. Here are two examples of well known evidence.

(a) QED in 4 dimensions. Noncompact lattice QED experiences a second order chiral phase transition at finite some bare coupling constant g, where the chiral condensate vanishes. The critical coupling and critical index determined by a m extrapolation of $\langle \bar{\psi}\psi \rangle$ are ambiguous. Detailed discussions can be found in Ref. [1].

(b) The one-flavor massless Schwinger model. In the continuum, as is analytically known, $\langle \bar{\psi}\psi \rangle_{\mathrm{cont}} \approx 0.16e$, where e is the electric charge. Unfortunately, a more careful study [2] indicates the value of the chiral condensate computed by mass extrapolation depends strongly on the mass range to extrapolate, and the fitting function mentioned above.

In Ref. [3], an alternative, the probability distribution function (p.d.f.) method, was proposed to investigate spontaneous chiral-symmetry breaking.[1] This method has been tested in the Schwinger model [3], and applied to the study of the spontaneous P and CT symmetry breaking [6] and theta-vacuum-like systems [7] as well as the phase transition of SU(2) lattice gauge theory at finite density [8].

In this paper, we will further explore the p.d.f. method by applying it to SU(3) lattice gauge theory with Kogut-Susskind (KS) fermions. The rest of the paper is organized as follows. In Sec. II, we elaborate the idea of the p.d.f. method and derive some relations between the eigenvalues of the Dirac operator and chiral condensate. In Sec. III, we present the results from numerical simulations.

II. p.d.f. OF THE CHIRAL CONDENSATE

Let us characterize each vacuum state by α and the chiral condensate by $\langle \bar{\psi}\psi \rangle_\alpha$. The p.d.f. of the chiral condensate in the Gibbs state is defined by

$$P(c) = \sum_\alpha w_\alpha \delta(c - \langle \bar{\psi}\psi \rangle_\alpha), \tag{2}$$

with w_α the weight to get the vacuum state α. $P(c)$ is the probability to get the value c for the chiral condensate from a randomly chosen vacuum state. If there is exact chiral symmetry in the ground state, $P(c) = \delta(c)$. If chiral symmetry is spontaneously broken, $P(c)$ will be a more complex function. Therefore, from the shape of the function $P(c)$ computed in the configurations generated by a chiral *symmetric* action with exact $m = 0$, one can qualitatively judge whether chiral symmetry is spontaneously broken.

In quantum field theory with fermions, chiral-symmetry breaking is dominated by the properties of the fermion fields

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[1]One can find an analogue in statistical physics, e.g., in the analysis of spin glasses [4,5]. However, to our knowledge, it is the first time in Ref. [3] such an idea has been applied to first principle quantum field theory, i.e., lattice gauge theory with fermions.

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under global chiral transformation $\psi \rightarrow \exp(i\boldsymbol{\alpha}\cdot\boldsymbol{\tau}\gamma_5)\psi$, with $\boldsymbol{\tau}$ the generator of the chiral symmetry group. From Eq. (2), one can define the p.d.f. of the chiral condensate for a single gauge configuration U:

$$P_U(c)=\frac{\int[d\bar{\psi}][d\psi]\exp(-S_f)\,\delta\left[c-\frac{1}{N_cV}\sum_x\bar{\psi}(x)\psi(x)\right]}{\int[d\bar{\psi}][d\psi]\exp(-S_f)},\tag{3}$$

where in "$\Sigma_x\bar{\psi}(x)\psi(x)$," summation over color, spin, and position indices is implied.

One can also define the p.d.f. for all gauge configurations

$$P(c)=\left\langle\delta\left(c-\frac{1}{N_cV}\sum_x\bar{\psi}(x)\psi(x)\right)\right\rangle,\tag{4}$$

where the expectation value "$\langle\cdots\rangle$" is computed with the integration measure associated with the partition function

$$\begin{aligned}Z&=\int[d\bar{\psi}][d\psi][dU]\exp(-S)\\&=\int[dU]\exp(-S_g+\ln\det\Delta),\end{aligned}\tag{5}$$

with Δ the fermionic matrix.

To study the chiral properties quantitatively, it is more convenient to employ the Fourier transformed p.d.f.

$$\tilde{P}_U(q)=\int_{-\infty}^{\infty}dc\,\exp(-iqc)P_U(c)\tag{6}$$

and

$$\tilde{P}(q)=\int_{-\infty}^{\infty}dc\,\exp(-iqc)P(c).\tag{7}$$

Inserting Eq. (4) into Eq. (7), one obtains

$$\begin{aligned}\tilde{P}(q)&=\int_{-\infty}^{\infty}dc\,\exp(-iqc)P(c)\\&=\frac{1}{Z}\int[d\bar{\psi}][d\psi][dU]\exp(-S_g-S_f)\\&\quad\times\int_{-\infty}^{\infty}dc\,\exp(-iqc)\,\delta\left(c-\frac{1}{N_cV}\sum_x\bar{\psi}(x)\psi(x)\right)\\&=\frac{1}{Z}\int[d\bar{\psi}][d\psi][dU]\\&\quad\times\exp\left[-S_g+\sum_{x,y}\bar{\psi}(x)\left(\Delta_{x,y}-i\frac{q}{N_cV}\delta_{x,y}\right)\psi(y)\right].\end{aligned}\tag{8}$$

Integrating out the fermion fields, Eq. (8) becomes

$$\begin{aligned}\tilde{P}(q)&=\frac{1}{Z}\int[dU]\det\left(\Delta-\frac{iq}{N_cV}I\right)\exp(-S_g)\\&=\frac{1}{Z}\int[dU]\frac{\det\left(\Delta-\frac{iq}{N_cV}I\right)}{\det\Delta}\exp(-S_g+\ln\det\Delta),\end{aligned}\tag{9}$$

where I is the identity matrix. Generally, a fermionic matrix Δ can be decomposed as

$$\Delta=mI+i\Gamma.\tag{10}$$

Denoting λ_j the jth positive eigenvalue of Γ, the determinants in Eq. (9) are

$$\begin{aligned}\det\Delta&=\prod_{j=1}^{N_cV/2}(\lambda_j^2+m^2),\\\det\left(\Delta-\frac{iq}{N_cV}I\right)&=\prod_{j=1}^{N_cV/2}\left(\lambda_j^2+m^2-\frac{q^2+2imqN_cV}{(N_cV)^2}\right).\end{aligned}\tag{11}$$

Substituting them into Eq. (9), one obtains

$$\begin{aligned}\tilde{P}(q)&=\frac{1}{Z}\int[dU]\exp(-S_g+\ln\det\Delta)\\&\quad\times\prod_{j=1}^{N_cV/2}\left(1-\frac{q^2+2imqN_cV}{(N_cV)^2(\lambda_j^2+m^2)}\right)\\&=\left\langle\prod_{j=1}^{N_cV/2}\left(1-\frac{q^2+2imqN_cV}{(N_cV)^2(\lambda_j^2+m^2)}\right)\right\rangle.\end{aligned}\tag{12}$$

From Eq. (12), we derive relations Eq. (16) and Eq. (21) between the chiral condensate and the eigenmodes of the Dirac operator.

A. First relation

According to the definition (7), the Fourier transformed p.d.f. of the chiral condensate can also be written as

$$\begin{aligned}\tilde{P}(q)&=\int_{-\infty}^{\infty}dc\,\exp(-iqc)P(c)\\&\int_{-\infty}^{\infty}dc\,\exp(-iqc)\left\langle\delta\left(c-\frac{1}{N_cV}\sum_x\bar{\psi}\psi\right)\right\rangle\\&=\left\langle\exp\left(-\frac{iq}{N_cV}\sum_x\bar{\psi}\psi\right)\right\rangle.\end{aligned}\tag{13}$$

Its derivative with respect to q at $q=0$ is

$$\left.\frac{\partial\tilde{P}(q)}{\partial q}\right|_{q=0}=-i\left\langle\frac{1}{N_cV}\sum_x\bar{\psi}\psi\right\rangle.\tag{14}$$

On the other hand, using Eq. (12), the derivative of $\tilde{P}(q)$ with respect to q at $q=0$ is

$$\left.\frac{\partial \tilde{P}(q)}{\partial q}\right|_{q=0} = -i\left\langle \frac{1}{N_c V}\sum_{j=1}^{NcV/2}\frac{2m}{\lambda_j^2+m^2}\right\rangle. \tag{15}$$

Comparing Eqs. (14) and (15), we have

$$\langle \bar{\psi}\psi\rangle = \frac{1}{N_c V}\left\langle \sum_{j=1}^{NcV/2}\frac{2m}{\lambda_j^2+m^2}\right\rangle. \tag{16}$$

In the derivation, we have not used the specific properties of lattice fermion formulation, just the standard one in the literature. The disadvantage is that to get the chiral condensate in the chiral limit $\lim_{m\to 0}\lim_{V\to\infty}\langle\bar{\psi}\psi\rangle$, it requires a m extrapolation, since $\langle\bar{\psi}\psi\rangle|_{m=0}=0$ on a finite lattice. As mentioned above, the result depends on the choice of the fitting function, in particular near the chiral phase transition. It also requires the calculation of all eigenvalues of the Dirac operator. When the lattice volume is large, the computational task is huge and not so feasible. From Eq. (16), one can also derive the so-called Banks-Casher formula

$$\lim_{m\to 0}\lim_{V\to\infty}\langle\bar{\psi}\psi\rangle = \lim_{\lambda\to 0}\pi\langle\rho(\lambda)\rangle, \tag{17}$$

which is also frequently used in the literature. Here $\rho(\lambda)$ is the eigenvalue density. This formula means that the eigenvalues relevant for chiral-symmetry breaking go to zero in the infinite volume limit. The disadvantage is that on a finite lattice, $\rho(0)=0$, it requires a $\lambda\to 0$ extrapolation using some modeled fitting function. Only in the infinite volume limit does the number of the eigenvalues approaching zero diverge, so that $\rho(0)\neq 0$.

B. Second relation

In a theory with continuous U(1) chiral symmetry (exactly when $m=0$), the vacuum is characterized by an angle $\alpha \in[-\pi,\pi]$ and the chiral condensate can be parametrized as $\langle\bar{\psi}\psi\rangle_\alpha = c_0\cos\alpha$, where c_0 is the amplitude of the chiral condensate corresponding to the spontaneously broken continuous U(1) symmetry. According to the definition (2), the p.d.f. of the chiral condensate is

$$\begin{aligned} P(c)|_{m=0} &= \sum_{\alpha} w_\alpha \delta(c-\langle\bar{\psi}\psi\rangle_\alpha) \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\alpha\,\delta(c-c_0\cos\alpha) \\ &= \begin{cases} \dfrac{1}{\pi\sqrt{c_0^2-c^2}}, & c\in[-c_0,c_0], \\ 0, & c<-c_0 \ \text{or}\ c>c_0. \end{cases} \end{aligned} \tag{18}$$

The Fourier transformed p.d.f. is then

$$\begin{aligned} \tilde{P}(q)|_{m=0} &= \int_{-\infty}^{\infty} dc\,\exp(-iqc)P(c) \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\alpha\int_{-\infty}^{\infty} dc\,\delta(c-c_0\cos\alpha)\exp(-iqc) \\ &= \frac{1}{2\pi}\int_{-\pi}^{\pi} d\alpha\,\exp(-iqc_0\cos\alpha) = J_0(qc_0), \end{aligned} \tag{19}$$

where J_0 is the zeroth order Bessel function of the first kind.

TABLE I. First 40 zeros of J_0.

j	$z(j)$
1	2.4048
2	5.5200
3	8.6540
4	11.7920
5	14.9310
6	18.0710
7	21.2120
8	24.3530
9	27.4940
10	30.6346
11	33.7758
12	36.9171
13	40.0584
14	43.1998
15	46.3412
16	49.4826
17	52.6241
18	55.7655
19	58.9070
20	62.0485
21	65.1900
22	68.3315
23	71.4730
24	74.6145
25	77.7562
26	80.8976
27	84.0391
28	87.1806
29	90.3222
30	93.4637
31	96.6053
32	99.7468
33	102.8884
34	106.0299
35	109.1715
36	112.3131
37	115.4546
38	118.5962
39	121.7377
40	124.8793

From above derivation, one sees that the p.d.f. depends on the symmetry group of the theory.

In the chiral limit, Eq. (12) becomes

$$\tilde{P}(q)|_{m=0} = \left\langle \prod_{j=1}^{N_c V/2} \left(1 - \left(\frac{q}{N_c V \lambda_j} \right)^2 \right) \right\rangle. \tag{20}$$

By computing the second derivative of Eq. (20) with respect to q, and comparing it to the second derivative of $J_0(qc_0)$, we have the following sum rule:

$$\lim_{m \to 0} \lim_{V \to \infty} \langle \bar{\psi}\psi \rangle = c_0 = \lim_{V \to \infty} \sqrt{ \frac{4}{N_c^2 V^2} \left\langle \sum_{j=1}^{NcV/2} \frac{1}{\lambda_j^2} \right\rangle }, \tag{21}$$

which agrees with the result from chiral perturbation theory [9] and chiral random matrix theory [10]. The advantage is that no λ extrapolation is necessary. The disadvantage is that all the eigenvalues of the massless Dirac operator have to be calculated as in Eq. (16). When V is large, the computational task is huge and not so feasible. Also, a very large lattice is required to get stable and consistent results.

C. Third relation

One can perform similar analysis for the p.d.f. of the chiral condensate for a single configuration, defined in Eq. (3). The Fourier transformed p.d.f. for this gauge configuration Eq. (6) is then

$$\tilde{P}_U(q) = \int_{-\infty}^{\infty} dc \exp(-iqc) P_U(c) = \prod_{j=1}^{N_c V/2} \left(1 - \frac{q^2 + 2imqN_c V}{(N_c V)^2 (\lambda_j^2(U) + m^2)} \right). \tag{22}$$

In the chiral limit, it becomes

$$\tilde{P}_U(q)|_{m=0} = \prod_{j=1}^{N_c V/2} \left[1 - \left(\frac{q}{N_c V \lambda_j(U)} \right)^2 \right]. \tag{23}$$

This equation is equal to zero at

$$q = N_c V \lambda_j(U), \quad j = 1, \dots, N_c V/2. \tag{24}$$

Performing similar procedures when deriving Eq. (19), one has for $\tilde{P}_U(q)|_{m=0}$

$$\tilde{P}_U(q)|_{m=0} = J_0[qc_0(U)]. \tag{25}$$

This equation is equal to zero at

$$q = \frac{z(j)}{c_0(U)}, \quad j = 1, \dots, \infty, \tag{26}$$

where $z(j)$ is the jth zero of J_0. In Table I, the first 40 zeros of J_0 are provided.

For $V \gg 1$, Eq. (24) should agree with Eq. (26) so that

$$c_0(U) = \frac{z(j)}{N_c V \lambda_j(U)}, \quad j = 1, \dots, \infty. \tag{27}$$

$c_0(U)$ is the amplitude of the chiral condensate for configuration U. Averaging it over gauge configurations with fermions, we obtain

$$C(j) = \langle c_0(U) \rangle = \frac{z(j)}{N_c V} \left\langle \frac{1}{\lambda_j} \right\rangle. \tag{28}$$

Neither m nor λ extrapolation is necessary. In the chiral-symmetry breaking phase, a plateau for $C(j) = \text{const}$ will develop, from which the chiral condensate in the chiral limit can be extracted.

The relation between eigenmodes and chiral-symmetry breaking is clear: if chiral symmetry is spontaneously broken, i.e., $c_0(U) \not\equiv 0$, according to Eqs. (27) and (28), λ_j should scale as $z(j)/V$. In the infinite volume limit $V \to \infty$, the eigenvalues relevant for chiral-symmetry breaking are those going to zero as $1/V$, which is consistent with Banks and Casher.

The advantage of Eq. (28) is that to extract the value of $C(j)$ from a plateau, only a few smallest eigenvalues are

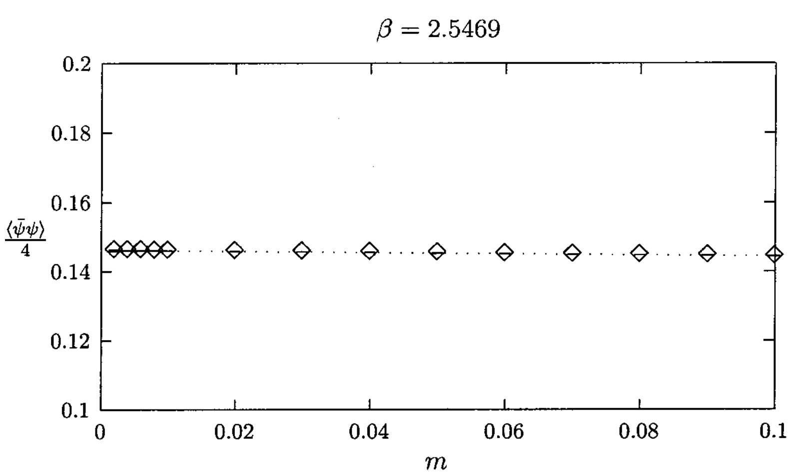

FIG. 1. $\langle \bar{\psi}\psi \rangle/4$ as a function of m for $\beta = 2.5469$ using Eq. (16). The dotted line is a linear fit of the data to the chiral limit.

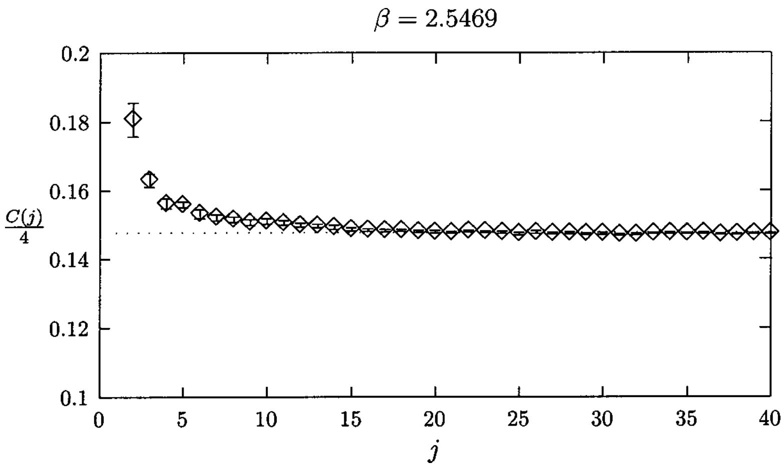

FIG. 2. $C(j)/4$ as a function of j for $\beta = 2.5469$ using Eq. (28). The dotted line stands for the mean value of data in the plateau.

needed for this calculation. Of course, finite size analysis $\lim_{m\to 0}\lim_{V\to\infty}\langle\bar{\psi}\psi\rangle = \lim_{V\to\infty}C(j)$ remains to be done, as in all approaches.

III. RESULTS IN QCD WITH KS QUARKS

The most interesting application of this method is QCD. Here we would like to present the first data for SU(3) lattice gauge theory with KS fermions, which has the action $S = S_g + S_f$:

$$S_g = -\frac{\beta}{N_c}\sum_p \mathrm{Re\,Tr}(U_p),$$

$$S_f = \sum_{x,y}\bar{\psi}(x)\Delta_{x,y}\psi(y),$$

$$U_p = U_\mu(x)U_\nu(x+\mu)U_\mu^\dagger(x+\nu)U_\nu^\dagger(x),$$

$$\Delta_{x,y} = m\delta_{x,y} + \sum_{\mu=1}^{4}\frac{1}{2}\eta_\mu(x)[U_\mu(x)\delta_{x,y-\hat{\mu}} - U_\mu^\dagger(x-\hat{\mu})\delta_{x,y+\hat{\mu}}],$$

$$\eta_\mu(x) = (-1)^{x_1+x_2+\cdots+x_{\mu-1}}, \tag{29}$$

where $\beta = 2N_c/g^2$. In the chiral limit $m=0$, a U(1) subgroup of the continuous chiral symmetry exists, i.e., S_f is invariant under the following transformation:

$$\psi(x) \to \exp[i\alpha(-1)^{x_1+x_2+x_3+x_4}]\psi(x),$$

$$\bar{\psi}(x) \to \bar{\psi}(x)\exp[i\alpha(-1)^{x_1+x_2+x_3+x_4}]. \tag{30}$$

All simulations are done on the $V=10^4$ lattice in the quenched SU(3) case. The pure SU(3) gauge fields are updated using the Cabibbo-Marinari quasiheat bath algorithm, followed by some over-relaxation sweeps. 100–400 independent configurations are used for the measurements.

Figure 1 shows the data for $\langle\bar{\psi}\psi\rangle$ at a stronger coupling $\beta = 2.5469$ using Eq. (16). A linear function is also used to extrapolate the data of $\langle\bar{\psi}\psi\rangle$ at nonzero fermion mass $m \in [0.005, 0.1]$ to the chiral limit. Figure 2 shows the result of $C(j)$ for the same β using Eq. (28); there is a nice plateau for $j \in [15,40]$. The linear extrapolation result from Eq. (16) is consistent with the mean value of Eq. (28) in the plateau.

The results at a weaker coupling $\beta = 5.6263$ are shown in Figs. 3 and 4. One sees there is a little change in the slope when using Eq. (16) to calculate $\langle\bar{\psi}\psi\rangle$ and the extrapolated value at $m=0$. In comparison, there is a wide plateau for $C(j)$ using Eq. (28). But both approaches still give consistent results.

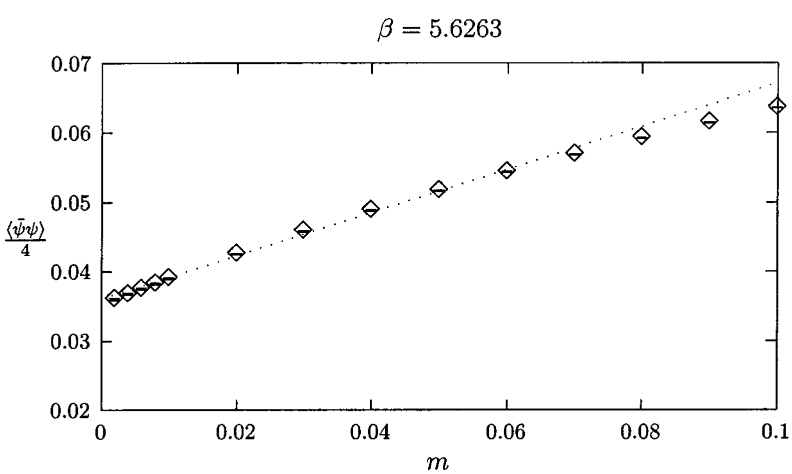

FIG. 3. $\langle\bar{\psi}\psi\rangle/4$ as a function of m for $\beta = 5.6263$ using Eq. (16). The dotted line is a linear fit of the data to the chiral limit.

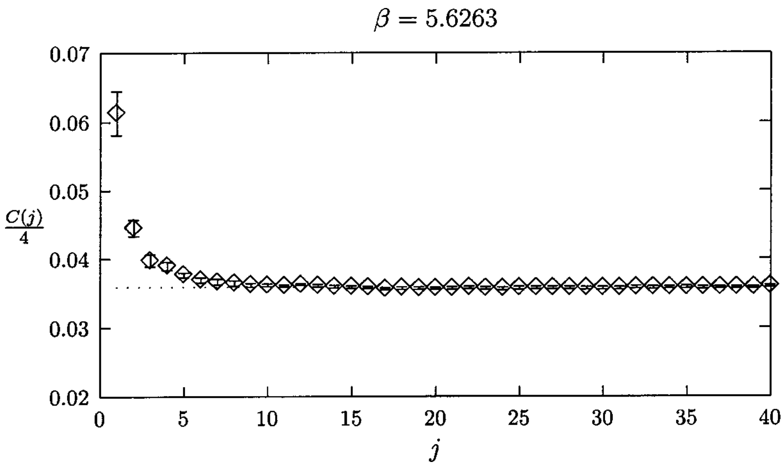

FIG. 4. $C(j)/4$ as a function of j for $\beta = 5.6263$ using Eq. (28). The dotted line stands for mean value of data in the plateau.

In conclusion, we have shown how the p.d.f. method for obtaining the chiral condensate in the exact chiral limit works in lattice QCD with quenched KS quarks. There are several advantages in using relation (28): only calculations of a small set of eigenvalues of the massless Dirac operator are necessary; there is no need for m or λ extrapolation. This might be an alternative efficient method for investigating the spontaneous chiral-symmetry breaking in lattice QCD. It would also be very interesting to see application of this approach to other fermion formulations, e.g., overlap fermions or domain wall fermions.

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