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We perform a nonperturbative determination of the $O(a)$-improvement coefficient c_{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_{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 β. Our analysis with a perturbatively modified improvement condition for c_{SW} suggests that finite volume effects in c_{SW} are not large on the $8^3 \times 16$ lattice. We investigate N_f dependence of c_{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_{SW} in two-flavor QCD at $\beta = 5.2$. At this β, several groups have carried out large-scale calculations of the hadron spectrum, while no systematic determination of c_{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_{SW}. However, c_{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_{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_{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_{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_{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_{SW}.

As a preparatory step toward this study, we also determine c_{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_{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 $c_{\rm SW}$ obtained by extrapolating ALPHA's formula. We, therefore, determine $c_{\rm SW}$ directly at $\beta = 5.2$ in order to see if the extrapolation of the formula to this value of β 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 nonpertubative tuning of $c_{\rm SW}$ 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 $c_{\rm SW}$, 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 $c_{\rm SW}$.

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:

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

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

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

$$S_g = \frac{\beta}{6}\sum_{x,\mu,\nu} \mathrm{Tr}[1 - U_{x,\mu\nu}], \tag{3}$$

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

$$U_{x,\mu\nu} = U_{x,\mu}U_{x+\hat{\mu},\nu}U^\dagger_{x+\hat{\nu},\mu}U^\dagger_{x,\nu}. \tag{4}$$

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

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

$$D_{xy} = \delta_{xy} - K\sum_\mu \{(1 - \gamma_\mu)U_{x,\mu}\delta_{x+\hat{\mu},y} + (1 + \gamma_\mu)U^\dagger_{x-\hat{\mu},\mu}\delta_{x-\hat{\mu},y}\} + \frac{i}{2}Kc_{\rm SW}\sigma_{\mu\nu}F_{x,\mu\nu}\delta_{xy}, \tag{6}$$

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

$$F_{x,\mu\nu} = \frac{1}{8}\{(U_{x,\mu\nu} + U_{x,\nu-\mu} + U_{x,-\mu-\nu} + U_{x,-\nu\mu}) - (\mathrm{h.c.})\}, \tag{7}$$

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 $c_{\rm SW}$ 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 $c_{\rm SW}$ 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 $c_{\rm SW}$ from the PCAC relation. In ALPHA Collaboration's studies, the counterterms are omitted except for a term

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

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 $c_{\rm SW}$ by imposing the validity of the PCAC relation

$$\frac{1}{2}(\partial_\mu + \partial^*_\mu)A^a_{{\rm imp},\mu} = 2mP^a, \tag{9}$$

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

$$P^a = \bar{\psi}\gamma_5\tau^a\psi, \tag{10}$$

$$A^a_{{\rm imp},\mu} = A^a_\mu + c_A\frac{1}{2}(\partial_\mu + \partial^*_\mu)P^a, \tag{11}$$

$$A^a_\mu = \bar{\psi}\gamma_\mu\gamma_5\tau^a\psi, \tag{12}$$

where ∂_μ and ∂^*_μ are the forward and backward lattice

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

We measure two correlation functions,

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

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

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

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

defined from the boundary fields

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

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):

$$m(x_0) = r(x_0) + c_A s(x_0), \tag{17}$$

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

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

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

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

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

using the source operator at the other boundary

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

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

The improvement condition to fix $c_{\rm SW}$ 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 $c_{\rm SW}$. To eliminate c_A from the process, it was proposed in Ref. [5] to use a modified definition of the quark mass

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

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

$$\Delta M(x_0, y_0) = M(x_0, y_0) - M'(x_0, y_0), \tag{24}$$

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 ΔM without arguments denote $M(T/2, T/4)$ and $\Delta M(3T/4, T/4)$, respectively.

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

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

where $\Delta M^{(0)}$ is the tree-level value of ΔM at the massless point $M = 0$ on the finite lattice volume $L^3 \times T$. We tune ΔM to $\Delta M^{(0)}$ but not to zero so that the weak coupling limit of the nonperturbatively determined $c_{\rm SW}$ 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 $c_{\rm SW}$ 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 $c_{\rm SW}$ in a range $c_{\rm SW} = 1.5$–3.0. We choose two to four values for the hopping parameter K at each $c_{\rm SW}$ so that we have data of ΔM 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 $c_{\rm SW}$ 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

$$||R_i||/||B|| < 10^{-14}, \tag{26}$$

where $R_i = DX_i - B$ is the residual vector and X_i is the estimate for the solution X in the ith 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 $\beta = 5.2$.

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

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

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

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

$$c_{\rm SW} = 1.908(64), \tag{29}$$

$$K_c = 0.1381(12). \tag{30}$$

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

$$a\Delta M = a'_M + b'_M (aM). \tag{31}$$

At $c_{\rm SW} = 1.90$ 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 $c_{\rm SW}$ dependence of ΔM at $M = 0$ which we parametrize by linear or quadratic forms

$$a\Delta M = a'_{\Delta M} + b'_{\Delta M} c_{\rm SW} + c'_{\Delta M} c_{\rm SW}^2. \tag{32}$$

By tuning ΔM to its tree-level value, we obtain $c_{\rm SW} = 1.979(68)$ 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 $c_{\rm SW}$ and K in simu-

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

$c_{\rm SW}$	K	aM	$a\Delta M$	$c_{\rm SW}$	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 $\beta = 5.2$.

χ^2/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)
χ^2/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)

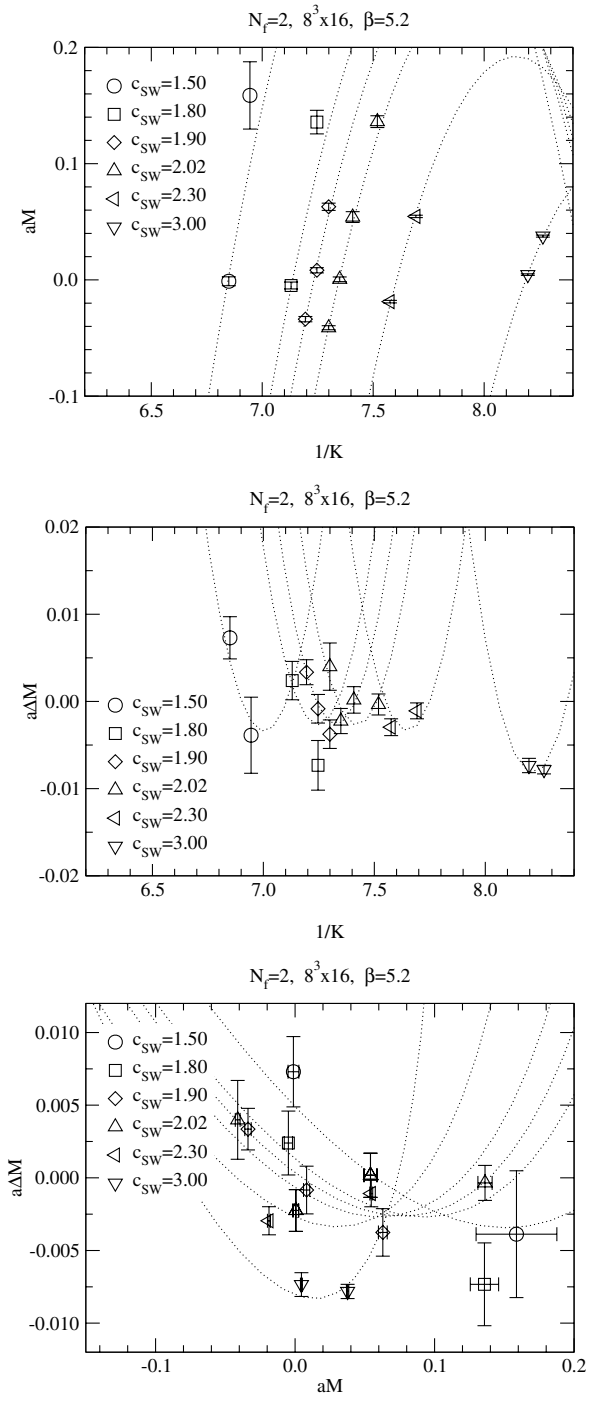

FIG. 1. Plots of M (top figure) and ΔM (middle figure) in two-flavor QCD at $\beta = 5.2$ as a function of $1/K$. The bottom figure shows ΔM as a function of M.

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

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

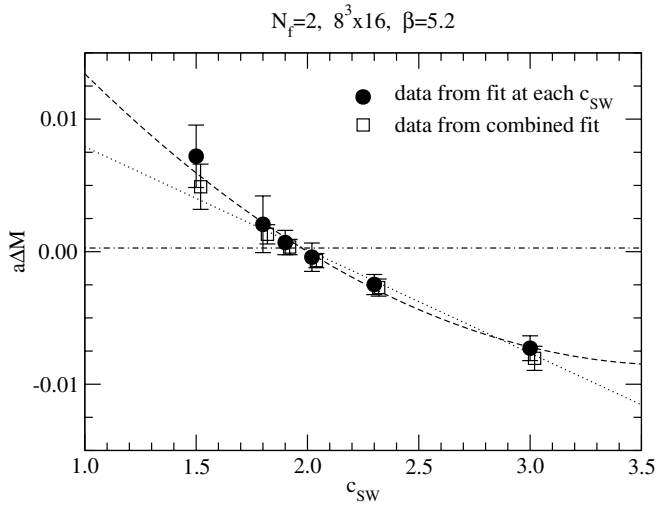

FIG. 2. Mass difference ΔM at $M = 0$ as a function of $c_{\rm SW}$. Filled and open symbols are obtained from the fit equation (31) and combined fit equations (27) and (28). Results from the combined fit are slightly shifted in the horizontal direction for better visibility. Dotted and dashed lines 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 β. 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 $c_{\rm SW}$ in three-flavor QCD at nine values of β in the range $\beta = 12.0$–5.2. Numerical simulations are carried out on a $8^3 \times 16$ lattice at four values of $c_{\rm SW}$ at each β, and three or four values of K at each $c_{\rm SW}$. 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.

$\beta = 12.0$							
$c_{\rm SW} = 1.08624$		$c_{\rm SW} = 1.12036$		$c_{\rm SW} = 1.15448$		$c_{\rm SW} = 1.18860$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
0.128 958	3000	0.128 958	3000	0.128 958	3000	0.128 958	3000
0.129 607	3000	0.129 607	3000	0.129 607	3000	0.129 607	3000
0.130 257	3000	0.130 257	3000	0.130 257	3000	0.130 257	3000
0.130 906	3000	0.130 906	3000	0.130 906	3000	0.130 906	3000
$\beta = 9.6$							
$c_{\rm SW} = 1.12990$		$c_{\rm SW} = 1.16539$		$c_{\rm SW} = 1.20089$		$c_{\rm SW} = 1.23638$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
0.130 43	7000	0.130 43	7000	0.130 43	7000	0.130 43	7000
0.131 09	7000	0.131 09	7000	0.131 09	7000	0.131 09	7000
0.131 75	7000	0.131 75	7000	0.131 75	7000	0.131 75	7000
0.132 40	7000	0.132 40	7000	0.132 30	1800	0.132 30	7000
$\beta = 7.4$							
$c_{\rm SW} = 1.2258$		$c_{\rm SW} = 1.2643$		$c_{\rm SW} = 1.3028$		$c_{\rm SW} = 1.3413$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
0.132 93	5400	0.132 93	5400	0.132 93	5400	0.132 93	5400
0.133 60	5400	0.133 60	5400	0.133 60	5400	0.133 60	5400
0.134 27	5400	0.134 27	5400	0.134 27	5400	0.133 93	400
0.134 94	5400	0.134 70	3400	···	···	0.134 27	5400
$\beta = 6.8$							
$c_{\rm SW} = 1.2783$		$c_{\rm SW} = 1.3184$		$c_{\rm SW} = 1.3586$		$c_{\rm SW} = 1.3987$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
0.133 91	4200	0.133 91	4200	0.133 91	4200	0.133 91	4200
0.134 59	4200	0.134 59	4200	0.134 59	4200	0.134 59	4200
0.135 26	4200	0.135 26	4200	0.135 26	4200	0.134 92	3700
0.135 94	4200	0.135 60	4200	0.135 40	3700	0.135 00	3150
$\beta = 6.3$							
$c_{\rm SW} = 1.3117$		$c_{\rm SW} = 1.3675$		$c_{\rm SW} = 1.4233$		$c_{\rm SW} = 1.4791$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
0.135 01	4600	0.135 01	4600	0.134 46	4600	0.134 46	4600
0.135 55	4600	0.135 55	4600	0.135 01	4600	0.135 01	4600
0.136 09	4600	0.136 09	4600	0.135 55	4600	0.135 30	1100
0.136 64	4600	0.136 64	4600	0.136 09	4600	0.135 55	4600
$\beta = 6.0$							
$c_{\rm SW} = 1.3237$		$c_{\rm SW} = 1.3801$		$c_{\rm SW} = 1.4364$		$c_{\rm SW} = 1.4927$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
0.135 52	4200	0.135 52	4200	0.134 98	4200	0.134 98	4200
0.136 07	4200	0.136 07	4200	0.135 52	4200	0.135 52	4200
0.136 61	4200	0.136 61	4200	0.136 07	4200	0.136 07	4200
0.137 16	4200	0.137 16	4200	0.136 61	4200	0.136 34	4200
$\beta = 5.7$							
$c_{\rm SW} = 1.5431$		$c_{\rm SW} = 1.6088$		$c_{\rm SW} = 1.6745$		$c_{\rm SW} = 1.7401$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
0.135 75	5000	0.135 41	5000	0.135 07	5000	0.134 00	4500
0.136 44	5000	0.136 10	5000	0.135 40	4400	0.134 50	4100
0.137 12	4700	0.136 44	3700	0.135 75	5000	0.134 73	5000
0.137 50	4500	0.136 78	5000	0.135 85	2700	0.135 00	4400
$\beta = 5.4$							
$c_{\rm SW} = 1.6$		$c_{\rm SW} = 1.7$		$c_{\rm SW} = 1.8$		$c_{\rm SW} = 1.9$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
0.137 50	9000	0.136 00	9000	0.134 80	9000	0.133 30	9000
0.138 10	9000	0.136 30	7900	0.135 20	9000	0.133 70	9000
0.138 25	7100	0.136 60	9000	0.135 60	9000	0.134 10	9000
0.138 40	8200	0.137 20	9000	0.135 80	7700	0.134 50	9000
$\beta = 5.2$							
$c_{\rm SW} = 1.70$		$c_{\rm SW} = 1.85$		$c_{\rm SW} = 2.00$		$c_{\rm SW} = 2.15$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
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

$$P_{\rm corr} = \det[W(D)] \tag{33}$$

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 $N_{\rm poly}$ 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 $N_{\rm traj}$ 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 $N_{\rm bin}$ is investigated in a range $N_{\rm bin} = 1$–$N_{\rm traj}/20$. We then adopt $N_{\rm bin}$ giving the maximum error in the jackknife procedure in the following analysis.

We determine $c_{\rm SW}$ 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 $c_{\rm SW}$ in three-flavor QCD

Numerical results of M and ΔM are summarized in Table VIII. In Fig. 3, we plot M and M' at several values of β 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 $c_{\rm SW}$ to the level of $\sim$5% even at our coarsest lattice spacing.

In order to parametrize the K and $c_{\rm SW}$ dependence of M and ΔM, 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 ΔM and their fit curves at several values of β. We observe that our data are well described by the combined fit. Consequently, as shown in Fig. 6, M dependence of ΔM is reproduced reasonably well by the fit. We fix $c_{\rm SW}$ and K_c satisfying the improvement condition

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

$c_{\rm SW} = 1.129\,90$		$c_{\rm SW} = 1.165\,39$		$c_{\rm SW} = 1.200\,89$		$c_{\rm SW} = 1.236\,38$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
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 $\beta = 9.6$.

$c_{\rm SW} = 1.129\,90$		$c_{\rm SW} = 1.165\,39$		$c_{\rm SW} = 1.200\,89$		$c_{\rm SW} = 1.236\,38$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
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 $\beta = 9.6$.

$c_{\rm SW} = 1.129\,90$		$c_{\rm SW} = 1.165\,39$		$c_{\rm SW} = 1.200\,89$		$c_{\rm SW} = 1.236\,38$	
K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$	K	$N_{\rm traj}$
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 $c_{\rm SW}$ 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 $c_{\rm SW}$ and K_c, and hence conclude that the systematic error due to the parametrization method for M and ΔM is small.

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

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

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

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

with $k^{(1)} = 0.00843986$. These fits reproduce our data reasonably well with χ^2/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 β dependence of $c_{\rm SW}$ and K_c in Fig. 7. While $c_{\rm SW}$ 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 $c_{\rm SW}$ in Eq. (34) is essential to remove the $O(a)$ effects in practical lattice calculations.

TABLE VIII. Quark mass M and its difference ΔM in three-flavor QCD.

$\beta = 12.0$

	$c_{\rm SW} = 1.086\,24$			$c_{\rm SW} = 1.120\,36$	
K	aM	$a\Delta M$	K	aM	$a\Delta M$
0.128 958	0.035 02(11)	0.001 07(13)	0.128 958	0.030 66(8)	0.000 67(10)
0.129 607	0.014 98(13)	0.000 99(12)	0.129 607	0.010 28(10)	0.000 72(16)
0.130 257	−0.005 44(10)	0.001 00(14)	0.130 257	−0.010 11(12)	0.000 40(12)
0.130 906	−0.025 91(11)	0.001 16(12)	0.130 906	−0.030 88(11)	0.000 52(12)
	$c_{\rm SW} = 1.154\,48$			$c_{\rm SW} = 1.188\,60$	
K	aM	$a\Delta M$	K	aM	$a\Delta M$
0.128 958	0.025 81(9)	0.000 27(12)	0.128 958	0.021 25(9)	−0.000 29(11)
0.129 607	0.005 61(11)	0.000 15(11)	0.129 607	0.000 76(10)	−0.000 27(11)
0.130 257	−0.015 12(14)	0.000 08(13)	0.130 257	−0.019 65(11)	−0.000 44(13)
0.130 906	−0.035 55(17)	0.000 25(13)	0.130 906	−0.040 41(12)	−0.000 43(14)

$\beta = 9.6$

	$c_{\rm SW} = 1.129\,90$			$c_{\rm SW} = 1.165\,39$	
K	aM	$a\Delta M$	K	aM	$a\Delta M$
0.130 43	0.038 18(12)	0.001 18(10)	0.130 43	0.032 26(9)	0.000 67(10)
0.131 09	0.018 05(9)	0.001 00(12)	0.131 09	0.011 87(10)	0.000 62(12)
0.131 75	−0.002 75(10)	0.001 04(14)	0.131 75	−0.008 71(12)	0.000 56(13)
0.132 40	−0.023 12(11)	0.001 04(13)	0.132 40	−0.029 48(11)	0.000 63(16)
	$c_{\rm SW} = 1.200\,89$			$c_{\rm SW} = 1.236\,38$	
K	aM	$a\Delta M$	K	aM	$a\Delta M$
0.130 43	0.025 96(11)	0.000 37(11)	0.130 43	0.019 95(9)	−0.000 37(14)
0.131 09	0.005 59(12)	0.000 14(13)	0.131 09	−0.000 91(10)	−0.000 12(9)
0.131 75	−0.015 22(11)	0.000 05(12)	0.131 75	−0.021 45(11)	−0.000 44(13)
0.132 30	−0.032 56(19)	0.000 33(24)	0.132 30	−0.039 34(13)	−0.000 54(14)

$\beta = 7.4$

	$c_{\rm SW} = 1.2258$			$c_{\rm SW} = 1.2643$	
K	aM	$a\Delta M$	K	aM	$a\Delta M$
0.132 93	0.041 47(22)	0.001 35(19)	0.132 93	0.032 65(15)	0.000 67(19)
0.133 60	0.021 34(21)	0.001 58(25)	0.133 60	0.012 09(23)	0.000 65(25)
0.134 27	0.000 79(21)	0.000 99(26)	0.134 27	−0.009 42(21)	0.001 02(23)
0.134 94	−0.020 65(24)	0.000 77(28)	0.134 70	−0.022 92(28)	0.000 89(34)
	$c_{\rm SW} = 1.3028$			$c_{\rm SW} = 1.3413$	
K	aM	$a\Delta M$	K	aM	$a\Delta M$
0.132 93	0.022 96(25)	0.000 35(24)	0.132 93	0.013 09(22)	0.000 04(23)
0.133 60	0.002 14(17)	0.000 18(19)	0.133 60	−0.007 56(21)	0.000 29(28)
0.134 27	−0.018 88(23)	0.000 52(22)	0.133 93	−0.017 74(64)	−0.000 18(68)
···	···	···	0.134 27	−0.028 67(26)	−0.000 48(36)

$\beta = 6.8$

	$c_{\rm SW} = 1.2783$			$c_{\rm SW} = 1.3184$	
K	aM	$a\Delta M$	K	aM	$a\Delta M$
0.133 91	0.044 62(36)	0.000 66(28)	0.133 91	0.033 42(33)	0.000 92(28)
0.134 59	0.024 57(29)	0.000 79(32)	0.134 59	0.013 58(28)	0.000 51(27)
0.135 26	0.003 38(33)	0.000 98(30)	0.135 26	−0.008 23(30)	0.000 65(40)
0.135 94	−0.018 24(30)	0.001 63(37)	0.135 60	−0.018 39(36)	0.000 54(39)
	$c_{\rm SW} = 1.3586$			$c_{\rm SW} = 1.3987$	
K	aM	$a\Delta M$	K	aM	$a\Delta M$
0.133 91	0.022 40(31)	0.000 49(26)	0.133 91	0.012 08(22)	−0.000 21(35)
0.134 59	0.001 75(31)	0.000 31(23)	0.134 59	−0.009 53(30)	−0.000 30(27)
0.135 26	−0.019 24(27)	0.000 33(34)	0.134 92	−0.019 56(58)	0.000 25(45)
0.135 40	−0.024 74(30)	0.000 58(46)	0.135 00	−0.022 71(43)	−0.000 14(34)

TABLE VIII. (*continued*)

$\beta = 6.3$

	$c_{SW} = 1.3117$			$c_{SW} = 1.3675$	
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)
	$c_{SW} = 1.4233$			$c_{SW} = 1.4791$	
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)

$\beta = 6.0$

	$c_{SW} = 1.3237$			$c_{SW} = 1.3801$	
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)
	$c_{SW} = 1.4364$			$c_{SW} = 1.4927$	
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)

$\beta = 5.7$

	$c_{SW} = 1.5431$			$c_{SW} = 1.6088$	
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)
	$c_{SW} = 1.6745$			$c_{SW} = 1.7401$	
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)

$\beta = 5.4$

	$c_{SW} = 1.6$			$c_{SW} = 1.7$	
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)
	$c_{SW} = 1.8$			$c_{SW} = 1.9$	
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*)

$\beta = 5.2$

	$c_{\rm SW} = 1.70$			$c_{\rm SW} = 1.85$	
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)
	$c_{\rm SW} = 2.00$			$c_{\rm SW} = 2.15$	
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 $c_{\rm SW}$ monotonously decreases as N_f increases at fixed β. 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 carefully, we determine $c_{\rm SW}$ 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 ΔM 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 $c_{\rm SW}$ and K_c summarized in Table XVII.

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

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

β	χ^2/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.

β	χ^2/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)

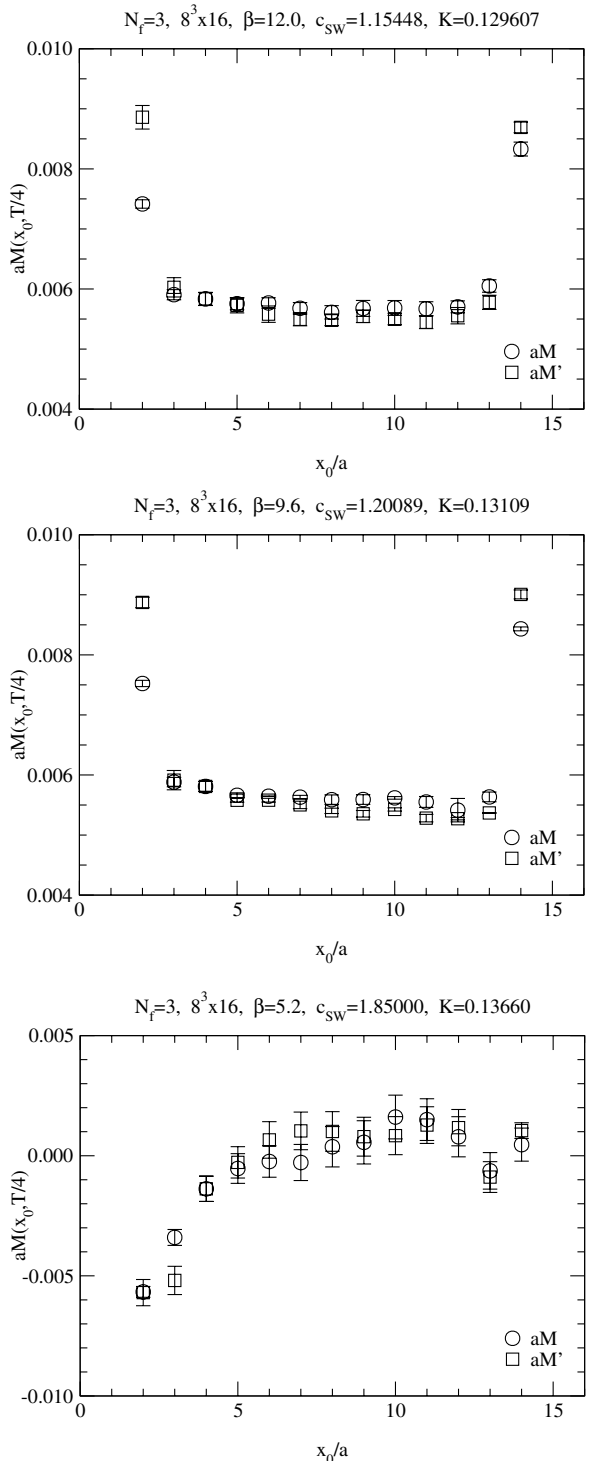

FIG. 3. Quark masses M and M' in three-flavor QCD as a function of x_0. Top, middle, and bottom figures show data at $\beta = 12.0$, 9.6, and 5.2, respectively.

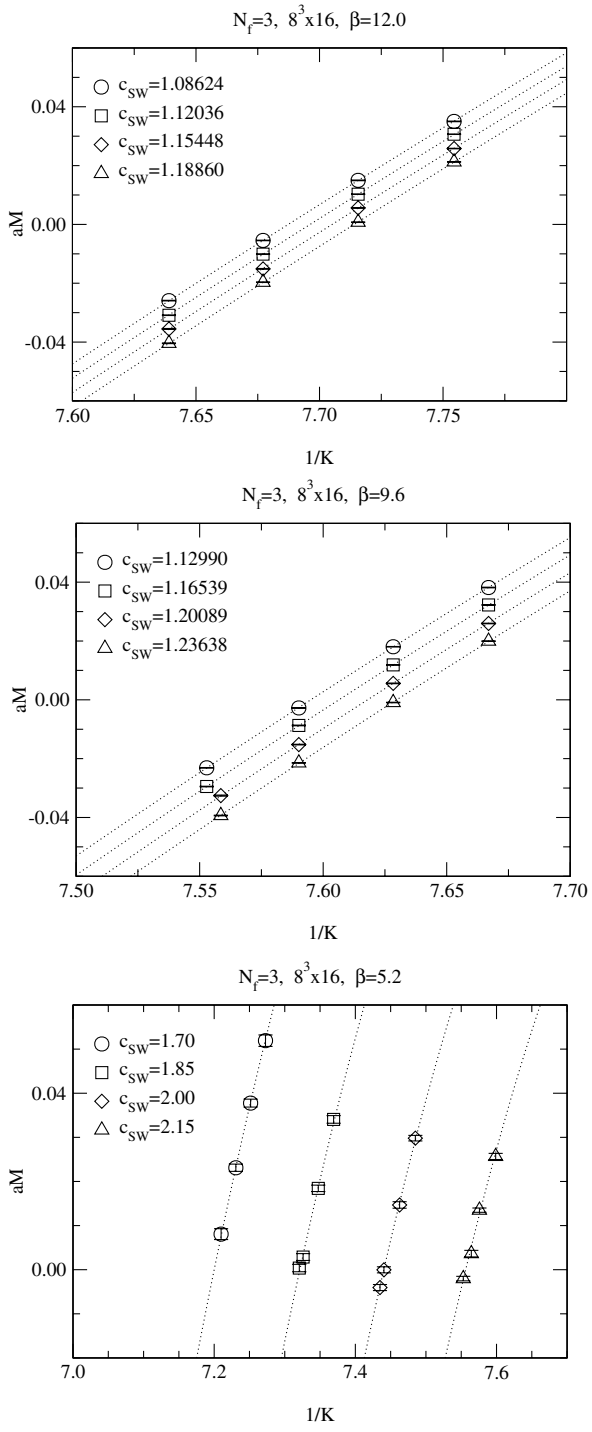

FIG. 4. Quark mass M as a function of $1/K$. Top, middle, and bottom figures show data at $\beta = 12.0$, 9.6, and 5.2, respectively. Dotted lines are fit curves of Eq. (27).

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

$$c_{\rm SW} = c_0 + c_1 g_0^4 N_f, \tag{36}$$

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

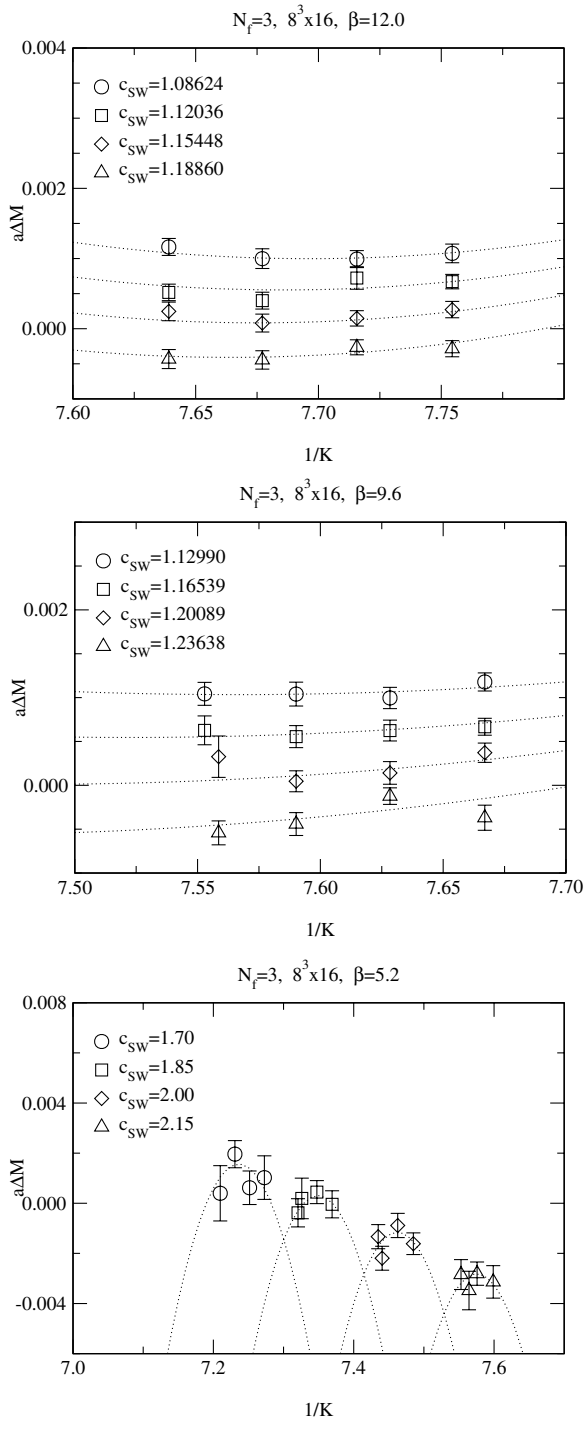

FIG. 5. Mass difference ΔM as a function of $1/K$. Top, middle, and bottom figures show data at $\beta = 12.0$, 9.6, and 5.2, respectively. Dotted lines are fit curves of Eq. (28).

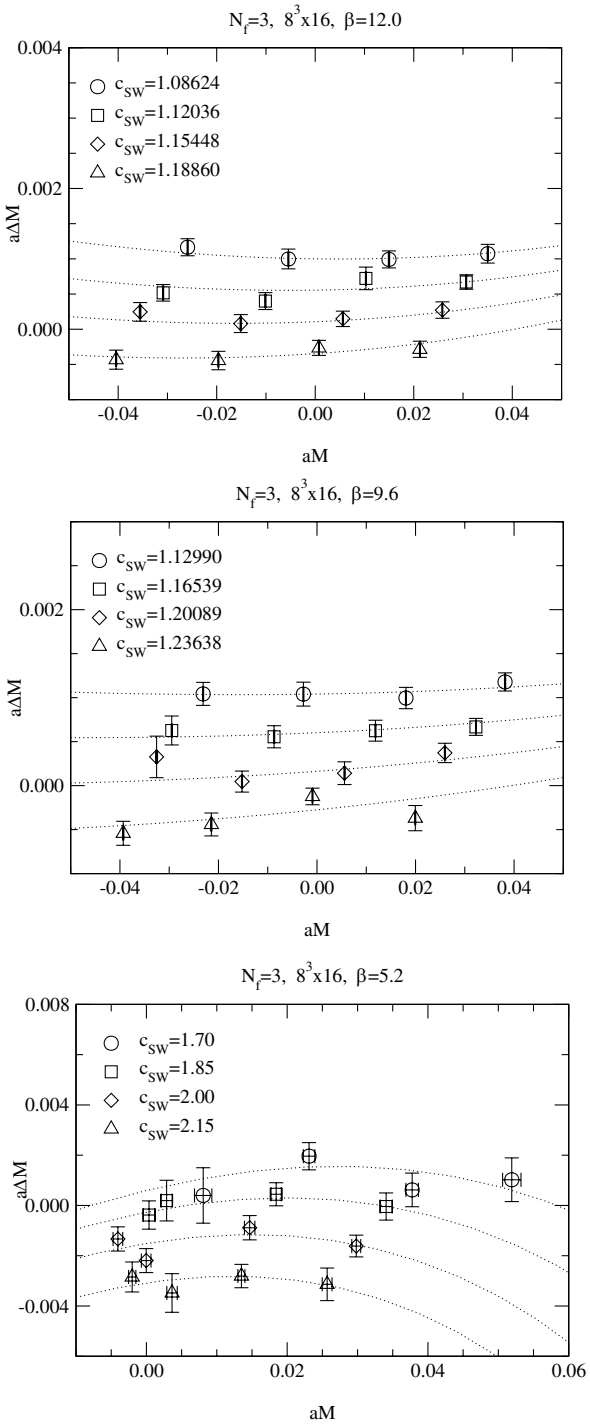

FIG. 6. Mass difference ΔM as a function of M in three-flavor QCD. Top, middle, and bottom figures show data at $\beta = 12.0$, 9.6, and 5.2, respectively. Dotted lines are fit curves reproduced from Eqs. (27) and (28).

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

Our nonperturbative estimate of $c_{\rm SW}$ 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 $c_{\rm SW}$ with the spatial size in lattice units L/a fixed to a constant value 8, the $O(a/L)$ dependence of $c_{\rm SW}$ induces $O(a)$ effects in observables. These effects can be removed by extrapolating $c_{\rm SW}$ 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 $c_{\rm SW}$ and K_c in three-flavor QCD obtained from tree-level improvement condition Eq. (25).

β	$c_{\rm SW}$	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 ΔM in four-flavor QCD at $\beta = 9.6$.

	$c_{\rm SW} = 1.129\,90$			$c_{\rm SW} = 1.165\,39$	
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)
	$c_{\rm SW} = 1.200\,89$			$c_{\rm SW} = 1.236\,38$	
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 $c_{\rm SW}$ 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 $c_{\rm SW}$ [5]. We extend this procedure to the one-loop level, namely, the one-loop correction to ΔM for the finite lattice volume $8^3 \times 16$ given by [24]

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

is incorporated into the improvement condition

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

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

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

	$c_{\rm SW} = 1.129\,90$			$c_{\rm SW} = 1.165\,39$	
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)
	$c_{\rm SW} = 1.200\,89$			$c_{\rm SW} = 1.236\,38$	
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)

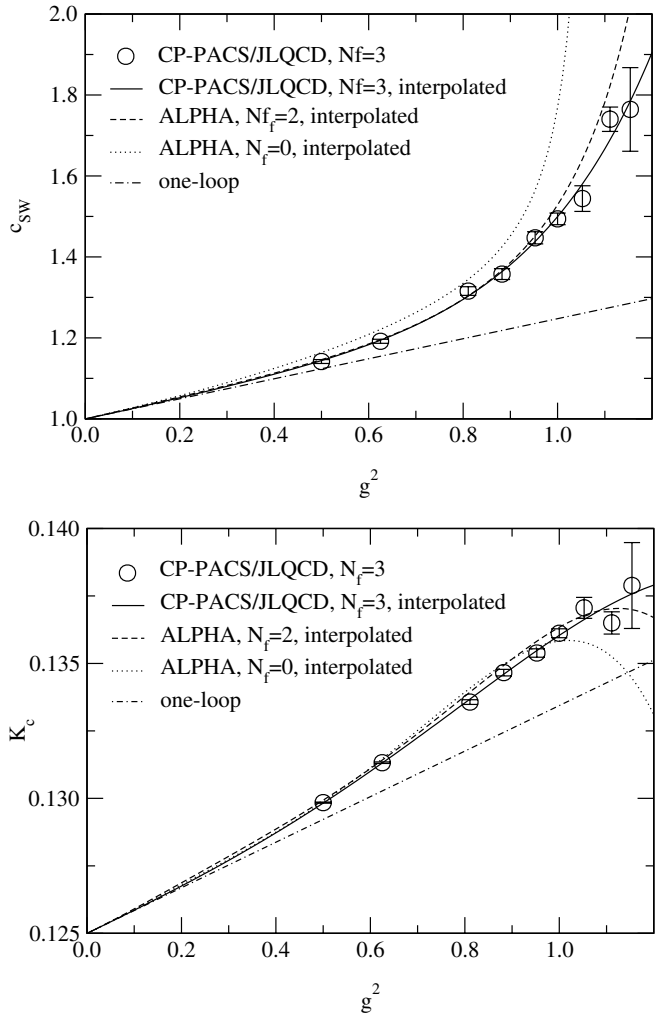

FIG. 7. Nonperturbatively determined c_{SW} (top figure) and K_c (bottom figure) as a function of g_0^2. For K_c in quenched QCD, author's interpolation of ALPHA's results is plotted.

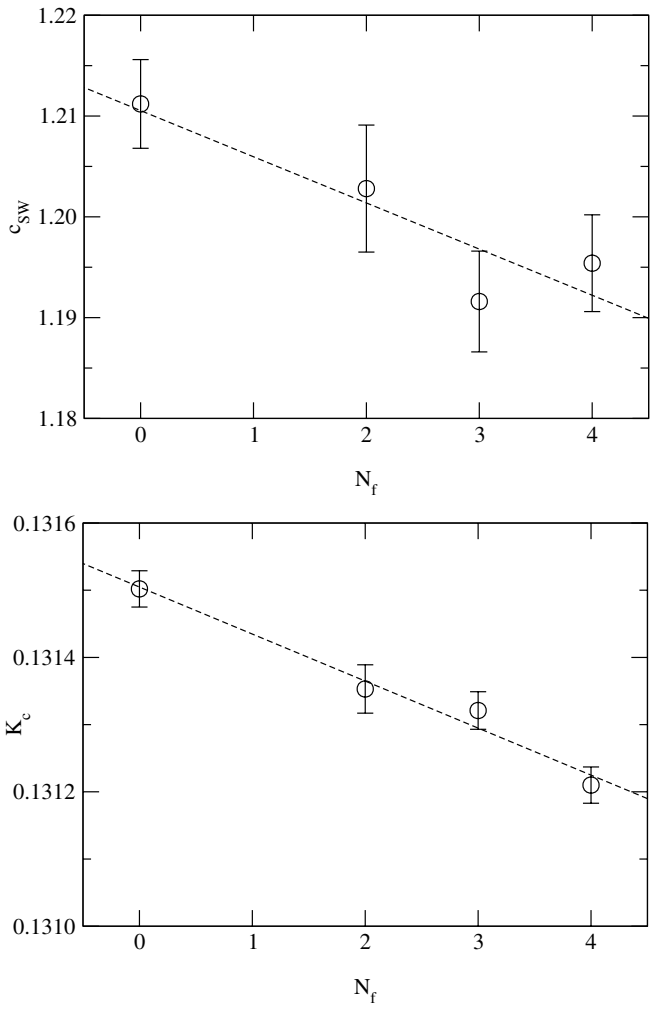

FIG. 8. Plots of c_{SW} (top figure), K_c (bottom figure) at $\beta = 9.6$ as a function of N_f. The dashed line shows a linear fit to data.

From the parametrization of Eqs. (27) and (28) and the modified improvement condition Eq. (38), we obtain c_{SW} and K_c summarized in Table XVIII. A comparison with Table XI shows that the modified and original improvement conditions give consistent results with each other for c_{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 ΔM in quenched QCD at $\beta = 9.6$.

	$c_{\mathrm{SW}} = 1.129\,90$			$c_{\mathrm{SW}} = 1.165\,39$	
K	aM	$a\Delta M$	K	aM	$a\Delta M$
0.130 43	0.046 46(7)	0.001 41(10)	0.130 43	0.040 59(8)	0.000 95(11)
0.131 09	0.026 79(8)	0.001 31(11)	0.131 09	0.020 64(8)	0.000 80(11)
0.131 75	0.006 56(7)	0.001 31(14)	0.131 75	0.000 41(7)	0.000 84(10)
0.132 40	−0.013 24(8)	0.001 32(10)	0.132 40	−0.019 78(8)	0.000 74(11)
	$c_{\mathrm{SW}} = 1.200\,89$			$c_{\mathrm{SW}} = 1.236\,38$	
K	aM	$a\Delta M$	K	aM	$a\Delta M$
0.130 43	0.034 58(9)	0.000 36(11)	0.130 43	0.028 40(8)	−0.000 15(10)
0.131 09	0.014 51(7)	0.000 34(12)	0.131 09	0.008 18(7)	0.000 06(10)
0.131 75	−0.005 80(8)	0.000 50(14)	0.131 75	−0.012 31(8)	−0.000 05(13)
0.132 40	−0.026 07(10)	0.000 53(16)	0.132 40	−0.032 47(10)	−0.000 13(21)

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

N_f	β	χ^2/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	β	χ^2/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 $c_{\rm SW}$ and K_c for $N_f = 4$, 2, and 0 obtained from tree-level improvement condition Eq. (25).

N_f	β	$c_{\rm SW}$	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 $c_{\rm SW}$ and K_c in three-flavor QCD obtained from one-loop level improvement condition Eq. (38).

β	$c_{\rm SW}$	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 $c_{\rm SW}$ 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 $c_{\rm SW}$ 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 $c_{\rm SW}$ 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 $c_{\rm SW}$ and K enable us to determine nonperturbative $c_{\rm SW}$ 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 $c_{\rm SW}$ is not large, this point should be confirmed by a direct determination of $c_{\rm SW}$ with varying L. A test of scaling properties of physical observables with our estimate of $c_{\rm SW}$ is an important next step toward an extensive simulation of three-flavor QCD with the plaquette gauge action.

We note that the range of β explored in this study is significantly higher than $\beta = 5.0$, where an artificial phase transition exists. Numerical studies at β 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].

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