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# Nonperturbative $O(a)$ improvement of Wilson quark action in three-flavor QCD with plaquette gauge action

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We perform a nonperturbative determination of the  $O(a)$ -improvement coefficient  $c_{\text{SW}}$  for the Wilson quark action in three-flavor QCD with the plaquette gauge action. Numerical simulations are carried out in a range of  $\beta = 12.0$ – $5.2$  on a single lattice size of  $8^3 \times 16$  employing the Schrödinger functional setup of lattice QCD. As our main result, we obtain an interpolation formula for  $c_{\text{SW}}$  and the critical hopping parameter  $K_c$  as a function of the bare coupling. This enables us to remove the  $O(a)$  scaling violation from physical observables in future numerical simulation in the wide range of  $\beta$ . Our analysis with a perturbatively modified improvement condition for  $c_{\text{SW}}$  suggests that finite volume effects in  $c_{\text{SW}}$  are not large on the  $8^3 \times 16$  lattice. We investigate  $N_f$  dependence of  $c_{\text{SW}}$  by additional simulations for  $N_f = 4, 2,$  and  $0$  at  $\beta = 9.6$ . As a preparatory step for this study, we also determine  $c_{\text{SW}}$  in two-flavor QCD at  $\beta = 5.2$ . At this  $\beta$ , several groups have carried out large-scale calculations of the hadron spectrum, while no systematic determination of  $c_{\text{SW}}$  has been performed.

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## I. INTRODUCTION

Recent large-scale simulations in two-flavor QCD have demonstrated that quenching artifacts found in various physical observables are reduced by dynamical effects of up and down quarks. There has been significant progress also in the algorithms for QCD with odd numbers of flavors: while the conventional Hybrid Monte Carlo (HMC) algorithm [1] is applicable only to even-flavor QCD, the exact algorithms, such as the Multi-Boson [2] and the polynomial HMC algorithms [3] capable of odd-flavor cases, have been developed. Clearly the time has come to undertake fully realistic and extensive simulations of QCD with dynamical up, down, and strange quarks.

Since simulations with dynamical quarks are computationally demanding, highly improved lattice actions should be employed in the three-flavor simulations. The leading cutoff effect in physical quantities is  $O(a)$  with the Wilson quark action, and this error can be removed by adding a single counterterm, the Sheikholeslami-Wohlert (SW) term [4], to the action with a nonperturbatively determined coefficient  $c_{\text{SW}}$ . However,  $c_{\text{SW}}$  has been determined only in quenched and two-flavor QCD so far [5,6].

In this article, we perform a nonperturbative determination of  $c_{\text{SW}}$  in three-flavor QCD with the plaquette gauge and the Wilson quark actions. In Refs. [7,8], however, we found that this theory has a nontrivial phase structure: there is an unphysical phase transition at  $\beta \approx 5.0$ , where the lattice cutoff  $a^{-1}$  is roughly 2.6 GeV. It is expected that the

phase transition strongly distorts scaling properties of physical observables. This transition is considered as an artifact due to the finite lattice spacing and can be removed by the use of improved gauge actions [7,8]. Therefore, there are two strategies for meaningful simulations in three-flavor QCD: (i) use the plaquette gauge action at  $\beta \gg 5.0$ , or (ii) use an improved gauge action, if simulations at  $a^{-1} \lesssim 2.6$  GeV are needed. We explore the former strategy in this article, and the latter possibility is studied in a separate publication [9].

In our determination of  $c_{\text{SW}}$ , we follow the method proposed by ALPHA Collaboration in Refs. [5,10]. We explore a wide range of  $\beta = 12.0$ – $5.2$ , which is significantly higher than the phase transition point  $\beta \approx 5.0$ , employing a single lattice size of  $8^3 \times 16$ . As our main result, we derive an interpolation formula for  $c_{\text{SW}}$  as a function of the bare coupling. The critical hopping parameter  $K_c$  in the  $O(a)$ -improved theory is also obtained as a by-product. We examine finite volume effects in  $c_{\text{SW}}$  by modifying the improvement condition at one-loop order of perturbation theory. Additional simulations in four-flavor, two-flavor, and quenched QCD at  $\beta = 9.6$  are carried out to investigate the  $N_f$  dependence of  $c_{\text{SW}}$ .

As a preparatory step toward this study, we also determine  $c_{\text{SW}}$  in two-flavor QCD at  $\beta = 5.2$ . In the previous work by ALPHA Collaboration [6], they carried out the nonperturbative tuning of  $c_{\text{SW}}$  at  $\beta \geq 5.4$ , and derived an interpolation formula of their result as a function of  $g_0^2$ .

However, due to the limitation of available computer power, recent large-scale simulations by UKQCD Collaboration[11] and JLQCD Collaboration [12] were performed at a lower value  $\beta = 5.2$  with  $c_{\text{SW}}$  obtained by extrapolating ALPHA's formula. We, therefore, determine  $c_{\text{SW}}$  directly at  $\beta = 5.2$  in order to see if the extrapolation of the formula to this value of  $\beta$  really works out, and to confirm that the  $O(a)$  scaling violation is absent in the UKQCD and JLQCD simulations.

This paper is organized as follows. In Sec. II, we briefly introduce the method for the nonperturbative tuning of  $c_{\text{SW}}$  employed in this study. Section III is devoted to detailed description of our numerical analysis and results in two-flavor QCD at  $\beta = 5.2$ . We present our results in three-flavor QCD and discuss its  $O(a/L)$  uncertainty in Sec. IV. Finally, our conclusion is given in Sec. V.

## II. IMPROVEMENT CONDITION FOR $O(a)$ IMPROVEMENT

In our determination of  $c_{\text{SW}}$ , we basically follow the method proposed in Refs. [5,10], which employs the Schrödinger functional (SF) setup of lattice QCD [13]. In this section, we briefly introduce the SF setup and the choice of the improvement condition to fix  $c_{\text{SW}}$ .

### A. SF setup

The SF is the generating functional of the field theory with the Dirichlet boundary condition imposed in the temporal direction. In this study, the spatial link variables at the boundaries are set to the following diagonal, constant SU(3) matrices:

$$\begin{aligned} U_k(\mathbf{x}, x_0)|_{x_0=0} &= \exp[aC_k], \\ U_k(\mathbf{x}, x_0)|_{x_0=T} &= \exp[aC'_k], \end{aligned} \quad (1)$$

$$C_k = \frac{i\pi}{6L_k} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad C'_k = \frac{i\pi}{6L_k} \begin{pmatrix} -5 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}, \quad (2)$$

where  $L_k (k = 1, 2, 3)$  and  $T$  are physical lattice sizes in the spatial and temporal directions. All quark fields at the boundaries are set to zero. In the spatial directions, the periodic boundary condition is imposed for both gauge and quark fields.

We use the plaquette gauge action

$$S_g = \frac{\beta}{6} \sum_{x,\mu,\nu} \text{Tr}[1 - U_{x,\mu\nu}], \quad (3)$$

where  $U_{x,\mu\nu}$  is the product of gauge link variables  $U_{x,\mu}$  around the plaquette

$$U_{x,\mu\nu} = U_{x,\mu} U_{x+\hat{\mu},\nu} U_{x+\hat{\mu},\mu}^\dagger U_{x,\nu}^\dagger. \quad (4)$$

The  $O(a)$ -improved Wilson quark action [4] is given by

$$S_q = \sum_{x,y} \bar{q}_x D_{xy} q_y, \quad (5)$$

$$\begin{aligned} D_{xy} &= \delta_{xy} - K \sum_{\mu} \{ (1 - \gamma_{\mu}) U_{x,\mu} \delta_{x+\hat{\mu},y} + (1 \\ &+ \gamma_{\mu}) U_{x-\hat{\mu},\mu}^\dagger \delta_{x-\hat{\mu},y} \} + \frac{i}{2} K c_{\text{SW}} \sigma_{\mu\nu} F_{x,\mu\nu} \delta_{xy}, \end{aligned} \quad (6)$$

with the field strength tensor  $F_{x,\mu\nu}$  defined by

$$\begin{aligned} F_{x,\mu\nu} &= \frac{1}{8} \{ (U_{x,\mu\nu} + U_{x,\nu-\mu} + U_{x,-\mu-\nu} + U_{x,-\nu\mu}) \\ &- (\text{h.c.}) \}, \end{aligned} \quad (7)$$

where (h.c.) denotes the Hermitian conjugate of the preceding bracket, and  $\sigma_{\mu\nu} = (i/2)[\gamma_{\mu}, \gamma_{\nu}]$ . The last term in Eq. (6) is the counterterm to remove  $O(a)$  effects in on-shell quantities. Its coefficient  $c_{\text{SW}}$  is set to unity to remove the tree-level  $O(a)$  scaling violation from physical observables. The main purpose of this article is nonperturbative tuning of  $c_{\text{SW}}$  for removal of all  $O(ag_0^n)$  scaling violation ( $n \geq 0$ ). For the  $O(a)$  improvement of the SF itself, we add counterterms made of the gauge and quark fields at boundaries to the lattice action. However, these counterterms affect the PCAC relation at order of  $a^2$  or higher, and hence are not necessary for determination of  $c_{\text{SW}}$  from the PCAC relation. In ALPHA Collaboration's studies, the counterterms are omitted except for a term

$$\delta S_g = \frac{\beta}{6} (c_t - 1) \sum_{\mathbf{x}, \mu (x_0=0, T-a)} \text{Tr}[1 - U_{x,\mu 0}], \quad (8)$$

which is made of the temporal plaquettes touching the boundaries. In this study, we also include this counterterm to the total lattice action  $S = S_g + \delta S_g + S_q$  so that we can directly compare our and ALPHA Collaboration's results. The coefficient of the counterterm  $c_t$  is set to the one-loop estimate in Ref. [14].

### B. Improvement condition

We determine  $c_{\text{SW}}$  by imposing the validity of the PCAC relation

$$\frac{1}{2} (\partial_{\mu} + \partial_{\mu}^*) A_{\text{imp},\mu}^a = 2mP^a, \quad (9)$$

up to order of  $a^2$ . The pseudoscalar operator and  $O(a)$ -improved and unimproved axial currents are given by

$$P^a = \bar{\psi} \gamma_5 \tau^a \psi, \quad (10)$$

$$A_{\text{imp},\mu}^a = A_{\mu}^a + c_A \frac{1}{2} (\partial_{\mu} + \partial_{\mu}^*) P^a, \quad (11)$$

$$A_{\mu}^a = \bar{\psi} \gamma_{\mu} \gamma_5 \tau^a \psi, \quad (12)$$

where  $\partial_{\mu}$  and  $\partial_{\mu}^*$  are the forward and backward lattice

derivatives and  $SU(N_f)$  generators  $\tau^a$  act on the flavor indices of the quark fields  $\bar{\psi}$  and  $\psi$ .

We measure two correlation functions,

$$f_A(x_0) = -\frac{1}{N_f^2 - 1} \langle A_0^a(x) \mathcal{O}^a \rangle, \quad (13)$$

$$f_P(x_0) = -\frac{1}{N_f^2 - 1} \langle P^a(x) \mathcal{O}^a \rangle, \quad (14)$$

where  $\langle \cdots \rangle$  denotes the expectation value after taking trace over color and spinor indices and summing over spatial coordinate  $\mathbf{x}$ . For the source operator, we take

$$\mathcal{O}^a = a^6 \sum_{\mathbf{y}, \mathbf{z}} \bar{\zeta}(\mathbf{y}) \gamma_5 \tau^a \zeta(\mathbf{z}), \quad (15)$$

defined from the boundary fields

$$\zeta(\mathbf{x}) = \frac{\delta}{\delta \bar{\rho}(\mathbf{x})}, \quad \bar{\zeta}(\mathbf{x}) = \frac{\delta}{\delta \rho(\mathbf{x})}, \quad (16)$$

where  $\rho(\mathbf{x})$  is the quark field at  $x_0 = 0$  and is set to zero in the calculation of  $f_A$  and  $f_P$ . The bare quark mass is then calculated from  $f_A$  and  $f_P$  through the PCAC relation equation (9):

$$m(x_0) = r(x_0) + c_A s(x_0), \quad (17)$$

$$r(x_0) = \frac{1}{4} (\partial_0 + \partial_0^*) f_A(x_0) / f_P(x_0), \quad (18)$$

$$s(x_0) = \frac{1}{2} a \partial_0 \partial_0^* f_P(x_0) / f_P(x_0). \quad (19)$$

We can calculate another set of  $m'$ ,  $r'$ , and  $s'$  from the correlation functions

$$f'_A(T - x_0) = +\frac{1}{N_f^2 - 1} \langle A_0^a(x) \mathcal{O}'^a \rangle, \quad (20)$$

$$f'_P(T - x_0) = -\frac{1}{N_f^2 - 1} \langle P^a(x) \mathcal{O}'^a \rangle, \quad (21)$$

using the source operator at the other boundary

$$\mathcal{O}'^a = a^6 \sum_{\mathbf{y}, \mathbf{z}} \bar{\zeta}'(\mathbf{y}) \gamma_5 \tau^a \zeta'(\mathbf{z}), \quad (22)$$

where  $\zeta'$  is the boundary field at  $x_0 = T$ .

The improvement condition to fix  $c_{\text{SW}}$  is obtained by requiring that quark masses calculated with different boundary conditions coincide with each other. However, a naive condition  $m(x_0) = m'(x_0)$  requires a nonperturbative tuning of  $c_A$  as well as  $c_{\text{SW}}$ . To eliminate  $c_A$  from the process, it was proposed in Ref. [5] to use a modified definition of the quark mass

$$M(x_0, y_0) = m(x_0) - \frac{m(y_0) - m'(y_0)}{s(y_0) - s'(y_0)} s(x_0), \quad (23)$$

and similarly defined  $M'(x_0, y_0)$ . Therefore,  $c_{\text{SW}}$  is tuned so that the following mass difference,

$$\Delta M(x_0, y_0) = M(x_0, y_0) - M'(x_0, y_0), \quad (24)$$

vanishes with a certain choice of  $(x_0, y_0)$ .

In principle, we can take an arbitrary choice for  $(x_0, y_0)$ , since a change of the choice leads to a difference in the  $O(a^2)$  scaling violation in physical observables. In this study, we take  $(x_0, y_0) = (3T/4, T/4)$  for  $\Delta M(x_0, y_0)$ , and  $(x_0, y_0) = (T/2, T/4)$  for  $M(x_0, y_0)$ . The latter is used to specify the massless point. We note that this choice is the same as that in ALPHA's studies in quenched and two-flavor QCD. From now on,  $M$  and  $\Delta M$  without arguments denote  $M(T/2, T/4)$  and  $\Delta M(3T/4, T/4)$ , respectively.

In practice,  $c_{\text{SW}}$  is determined by demanding that  $M$  and  $\Delta M$  satisfy the following improvement condition,

$$\begin{cases} M &= 0, \\ \Delta M &= \Delta M^{(0)}, \end{cases} \quad (25)$$

where  $\Delta M^{(0)}$  is the tree-level value of  $\Delta M$  at the massless point  $M = 0$  on the finite lattice volume  $L^3 \times T$ . We tune  $\Delta M$  to  $\Delta M^{(0)}$  but not to zero so that the weak coupling limit of the nonperturbatively determined  $c_{\text{SW}}$  is exactly unity. On our lattice size of  $8^3 \times 16$ ,  $a\Delta M^{(0)} = 0.000277$  [5]. We also note that the tuning of  $M$  to the massless point provides a nonperturbative estimate of the critical hopping parameter  $K_c$  in the  $O(a)$ -improved theory.

### III. TWO-FLAVOR QCD AT $\beta = 5.2$

#### A. Simulation method

In this section, we report the determination of  $c_{\text{SW}}$  in two-flavor QCD at  $\beta = 5.2$ .

Our numerical simulations are carried out on a  $8^3 \times 16$  lattice at six values of  $c_{\text{SW}}$  in a range  $c_{\text{SW}} = 1.5\text{--}3.0$ . We choose two to four values for the hopping parameter  $K$  at each  $c_{\text{SW}}$  so that we have data of  $\Delta M$  at both positive and negative values of  $M$ , and/or at  $M$  close to the massless point ( $|aM| \leq 0.01$  in our study). This enables us to tune  $(M, \Delta M)$  to  $(0, \Delta M^{(0)})$  by an interpolation or short extrapolation. The simulated values of  $c_{\text{SW}}$  and  $K$  are summarized in Table I.

We use the standard HMC algorithm with the asymmetric even-odd preconditioning described in Refs. [15,16] for the determinant of the quark matrix  $D$ . We solve the linear equation  $DX = B$  using the BiCGStab algorithm [17] with the stopping condition

$$\|R_i\|/\|B\| < 10^{-14}, \quad (26)$$

where  $R_i = DX_i - B$  is the residual vector and  $X_i$  is the estimate for the solution  $X$  in the  $i$ th BiCGStab iteration. The HMC trajectory length is fixed to the unit length. We set the number of the molecular dynamics steps to 60–80, which achieves the acceptance rate higher than 80%.

TABLE I. Simulation parameters in two-flavor QCD at  $\beta = 5.2$ .

$c_{\text{SW}}$	$K$	$N_{\text{traj}}$	$c_{\text{SW}}$	$K$	$N_{\text{traj}}$	$c_{\text{SW}}$	$K$	$N_{\text{traj}}$
1.50	0.144 00	6400	1.90	0.138 00	5600	2.02	0.137 00	4800
1.50	0.146 00	6200	1.90	0.139 00	6387	2.30	0.130 00	3200
1.80	0.138 00	6400	2.02	0.133 00	8000	2.30	0.132 00	4000
1.80	0.140 25	6400	2.02	0.135 00	2176	3.00	0.121 00	4000
1.90	0.137 00	6400	2.02	0.136 07	6400	3.00	0.122 00	4000

After the thermalization of 500 HMC trajectories, we accumulate the statistics  $N_{\text{traj}}$  summarized in Table I. The correlators  $f_X$  and  $f'_X (X = A, P)$  are measured at every trajectory. We use the jackknife method to estimate statistical errors of  $f_X, f'_X$  and all results derived from them.

### B. Numerical results

Numerical results of  $M$  and  $\Delta M$  are summarized in Table II. In order to fix  $c_{\text{SW}}$  and  $K_c$  satisfying the improvement condition Eq. (25), we parametrize  $M$  and  $\Delta M$  by a simultaneous fit in terms of  $1/K$  and  $c_{\text{SW}}$ :

$$aM = a_M + \frac{b_M^{(1)}}{K} + \frac{b_M^{(2)}}{K^2} + c_M^{(1)}c_{\text{SW}} + c_M^{(2)}c_{\text{SW}}^2 + \frac{d_M}{K}c_{\text{SW}}, \quad (27)$$

$$a\Delta M = a_{\Delta M} + \frac{b_{\Delta M}^{(1)}}{K} + \frac{b_{\Delta M}^{(2)}}{K^2} + c_{\Delta M}^{(1)}c_{\text{SW}} + c_{\Delta M}^{(2)}c_{\text{SW}}^2 + \frac{d_{\Delta M}}{K}c_{\text{SW}}. \quad (28)$$

Fit parameters are summarized in Table III. Figure 1 shows  $1/K$  dependence of  $M$  and  $\Delta M$ , and  $M$  dependence of  $\Delta M$  at each  $c_{\text{SW}}$ . By interpolating  $(M, \Delta M)$  to  $(0, \Delta M^{(0)})$  with

this parametrization, we obtain

$$c_{\text{SW}} = 1.908(64), \quad (29)$$

$$K_c = 0.1381(12). \quad (30)$$

We also test another method for the parametrization of  $M$  and  $\Delta M$  in order to estimate the systematic error due to the simultaneous fit equations (27) and (28). At each  $c_{\text{SW}}$ , we determine  $\Delta M$  at  $M = 0$  by a linear fit

$$a\Delta M = a'_M + b'_M(aM). \quad (31)$$

At  $c_{\text{SW}} = 1.90$  and  $2.02$  where we simulate more than two values for  $K$ , we also test a quadratic form and find that the higher order contribution is small and can be safely neglected in this analysis. Figure 2 shows  $c_{\text{SW}}$  dependence of  $\Delta M$  at  $M = 0$  which we parametrize by linear or quadratic forms

$$a\Delta M = a'_{\Delta M} + b'_{\Delta M}c_{\text{SW}} + c'_{\Delta M}c_{\text{SW}}^2. \quad (32)$$

By tuning  $\Delta M$  to its tree-level value, we obtain  $c_{\text{SW}} = 1.979(68)$  from the linear fit as reported in Ref. [12], and  $1.975(50)$  from the quadratic one. These are consistent with the result from the combined fit. This good agreement originates from our careful choice of  $c_{\text{SW}}$  and  $K$  in simu-

TABLE II. Quark mass  $M$  and its difference  $\Delta M$  in two-flavor QCD at  $\beta = 5.2$ .

$c_{\text{SW}}$	$K$	$aM$	$a\Delta M$	$c_{\text{SW}}$	$K$	$aM$	$a\Delta M$
1.50	0.144 00	0.159(29)	-0.0039(44)	2.02	0.135 00	0.0541(47)	0.0002(15)
1.50	0.146 00	-0.0012(39)	0.0073(24)	2.02	0.136 07	0.0005(20)	-0.0022(14)
1.80	0.138 00	0.136(10)	-0.0073(28)	2.02	0.137 00	-0.0411(17)	0.0040(27)
1.80	0.140 25	-0.0048(29)	0.0024(22)	2.30	0.130 00	0.0546(10)	-0.001 08(91)
1.90	0.137 00	0.0629(31)	-0.0038(16)	2.30	0.132 00	-0.0187(11)	-0.002 96(97)
1.90	0.138 00	0.0083(22)	-0.0008(16)	3.00	0.121 00	0.03767(84)	-0.007 82(49)
1.90	0.139 00	-0.0338(23)	0.0033(14)	3.00	0.122 00	0.00455(71)	-0.007 35(82)
2.02	0.133 00	0.1361(51)	-0.0003(12)	...	...	...	...

TABLE III. Fit parameters for Eqs. (27) and (28) in two-flavor QCD at  $\beta = 5.2$ .

$\chi^2/\text{dof}$	$a_M$	$b_M^{(1)}$	$b_M^{(2)}$	$c_M^{(1)}$	$c_M^{(2)}$	$d_M$
6.37	-28.8(7.1)	8.9(2.5)	-0.67(22)	-6.3(2.2)	-0.15(17)	0.83(39)
$\chi^2/\text{dof}$	$a_{\Delta M}$	$b_{\Delta M}^{(1)}$	$b_{\Delta M}^{(2)}$	$c_{\Delta M}^{(1)}$	$c_{\Delta M}^{(2)}$	$d_{\Delta M}$
1.88	11.2(3.2)	-3.9(1.1)	0.336(98)	3.16(95)	0.214(71)	-0.54(17)

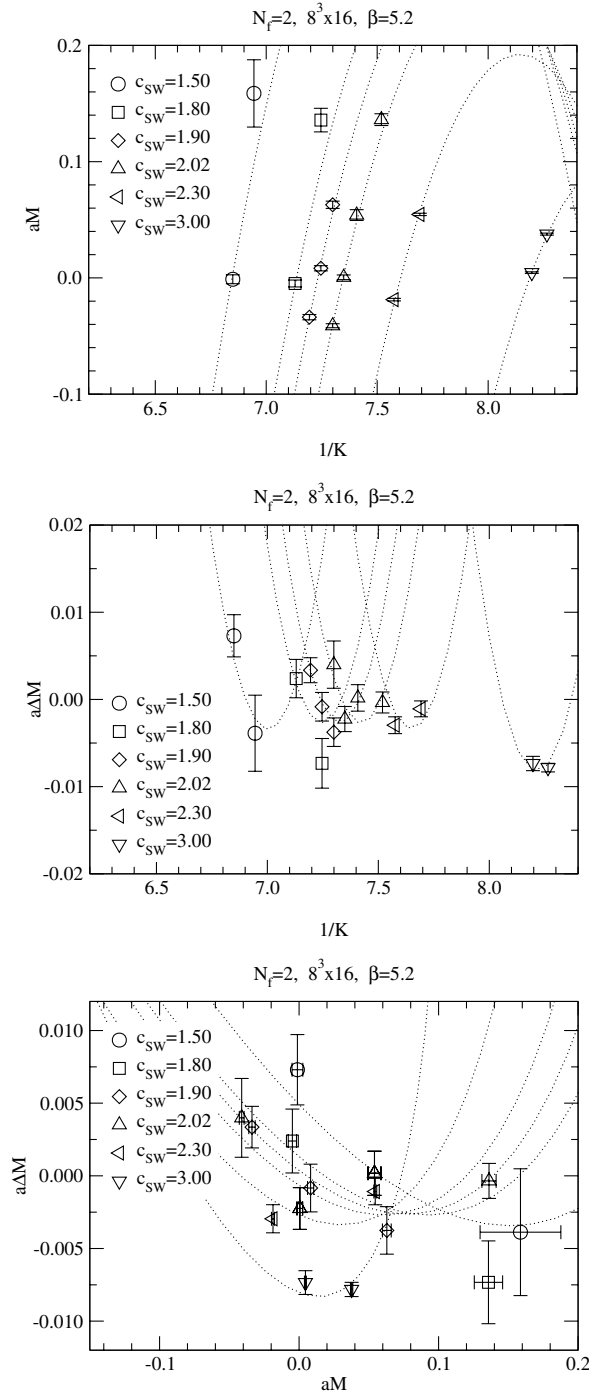


FIG. 1. Plots of  $M$  (top figure) and  $\Delta M$  (middle figure) in two-flavor QCD at  $\beta = 5.2$  as a function of  $1/K$ . The bottom figure shows  $\Delta M$  as a function of  $M$ .

lations: since we choose these parameters so that the region of  $(M, \Delta M)$  contains  $(0, \Delta M^{(0)})$  as shown in Fig. 1,  $c_{\text{SW}}$  can be fixed by a short interpolation for which the uncertainty due to the choice of the parametrization function for  $M$  and  $\Delta M$  is not large.

ALPHA's interpolation formula in Ref. [6] gives  $c_{\text{SW}} = 2.017$  at  $\beta = 5.2$ , which is consistent with our results. This

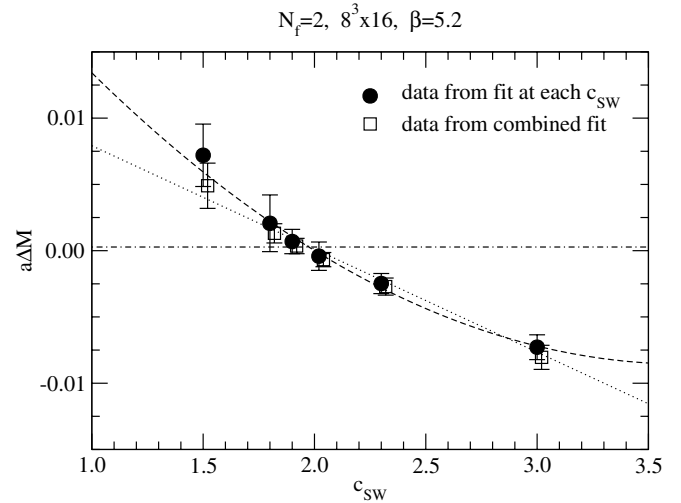


FIG. 2. Mass difference  $\Delta M$  at  $M = 0$  as a function of  $c_{\text{SW}}$ . Filled and open symbols are obtained from the fit equation (31) and combined fit equations (27) and (28). Results from the combined fit are slightly shifted in the horizontal direction for better visibility. Dotted and dashed lines show linear and quadratic fit equation (32). The dot-dashed line shows the tree-level value  $\Delta M^{(0)} = 0.000277$ .

confirms that ALPHA's formula can be used down to  $\beta = 5.2$  as in the UKQCD [11] and JLQCD simulations [12].

However, as pointed out in Ref. [18], there are large cutoff effects in the PCAC quark mass  $m$  and the mass dependence of the Sommer scale  $r_0$  [19] around  $\beta = 5.2$ . There is a possibility that the improvement condition Eq. (25) adopted in this and ALPHA's previous studies leaves unexpectedly large  $O(a^2)$  scaling violations in physical observables around this value of  $\beta$ . Therefore, a test of alternative improvement conditions and scaling properties of physical observables is an important subject to avoid the large cutoff effects in future lattice calculations.

## IV. THREE-FLAVOR QCD

### A. Simulation method

We determine  $c_{\text{SW}}$  in three-flavor QCD at nine values of  $\beta$  in the range  $\beta = 12.0-5.2$ . Numerical simulations are carried out on a  $8^3 \times 16$  lattice at four values of  $c_{\text{SW}}$  at each  $\beta$ , and three or four values of  $K$  at each  $c_{\text{SW}}$ . These values are carefully chosen so that the region of  $(M, \Delta M)$  contains or is sufficiently close to the point  $(0, \Delta M^{(0)})$  which satisfies the improvement condition Eq. (25). These simulation parameters are summarized in Table IV.

In our simulations, we adopt the standard HMC algorithm for two-flavors of dynamical quarks and a polynomial HMC algorithm developed in Ref. [16] for the remaining one-flavor. We employ the symmetric even-odd preconditioning in Refs. [15,16] for the quark matrix  $D$ . As in the two-flavor simulations at  $\beta = 5.2$ , we calcu-

TABLE IV. Simulation parameters in three-flavor QCD.

$\beta = 12.0$							
$c_{\text{SW}} = 1.08624$	$c_{\text{SW}} = 1.12036$	$c_{\text{SW}} = 1.15448$	$c_{\text{SW}} = 1.18860$				
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.128958	3000	0.128958	3000	0.128958	3000	0.128958	3000
0.129607	3000	0.129607	3000	0.129607	3000	0.129607	3000
0.130257	3000	0.130257	3000	0.130257	3000	0.130257	3000
0.130906	3000	0.130906	3000	0.130906	3000	0.130906	3000
$\beta = 9.6$							
$c_{\text{SW}} = 1.12990$	$c_{\text{SW}} = 1.16539$	$c_{\text{SW}} = 1.20089$	$c_{\text{SW}} = 1.23638$				
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.13043	7000	0.13043	7000	0.13043	7000	0.13043	7000
0.13109	7000	0.13109	7000	0.13109	7000	0.13109	7000
0.13175	7000	0.13175	7000	0.13175	7000	0.13175	7000
0.13240	7000	0.13240	7000	0.13230	1800	0.13230	7000
$\beta = 7.4$							
$c_{\text{SW}} = 1.2258$	$c_{\text{SW}} = 1.2643$	$c_{\text{SW}} = 1.3028$	$c_{\text{SW}} = 1.3413$				
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.13293	5400	0.13293	5400	0.13293	5400	0.13293	5400
0.13360	5400	0.13360	5400	0.13360	5400	0.13360	5400
0.13427	5400	0.13427	5400	0.13427	5400	0.13393	400
0.13494	5400	0.13470	3400	...	...	0.13427	5400
$\beta = 6.8$							
$c_{\text{SW}} = 1.2783$	$c_{\text{SW}} = 1.3184$	$c_{\text{SW}} = 1.3586$	$c_{\text{SW}} = 1.3987$				
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.13391	4200	0.13391	4200	0.13391	4200	0.13391	4200
0.13459	4200	0.13459	4200	0.13459	4200	0.13459	4200
0.13526	4200	0.13526	4200	0.13526	4200	0.13492	3700
0.13594	4200	0.13560	4200	0.13540	3700	0.13500	3150
$\beta = 6.3$							
$c_{\text{SW}} = 1.3117$	$c_{\text{SW}} = 1.3675$	$c_{\text{SW}} = 1.4233$	$c_{\text{SW}} = 1.4791$				
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.13501	4600	0.13501	4600	0.13446	4600	0.13446	4600
0.13555	4600	0.13555	4600	0.13501	4600	0.13501	4600
0.13609	4600	0.13609	4600	0.13555	4600	0.13530	1100
0.13664	4600	0.13664	4600	0.13609	4600	0.13555	4600
$\beta = 6.0$							
$c_{\text{SW}} = 1.3237$	$c_{\text{SW}} = 1.3801$	$c_{\text{SW}} = 1.4364$	$c_{\text{SW}} = 1.4927$				
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.13552	4200	0.13552	4200	0.13498	4200	0.13498	4200
0.13607	4200	0.13607	4200	0.13552	4200	0.13552	4200
0.13661	4200	0.13661	4200	0.13607	4200	0.13607	4200
0.13716	4200	0.13716	4200	0.13661	4200	0.13634	4200
$\beta = 5.7$							
$c_{\text{SW}} = 1.5431$	$c_{\text{SW}} = 1.6088$	$c_{\text{SW}} = 1.6745$	$c_{\text{SW}} = 1.7401$				
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.13575	5000	0.13541	5000	0.13507	5000	0.13400	4500
0.13644	5000	0.13610	5000	0.13540	4400	0.13450	4100
0.13712	4700	0.13644	3700	0.13575	5000	0.13473	5000
0.13750	4500	0.13678	5000	0.13585	2700	0.13500	4400
$\beta = 5.4$							
$c_{\text{SW}} = 1.6$	$c_{\text{SW}} = 1.7$	$c_{\text{SW}} = 1.8$	$c_{\text{SW}} = 1.9$				
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.13750	9000	0.13600	9000	0.13480	9000	0.13330	9000
0.13810	9000	0.13630	7900	0.13520	9000	0.13370	9000
0.13825	7100	0.13660	9000	0.13560	9000	0.13410	9000
0.13840	8200	0.13720	9000	0.13580	7700	0.13450	9000
$\beta = 5.2$							
$c_{\text{SW}} = 1.70$	$c_{\text{SW}} = 1.85$	$c_{\text{SW}} = 2.00$	$c_{\text{SW}} = 2.15$				
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.1375	7800	0.1357	7800	0.1336	7800	0.1316	7800
0.1379	7800	0.1361	7800	0.1340	7800	0.1320	7800
0.1383	7800	0.1365	7800	0.1344	7800	0.1322	5500
0.1387	6300	0.1366	7400	0.1345	7400	0.1324	7800

late  $D^{-1}$  using the BiCGStab algorithm with the tolerance parameter  $\|R_i\|/\|B\| < 10^{-14}$ . We set the number of the molecular dynamics steps to 80. This achieves the acceptance rate of about 90% or higher.

In the PHMC algorithm, we use the Chebyshev polynomial  $P[D]$  to approximate  $D^{-1}$ . In order to make this algorithm exact, the correction factor

$$P_{\text{corr}} = \det[W(D)] \quad (33)$$

with  $W[D] = P[D]D$  is taken into account by the noisy Metropolis method [20]. We calculate the square root of  $W[D]$ , which is required in the Metropolis test, with an accuracy of  $10^{-14}$  using the Taylor expansion of  $W[D]$  [16]. The order of the polynomial  $N_{\text{poly}}$  is chosen so that we achieve the acceptance rate of about 90% or higher for the Metropolis test.

We note that, even with the SF setup, there is a difficulty in simulating massless or negative quark masses in three-flavor QCD. In the strong coupling region, eigenvalues of  $D$  have large fluctuations and they can take values outside the radius of convergence of  $P[D]$ . If this happens, the polynomial approximation  $P[D]$  and Taylor expansion of  $W[D]$  break down. For this reason, our simulations in the strong coupling region are performed only down to  $M \simeq 0$ , while negative quark masses  $M \simeq -0.03$  are simulated in the weak coupling region  $\beta \simeq 12$ .

We accumulate statistics  $N_{\text{traj}}$  summarized in Table IV, and measure the correlators  $f_X$  and  $f'_X (X = A, P)$  at every trajectory. The dependence of the jackknife error of  $M$  on the bin size  $N_{\text{bin}}$  is investigated in a range  $N_{\text{bin}} = 1 - N_{\text{traj}}/20$ . We then adopt  $N_{\text{bin}}$  giving the maximum error in the jackknife procedure in the following analysis.

We determine  $c_{\text{SW}}$  and  $K_c$  nonperturbatively also in four-flavor, two-flavor, and quenched QCD at  $\beta = 9.6$  to study their  $N_f$  dependence. The simulation method is similar to that in three-flavor QCD, except that we use the standard HMC algorithm in these cases. Simulation parameters are summarized in Tables V, VI, and VII.

## B. Nonperturbative $c_{\text{SW}}$ in three-flavor QCD

Numerical results of  $M$  and  $\Delta M$  are summarized in Table VIII. In Fig. 3, we plot  $M$  and  $M'$  at several values of  $\beta$  as a function of  $x_0$ . With our statistics,  $aM$ ,  $aM'$ , and hence  $a\Delta M$  have an accuracy of  $10^{-3}$  at all simulation parameters. These accurate data enable us to reduce the statistical error of  $c_{\text{SW}}$  to the level of  $\sim 5\%$  even at our coarsest lattice spacing.

In order to parametrize the  $K$  and  $c_{\text{SW}}$  dependence of  $M$  and  $\Delta M$ , we use the combined fit of Eqs. (27) and (28). Fit parameters are summarized in Tables IX and X. Figs. 4 and 5 show  $M$  and  $\Delta M$  and their fit curves at several values of  $\beta$ . We observe that our data are well described by the combined fit. Consequently, as shown in Fig. 6,  $M$  dependence of  $\Delta M$  is reproduced reasonably well by the fit. We fix  $c_{\text{SW}}$  and  $K_c$  satisfying the improvement condition

TABLE V. Simulation parameters in four-flavor QCD at  $\beta = 9.6$ .

$c_{\text{SW}} = 1.129\,90$		$c_{\text{SW}} = 1.165\,39$		$c_{\text{SW}} = 1.200\,89$		$c_{\text{SW}} = 1.236\,38$	
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.130 43	5000	0.130 43	5000	0.130 43	5000	0.130 43	5000
0.131 09	5000	0.131 09	5000	0.131 09	5000	0.131 09	5000
0.131 75	5000	0.131 75	5000	0.131 75	5000	0.131 75	5000
0.132 40	5000	0.132 40	5000	0.132 40	5000	0.132 40	5000

TABLE VI. Simulation parameters in two-flavor QCD at  $\beta = 9.6$ .

$c_{\text{SW}} = 1.129\,90$		$c_{\text{SW}} = 1.165\,39$		$c_{\text{SW}} = 1.200\,89$		$c_{\text{SW}} = 1.236\,38$	
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.130 43	5000	0.130 43	5000	0.130 43	5000	0.130 43	5000
0.131 09	5000	0.131 09	5000	0.131 09	5000	0.131 09	5000
0.131 75	5000	0.131 75	5000	0.131 75	5000	0.131 75	5000
0.132 40	5000	0.132 40	5000	0.132 40	5000	0.132 40	5000

TABLE VII. Simulation parameters in quenched QCD at  $\beta = 9.6$ .

$c_{\text{SW}} = 1.129\,90$		$c_{\text{SW}} = 1.165\,39$		$c_{\text{SW}} = 1.200\,89$		$c_{\text{SW}} = 1.236\,38$	
$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$	$K$	$N_{\text{traj}}$
0.130 43	8000	0.130 43	8000	0.130 43	8000	0.130 43	8000
0.131 09	8000	0.131 09	8000	0.131 09	8000	0.131 09	8000
0.131 75	8000	0.131 75	8000	0.131 75	8000	0.131 75	8000
0.132 40	8000	0.132 40	8000	0.132 40	8000	0.132 40	8000

Eq. (25) using this parametrization. Numerical results for the nonperturbatively tuned  $c_{\text{SW}}$  and  $K_c$  are summarized in Table XI.

As in the analysis in two-flavor QCD at  $\beta = 5.2$ , we test Eqs. (31) and (32) as the alternative method for the

parametrization. We confirm that the two methods give consistent results both for  $c_{\text{SW}}$  and  $K_c$ , and hence conclude that the systematic error due to the parametrization method for  $M$  and  $\Delta M$  is small.

We fit  $c_{\text{SW}}$  to a rational function of  $g_0^2$  and obtain the following interpolation formula,

$$c_{\text{SW}} = \frac{1 - 0.194785g^2 - 0.110781g^4 - 0.0230239g^6 + 0.137401g^8}{1 - 0.460685g^2}. \quad (34)$$

The interpolation formula for  $K_c$  is obtained in a polynomial form,

$$K_c = 1/8 + k^{(1)}g_0^2 + 0.000964911g_0^4 + 0.00298136g_0^6 + 0.00100995g_0^8 - 0.00235564g_0^{10}, \quad (35)$$

with  $k^{(1)} = 0.00843986$ . These fits reproduce our data reasonably well with  $\chi^2/\text{dof}$  of around 1.6. We also note that the coefficients of  $O(g_0^2)$  terms in these fits are constrained so that these expressions coincide with their one-loop estimates [21,22] up to  $O(g_0^2)$ .

We plot the  $\beta$  dependence of  $c_{\text{SW}}$  and  $K_c$  in Fig. 7. While  $c_{\text{SW}}$  in three-flavor QCD is well approximated by the

one-loop estimate in the weak coupling region of  $g_0^2 < 0.4$  ( $\beta > 15$ ), it develops a significant deviation toward the strong coupling. Similar deviation is also observed in  $K_c$ . It is possible that these deviations are partly compensated by a better choice of the expansion parameter for lattice perturbation theory [23]. However, the large deviation at the strong coupling  $g_0^2 \lesssim 1.0$  suggests that one-loop  $O(a)$ -improved Wilson quark action leads to a significant  $O(a)$  scaling violation in physical observables at the strong coupling region, where high statistics simulations are feasible with currently available computer resources. Therefore, the use of  $c_{\text{SW}}$  in Eq. (34) is essential to remove the  $O(a)$  effects in practical lattice calculations.



TABLE VIII. Quark mass  $M$  and its difference  $\Delta M$  in three-flavor QCD.

$\beta = 12.0$					
$K$	$c_{\text{SW}} = 1.08624$ $aM$	$a\Delta M$	$K$	$c_{\text{SW}} = 1.12036$ $aM$	$a\Delta M$
0.128958	0.03502(11)	0.00107(13)	0.128958	0.03066(8)	0.00067(10)
0.129607	0.01498(13)	0.00099(12)	0.129607	0.01028(10)	0.00072(16)
0.130257	-0.00544(10)	0.00100(14)	0.130257	-0.01011(12)	0.00040(12)
0.130906	-0.02591(11)	0.00116(12)	0.130906	-0.03088(11)	0.00052(12)
$K$	$c_{\text{SW}} = 1.15448$ $aM$	$a\Delta M$	$K$	$c_{\text{SW}} = 1.18860$ $aM$	$a\Delta M$
0.128958	0.02581(9)	0.00027(12)	0.128958	0.02125(9)	-0.00029(11)
0.129607	0.00561(11)	0.00015(11)	0.129607	0.00076(10)	-0.00027(11)
0.130257	-0.01512(14)	0.00008(13)	0.130257	-0.01965(11)	-0.00044(13)
0.130906	-0.03555(17)	0.00025(13)	0.130906	-0.04041(12)	-0.00043(14)
$\beta = 9.6$					
$K$	$c_{\text{SW}} = 1.12990$ $aM$	$a\Delta M$	$K$	$c_{\text{SW}} = 1.16539$ $aM$	$a\Delta M$
0.13043	0.03818(12)	0.00118(10)	0.13043	0.03226(9)	0.00067(10)
0.13109	0.01805(9)	0.00100(12)	0.13109	0.01187(10)	0.00062(12)
0.13175	-0.00275(10)	0.00104(14)	0.13175	-0.00871(12)	0.00056(13)
0.13240	-0.02312(11)	0.00104(13)	0.13240	-0.02948(11)	0.00063(16)
$K$	$c_{\text{SW}} = 1.20089$ $aM$	$a\Delta M$	$K$	$c_{\text{SW}} = 1.23638$ $aM$	$a\Delta M$
0.13043	0.02596(11)	0.00037(11)	0.13043	0.01995(9)	-0.00037(14)
0.13109	0.00559(12)	0.00014(13)	0.13109	-0.00091(10)	-0.00012(9)
0.13175	-0.01522(11)	0.00005(12)	0.13175	-0.02145(11)	-0.00044(13)
0.13230	-0.03256(19)	0.00033(24)	0.13230	-0.03934(13)	-0.00054(14)
$\beta = 7.4$					
$K$	$c_{\text{SW}} = 1.2258$ $aM$	$a\Delta M$	$K$	$c_{\text{SW}} = 1.2643$ $aM$	$a\Delta M$
0.13293	0.04147(22)	0.00135(19)	0.13293	0.03265(15)	0.00067(19)
0.13360	0.02134(21)	0.00158(25)	0.13360	0.01209(23)	0.00065(25)
0.13427	0.00079(21)	0.00099(26)	0.13427	-0.00942(21)	0.00102(23)
0.13494	-0.02065(24)	0.00077(28)	0.13470	-0.02292(28)	0.00089(34)
$K$	$c_{\text{SW}} = 1.3028$ $aM$	$a\Delta M$	$K$	$c_{\text{SW}} = 1.3413$ $aM$	$a\Delta M$
0.13293	0.02296(25)	0.00035(24)	0.13293	0.01309(22)	0.00004(23)
0.13360	0.00214(17)	0.00018(19)	0.13360	-0.00756(21)	0.00029(28)
0.13427	-0.01888(23)	0.00052(22)	0.13393	-0.01774(64)	-0.00018(68)
...	...	...	0.13427	-0.02867(26)	-0.00048(36)
$\beta = 6.8$					
$K$	$c_{\text{SW}} = 1.2783$ $aM$	$a\Delta M$	$K$	$c_{\text{SW}} = 1.3184$ $aM$	$a\Delta M$
0.13391	0.04462(36)	0.00066(28)	0.13391	0.03342(33)	0.00092(28)
0.13459	0.02457(29)	0.00079(32)	0.13459	0.01358(28)	0.00051(27)
0.13526	0.00338(33)	0.00098(30)	0.13526	-0.00823(30)	0.00065(40)
0.13594	-0.01824(30)	0.00163(37)	0.13560	-0.01839(36)	0.00054(39)
$K$	$c_{\text{SW}} = 1.3586$ $aM$	$a\Delta M$	$K$	$c_{\text{SW}} = 1.3987$ $aM$	$a\Delta M$
0.13391	0.02240(31)	0.00049(26)	0.13391	0.01208(22)	-0.00021(35)
0.13459	0.00175(31)	0.00031(23)	0.13459	-0.00953(30)	-0.00030(27)
0.13526	-0.01924(27)	0.00033(34)	0.13492	-0.01956(58)	0.00025(45)
0.13540	-0.02474(30)	0.00058(46)	0.13500	-0.02271(43)	-0.00014(34)

TABLE VIII. (continued)

$\beta = 6.3$					
$c_{\text{SW}} = 1.3117$			$c_{\text{SW}} = 1.3675$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.135 01	0.053 92(55)	0.000 85(50)	0.135 01	0.036 77(44)	0.000 97(29)
0.135 55	0.037 66(40)	0.001 07(32)	0.135 55	0.020 65(30)	0.000 63(33)
0.136 09	0.021 52(36)	0.000 80(38)	0.136 09	0.003 53(36)	0.000 58(32)
0.136 64	0.004 03(41)	0.001 75(34)	0.136 64	-0.013 45(53)	0.001 68(41)
$c_{\text{SW}} = 1.4233$			$c_{\text{SW}} = 1.4791$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.134 46	0.036 35(37)	0.000 70(37)	0.134 46	0.018 34(37)	-0.000 34(33)
0.135 01	0.019 15(34)	0.000 28(37)	0.135 01	0.001 98(38)	0.000 06(30)
0.135 55	0.002 84(43)	0.000 92(33)	0.135 30	-0.008 07(57)	0.000 75(47)
0.136 09	-0.014 97(43)	0.000 50(37)	0.135 55	-0.015 99(41)	-0.000 39(51)
$\beta = 6.0$					
$c_{\text{SW}} = 1.3237$			$c_{\text{SW}} = 1.3801$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.135 52	0.076 08(51)	0.001 54(39)	0.135 52	0.058 26(50)	0.001 56(37)
0.136 07	0.060 56(57)	0.001 75(43)	0.136 07	0.041 82(39)	0.001 24(44)
0.136 61	0.044 11(52)	0.001 20(48)	0.136 61	0.024 00(46)	0.000 77(40)
0.137 16	0.027 55(53)	0.002 41(53)	0.137 16	0.008 43(50)	0.002 59(53)
$c_{\text{SW}} = 1.4364$			$c_{\text{SW}} = 1.4927$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.134 98	0.054 92(48)	0.000 54(40)	0.134 98	0.036 35(37)	-0.000 60(60)
0.135 52	0.038 93(49)	0.000 35(54)	0.135 52	0.018 78(41)	0.000 30(45)
0.136 07	0.022 21(48)	0.001 07(44)	0.136 07	0.002 35(45)	-0.000 05(48)
0.136 61	0.005 62(49)	0.000 31(50)	0.136 34	-0.006 92(49)	0.000 76(39)
$\beta = 5.7$					
$c_{\text{SW}} = 1.5431$			$c_{\text{SW}} = 1.6088$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.135 75	0.043 54(59)	0.000 79(42)	0.135 41	0.027 48(50)	-0.000 68(47)
0.136 44	0.020 91(55)	-0.000 39(51)	0.136 10	0.006 95(130)	0.000 53(54)
0.137 12	-0.001 81(57)	0.000 72(53)	0.136 44	-0.005 87(70)	-0.000 87(64)
0.137 50	-0.013 86(70)	0.000 07(72)	0.136 78	-0.017 02(60)	-0.000 89(65)
$c_{\text{SW}} = 1.6745$			$c_{\text{SW}} = 1.7401$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.135 07	0.013 31(69)	-0.000 81(51)	0.134 00	0.022 29(42)	-0.001 40(52)
0.135 40	0.002 78(64)	-0.000 22(61)	0.134 50	0.005 21(59)	-0.001 04(39)
0.135 75	-0.009 47(54)	-0.000 78(43)	0.134 73	-0.001 73(44)	-0.000 82(42)
0.135 85	-0.011 24(62)	-0.001 15(51)	0.135 00	-0.011 53(59)	-0.001 72(69)
$\beta = 5.4$					
$c_{\text{SW}} = 1.6$			$c_{\text{SW}} = 1.7$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.137 50	0.033 10(70)	0.000 15(43)	0.136 00	0.035 92(56)	-0.000 31(40)
0.138 10	0.012 45(75)	0.000 83(52)	0.136 30	0.026 22(54)	0.000 32(52)
0.138 25	0.006 84(78)	0.000 53(62)	0.136 60	0.016 53(48)	0.000 30(46)
0.138 40	0.003 82(124)	0.001 00(49)	0.137 20	-0.005 89(52)	0.001 06(57)
$c_{\text{SW}} = 1.8$			$c_{\text{SW}} = 1.9$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.134 80	0.030 73(51)	-0.001 29(56)	0.133 30	0.036 00(40)	-0.001 49(40)
0.135 20	0.016 50(50)	-0.000 48(49)	0.133 70	0.022 50(34)	-0.001 67(51)
0.135 60	0.003 73(52)	0.000 10(47)	0.134 10	0.008 71(47)	-0.001 10(40)
0.135 80	-0.004 26(70)	-0.000 62(53)	0.134 50	-0.005 08(51)	-0.001 94(51)

TABLE VIII. (*continued*)

$\beta = 5.2$					
$c_{\text{SW}} = 1.70$			$c_{\text{SW}} = 1.85$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.1375	0.051 91(131)	0.001 02(87)	0.1357	0.034 06(87)	-0.000 04(54)
0.1379	0.037 76(89)	0.000 62(67)	0.1361	0.018 44(73)	0.000 45(46)
0.1383	0.023 11(82)	0.001 96(54)	0.1365	0.002 87(78)	0.000 19(81)
0.1387	0.008 07(123)	0.000 40(110)	0.1366	0.000 37(84)	-0.000 38(56)
$c_{\text{SW}} = 2.00$			$c_{\text{SW}} = 2.15$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.1336	0.029 82(64)	-0.001 61(43)	0.1316	0.025 68(70)	-0.003 14(65)
0.1340	0.014 67(74)	-0.000 89(48)	0.1320	0.013 50(49)	-0.002 81(46)
0.1344	-0.000 03(68)	-0.002 19(48)	0.1322	0.003 64(74)	-0.003 48(77)
0.1345	-0.004 05(69)	-0.001 33(48)	0.1324	-0.002 02(51)	-0.002 84(60)

### C. $N_f$ dependence

In Fig. 7, a comparison of our interpolation formula and those by ALPHA Collaboration in two-flavor and quenched QCD suggests that  $c_{\text{SW}}$  monotonously decreases as  $N_f$  increases at fixed  $\beta$ . However, the difference between two- and three-flavor QCD is not large. This comparison may also suffer from the systematic error due to the difference in the analysis method between the two collaborations. In order to study the  $N_f$  dependence more care-

fully, we determine  $c_{\text{SW}}$  and  $K_c$  for  $N_f = 4, 2$ , and 0 at  $\beta = 9.6$  with an analysis method similar to that for  $N_f = 3$ . We obtain  $M$  and  $\Delta M$  summarized in Tables XII, XIII, and XIV. A fit to Eqs. (27) and (28) results in parameters given in Tables XV and XVI. Using the improvement condition Eq. (25), we obtain  $c_{\text{SW}}$  and  $K_c$  summarized in Table XVII.

Figure 8 shows  $c_{\text{SW}}$  and  $K_c$  at  $\beta = 9.6$  as a function of  $N_f$ . While  $K_c$  has an evident  $N_f$  dependence, that for  $c_{\text{SW}}$  is

TABLE IX. Fit parameters for Eq. (27) in three-flavor QCD.

$\beta$	$\chi^2/\text{dof}$	$a_M$	$b_M^{(1)}$	$b_M^{(2)}$	$c_M^{(1)}$	$c_M^{(2)}$	$d_M$
12.0	0.96	-10.9(1.1)	2.40(28)	-0.125(18)	-0.47(13)	-0.012(23)	0.046(16)
9.6	1.41	-13.1(1.1)	3.02(30)	-0.168(20)	-0.64(14)	-0.047(22)	0.076(17)
7.4	1.17	-15.9(2.9)	3.90(81)	-0.233(55)	-0.90(34)	-0.057(39)	0.106(46)
6.8	1.57	-24.9(4.3)	6.6(1.2)	-0.430(85)	-2.30(47)	0.016(53)	0.266(68)
6.3	0.66	-19.0(5.8)	5.0(1.7)	-0.33(12)	-1.99(66)	-0.094(40)	0.262(97)
6.0	1.19	-12.2(6.6)	3.2(1.9)	-0.20(13)	-1.75(64)	-0.111(40)	0.234(92)
5.7	1.16	-7.6(9.5)	1.6(3.0)	-0.07(23)	-0.4(1.8)	-0.007(99)	0.005(280)
5.4	0.92	-27(11)	8.0(3.7)	-0.58(30)	-5.0(2.7)	-0.19(17)	0.70(45)
5.2	1.42	-38(22)	11.9(7.4)	-0.91(62)	-8.0(5.5)	-0.32(35)	1.17(93)

TABLE X. Fit parameters for Eq. (28) in three-flavor QCD.

$\beta$	$\chi^2/\text{dof}$	$a_{\Delta M}$	$b_{\Delta M}^{(1)}$	$b_{\Delta M}^{(2)}$	$c_{\Delta M}^{(1)}$	$c_{\Delta M}^{(2)}$	$d_{\Delta M}$
12.0	0.59	1.6(1.2)	-0.41(32)	0.025(21)	-0.12(16)	-0.008(26)	0.016(19)
9.6	0.91	0.6(1.3)	-0.14(35)	0.008(23)	-0.14(16)	-0.007(25)	0.019(19)
7.4	1.13	-3.1(3.4)	0.82(93)	-0.053(64)	0.09(38)	0.025(44)	-0.022(51)
6.8	0.40	6.2(4.4)	-1.7(1.2)	0.109(84)	-0.06(50)	-0.051(49)	0.025(66)
6.3	1.14	7.1(5.3)	-2.0(1.5)	0.14(11)	0.49(61)	-0.012(38)	-0.062(91)
6.0	1.28	8.7(6.3)	-2.5(1.8)	0.18(13)	0.78(60)	0.003(37)	-0.108(84)
5.7	1.06	-4.8(8.7)	1.5(2.7)	-0.11(21)	-0.7(1.5)	0.008(80)	0.09(23)
5.4	0.53	-6.9(10.8)	2.4(3.6)	-0.21(29)	-2.1(2.6)	-0.18(16)	0.38(43)
5.2	0.67	-26(16)	8.7(5.4)	-0.73(45)	-6.6(4.0)	-0.42(25)	1.10(67)

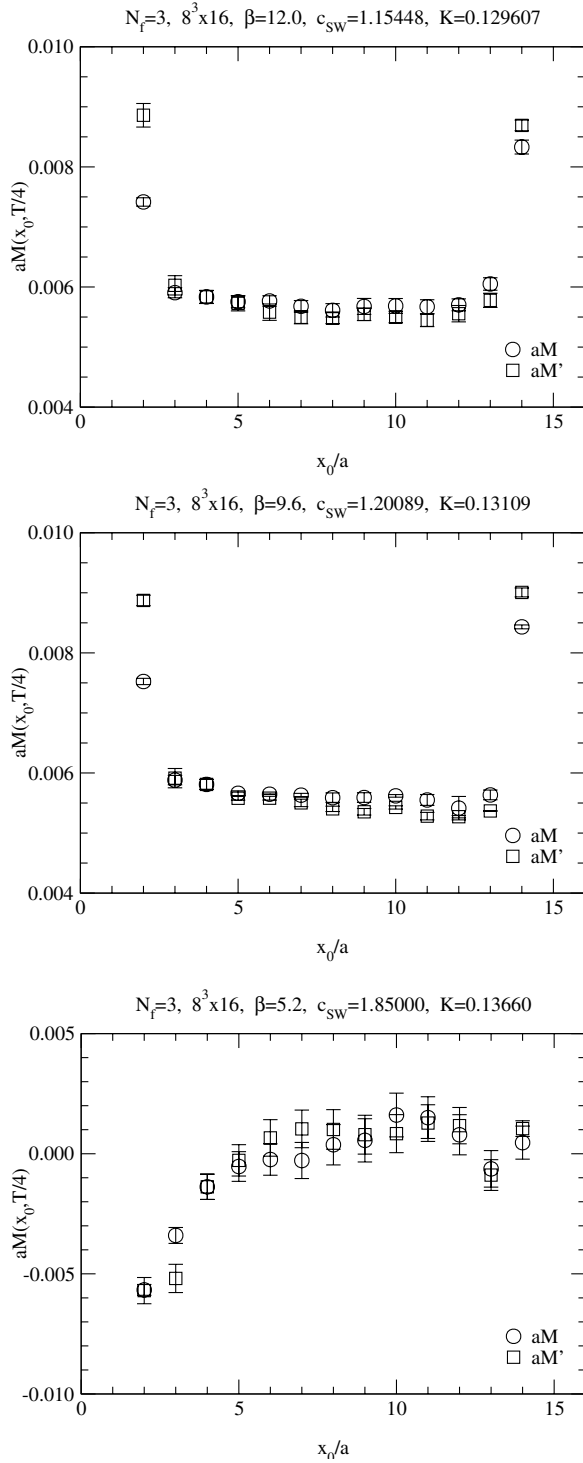


FIG. 3. Quark masses  $M$  and  $M'$  in three-flavor QCD as a function of  $x_0$ . Top, middle, and bottom figures show data at  $\beta = 12.0, 9.6,$  and  $5.2,$  respectively.

not so clear. The leading  $N_f$  dependence of  $c_{SW}$  is of order  $g_0^4 N_f$ . By fitting our results to a linear form in  $N_f$

$$c_{SW} = c_0 + c_1 g_0^4 N_f, \quad (36)$$

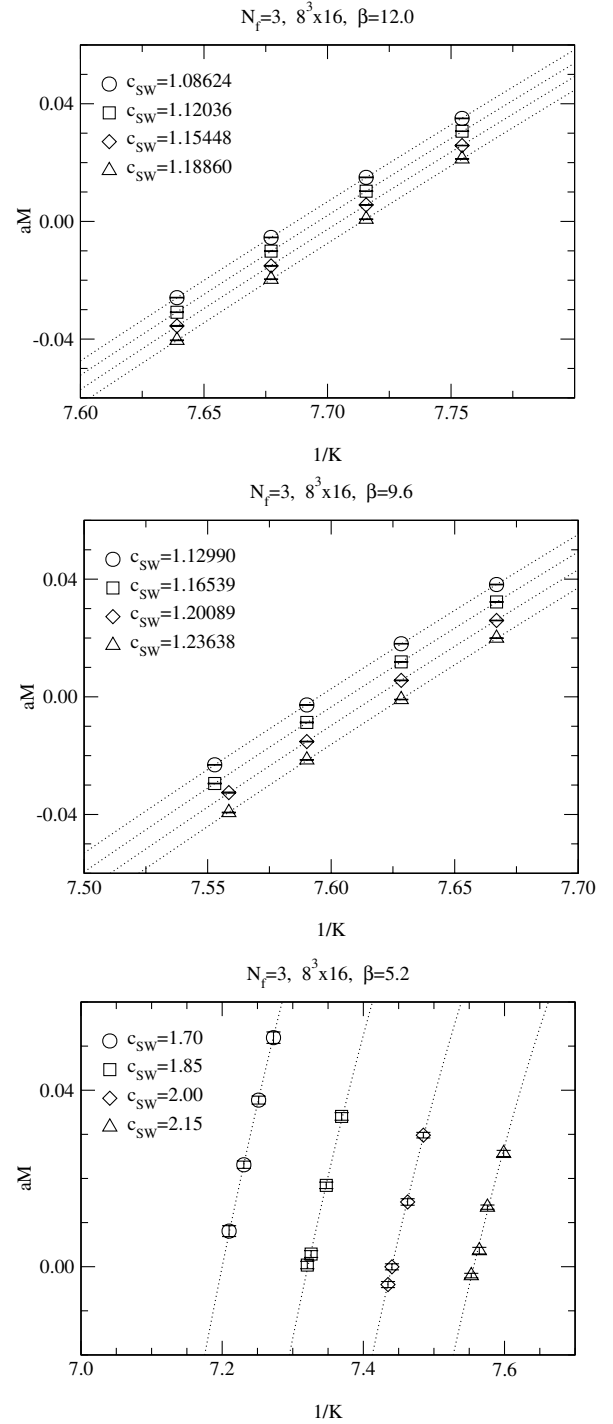


FIG. 4. Quark mass  $M$  as a function of  $1/K$ . Top, middle, and bottom figures show data at  $\beta = 12.0, 9.6,$  and  $5.2,$  respectively. Dotted lines are fit curves of Eq. (27).

we obtain  $c_1 = -0.0117(40)$  which suggests that the two-loop  $N_f$  dependence is significant also in  $c_{SW}$  at the relatively weak coupling  $\beta = 9.6$ . If a two-loop perturbative calculation of  $c_{SW}$  becomes available in the future, it will be interesting to compare the above estimate of  $c_1$  to the perturbative estimate.

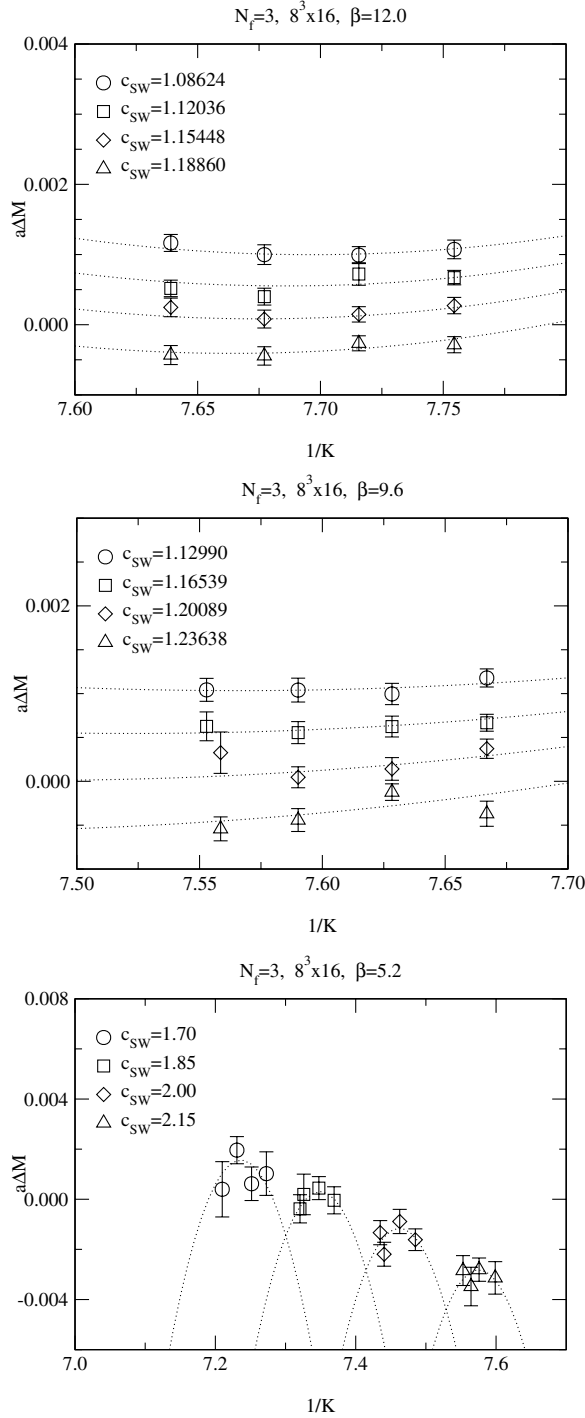


FIG. 5. Mass difference  $\Delta M$  as a function of  $1/K$ . Top, middle, and bottom figures show data at  $\beta = 12.0$ , 9.6, and 5.2, respectively. Dotted lines are fit curves of Eq. (28).

**D.  $O(a/L)$  uncertainty in  $c_{SW}$**

Our nonperturbative estimate of  $c_{SW}$  has  $O(a/L)$  uncertainties, which affects physical observables at  $O(a^2)$  when the spatial lattice size  $L$  is fixed. However, since we calculate  $c_{SW}$  with the spatial size in lattice units  $L/a$  fixed to a constant value 8, the  $O(a/L)$  dependence of  $c_{SW}$  induces

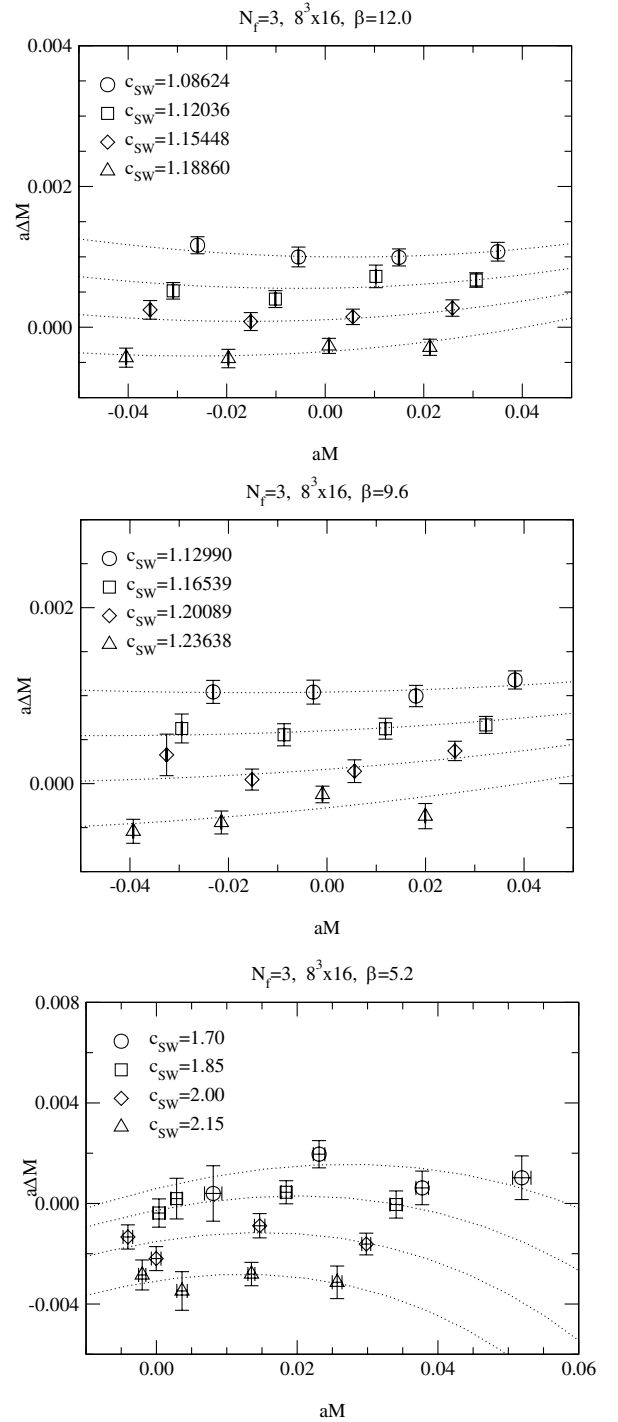


FIG. 6. Mass difference  $\Delta M$  as a function of  $M$  in three-flavor QCD. Top, middle, and bottom figures show data at  $\beta = 12.0$ , 9.6, and 5.2, respectively. Dotted lines are fit curves reproduced from Eqs. (27) and (28).

$O(a)$  effects in observables. These effects can be removed by extrapolating  $c_{SW}$  to the infinite volume limit, or interpolating to a fixed physical size in the whole region of  $g_0$ . However, we are not able to do that in the present work, since our data are taken at a single lattice size at each  $g_0$ .

TABLE XI. Nonperturbative estimate of  $c_{\text{SW}}$  and  $K_c$  in three-flavor QCD obtained from tree-level improvement condition Eq. (25).

$\beta$	$c_{\text{SW}}$	$K_c$
12.0	1.1415(48)	0.129 841(21)
9.6	1.1916(50)	0.131 321(28)
7.4	1.316(11)	0.133 567(87)
6.8	1.358(13)	0.134 66(12)
6.3	1.447(15)	0.135 39(16)
6.0	1.494(14)	0.136 12(16)
5.7	1.544(32)	0.137 06(39)
5.4	1.740(30)	0.136 50(41)
5.2	1.764(103)	0.137 89(159)

TABLE XII. Quark mass  $M$  and its difference  $\Delta M$  in four-flavor QCD at  $\beta = 9.6$ .

$c_{\text{SW}} = 1.129 90$			$c_{\text{SW}} = 1.165 39$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.130 43	0.035 30(11)	0.001 11(14)	0.130 43	0.029 55(11)	0.000 50(11)
0.131 09	0.015 27(12)	0.001 18(15)	0.131 09	0.008 92(12)	0.000 68(13)
0.131 75	-0.005 22(12)	0.001 10(12)	0.131 75	-0.011 58(11)	0.000 69(12)
0.132 40	-0.026 11(13)	0.001 23(12)	0.132 40	-0.032 56(14)	0.000 61(13)
$c_{\text{SW}} = 1.200 89$			$c_{\text{SW}} = 1.236 38$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.130 43	0.023 28(12)	0.000 18(11)	0.130 43	0.017 23(12)	-0.000 32(14)
0.131 09	0.002 80(14)	0.000 28(13)	0.131 09	-0.003 64(12)	-0.000 21(11)
0.131 75	-0.018 25(10)	0.000 28(15)	0.131 75	-0.024 62(17)	-0.000 35(15)
0.132 40	-0.039 03(15)	0.000 04(15)	0.132 40	-0.045 92(14)	-0.000 23(13)

We estimate the magnitude of  $O(a/L)$  uncertainty in  $c_{\text{SW}}$  by using a modified improvement condition. In our study as well as in ALPHA's, the improvement condition Eq. (25) is adopted instead of  $\Delta M = 0$  in order to remove the tree-level  $O(a/L)$  correction to  $c_{\text{SW}}$  [5]. We extend this procedure to the one-loop level, namely, the one-loop correction to  $\Delta M$  for the finite lattice volume  $8^3 \times 16$  given by [24]

$$a\Delta M^{(1)} = -(0.00004839 + 0.00006455N_f) \quad (37)$$

is incorporated into the improvement condition

$$\begin{cases} M &= 0, \\ \Delta M &= \Delta M^{(0)} + g_0^2 \Delta M^{(1)} \end{cases} \quad (38)$$

in order to remove the  $O(g_0^2 a/L)$  correction from  $c_{\text{SW}}$ .

TABLE XIII. Quark mass  $M$  and its difference  $\Delta M$  in two-flavor QCD at  $\beta = 9.6$ .

$c_{\text{SW}} = 1.129 90$			$c_{\text{SW}} = 1.165 39$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.130 43	0.040 89(10)	0.001 27(13)	0.130 43	0.035 08(10)	0.000 85(12)
0.131 09	0.020 85(10)	0.001 19(13)	0.131 09	0.014 82(12)	0.000 53(16)
0.131 75	0.000 47(12)	0.001 02(16)	0.131 75	-0.005 85(13)	0.000 70(14)
0.132 40	-0.019 98(13)	0.001 04(13)	0.132 40	-0.026 46(15)	0.000 68(15)
$c_{\text{SW}} = 1.200 89$			$c_{\text{SW}} = 1.236 38$		
$K$	$aM$	$a\Delta M$	$K$	$aM$	$a\Delta M$
0.130 43	0.028 84(12)	0.000 13(13)	0.130 43	0.022 59(10)	-0.000 21(13)
0.131 09	0.008 55(11)	0.000 45(14)	0.131 09	0.002 18(10)	-0.000 03(12)
0.131 75	-0.012 25(13)	0.000 13(19)	0.131 75	-0.018 57(13)	-0.000 00(13)
0.132 40	-0.032 70(12)	0.000 32(22)	0.132 40	-0.039 27(11)	-0.000 24(16)

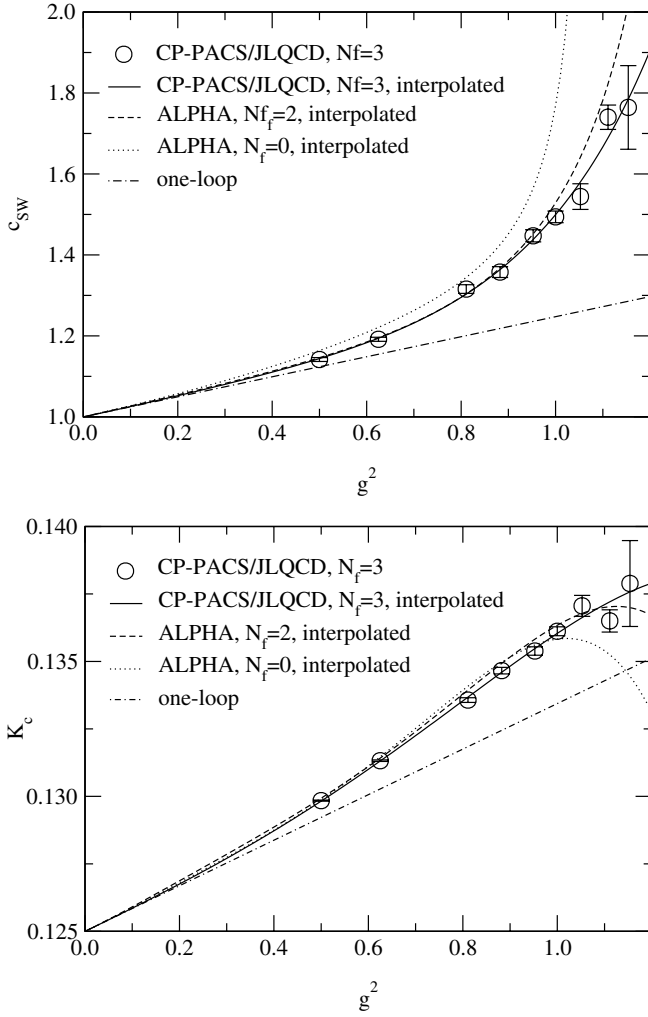


FIG. 7. Nonperturbatively determined  $c_{\text{SW}}$  (top figure) and  $K_c$  (bottom figure) as a function of  $g_0^2$ . For  $K_c$  in quenched QCD, author's interpolation of ALPHA's results is plotted.

From the parametrization of Eqs. (27) and (28) and the modified improvement condition Eq. (38), we obtain  $c_{\text{SW}}$  and  $K_c$  summarized in Table XVIII. A comparison with Table XI shows that the modified and original improve-

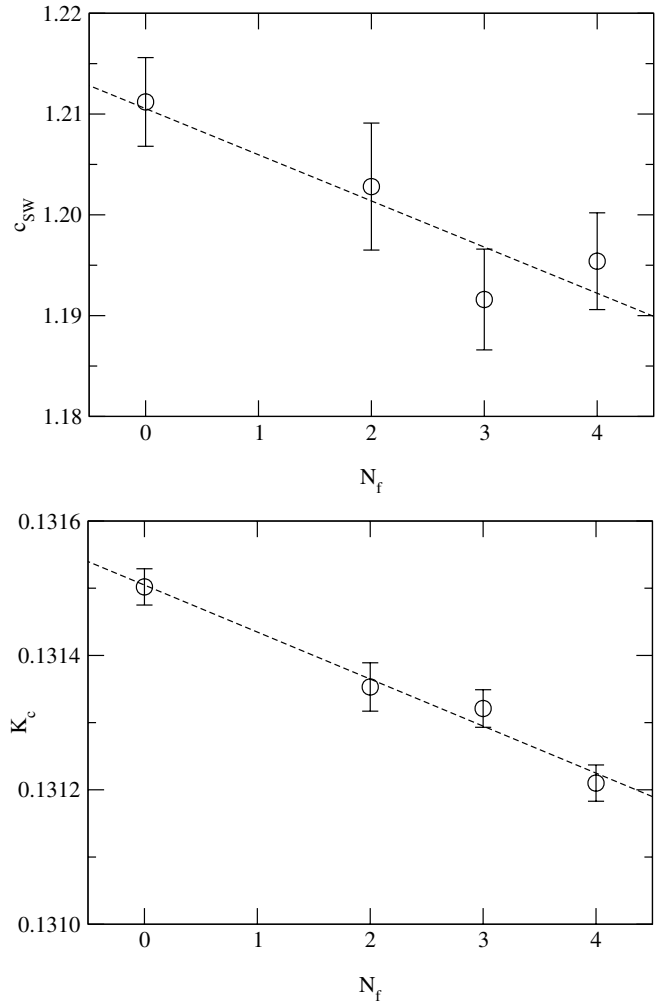


FIG. 8. Plots of  $c_{\text{SW}}$  (top figure),  $K_c$  (bottom figure) at  $\beta = 9.6$  as a function of  $N_f$ . The dashed line shows a linear fit to data.

ment conditions give consistent results with each other for  $c_{\text{SW}}$ , and hence that the  $O(g_0^2 a/L)$  correction is small in our results.

In Fig. 3, we observe that  $M$  and  $M'$  have a mild  $x_0$  dependence at  $4a < x_0 < 14a$ . This may suggest that dif-

TABLE XIV. Quark mass  $M$  and its difference  $\Delta M$  in quenched QCD at  $\beta = 9.6$ .

$K$	$c_{\text{SW}} = 1.12990$		$K$	$c_{\text{SW}} = 1.16539$	
	$aM$	$a\Delta M$		$aM$	$a\Delta M$
0.13043	0.04646(7)	0.00141(10)	0.13043	0.04059(8)	0.00095(11)
0.13109	0.02679(8)	0.00131(11)	0.13109	0.02064(8)	0.00080(11)
0.13175	0.00656(7)	0.00131(14)	0.13175	0.00041(7)	0.00084(10)
0.13240	-0.01324(8)	0.00132(10)	0.13240	-0.01978(8)	0.00074(11)
$K$	$c_{\text{SW}} = 1.20089$		$K$	$c_{\text{SW}} = 1.23638$	
	$aM$	$a\Delta M$		$aM$	$a\Delta M$
0.13043	0.03458(9)	0.00036(11)	0.13043	0.02840(8)	-0.00015(10)
0.13109	0.01451(7)	0.00034(12)	0.13109	0.00818(7)	0.00006(10)
0.13175	-0.00580(8)	0.00050(14)	0.13175	-0.01231(8)	-0.00005(13)
0.13240	-0.02607(10)	0.00053(16)	0.13240	-0.03247(10)	-0.00013(21)

TABLE XV. Fit parameters in Eq. (27) for  $N_f = 4, 2$ , and 0.

$N_f$	$\beta$	$\chi^2/\text{dof}$	$a_M$	$b_M^{(1)}$	$b_M^{(2)}$	$c_M^{(1)}$	$c_M^{(2)}$	$d_M$
4	9.6	0.96	-14.7(1.3)	3.52(33)	-0.206(22)	-1.14(15)	-0.041(25)	0.140(19)
2	9.6	0.48	-13.5(1.2)	3.15(31)	-0.177(20)	-0.64(14)	-0.052(23)	0.077(17)
0	9.6	1.03	-11.71(80)	2.70(21)	-0.150(14)	-0.80(10)	-0.040(16)	0.094(12)

TABLE XVI. Fit parameters in Eq. (28) for  $N_f = 4, 2$ , and 0.

$N_f$	$\beta$	$\chi^2/\text{dof}$	$a_{\Delta M}$	$b_{\Delta M}^{(1)}$	$b_{\Delta M}^{(2)}$	$c_{\Delta M}^{(1)}$	$c_{\Delta M}^{(2)}$	$d_{\Delta M}$
4	9.6	0.42	-1.2(1.3)	0.33(34)	-0.023(22)	-0.14(16)	0.015(26)	0.012(19)
2	9.6	0.80	-1.0(1.4)	0.24(38)	-0.014(25)	0.15(17)	0.013(28)	-0.026(21)
0	9.6	0.53	-0.3(1.2)	0.06(31)	-0.002(20)	0.11(14)	0.012(23)	-0.020(18)

TABLE XVII. Nonperturbative estimate of  $c_{\text{SW}}$  and  $K_c$  for  $N_f = 4, 2$ , and 0 obtained from tree-level improvement condition Eq. (25).

$N_f$	$\beta$	$c_{\text{SW}}$	$K_c$
4	9.6	1.1954(48)	0.131 210(27)
2	9.6	1.2028(63)	0.131 353(36)
0	9.6	1.2112(44)	0.131 502(25)

TABLE XVIII. Nonperturbative estimate of  $c_{\text{SW}}$  and  $K_c$  in three-flavor QCD obtained from one-loop level improvement condition Eq. (38).

$\beta$	$c_{\text{SW}}$	$K_c$
12.0	1.1507(46)	0.129 801(20)
9.6	1.2039(46)	0.131 252(26)
7.4	1.336(14)	0.133 40(12)
6.8	1.378(12)	0.134 47(11)
6.3	1.470(16)	0.135 15(17)
6.0	1.508(17)	0.135 96(20)
5.7	1.569(27)	0.136 76(32)
5.4	1.770(26)	0.136 09(35)
5.2	1.811(67)	0.1372(10)

ferent choices of  $x_0$  for the improvement condition Eqs. (25) and (38) lead to a small difference in  $c_{\text{SW}}$  and hence its  $O(a/L)$  ambiguity is not large.

From these observations, we expect that  $O(g_0^n a/L)$  corrections are not large at  $L/a = 8$ , and that  $c_{\text{SW}}$  in the infinite volume limit is well approximated by our results. It is an important subject in future studies to confirm this point by a direct calculation of  $c_{\text{SW}}$  with varying  $L$ .

## V. CONCLUSION

In this paper, we have performed a nonperturbative  $O(a)$  improvement of the Wilson quark action in three-flavor QCD with the plaquette gauge action. Our high statistics at

carefully chosen simulation parameters  $c_{\text{SW}}$  and  $K$  enable us to determine nonperturbative  $c_{\text{SW}}$  with an accuracy of  $\sim 5\%$  level in the wide range of  $\beta = 12.0-5.2$ . The main result of this study is the interpolation formula equation (34), with which the  $O(a)$  scaling violation in physical observables can be removed in future simulations at  $\beta \geq 5.2$ . As a by-product, we also obtain the interpolation formula for  $K_c$ , which is useful to locate simulation points.

While it is expected that  $O(a/L)$  uncertainty in  $c_{\text{SW}}$  is not large, this point should be confirmed by a direct determination of  $c_{\text{SW}}$  with varying  $L$ . A test of scaling properties of physical observables with our estimate of  $c_{\text{SW}}$  is an important next step toward an extensive simulation of three-flavor QCD with the plaquette gauge action.



We note that the range of  $\beta$  explored in this study is significantly higher than  $\beta = 5.0$ , where an artificial phase transition exists. Numerical studies at  $\beta$  below our range would possibly suffer from large distortion of scaling properties of physical observables. The use of improved gauge actions removes the lattice artifact and can push simulations toward coarser lattice spacings. This possibility is explored in a separate publication [9].

## ACKNOWLEDGMENTS

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