

QCD phase diagram for three-flavor Möbius domain-wall fermions

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We investigate the phase transition of quantum chromodynamics (QCD) with three degenerate quark flavors at zero baryon chemical potential. Using Möbius domain-wall fermions as the lattice fermion formulation, we ensure excellent chiral symmetry preservation. Our simulations are performed at three different temporal lattice extents, $N_t = 6, 8, 12$, with a fixed lattice spacing $a = 0.1361(20)$ fm, corresponding to temperatures of 242(4), 181(3), and 121(2) MeV, respectively. We explore a range of quark masses and spatial volumes with aspect ratios N_s/N_t spanning from 2 to 4. By analyzing the mass and volume dependencies of the plaquette, plaquette susceptibility, chiral condensate, chiral susceptibilities, and Binder cumulant, we identify the pseudocritical transition quark masses from our largest lattice volumes. For $N_t = 6$, this is 184(10) MeV (determined from the plaquette susceptibility), corresponding to $m_\pi \simeq 0.96$ GeV. For $N_t = 8$ and 12, the transition points vary slightly depending on whether the total or disconnected chiral susceptibility is used, yielding ranges of 36(1)–39.1(9) MeV and 3.5(3)–3.7(2) MeV, respectively, in the $\overline{\text{MS}}$ scheme at a scale of $\mu = 2$ GeV. In terms of the pseudoscalar mass, these correspond to $m_\pi \simeq 427$ –445 MeV and 133–137 MeV. The negligible volume dependence at $N_t = 6$ and 8, combined with finite-size scaling analysis at $N_t = 12$ revealing volume growth significantly weaker than expected for a first- or second-order phase transition, points to a continuous crossover at these specific quark mass points. Additionally, we study the effects of residual chiral symmetry breaking on the chiral condensate and chiral susceptibilities using two different values of L_s .

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I. INTRODUCTION

The nature of the finite-temperature QCD phase transition at zero baryon chemical potential depends on the number of quark flavors and their masses, a dependence summarized classically in the Columbia plot [1]. At physical quark masses, it is well established that the transition is an analytic crossover [2], occurring at a pseudocritical temperature T_{pc} of approximately 156 MeV [3–6]. The order of the transition in the various limiting corners of the Columbia plot, by contrast, has remained a long-standing and challenging problem for

decades. This work addresses the corner of three degenerate light quarks ($N_f = 3$), located in the bottom left of the plot.

It is useful first to recall the two-flavor case ($N_f = 2$), which introduces the concept central to what follows. Here, the order of the chiral transition is governed by the strength of $U(1)_A$ symmetry breaking at the critical temperature T_c [7]. If $U(1)_A$ remains significantly broken, the transition is expected to be second order, in the $O(4)$ universality class; if $U(1)_A$ is effectively restored, it could instead be first order or second order in the $U(2)_L \times U(2)_R \rightarrow U(2)_V$ universality class [7–10]. Determining which scenario is realized in QCD has remained elusive due to the severe challenges of performing continuum and chiral extrapolations near the critical temperature in lattice QCD calculations [4,11–22]. Recent lattice calculations have begun to address the fate of $U(1)_A$ directly. A study using the highly improved staggered quark (HISQ) action in $N_f = 2 + 1$ QCD found that $U(1)_A$ remains effectively broken even after continuum and chiral extrapolations at $1.6T_c$, where $T_c \simeq 132$ MeV [23,24], pointing to a second-order $O(4)$

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transition in the chiral limit at the physical strange quark mass [25]. A subsequent HISQ study confirmed that $U(1)_A$ stays broken at T_c in the chiral and continuum limits of $N_f = 2 + 1$ QCD [26]. Another study using Möbius domain-wall fermions observed a strong suppression of the $U(1)_A$ susceptibility in the chiral limit at temperatures of 153–204 MeV, while it remained nonzero at 136 MeV [27].

For the $N_f = 3$ chiral limit—the subject of this work—the theoretical predictions themselves are in conflict. The universality argument of Pisarski and Wilczek [7] predicts a first-order transition. Away from the chiral limit, explicit chiral symmetry breaking weakens this first-order transition, which eventually terminates at a second-order critical line in the three-dimensional $Z(2)$ universality class. The location of this critical line is of particular importance: its extension into the plane of nonzero baryon chemical potential determines the curvature of the $Z(2)$ critical surface and thereby influences the location—or even the existence—of the critical end point in the T – μ_B QCD phase diagram at the physical point, a central target of both theoretical [6,28–33] and experimental [34] efforts.

The first-order prediction has, however, been increasingly challenged. While the ϵ -expansion of RG flows in $d = 4 - \epsilon$ dimensions [7] and early $d = 3$ analyses—both perturbative [8] and via the nonperturbative functional renormalization group (FRG) [35]—supported a first-order transition (no infrared-stable fixed point being found, regardless of the status of $U(1)_A$), a renewed $d = 3$ FRG treatment that includes all relevant operators [36,37], together with conformal bootstrap studies [38], has identified an infrared-stable fixed point. This suggests a possible second-order transition, provided $U(1)_A$ is effectively restored at the critical point. Recent conjectures [39] and extended linear sigma model analyses [40] further emphasize that a vanishing 't Hooft determinant is necessary for a second-order transition in massless $N_f = 3$ QCD. These findings collectively point to the possibility of a second-order transition in the $m_{u,d} = 0$ limit for all values of the strange quark mass, though the universality class differs between the $N_f = 2$ and $N_f = 3$ chiral limits; in these frameworks, the fate of $U(1)_A$ plays a crucial role in determining the order of the phase transition and the universality class for $N_f = 3$ massless QCD. Adding to the complexity, a truncated Dyson-Schwinger study predicts a second-order transition in the $N_f = 3$ chiral limit irrespective of the fate of $U(1)_A$ at T_c [41]. In addition, recent theoretical work revisited the QCD chiral phase transition by emphasizing additional 't Hooft anomaly constraints. It argued that, if the chiral phase transition is second order or very weakly first order for $N_f \geq 2$, the conventional Ginzburg-Landau picture is strongly constrained, and a beyond-Ginzburg-Landau conformal-manifold scenario may be a viable possibility, particularly for $N_f \geq 3$ [42]. While these theoretical approaches

provide valuable qualitative insight, their predictions do not agree.

The key open questions can therefore be stated plainly. Does a first-order region exist in the $N_f = 3$ chiral limit? If not, what is the corresponding universality class? If it does exist, what is the critical mass separating the first-order and crossover regions? Answering these questions requires nonperturbative lattice QCD simulations.

Pinpointing the transition in the $N_f = 3$ chiral region on the lattice is difficult, however, owing to the high computational cost at small quark masses and the sensitivity to cutoff effects. Early studies with staggered [43–46] and Wilson fermions [47], as well as $\mathcal{O}(a)$ -improved Wilson fermions [48], identified a first-order chiral phase transition region on coarse lattices. Subsequent studies, however, revealed that the critical pion mass extracted from such coarse lattices depends heavily on both the lattice action and the lattice spacing [30,49–56]: for both formulations the critical pion mass decreases as the lattice spacing is reduced. Moreover, a systematic discrepancy persists between them, with Wilson-type fermions consistently yielding larger critical pion masses than staggered fermions—a difference likely due to the substantial chiral symmetry breaking inherent in Wilson fermions. A similar trend appears in $N_f = 4$ QCD, where the critical pion mass shows strong cutoff effects for both staggered [57] and Wilson fermions [58], even approaching zero as the lattice spacing decreases. More recently, an $\mathcal{O}(a)$ -improved Wilson study placed an upper bound $m_\pi^c \lesssim 110$ MeV in the continuum limit of $N_f = 3$ QCD [56], a tricritical-scaling analysis with unimproved staggered fermions found evidence of a second-order transition in the chiral and continuum limits—the same conclusion was reached when the analysis of Ref. [59] was applied to the improved Wilson data of [56]—and a HISQ study likewise suggested a second-order transition in the chiral limit [60]. These results leave little room for a first-order region, though they do not rule it out entirely. Crucially, all existing results come from staggered or Wilson-type fermions, which break chiral symmetry partially or completely, with full restoration only in the continuum limit. This underscores the need to explore the $N_f = 3$ chiral phase transition using a chiral fermion formulation in order to achieve a more comprehensive understanding.

In this work, we present the first investigation of the finite-temperature phase transition in $N_f = 3$ QCD using Möbius domain wall fermions [61], a generalization of the Shamir domain wall fermion formulation. This formulation precisely preserves chiral symmetry at finite lattice spacing when the fifth dimension is sufficiently large, while significantly reducing residual chiral symmetry breaking even for smaller extents than Shamir domain wall fermions. Preliminary results from this work have been reported in previous lattice conference proceedings [62–65]. The paper is organized as follows. In Sec. II, we introduce the

observables used for determining the finite-temperature phase transition in $N_f = 3$ QCD. In Sec. III, we provide details of the simulation parameters. Sections IV and V present our numerical results at zero and finite temperature, respectively. Finally, we summarize our findings and discuss future prospects in Sec. VI. Additional details on the Möbius domain-wall fermion action and the axial Ward-Takahashi identity are collected in Appendix A, simulation parameters are compiled in Appendix B, the rational function reweighting procedure is described in Appendix C, and additional residual mass and pion screening mass results are presented in Appendix D.

II. OBSERVABLES

The Möbius domain-wall fermion action used in this work is detailed in Appendix A. Based on this action, we compute several key physical quantities in this section to quantify the residual chiral symmetry breaking and the nature of the QCD phase transition.

A. Residual mass

The Möbius domain-wall fermion formulation with a finite fifth dimension L_s allows mixing between the left- and right-handed modes, leading to residual chiral symmetry breaking. At leading order in the lattice spacing expansion, this breaking is characterized by a mass-independent residual mass m_{res} , which acts as an additive renormalization to the bare quark mass, giving the total quark mass $m = m_q + m_{\text{res}}$. In practice, m_{res} is determined nonperturbatively from the Ward-Takahashi identity of the axial current, as shown in Eq. (A15) in Appendix A. In this identity, m_q denotes the input bare quark mass, and J_5^a represents the pseudoscalar density constructed from the quark fields on the boundaries of the fifth dimension, given by

$$J_5^a(x) = \bar{\Psi}_{x,0} \lambda^a D_-^{(0)} P_+ \Psi_{x,L_s-1} - \bar{\Psi}_{x,L_s-1} \lambda^a D_-^{(L_s-1)} P_- \Psi_{x,0}, \quad (1)$$

where $P_{\pm} = \frac{1}{2}(1 \pm \gamma_5)$ are the chiral projection operators.

An additional current, the midpoint current J_{5q}^a , is built from the quark fields at $L_s/2$ and $L_s/2 - 1$:

$$J_{5q}^a(x) = \bar{\Psi}_{x,L_s/2} \lambda^a D_-^{(L_s/2)} P_+ \Psi_{x,L_s/2-1} - \bar{\Psi}_{x,L_s/2-1} \lambda^a D_-^{(L_s/2-1)} P_- \Psi_{x,L_s/2}. \quad (2)$$

The midpoint current J_{5q}^a represents an additional contribution to the continuum Ward-Takahashi identity, which is recovered only in the $L_s \rightarrow \infty$ limit for the nonsinglet flavor. The residual mass m_{res} can be determined from this midpoint current.

At large source-sink separations t , the ratio of the midpoint correlation function to the pion correlation

function,

$$R(t) = \frac{\langle \sum_{\vec{x}} J_{5q}^a(\vec{x}, t) J_5^a(\vec{0}, 0) \rangle}{\langle \sum_{\vec{x}} J_5^a(\vec{x}, t) J_5^a(\vec{0}, 0) \rangle}, \quad (3)$$

converges to a plateau value, denoted as $m_{\text{res}}(m_q)$, which depends weakly on m_q . This mass dependence is a lattice artifact arising from higher-dimension operators in the axial current divergence and represents an $\mathcal{O}(a^2)$ contribution [66,67].

The above determination ensures that m_{π} vanishes when $m_q + m_{\text{res}}(m_q) = 0$. The chiral limit is defined by vanishing total quark mass, $m_q + m_{\text{res}} = 0$, or equivalently $m_q = -m_{\text{res}}$, where m_{res} denotes a mass-independent constant. To obtain this constant, a natural approach is to extrapolate $m_{\text{res}}(m_q)$ to the chiral limit, yielding a value denoted as $m_{\text{res}}(-m_{\text{res}})$. Another popular choice is to use $m_{\text{res}}(0)$. We will use the latter throughout this work.

B. Chiral condensate, chiral susceptibilities, and Binder cumulant

The chiral condensate $\langle \bar{\psi} \psi \rangle$ serves as the order parameter for the QCD chiral phase transition, with its value being zero in the chirally symmetric phase and nonzero in the chirally broken phase. In the Möbius domain wall formulation, the physical 4D quark fields, ψ and $\bar{\psi}$, are constructed from the chiral modes localized on opposite boundaries of the fifth dimension as follows:

$$\psi_x = P_- \Psi_{x,0} + P_+ \Psi_{x,L_s-1} = [\mathcal{P}^\dagger \Psi]_{x,0}, \quad (4)$$

$$\bar{\psi}_x = \bar{\Psi}_{x,0} (-D_-^{(0)}) P_+ + \bar{\Psi}_{x,L_s-1} (-D_-^{(L_s-1)}) P_- = [\bar{\Psi} (-D_-) \mathcal{P}]_{x,L_s-1}. \quad (5)$$

Here, $\mathcal{P}$ is a permutation matrix defined as $\mathcal{P}_{ss'} = \delta_{ss'} P_- + \delta_{s',(s+1) \bmod L_s} P_+$. The quark mass m_q enters the fermion action through the coupling between the boundaries of the fifth dimension, as shown in the last two terms of Eq. (A1). Here, $D_-^{(s)}$ is related to the Wilson Dirac matrix operator (for details, please see Appendix A).

To calculate the fermionic observables, we first consider the quark propagator in a fixed gauge background U . In the fermionic path integral formalism, it is given by

$$\langle \psi_x \bar{\psi}_y \rangle_F = \frac{1}{Z_F(U)} \int \mathcal{D}\Psi \mathcal{D}\bar{\Psi} \mathcal{D}\Phi \mathcal{D}\bar{\Phi} \psi_x \bar{\psi}_y \times e^{-\bar{\Psi} D_{\text{MDWF}}(m_q, U) \Psi - \bar{\Phi} D_{\text{MDWF}}(1, U) \Phi}, \quad (6)$$

where $Z_F(U)$ is the fermionic partition function in the fixed gauge background U , and $\Phi_{x,s}, \bar{\Phi}_{x,s}$ are the 5D bosonic Pauli-Villars fields. Integrating out the fermion and Pauli-Villars fields yields

$$\langle \psi_x \bar{\psi}_y \rangle_F = \frac{1}{1 - m_q} ([D_{\text{ov}}^{L_s}(m_q)]_{x,y}^{-1} - \delta_{x,y}). \quad (7)$$

For notational convenience, we define the operator $\tilde{D}_{\text{ov}}^{L_s}(m_q)$ by

$$[\tilde{D}_{\text{ov}}^{L_s}(m_q)]_{x,y}^{-1} = \frac{1}{1 - m_q} ([D_{\text{ov}}^{L_s}(m_q)]_{x,y}^{-1} - \delta_{x,y}). \quad (8)$$

$D_{\text{ov}}^{L_s}$ is the 4D effective overlap operator utilizing the polar approximation to the sign function, given by [61]

$$D_{\text{ov}}^{L_s}(m_q) = \frac{1 + m_q}{2} + \frac{1 - m_q}{2} \gamma_5 \epsilon_{L_s}[H] \quad \text{with} \quad \epsilon_{L_s}[H] = \frac{(1 + H)^{L_s} - (1 - H)^{L_s}}{(1 + H)^{L_s} + (1 - H)^{L_s}}. \quad (9)$$

Here, $H = \gamma_5 D^{\text{Möbius}}(M_s)$, with $D^{\text{Möbius}}(M_s)$ being the Möbius kernel, whose explicit form is given in Eq. (A3) of Appendix A. In the limit $L_s \rightarrow \infty$, $\epsilon_{L_s}[H]$ converges to $\text{sign}(H)$, recovering the exact overlap operator. The exact mapping between the 4D effective operators and the 5D Möbius domain wall fermion operators is given by

$$D_{\text{ov}}^{L_s}(m_q) = \mathcal{P}^\dagger D_{\text{MDWF}}^{-1}(1) D_{\text{MDWF}}(m_q) \mathcal{P}. \quad (10)$$

The corresponding 4D quark propagator is then obtained from the inverse of the 5D Dirac operator through the relation:

$$[\tilde{D}_{\text{ov}}^{L_s}(m_q)]^{-1} = \mathcal{P}^\dagger D_{\text{MDWF}}^{-1}(m_q) (-D_-) \mathcal{P} \quad (11)$$

where $D_{\text{MDWF}}^{-1}(m_q) \equiv \langle \Psi \bar{\Psi} \rangle$. It should be noted that, because directly inverting the 4D effective overlap operator is computationally expensive, we instead construct a 5D source vector, $\xi_{\text{MDWF},0} = -D_- \mathcal{P}^\dagger \xi_0$, from the 4D source ξ_0 . We then invert the 5D Möbius domain wall fermion Dirac operator by solving $G = D_{\text{MDWF}}^{-1}(m_q) \xi_{\text{MDWF},0}$ using the even-odd preconditioned conjugate gradient method. Finally, the 5D solution G is projected back to 4D via $\mathcal{P}^\dagger G$ to yield the physical propagator $[\tilde{D}_{\text{ov}}^{L_s}(m_q)]_{x,y}^{-1}$.

The N_f -flavor Möbius domain wall fermion chiral condensate is then defined as

$$\langle \bar{\psi} \psi \rangle = \frac{T}{V} \frac{\partial \ln Z}{\partial m_q} = \frac{N_f}{N_s^3 N_t} \langle \text{Tr}(\tilde{D}_{\text{ov}}^{L_s}(m_q))^{-1} \rangle \quad (12)$$

To ensure that $\langle \bar{\psi} \psi \rangle$, as computed in Eq. (12), is finite and well-defined in the continuum limit, both additive and multiplicative renormalizations have to be applied when the quark mass is finite. The dominant ultraviolet divergence, which necessitates an additive renormalization, is a power-law term of the form $C^D(m_q + x m_{\text{res}})/a^2$, where C^D and

$x = O(1)$ are *a priori* unknown coefficients [68]. Here the $x m_{\text{res}} a^{-2}$ term arises from the finite extent L_s of the fifth dimension: the residual violation of chiral symmetry induces a similar effect to that of the quark mass term. A subleading logarithmic divergence also exists, but its contribution is highly suppressed and can be safely ignored [3]. Therefore, the chiral condensate behaves as

$$\langle \bar{\psi} \psi \rangle|_{\text{DWF}} \sim C^D \frac{m_q + x m_{\text{res}}}{a^2} + \langle \bar{\psi} \psi \rangle|_{\text{cont}} + \dots \quad (13)$$

Since $x \neq 1$, if we perform an extrapolation to the chiral limit $m_q + m_{\text{res}} = 0$ as one usually does for low-energy physics, a UV-divergent piece still remains and behaves as $C^D \frac{(x-1)m_{\text{res}}}{a^2}$. This unwanted contribution can only be effectively controlled by increasing L_s . On the one hand, if we know the value of C^D and x , we can remove the additive divergence part explicitly; on the other hand, because the UV divergence term $C^D \frac{m_q + x m_{\text{res}}}{a^2}$ is temperature independent, it can be canceled by subtracting the zero-temperature condensate $\langle \bar{\psi} \psi \rangle^{T=0}$ from the finite-temperature one $\langle \bar{\psi} \psi \rangle^{T>0}$ at the same bare parameters.

To eliminate the remaining multiplicative divergence, we multiply by the scalar density renormalization factor $Z_s^{\text{MS}}(\mu = 2 \text{ GeV}) = 1/Z_m^{\text{MS}}(\mu = 2 \text{ GeV})$, where $Z_m^{\text{MS}}(\mu = 2 \text{ GeV})$ is the quark mass renormalization constant obtained from next-to-next-to-next-to-leading order running [69]. The two renormalized chiral condensates are then defined as

$$\frac{\langle \bar{\psi} \psi \rangle^{T>0} - \langle \bar{\psi} \psi \rangle^{T=0}}{Z_m^{\text{MS}}(\mu = 2 \text{ GeV})} = [\langle \bar{\psi} \psi \rangle^{T>0} - \langle \bar{\psi} \psi \rangle^{T=0}]^{\text{MS}}(\mu = 2 \text{ GeV}), \quad (14)$$

$$\begin{aligned} & \frac{\langle \bar{\psi} \psi \rangle}{Z_m^{\text{MS}}(\mu = 2 \text{ GeV})} - C^D \frac{m_q + x m_{\text{res}}}{a^2} Z_m^{\text{MS}}(\mu = 2 \text{ GeV}) \\ &= \left[\langle \bar{\psi} \psi \rangle - C^D \frac{m_q + x m_{\text{res}}}{a^2} \right]^{\text{MS}}(\mu = 2 \text{ GeV}). \end{aligned} \quad (15)$$

The total chiral susceptibility χ_{tot} measures the response of the chiral condensate to a small change in the quark mass, and is defined as

$$\chi_{\text{tot}} = \frac{\partial \langle \bar{\psi} \psi \rangle}{\partial m_q}. \quad (16)$$

It contains two parts: the quark-line disconnected part χ_{disc} , which describes the fluctuations of the chiral condensate:

$$\chi_{\text{disc}} = \frac{N_f^2}{N_s^3 N_t} \{ \langle [\text{Tr}(\tilde{D}_{\text{ov}}^{L_s}(m_q))^{-1}]^2 \rangle - \langle \text{Tr}(\tilde{D}_{\text{ov}}^{L_s}(m_q))^{-1} \rangle^2 \}, \quad (17)$$

and the quark-line connected part χ_{con} (also denoted χ_δ):

$$\chi_\delta = -\frac{N_f}{N_s^3 N_t} \langle \text{Tr}[(\tilde{D}_{\text{ov}}^{L_s}(m_q))^{-2}] \rangle. \quad (18)$$

Alternatively, χ_δ can also be written in terms of the integrated two-point flavor nonsinglet scalar correlator:

$$\chi_\delta = -N_f \sum_x \langle \text{tr}[(\tilde{D}_{\text{ov}}^{L_s})^{-1}(x, 0)(\tilde{D}_{\text{ov}}^{L_s})^{-1}(0, x)] \rangle. \quad (19)$$

Here, tr denotes a trace over spinor and color indices only, while Tr indicates a trace that additionally includes the space-time volume. We employ stochastic trace estimation to calculate the chiral condensate and its fluctuations. To determine the connected chiral susceptibility, we utilize the integrated two-point flavor nonsinglet scalar correlator, which is readily available from the two-point correlator measurements performed for all gamma matrix insertions in the residual mass calculation.

The disconnected chiral susceptibility χ_{disc} serves as a sensitive probe of the chiral phase transition. In the chiral and infinite-volume limits, χ_{disc} diverges at the critical point, whereas χ_δ remains finite. At finite quark mass, this divergence is smoothed into a peak that reaches its maximum at the pseudocritical temperature. Unlike the connected part, χ_{disc} does not exhibit an additive divergence but requires multiplicative renormalization [3]. This is achieved using $Z_m^{\text{MS}}(\mu = 2 \text{ GeV})$ as follows:

$$\chi_{\text{disc}}^{\text{MS}}(\mu = 2 \text{ GeV}) = \frac{\chi_{\text{disc}}}{(Z_m^{\text{MS}}(\mu = 2 \text{ GeV}))^2}. \quad (20)$$

The connected chiral susceptibility, originating from the explicit quark mass dependence of the chiral condensate, requires both additive and multiplicative renormalization. Its additive divergence, which behaves as C^D/a^2 , can be removed either by subtracting the vacuum expectation value or, if C^D is known, by explicit subtraction. The multiplicative renormalization can be addressed in the same manner as for χ_{disc} .

To determine the order of the phase transition, we measure the Binder cumulant of the chiral condensate [70]. For each gauge configuration U we construct the fermion-integrated condensate

$$M(U) = \frac{N_f}{N_s^3 N_t} \text{Tr}[\tilde{D}_{\text{ov}}^{L_s}(m_q)]^{-1}(U), \quad (21)$$

the configuration-wise, c-number representative of $\bar{\psi}\psi$, so that $\langle \bar{\psi}\psi \rangle = \langle M \rangle_U$ with $\langle \cdots \rangle_U$ the gauge-ensemble average [cf., Eq. (12)]. The Binder cumulant is then

$$B_4(\bar{\psi}\psi) = \frac{\langle (\delta M)^4 \rangle_U}{\langle (\delta M)^2 \rangle_U^2}, \quad \delta M = M(U) - \langle M \rangle_U, \quad (22)$$

i.e., the Binder cumulant of the gauge-ensemble probability distribution $P(M)$ of the chiral order parameter, built from the quark-line disconnected moments.¹

To compute $B_4(\bar{\psi}\psi)$ accurately, we use an unbiased stochastic estimation method with a set of $N = 10$ independent Z_2 noise vectors. Letting $O_i = \frac{N_f}{N_s^3 N_t} \xi_i^\dagger [\tilde{D}_{\text{ov}}^{L_s}(m_q)]^{-1} \xi_i$ be the estimate from a single noise vector, the required moments are constructed by averaging over all unique combinations of these individual estimators [71]. This approach is crucial for eliminating statistical bias that would arise from reusing noise vectors within a product. For a fixed gauge configuration, the unbiased stochastic estimators of the first four powers of $M(U)$ are

$$\overline{M} = \frac{1}{\binom{10}{1}} \sum_{i=1}^{10} O_i, \quad (23)$$

$$\overline{M^2} = \frac{1}{\binom{10}{2}} \sum_{1 \leq i < j \leq 10} O_i O_j, \quad (24)$$

$$\overline{M^3} = \frac{1}{\binom{10}{3}} \sum_{1 \leq i < j < k \leq 10} O_i O_j O_k, \quad (25)$$

$$\overline{M^4} = \frac{1}{\binom{10}{4}} \sum_{1 \leq i < j < k < l \leq 10} O_i O_j O_k O_l, \quad (26)$$

where the overline denotes the average over the noise vectors on a fixed gauge configuration and the indices i, j, k, l label these vectors, not quark flavors. The gauge-ensemble average is performed subsequently. We can distinguish different types of phase transitions by the result of $B_4(\bar{\psi}\psi)$. In the thermodynamic limit, $B_4(\bar{\psi}\psi) = 1$ represents a first-order phase transition; $B_4(\bar{\psi}\psi) = 3$ corresponds to a smooth crossover; and $B_4(\bar{\psi}\psi) = 1.604$ indicates a second-order phase transition belonging to the 3D $Z(2)$ universality class [72]. However, at finite volume, $B_4(\bar{\psi}\psi)$ deviates from its infinite-volume limits ($B_4(\bar{\psi}\psi) = 1$ for a first-order transition and $B_4(\bar{\psi}\psi) = 3$ for a crossover) due to finite-volume corrections, approaching these values only in the thermodynamic limit. In contrast, at a second-order critical point, the $B_4(\bar{\psi}\psi)$ curves for different volumes are expected to intersect in the vicinity of the critical point for sufficiently large volumes. Our goal is to determine the order of the phase transition at

¹The cumulants of the microscopic condensate operator, given by $\partial^n \ln Z / \partial m_q^n$, contain in addition quark-line connected contributions; at second order this is the decomposition $\chi_{\text{tot}} = \chi_{\text{disc}} + \chi_\delta$ of Eqs. (17) and (18). The connected contributions are subleading near the chiral critical point and regular away from it, so that the limiting values of $B_4(\bar{\psi}\psi)$ given below are the same for either definition.

the transition mass point for a fixed temperature via measurements of the Binder cumulant.

III. LATTICE PARAMETERS AND SIMULATION DETAILS

We perform $N_f = 3$ QCD simulations using the tree-level improved Symanzik gauge action and the Möbius domain-wall fermion action with three steps of stout smearing [62,63]. The simulations are carried out with the Grid code, using a version optimized for the A64FX architecture of the Fugaku supercomputer [73]. We choose a fixed gauge coupling of $\beta = 4.0$, corresponding to a lattice spacing of $a = 0.1361(20)$ fm. The lattice spacing is determined from the Wilson-flow scale t_0 , defined by the condition $t^2 \langle E(t) \rangle|_{t=t_0} = 0.3$, with $\sqrt{t_0}$ set to its physical value of $0.1465(21)(13)$ fm as obtained in $N_f = 2 + 1$ QCD [74]. The calculations are carried out on lattices of size $N_s^3 \times N_t \times L_s = N_s^3 \times 6 \times 16$ with $N_s = 12, 16, N_s^3 \times 8 \times 16$ with $N_s = 16, 24$; as well as $N_s^3 \times 12 \times 16$ with $N_s = 24, 36$ and 48 . These temporal extents $N_t = 6, 8, 12$ correspond to temperatures of $242(4)$, $181(3)$, and $121(2)$ MeV, respectively, and encompass a range of quark masses. Specifically, we simulated 41 and 21 quark masses within $am_q \in [0, 0.4]$ and $[0.05, 0.25]$ for the $12^3 \times 6 \times 16$ and $16^3 \times 6 \times 16$ ensembles, respectively; 11 and 15 quark masses within $am_q \in [0, 0.2]$ and $[0, 0.14]$ for the $16^3 \times 8 \times 16$ and $24^3 \times 8 \times 16$ ensembles, respectively; 26 quark masses within $am_q \in [-0.006, 0.1]$ for $24^3 \times 12 \times 16$ ensembles, 7 quark masses within $am_q \in [-0.005, 0.001]$ for $36^3 \times 12 \times 16$ ensembles, and $am_q = -0.003$ and -0.004 for $48^3 \times 12 \times 16$ ensembles. L_s is 16 for all the above ensembles. To check the residual chiral symmetry breaking effect and the stability of the molecular dynamics evolution in the hybrid Monte Carlo simulation for the above $N_t = 12$, $L_s = 16$ ensembles, we generated $24^3 \times 12 \times 32$ ensembles with five quark masses in the range between -0.001 and 0.003 . For each parameter set, we accumulate between $\sim 10^4$ and $\sim 10^5$ trajectories, performing measurements every 10 trajectories, except for the $N_t = 8$ ensembles, where configurations were analyzed every 100 trajectories. Further details are given in Tables II–IV of Appendix B.

Apart from the finite temperature ensembles, we also generated zero-temperature ensembles at several gauge couplings: $\beta = 4.0$ and 4.1 on $24^3 \times 48 \times 16$ ensembles, and $\beta = 4.17$ on $32^3 \times 64 \times 16$ ensembles, each with several quark masses (see Table V in Appendix B). These zero-temperature ensembles are utilized to calculate the lattice spacing, pion mass, residual mass, and the zero-temperature chiral condensate, which is used to subtract the UV divergence present in the finite-temperature chiral condensate. For the stochastic estimation of the chiral condensate, $N_{src} = 10$ noise vectors were used per

configuration. While the random seeds remained independent for every measurement within an individual stream, for ensembles with multiple streams, the seeds were identical across different streams for the same trajectory number. To ensure this correlation across streams did not introduce significant bias, we performed a cross-check on a representative ensemble using independent random seeds for all measurements. The results were found to be consistent within statistical errors. Since the configuration generation process utilized independent seeds and was not affected, we retain the original results to avoid additional computational cost.

Our Möbius domain-wall fermion configurations are generated using the same algorithmic setup as in $N_f = 2 + 1$ QCD simulations implemented in the Grid code. In this setup, the two degenerate light flavors are simulated using the standard hybrid Monte Carlo (HMC) algorithm, while the remaining single flavor is simulated using the rational hybrid Monte Carlo (RHMC) algorithm. In the present $N_f = 3$ degenerate case, we set $m_s = m_l = m_q$, so the product of the two-flavor HMC determinant and the one-flavor RHMC determinant reproduces the desired $\det[D_{\text{MDWF}}^\dagger(m_q)D_{\text{MDWF}}(m_q)]^{3/2}$. After integrating out the Grassmann-valued fermions and Pauli-Villars fields, the fractional power appears only in the one-flavor RHMC factor. Introducing bosonic pseudofermion fields ϕ_l and ϕ_s for the two-flavor HMC and one-flavor RHMC sectors, respectively, the determinant ratio can be represented as

$$\frac{\det[D_{\text{MDWF}}^\dagger(m_q)D_{\text{MDWF}}(m_q)]^{3/2}}{\det[D_{\text{MDWF}}^\dagger(1)D_{\text{MDWF}}(1)]^{3/2}} = \int \mathcal{D}\phi_l^\dagger \mathcal{D}\phi_l \mathcal{D}\phi_s^\dagger \mathcal{D}\phi_s e^{-S_{pf}}, \quad (27)$$

where the pseudofermion action is given by

$$S_{pf} = \phi_l^\dagger \left(\frac{D_{\text{MDWF}}^\dagger(m_q)D_{\text{MDWF}}(m_q)}{D_{\text{MDWF}}^\dagger(1)D_{\text{MDWF}}(1)} \right)^{-1} \phi_l + \phi_s^\dagger \left(\frac{D_{\text{MDWF}}^\dagger(m_q)D_{\text{MDWF}}(m_q)}{D_{\text{MDWF}}^\dagger(1)D_{\text{MDWF}}(1)} \right)^{-1/2} \phi_s. \quad (28)$$

The fractional power in the one-flavor RHMC part is approximated using a rational function, written in the partial fraction form $x^{-1/2} \simeq a_0 + \sum_{i=1}^n \frac{a_i}{x+b_i}$. The multishift solver solves the set of linear systems $(D_{\text{MDWF}}^\dagger(m_q)D_{\text{MDWF}}(m_q) + b_i)v_i = \phi_s$ for all shifts b_i simultaneously, requiring essentially the same number of applications as for a single matrix inversion using the conjugate gradient method [75].

In our $N_f = 3$ simulations on $36^3 \times 12 \times 16$ ensembles, the number of terms used in the rational function was found to be insufficient. This limited precision causes the generated gauge configurations to deviate slightly from the

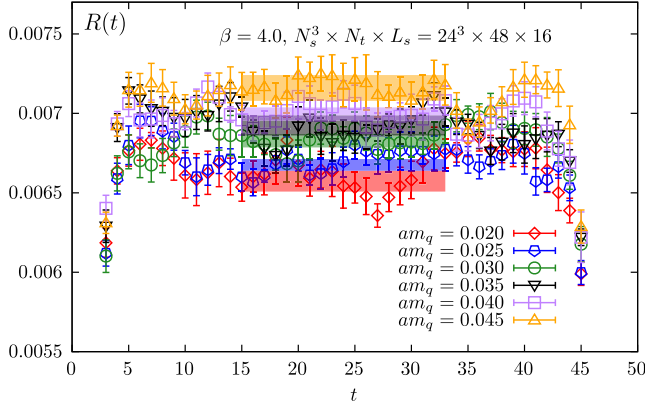


FIG. 1. The ratio $R(t)$ of the midpoint correlator to the pion correlator as a function of source-sink separation t on zero-temperature $24^3 \times 48 \times 16$ ensembles at $\beta = 4.0$ with several quark masses. The horizontal bands indicate constant fits over $15 \leq t \leq 33$, from which $am_{\text{res}}(am_q)$ is determined.

target distribution. To correct for this, we employ a rational function reweighting procedure. Further details regarding this reweighting can be found in Appendix C.

IV. ZERO-TEMPERATURE OBSERVABLES

A. The residual mass

To quantify the residual chiral symmetry breaking of Möbius domain-wall fermions with finite L_s , we measure m_{res} using the ratio $R(t)$ in Eq. (3). The correlation functions are computed using a Z_2 wall source. The ratio $R(t)$ is shown in Fig. 1 for the zero-temperature $24^3 \times 48 \times 16$ ensembles at $\beta = 4.0$ with several different quark masses. In this plot, the horizontal bands denote fits to a constant over the range $15 \leq t \leq 33$ with jackknife errors, from which am_{res} is determined for each am_q .

Although am_{res} should be a constant providing a universal description of residual chiral symmetry breaking effects on long-distance observables, the estimator defined in Eq. (3) depends on the input quark mass.

Figure 2 shows the residual mass as a function of bare input quark mass am_q for zero-temperature ensembles at $\beta = 4.0, 4.1$, and 4.17 . The dash-dotted lines represent the linear fits that describe the data well. This linear quark mass dependence is understood as a lattice artifact [68,76]: $am_{\text{res}}(am_q) = am_{\text{res}}(am_q = 0)[1 + \mathcal{O}((am_q)(a\Lambda))]$. We extrapolate am_{res} to the zero input quark mass limit and obtain $am_{\text{res}}(0) = 0.00613(9)$, $0.00090(3)$, and $0.00025(1)$ at $\beta = 4.0, 4.1$ and 4.17 , respectively.

These values strongly depend on β , as shown in Fig. 3. We find that am_{res} increases exponentially as β decreases. This can be understood by the appearance of more localized lattice dislocations toward the coarser lattices [12]. We also verify that extrapolating to $m_q = 0$ and $m_q = -m_{\text{res}}$ yields consistent results within errors, as shown in Fig. 21.

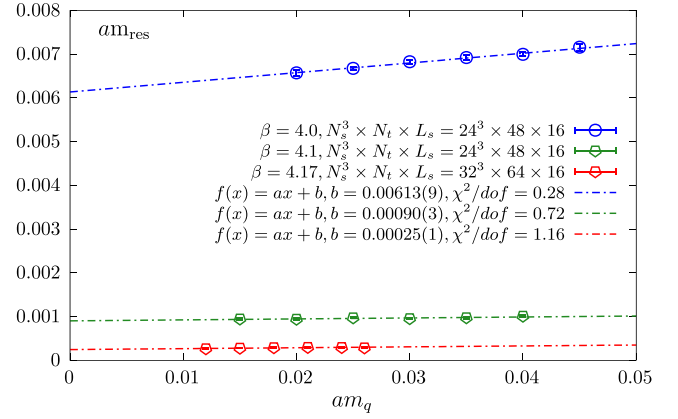


FIG. 2. The residual mass as a function of the bare input quark mass for zero-temperature ensembles at $\beta = 4.0, 4.1$, and 4.17 . The dash-dotted lines represent linear fits $f(x) = ax + b$, with the intercept b giving $am_{\text{res}}(0)$.

B. Chiral condensate

The left panel of Fig. 4 shows the chiral condensate $\langle \bar{\psi}\psi \rangle$, renormalized in the $\overline{\text{MS}}$ scheme at $\mu = 2$ GeV, as a function of the renormalized quark mass

$$\begin{aligned} m_R &\equiv (m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) \\ &= Z_m^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})(m_q + m_{\text{res}}) \end{aligned}$$

for $\beta = 4.0, 4.1$, and 4.17 , with dashed lines showing quadratic fits. Even after multiplicative renormalization, the chiral condensate contains an additive UV-divergent contribution proportional to the quark mass, whose coefficient diverges as $1/a^2$. To separate this UV-divergent contribution from the regular mass dependence, we study the mass dependence of $\langle \bar{\psi}\psi \rangle$ at several lattice spacings. For each lattice spacing a_i , the condensate is fitted as

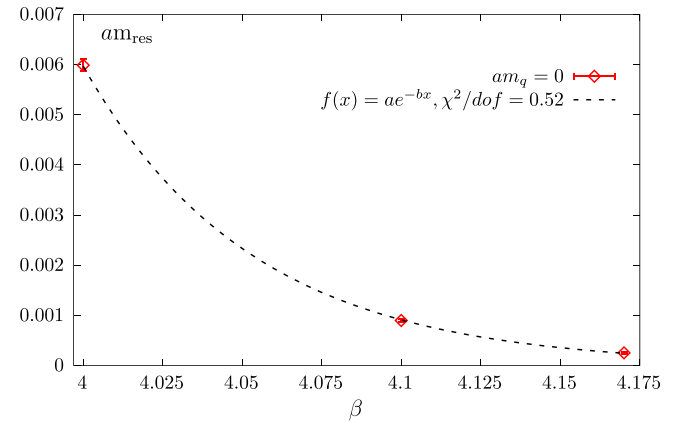


FIG. 3. The residual mass $am_{\text{res}}(0)$ extrapolated to zero input quark mass as a function of the gauge coupling β . The dashed line shows an exponential fit $f(\beta) = ae^{-b\beta}$, where am_{res} decreases exponentially as β increases.

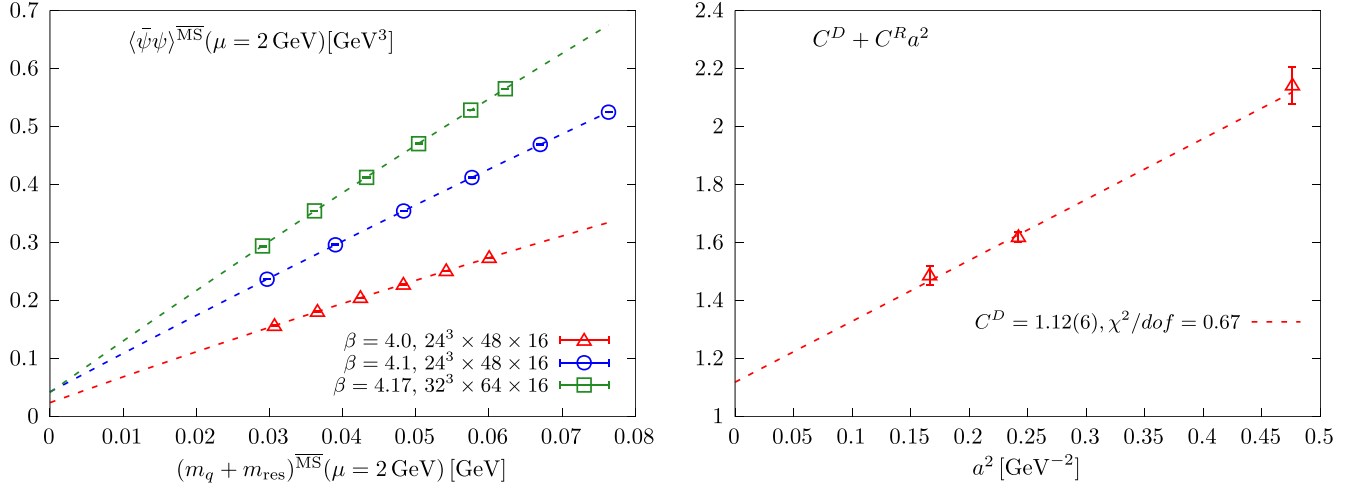


FIG. 4. Left: The multiplicatively renormalized chiral condensate $\langle \bar{\psi}\psi \rangle^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ as a function of the renormalized quark mass $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ on zero-temperature ensembles at $\beta = 4.0, 4.1$, and 4.17 . The ensemble sizes shown in the legend are given as $N_s^3 \times N_t \times L_s$. The dashed curves show quadratic fits of the form $\langle \bar{\psi}\psi \rangle(m_R, a_i) = A_i m_R^2 + B_i m_R + C_i$. Right: The corresponding dimensionless linear coefficients $a_i^2 B_i = C^D + C^R a_i^2$ are plotted as a function of a_i^2 . The dashed line shows a linear extrapolation to the continuum limit, yielding $C^D = 1.12(6)$.

$$\begin{aligned}
 \langle \bar{\psi}\psi \rangle(m_R, a_i) &= \langle \bar{\psi}\psi \rangle(0, a_i) + C^D \frac{m_R + (x-1)m_{\text{res},R}}{a_i^2} \\
 &\quad + C^R m_R + A_i m_R^2 \\
 &= \underbrace{\left[\langle \bar{\psi}\psi \rangle(0, a_i) + C^D \frac{(x-1)m_{\text{res},R}}{a_i^2} \right]}_{C_i} \\
 &\quad + \underbrace{\left[\frac{C^D + C^R a_i^2}{a_i^2} \right]}_{B_i} m_R + A_i m_R^2, \quad (29)
 \end{aligned}$$

where $m_{\text{res},R} = \overline{m}_m^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) m_{\text{res}}$. The key point of Eq. (29) is that the coefficient of the term linear in the quark mass (B_i) contains two contributions: the additive UV-divergent part, C^D/a_i^2 , and the regular part, C^R . Equivalently, $a_i^2 B_i = C^D + C^R a_i^2$, which is the dimensionless quantity plotted in the right panel of Fig. 4 as a function of the squared lattice spacing a_i^2 . Fitting $a_i^2 B_i$ linearly in a_i^2 and extrapolating to the continuum limit, we cleanly isolate the UV-divergent coefficient, yielding $C^D = 1.12(6)$.

In Fig. 5, we show the pion mass squared as a function of the renormalized quark mass on zero-temperature ensembles for three different β values. The results exhibit good linearity, as indicated by the dash-dotted lines. This behavior is consistent with the leading order prediction of chiral perturbation theory, where $m_\pi^2 \propto m_q + m_{\text{res}}$. As expected, m_π^2 approaches zero in the chiral limit, demonstrating the excellent chiral properties of Möbius domain-wall fermions. However, m_π^2 does not reach exactly zero, which could be due to finite-volume effects or the absence of chiral logarithm corrections in the linear fit ansatz.

V. FINITE-TEMPERATURE OBSERVABLES

A. Plaquette and plaquette susceptibility

We utilize the plaquette expectation value $\langle P \rangle$ and its susceptibility χ_P to determine the transition point. These quantities are defined as follows:

$$\langle P \rangle = \frac{1}{6N_s^3 N_t} \sum_{\vec{x}, t} \sum_{\mu < \nu} \left[1 - \frac{1}{3} \text{ReTr} U_{\mu\nu}(\vec{x}, t) \right], \quad (30)$$

$$\chi_P = N_s^3 N_t (\langle P^2 \rangle - \langle P \rangle^2). \quad (31)$$

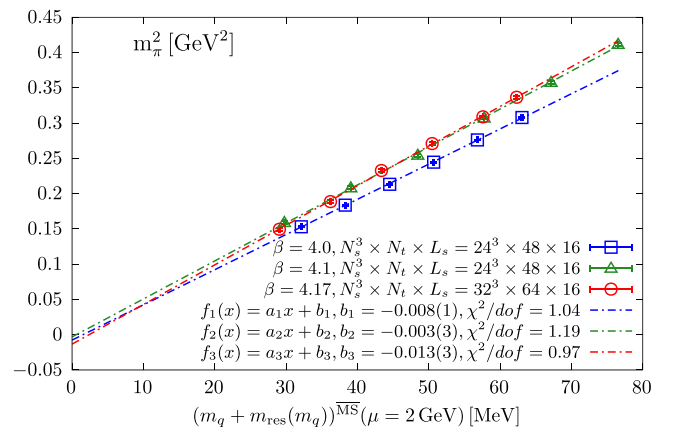


FIG. 5. The pion mass squared m_π^2 , calculated from the pion correlator $\langle \pi^a(x) \pi^a(0) \rangle$, as a function of the renormalized quark mass $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ on zero-temperature ensembles at three different β values. The dash-dotted lines represent linear fits.

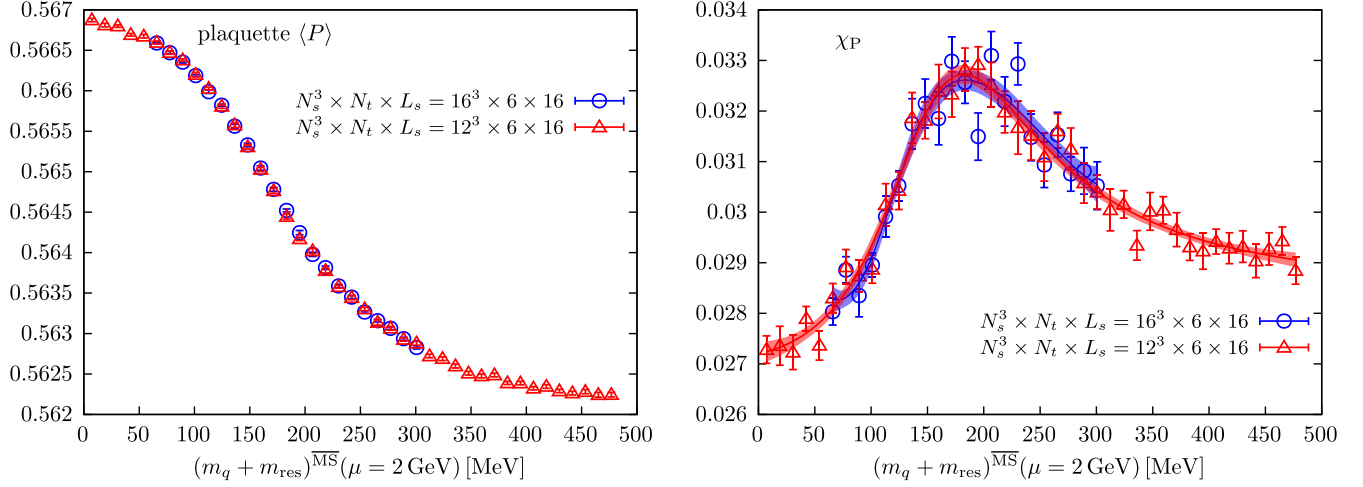


FIG. 6. Left: the plaquette expectation value $\langle P \rangle$ as a function of the renormalized quark mass for $N_t = 6$, corresponding to a temperature of $T = 242(4)$ MeV, with two different volumes. Right: the corresponding plaquette susceptibility χ_P . The continuous bands in the right panel are obtained from a Padé fit of order $[3/2]$. The susceptibility peaks provide estimates of the pseudocritical quark masses, $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) = 182(5) \text{ MeV}$ and $184(10) \text{ MeV}$ for the $12^3 \times 6 \times 16$ and $16^3 \times 6 \times 16$ ensembles, respectively, corresponding in both cases to $m_\pi \simeq 0.96 \text{ GeV}$.

Figure 6 shows the plaquette and its susceptibility plotted as a function of the renormalized quark mass at $N_t = 6$ and $\beta = 4.0$, corresponding to the temperature of $242(4)$ MeV, for two different volumes. The region of rapid change in the plaquette aligns with a peak in the susceptibility. As shown in the right panel, the peaks of χ_P are located at $182(5) \text{ MeV}$ and $184(10) \text{ MeV}$ on the $12^3 \times 6 \times 16$ and $16^3 \times 6 \times 16$ lattices, respectively, providing estimates of the pseudocritical quark masses, corresponding in both cases to $m_\pi \simeq 0.96 \text{ GeV}$. The continuous bands are obtained from a

Padé fit of order $[3/2]$. The negligible volume dependence of the χ_P peak height suggests a crossover transition.

B. Chiral condensate

The left panel of Fig. 7 depicts the multiplicatively renormalized chiral condensate $\langle \bar{\psi}\psi \rangle^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$, without subtracting the additive divergence, as a function of the renormalized quark mass. The data are obtained on zero-temperature lattices and finite-temperature lattices with

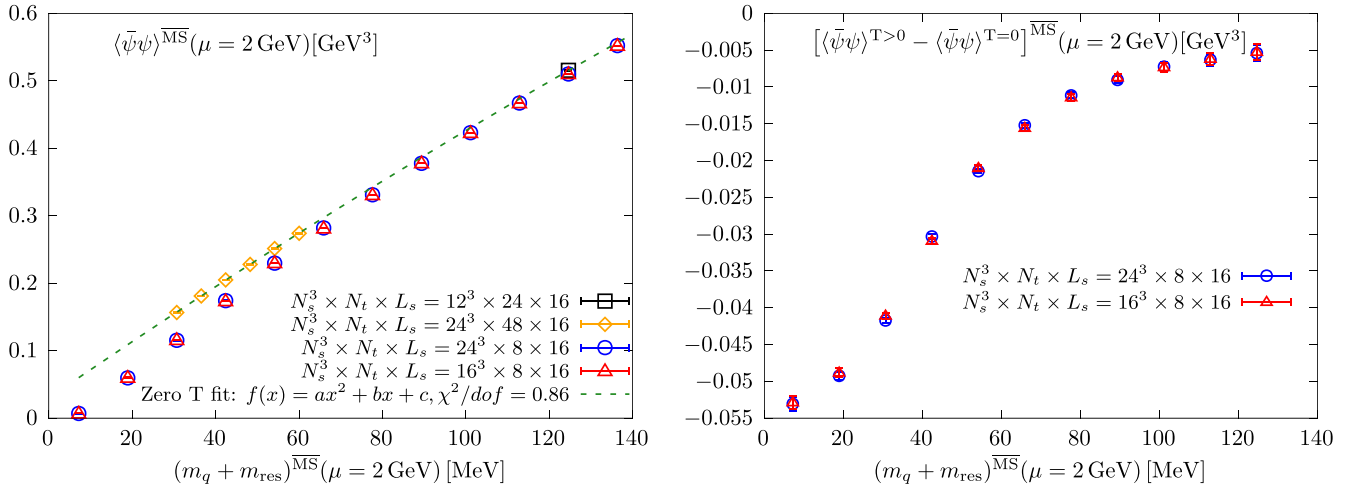


FIG. 7. Left: the multiplicatively renormalized chiral condensate on finite-temperature lattices ($16^3 \times 8$, $24^3 \times 8$) and zero-temperature lattices ($12^3 \times 24$, $24^3 \times 48$) for $\beta = 4.0$ is shown as a function of the renormalized quark mass. The dashed curve is a quadratic fit to the zero-temperature data, including the $12^3 \times 24$ point at $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) = 125 \text{ MeV}$, which constrains the fit at large quark mass; this is the same fit used for the subtraction shown in the right panel. Right: the subtracted chiral condensate $[\langle \bar{\psi}\psi \rangle^{T>0} - \langle \bar{\psi}\psi \rangle^{T=0}]^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ as a function of the renormalized quark mass for lattices of size $16^3 \times 8 \times 16$ and $24^3 \times 8 \times 16$.

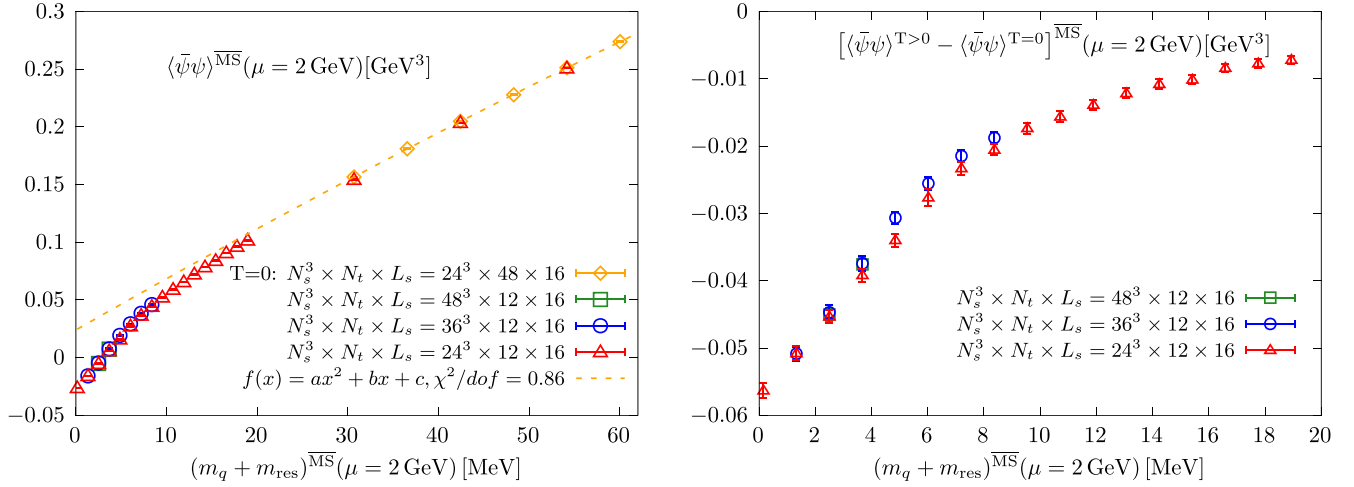


FIG. 8. Same as Fig. 7, but for finite-temperature ensembles with $N_t = 12$ (volumes $24^3 \times 12$, $36^3 \times 12$, and $48^3 \times 12$) at $\beta = 4.0$. Zero-temperature data are from the $24^3 \times 48 \times 16$ ensembles. The dashed curve in the left panel represents the extrapolation of the zero-temperature chiral condensate. Right: the subtracted chiral condensate $[\langle \bar{\psi}\psi \rangle^{T>0} - \langle \bar{\psi}\psi \rangle^{T=0}]^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ as a function of the renormalized quark mass for $N_t = 12$ ensembles.

$N_t = 8$, both at $\beta = 4.0$, where the finite-temperature lattices span two different volumes with aspect ratios $N_s/N_t = 2$ and 3. We observe that $\langle \bar{\psi}\psi \rangle^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ on the $N_t = 8$ lattices vanishes at a positive value of quark mass. This is because $x \neq 1$: the UV-divergent term $C^D(m_q + xm_{\text{res}})a^{-2}$ vanishes at $m_q = -xm_{\text{res}}$, rather than at the chiral limit $m_q = -m_{\text{res}}$. Therefore, at $m_q + m_{\text{res}} = 0$, the unsubtracted chiral condensate still contains a residual contribution $C^D(x-1)m_{\text{res}}/a^2$. As will be shown below, $x < 1$, so this residual term is negative and shifts the zero of the unsubtracted chiral condensate to a positive renormalized quark mass.

The UV divergence can be eliminated by subtracting the zero-temperature chiral condensate from the finite-temperature data at the same quark mass. However, this requires zero-temperature lattices at $\beta = 4.0$ with the same quark masses as the finite-temperature ensembles, and some of these masses are not available in our zero-temperature simulations. To address this, we perform a quadratic extrapolation of the zero-temperature chiral condensate, shown as the dashed line in the left panel of Fig. 7. This procedure yields the additively and multiplicatively renormalized chiral condensate $[\langle \bar{\psi}\psi \rangle^{T>0} - \langle \bar{\psi}\psi \rangle^{T=0}]^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$, presented in the right panel of Fig. 7.

We observe volume independence of the chiral condensate for lattices of size $24^3 \times 8$ and $16^3 \times 8$ in both panels, since the UV divergence term is volume independent. The right panel shows a smooth, monotonic increase of the subtracted condensate toward zero as the renormalized quark mass increases, with no sign of a discontinuity. This indicates that the transition is an analytic crossover. A precise determination of the transition quark mass from the chiral condensate alone is difficult due to its gradual

variation; we therefore defer to the chiral susceptibility, which exhibits a peak that defines the crossover location.

In Fig. 8, we present the same quantities as in Fig. 7, but for the $N_t = 12$ ensembles. In the left panel, the unsubtracted chiral condensate becomes negative near the chiral limit. This negative value arises from the residual additive UV-divergent contribution, $C^D(x-1)m_{\text{res}}a^{-2}$. In the right panel, the zero-temperature subtraction removes this additive UV-divergent contribution. The subtracted condensate remains negative near the chiral limit because the finite-temperature condensate is smaller than the zero-temperature condensate. At larger quark masses, the chiral condensate becomes less sensitive to finite-temperature effects, so the finite- and zero-temperature condensates become closer and the subtracted condensate moves toward zero. We observe visible finite-volume effects around $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) \sim 4\text{--}9 \text{ MeV}$. It is difficult to determine whether this is a crossover or a true phase transition, and the inflection point is also hard to locate just from the chiral condensate itself. To address this, we calculate the disconnected chiral susceptibility and total chiral susceptibility.

To study the $N_f = 3$ QCD phase transition in the chiral region, small quark mass ($m = m_q + m_{\text{res}}$) simulations are needed. The simplest way to achieve this is to use a negative input quark mass m_q ; however, this carries the risk of inducing singularities in the Dirac operator during the dynamical evolution when the magnitude of the negative input quark mass exceeds the corresponding residual mass [12]. In our simulations, the magnitude of the most negative input quark mass we used was roughly comparable to the residual mass, and we did not observe any singularity issues. Another way of achieving the target small value of

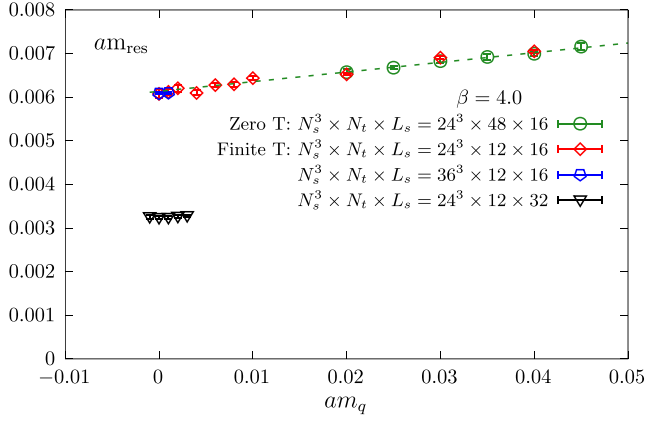


FIG. 9. am_{res} as a function of the bare input quark mass for the zero-temperature lattices with $L_s = 16$ and the finite-temperature lattices with $L_s = 16$ and $L_s = 32$.

the total quark mass is by increasing the value of L_s , since m_{res} decreases as L_s is increased.

Since simulations with negative input quark masses are uncommon for Möbius domain-wall fermions, we performed an additional cross-check by generating $24^3 \times 12 \times 32$ ensembles to assess residual chiral symmetry breaking effects and the reliability of the large negative input quark masses used for the $N_t = 12$, $L_s = 16$ ensembles. The input quark masses for these $L_s = 32$ ensembles were chosen to target approximately the same total quark mass as the corresponding $L_s = 16$ ensembles. We measured m_{res} using the ratio of spatially separated midpoint correlation functions to pion correlation functions, as opposed to the temporally separated ones used in Eq. (3), since the temporal extent is rather short at finite temperature. As shown in Fig. 9, m_{res} for $L_s = 32$ is reduced by a factor of two relative to $L_s = 16$, consistent with the expected $1/L_s$ dependence. At strong gauge coupling, this behavior is

expected because m_{res} receives significant contributions from near-zero eigenmodes, which yield a power-law dependence of $1/L_s$ due to the presence of gauge field dislocations [77]. Figure 9 also demonstrates that the values of m_{res} for $L_s = 16$, computed at a fixed $\beta = 4.0$, are consistent between zero-temperature and finite-temperature ensembles, showing no volume dependence.

More importantly, after explicitly subtracting the additive UV-divergent contribution $C^D(m_q + xm_{\text{res}})/a^2$ from the chiral condensate, the renormalized subtracted condensates from the $L_s = 16$ and $L_s = 32$ ensembles agree at the same total quark mass, as shown in the right panel of Fig. 10. This agreement, together with the consistency of the chiral susceptibilities, confirms the reliability of the $N_t = 12$, $L_s = 16$ simulations with negative input quark masses.

From the left panel of Fig. 10, we observe that close to the chiral limit, the chiral condensate is negative for the $24^3 \times 12 \times 16$ ensemble. This is due to the lack of exact chiral symmetry, as shown by the expression: $\lim_{m_q + m_{\text{res}} \rightarrow 0} \langle \bar{\psi}\psi \rangle|_{\text{DWF}} \sim C^D \frac{(x-1)m_{\text{res}}}{a^2} + \langle \bar{\psi}\psi \rangle|_{\text{cont}} + \dots$. The negativity of the chiral condensate implies $x < 1$. We also see that increasing L_s from 16 to 32 while keeping the total quark masses roughly the same causes an increase in the chiral condensate. This behavior is straightforward to understand by rewriting Eq. (13) as $\langle \bar{\psi}\psi \rangle|_{\text{DWF}} \sim C^D \left(\frac{(x-1)m_{\text{res}}}{a^2} + \frac{m_q + m_{\text{res}}}{a^2} \right) + \langle \bar{\psi}\psi \rangle|_{\text{cont}} + \dots$. Since m_{res} is smaller for $L_s = 32$ than $L_s = 16$ and $x < 1$, for similar total quark masses, the chiral condensate result for $L_s = 32$ is always larger than for $L_s = 16$. We expect that with $L_s = 32$, the residual chiral symmetry breaking effect will become smaller, and this can be seen if we do the extrapolation to the chiral limit.

The unwanted UV divergence component, $C^D \frac{m_q + xm_{\text{res}}}{a^2}$, can be removed explicitly without contaminating the

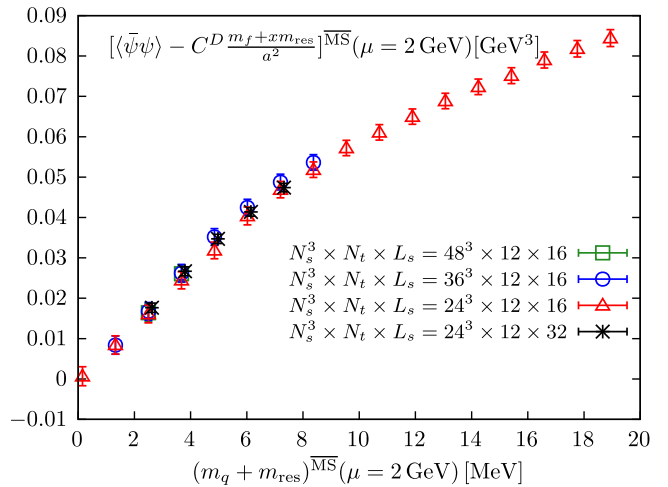
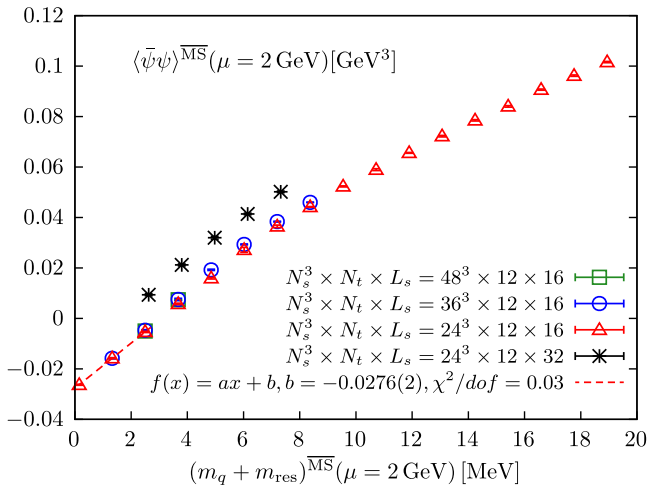


FIG. 10. The multiplicatively renormalized chiral condensate (left) and the additively and multiplicatively renormalized chiral condensate (right) as functions of the renormalized quark mass for $N_t = 12$ lattices with $L_s = 16$ and $L_s = 32$.

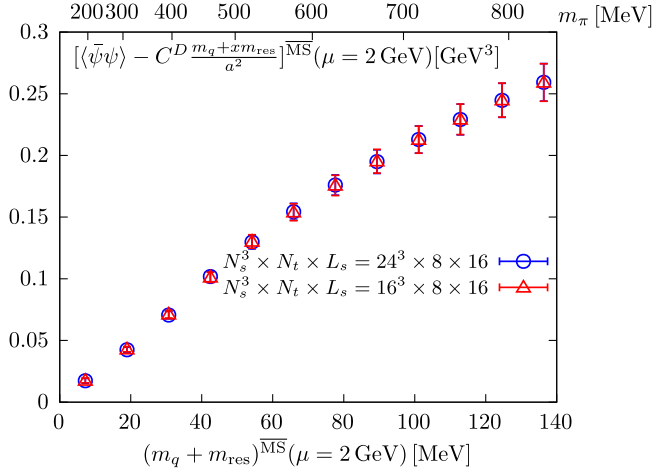


FIG. 11. The renormalized subtracted chiral condensate for $N_t = 8$ lattices with two different volumes. The upper axis indicates the corresponding pseudoscalar mass; these are leading-order estimates meant for orientation only, see the beginning of Appendix B.

regular part contribution if the value of x is known. The value of x can be estimated using the finite-temperature chiral condensate results on $24^3 \times 12 \times 16$ lattices, evaluated at quark masses close to the chiral limit. In the chiral limit, the chiral condensate takes the form: $\lim_{m_q + m_{\text{res}} \rightarrow 0} \langle \bar{\psi}\psi \rangle|_{\text{DWF}} \sim \langle \bar{\psi}\psi \rangle|_{\text{cont}} + C^D \frac{(x-1)m_{\text{res}}}{a^2}$. We believe that at this temperature, $T = 121(2)$ MeV, chiral symmetry is already restored in the chiral limit, according to the estimate $T_c = 98_{-6}^{+3}$ MeV for $N_t = 8$ [60], and therefore assume $\langle \bar{\psi}\psi \rangle|_{\text{cont}} = 0$. Using the linear fit result in the chiral limit—indicated by the intercept of the dashed line,

which equals $C^D \frac{(x-1)m_{\text{res}}}{a^2}$ —together with the known value of m_{res} for $L_s = 16$ and C^D , we obtain $x = -0.6(1)$. With the knowledge of m_{res} for $L_s = 32$, and assuming that x is independent of L_s at fixed gauge coupling, we can now effectively eliminate the additive UV divergence term for both the $L_s = 16$ and $L_s = 32$ lattices. The right panel of Fig. 10 displays the renormalized subtracted chiral condensate results.

We observe that the results from the $24^3 \times 12 \times 16$ and $24^3 \times 12 \times 32$ lattices exhibit consistency, with some minor discrepancies likely attributed to slight differences in total quark mass. This observation implies that the UV divergence term, which includes the residual chiral symmetry breaking effect, has been successfully subtracted from the chiral condensate.

Figure 11 shows the renormalized subtracted chiral condensate for $N_t = 8$ lattices. A simple linear extrapolation would show that the renormalized subtracted chiral condensate vanishes in the chiral limit. This is expected since the current temperature is safely above the critical temperature.

C. Chiral susceptibility

On our finite-temperature lattices, we calculate the chiral condensate using ten stochastic noise vectors for each gauge configuration. This allows us to estimate the fluctuations of the chiral condensate—in other words, the disconnected chiral susceptibility—in an unbiased way.

The left and right panels of Fig. 12 show the renormalized disconnected chiral susceptibility $\chi_{\text{disc}}^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ and the multiplicatively renormalized total chiral susceptibility $\chi_{\text{tot}}^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ as functions of the renormalized

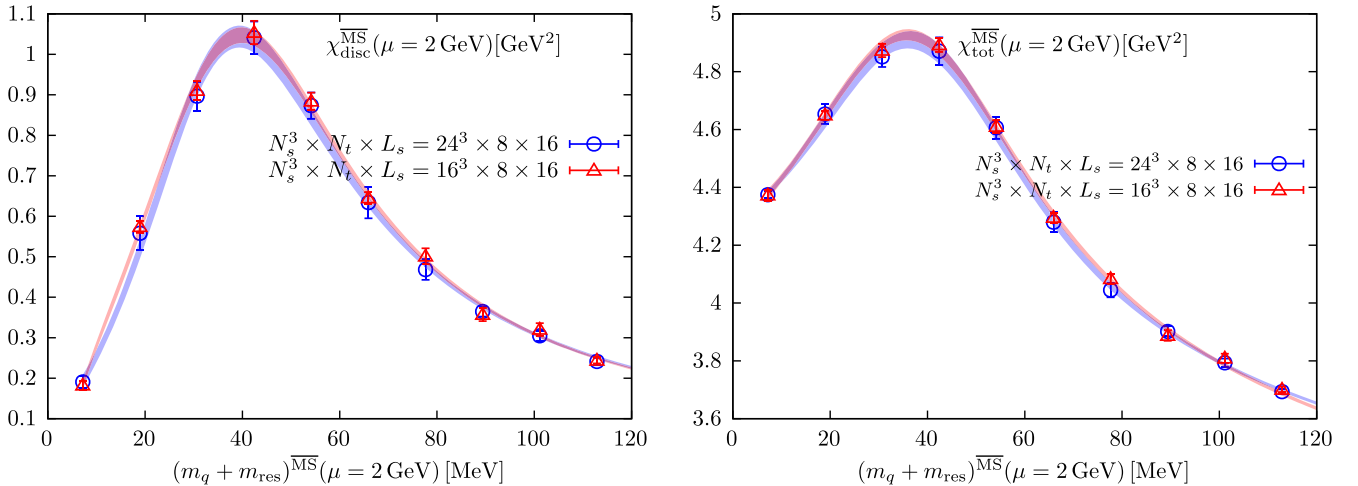


FIG. 12. The renormalized disconnected chiral susceptibility (left) and the multiplicatively renormalized total chiral susceptibility (right) as functions of the renormalized quark mass for $N_t = 8$ lattices, corresponding to $T = 181(3)$ MeV, with two different volumes, along with their Padé fits. The susceptibility peaks give pseudocritical quark masses of $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) = 39.1(9)$ – $40.2(6)$ MeV (disconnected) and $36(1)$ – $36.1(7)$ MeV (total), for the $24^3 \times 8 \times 16$ and $16^3 \times 8 \times 16$ ensembles, respectively, i.e., $m_{\pi} \simeq 445$ – 451 MeV (disconnected) and $\simeq 427$ MeV (total).

quark mass for lattices of size $N_s^3 \times 8$ with $N_s = 16$ and 24 , respectively. The total susceptibility still suffers from the additive divergence. However, since we are using a fixed lattice spacing, the additive divergence is identical across different volumes and therefore does not affect our analysis of the critical behavior. The bands represent Padé fits. We observe that both chiral susceptibilities exhibit no significant volume dependence, which indicates an analytic crossover. The disconnected susceptibility exhibits a pronounced peak at a quark mass of $40.2(6)$ MeV for $16^3 \times 8$ lattices and $39.1(9)$ MeV for $24^3 \times 8$ lattices, while the total susceptibility develops a peak at $36.1(7)$ MeV for $16^3 \times 8$ lattices and $36(1)$ MeV for $24^3 \times 8$ lattices. Since the transition region is broad for a crossover, the pseudocritical point determined from different observables can differ.

D. Quark mass reweighting

Generating gauge configurations with Möbius domain-wall fermions is computationally expensive for large volumes and light quark masses. Due to limited computational resources, we simulated only two mass points for $48^3 \times 12 \times 16$ lattices, positioned near the transition region. To precisely locate the transition point, additional mass points are required. Instead of generating new gauge configurations, we employ reweighting of the sea quark mass, which is significantly cheaper. This technique reuses an ensemble generated at one quark mass to obtain predictions at a different mass. The accessible quark mass range via reweighting is constrained by the overlap in configuration space between the generated and target ensembles; if the overlap is too small, the reweighting factor exhibits large fluctuations.

Quark mass reweighting requires computing a reweighting factor for each gauge configuration. In this work, we use three degenerate flavors of Möbius domain-wall fermions. For an ensemble of gauge configurations generated at sea quark mass m_1 , we can reweight it to an ensemble with sea quark mass m_2 using a reweighting factor $w(U; m_1, m_2)$, defined as the ratio of fermion determinants [78,79]:

$$\begin{aligned} w(U; m_1, m_2) &= \left(\frac{\det[D_{\text{MDWF}}^\dagger(U, m_2) D_{\text{MDWF}}(U, m_2)]}{\det[D_{\text{MDWF}}^\dagger(U, m_1) D_{\text{MDWF}}(U, m_1)]} \right)^{3/2} \\ &= \left(\frac{1}{\det A} \right)^{3/2}, \end{aligned} \quad (32)$$

where $D_{\text{MDWF}}(U, m_1)$ is the Möbius domain-wall fermion Dirac operator with fermion mass m_1 , and the matrix A is defined as $A = D_{\text{MDWF}}^\dagger(m_1) D_{\text{MDWF}}^\dagger(m_2)^{-1} D_{\text{MDWF}}(m_2)^{-1} D_{\text{MDWF}}(m_1)$. Since an exact computation of the reweighting factor is prohibitively expensive, we employ stochastic estimation with Gaussian noise vectors:

$$\begin{aligned} w(U; m_1, m_2) &= \left(\frac{\int \mathcal{D}\xi^\dagger \mathcal{D}\xi e^{-\xi^\dagger \xi} e^{-\xi^\dagger (A-I)\xi}}{\int \mathcal{D}\xi^\dagger \mathcal{D}\xi e^{-\xi^\dagger \xi}} \right)^{3/2} \\ &= \langle e^{-\xi^\dagger (A-I)\xi} \rangle_\xi^{3/2}. \end{aligned} \quad (33)$$

The expectation value of an observable O at the target sea quark mass m_2 is then obtained by computing the weighted average over the N configurations generated at m_1 :

$$\begin{aligned} \langle O \rangle_2 &= \frac{\langle Ow(m_1, m_2) \rangle_1}{\langle w(m_1, m_2) \rangle_1} \\ &\approx \frac{\sum_{i=1}^N w(U_i; m_1, m_2) O(U_i)}{\sum_{i=1}^N w(U_i; m_1, m_2)}. \end{aligned} \quad (34)$$

Having calculated the reweighting factors configuration by configuration, we can obtain the reweighted physical quantity of interest. We performed simulations at two bare input quark masses, $am_q = -0.003$ and -0.004 , on the $48^3 \times 12 \times 16$ lattices. Since these two points are not enough to locate the transition mass point, we resorted to sea quark mass reweighting. We have seven mass points reweighted from $am_q = -0.003$ and three mass points reweighted from $am_q = -0.004$ in order to cover the transition range.

In the left panel of Fig. 13, $\chi_{\text{disc}}^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ shows a sizeable finite-volume effect for $N_s^3 \times 12 \times 16$ lattices with $N_s = 24, 36, 48$ over a broad range of $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) \sim 2\text{--}6$ MeV, which is near the transition range. In the right panel of Fig. 13, we observe a slightly smaller finite-volume effect for $(\chi_{\text{tot}}^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) - C^D a^{-2})[\text{GeV}^2]$ at quark masses around $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) \sim 2\text{--}5$ MeV for the same lattices. Here, the large, volume-independent UV divergence term C^D/a^2 is subtracted to prevent its constant background from obscuring the finite-size effects. The transition mass points determined from the pronounced peaks of $\chi_{\text{disc}}^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ and $(\chi_{\text{tot}}^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) - \frac{C^D}{a^2})[\text{GeV}^2]$ for our largest volume ($48^3 \times 12 \times 16$) are $3.7(2)$ MeV and $3.5(3)$ MeV, respectively, in the $\overline{\text{MS}}$ scheme at a scale of $\mu = 2 \text{ GeV}$, corresponding to $m_\pi \simeq 137$ and 133 MeV. At a genuine chiral phase transition in the thermodynamic limit, these two determinations are expected to coincide.

For a crossover transition, the peak height of chiral susceptibilities should be volume independent for large volumes. However, we observe that the peak height continues to increase up to our largest volume, $48^3 \times 12 \times 16$. According to the finite-size scaling analysis, the peak height of the renormalized total susceptibility is expected to be proportional to N_s^3 for a first-order phase transition and $N_s^{1.966}$ for a $Z(2)$ second-order phase transition. However, as shown in the left plot of Fig. 14, the change in peak height for the total chiral susceptibility is

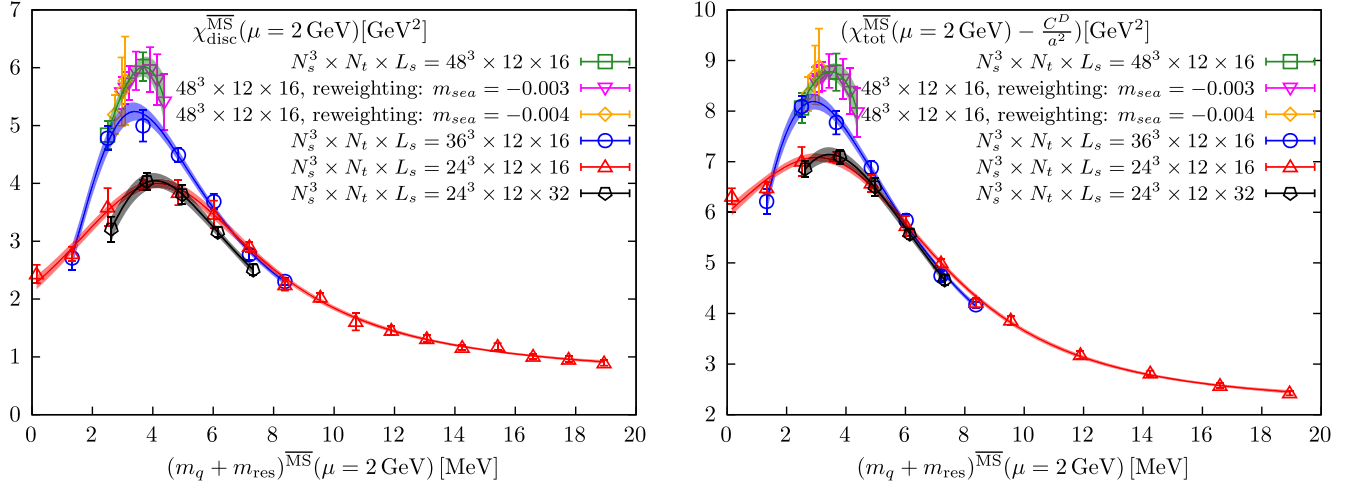


FIG. 13. The renormalized disconnected chiral susceptibility (left) and total susceptibility (right) as functions of the renormalized quark mass for $N_t = 12$ lattices with $L_s = 16$ and $L_s = 32$. The bands are from Padé fits.

not as large as anticipated from either a first-order or $Z(2)$ second-order phase transition. The observed $N_s^{0.39(4)}$ growth remains puzzling. Instead, we also consider a finite-volume effect that is exponentially suppressed as $e^{-am_{\pi}}$ at large volumes. The exponent must be controlled by the lightest degree of freedom in the system. Given that we only have three different volumes, we fix the mass in the exponent to the measured pion screening mass near the transition region, $m_{\pi} \approx 200 \text{ MeV}$, as shown in Fig. 22, and apply an exponential fit. This fit describes the data reasonably well, as shown in the right plot of Fig. 14. An exponential volume dependence of the chiral susceptibility for a crossover has also been observed in Ref. [80] using stout staggered fermions; however, in their study, the peak height decreases to reach a plateau at large volumes, whereas our results show an increase toward saturation. Taken together, the lack of expected power-law growth and

the exponential saturation of the peak height most likely indicate an analytic crossover rather than a true phase transition.

Unlike the chiral condensate, the disconnected and total chiral susceptibilities exhibit a clear dependence on the total quark mass. As shown in Fig. 13, at approximately equal total quark masses, the disconnected and total chiral susceptibilities obtained with $L_s = 32$ closely agree with those obtained with $L_s = 16$ on the $24^3 \times 12$ lattices, despite the substantial difference in the relative magnitudes of the residual mass and the input quark mass. This behavior is expected because, upon differentiating the chiral condensate with respect to the input quark mass, both the additive UV-divergent term and the regular term linear in the quark mass become mass-independent constants, whereas the higher-order terms retain their dependence on the total quark mass. We also obtain consistent

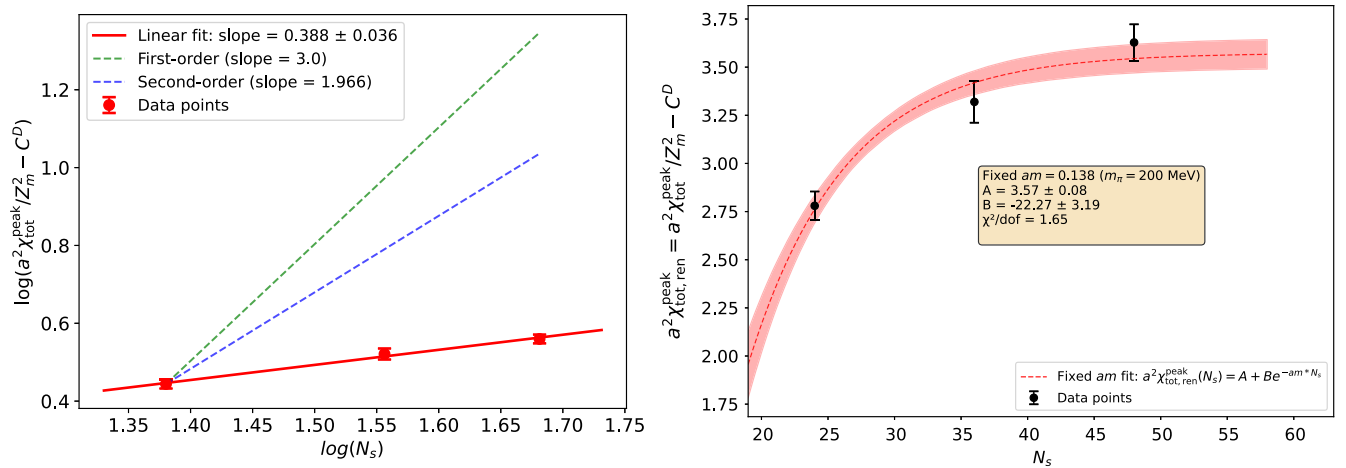


FIG. 14. Left: logarithm of the peak height of the total chiral susceptibility as a function of the logarithm of the spatial extent N_s . Right: the exponential fit of the total chiral susceptibility as a function of N_s .

TABLE I. Pseudocritical quark mass $(m_q + m_{\text{res}})^{\overline{\text{MS}}}$ at $\mu = 2$ GeV, obtained from the susceptibility peaks, together with the observable used and the corresponding pseudoscalar mass.

N_t	T (MeV)	Volume	Observable	$(m_q + m_{\text{res}})^{\overline{\text{MS}}}$ (MeV)	m_π (MeV)
6	242(4)	$16^3 \times 6 \times 16$	χ_P	184(10)	$\simeq 960$
8	181(3)	$24^3 \times 8 \times 16$	$\chi_{\text{disc}}^{\overline{\text{MS}}}, \chi_{\text{tot}}^{\overline{\text{MS}}}$	39.1(9), 36(1)	$\simeq 445, 427$
12	121(2)	$48^3 \times 12 \times 16$	$\chi_{\text{disc}}^{\overline{\text{MS}}}, \chi_{\text{tot}}^{\overline{\text{MS}}}$	3.7(2), 3.5(3)	$\simeq 137, 133$

pseudocritical quark masses on the $24^3 \times 12 \times 16$ and $24^3 \times 12 \times 32$ lattices. This agreement provides an encouraging consistency check on the use of relatively large negative input quark masses for the $L_s = 16$ ensembles.

Table I summarizes the pseudocritical quark masses obtained from the susceptibility peaks discussed in Sec. V, using the largest available volume at each temperature.

E. Binder cumulant

Examining the distribution of the chiral condensate provides additional evidence for the nature of the phase transition. For example, if the transition were first-order, one would expect the histogram of the chiral condensate to develop a double-peak structure at the transition point. In

Fig. 15, we show normalized histograms of the chiral condensate for ensembles located closest to the transition mass points determined from the peaks of the disconnected chiral susceptibility for $N_t = 8$ and $N_t = 12$. These correspond to $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) \simeq 42$ and 3.6 MeV, respectively.

No pronounced evidence of a double-peak structure is observed as the volume increases. Instead, the histograms of the chiral condensate behave like a Gaussian distribution across different volumes at the simulated mass points, providing further evidence for a crossover transition.

We also measured the Binder cumulant to determine the order of the phase transition at the transition mass point. In Fig. 16, we present the Binder cumulant $B_4(\bar{\psi}\psi)$

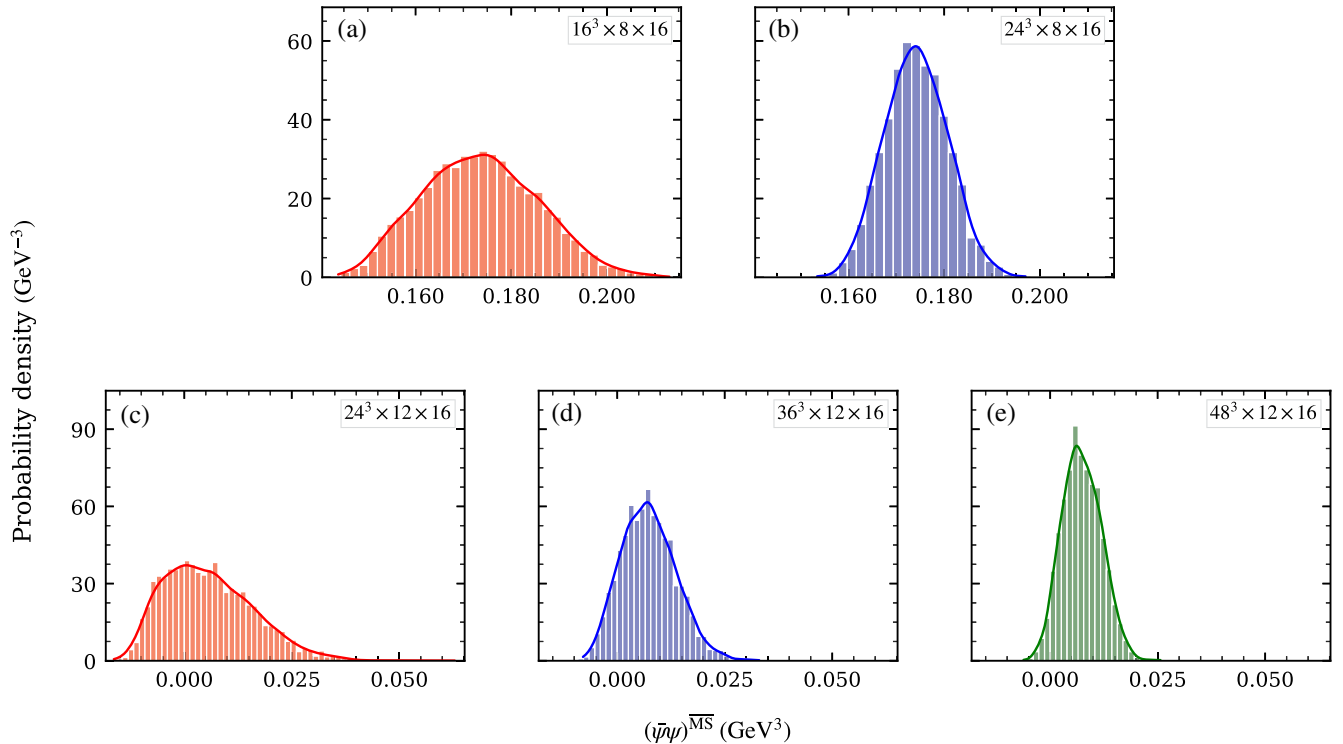


FIG. 15. Probability-density histograms of the chiral condensate, multiplicatively renormalized in the $\overline{\text{MS}}$ scheme at $\mu = 2$ GeV, near the transition-mass points. Panels (a) and (b) show the $N_t = 8$ ensembles at $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) \simeq 42$ MeV, while panels (c)–(e) show the $N_t = 12$ ensembles at $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) \simeq 3.6$ MeV. The lattice dimensions are indicated in each panel. Within each N_t group, common bin edges and common axis ranges are used for all spatial volumes. Each histogram is normalized to unit area. The solid curves are kernel-density estimates shown as guides to the eye.

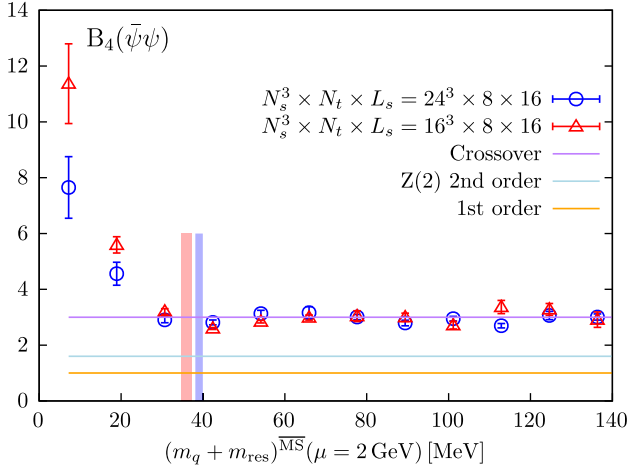


FIG. 16. Binder cumulant of the chiral condensate as a function of the renormalized quark mass evaluated on $N_s^3 \times 8 \times 16$ lattices with $N_s = 16$ and 24 . The horizontal lines represent the universal values for different types of phase transitions. The vertical bands represent the transition regions determined from the 1σ error bounds (mean $\pm$ error) of the pseudocritical masses for the disconnected and total chiral susceptibilities, using only our largest volume ($24^3 \times 8 \times 16$).

evaluated on $16^3 \times 8 \times 16$ and $24^3 \times 8 \times 16$ lattices at $\beta = 4.0$ as a function of the renormalized quark mass. The vertical bands indicate the transition regions at this fixed temperature, representing the 1σ error bounds of the pseudocritical masses determined from both the disconnected and the total chiral susceptibilities for our largest volume ($24^3 \times 8 \times 16$). The value of B_4 in these transition regions is consistent with 3, indicating a crossover transition. This conclusion aligns with the finding obtained from the volume independence of the chiral condensate and chiral susceptibilities, as illustrated in Figs. 7, 11, and 12.

In Fig. 17, we present a plot similar to Fig. 16, but for $N_t = 12$ lattices with $L_s = 16$ and $L_s = 32$. The vertical bands indicate the transition mass regions, representing the 1σ error bounds of the pseudocritical masses determined from both the disconnected and total chiral susceptibilities for our largest volume ($48^3 \times 12 \times 16$). Within these regions, the value of $B_4(\bar{\psi}\psi)$ is found to be close to 3 at $T = 121(2)$ MeV. This further supports the crossover scenario.

VI. SUMMARY AND OUTLOOK

We initiated a pioneering investigation of the nature of the three-flavor QCD phase transition toward the chiral limit using Möbius domain-wall fermions. We performed simulations at a fixed lattice spacing, $a = 0.1361(20)$ fm, on lattices with temporal extents $N_t = 6, 8$, and 12 , corresponding to temperatures of $242(4)$, $181(3)$, and $121(2)$ MeV, respectively. At each temperature, we

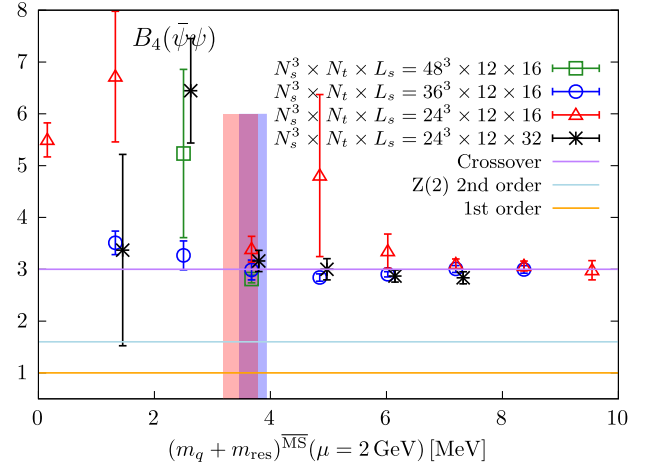


FIG. 17. The Binder cumulant as a function of the renormalized quark mass for $N_t = 12$ lattices with $L_s = 16$ and $L_s = 32$. The vertical bands indicate the transition mass regions, representing the 1σ error bounds (mean $\pm$ error) of the pseudocritical masses determined from the disconnected and total chiral susceptibilities for our largest volume ($48^3 \times 12 \times 16$).

explored a wide range of quark masses and several spatial volumes. By evaluating the plaquette, plaquette susceptibility, chiral condensate, chiral susceptibilities, and Binder cumulant at different quark masses and volumes, we have estimated the pseudocritical quark masses at the two higher temperatures. On our largest simulated volumes, the pseudocritical mass at $T = 242(4)$ MeV, determined from the plaquette susceptibility, is

$$(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) \simeq 184(10) \text{ MeV},$$

corresponding to $m_\pi \simeq 0.96 \text{ GeV}$, while at $T = 181(3)$ MeV the peaks of the disconnected and total chiral susceptibilities give

$$(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) \simeq 39.1(9) \text{ MeV} \quad \text{and} \quad 36(1) \text{ MeV},$$

i.e., $m_\pi \simeq 445$ and 427 MeV, respectively. These pseudocritical points lie unequivocally within the crossover region.

For $T = 121(2)$ MeV, the pseudocritical quark masses determined from the peaks of the disconnected and total chiral susceptibilities on the largest volume are

$$(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV}) \simeq 3.7(2) \text{ MeV} \quad \text{and} \quad 3.5(3) \text{ MeV},$$

i.e., $m_\pi \simeq 137$ and 133 MeV, respectively. In contrast to the behavior at $T = 181(3)$ MeV, where no significant volume dependence is observed, the peak height of the total chiral

susceptibility at $T = 121(2)$ MeV increases with increasing volume. However, this growth is substantially weaker than the power-law behavior anticipated for either a first-order or a $Z(2)$ second-order phase transition. The chiral condensate histograms and Binder cumulants also do not show definitive signatures of a true phase transition. Instead, the volume dependence of the susceptibility peak is well described by an exponential ansatz with saturation at large volumes, which is characteristic of a crossover. Nevertheless, since the peak height has not fully saturated across our simulated volumes, the possibility of a weak first-order phase transition cannot be completely ruled out. Our results therefore suggest that, if a first-order region exists in the lower-left corner of the Columbia plot, the corresponding $Z(2)$ critical boundary mass is likely below $3.7(2)$ MeV, close to the physical light-quark mass [81], i.e., $m_\pi \lesssim 137$ MeV. This finding is consistent with results obtained using Wilson and staggered-type fermions.

As a cross-check of the $N_t = 12$, $L_s = 16$ ensembles with negative input quark masses, we performed additional simulations on $24^3 \times 12 \times 32$ lattices. Comparing the $L_s = 16$ and $L_s = 32$ results, we find that the residual chiral symmetry breaking contribution to the chiral condensate is reduced at larger L_s , as expected, while the chiral susceptibilities remain consistent when compared at approximately the same total quark mass, $m_q + m_{\text{res}}$. This indicates that the chiral susceptibilities are primarily controlled by the total quark mass, rather than by the individual values of m_q and m_{res} .

From fits to the zero- and finite-temperature chiral-condensate data, we extract the coefficients C^D and x that enter the additive UV-divergent term $C^D(m_q + xm_{\text{res}})/a^2$. We then explicitly subtract this contribution from the domain-wall-fermion chiral condensate. To our knowledge, this is the first explicit determination of both C^D and x , and the first explicit subtraction of the additive UV-divergent contribution for domain-wall fermions. After this subtraction, the renormalized subtracted chiral condensates from the $L_s = 16$ and $L_s = 32$ ensembles agree when compared at the same total quark mass. Together with the consistency of the chiral susceptibilities, these observations support the robustness of the large negative input quark masses used for the $N_t = 12$, $L_s = 16$ ensembles.

In the case of a crossover transition, the peak height of the chiral susceptibilities should be volume independent for large volumes. For $N_t = 12$ lattices, however, we have observed significant volume dependence in the chiral susceptibilities, though the effect is not as strong as one would expect for a true phase transition. To further clarify this ambiguity at $N_t = 12$, future studies will require simulations on even larger spatial volumes (e.g., $N_s \geq 64$) to determine whether the peak height ultimately saturates in the thermodynamic limit, confirming

a crossover, or continues to diverge, signaling a potentially weak true phase transition. Furthermore, to map out the broader phase structure and directly search for the first-order region, if it exists, exploring even lower temperatures corresponding to a lighter quark mass transition point remains a critical direction. In particular, extending these Möbius domain-wall fermion simulations to $N_t = 14$ lattices, which would correspond to a temperature of $104(2)$ MeV, would be highly valuable. Such studies would provide an essential cross-check of a recent HISQ investigation that suggested a continuous chiral phase transition with a transition temperature of 98_{-6}^{+3} MeV at a finite lattice spacing corresponding to $N_t = 8$ [60], and would further sharpen the constraints on the lower-left corner of the Columbia plot.

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DATA AVAILABILITY

The numerical data that support the findings of this article are openly available in Zenodo [85].

APPENDIX A: THE MÖBIUS DOMAIN WALL FERMION

In this work, we employ the Möbius domain-wall fermion action, expressed in terms of five-dimensional Möbius domain-wall fermion fields Ψ and $\bar{\Psi}$ as [61]

$$\begin{aligned}
S_{\text{MDWF}}(\bar{\Psi}, \Psi, U) &= \bar{\Psi} D_{\text{MDWF}}(m_q) \Psi \\
&= \sum_{s=0}^{L_s-1} \bar{\Psi}_s D_+^{(s)} \Psi_s + \sum_{s=1}^{L_s-1} \bar{\Psi}_s D_-^{(s)} P_+ \Psi_{s-1} \\
&\quad + \sum_{s=0}^{L_s-2} \bar{\Psi}_s D_-^{(s)} P_- \Psi_{s+1} \\
&\quad - m_q \bar{\Psi}_0 D_-^{(0)} P_+ \Psi_{L_s-1} \\
&\quad - m_q \bar{\Psi}_{L_s-1} D_-^{(L_s-1)} P_- \Psi_0, \tag{A1}
\end{aligned}$$

where L_s is the size of the fifth dimension, and m_q is the input bare quark mass. Here, $D_+^{(s)} = b_5(s) D^{\text{Wilson}}(M_5) + 1$, $D_-^{(s)} = c_5(s) D^{\text{Wilson}}(M_5) - 1$, and $P_{\pm} = \frac{1}{2}(\mathbb{1} \pm \gamma_5)$. The four-dimensional Wilson-Dirac operator is defined as

$$\begin{aligned}
D_{x,y}^{\text{Wilson}}(U, M_5) &= (4 + M_5) \delta_{x,y} - \frac{1}{2} [(1 - \gamma_\mu) U_\mu(x) \delta_{x+\mu, y} \\
&\quad + (1 + \gamma_\mu) U_\mu^\dagger(y) \delta_{x, y+\mu}], \tag{A2}
\end{aligned}$$

where M_5 is the domain-wall height.

Considering the polar decomposition to the sign function, it suffices to select constant coefficients $b_5(s) = b_5$ and $c_5(s) = c_5$. Using the real Möbius transformation of the Wilson-Dirac operator, the Möbius kernel can be expressed as

$$D^{\text{Möbius}}(M_5) = \frac{(b_5 + c_5) D^{\text{Wilson}}(M_5)}{2 + (b_5 - c_5) D^{\text{Wilson}}(M_5)}. \tag{A3}$$

When $b_5 = a_5$ and $c_5 = 0$, the Möbius kernel reduces to the Shamir kernel, so

$$D^{\text{Shamir}}(M_5) = \frac{a_5 D^{\text{Wilson}}(M_5)}{2 + a_5 D^{\text{Wilson}}(M_5)} \tag{A4}$$

If we consider the Shamir parameter a_5 fixed such that $a_5 = b_5 - c_5$, then the Möbius kernel is just a rescaled version of the Shamir kernel with a scaling factor $\alpha = (b_5 + c_5)/a_5$,

$$D^{\text{Möbius}}(M_5) = \alpha D^{\text{Shamir}}(M_5) \tag{A5}$$

The Möbius domain-wall fermion formulation has smaller residual chiral symmetry breaking effects than the Shamir domain-wall fermion. As demonstrated in [61], the scaling factor α exponentially enhances the reduction of the residual chiral symmetry breaking effect.

The Möbius domain-wall fermion action with degenerate quark masses is invariant under a global $U(N_f)$ flavor symmetry. This symmetry allows for the definition of a five-dimensional conserved vector current:

$$\begin{aligned}
j_\mu^{a, \text{MDWF}}(x, s) &= b_5 \bar{\Psi}_s \lambda^a \mathcal{V}_\mu(x) \Psi_s + c_5 \bar{\Psi}_s \lambda^a \mathcal{V}_\mu(x) P_- \Psi_{s+1} + c_5 \bar{\Psi}_s \lambda^a \mathcal{V}_\mu(x) P_+ \Psi_{s-1} \\
&\quad - c_5 (1 + m_q) \bar{\Psi}_0 \lambda^a \mathcal{V}_\mu(x) P_+ \Psi_{L_s-1} \delta_{s,0} - c_5 (1 + m_q) \bar{\Psi}_{L_s-1} \lambda^a \mathcal{V}_\mu(x) P_- \Psi_0 \delta_{s, L_s-1}, \tag{A6}
\end{aligned}$$

for $\mu = 1, \dots, 4$, and $0 \leq s \leq L_s - 1$. The fifth component of the current is

$$j_5^{a, \text{MDWF}}(x, s) = \begin{cases} \bar{\Psi}_{x, s+1} \lambda^a D_-^{(s+1)} P_+ \Psi_{x, s} - \bar{\Psi}_{x, s} \lambda^a D_-^{(s)} P_- \Psi_{x, s+1}, & 0 \leq s < L_s - 1, \\ \bar{\Psi}_{x, 0} \lambda^a D_-^{(0)} P_+ \Psi_{x, L_s-1} - \bar{\Psi}_{x, L_s-1} \lambda^a D_-^{(L_s-1)} P_- \Psi_{x, 0}, & s = L_s - 1. \end{cases} \tag{A7}$$

Here, $\mathcal{V}_\mu(x) = \frac{\gamma_\mu - 1}{2} U_\mu(x) + \frac{\gamma_\mu + 1}{2} U_\mu^\dagger(x)$. The five-dimensional theory is anomaly-free, so the divergence equation satisfies

$$\sum_{\mu=1}^4 \Delta_\mu j_\mu^{a, \text{MDWF}}(x, s) + \Delta_5 j_5^{a, \text{MDWF}}(x, s) = 0. \tag{A8}$$

Written out explicitly, this becomes

$$\sum_{\mu=1}^4 \Delta_\mu j_\mu^{a, \text{MDWF}}(x, s) = \begin{cases} -j_5^a(x, 0) - m_q j_5^a(x, L_s - 1), & s = 0, \\ -\Delta_5 j_5^a(x, s), & 0 < s < L_s - 1, \\ j_5^a(x, L_s - 2) + m_q j_5^a(x, L_s - 1), & s = L_s - 1. \end{cases} \tag{A9}$$

Here,

$$\Delta_5 f(x, s) = f(x, s) - f(x, s-1). \quad (\text{A10})$$

One then defines a conserved four-dimensional vector current by summing over the fifth dimension

$$J_\mu^{a, \text{MDWF}}(x) = \sum_{s=0}^{L_s-1} j_\mu^{a, \text{MDWF}}(x, s) \quad (\text{A11})$$

since no current escapes through the fifth dimension,

$$\sum_{s=0}^{L_s-1} \Delta_5 j_5^{a, \text{MDWF}}(x, s) = 0. \quad (\text{A12})$$

The four-dimensional axial current is defined by splitting the left- and right-handed currents in the fifth dimension with opposite signs:

$$\mathcal{A}_\mu^a(x) = \sum_{s=0}^{L_s-1} \text{sign}\left(s - \frac{L_s-1}{2}\right) j_\mu^{a, \text{MDWF}}(x, s). \quad (\text{A13})$$

The divergence of the four-dimensional axial current satisfies

$$\sum_{\mu=1}^4 \Delta_\mu \mathcal{A}_\mu^a(x) = 2m_q J_5^{a, \text{MDWF}}(x) + 2J_{5q}^{a, \text{MDWF}}(x), \quad (\text{A14})$$

where $J_5^{a, \text{MDWF}}(x)$ and $J_{5q}^{a, \text{MDWF}}(x)$ are the pseudoscalar densities defined in Eqs. (1) and (2), respectively.

Under the axial current transformation, the change in the Möbius domain-wall fermion action comes from two sides: one is the coupling between $s = L_s/2 - 1$ and $s = L_s/2$ layers, which persists even when $m_q = 0$, and the other one comes from the coupling between $s = 0$ and $s = L_s - 1$, which vanishes when $m_q = 0$.

The corresponding axial Ward-Takahashi identity is [86]

$$\begin{aligned} \sum_{\mu=1}^4 \Delta_\mu \langle \mathcal{A}_\mu^a(x) O(y) \rangle \\ = 2m_q \langle J_5^a(x) O(y) \rangle + 2 \langle J_{5q}^a(x) O(y) \rangle + i \langle \delta^a O(y) \rangle. \end{aligned} \quad (\text{A15})$$

It is shown in [86] that if the operator O only involves the four-dimensional quark field as defined in Eqs. (4) and (5), then the correlation function $\langle J_{5q}^a(x) O(y) \rangle$ will tend to zero as $L_s \rightarrow \infty$. This implies that as the scale of the fifth dimension tends to infinity, we can obtain the expected Ward identity.

When $O(y) = J_5^b(y) = \bar{\psi}_y \gamma_5 \lambda^b \psi_y$, the corresponding Ward identity is

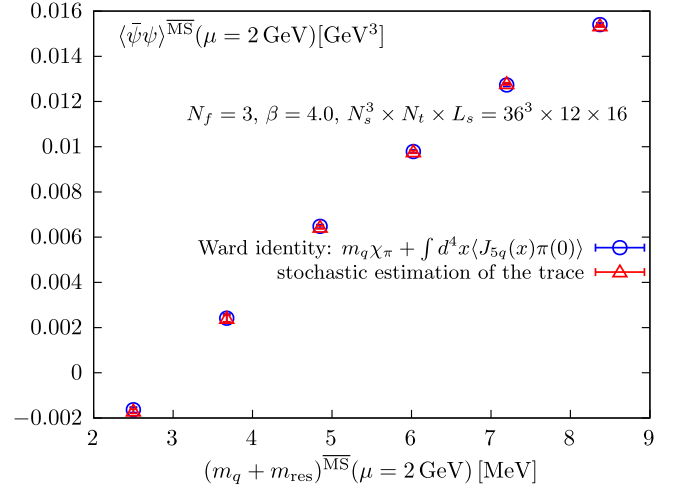


FIG. 18. Numerical verification of the integrated axial Ward-Takahashi identity as shown in Eq. (A18) for $36^3 \times 12 \times 16$ lattices. The renormalized chiral condensate obtained using the Ward identity $m_q \chi_\pi + \int d^4x \langle J_{5q}^a(x) \pi(0) \rangle$ (circles) and stochastic estimator (triangles) are shown as a function of the renormalized quark mass.

$$\begin{aligned} \sum_{\mu=1}^4 \Delta_\mu \langle \mathcal{A}_\mu^a(x) J_5^b(y) \rangle \\ = 2m_q \langle J_5^a(x) J_5^b(y) \rangle + 2 \langle J_{5q}^a(x) J_5^b(y) \rangle \\ - \delta_{x,y} \langle \bar{\psi}_y \{ \lambda^a, \lambda^b \} \psi_y \rangle, \end{aligned} \quad (\text{A16})$$

where λ^a is a flavor symmetry generator, and $\{ \lambda^a, \lambda^b \} = 2\delta^{ab} \mathbb{1}$.

Summing over all lattice points gives [87,88]

$$\begin{aligned} 0 &= \int d^4x \sum_{\mu=1}^4 \Delta_\mu \langle \mathcal{A}_\mu^a(x) J_5^b(y) \rangle \\ &= \int d^4x (2m_q \langle J_5^a(x) J_5^b(y) \rangle + 2 \langle J_{5q}^a(x) J_5^b(y) \rangle \\ &\quad - \delta_{x,y} \langle \bar{\psi}_y \{ \lambda^a, \lambda^b \} \psi_y \rangle) \\ &= 2m_q \chi_\pi + 2\Delta_{\text{mp}} - 2 \langle \bar{\psi}\psi \rangle, \end{aligned} \quad (\text{A17})$$

yielding

$$m_q \chi_\pi + \Delta_{\text{mp}} = \langle \bar{\psi}\psi \rangle, \quad (\text{A18})$$

which we will refer to as the integrated axial Ward-Takahashi identity. Here,

$$\Delta_{\text{mp}} = \int d^4x \langle J_{5q}^a(x) J_5^b(y) \rangle. \quad (\text{A19})$$

In Fig. 18, we numerically verify the integrated axial Ward-Takahashi identity, Eq. (A18), by comparing two independent determinations of the chiral condensate: one obtained

from the Ward identity and the other from the stochastic estimator. The excellent agreement between the two determinations confirms the validity of the identity.

APPENDIX B: DETAILS ON SIMULATION PARAMETERS

In Tables III and IV we also quote the pseudoscalar mass, obtained from $m_\pi^2 = 2B(m_q + m_{\text{res}})$ with $am_{\text{res}} = 0.00613$ for $L_s = 16$ and 0.00324 for $L_s = 32$, and $2B$ determined in the same convention from the $\beta = 4.0$ zero-temperature data of Fig. 5, constrained to pass through the origin. These values are leading-order estimates meant as guidance; no value is quoted when the renormalized quark mass is consistent with zero.

TABLE II. Simulation parameters and statistics for the $N_t = 6$ finite-temperature ensembles at $\beta = 4.0$, corresponding to $T = 242(4)$ MeV. Each quark mass was simulated with several independent streams; the first 1000 trajectories of each stream were discarded for thermalization, and configurations were sampled every 10 trajectories.

am_q	#streams	#conf	am_q	#streams	#conf
$12^3 \times 6 \times 16$					
0.000	8	10336	0.210	8	10420
0.010	8	10300	0.220	8	10431
0.020	8	10434	0.230	8	10419
0.030	8	10468	0.240	8	10337
0.040	8	10399	0.250	8	10257
0.050	8	10398	0.260	8	10397
0.060	8	10426	0.270	8	10243
0.070	8	10277	0.280	8	10129
0.080	8	10326	0.290	8	10377
0.090	8	10440	0.300	8	10350
0.100	8	10398	0.310	8	10115
0.110	8	10402	0.320	8	10425
0.120	8	10454	0.330	8	10466
0.130	8	10374	0.340	8	10401
0.140	8	10428	0.350	8	10492
0.150	8	10440	0.360	8	10280
0.160	8	10228	0.370	8	10438
0.170	8	10421	0.380	8	10422
0.180	7	9097	0.390	8	10479
0.190	6	7657	0.400	8	10441
0.200	8	10383			
$16^3 \times 6 \times 16$					
0.050	10	9907	0.160	10	8910
0.060	10	9910	0.170	10	8027
0.070	10	9410	0.180	8	7119
0.080	10	8910	0.190	8	7120
0.090	10	8910	0.200	10	8910
0.100	10	8910	0.210	10	8906
0.110	10	8910	0.220	10	8910
0.120	10	8910	0.230	10	9010
0.130	10	8910	0.240	10	9110
0.140	10	8910	0.250	10	9810
0.150	10	8910			

TABLE III. Simulation parameters and statistics for the finite-temperature ensembles at $N_t = 8$. The lattice spacing is fixed at $a = 0.1361(20)$ fm, with the temperature determined via $T = 1/(N_t a)$. The first 1100 trajectories were discarded for thermalization. Configurations were sampled every 100 trajectories across 10 streams.

β	T (MeV)	$N_s^3 \times N_t \times L_s$	am_q	m_π (MeV)	#conf
4	181(3)	$16^3 \times 8 \times 16$	0	191	95
			0.02	394	106
			0.04	523	98
			0.06	627	108
			0.08	715	113
			0.10	794	116
			0.12	865	115
			0.14	932	119
			0.16	993	124
			0.18	1051	125
			0.20	1106	123
4	181(3)	$24^3 \times 8 \times 16$	0	191	51
			0.01	310	56
			0.02	394	42
			0.03	463	41
			0.04	523	60
			0.05	577	60
			0.06	627	60
			0.07	672	60
			0.08	715	60
			0.09	756	60
			0.10	794	57
			0.11	830	60
			0.12	865	60
			0.13	899	59
			0.14	932	60

APPENDIX C: REWEIGHTING OF THE RATIONAL FUNCTIONS

1. Rational approximation

For simplicity, we illustrate the reweighting of the rational functions for the case of a single flavor of domain-wall fermions. The pseudofermion action for one flavor, approximated by a rational function, reads

$$S_{pf} = \phi^\dagger \mathcal{D}(1)^{1/4} \mathcal{D}(m_q)^{-1/2} \mathcal{D}(1)^{1/4} \phi \quad (\text{C1})$$

$$\approx \phi^\dagger \left(a_0 + \sum_i \frac{a_i}{\mathcal{D}(1) + b_i} \right) \left(\tilde{a}_0 + \sum_i \frac{\tilde{a}_i}{\mathcal{D}(m_q) + \tilde{b}_i} \right) \times \left(a_0 + \sum_i \frac{a_i}{\mathcal{D}(1) + b_i} \right) \phi, \quad (\text{C2})$$

where $\mathcal{D}(m_q) = D_{\text{MDWF}}^\dagger(m_q) D_{\text{MDWF}}(m_q)$ is the hermitian two-flavor Möbius domain-wall Dirac operator with fermion mass m_q . The coefficients (a_0, a_i, b_i) and $(\tilde{a}_0, \tilde{a}_i, \tilde{b}_i)$ are the rational approximation coefficients for $\mathcal{D}(1)^{1/4}$ and

TABLE IV. Simulation parameters and statistics for $N_t = 12$ finite-temperature ensembles. The first 500–800 trajectories were discarded for thermalization. Configurations are stored every 10 trajectories.

β	T (MeV)	$N_s^3 \times N_t \times L_s$	am_q	m_π (MeV)	#conf
4.0	121(2)	$24^3 \times 12 \times 16$	0.1	794	2452
			0.090	756	2374
			0.080	715	2361
			0.070	672	2332
			0.060	627	2063
			0.050	577	2033
			0.040	523	2034
			0.030	463	1758
			0.020	394	1604
			0.010	310	1366
			0.009	300	1357
			0.008	290	1329
			0.007	279	1322
			0.006	268	1330
			0.005	257	1076
			0.004	245	1116
			0.003	233	984
			0.002	220	1023
			0.001	206	1628
			0	191	1445
			-0.001	175	631
			-0.002	157	3183
			-0.003	136	3032
			-0.004	112	2772
			-0.005	82	2238
			-0.006	—	2057
4.0	121(2)	$36^3 \times 12 \times 16$	0.001	206	3734
			0	191	4034
			-0.001	175	4307
			-0.002	157	3859
			-0.003	136	2173
			-0.004	112	2229
4.0	121(2)	$48^3 \times 12 \times 16$	-0.003	136	1915
			-0.004	112	1986
4.0	121(2)	$24^3 \times 12 \times 32$	0.003	192	1786
			0.002	176	1656
			0.001	159	1870
			0	139	1641
			-0.001	115	1614

$\mathcal{D}(m_q)^{-1/2}$, respectively. Integrating out the pseudofermion fields yields the fermion determinant:

$$\begin{aligned}
& \int D\phi^\dagger D\phi e^{-\phi^\dagger \mathcal{D}(1)^{1/4} \mathcal{D}(m_q)^{-1/2} \mathcal{D}(1)^{1/4} \phi} \\
&= \det(\mathcal{D}(1)^{-1/4} \mathcal{D}(m_q)^{1/2} \mathcal{D}(1)^{-1/4}) \\
&= \det\left(\frac{\mathcal{D}(m_q)}{\mathcal{D}(1)}\right)^{1/2}. \tag{C3}
\end{aligned}$$

TABLE V. Simulation parameters and statistics for the zero-temperature ensembles. The first 300–450 trajectories were discarded for thermalization. Configurations for the $12^3 \times 24 \times 16$ ensemble were sampled every 100 trajectories, while for all other ensembles, configurations were sampled every 10 trajectories. In contrast to Tables III and IV, the pseudoscalar masses quoted here are measured directly on these ensembles; the quoted errors are statistical.

β	a^{-1} (GeV)	$N_s^3 \times N_t \times L_s$	am_q	m_π (MeV)	#conf
4.0	1.449	$12^3 \times 24 \times 16$	0.1	822.7(22)	69
			0.2	1189.0(10)	69
			0.3	1491.1(9)	70
4.0	1.449	$24^3 \times 48 \times 16$	0.020	391.1(5)	78
			0.025	428.5(9)	95
			0.030	461.7(8)	100
			0.035	494.5(8)	152
			0.040	525.4(6)	109
			0.045	554.8(9)	109
4.1	2.033	$24^3 \times 48 \times 16$	0.015	398.9(32)	362
			0.020	456.3(20)	427
			0.025	504.4(23)	457
			0.030	554.2(14)	467
			0.035	598.1(16)	511
			0.040	641.5(17)	539
4.17	2.453	$32^3 \times 64 \times 16$	0.012	386.5(22)	166
			0.015	434.4(20)	181
			0.018	482.3(17)	190
			0.021	520.5(16)	220
			0.024	555.6(14)	247
			0.026	580.1(17)	253

The pseudofermion field ϕ is generated from a Gaussian stochastic noise field ξ satisfying $\langle \xi_i^\dagger \xi_j \rangle = \delta_{ij}$ via

$$\phi = \mathcal{D}(1)^{-1/4} \mathcal{D}(m_q)^{1/4} \xi, \tag{C4}$$

which, in the rational approximation, reads

$$\phi \approx \left(\alpha_0 + \sum_i \frac{\alpha_i}{\mathcal{D}(1) + \beta_i} \right) \left(\tilde{\alpha}_0 + \sum_i \frac{\tilde{\alpha}_i}{\mathcal{D}(m_q) + \tilde{\beta}_i} \right) \xi, \tag{C5}$$

where $(\alpha_0, \alpha_i, \beta_i)$ and $(\tilde{\alpha}_0, \tilde{\alpha}_i, \tilde{\beta}_i)$ are the rational approximation coefficients for $\mathcal{D}(1)^{-1/4}$ and $\mathcal{D}(m_q)^{1/4}$, respectively. Changing the integration variable from ϕ to ξ via Eq. (C4) in Eq. (C3) then yields

$$\int D\xi^\dagger D\xi \left(\det \frac{\mathcal{D}(m_q)}{\mathcal{D}(1)} \right)^{1/2} e^{-\xi^\dagger \xi}. \tag{C6}$$

For each operator, $\mathcal{D}(m_q)$ and $\mathcal{D}(1)$, we need two rational approximations. The rational approximations should satisfy the following conditions:

- (i) The rational approximation in Eq. (C2) should accurately reproduce $\mathcal{D}(1)^{1/4}\mathcal{D}(m_q)^{-1/2}\mathcal{D}(1)^{1/4}$ in calculating the final Hamiltonian.
- (ii) For $\xi^\dagger\xi$ to give the initial pseudofermion action, the approximation should satisfy the following condition, obtained by substituting Eq. (C5) into Eq. (C1):

$$\begin{aligned}
1 = & \left(\tilde{\alpha}_0 + \sum_i \frac{\tilde{\alpha}_i}{\mathcal{D}(m_q) + \tilde{\beta}_i} \right) \left(\alpha_0 + \sum_i \frac{\alpha_i}{\mathcal{D}(1) + \beta_i} \right) \\
& \times \left(a_0 + \sum_i \frac{a_i}{\mathcal{D}(1) + b_i} \right) \left(\tilde{a}_0 + \sum_i \frac{\tilde{a}_i}{\mathcal{D}(m_q) + \tilde{b}_i} \right) \\
& \times \left(a_0 + \sum_i \frac{a_i}{\mathcal{D}(1) + b_i} \right) \\
& \times \left(\alpha_0 + \sum_i \frac{\alpha_i}{\mathcal{D}(1) + \beta_i} \right) \left(\tilde{\alpha}_0 + \sum_i \frac{\tilde{\alpha}_i}{\mathcal{D}(m_q) + \tilde{\beta}_i} \right).
\end{aligned} \tag{C7}$$

- (iii) During the molecular dynamics, the accuracy of the rational approximation is not very important as long as the reversibility is kept.

If the condition for the pseudofermion is violated, the reversibility is lost. It is expensive to monitor directly the reversibility during production runs, but we can monitor its violation by checking if $\langle \exp(-dH) \rangle = 1$ is satisfied. If the approximation for the final Hamiltonian is poor, the distribution of the configuration is skewed. It should be accurate enough to resolve dH in the Metropolis test.

The older version of Grid appears to use Eq. (C2) instead of $\xi^\dagger\xi$ to calculate the initial action so that the reversibility is fine. But the poor accuracy of the approximation implies that the connection to the Gaussian distribution is poor, and the distribution of the pseudofermion becomes inaccurate.

There are three sources that cause poor accuracy in the rational approximation:

- (i) The eigenvalues spread beyond the support of the approximation. In the case of Grid, it sometimes checks the bound of the eigenvalues and RHMC stops if it goes outside of the support.
- (ii) On the support, the rational function approximates the target function within a certain finite precision. We need a sufficient number of terms to realize the precision we need.
- (iii) The precision of the solvers is also relevant.

Assuming the range of the eigenvalues is valid, the precision of the rational function or the solver governs the accuracy of the rational approximation. If the number of terms is not large enough but the solver is precise so that dH makes sense, we can conclude that the RHMC generates configurations with a slightly different weight.

The effect of the solver precision is more involved in practice. Even if the precision of one term $(\mathcal{D}(1) + b_i)^{-1}$, for example, is poor, if the coefficient of this term a_i is

small its effect on the result is limited. For a given target tolerance, the solutions of the multishift solver tend to yield more accurate solutions for larger shift b_i . The coefficient a_i in the rational function becomes larger as the shift b_i becomes larger. As a result, one can expect better accuracy than the target tolerance passed to the multishift solver.

Let us denote the rational function that approximates x^p by $f_p(x)$ and a less accurate approximation by $f_p^{\text{poor}}(x)$. We summarize the situation below.

What we want:

- (i) pseudofermion: $\phi = f_{-1/4}(\mathcal{D}(1))f_{1/4}(\mathcal{D}(m_q))\xi$
- (ii) initial action: $\xi^\dagger\xi$
- (iii) action for MD: $\phi^\dagger f_{1/4}(\mathcal{D}(1))f_{-1/2}(\mathcal{D}(m_q))f_{1/4}(\mathcal{D}(1))\phi$
- (iv) final action: $\phi^\dagger f_{1/4}(\mathcal{D}(1))f_{-1/2}(\mathcal{D}(m_q))f_{1/4}(\mathcal{D}(1))\phi$

What we actually did:

- (i) pseudofermion: $\tilde{\phi} = f_{-1/4}^{\text{poor}}(\mathcal{D}(1))f_{1/4}^{\text{poor}}(\mathcal{D}(m_q))\xi$
- (ii) initial action: $\xi^\dagger\xi$ or $\tilde{\phi}^\dagger f_{1/4}^{\text{poor}}(\mathcal{D}(1))f_{-1/2}^{\text{poor}}(\mathcal{D}(m_q))f_{1/4}^{\text{poor}}(\mathcal{D}(1))\tilde{\phi}$
- (iii) action for MD: $S^{\text{poor}} = \tilde{\phi}^\dagger f_{1/4}^{\text{poor}}(\mathcal{D}(1))f_{-1/2}^{\text{poor}}(\mathcal{D}(m_q))f_{1/4}^{\text{poor}}(\mathcal{D}(1))\tilde{\phi}$
- (iv) final action: $\tilde{\phi}^\dagger f_{1/4}^{\text{poor}}(\mathcal{D}(1))f_{-1/2}^{\text{poor}}(\mathcal{D}(m_q))f_{1/4}^{\text{poor}}(\mathcal{D}(1))\tilde{\phi}$

2. Reweighting to correct the rational function

For $36^3 \times 12 \times 16$ runs, it turned out that the number of terms for the rational function is not large enough. The following numbers come from a run for $36^3 \times 12 \times 16$ configurations with 12 poles for the rational functions:

- (i) the errors are $1.387188049647018 \times 10^{-6}$ ($x^{1/2}$ and $x^{-1/2}$), and $9.662807343093718 \times 10^{-7}$ ($x^{1/4}$ and $x^{-1/4}$)
- (ii) the size of the pseudofermion action: 5.37×10^7
- (iii) the target solver tolerance: 1.0×10^{-7}

The observed ΔH distribution is reasonable and satisfies $\langle e^{-\Delta H} \rangle \simeq 1$, indicating that the HMC evolution is valid for the approximate rational action. However, the finite error of the rational approximation slightly modifies the target distribution. We therefore apply rational-function reweighting to correct this difference.

An older version of the Grid code uses S^{poor} to estimate the initial action. We denote the relation between the correct pseudofermion ϕ and the one we actually used $\tilde{\phi}$ as

$$\tilde{\phi} = C\phi. \tag{C8}$$

Then, both the initial and final action as well as the MD process use

$$\tilde{S}_C = \phi^\dagger C^\dagger f_{1/4}^{\text{poor}}(\mathcal{D}(1))f_{-1/2}^{\text{poor}}(\mathcal{D}(m_q))f_{1/4}^{\text{poor}}(\mathcal{D}(1))C\phi \tag{C9}$$

and the fermion determinant

$$\det [C^\dagger f_{1/4}^{\text{poor}}(\mathcal{D}(1)) f_{-1/2}^{\text{poor}}(\mathcal{D}(m_q)) f_{1/4}^{\text{poor}}(\mathcal{D}(1)) C]^{-1}. \quad (\text{C10})$$

As

$$C = f_{-1/4}^{\text{poor}}(\mathcal{D}(1)) f_{1/4}^{\text{poor}}(\mathcal{D}(m_q)) f_{-1/4}^{\text{poor}}(\mathcal{D}(m_q)) f_{1/4}^{\text{poor}}(\mathcal{D}(1)), \quad (\text{C11})$$

$$\begin{aligned} w &= \det \left[\frac{C^\dagger f_{1/4}^{\text{poor}}(\mathcal{D}(1)) f_{-1/2}^{\text{poor}}(\mathcal{D}(m_q)) f_{1/4}^{\text{poor}}(\mathcal{D}(1)) C}{f_{1/4}^{\text{poor}}(\mathcal{D}(1)) f_{-1/2}^{\text{poor}}(\mathcal{D}(m_q)) f_{1/4}^{\text{poor}}(\mathcal{D}(1))} \right] \\ &= \det [f_{-1/4}^{\text{poor}}(\mathcal{D}(1)) f_{1/4}^{\text{poor}}(\mathcal{D}(1)) f_{1/4}^{\text{poor}}(\mathcal{D}(m_q)) \\ &\quad \times f_{-1/2}^{\text{poor}}(\mathcal{D}(m_q)) f_{1/4}^{\text{poor}}(\mathcal{D}(m_q)) f_{1/4}^{\text{poor}}(\mathcal{D}(1)) f_{-1/4}^{\text{poor}}(\mathcal{D}(1))] \\ &= \det \Omega. \end{aligned} \quad (\text{C12})$$

the reweighting factor is

In general,

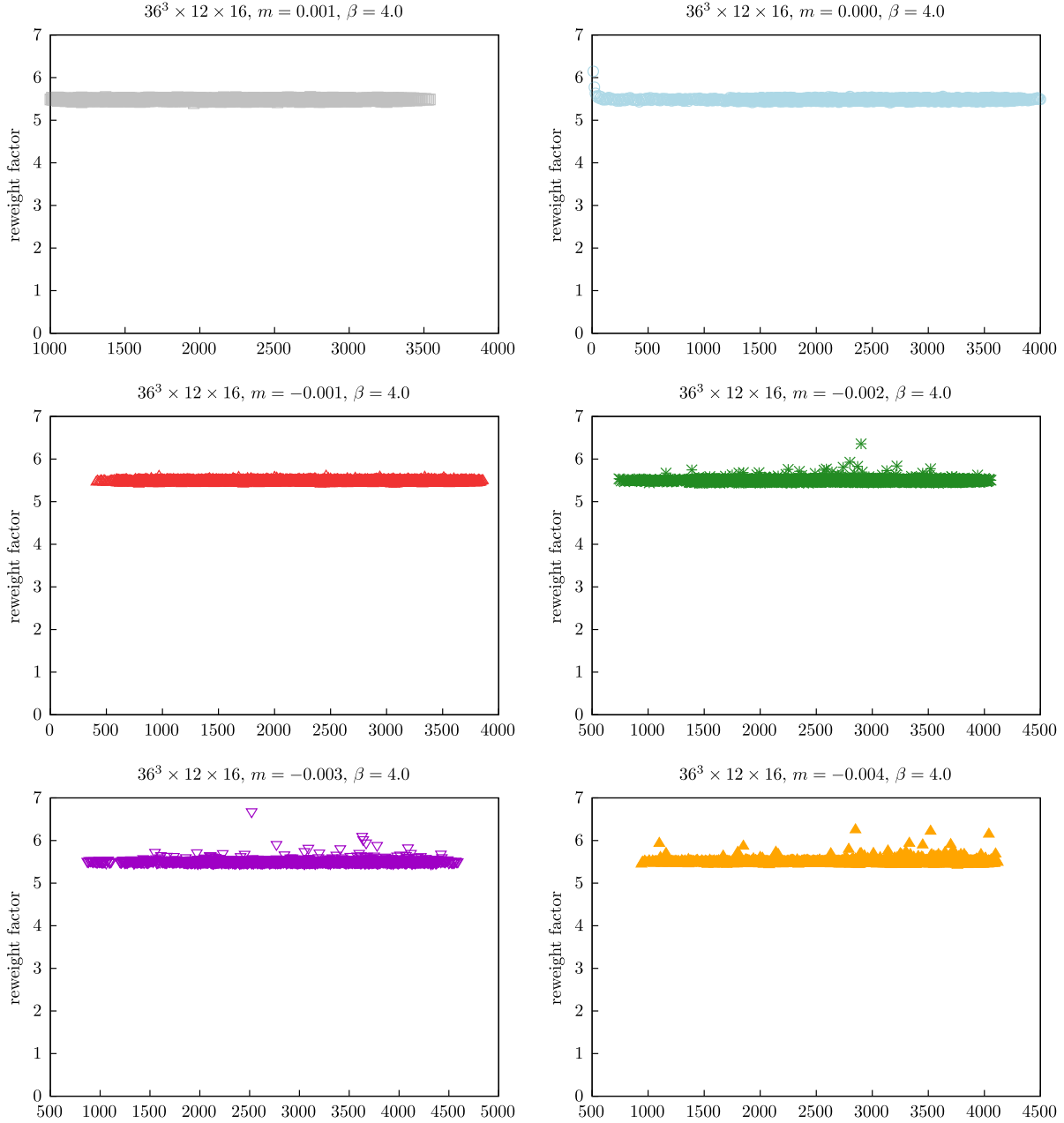


FIG. 19. The reweighting factors for the rational function reweighting on the $36^3 \times 12 \times 16$ ensembles at $\beta = 4.0$, for quark masses $m_q = 0.001, 0.000, -0.001, -0.002, -0.003, -0.004$. The reweighting factors are stable throughout the Monte Carlo history with no large fluctuations, indicating that the reweighting is well under control and can be safely applied to correct for the poor rational function approximation used in the original runs.

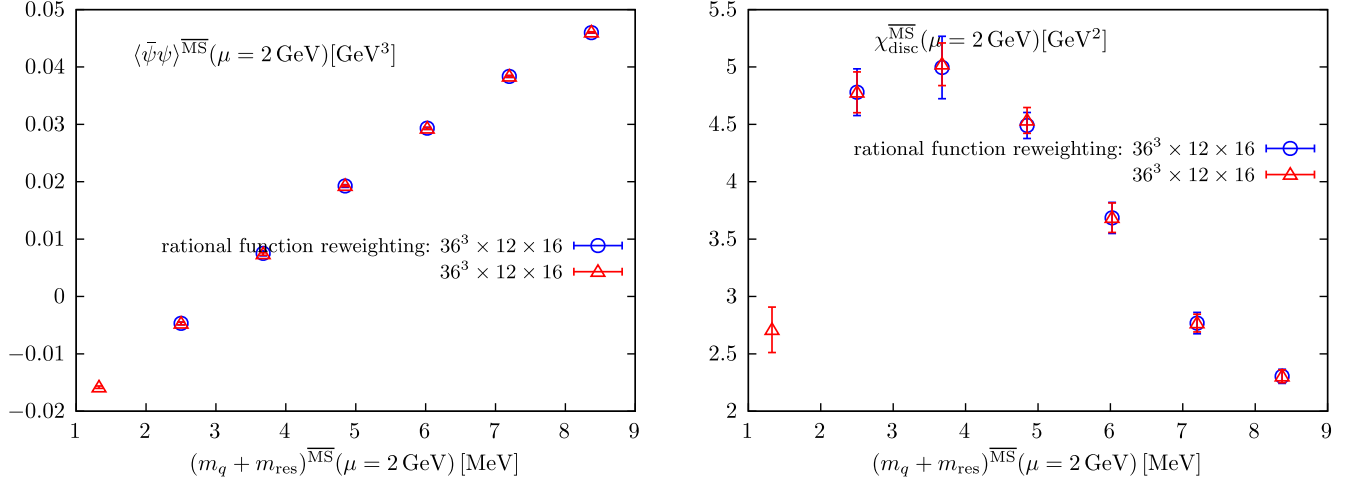


FIG. 20. Comparison of the chiral condensate $\langle \bar{\psi}\psi \rangle^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ (left) and the disconnected chiral susceptibility $\chi_{\text{disc}}^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ (right) on the $36^3 \times 12 \times 16$, $\beta = 4.0$ ensembles, before (red triangles) and after (blue circles) applying the rational function reweighting, as a function of the renormalized quark mass $(m_q + m_{\text{res}})^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$.

$$\begin{aligned} \frac{1}{\det \Omega} &= \frac{\int d\xi \exp(-\xi^\dagger \Omega \xi)}{\int d\xi \exp(-\xi^\dagger \xi)} \\ &= \frac{\int d\xi \exp(-\xi^\dagger (\Omega - 1) \xi) \exp(-\xi^\dagger \xi)}{\int d\xi \exp(-\xi^\dagger \xi)}, \end{aligned} \quad (\text{C13})$$

therefore, using a Gaussian noise vector ξ , we can estimate the above as a noise average

$$\frac{1}{\det \Omega} = \langle \exp(-\xi^\dagger (\Omega - 1) \xi) \rangle_\xi. \quad (\text{C14})$$

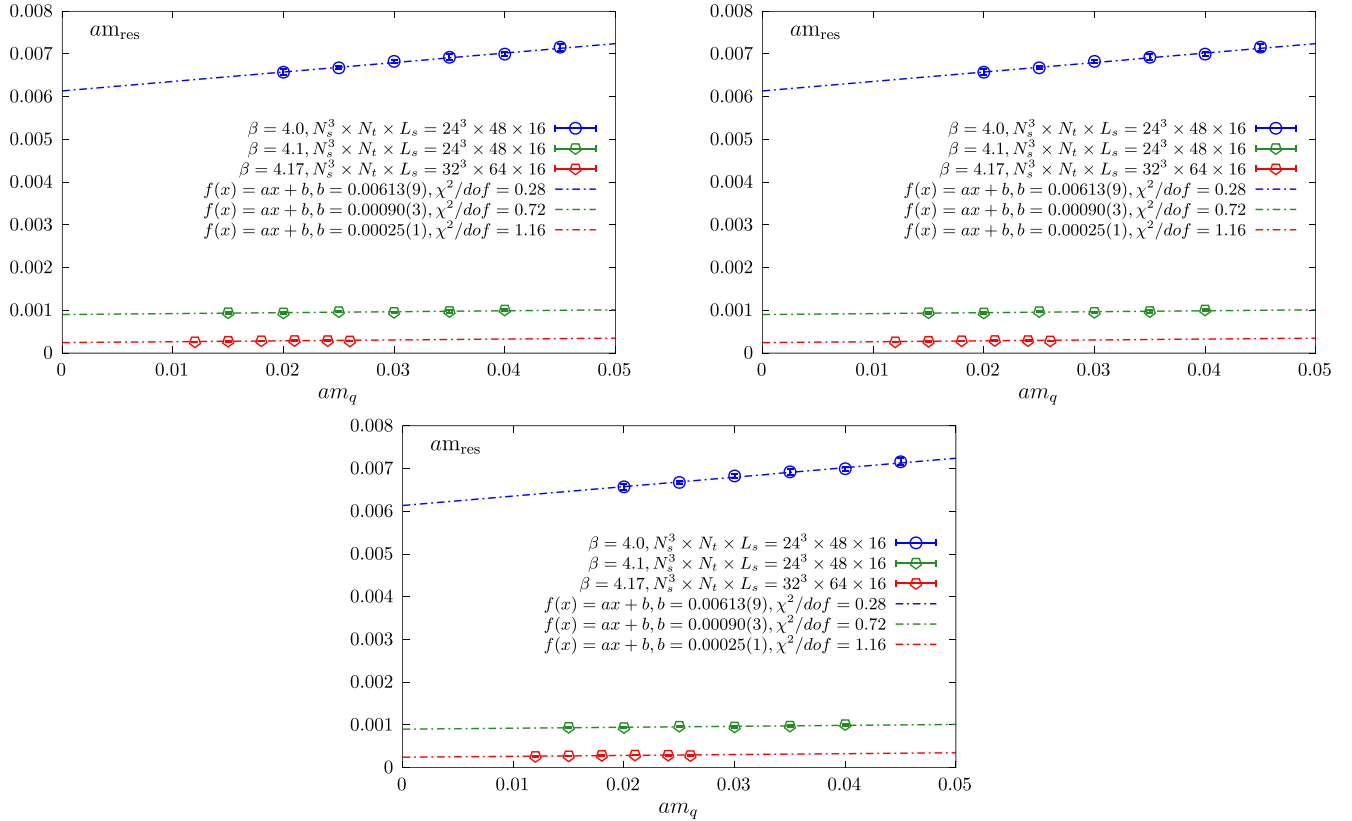


FIG. 21. Residual mass m_{res} as a function of the input quark mass, determined from the ratio of matrix elements of J_{5q} and J_5 . Results are shown for $\beta = 4.0$ (left), $\beta = 4.10$ (right), and $\beta = 4.17$ (bottom). Dash-dotted lines indicate linear fits. The residual masses extrapolated to bare input quark mass 0 and $-m_{\text{res}}$ are shown. The two results are consistent within errors for all three β values.

The reweighting factor is evaluated by using a Gaussian noise vector $|\xi\rangle$ as

$$\begin{aligned} |v_1\rangle &= f_{1/4}^{\text{poor}}(\mathcal{D}(m_q)) f_{1/4}^{\text{poor}}(\mathcal{D}(1)) f_{-1/4}^{\text{poor}}(\mathcal{D}(1)) |\xi\rangle, \\ |v_2\rangle &= f_{-1/2}^{\text{poor}} \mathcal{D}(m_q) |v_1\rangle, \\ \frac{1}{w} &= \exp[-(\omega - \xi_2)], \omega \equiv \langle v_1 | v_2 \rangle, \quad \xi_2 \equiv \langle \xi | \xi \rangle. \end{aligned} \quad (\text{C15})$$

3. Results

Figure 19 shows the reweighting factors for configurations generated with the earlier version of Grid. Their stability throughout the Monte Carlo history indicates that the reweighting can be safely applied. We can also estimate the magnitude of the reweighting factors. By neglecting the difference between $D_{\text{MDWF}}(1)$ and $D_{\text{MDWF}}(m_q)$, the correction to the fermion action is

$$\begin{aligned} \int dx \rho(x) [f_{1/4}^{\text{poor}}(x) f_{1/4}^{\text{poor}}(x) f_{1/4}^{\text{poor}}(x) f_{1/4}^{\text{poor}}(x) \\ \times f_{1/2}^{\text{poor}}(x) f_{1/4}^{\text{poor}}(x) f_{1/4}^{\text{poor}}(x) - 1] \end{aligned} \quad (\text{C16})$$

where $\rho(x)$ is the spectral density of the matrix. Assuming that $\rho(x)$ is constant, integration over the range $10^{-4} \leq x \leq 100$ gives 1.4×10^{-8} . Since the magnitude of the pseudo-fermion action is 5.37×10^7 , the resulting correction to the action is estimated to be $1.4 \times 10^{-8} \times 5.37 \times 10^7 = 0.75$, which provides an estimate of the logarithm of the reweighting factor. The actual value $\sim \log 6 = 1.8$ is larger but of the same order of magnitude.

Figure 20 shows the comparison of the chiral condensate $\langle \bar{\psi}\psi \rangle^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ and the disconnected chiral

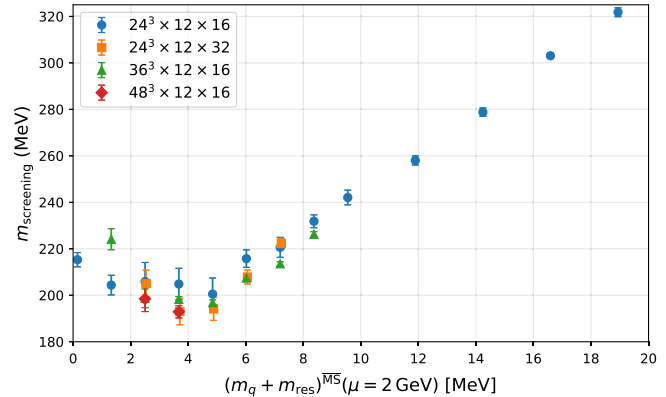


FIG. 22. The pion screening mass as a function of the renormalized quark mass for all $N_t = 12$ lattices.

susceptibility $\chi_{\text{disc}}^{\overline{\text{MS}}}(\mu = 2 \text{ GeV})$ before and after rational function reweighting on the $36^3 \times 12 \times 16$, $\beta = 4.0$ ensembles. The two results are in good agreement within statistical errors, as expected from Fig. 19, where the reweighting factors are seen to remain stable along the Monte Carlo history. We have found no case in which the reweighting changes a result beyond its statistical uncertainty; it is nevertheless included throughout for consistency.

APPENDIX D: RESIDUAL AND PION SCREENING MASSES

The residual-mass extrapolations to the bare input quark masses $m_q = 0$ and $m_q = -m_{\text{res}}$ for three values of β are shown in Fig. 21.

The pion screening masses used to fix the exponential scale in the finite-volume fit are summarized in Fig. 22.

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