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Nonperturbative $O(a)$ improvement of the Wilson quark action with the renormalization-group-improved gauge action using the Schrödinger functional method

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We perform a nonperturbative determination of the $O(a)$-improvement coefficient c_{SW} and the critical hopping parameter κ_c for $N_f = 3$, 2, and 0 flavor QCD with the (RG) renormalization-group-improved gauge action using the Schrödinger functional method. In order to interpolate c_{SW} and κ_c as a function of the bare coupling, a wide range of β from the weak coupling region to the moderately strong coupling points used in large-scale simulations is studied. Corrections at finite lattice size of $O(a/L)$ turned out to be large for the RG-improved gauge action, and hence we make the determination at a size fixed in physical units using a modified improvement condition. This enables us to avoid $O(a)$ scaling violations which would remain in physical observables if c_{SW} determined for a fixed lattice size L/a is used in numerical simulations.

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I. INTRODUCTION

Fully unquenched simulations of QCD with dynamical up, down, and strange quarks have become feasible [1] thanks to the recent development of algorithms [2] and computational facilities. However, it is still very demanding to control discretization errors below a few percent level in dynamical QCD simulations. Thus highly improved lattice actions are desirable to accelerate the approach to the continuum limit.

The on-shell improvement of the Wilson quark action through $O(a)$ requires only a single additional term, i.e. the Sheikholeslami-Wohlert (SW) term [3]. In Ref. [4], we determined c_{SW} in three-flavor QCD for the plaquette gauge action, using the Schrödinger functional (SF) method [5–8]. Applications of the resulting $O(a)$ improved Wilson-clover quark action in combination with the plaquette gauge action suffer from a serious problem, however, since it was found in Ref. [9] that this action combination exhibits an unphysical first-order phase transition at zero temperature in the strong coupling regime ($\beta \leq 5.0$).

We also found in Ref. [9] that such a phase transition weakens, and possibly disappears, when the gauge action is improved. In this work, motivated by this observation, we extend the determination of c_{SW} for the case of the (RG) renormalization-group-improved action [10] for gluons for $N_f = 3$, 2, and 0 flavor QCD.

We explore a wide range of β to work out the interpolation formula as a function of the bare coupling. The critical hopping parameter κ_c in the $O(a)$-improved theory is also obtained.

In the Schrödinger functional method, c_{SW} is determined such that the axial Ward-Takahashi identity is satisfied for a given finite volume. Since the linear extent L of a finite lattice provides an energy scale $1/L$, a determination of c_{SW} generally involves corrections of order a/L. We find that this correction is sizable for the RG-improved gauge action. If the determination of c_{SW} is made for a fixed value of L/a, observables calculated in subsequent simulations using such c_{SW} would suffer from $O(a)$ scaling violations. To avoid this problem, we modify the standard improvement condition and determine c_{SW} at a *fixed physical size* L. Similar considerations have been made in the determinations of some other $O(a)$ improvement coefficients in Refs. [11,12].

This paper is organized as follows. In Sec. II, we briefly recall the Schrödinger functional method, mainly to fix notations. In Sec. III, corrections at the finite lattice size of $O(a/L)$ that affect c_{SW} are discussed, and our modified method and one-loop calculations relevant for the subsequent analyses are given. Section IV is devoted to describing our numerical results, and Sec. V to systematic uncertainties in them. Our conclusions are given in Sec. VI. A preliminary report of this work was made in Ref. [13].

II. SCHRÖDINGER FUNCTIONAL METHOD FOR THE DETERMINATION OF $c_{\rm SW}$

We briefly introduce the setup of the SF method and the improvement condition developed in Refs. [5–8].

A. SF setup

Consider the SF defined on a four dimensional hypercubic lattice with a volume $L^3 \times T$ and the cylindrical geometry, i.e., the periodic boundary condition is imposed in the spatial directions and the Dirichlet one in the temporal direction for both gauge and quark fields. At the temporal boundaries $x_0 = 0$ and T, the following conditions are imposed on the link variables and the quark fields: the spatial link variables on the boundaries are fixed to the diagonal, constant $SU(3)$ matrices given by

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

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

while all quark fields on the boundaries are set to zero.

We use the RG-improved gauge action [10] given by

$$S_g = \frac{2}{g^2}\Big[\sum_x w^P_{\mu\nu}(x_0)\mathrm{Re\,Tr}(1 - P_{\mu,\nu}(x)) + \sum_x w^R_{\mu\nu}(x_0)\mathrm{Re\,Tr}(1 - R^{(1\times 2)}_{\mu,\nu}(x))\Big], \tag{3}$$

where $P_{\mu,\nu}(x)$ denotes a 1×1 Wilson loop on the μ-ν plane starting and ending at x, and $R^{(1\times 2)}_{\mu,\nu}(x)$ a 1×2 rectangular loop with the side of length 2 in the ν direction. These terms are added up with proper weights, $w^P_{\mu\nu}(x_0)$ and $w^R_{\mu\nu}(x_0)$, respectively. In ordinary simulations with the periodic boundary condition in the temporal direction, the weights are given by $w^P_{\mu\nu} = 3.648$ and $w^R_{\mu\nu} = -0.331$ independently of x_0. In the SF, these weights are modified. Among several possible choices, we select choice B defined in Ref. [14] in this work,

$$w^P_{\mu\nu}(x_0) = \begin{cases} \frac{1}{2} \times (3.648) & \text{at } t = 0 \text{ or } T \text{ and } \mu, \nu \neq 4, \\ 3.648 & \text{otherwise,} \end{cases} \tag{4}$$

$$w^R_{\mu\nu}(x_0) = \begin{cases} 0 & \text{at } t = 0 \text{ or } T \text{ and } \mu, \nu \neq 4, \\ \frac{3}{2} \times (-0.331) & \text{at } t = 0 \text{ or } T \text{ and } \mu = 4, \\ -0.331 & \text{otherwise.} \end{cases} \tag{5}$$

The $O(a)$-improved Wilson quark action [3] is given by

$$S_q = \sum_{x,y} \bar{q}_x D_{xy} q_y, \tag{6}$$

$$D_{xy} = \delta_{xy} - \kappa \sum_\mu \{(1 - \gamma_\mu)U_{x,\mu}\delta_{x+\hat{\mu},y} + (1 + \gamma_\mu)U^\dagger_{x-\hat{\mu},\mu}\delta_{x-\hat{\mu},y}\} + \frac{i}{2}\kappa c_{\rm SW}\sigma_{\mu\nu}F_{x,\mu\nu}\delta_{xy}, \tag{7}$$

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

$$F_{x,\mu\nu} = \tfrac{1}{8}\{(P_{\mu,\nu}(x) + P_{\nu,-\mu}(x) + P_{-\mu,-\nu}(x) + P_{-\nu,\mu}(x)) - (\mathrm{H.c.})\}, \tag{8}$$

and $\sigma_{\mu\nu} = (i/2)[\gamma_\mu, \gamma_\nu]$. The last term in Eq. (7) is the only counterterm to get rid of $O(a)$ errors present for on-shell quantities on the lattice. At tree level, $c_{\rm SW} = 1$. For the $O(a)$ improvement of the SF, we need to add extra terms made of the gauge and quark fields at boundaries to the lattice action. However, since these counterterms affect the PCAC relation used in the following calculations only at $O(a^2)$ or higher, they are not necessary for the determination of $c_{\rm SW}$.

B. PCAC relation

We determine $c_{\rm SW}$ by imposing the PCAC relation

$$\tfrac{1}{2}(\partial_\mu + \partial^*_\mu)A^a_{\mathrm{imp},\mu} = 2m_q P^a, \tag{9}$$

up to $O(a^2)$ corrections. The pseudoscalar density operator, axial vector current, and its $O(a)$-improved version are given by

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

$$A^a_\mu = \bar{\psi}\gamma_\mu\gamma_5\tau^a\psi, \tag{11}$$

$$A^a_{\mathrm{imp},\mu} = A^a_\mu + c_A\tfrac{1}{2}(\partial_\mu + \partial^*_\mu)P^a, \tag{12}$$

where ∂_μ and ∂^*_μ are the forward and backward lattice derivatives, and τ^a denotes the generator of $SU(N_f)$ flavor symmetry acting on the flavor indices of the quark fields $\bar{\psi}$ and ψ.

We measure two correlation functions,

$$f_A(x_0) = -\frac{1}{N_f^2 - 1}\langle A^a_0(x)\mathcal{O}^a\rangle, \tag{13}$$

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

where $x = (x_0, \mathbf{x})$, and $\langle\cdots\rangle$ represents the expectation value after taking trace over color and spinor indices and summing over spatial coordinate $\mathbf{x}$. The source operator is given by

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

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

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 PCAC quark mass is then calculated using f_A and f_P through the PCAC relation Eq. (9) as

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

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

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

Using the source operator on the other boundary

$$\mathcal{O}'^{,a} = a^6 \sum_{\mathbf{y},\mathbf{z}} \bar{\zeta}'(\mathbf{y}) \gamma_5 \tau^a \zeta'(\mathbf{z}), \tag{20}$$

where ζ' is the boundary field at $x_0 = T$, we can calculate another set of quantities $m'(x_0)$, $r'(x_0)$, and $s'(x_0)$ from the correlation functions defined by

$$f_A'(T - x_0) = +\frac{1}{N_f^2 - 1} \langle A_0^a(x) \mathcal{O}'^{,a} \rangle, \tag{21}$$

$$f_P'(T - x_0) = -\frac{1}{N_f^2 - 1} \langle P^a(x) \mathcal{O}'^{,a} \rangle. \tag{22}$$

A naive improvement condition would be $m(x_0) = m'(x_0)$. However, this condition requires a nonperturbative tuning of c_A as well as of $c_{\rm SW}$. To eliminate c_A from the determination, it was proposed in Ref. [7] to use an alternative definition of the quark mass given by

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

$$M'(x_0, y_0) = m'(x_0) - \frac{m'(y_0) - m(y_0)}{s'(y_0) - s(y_0)} s'(x_0), \tag{24}$$

with which $c_{\rm SW}$ is obtained at the point where the mass difference

$$\Delta M(x_0, y_0) = M(x_0, y_0) - M'(x_0, y_0) \tag{25}$$

vanishes. In principle, we can take an arbitrary choice for (x_0, y_0), since different choices result only in $O(a^2)$ differences in physical observables. We follow the ALPHA Collaboration and use $(x_0, y_0) = (3T/4, T/4)$ for ΔM, and $(T/2, T/4)$ for M. In the following, M and ΔM without arguments denote $M(T/2, T/4)$ and $\Delta M(3T/4, T/4)$, respectively.

In previous studies, $c_{\rm SW}$ has been determined through the conditions

$$\begin{cases} M(g_0^2, L/a) & = 0, \\ \Delta M(g_0^2, L/a) & = \Delta M(0, L/a), \end{cases} \tag{26}$$

at a given g_0^2 and L/a. $\Delta M(0, L/a)$ on the right-hand side, which is the tree-level value of $\Delta M(g_0^2, L/a)$ at the massless point, is necessary in order that the resulting $c_{\rm SW}$ reproduces its tree-level value ($c_{\rm SW} = 1$) in the weak coupling limit. In the next section, we address the issue of corrections at finite lattice size and propose a new condition to avoid the problem.

III. CORRECTIONS AT FINITE LATTICE SIZE AND MODIFIED IMPROVEMENT CONDITIONS

A. Corrections at finite lattice size

In the standard approach, we first calculate $M(g_0^2, L/a)$ and $\Delta M(g_0^2, L/a)$ for a set of values of $c_{\rm SW}$ and κ. The results are fitted as a function of $c_{\rm SW}$ and κ to find $c_{\rm SW}(g_0^2, L/a)$ and $\kappa_c(g_0^2, L/a)$ satisfying Eq. (26) at a given value of g_0^2 and L/a. The asymptotic a dependence of $c_{\rm SW}(g_0^2, L/a)$ and $\kappa_c(g_0^2, L/a)$ obtained in such a way is expected to be

$$\begin{aligned} c_{\rm SW}(g_0^2, L/a) = {} & c_{\rm SW}(g_0^2, \infty) + c_L \cdot (a/L) + c_\Lambda \cdot (a\Lambda_{\rm QCD}) \\ & + O((a/L)^2, (a^2\Lambda_{\rm QCD}/L), (a\Lambda_{\rm QCD})^2), \end{aligned} \tag{27}$$

$$\begin{aligned} \kappa_c(g_0^2, L/a) = {} & \kappa_c(g_0^2, \infty) + k_L \cdot (a/L) + k_\Lambda \cdot (a\Lambda_{\rm QCD}) \\ & + O((a/L)^2, (a^2\Lambda_{\rm QCD}/L), (a\Lambda_{\rm QCD})^2), \end{aligned} \tag{28}$$

where c_L, c_Λ, k_L, and k_Λ are unknown coefficients. (In practice, a logarithmic dependence on a/L also appears, but it does not alter the following discussion, and hence is not written explicitly.)

Consider an on-shell physical quantity Q, and let $Q^{\rm latt}(a)$ be the value obtained on a lattice with lattice spacing a using the SW quark action with a choice of the improvement coefficient $c_{\rm SW}^{\rm sim}$. We expect the discrepancy between Q and $Q^{\rm latt}(a)$ in the measured value to be

$$\begin{aligned} Q - Q^{\rm latt}(a) = {} & q \cdot (c_{\rm SW}^{\rm sim} - c_{\rm SW}(g_0^2, \infty)) \cdot (a\Lambda_{\rm QCD}) \\ & + O(a^2\Lambda_{\rm QCD}^2), \end{aligned} \tag{29}$$

where q is an unknown constant assumed to be $O(1)$. Hence, if one uses $c_{\rm SW}^{\rm sim} = c_{\rm SW}(g_0^2, \infty)$ in the simulation, the $O(a)$ error is absent, while if one uses $c_{\rm SW}(g_0^2, L/a)$ in Eq. (27), the above expression results in

$$\begin{aligned} Q - Q^{\rm latt}(a) = {} & q \cdot c_L \cdot (a/L) \cdot (a\Lambda_{\rm QCD}) + O(a^2\Lambda_{\rm QCD}^2) \\ & + O(a\Lambda_{\rm QCD}(a/L)^2). \end{aligned} \tag{30}$$

While the scaling violation appears to start from $O(a^2)$, *it is actually linear in the lattice spacing if one determines* $c_{\rm SW}(g_0^2, L/a)$ *with a fixed value of* a/L. Indeed, previous

studies determining $c_{\rm SW}$ have used certain fixed values of L/a, e.g. 8, independently of β.

In Ref. [4], we studied the magnitude of the corrections at finite lattice size in $c_{\rm SW}$ for the plaquette gauge action. The coefficient c_L defined in Eq. (27) was evaluated in one-loop perturbation theory in the same SF setup, and it was found that the effect on $c_{\rm SW}$ does not exceed 3% when $L/a = 8$ for $\beta \geq 5.2$. We have repeated the same perturbative analysis with the RG-improved action, and observed a sizable effect of about 15% at $\beta = 1.9$, around which large-scale simulations are carried out. This enhancement of the one-loop correction for the RG-improved action is mainly due to the larger value of the bare coupling compared to that for the plaquette gauge action for realizing the same value of the lattice spacing.

B. Modified improvement condition

We propose to resolve the problem due to the sizable corrections explained above by introducing a fixed physical length L^*, and determining $c_{\rm SW}$ at the fixed physical volume $L^{*3} \times T^*$ ($T^* = 2L^*$). If one uses $c_{\rm SW}$ thus determined, L in (30) is replaced by L^* and scaling violations are $O(a^2)$.

The actual procedure we use runs as follows. Instead of Eq. (26), we impose a modified improvement condition given by

$$\begin{cases} M(g_0^2, L/a) & = 0, \\ \Delta M(g_0^2, L/a) & = 0, \end{cases} \tag{31}$$

to calculate $c_{\rm SW}(g_0^2, L/a)$ and $\kappa_c(g_0^2, L/a)$. The results are converted to $c_{\rm SW}(g_0^2, L^*/a)$ and $\kappa_c(g_0^2, L^*/a)$. To do so, we must know the value of L^*/a or $1/a$ at that value of g_0^2, which we obtain through the two-loop β function,

$$a\Lambda_L = \exp\left(-\frac{1}{2b_0 g_0^2}\right)(b_0 g_0^2)^{-b_1/2b_0^2}, \tag{32}$$

$$b_0 = \frac{1}{(4\pi)^2}\left(\frac{11}{3}N_c - \frac{2}{3}N_f\right), \tag{33}$$

$$b_1 = \frac{1}{(4\pi)^4}\left(\frac{34}{3}N_c^2 - N_f\left(\frac{13}{3}N_c - \frac{1}{N_c}\right)\right). \tag{34}$$

The transformation from $c_{\rm SW}(g_0^2, L/a)$ and $\kappa_c(g_0^2, L/a)$ to those at L^*/a are made through

$$c_{\rm SW}(g_0^2, L^*/a) = c_{\rm SW}(g_0^2, L/a) + \delta c_{\rm SW}(g_0^2, L/a; L^*/a), \tag{35}$$

$$\kappa_c(g_0^2, L^*/a) = \kappa_c(g_0^2, L/a) + \delta\kappa_c(g_0^2, L/a; L^*/a), \tag{36}$$

where

$$\delta c_{\rm SW}(g_0^2, L/a; L^*/a) = -c_{\rm SW}^{\rm PT}(g_0^2, L/a) + c_{\rm SW}^{\rm PT}(g_0^2, L^*/a), \tag{37}$$

$$\delta\kappa_c(g_0^2, L/a; L^*/a) = -\kappa_c^{\rm PT}(g_0^2, L/a) + \kappa_c^{\rm PT}(g_0^2, L^*/a), \tag{38}$$

and $c_{\rm SW}^{\rm PT}(g_0^2, L/a)$ and $\kappa_c^{\rm PT}(g_0^2, L/a)$ are calculated at the one-loop level for the same SF setup at the given value of L/a.

It turned out that the tree and the one-loop coefficients for $c_{\rm SW}$ and κ_c have a significant a/L dependence. To describe this dependence precisely we fit them to a Padé or a polynomial-like function of a/L as

$$c_{\rm SW}^{(0)}(L/a) = \frac{1 + a_1(a/L) + a_2(a/L)^2 + a_3(a/L)^3}{1 + b_1(a/L)}, \tag{39}$$

$$c_{\rm SW}^{(1)}(L/a) = 0.113 + (c_1 - d_1\ln(L/a))(a/L) + (c_2 - d_2\ln(L/a))(a/L)^2, \tag{40}$$

TABLE I. Finite-size coefficients in Eqs. (39)–(42).

$c_{\rm SW}^{(0)}$		$c_{\rm SW}^{(1)}$			
			$N_f = 0$	$N_f = 2$	$N_f = 3$
a_1	-3.4415	c_1	-4.5736	-6.2641	-7.1094
a_2	-5.0248	c_2	-3.3402	-8.0488	-10.403
a_3	11.1475	d_1	-1.1681	-1.5466	-1.7359
b_1	-3.9702	d_2	-8.9448	-14.306	-16.987
$\kappa_c^{(0)}$				$\kappa_c^{(1)}$	
			$N_f = 0$	$N_f = 2$	$N_f = 3$
k_1	$0.260\,982 \times 10^{-6}$	l_1	$0.101\,302 \times 10^{-2}$	$-0.224\,650 \times 10^{-2}$	$-0.387\,626 \times 10^{-2}$
k_2	$-0.845\,333 \times 10^{-5}$	l_2	$0.162\,496 \times 10^{-1}$	$0.862\,878 \times 10^{-2}$	$0.481\,835 \times 10^{-2}$
k_3	$-0.103\,610 \times 10^{-1}$	m_1	$0.547\,826 \times 10^{-3}$	$-0.507\,665 \times 10^{-3}$	$-0.155\,835 \times 10^{-3}$
k_4	$0.751\,742 \times 10^{-2}$	m_2	$0.882\,220 \times 10^{-2}$	$-0.136\,413 \times 10^{-2}$	$-0.645\,729 \times 10^{-2}$

TABLE II. Inverse coupling β and lattice size L/a chosen for the three-flavor QCD simulation. L^*/a is estimated by the two-loop β function assuming $L^*/a = 6$ at $\beta = 1.9$. Finite-size corrections $\delta c_{\rm SW}$ and $\delta\kappa_c$ calculated with Eqs. (37) and (38) are also shown.

β	L/a	L^*/a	$\delta c_{\rm SW}(g_0^2, L/a; L^*/a)$	$\delta\kappa_c(g_0^2, L/a; L^*/a)$
12.00	8	7.51×10^6	5.51×10^{-3}	6.35×10^{-5}
8.85	8	8.46×10^4	1.42×10^{-2}	7.95×10^{-5}
5.00	8	3.81×10^2	5.14×10^{-2}	1.23×10^{-4}
3.00	8	2.50×10^1	1.14×10^{-1}	6.80×10^{-5}
2.60	8	1.48×10^1	1.08×10^{-1}	1.34×10^{-5}
2.40	8	1.14×10^1	8.70×10^{-2}	-8.82×10^{-6}
2.20	8	8.78	3.42×10^{-2}	-9.84×10^{-6}
2.10	8	7.73	-1.59×10^{-2}	5.70×10^{-6}
2.00	8	6.81	-9.36×10^{-2}	3.85×10^{-5}
2.00	6	6.81	1.10×10^{-1}	-5.08×10^{-5}
1.90	6	6	0	0

$$\kappa_c^{(0)}(L/a) = \tfrac{1}{8} + k_1(a/L) + k_2(a/L)^2 + k_3(a/L)^3 + k_4(a/L)^4, \quad (41)$$

$$\kappa_c^{(1)}(L/a) = 0.002\,760\,894 + (l_1 - m_1 \ln(L/a))(a/L) + (l_2 - m_2 \ln(L/a))(a/L)^2. \quad (42)$$

The coefficients are given in Table I. We note that the one-loop coefficients have an N_f dependence due to the tadpole diagram, although it vanishes in the large volume limit.

In our actual determination, we define L^* by $L^*/a = 6$ at $\beta = 1.9$, $L^*/a = 6$ at $\beta = 2.0$, and $L^*/a = 6$ at $\beta = 2.6$ for $N_f = 3$, 2, and 0 flavor QCD, respectively. In Tables II, III, and IV numerical values of $\beta = 6/g_0^2$, L/a, and L^*/a in our simulations for $N_f = 3$, 2, and 0 cases are summarized. In these tables, we also show the numerical values of $\delta c_{\rm SW}(g_0^2, L/a; L^*/a)$ and $\delta\kappa_c(g_0^2, L/a; L^*/a)$. For large values of β, the perturbative corrections are small and hence reliable. On the other hand, if L/a are close to L^*/a, the corrections needed for the conversion from L to L^* should again be small. Since we fix L^* at strong coupling, the corrections, Eqs. (37) and (38), are small at both ends of our range of β as one can see in the tables.

TABLE III. Same as Table II, but for two-flavor QCD.

β	L/a	L^*/a	$\delta c_{\rm SW}(L/a; L^*/a)$	$\delta\kappa(L/a; L^*/a)$
12.00	8	2.35×10^6	2.43×10^{-3}	5.93×10^{-5}
8.85	8	3.66×10^4	1.01×10^{-2}	7.38×10^{-5}
5.00	8	2.45×10^2	4.63×10^{-2}	1.08×10^{-4}
3.00	8	1.98×10^1	9.51×10^{-2}	2.69×10^{-5}
2.60	8	1.22×10^1	7.84×10^{-2}	-1.81×10^{-5}
2.20	8	7.58	-2.11×10^{-2}	1.41×10^{-5}
2.10	8	6.74	-8.24×10^{-2}	6.14×10^{-5}
2.10	6	6.74	8.37×10^{-2}	-7.04×10^{-5}
2.00	6	6	0	0

TABLE IV. Same as Table II, but for quenched QCD.

β	L/a	L^*/a	$\delta c_{\rm SW}(L/a; L^*/a)$	$\delta\kappa(L/a; L^*/a)$
24.00	8	3.09×10^{11}	-1.11×10^{-2}	3.47×10^{-5}
12.00	8	2.41×10^5	-3.70×10^{-3}	5.08×10^{-5}
8.85	8	6.33×10^3	2.24×10^{-3}	6.18×10^{-5}
5.00	8	8.04×10^1	3.80×10^{-2}	6.29×10^{-5}
3.00	8	9.12	2.07×10^{-2}	-2.68×10^{-5}
2.70	8	6.66	-4.81×10^{-2}	8.79×10^{-5}
2.70	6	6.66	3.98×10^{-2}	-8.40×10^{-5}
2.60	6	6	0	0

IV. NUMERICAL SIMULATIONS

A. Parameters and algorithm

The numerical simulations are performed with $N_f = 3$, 2, and 0 degenerate dynamical quarks on a $(L/a)^3 \times 2(L/a)$ ($L/a = 8$ or 6) lattice for a wide range of β. The simulation parameters are summarized in Tables II, III, and IV for $N_f = 3$, 2, and 0, respectively.

We employ the symmetric even-odd preconditioning introduced in Refs. [15,16] for the quark matrix D. Calculation of D^{-1} is made with the BiCGStab algorithm with the tolerance parameter $\|R_i\|/\|B\| < 10^{-14}$, where $R_i = DX_i - B$ is the residual vector and X_i is an estimate for the solution X in the ith BiCGStab iteration.

We adopt the standard hybrid Monte Carlo (HMC) algorithm [17] for the $N_f = 2$ and 0 flavor cases. For the three-flavor case, the polynomial HMC (PHMC) algorithm [16,18] is applied to describe the third flavor, employing the Chebyshev polynomial $P[D]$ to approximate D^{-1}. In order to make the PHMC algorithm exact, the correction factor $P_{\rm corr} = \det[W[D]]$ with $W[D] = P[D]D$ is taken into account by the noisy Metropolis method [19]. The square root of $W[D]$, which is required in the Metropolis test, is evaluated with an accuracy of 10^{-14} using a Taylor expansion of $W[D]$ [16]. The order of the polynomial $N_{\rm poly}$ is chosen so that an acceptance rate of about 70% or higher is achieved for the Metropolis test.

In the calculations of aM and $a\Delta M$, f_X and f'_X ($X = A$ or P) are first evaluated at every trajectory, and they are combined to produce aM and $a\Delta M$. The bin size dependence of the jackknife error of aM is investigated in the range $N_{\rm bin} = 1$–$N_{\rm traj}/20$. We adopt $N_{\rm bin}$ giving the maximum error in this range in the error analyses in the following.

B. Results

The trial values of $c_{\rm SW}$ and κ at which simulations are made are summarized in Tables V, VI, and VII for $N_f = 3$, 2, and 0, respectively, together with the results for aM and

TABLE V. Results for aM and $a\Delta M$ for three-flavor QCD. The acceptance rates for the molecular dynamics (MD) and the noisy Metropolis test are shown together with the number of MD steps per trajectory and the order of the polynomial $N_{\rm poly}$ used in the noisy Metropolis test. The final column gives the number of trajectories accumulated.

$c_{\rm SW}$	κ	aM	$a\Delta M$	$P_{\rm acc}[N_{\rm MD}]$	$P_{\rm corr}[N_{\rm poly}]$	$N_{\rm traj}$
			$\beta = 12.00,\ L/a = 8$			
1.00	0.126 59	0.012 35(13)	0.001 01(13)	0.73(2)[100]	0.983(5)[100]	1600
	0.126 76	0.006 906(91)	0.000 72(13)	0.75(1)[100]	0.979(4)[100]	1600
	0.126 93	0.001 49(13)	0.000 87(14)	0.73(2)[100]	0.973(5)[100]	1600
	0.127 09	−0.003 68(13)	0.000 92(16)	0.75(1)[100]	0.970(5)[100]	1600
1.05	0.126 59	0.008 565(98)	−0.00009(18)	0.72(2)[100]	0.984(4)[100]	1600
	0.126 76	0.002 83(11)	−0.000 03(13)	0.74(1)[100]	0.968(6)[100]	1600
	0.126 93	−0.002 21(11)	0.000 04(17)	0.72(3)[100]	0.969(6)[100]	1600
	0.127 09	−0.007 708(89)	0.000 23(10)	0.74(2)[100]	0.955(5)[100]	1600
1.10	0.126 59	0.004 60(12)	−0.000 76(13)	0.72(2)[100]	0.981(4)[100]	1600
	0.126 76	−0.000 97(15)	−0.000 69(22)	0.71(3)[100]	0.972(4)[100]	1600
	0.126 93	−0.006 25(21)	−0.000 73(16)	0.74(2)[100]	0.953(9)[100]	1600
	0.127 09	−0.011 61(17)	−0.000 70(13)	0.73(2)[100]	0.94(2)[100]	1600
			$\beta = 8.85,\ L/a = 8$			
1.0141	0.126 98	0.023 16(13)	0.000 94(15)	0.68(2)[80]	0.989(3)[100]	2000
	0.127 30	0.013 11(11)	0.001 04(18)	0.66(2)[80]	0.988(4)[100]	2000
	0.127 62	0.003 09(12)	0.001 02(15)	0.71(2)[80]	0.969(5)[100]	2000
	0.128 26	−0.017 34(10)	0.000 92(16)	0.70(1)[80]	0.943(6)[110]	2000
1.0350	0.126 98	0.021 21(11)	0.000 60(12)	0.70(2)[80]	0.990(2)[100]	2000
	0.127 30	0.011 19(16)	0.000 57(17)	0.71(1)[80]	0.985(3)[100]	2000
	0.127 62	0.000 80(13)	0.000 60(16)	0.70(2)[80]	0.972(4)[100]	2000
	0.128 26	−0.019 48(13)	0.000 55(15)	0.71(2)[80]	0.937(6)[110]	2000
1.0559	0.126 98	0.019 03(14)	0.000 13(14)	0.69(2)[80]	0.987(4)[100]	2000
	0.127 30	0.008 96(11)	0.000 33(10)	0.68(1)[80]	0.975(4)[100]	2000
	0.127 62	−0.001 30(11)	0.000 24(20)	0.69(2)[80]	0.964(5)[100]	2000
	0.128 26	−0.021 66(13)	0.000 39(10)	0.70(2)[80]	0.928(7)[110]	2000
1.0800	0.127 19	0.009 83(15)	−0.000 13(15)	0.69(2)[80]	0.990(2)[120]	2000
	0.127 53	−0.000 78(11)	0.000 07(12)	0.68(2)[80]	0.989(3)[130]	2000
1.1000	0.127 13	0.009 82(35)	−0.000 41(19)	0.68(2)[80]	0.990(3)[110]	2000
	0.127 47	−0.001 21(11)	−0.000 39(14)	0.69(1)[80]	0.986(3)[120]	2000
			$\beta = 5.00,\ L/a = 8$			
1.08	0.129 58	0.010 31(33)	0.000 73(22)	0.72(1)[64]	0.982(3)[100]	2200
	0.129 74	0.005 53(17)	0.000 82(29)	0.77(2)[64]	0.968(4)[100]	2200
	0.129 89	0.000 49(35)	0.000 60(25)	0.74(2)[64]	0.970(4)[100]	2200
	0.130 04	−0.003 77(20)	0.000 70(19)	0.74(2)[64]	0.962(5)[100]	2200
1.13	0.129 32	0.010 27(26)	0.000 39(22)	0.73(1)[64]	0.976(6)[100]	2200
	0.129 48	0.005 41(24)	0.000 43(27)	0.73(1)[64]	0.975(4)[100]	2200
	0.129 63	0.000 30(24)	0.000 24(21)	0.77(1)[64]	0.964(7)[100]	2200
	0.129 78	−0.004 28(29)	0.000 42(37)	0.74(1)[64]	0.950(6)[100]	2200
1.18	0.129 07	0.010 02(22)	−0.000 71(20)	0.76(2)[64]	0.982(3)[100]	2200
	0.129 22	0.004 89(25)	−0.001 05(22)	0.73(2)[64]	0.974(4)[100]	2200
	0.129 37	0.000 43(43)	−0.000 74(21)	0.75(1)[64]	0.970(4)[100]	2200
	0.129 52	−0.004 41(28)	−0.000 89(21)	0.76(1)[64]	0.958(6)[100]	2200
			$\beta = 3.00,\ L/a = 8$			
1.20	0.132 81	0.027 98(33)	0.000 99(26)	0.770(9)[50]	0.988(2)[100]	4300
	0.133 11	0.017 69(47)	0.000 36(57)	0.77(1)[50]	0.978(3)[100]	4000
	0.133 41	0.008 13(46)	0.000 44(33)	0.78(1)[50]	0.960(4)[100]	4000
	0.133 70	−0.000 36(41)	0.001 04(40)	0.77(1)[50]	0.937(5)[100]	3800
1.25	0.132 35	0.027 74(42)	−0.000 15(61)	0.78(1)[50]	0.986(4)[100]	4200
	0.132 65	0.018 20(52)	0.000 03(40)	0.76(1)[50]	0.980(3)[100]	3800

TABLE V. (*Continued*)

c_{SW}	κ	aM	$a\Delta M$	$P_{acc}[N_{MD}]$	$P_{corr}[N_{poly}]$	N_{traj}
	0.132 94	0.009 40(38)	0.000 04(36)	0.77(1)[50]	0.960(3)[100]	4200
	0.133 24	−0.000 27(40)	−0.000 29(34)	0.773(9)[50]	0.948(5)[100]	3900
1.30	0.131 90	0.027 42(65)	−0.000 52(28)	0.76(1)[50]	0.990(2)[100]	4200
	0.132 19	0.017 13(64)	−0.000 40(36)	0.77(2)[50]	0.980(2)[100]	4200
	0.132 48	0.009 15(54)	−0.000 66(67)	0.78(2)[50]	0.962(3)[100]	3900
	0.132 78	−0.000 08(41)	0.000 31(64)	0.77(1)[50]	0.945(6)[100]	4000
1.35	0.131 45	0.026 97(35)	−0.000 98(46)	0.77(1)[50]	0.988(3)[100]	4300
	0.131 74	0.016 43(70)	−0.000 75(44)	0.770(8)[50]	0.979(4)[100]	4100
	0.132 03	0.008 00(43)	−0.000 92(58)	0.76(1)[50]	0.972(3)[100]	4100
	0.132 32	−0.000 79(38)	−0.001 09(38)	0.77(1)[50]	0.947(4)[100]	4000
			$\beta = 2.60$, $L/a = 8$			
1.20	0.135 31	0.021 10(64)	0.001 68(38)	0.878(9)[64]	0.979(3)[110]	4500
	0.135 50	0.015 28(44)	0.001 42(85)	0.879(6)[64]	0.972(3)[110]	4500
	0.135 74	0.008 10(69)	0.001 70(43)	0.87(1)[64]	0.966(6)[120]	4500
	0.135 94	0.001 40(72)	0.001 58(62)	0.882(7)[64]	0.965(8)[130]	4500
1.27	0.134 54	0.020 61(53)	0.000 73(91)	0.870(6)[64]	0.983(2)[110]	4500
	0.134 73	0.015 12(73)	0.002 18(47)	0.881(6)[64]	0.978(2)[110]	4500
	0.134 96	0.007 21(52)	0.001 02(48)	0.883(10)[64]	0.971(5)[120]	4500
	0.135 16	0.003 27(73)	0.000 39(53)	0.883(6)[64]	0.972(3)[130]	4500
1.34	0.133 78	0.021 77(75)	−0.000 06(57)	0.883(6)[64]	0.984(2)[110]	4500
	0.134 20	0.008 30(57)	−0.000 04(45)	0.872(6)[64]	0.972(3)[120]	4500
	0.134 40	0.001 8(11)	0.000 31(44)	0.876(9)[64]	0.975(2)[130]	4500
	0.134 73	−0.009 68(93)	−0.000 07(34)	0.880(6)[64]	0.903(5)[110]	4500
1.41	0.133 03	0.020 40(50)	−0.000 55(43)	0.874(7)[64]	0.983(2)[110]	4500
	0.133 22	0.013 75(64)	−0.000 42(67)	0.874(7)[64]	0.979(3)[110]	4500
	0.133 44	0.007 92(81)	−0.000 64(37)	0.873(9)[64]	0.975(3)[120]	4500
	0.133 64	0.001 16(66)	−0.000 22(50)	0.882(6)[64]	0.964(3)[130]	4500
1.48	0.132 77	0.003 6(10)	−0.001 09(49)	0.883(6)[64]	0.978(3)[130]	5000
	0.133 01	−0.003 16(79)	−0.000 85(34)	0.872(6)[64]	0.979(2)[150]	5000
1.55	0.132 02	0.004 76(58)	−0.002 18(36)	0.873(7)[64]	0.980(2)[130]	5000
	0.132 26	−0.002 70(73)	−0.001 95(48)	0.879(10)[64]	0.973(3)[140]	5000
			$\beta = 2.40$, $L/a = 8$			
1.3	0.135 917	0.021 1(39)	0.001 62(74)	0.819(7)[50]	0.974(2)[110]	10 000
	0.136 152	0.011 46(50)	0.000 11(100)	0.819(5)[50]	0.971(2)[120]	10 000
	0.136 387	0.002 76(49)	0.001 00(29)	0.82(1)[50]	0.947(2)[120]	10 000
1.4	0.134 882	0.012 07(50)	0.000 22(60)	0.815(5)[50]	0.974(2)[120]	10 000
	0.135 113	0.004 66(45)	0.000 34(50)	0.828(5)[50]	0.954(2)[120]	10 000
1.5	0.133 410	0.020 6(10)	−0.000 40(30)	0.823(4)[50]	0.983(2)[110]	10 000
	0.133 636	0.013 00(56)	0.000 27(68)	0.828(5)[50]	0.979(2)[120]	10 000
	0.133 862	0.005 84(49)	−0.000 95(39)	0.827(5)[50]	0.966(2)[120]	10 000
1.6	0.132 400	0.015 1(12)	−0.002 10(81)	0.82(1)[50]	0.980(2)[120]	11 900
	0.132 680	0.005 67(70)	−0.001 94(55)	0.825(5)[50]	0.966(2)[120]	11 900
1.7	0.131 230	0.013 85(71)	−0.002 36(54)	0.888(5)[64]	0.983(1)[120]	10 700
	0.131 510	0.004 7(13)	−0.003 21(28)	0.886(7)[64]	0.978(1)[130]	10 700
			$\beta = 2.20$, $L/a = 8$			
1.3	0.138 247	0.016 85(90)	0.001 61(63)	0.840(5)[50]	0.958(2)[120]	16 500
	0.138 487	0.010 0(15)	0.001 44(36)	0.836(3)[50]	0.946(3)[130]	16 500
	0.138 729	0.001 28(62)	0.001 49(45)	0.843(4)[50]	0.919(3)[140]	16 500
1.5	0.135 400	0.018 77(64)	−0.000 28(38)	0.844(4)[50]	0.973(1)[120]	16 000
	0.135 654	0.010 83(46)	−0.000 04(36)	0.844(4)[50]	0.965(2)[130]	16 500
	0.135 885	0.002 85(55)	0.000 79(51)	0.841(4)[50]	0.951(2)[140]	16 500
1.7	0.132 712	0.019 13(70)	−0.001 48(29)	0.846(5)[50]	0.983(1)[120]	16 500

TABLE V. (*Continued*)

c_{SW}	κ	aM	$a\Delta M$	$P_{acc}[N_{MD}]$	$P_{corr}[N_{poly}]$	N_{traj}
	0.132 934	0.012 26(45)	−0.001 98(45)	0.844(8)[50]	0.977(2)[130]	16 500
	0.133 156	0.004 94(49)	−0.002 05(50)	0.834(5)[50]	0.968(2)[140]	16 500
1.9	0.130 170	0.020 45(54)	−0.003 85(32)	0.843(6)[50]	0.984(1)[120]	16 100
	0.130 370	0.012 48(76)	−0.003 42(30)	0.840(4)[50]	0.984(2)[130]	16 100
	0.130 570	0.005 61(55)	−0.003 22(32)	0.841(4)[50]	0.977(1)[140]	16 100
			$\beta = 2.10,\ L/a = 8$			
1.5	0.1355	0.057 9(12)	0.000 66(57)	0.850(4)[50]	0.979(3)[80]	14 500
	0.1358	0.050 0(15)	0.000 11(44)	0.847(4)[50]	0.9877(10)[100]	14 500
	0.1360	0.043 80(77)	0.000 33(44)	0.855(4)[50]	0.984(1)[100]	14 400
	0.1362	0.038 6(10)	0.000 47(56)	0.851(6)[50]	0.978(2)[100]	14 500
1.6	0.1340	0.061 67(75)	−0.000 27(49)	0.854(5)[50]	0.986(2)[80]	14 500
	0.1344	0.0481 1(59)	0.000 39(83)	0.848(5)[50]	0.9888(10)[100]	14 500
	0.1346	0.041 79(72)	−0.000 35(76)	0.850(4)[50]	0.985(1)[100]	14 500
1.7	0.1326	0.059 64(58)	−0.001 32(47)	0.853(5)[50]	0.987(1)[80]	14 500
	0.1329	0.049 52(50)	−0.001 28(33)	0.850(4)[50]	0.987(2)[90]	14 500
	0.1331	0.043 93(48)	−0.001 45(32)	0.854(3)[50]	0.988(1)[100]	14 500
	0.1333	0.037 52(54)	−0.000 18(31)	0.849(3)[50]	0.982(2)[100]	14 500
	0.1335	0.029 76(87)	−0.000 96(31)	0.856(3)[50]	0.974(1)[100]	14 500
1.8	0.1315	0.050 54(44)	−0.001 92(33)	0.850(4)[50]	0.9889(9)[90]	14 500
	0.1318	0.041 01(59)	−0.001 82(35)	0.844(3)[50]	0.9883(10)[100]	14 500
	0.1321	0.031 49(47)	−0.001 76(41)	0.847(4)[50]	0.983(2)[110]	14 500
	0.1324	0.019 56(59)	−0.001 48(33)	0.850(4)[50]	0.980(1)[120]	14 500
			$\beta = 2.00,\ L/a = 8$			
1.5	0.138 355 0	0.027 6(15)	0.000 20(44)	0.863(3)[50]	0.961(2)[130]	24 500
	0.138 667 2	0.017 6(12)	0.000 82(56)	0.857(3)[50]	0.928(2)[140]	21 500
	0.138 800 0	0.013 8(13)	0.000 34(58)	0.853(3)[50]	0.914(7)[160]	21 200
1.6	0.136 431 0	0.036 0(10)	0.000 36(60)	0.858(4)[50]	0.9912(9)[140]	20 000
	0.136 750 0	0.026 18(98)	−0.001 1(10)	0.857(4)[50]	0.982(1)[150]	20 000
	0.137 070 0	0.015 6(12)	0.000 49(52)	0.857(7)[50]	0.961(2)[160]	20 000
1.7	0.134 874 0	0.037 23(61)	−0.001 34(41)	0.856(3)[50]	0.9932(9)[140]	20 000
	0.135 430 9	0.015 88(70)	−0.000 73(30)	0.861(3)[50]	0.950(2)[130]	24 500
	0.135 498 0	0.014 35(93)	−0.000 37(46)	0.859(3)[50]	0.971(1)[160]	20 000
	0.135 600 0	0.010 43(82)	−0.000 72(58)	0.861(4)[50]	0.951(2)[150]	20 300
1.8	0.133 352 0	0.035 33(61)	−0.000 95(40)	0.859(3)[50]	0.9936(6)[140]	20 000
	0.133 657 0	0.024 41(57)	−0.001 29(33)	0.863(3)[50]	0.9899(8)[150]	20 000
	0.133 962 0	0.013 74(65)	−0.000 50(51)	0.853(5)[50]	0.978(1)[160]	20 000
1.9	0.132 057 8	0.028 43(57)	−0.002 37(38)	0.860(3)[50]	0.977(1)[110]	24 500
	0.132 342 2	0.019 18(68)	−0.001 66(42)	0.860(2)[50]	0.976(1)[130]	24 500
	0.132 627 8	0.010 16(60)	−0.001 83(39)	0.858(3)[50]	0.945(2)[130]	24 500
2.0	0.130 830 0	0.020 8(13)	−0.003 57(75)	0.853(6)[50]	0.989(2)[150]	5 400
	0.131 110 0	0.012 08(82)	−0.003 10(40)	0.860(7)[50]	0.983(2)[160]	7 300
2.1	0.129 380 0	0.025 89(84)	−0.003 91(65)	0.859(8)[50]	0.996(2)[150]	5 400
	0.129 660 0	0.014 83(96)	−0.004 06(79)	0.855(5)[50]	0.988(2)[160]	7 300
			$\beta = 2.00,\ L/a = 6$			
1.30	0.1400	0.100 2(43)	0.005 5(15)	0.925(3)[50]	0.9998(2)[120]	11 200
	0.1400	0.101 7(33)	0.003 46(89)	0.926(3)[50]	1.0000(0)[120]	11 200
	0.1405	0.087 1(30)	0.003 90(95)	0.923(2)[50]	0.9993(2)[120]	14 500
	0.1405	0.089 0(29)	0.003 0(11)	0.926(2)[50]	0.9991(5)[120]	14 500
	0.1410	0.066 9(28)	0.003 3(11)	0.922(3)[50]	0.9974(6)[120]	15 000
	0.1410	0.072 1(30)	0.004 5(15)	0.922(2)[50]	0.9974(8)[120]	15 000
	0.1415	0.050 5(26)	0.003 7(11)	0.922(4)[50]	0.990(1)[120]	15 100
	0.1415	0.050 8(24)	0.004 8(12)	0.923(2)[50]	0.990(1)[120]	15 100

TABLE V. (*Continued*)

c_{SW}	κ	aM	$a\Delta M$	$P_{acc}[N_{MD}]$	$P_{corr}[N_{poly}]$	N_{traj}
1.45	0.1380	0.075 2(22)	0.001 53(95)	0.925(3)[50]	0.9995(2)[120]	14 900
	0.1380	0.078 4(17)	0.001 26(66)	0.925(3)[50]	0.9994(3)[120]	14 900
	0.1385	0.056 4(17)	0.002 24(73)	0.921(3)[50]	0.9985(4)[120]	14 900
	0.1385	0.056 8(24)	0.000 94(76)	0.922(4)[50]	0.9979(5)[120]	14 900
	0.1390	0.040 1(20)	−0.000 1(12)	0.921(2)[50]	0.994(1)[120]	15 000
	0.1390	0.041 7(21)	0.001 73(83)	0.921(3)[50]	0.993(1)[120]	15 000
	0.1395	0.023 1(17)	0.001 28(80)	0.923(5)[50]	0.982(2)[120]	15 100
	0.1395	0.024 5(23)	0.002 38(83)	0.926(3)[50]	0.981(1)[120]	15 100
1.60	0.1355	0.067 3(20)	0.002 1(16)	0.925(4)[50]	0.9994(2)[120]	11 200
	0.1355	0.069 8(16)	−0.000 90(78)	0.924(3)[50]	0.9998(2)[120]	11 200
	0.1360	0.053 0(17)	−0.000 53(56)	0.920(3)[50]	0.9983(6)[120]	15 000
	0.1360	0.053 5(14)	−0.000 4(14)	0.925(3)[50]	0.9990(3)[120]	15 000
	0.1365	0.034 0(19)	0.000 8(10)	0.926(2)[50]	0.9957(8)[120]	15 000
	0.1365	0.034 7(15)	0.000 78(62)	0.925(3)[50]	0.9971(5)[120]	15 000
	0.1370	0.016 5(14)	−0.000 13(69)	0.922(3)[50]	0.988(1)[120]	15 000
	0.1370	0.017 1(16)	−0.000 4(12)	0.923(2)[50]	0.9888(10)[120]	15 000
1.75	0.1330	0.068 2(37)	−0.002 23(95)	0.920(7)[50]	1.0000(0)[120]	3 400
	0.1330	0.068 3(20)	−0.001 6(10)	0.927(7)[50]	0.9997(3)[120]	3 400
	0.1335	0.050 35(96)	−0.002 93(66)	0.925(3)[50]	0.9996(3)[120]	14 500
	0.1335	0.052 42(96)	−0.001 87(64)	0.923(3)[50]	0.9995(2)[120]	14 500
	0.1340	0.033 9(10)	−0.000 88(59)	0.927(3)[50]	0.9985(5)[120]	15 000
	0.1340	0.035 0(11)	−0.002 5(13)	0.924(3)[50]	0.9983(5)[120]	15 000
	0.1345	0.016 4(15)	−0.002 6(10)	0.920(3)[50]	0.9948(6)[120]	15 000
	0.1345	0.019 7(15)	−0.000 95(70)	0.920(3)[50]	0.994(1)[120]	15 000
			$\beta = 1.90$, $L/a = 6$			
1.4	0.1410	0.131 5(62)	0.001 12(92)	0.930(2)[50]	0.999 7(1)[120]	24 000
	0.1410	0.133 8(41)	0.000 8(13)	0.923(2)[50]	0.999 7(1)[120]	23 900
	0.1415	0.110 3(64)	0.000 6(12)	0.928(2)[50]	0.998 5(4)[120]	24 000
	0.1415	0.113 6(36)	0.001 44(94)	0.927(2)[50]	0.998 9(2)[120]	24 000
	0.1420	0.085 7(25)	0.002 8(10)	0.930(3)[50]	0.993 0(8)[120]	24 100
	0.1420	0.087 6(31)	0.001 66(90)	0.923(2)[50]	0.994 5(5)[120]	24 100
1.8	0.1340	0.087 8(25)	−0.000 21(84)	0.929(3)[50]	1.000 0(0)[120]	15 100
	0.1340	0.090 0(21)	−0.001 74(58)	0.928(3)[50]	1.000 0(0)[120]	15 100
	0.1345	0.071 0(21)	−0.001 59(69)	0.926(3)[50]	0.999 4(2)[120]	24 000
	0.1345	0.073 3(14)	−0.001 93(55)	0.929(2)[50]	0.999 5(3)[120]	24 000
	0.1350	0.052 0(24)	−0.001 36(59)	0.929(2)[50]	0.997 3(3)[120]	24 100
	0.1350	0.053 5(21)	−0.000 45(76)	0.928(2)[50]	0.997 6(6)[120]	24 100
	0.1355	0.030 7(16)	−0.001 02(68)	0.926(2)[50]	0.988 8(7)[120]	24 100
	0.1355	0.030 9(14)	−0.001 08(55)	0.926(2)[50]	0.989 5(8)[120]	24 100
2.2	0.1280	0.061 46(84)	−0.006 01(53)	0.928(2)[50]	0.999 91(9)[120]	22 700
	0.1280	0.063 03(92)	−0.006 99(67)	0.926(2)[50]	0.999 8(1)[120]	22 700
	0.1285	0.043 76(79)	−0.007 34(52)	0.928(2)[50]	0.999 3(2)[120]	23 600
	0.1285	0.044 34(83)	−0.005 94(51)	0.928(2)[50]	0.999 6(1)[120]	23 600
	0.1290	0.025 40(87)	−0.006 81(84)	0.929(2)[50]	0.997 6(6)[120]	24 100
	0.1290	0.026 07(99)	−0.005 85(67)	0.924(2)[50]	0.997 6(4)[120]	24 100
	0.1295	0.007 47(99)	−0.004 4(16)	0.925(2)[50]	0.991 6(8)[120]	24 100
	0.1295	0.008 4(15)	−0.006 49(46)	0.928(2)[50]	0.992 2(6)[120]	24 100
2.5	0.1240	0.053 5(12)	−0.010 90(60)	0.926(2)[50]	0.999 90(7)[120]	22 200
	0.1240	0.053 9(12)	−0.010 76(50)	0.927(2)[50]	0.999 7(2)[120]	22 200
	0.1245	0.037 2(13)	−0.010 83(49)	0.929(2)[50]	0.999 6(1)[120]	24 000
	0.1250	0.019 13(94)	−0.011 52(87)	0.926(2)[50]	0.998 5(3)[120]	24 000
	0.1250	0.019 8(11)	−0.011 44(38)	0.925(2)[50]	0.998 6(3)[120]	24 100
	0.1255	0.002 01(98)	−0.011 60(49)	0.924(2)[50]	0.993 7(7)[120]	24 100
	0.1255	−0.000 14(87)	−0.011 00(44)	0.923(2)[50]	0.993 2(8)[120]	24 100

TABLE VI. Same as Table V for two-flavor QCD.

$c_{\rm SW}$	κ	aM	$a\Delta M$	$P_{\rm acc}[N_{\rm MD}]$	$N_{\rm traj}$
		$\beta = 12.00,\ L/a = 8$			
1.00	0.126 59	0.012 66(15)	0.000 82(16)	0.75(3)[100]	1500
	0.126 76	0.007 137(77)	0.000 83(14)	0.74(2)[100]	1500
	0.126 93	0.001 80(16)	0.001 15(16)	0.73(2)[100]	1500
	0.127 09	−0.003 231(98)	0.000 70(13)	0.75(2)[100]	1500
1.05	0.126 59	0.008 82(14)	0.000 03(20)	0.71(3)[100]	1500
	0.126 76	0.003 17(11)	0.000 19(14)	0.73(2)[100]	1500
	0.126 93	−0.001 99(11)	0.000 16(14)	0.70(2)[100]	1500
	0.127 09	−0.007 35(16)	−0.000 08(12)	0.72(2)[100]	1500
1.10	0.126 59	0.004 98(12)	−0.000 61(11)	0.74(2)[100]	1500
	0.126 76	−0.000 42(12)	−0.000 65(15)	0.73(1)[100]	1500
	0.126 93	−0.005 81(11)	−0.000 69(12)	0.71(2)[100]	1500
	0.127 09	−0.011 19(15)	−0.000 70(12)	0.74(2)[100]	1500
		$\beta = 8.85,\ L/a = 8$			
1.040	0.1270	0.020 524(91)	0.000 36(11)	0.72(2)[80]	2100
	0.1274	0.007 94(13)	0.000 56(11)	0.72(2)[80]	2100
	0.1278	−0.004 70(14)	0.000 52(15)	0.70(1)[80]	2100
	0.1282	−0.017 306(94)	0.000 43(14)	0.70(1)[80]	2000
1.055	0.1270	0.019 165(83)	0.000 44(14)	0.70(2)[80]	2000
	0.1274	0.006 65(14)	0.000 42(16)	0.70(2)[80]	2000
	0.1278	−0.006 28(12)	0.000 32(18)	0.67(2)[80]	2000
	0.1282	−0.019 00(12)	0.000 25(16)	0.70(2)[80]	2000
1.070	0.1270	0.017 58(10)	0.000 02(15)	0.70(1)[80]	2000
	0.1274	0.005 05(12)	0.000 01(18)	0.70(1)[80]	2000
	0.1278	−0.007 54(14)	0.000 27(14)	0.69(2)[80]	2000
	0.1282	−0.020 57(17)	0.000 12(11)	0.70(2)[80]	2000
		$\beta = 5.00,\ L/a = 8$			
1.09	0.129 54	0.012 04(16)	0.000 54(26)	0.75(1)[64]	2300
	0.129 70	0.006 92(23)	0.000 68(21)	0.76(2)[64]	2300
	0.129 86	0.001 98(25)	0.000 41(21)	0.74(1)[64]	2300
	0.130 02	−0.003 08(18)	0.000 86(43)	0.74(1)[64]	2300
1.13	0.129 33	0.011 67(21)	−0.000 05(31)	0.74(2)[64]	2300
	0.129 49	0.006 91(21)	−0.000 14(24)	0.75(1)[64]	2300
	0.129 65	0.001 74(15)	0.000 41(19)	0.75(1)[64]	2300
	0.129 81	−0.003 07(24)	−0.000 13(20)	0.75(1)[64]	2300
1.17	0.129 12	0.011 64(26)	−0.000 63(18)	0.76(2)[64]	2300
	0.129 28	0.006 67(27)	−0.000 31(28)	0.74(2)[64]	2300
	0.129 43	0.001 75(32)	−0.000 76(20)	0.75(1)[64]	2300
	0.129 59	−0.003 38(19)	−0.000 20(33)	0.75(1)[64]	2300
		$\beta = 3.00,\ L/a = 8$			
1.20	0.133 210 0	0.021 95(25)	0.000 69(38)	0.780(5)[50]	10 500
	0.133 370 0	0.016 74(36)	0.000 86(22)	0.767(7)[50]	10 500
	0.133 540 0	0.011 65(34)	0.000 44(28)	0.77(1)[50]	10 500
	0.133 700 0	0.006 85(22)	0.000 68(28)	0.762(5)[50]	10 500
1.28	0.132 470 0	0.021 75(35)	−0.000 13(29)	0.774(6)[50]	10 500
	0.132 630 0	0.016 68(33)	−0.000 07(21)	0.773(6)[50]	10 500
	0.132 790 0	0.011 68(30)	−0.000 08(40)	0.781(8)[50]	10 500
	0.132 950 0	0.006 49(35)	0.000 21(22)	0.766(5)[50]	10 500
1.36	0.131 730 0	0.021 46(39)	−0.000 79(21)	0.769(7)[50]	10 500
	0.131 890 0	0.016 44(30)	−0.000 68(24)	0.771(7)[50]	10 500
	0.132 040 0	0.011 56(37)	−0.000 99(28)	0.777(7)[50]	10 500
	0.132 200 0	0.006 75(30)	−0.000 92(22)	0.779(6)[50]	10 500

TABLE VI. (*Continued*)

c_{SW}	κ	aM	$a\Delta M$	$P_{acc}[N_{MD}]$	N_{traj}
		$\beta = 2.60,\ L/a = 8$			
1.20	0.135 574	0.024 73(74)	0.001 04(62)	0.809(7)[50]	4500
	0.135 738	0.019 1(12)	0.001 61(59)	0.800(8)[50]	4500
	0.135 903	0.015 22(75)	0.002 09(53)	0.808(7)[50]	4500
	0.136 068	0.010 02(58)	0.001 43(93)	0.806(8)[50]	4500
1.25	0.135 020	0.024 24(81)	0.001 5(10)	0.80(1)[50]	4500
	0.135 180	0.019 12(58)	0.001 49(49)	0.811(8)[50]	4500
	0.135 340	0.015 06(67)	0.001 56(56)	0.810(8)[50]	4500
	0.135 510	0.009 82(59)	0.001 50(82)	0.812(7)[50]	4500
1.30	0.134 470	0.024 92(54)	−0.000 4(11)	0.800(8)[50]	4500
	0.134 630	0.019 50(73)	0.001 75(52)	0.814(8)[50]	4500
	0.134 790	0.014 74(63)	−0.000 07(49)	0.803(7)[50]	4500
	0.134 950	0.009 49(53)	0.000 38(65)	0.804(8)[50]	4500
1.35	0.133 920	0.023 69(45)	0.000 44(47)	0.82(1)[50]	4500
	0.134 080	0.019 0(10)	−0.000 40(73)	0.803(7)[50]	4500
	0.134 240	0.014 26(70)	0.000 11(93)	0.82(1)[50]	4500
	0.134 400	0.009 07(51)	−0.000 44(57)	0.81(1)[50]	4500
		$\beta = 2.20,\ L/a = 8$			
1.35	0.138 68	0.012 52(59)	0.001 82(70)	0.828(3)[50]	37 300
	0.139 14	−0.003 10(93)	0.001 30(87)	0.834(2)[50]	35 900
1.50	0.136 54	0.008 38(96)	0.000 71(72)	0.834(2)[50]	41 100
	0.136 93	−0.004 33(75)	0.000 03(62)	0.833(2)[50]	39 600
1.60	0.135 00	0.010 12(23)	−0.000 60(39)	0.839(2)[50]	39 900
	0.135 43	−0.004 83(38)	−0.000 76(68)	0.832(2)[50]	38 000
		$\beta = 2.10,\ L/a = 8$			
1.38	0.140 40	0.005 98(95)	0.000 7(11)	0.811(2)[50]	145 700
	0.140 92	−0.010 94(54)	0.001 88(56)	0.810(2)[50]	167 500
1.53	0.137 41	0.021 24(23)	0.000 62(65)	0.829(2)[50]	67 800
	0.138 37	−0.008 72(53)	0.000 74(92)	0.822(2)[50]	58 900
1.63	0.135 99	0.013 71(17)	0.000 30(58)	0.830(2)[50]	66 400
	0.136 48	−0.001 8(11)	0.000 20(57)	0.828(2)[50]	62 900
1.73	0.134 51	0.011 52(32)	−0.000 08(48)	0.836(1)[50]	104 400
	0.134 97	−0.003 17(40)	−0.001 8(12)	0.833(2)[50]	137 100
		$\beta = 2.10,\ L/a = 6$			
1.2	0.143 47	0.007 7(22)	0.006 3(21)	0.864(3)[40]	21 600
	0.143 91	−0.002 5(21)	0.007 9(24)	0.865(4)[40]	26 000
1.4	0.139 87	0.012 5(18)	0.003 0(11)	0.868(4)[40]	26 000
	0.140 21	0.004 3(14)	0.003 2(17)	0.864(3)[40]	26 000
	0.140 56	−0.009 0(23)	0.002 5(14)	0.862(4)[40]	26 000
1.6	0.136 60	0.007 3(13)	0.001 4(10)	0.869(7)[40]	25 200
	0.136 83	0.000 65(93)	−0.000 42(78)	0.868(3)[40]	26 000
	0.137 25	−0.013 6(16)	−0.000 2(11)	0.863(2)[40]	25 200
1.8	0.133 35	0.008 25(67)	−0.004 38(74)	0.867(4)[40]	26 000
	0.133 62	−0.001 69(79)	−0.002 14(84)	0.870(2)[40]	26 000
	0.133 89	−0.010 2(10)	−0.002 78(77)	0.867(4)[40]	28 000
2.0	0.130 59	−0.000 1(14)	−0.006 85(74)	0.870(3)[40]	21 600
	0.130 90	−0.012 7(12)	−0.007 1(10)	0.870(3)[40]	21 600
2.4	0.125 00	0.002 2(17)	−0.012 83(75)	0.873(3)[40]	21 600
	0.125 50	−0.014 8(31)	−0.013 3(12)	0.865(3)[40]	21 600
		$\beta = 2.00,\ L/a = 6$			
1.4	0.142 79	0.012 5(26)	0.006 8(17)	0.906(4)[50]	20 000

TABLE VI. (*Continued*)

$c_{\rm SW}$	κ	aM	$a\Delta M$	$P_{\rm acc}[N_{\rm MD}]$	$N_{\rm traj}$
	0.143 62	−0.013 5(21)	0.003 3(33)	0.902(3)[50]	25 000
1.6	0.139 01	0.013 1(17)	0.003 4(21)	0.914(2)[50]	25 000
	0.139 36	0.003 5(16)	0.003 30(91)	0.907(3)[50]	25 000
	0.139 71	−0.008 8(16)	0.000 9(26)	0.906(4)[50]	25 000
1.8	0.135 36	0.011 3(15)	0.000 2(13)	0.918(2)[50]	25 000
	0.135 88	−0.006 9(12)	−0.001 3(22)	0.909(4)[50]	25 000
	0.136 27	−0.019 8(45)	0.000 6(24)	0.907(7)[50]	25 000
2.0	0.131 92	0.011 6(11)	−0.004 90(92)	0.918(3)[50]	25 000
	0.132 21	0.001 5(18)	−0.004 1(14)	0.916(4)[50]	25 000
	0.132 50	−0.010 6(12)	−0.003 3(11)	0.915(2)[50]	25 000
2.2	0.128 39	0.020 7(11)	−0.007 4(11)	0.921(3)[50]	20 000
	0.129 02	−0.000 8(18)	−0.007 8(12)	0.919(2)[50]	20 000
2.6	0.122 95	0.013 99(86)	−0.013 30(73)	0.918(3)[50]	21 000
	0.123 53	−0.009 3(14)	−0.012 04(69)	0.921(3)[50]	21 000

TABLE VII. Same as Table V for quenched QCD.

$c_{\rm SW}$	κ	aM	$a\Delta M$	$P_{\rm acc}[N_{\rm MD}]$	$N_{\rm traj}$
		$\beta = 24.00$, $L/a = 8$			
1.00	0.125 67	0.009 136(59)	0.000 714(97)	0.67(1)[128]	3100
	0.125 84	0.003 733(51)	0.000 545(69)	0.67(1)[128]	3100
	0.126 00	−0.001 39(11)	0.000 525(96)	0.65(2)[128]	3100
	0.126 17	−0.006 783(76)	0.000 567(79)	0.66(1)[128]	3100
1.03	0.125 67	0.007 822(63)	0.000 078(90)	0.67(1)[128]	3100
	0.125 84	0.002 319(54)	0.000 054(70)	0.67(1)[128]	3100
	0.126 00	−0.002 756(68)	0.000 167(81)	0.67(1)[128]	3100
	0.126 17	−0.008 282(63)	−0.000 028(77)	0.67(1)[128]	3100
1.06	0.125 67	0.006 427(46)	−0.000 334(63)	0.67(1)[128]	3100
	0.125 84	0.000 984(78)	−0.000 317(76)	0.68(1)[128]	3100
	0.126 00	−0.004 01(10)	−0.000 293(75)	0.65(2)[128]	3100
	0.126 17	−0.009 544(91)	−0.000 295(78)	0.66(1)[128]	3100
		$\beta = 12.00$, $L/a = 8$			
1.00	0.126 59	0.013 236(96)	0.000 80(17)	0.74(2)[100]	1600
	0.126 76	0.007 870(89)	0.000 86(11)	0.73(3)[100]	1600
	0.126 93	0.002 46(14)	0.000 86(17)	0.72(1)[100]	1600
	0.127 09	−0.002 61(10)	0.001 07(15)	0.73(2)[100]	1600
1.05	0.126 59	0.009 444(92)	0.000 23(14)	0.74(2)[100]	1600
	0.126 76	0.004 108(91)	0.000 12(12)	0.72(2)[100]	1600
	0.126 93	−0.001 424(88)	−0.000 00(15)	0.70(2)[100]	1600
	0.127 09	−0.006 318(91)	0.000 214(98)	0.72(2)[100]	1600
1.10	0.126 59	0.005 635(81)	−0.000 43(13)	0.73(2)[100]	1600
	0.126 76	0.000 26(16)	−0.000 48(11)	0.74(1)[100]	1600
	0.126 93	−0.005 07(15)	−0.000 53(10)	0.73(2)[100]	1600
	0.127 09	−0.010 21(11)	−0.000 69(16)	0.75(2)[100]	1600
		$\beta = 8.85$, $L/a = 8$			
1.05	0.1261	0.048 752(68)	0.000 670(83)	0.70(1)[80]	3500
	0.1266	0.033 381(77)	0.000 472(91)	0.70(1)[80]	3500
	0.1271	0.017 522(76)	0.000 515(90)	0.69(1)[80]	3500
	0.1276	0.001 942(99)	0.000 34(11)	0.69(1)[80]	3500
1.07	0.1260	0.049 789(63)	0.000 197(85)	0.70(1)[80]	3500
	0.1265	0.034 276(80)	0.000 152(88)	0.68(1)[80]	3500

TABLE VII. (*Continued*)

c_{SW}	κ	aM	$a\Delta M$	$P_{acc}[N_{MD}]$	N_{traj}
	0.1270	0.018 797(76)	0.000 27(12)	0.70(1)[80]	3500
	0.1275	0.003 24(11)	0.000 19(12)	0.69(1)[80]	3500
1.09	0.1259	0.051 029(60)	−0.000 008(97)	0.69(1)[80]	3500
	0.1264	0.035 509(77)	−0.000 033(81)	0.70(1)[80]	3500
	0.1269	0.019 930(91)	−0.000 06(12)	0.71(1)[80]	3500
	0.1274	0.004 27(13)	0.000 05(12)	0.70(1)[80]	3500
			$\beta = 5.00,\ L/a = 8$		
1.08	0.129 54	0.017 59(11)	0.000 80(14)	0.762(10)[64]	4800
	0.129 70	0.012 54(13)	0.000 75(25)	0.751(9)[64]	3500
	0.129 79	0.009 91(18)	0.000 57(17)	0.73(1)[64]	3500
	0.129 86	0.007 67(17)	0.001 00(16)	0.754(9)[64]	3500
	0.129 95	0.004 80(21)	0.001 15(19)	0.75(1)[64]	3500
	0.130 02	0.002 80(14)	0.000 83(25)	0.75(1)[64]	3500
	0.130 11	−0.000 14(16)	0.000 94(27)	0.738(9)[64]	3500
	0.130 27	−0.005 08(20)	0.000 69(27)	0.76(1)[64]	3500
1.13	0.129 51	0.010 03(15)	−0.000 02(18)	0.75(2)[64]	3500
	0.129 54	0.009 028(95)	0.000 41(12)	0.747(9)[64]	3500
	0.129 67	0.005 06(12)	0.000 12(26)	0.75(1)[64]	3500
	0.129 70	0.004 13(13)	−0.000 09(29)	0.725(10)[64]	3500
	0.129 83	0.000 26(12)	0.000 48(18)	0.74(1)[64]	3500
	0.129 86	−0.000 82(15)	0.000 06(25)	0.75(2)[64]	3500
	0.129 99	−0.004 89(18)	0.000 38(23)	0.733(10)[64]	3500
	0.130 02	−0.005 76(11)	0.000 19(20)	0.747(9)[64]	3500
1.18	0.129 24	0.009 95(12)	−0.000 52(19)	0.74(1)[64]	3500
	0.129 40	0.005 00(16)	−0.000 23(25)	0.75(2)[64]	3500
	0.129 54	0.000 75(15)	−0.000 12(21)	0.742(10)[64]	3500
	0.129 56	0.000 10(14)	−0.000 05(20)	0.75(1)[64]	3500
	0.129 70	−0.004 29(23)	−0.000 19(32)	0.73(2)[64]	3500
	0.129 72	−0.005 15(16)	−0.000 54(22)	0.75(1)[64]	3500
	0.129 86	−0.009 33(13)	−0.000 18(27)	0.74(2)[64]	3500
	0.130 02	−0.014 66(12)	−0.000 32(17)	0.755(9)[64]	3500
			$\beta = 3.00,\ L/a = 8$		
1.20	0.133 93	0.015 24(24)	0.000 83(26)	0.785(6)[50]	8100
	0.134 10	0.010 10(25)	0.001 44(32)	0.789(6)[50]	8100
	0.134 28	0.004 61(25)	0.001 52(41)	0.786(8)[50]	8100
	0.134 40	0.001 20(27)	0.001 32(59)	0.778(6)[50]	8100
1.28	0.133 15	0.015 62(28)	0.000 57(29)	0.77(1)[50]	8100
	0.133 32	0.010 53(18)	0.000 10(29)	0.782(8)[50]	8100
	0.133 49	0.005 20(30)	0.001 22(38)	0.782(7)[50]	8100
	0.133 63	0.001 10(23)	0.000 03(36)	0.777(7)[50]	8100
1.36	0.132 39	0.014 22(36)	−0.000 45(27)	0.777(7)[50]	8100
	0.132 55	0.009 41(29)	−0.000 50(34)	0.776(7)[50]	8100
	0.132 72	0.004 14(21)	0.000 08(33)	0.777(8)[50]	8100
	0.132 86	−0.000 33(36)	−0.000 49(35)	0.776(9)[50]	8100
			$\beta = 2.70,\ L/a = 8$		
1.2	0.136 05	0.013 02(55)	0.002 76(40)	0.803(4)[50]	15 000
	0.136 42	0.002 35(76)	0.002 70(50)	0.803(4)[50]	15 000
	0.136 80	−0.010 13(71)	0.002 9(12)	0.797(4)[50]	15 000
1.3	0.134 72	0.018 45(90)	0.001 87(60)	0.798(8)[50]	15 000
	0.135 26	0.002 07(59)	0.001 58(62)	0.797(4)[50]	15 000
	0.135 44	−0.003 05(17)	0.001 50(24)	0.800(5)[50]	15 000
1.4	0.133 56	0.018 33(30)	0.000 15(50)	0.805(4)[50]	15 000

TABLE VII. (*Continued*)

$c_{\rm SW}$	κ	aM	$a\Delta M$	$P_{\rm acc}[N_{\rm MD}]$	$N_{\rm traj}$
	0.134 12	0.001 59(30)	0.001 13(48)	0.798(8)[50]	15 000
	0.134 28	−0.004 05(34)	0.000 47(52)	0.799(7)[50]	15 000
1.5	0.132 64	0.010 93(29)	−0.001 13(28)	0.800(5)[50]	15 000
	0.132 81	0.005 62(27)	−0.001 07(37)	0.805(4)[50]	15 000
	0.132 98	−0.000 9(12)	−0.000 76(43)	0.799(7)[50]	15 000
1.6	0.131 43	0.012 54(23)	−0.003 7(14)	0.797(4)[50]	15 000
	0.131 80	0.000 22(23)	−0.002 02(31)	0.815(6)[50]	15 000
		$\beta = 2.70,\ L/a = 6$			
1.2	0.136 05	0.010 09(38)	0.003 23(43)	0.888(3)[50]	15 000
	0.136 42	−0.000 71(39)	0.003 24(48)	0.888(3)[50]	15 000
	0.136 80	−0.010 69(42)	0.002 98(64)	0.890(4)[50]	15 000
1.3	0.134 72	0.016 51(28)	0.001 06(46)	0.890(3)[50]	15 000
	0.135 26	0.000 90(34)	0.000 97(53)	0.890(4)[50]	15 000
	0.135 44	−0.004 99(36)	0.001 37(44)	0.889(6)[50]	15 000
1.4	0.133 56	0.016 95(39)	−0.001 02(36)	0.889(3)[50]	15 000
	0.134 12	0.000 17(32)	−0.000 88(53)	0.890(3)[50]	15 000
	0.134 28	−0.004 64(39)	−0.000 70(51)	0.890(3)[50]	15 000
1.5	0.132 64	0.009 59(32)	−0.002 61(41)	0.889(6)[50]	15 000
	0.132 98	−0.000 68(35)	−0.002 67(42)	0.890(3)[50]	15 000
1.6	0.131 43	0.010 83(32)	−0.005 04(54)	0.890(4)[50]	15 000
		$\beta = 2.60,\ L/a = 6$			
1.2	0.136 98	0.009 83(59)	0.004 69(88)	0.896(3)[50]	15 000
	0.137 30	0.000 64(65)	0.004 82(99)	0.896(3)[50]	15 000
	0.137 49	−0.005 50(60)	0.004 9(11)	0.893(7)[50]	15 000
1.3	0.135 74	0.010 57(49)	0.002 81(79)	0.893(7)[50]	15 000
	0.136 16	−0.001 98(52)	0.001 70(81)	0.894(3)[50]	15 000
1.4	0.134 63	0.007 50(57)	−0.000 51(53)	0.894(3)[50]	15 000
	0.134 94	−0.001 87(34)	0.000 68(58)	0.894(3)[50]	15 000
1.5	0.133 31	0.010 48(54)	−0.002 49(50)	0.891(3)[50]	15 000
	0.133 67	−0.000 05(38)	−0.001 76(56)	0.893(3)[50]	15 000
1.6	0.132 15	0.007 74(45)	−0.003 42(50)	0.894(3)[50]	15 000
1.8	0.129 53	0.012 42(62)	−0.007 78(50)	0.893(3)[50]	15 000

$a\Delta M$ and the number of trajectories accumulated. In order to obtain $c_{\rm SW}(g_0^2, L/a)$ and $\kappa_c(g_0^2, L/a)$ satisfying Eq. (31) at each β, we make fits of those data using the functional forms,

$$aM = a_M + \frac{b_M^{(1)}}{\kappa} + \frac{b_M^{(2)}}{\kappa^2} + c_M^{(1)} c_{\rm SW} + c_M^{(2)} c_{\rm SW}^2 + \frac{d_M}{\kappa} c_{\rm SW}, \tag{43}$$

$$a\Delta M = a_{\Delta M} + \frac{b_{\Delta M}^{(1)}}{\kappa} + \frac{b_{\Delta M}^{(2)}}{\kappa^2} + c_{\Delta M}^{(1)} c_{\rm SW} + c_{\Delta M}^{(2)} c_{\rm SW}^2 + \frac{d_{\Delta M}}{\kappa} c_{\rm SW}. \tag{44}$$

The results for $c_{\rm SW}(g_0^2, L/a)$ and $\kappa_c(g_0^2, L/a)$ obtained with the fits, and the adopted functional form are tabulated in Tables VIII, IX, and X. The details of the fit procedure are as follows. In Figs. 1–3 we plot data on the $(aM, a\Delta M)$ plane for $N_f = 3$, 2, and 0, respectively. For those data for which the origin (0, 0) is contained in or close to the data

TABLE VIII. Numerical values of $c_{\rm SW}(g_0^2, L/a)$ and $\kappa(g_0^2, L/a)$ satisfying Eq. (31) in three-flavor QCD.

β	L/a	Function	$c_{\rm SW}(g_0^2, L/a)$	$\kappa(g_0^2, L/a)$
12.00	8	Linear	1.0546(25)	0.126 842 1(61)
8.85	8	Linear	1.0761(32)	0.127 513(10)
5.00	8	Linear	1.1311(48)	0.129 641(26)
3.00	8	Linear	1.254(15)	0.133 18(14)
2.60	8	Linear	1.359(13)	0.134 23(14)
2.40	8	Linear	1.384(23)	0.135 45(29)
2.20	8	Linear	1.508(29)	0.135 87(39)
2.10	8	Linear	1.649(58)	0.135 21(85)
2.00	8	Quadratic	1.670(56)	0.136 39(89)
2.00	6	Quadratic	1.632(45)	0.136 96(77)
1.90	6	Quadratic	1.739(53)	0.137 41(98)

TABLE IX. Same as Table VIII, but for two-flavor QCD.

β	L/a	Function	$c_{\rm SW}(g_0^2, L/a)$	$\kappa(g_0^2, L/a)$
12.00	8	Linear	1.0558(27)	0.126 850 9(66)
8.85	8	Linear	1.0818(85)	0.127 519(27)
5.00	8	Linear	1.1334(62)	0.129 686(34)
3.00	8	Linear	1.276(20)	0.133 20(19)
2.60	8	Linear	1.327(49)	0.134 96(55)
2.20	8	Linear	1.519(32)	0.136 49(48)
2.10	8	Linear	1.672(65)	0.135 8(10)
2.10	6	Linear	1.598(19)	0.136 89(31)
2.00	6	Linear	1.777(27)	0.136 12(47)

TABLE X. Same as Table VIII, but for quenched QCD.

β	L/a	Function	$c_{\rm SW}(g_0^2, L/a)$	$\kappa(g_0^2, L/a)$
24.00	8	Linear	1.0375(16)	0.125 902 6(23)
12.00	8	Linear	1.0627(27)	0.126 857 4(65)
8.85	8	Linear	1.0829(47)	0.127 565(15)
5.00	8	Linear	1.1540(42)	0.129 701(23)
3.00	8	Linear	1.338(20)	0.133 08(19)
2.70	8	Linear	1.429(10)	0.133 80(12)
2.70	6	Linear	1.3608(79)	0.134 554(92)
2.60	6	Linear	1.414(14)	0.134 70(17)

region, we make a fit leaving only the constant and linear terms in Eqs. (43) and (44). This applies to all cases except for the three-flavor simulations at $\beta \leq 2.2$, and the dotted lines in the figures show the fit results.

In the three-flavor simulations at $\beta \leq 2.2$, the region of negative aM is not covered, and the origin is missed by the data. This happens because the PHMC algorithm tends to fail at vanishing or negative PCAC quark masses at low β due to large quantum fluctuations. Thus, at $\beta \leq 2.2$, we are forced to extrapolate the data. In the extrapolation, three functional forms are examined: (i) linear, (ii) quadratic without the cross terms, and (iii) quadratic with the cross terms. At $\beta = 2.20$ and 2.10, a linear function well fits the data, and we take this in the following analysis. The data at $\beta = 2.00$ and 1.90 require the quadratic term, but it turns out that including the cross terms does not reduce χ^2/d.o.f. significantly from that without the cross terms, and leads to $c_{\rm SW}(g_0^2, L/a)$ and $\kappa_c(g_0^2, L/a)$ consistent within 1 standard deviation. Thus, we adopt the quadratic function without the cross terms at these β, and d_M and $d_{\Delta M}$ are always set to zero throughout this analysis.

Next, $c_{\rm SW}(g_0^2, L/a)$ and $\kappa_c(g_0^2, L/a)$ are transformed into those for the desired lattice volume, $(L^*/a)^3 \times 2(L^*/a)$, along the line presented in Sec. III B. Using

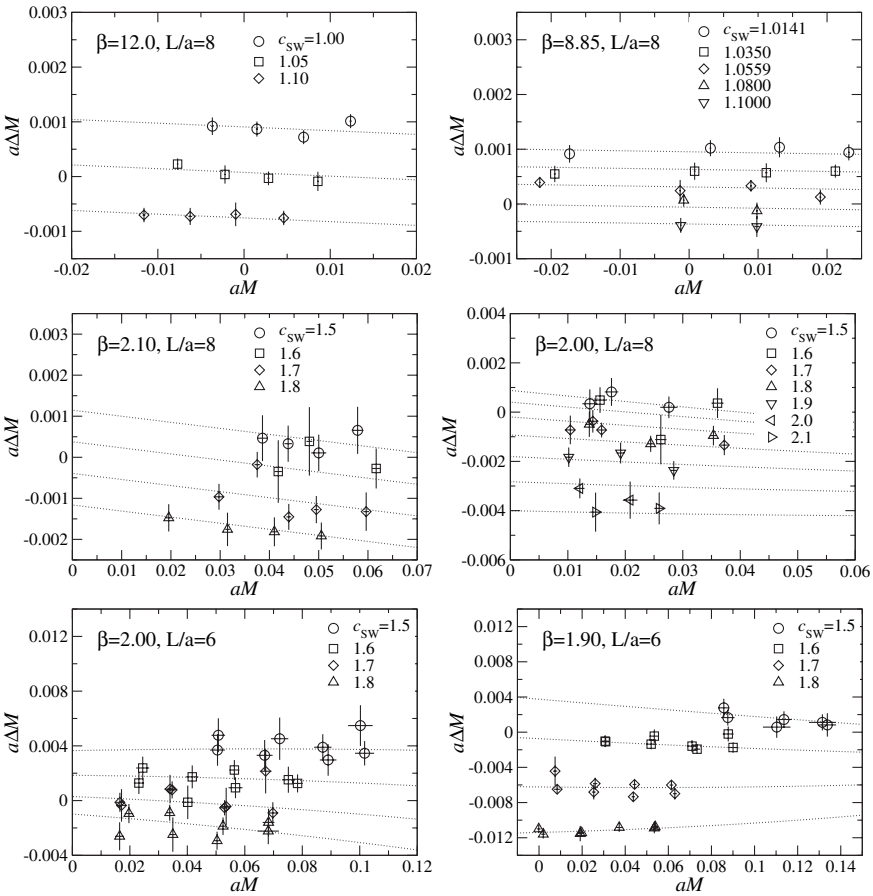

FIG. 1. aM dependence of $a\Delta M$ in three-flavor QCD.

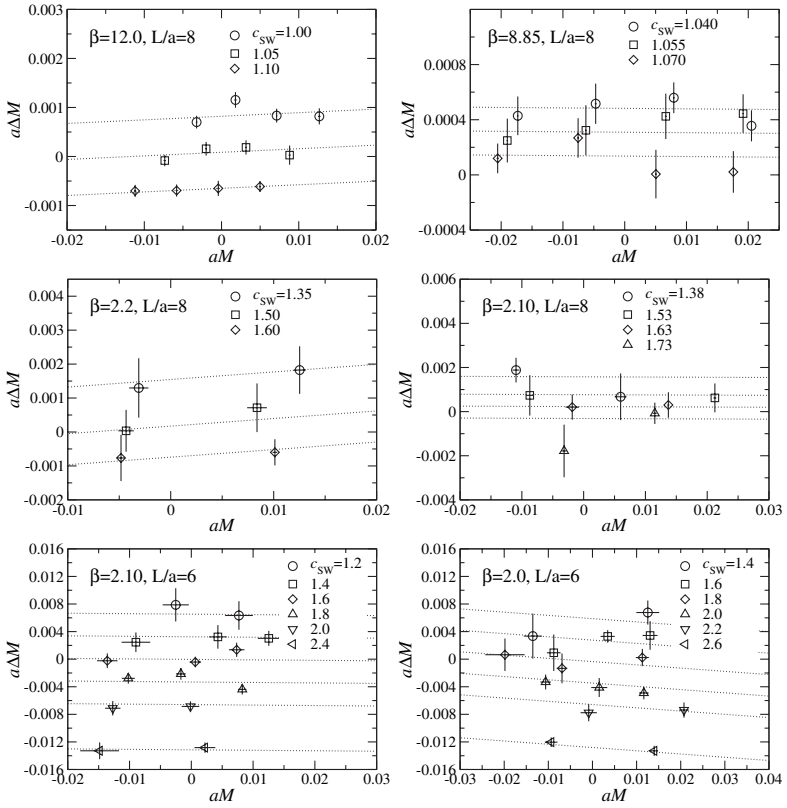

FIG. 2. Same as Fig. 1, but in two-flavor QCD.

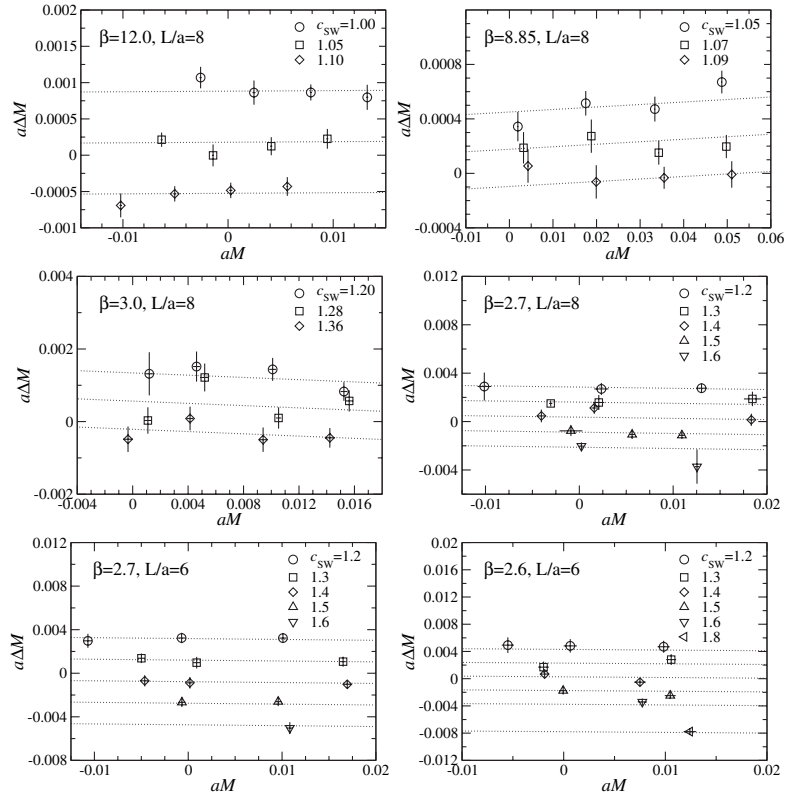

FIG. 3. Same as Fig. 1, but in quenched QCD.

TABLE XI. Final results for $c_{\rm SW}(g_0^2, L^*/a)$ and $\kappa(g_0^2, L^*/a)$ for fixed physical size L^* for three-flavor QCD.

β	L/a	L^*/a	$c_{\rm SW}(g_0^2, L^*/a)$	$\kappa_c(g_0^2, L^*/a)$
12.00	8	$7.508\,095 \times 10^6$	1.0601(25)	0.126 906 0(61)
8.85	8	$8.462\,365 \times 10^4$	1.0903(32)	0.127 592(10)
5.00	8	$3.807\,760 \times 10^2$	1.1825(48)	0.129 764(26)
3.00	8	$2.502\,040 \times 10^1$	1.368(15)	0.133 25(14)
2.60	8	$1.475\,172 \times 10^1$	1.467(13)	0.134 24(14)
2.40	8	$1.136\,512 \times 10^1$	1.471(23)	0.135 44(29)
2.20	8	8.780 129	1.542(29)	0.135 86(39)
2.10	8	7.726 477	1.633(58)	0.135 21(85)
2.00	8	6.805 369	1.576(56)	0.136 42(89)
2.00	6	6.805 369	1.742(45)	0.136 91(77)
2.00	6.805 369	6.805 369	1.650(51)	0.136 69(83)
1.90	6	6	1.739(53)	0.137 41(98)

Eqs. (35) and (36) and the $\delta c_{\rm SW}$ and $\delta\kappa_c$ given in Tables II, III, and IV, we obtain $c_{\rm SW}(g_0^2, L^*/a)$ and $\kappa_c(g_0^2, L^*/a)$ shown in Tables XI, XII, and XIII. Notice that in Table XI there are three results for $\beta = 2.0$. The first and second ones are obtained by transforming the data with $8^3 \times 16$ and $6^3 \times 12$ to those for $L^*/a \sim 6.805$, respectively, and the third one is obtained by simply interpolating the two raw values at $L/a = 8$ and 6 in Table VIII to $L^*/a \sim 6.805$, for which the corrections at finite lattice size are essentially corrected nonperturbatively. The two raw values, 1.670(56) at $L/a = 8$ and 1.632(45) at $L/a = 6$, are very close to each other and consistent within the error, and hence the linear interpolation to $L^*/a \sim 6.805$ is more reliable than the perturbative procedure. Similar observations are made at the second smallest β in each N_f flavor simulation, namely, at $\beta = 2.10$ for $N_f = 2$ and at $\beta = 2.70$ for $N_f = 0$. Thus, at these β the result interpolated to L^*/a is adopted as our final result, and used in the following analysis. At the same time, it is worth noting that in all three cases the one-loop corrections have the right sign, which indicates that the one-loop correction dominates over higher loop corrections. Furthermore, the discrepancy between the results corrected perturbatively and nonperturbatively is found to be 5%, 3%, and less than 1% for the $N_f = 3$, 2, and 0 cases, respectively, while the size of the one-loop correction itself at these β is 6%–7%, 5%, and 2%–3%. From this observation, we expect that the size of the one-loop correction gives a conservative estimate for the unknown higher loop corrections for all β.

TABLE XII. Same as Table XI, but for two-flavor QCD.

β	L/a	L^*/a	$c_{\rm SW}(g_0^2, L^*/a)$	$\kappa(g_0^2, L^*/a)$
12.00	8	$2.350\,129 \times 10^6$	1.0583(27)	0.126 910 0(66)
8.85	8	$3.656\,026 \times 10^4$	1.0919(85)	0.127 592(27)
5.00	8	$2.446\,546 \times 10^2$	1.1797(62)	0.129 794(34)
3.00	8	$1.982\,120 \times 10^1$	1.371(20)	0.133 23(19)
2.60	8	$1.219\,378 \times 10^1$	1.405(49)	0.134 95(55)
2.20	8	7.575 548	1.498(32)	0.136 51(48)
2.10	8	6.738 767	1.590(65)	0.135 8(10)
2.10	6	6.738 767	1.682(19)	0.136 80(31)
2.10	6.738 767	6.738 767	1.631(39)	0.136 38(63)
2.00	6	6	1.777(27)	0.136 12(47)

TABLE XIII. Same as Table XI, but for quenched QCD.

β	L/a	L^*/a	$c_{\rm SW}(g_0^2, L^*/a)$	$\kappa(g_0^2, L^*/a)$
24.00	8	$3.088\,560 \times 10^{11}$	1.0264(16)	0.125 937 0(23)
12.00	8	$2.409\,888 \times 10^5$	1.0590(27)	0.126 908 0(65)
8.85	8	$6.326\,167 \times 10^3$	1.0852(47)	0.127 627(15)
5.00	8	$8.042\,260 \times 10^1$	1.1921(42)	0.129 763(23)
3.00	8	9.115 448	1.359(20)	0.133 05(19)
2.70	8	6.655 769	1.381(10)	0.133 89(12)
2.70	6	6.655 769	1.4006(79)	0.134 470(92)
2.70	6.655 769	6.655 769	1.388(9)	0.134 26(10)
2.60	6	6	1.414(14)	0.134 70(17)

C. Interpolation formula

Our final results for $c_{\rm SW}(g_0^2, L^*)$ as a function of g_0^2 are shown in Fig. 4 for $N_f = 3$, 2, and 0 flavor QCD. When we interpolate $c_{\rm SW}$, not all available data are used in the fit. As mentioned in Sec. III B, the corrections at finite lattice size estimated perturbatively are small only around the high and low ends of β due to our choice of L^*, while in the middle range corrections may be significant. Therefore, we use data only if the correction is less than 5%. In the three-flavor case, the data at $\beta = 12.0$, 8.85, 2.2, 2.1, 2.0, and 1.9 are employed. As a consequence, we obtain the following interpolation formula:

$$c_{\rm SW}(g_0^2, L^*) = 1 + 0.113 g_0^2 + 0.0209(72)(g_0^2)^2 + 0.0047(27)(g_0^2)^3, \quad (45)$$

$(\chi^2/\text{d.o.f.} = 0.58)$.

For κ_c shown in Fig. 5, the corrections are smaller than 5% for all values of β. Including all data in the fit we obtain

$$\kappa_c(g_0^2, L^*) = 1/8 + 0.003\,681\,192 g_0^2 + 0.000\,211(43)(g_0^2)^2 + 0.000\,067(66)(g_0^2)^3 - 0.000\,038(21)(g_0^2)^4,$$

$(\chi^2/\text{d.o.f.} = 1.1)$. (46)

When performing the above fits, the tree and one-loop coefficients are fixed to the perturbative values at infinite volume. This is justified since, as seen in Table II, L^*/a grows very rapidly with β, and hence a/L^* corrections in Eqs. (39)–(42) are all negligibly small near the continuum limit. We also note that the tree and one-loop coefficients in the infinite volume limit do not depend on N_f, and hence the same values are used in the analysis for the $N_f = 2$ and 0 cases given below.

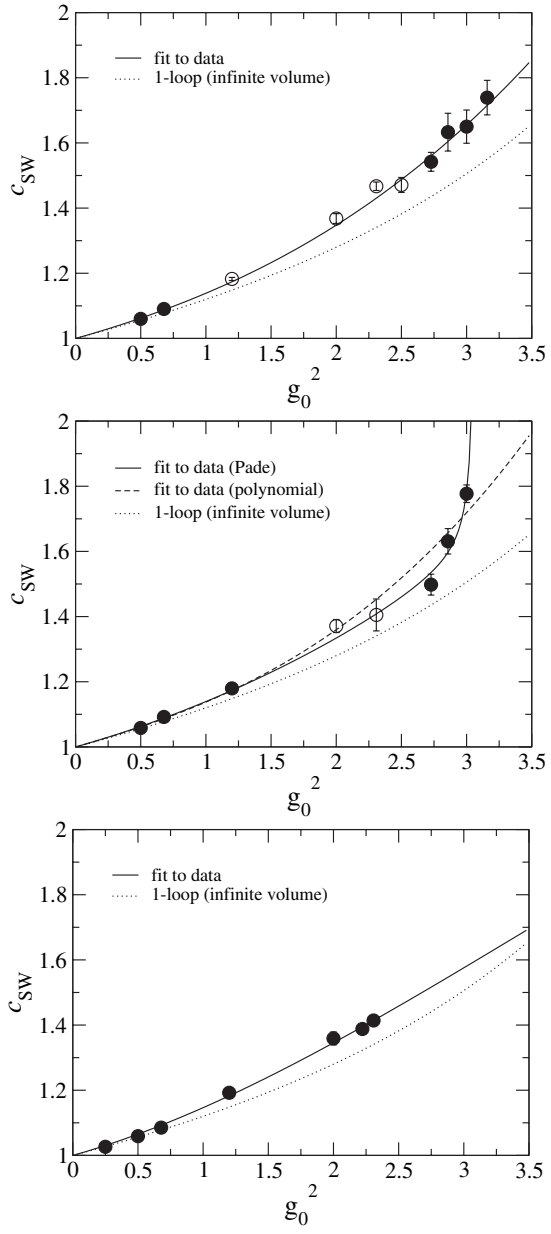

FIG. 4. g_0^2 dependence of $c_{\rm SW}^{\rm NP}(g_0^2, L^*/a)$ in $N_f = 3$, 2, and 0 flavor QCD from top to bottom. Filled symbols are used for curve fitting.

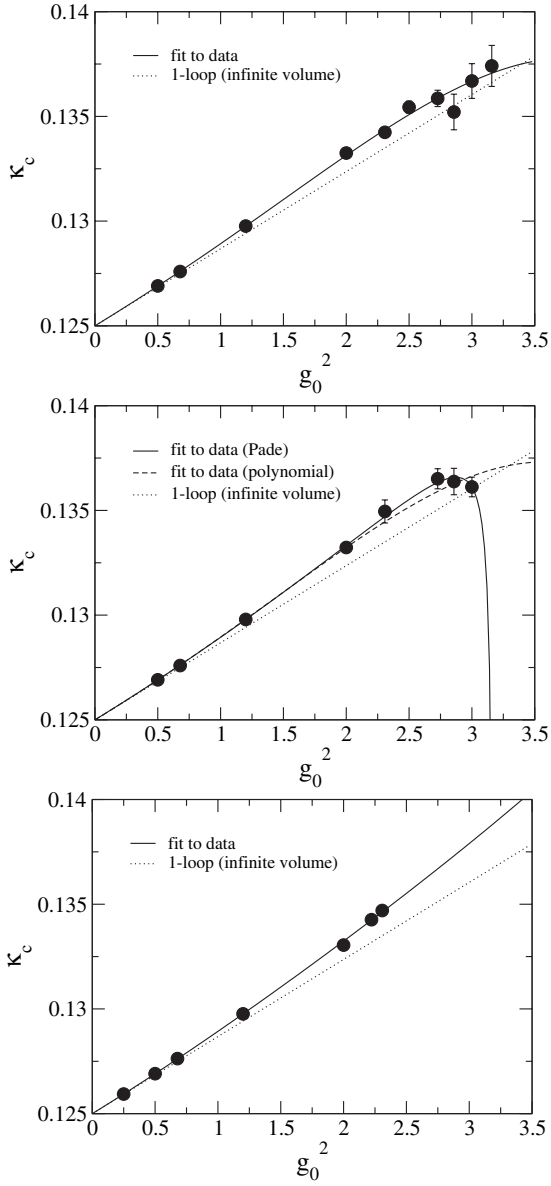

FIG. 5. g_0^2 dependence of $\kappa_c(g_0^2, L^*/a)$ in $N_f = 3$, 2, and 0 flavor QCD from top to bottom.

The interpolation formula for $c_{\rm SW}$ in two-flavor QCD is calculated in the same fashion as in the three-flavor case. In this case, the sizes of the corrections at finite lattice size are acceptable ($\leq 5\%$) at $\beta = 12.0, 8.85, 5{,}0, 2.2, 2.1$, and 2.0. We first try a polynomial form as before, and obtain

$$c_{\rm SW}(g_0^2, L^*) = 1 + 0.113 g_0^2 + 0.0158(63)(g_0^2)^2 + 0.0088(24)(g_0^2)^3, \quad (47)$$

$(\chi^2/\text{d.o.f.} = 4.68)$,

which is denoted by a dashed line in Fig. 4. A sharp rise of the data points near $g_0^2 = 3.0$ is not described well by this polynomial form, while in the three-flavor case the polynomial worked well over the whole range of β we studied. An alternative is a Padé function, with which we obtain

$$c_{\rm SW}(g_0^2, L^*) = \frac{1 - 0.212(9) g_0^2 - 0.0108(38)(g_0^2)^2 - 0.0083(19)(g_0^2)^3}{1 - 0.325(9) g_0^2}, \quad (48)$$

$(\chi^2/\text{d.o.f.} = 2.11)$.

This fit, denoted by a solid line in the middle panel of Fig. 4, interpolates our data very well. Since this formula has a pole at $g_0^2 = 3.08(8)$, its use is restricted to $g_0^2 \lesssim 3.0$. For κ_c, we use all available data to obtain

$$\kappa_c(g_0^2, L^*) = 1/8 + 0.003\,681\,192 g_0^2 + 0.000\,227(58)(g_0^2)^2 + 0.000\,093(84)(g_0^2)^3 - 0.000\,049(24)(g_0^2)^4, \quad (\chi^2/\text{d.o.f.} = 0.98), \tag{49}$$

for a polynomial, and

$$\kappa_c(g_0^2, L^*) = \frac{1/8 - 0.0356(23) g_0^2 - 0.000\,89(8)(g_0^2)^2 - 0.000\,09(6)(g_0^2)^3}{1 - 0.314(18) g_0^2}, \qquad (\chi^2/\text{d.o.f.} = 0.35), \tag{50}$$

for a Padé function. These results appear in the middle panel of Fig. 5 as a dashed and a solid line, respectively. It is interesting that the pole positions for $c_{\rm SW}$ and κ_c are consistent with each other. This seems to indicate that above $g_0^2 \sim 3.0$ the Wilson quark action cannot be improved in this fashion consistently for the $N_f = 2$ case. All in all the Padé fits provide a more satisfactory interpolation of the $N_f = 2$ data, and we take them as the main result for the $N_f = 2$ case. We have also applied a Padé function for $c_{\rm SW}$ in the $N_f = 3$ case. However, in this case the resulting fit lies on top of that for a polynomial over the range of β we used, and the position of the pole can be determined only poorly. Hence there seems no reason to favor the Padé fit over the polynomial for interpolating the data. The differences between the $N_f = 2$ and 3 cases probably arise from the fact, empirically known, that the $N_f = 2$ lattice is coarser than the $N_f = 3$ lattice at the same value of g_0^2. Indeed, a sharp rise of improvement coefficients was previously seen for the plaquette gauge action toward coarse lattices [7,8].

In quenched QCD, the size of the correction is smaller than 5% for all available data, and we use all data to obtain

$$c_{\rm SW}(g_0^2, L^*) = 1 + 0.113 g_0^2 + 0.0371(54)(g_0^2)^2 - 0.0036(26)(g_0^2)^3, \quad (\chi^2/\text{d.o.f.} = 4.09), \tag{51}$$

$$\kappa_c(g_0^2, L^*) = 1/8 + 0.003\,681\,192 g_0^2 + 0.000\,293(37)(g_0^2)^2 - 0.000\,053(65)(g_0^2)^3 + 0.000\,008(24)(g_0^2)^4, \quad (\chi^2/\text{d.o.f.} = 0.46). \tag{52}$$

In Ref. [20], the authors performed a one-loop determination of $c_{\rm SW}^{(1)}$ with conventional perturbation theory, and reported a very precise value $c_{\rm SW}^{(1)} = 0.113\,005\,91(1)$ in the infinite volume limit. Changes in our results due to the use of this value in the above analyses are expected to be negligibly small.

V. SYSTEMATIC ERRORS

There are two sources of systematic errors in our analysis, both related to the conversion to a fixed physical length scale L^*, one being the use of the two-loop β function to estimate L^* as a function of g_0^2, and the second being the use of the one-loop perturbation theory for correcting the value of $c_{\rm SW}$ from L to L^*.

In order to examine the magnitude of uncertainties from the first error, we go through the analysis using the three-loop β function. Since the three-loop term of the lattice β function is not available for the RG-improved gauge action, we take the value for the plaquette gauge action. Thus the following argument is only semiquantitatively valid. In this case, Eq. (32) is replaced with

$$a\Lambda_L = \exp\left(-\frac{1}{2b_0 g_0^2}\right)(b_0 g_0^2)^{-b_1/2b_0^2} \times (1 + q g_0^2), \tag{53}$$

where $q = 0.189\,603\,50(1)$, 0.4529(1), and 0.6138(2) for $N_f = 0$, 2, and 3 [21], respectively. With this function, we estimate L^*/a, $\delta c_{\rm SW}$, and $\delta\kappa_c$ with $N_f = 3$, which are tabulated in Table XIV. Comparing with Table II, it is found that L^*/a changes significantly while the changes in $\delta c_{\rm SW}$ and $\delta\kappa_c$ are at most a few percent and hence small. Thus we conclude that the uncertainty from the scaling violation in the lattice spacing is negligible.

In order to discuss the uncertainty of one-loop corrections, we write $c_{\rm SW}(g_0^2, L^*)$ determined through our procedure as

$$c_{\rm SW}(g_0^2, L^*) = c_{\rm SW}(g_0^2, \infty) + c^{(0)}(a/L^*) + g_0^2 c^{(1)}(a/L^*) + g_0^4 c^{(2)}(a/L^*) + g_0^4 (c^{(2)}(a/L) - c^{(2)}(a/L^*)) + O(g_0^6). \tag{54}$$

In other words, Eq. (54) represents the difference between $c_{\rm SW}(g_0^2, L^*)$ and $c_{\rm SW}(g_0^2, \infty)$ in terms of the perturbative series with coefficients $c^{(i)}(a/L)$, where $c^{(i)}(a/L)$ vanishes as $L \to \infty$. Since we have corrected the mismatch between $c_{\rm SW}(g_0^2, L/a)$ and $c_{\rm SW}(g_0^2, L^*/a)$ only at the tree and one-loop level, the unwanted a/L dependence remains at two-loop and higher. Replacing $c_{\rm SW}^{\rm sim}$ in Eq. (29) with Eq. (54), we obtain

$$Q - Q^{\rm latt}(a) = (c^{(0)}(a/L^*) + g_0^2 c^{(1)}(a/L^*) + g_0^4 c^{(2)}(a/L^*)) \cdot (a\Lambda_{\rm QCD}) + g_0^4 (c^{(2)}(a/L) - c^{(2)}(a/L^*)) \cdot (a\Lambda_{\rm QCD}) + O(g_0^6 a\Lambda_{\rm QCD} a/L) + O(a^2\Lambda_{\rm QCD}^2), \tag{55}$$

where we omit an unknown $O(1)$ overall coefficient q, because it is not relevant in the following discussion. If you expand $c^{(i)}(a/L^{(*)})$ around $a/L^{(*)} = 0$, the first term in Eq. (55) behaves $\sim a^2\Lambda_{\rm QCD}/L^* \sim O(a^2)$ because L^* is fixed. The second term behaves like $\sim g_0^4(a/L - a/L^*) \times (a\Lambda_{\rm QCD})$, which gives $O(a)$ scaling violation because a/L

TABLE XIV. L^*/a, $\delta c_{\rm SW}$, and $\delta\kappa_c$ with the three-loop β function Eq. (53).

β	L/a	L^*/a	$\delta c_{\rm SW}(g_0^2, L/a; L^*/a)$	$\delta\kappa_c(g_0^2, L/a; L^*/a)$
12.00	8	$1.688\,064 \times 10^{7}$	$5.509\,123 \times 10^{-3}$	$6.348\,932 \times 10^{-5}$
8.85	8	$1.755\,852 \times 10^{5}$	$1.412\,367 \times 10^{-2}$	$7.951\,364 \times 10^{-5}$
5.00	8	$6.442\,878 \times 10^{2}$	$4.794\,420 \times 10^{-2}$	$1.251\,814 \times 10^{-4}$
3.00	8	$3.300\,322 \times 10^{1}$	$1.179\,115 \times 10^{-1}$	$9.547\,393 \times 10^{-5}$
2.60	8	$1.793\,750 \times 10^{1}$	$1.198\,918 \times 10^{-1}$	$3.523\,283 \times 10^{-5}$
2.40	8	$1.317\,591 \times 10^{1}$	$1.058\,685 \times 10^{-1}$	$1.836\,828 \times 10^{-6}$
2.20	8	9.648 020	$6.105\,866 \times 10^{-2}$	$-1.406\,025 \times 10^{-5}$
2.10	8	8.244 442	$1.257\,961 \times 10^{-2}$	$-4.125\,600 \times 10^{-6}$
2.00	8	7.037 491	$-7.046\,997 \times 10^{-2}$	$2.824\,179 \times 10^{-5}$
2.00	6	7.037 491	$1.335\,089 \times 10^{-1}$	$-6.098\,453 \times 10^{-5}$
1.90	6	6	0	0

is fixed. As a result, the leading scaling violation could be $O(a)$ rather than $O(a^2)$. However it should be emphasized that when we obtain the interpolation formula we used only the weak coupling and the strong coupling regions because in these regions the perturbative errors are expected to be under control for the following reasons. In the weak coupling region, L/a and L^*/a are different by several orders of magnitude, but the coupling is very small, and hence the size of $O(g^4(a/L - a/L^*)(a\Lambda_{\rm QCD}))$ is expected to be as small as the size of the one-loop corrections. On the other hand, in the strong coupling region, L/a and L^*/a are close to each other, and again the remaining $O(a)$ scaling violation, $O(g^4(a/L - a/L^*)(a\Lambda_{\rm QCD}))$, should be small. We also saw in Sec. IV B that the size of the perturbative errors is roughly the same as that of the one-loop correction itself.

Most importantly, at our strongest and the second strongest couplings around which large-scale simulations are performed, there are no perturbative errors in $c_{\rm SW}$ due to our choice of L^* and interpolation to L^* at the second strongest couplings. Thus we believe $O(a)$ scaling violations are well below $O(a^2)$, though we need to check this in future work.

VI. CONCLUSION

In this work, we have performed a nonperturbative determination of the $O(a)$-improvement coefficient $c_{\rm SW}$ of the Wilson quark action with the RG-improved gauge action for $N_f = 3$, 2, and 0 flavor QCD. The corrections at the finite lattice size turn out to be sizable and are taken into account by modifying the improvement condition and carrying out the determination at a fixed physical length scale of L^*. While we have to resort to perturbation theory to incorporate the corrections, we have attempted to choose L^* at a moderately strong coupling, close to the range of lattice sizes of order $a^{-1} \sim 2$ GeV where physics simulations are practically made, so that their magnitudes are reasonably under control.

Using the data for $c_{\rm SW}$ thus obtained over a wide range of β, we have determined the interpolation formulas, given in Eqs. (45), (48), and (51), which represent the main results of this work. These results do depend on L^* chosen, but the removal of $O(a)$ scaling violations in physical observables holds independent of the value of L^*.

As a by-product, we have also obtained the interpolation formula for κ_c, Eqs. (46), (50), and (52), which may be useful to locate simulation points.

The three-flavor results reported here are already being used in a large-scale simulation aiming to carry out a systematic evaluation of hadronic observables for the realistic quark spectrum incorporating the dynamical up, down, and strange quarks. The preliminary results have been reported in Ref. [22].

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