PROCEEDINGS OF SCIENCE

Chiral susceptibility and axial U(1) anomaly near the (pseudo-)critical temperature

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We investigate relations between the chiral susceptibility and axial $U(1)$ anomaly in lattice QCD at high temperatures. Employing the exactly chiral symmetric Dirac operator, we separate the purely axial $U(1)$ breaking effect in the connected and disconnected chiral susceptibilites in a theoretically clean manner. Preliminary results for two-flavor lattice QCD near the critical temperature are presented.

The 40th International Symposium on Lattice Field Theory (Lattice 2023)
July 31st - August 4th, 2023
Fermi National Accelerator Laboratory

[*] Speaker

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1. Introduction

In the current universe, the chiral $SU(2)_L \times SU(2)_R$ symmetry is spontaneously broken, which explains the origin of the hadron masses as well as the special role of the pion as the (pseudo) Nambu-Goldstone boson. It is widely believed that at the critical temperature $T_c \sim 150$ MeV, the chiral symmetry is recovered. This is the so-called chiral phase transition our universe experienced just 10 μs after the Big-Bang. The chiral condensate $\langle \bar{q}q \rangle$ is considered to be the order parameter of the phase transition of QCD.

The QCD partition function at temperature T is given by a functional integral over the gluon field A,

$$Z(m,T) = \int [dA] \det(D(A,T) + m)^{N_f} e^{-S_G(A,T)}, \tag{1}$$

where $D(A,T)$ denotes the Dirac operator of quarks and $S_G(A,T)$ is the Yang-Mills acion of gauge fields. The T dependence is encoded as a finite temporal direction size $L_t = 1/T$ with the periodic boundary condition for gluons and anti-periodic one for quarks. We take $N_f = 2$ with degenerate up and down quark masses $m_u = m_d = m$ and take the strange and heavier quarks just as spectators. The chiral condensate is equivalent to the first derivative of $Z(m,T)$ with respect to m,

$$\Sigma(m,T) = -\langle \bar{q}q \rangle_{m,T} = \frac{1}{N_f V} \frac{\partial}{\partial m} \ln Z(m,T), \tag{2}$$

where V is the volume of the Euclidean spacetime. In this work, we focus on the second derivative,

$$\chi(m,T) = \frac{\partial}{\partial m} \Sigma(m,T), \tag{3}$$

which is known as the chiral susceptibility (See recent developments in [1–5]).

In Fig. 1 we illustrate how the chiral condensate and susceptiblity depend on T and m in the typical scinario of the second-order phase transition. At $m = 0$, the condensate continuously disappears at $T = T_c$, while it becomes a crossover for $m > 0$. It is, therefore, important to trace the quark mass dependence of the condensate at fixed temperatures marked by the color symbols at the top-left panel. As the top-right panel shows, while a rather mild quark mass dependence to a nonzero value at $m = 0$ is expected for lower temperatures than T_c, while the higher T curves show a steep drop to zero near the chiral limit $m = 0$. This drop should be reflected to the peaks of the chiral susceptibility $\chi(m,T)$ as the bottom-right panel presents.

When the phase transition is the first order, the T dependence becomes discontinuous at $T = T_c$ but in lattice QCD in a finite volume the discontinuity is smoothed and the situation will not be much different from Fig. 1.

The chiral condensate is a probe of the $SU(2)_L \times SU(2)_R$ chiral symmetry breaking or restoration. But the operator condensate $\langle \bar{q}q \rangle$ also breaks the axial $U(1)$ symmetry or $U(1)_A$ in short. In this talk we would like to discuss how much the $U(1)_A$ part contributes to the phase transition.

Since the anomaly is an explicit breaking in the theory given at the cutoff scale, it is natural to assume that the axial $U(1)$ is broken at any energy scale, and it is insensitive to the infra-red scales m and T. If this is true, the m and T dependence of the chiral condensate or chiral susceptibility should reflect the $SU(2)_L \times SU(2)_R$ breaking/restoration rather than that of $U(1)_A$.

A different scinario is possible if the topological excitations or instantons of the gluons are responsible for the low energy dynamics of QCD. In a paper by Callan, Dashen and Gross [6], they computed how much the instantons enhances the $U(1)_A$ anomaly as a trigger for the spontaneous $SU(2)_L \times SU(2)_R$ breaking (see also [7]). In this case, it is natural to assume that at $T = T_c$, the instantons disappear, reducing the $U(1)_A$ breaking effect, which makes the $SU(2)_L \times SU(2)_R$ to be recovered.

It has been a difficult issue in QCD to confirm either of the two scinarios near $T = T_c$. In analytic studies, it was found that the semiclassical QCD instanton configurations are not enough to quantitatively describe the low-energy dynamics of QCD. In lattice QCD simulations, it was difficult to treat chiral symmetries in a theoretically controled manner. The $SU(2)_L \times SU(2)_R \times U(1)_A$ symmetry is explicitly broken down to an axial $U(1)'$ subgroup (different from $U(1)_A$) symmetry in the staggered fermion formulation or down to a vectorlike $SU(2)$ symmetry in the Wilson fermon formulation.

In this work, we study the chiral condensate and its susceptibility in 2- and 2 + 1-flavor QCD with chiral symmetric Dirac operator on a lattice [8]. We separate the $U(1)_A$ breaking effect or topological effect in particular, from others in a theoretically clean way [9–12].

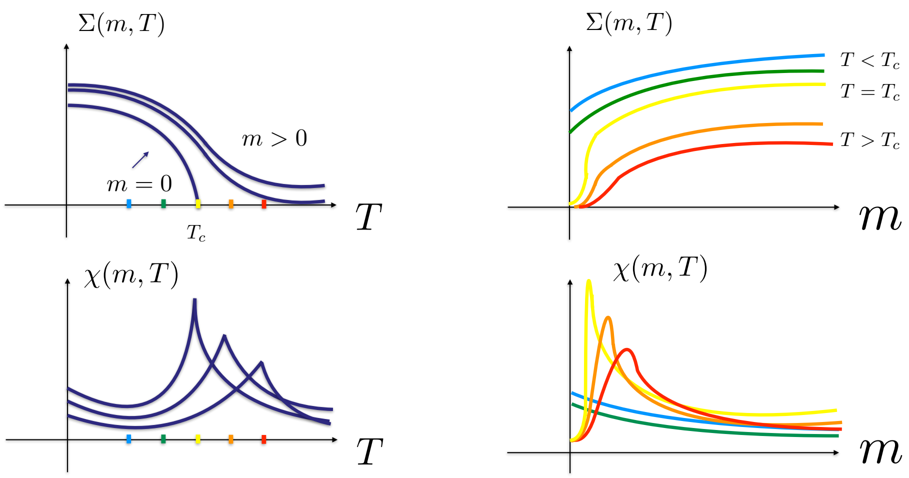

Figure 1: Schematic picture of the chiral condensate (top panels) and susceitpibility (bottom). The temperature T dependence (left panels) and and that on the quark mass m (right) at fixed temperatures marked by colored symbols are shown.

2. $U(1)_A$ contribution to chiral susceptibility

In this work, we formally rewrite the quark determinant in the QCD partition function by the eigenvalues λ of the Dirac operator. Then the chiral condensate is a configuration average of the summation over eigenvalues

$$\Sigma(m,T) = \frac{1}{N_f V}\frac{\partial}{\partial m}\ln Z(m) = \frac{1}{V}\left\langle \sum_\lambda \frac{1}{i\lambda(A)+m}\right\rangle, \tag{4}$$

and the chiral susceptibility is decomposed into the connected part given by the derivative with respect to the valence mass, and the disconnected part expressed by the derivative with respect to the sea quark mass:

$$\chi^{\text{con.}}(m) = \frac{\partial}{\partial m_{\text{valence}}}, \Sigma(m,T)\bigg|_{m_{\text{valence}}=m} \tag{5}$$

$$\chi^{\text{dis.}}(m) = \frac{\partial}{\partial m_{\text{sea}}}\Sigma(m,T)\bigg|_{m_{\text{sea}}=m}. \tag{6}$$

We relate the chiral susceptibility to a set of the other susceptibilites made of the scalar and pseudoscalar singlet operators : $S^0(x) = \bar{q}q(x)$ and $P^0(x) = \bar{q}i\gamma_5 q(x)$ where $q(x) = (u,d)^T$ denotes the up and down isospin doublet and those triplets: $S^a(x) = \bar{q}\tau^a q(x)$ and $P^a(x) = \bar{q}i\gamma_5\tau^a q(x)$, where τ^a denotes the a-th isospin generator or the Pauli matrix. These operators are connected by the $SU(2)_L \times SU(2)_R$ transformation $\exp(i\pi\gamma_5\tau^a/2)$ and the $U(1)_A$ one $\exp(i\pi\gamma_5/2)$.

By definition, the chiral susceptibility is equal to the singlet scalar susceptibility

$$\chi(m) = -\sum_x \langle S^0(x)S^0(0)\rangle - V\langle S^0\rangle^2. \tag{7}$$

Adding the θ term and absorbing it into the pseudoscalar mass term by the $U(1)_A$ rotation, we can relate the topological susceptibility to the pseusoscalar correlators,

$$\frac{N_f}{m^2}\chi_{\text{top.}}(m) = -\sum_x \langle P^0(x)P^0(0)\rangle + \frac{\Sigma(m,T)}{m}. \tag{8}$$

From the Ward-Takahashi identity about the $SU(2)_L \times SU(2)_R$ transformation of the $P^a(x)$, we have

$$m\sum_x \langle P^a(x)P^a(0)\rangle + \langle S^0\rangle = 0. \tag{9}$$

Recombining the above identities we obtain

$$\chi^{\text{con.}}(m) = \underbrace{-\Delta_{U(1)}(m) + \frac{\langle |Q(A)|\rangle}{m^2 V}}_{U(1)_A \text{ breaking}} + \underbrace{\frac{\Sigma_{\text{sub.}}(m,T)}{m}}_{\text{mixed.}}, \tag{10}$$

$$\chi^{\text{dis.}}(m) = \underbrace{\frac{N_f}{m^2}\chi_{\text{top.}}(m)}_{U(1)_A \text{ breaking}} + \underbrace{\Delta^{(1)}_{SU(2)}(m) - \Delta^{(2)}_{SU(2)}(m)}_{SU(2)_L\times SU(2)_R \text{ breaking}}, \tag{11}$$

where $Q(A)$ denotes the topological charge or the index of the Dirac operator. As indicated in the equations, the axial $U(1)$ susceptibility

$$\Delta_{U(1)}(m) \equiv \sum_x \langle P^a(x)P^a(0) - S^a(x)S^a(0)\rangle, \tag{12}$$

measures a purely $U(1)_A$ breaking effect, while the other two susceptibilities

$$\Delta^{(1)}_{SU(2)}(m) \equiv \sum_x \langle S^0(x)S^0(0) - P^a(x)P^a(0)\rangle, \quad \Delta^{(2)}_{SU(2)}(m) \equiv \sum_x \langle S^a(x)S^a(0) - P^0(x)P^0(0)\rangle, \tag{13}$$

are the probes for the $SU(2)_L \times SU(2)_R$ breaking. Note that we have subtracted the chiral condensate at a reference quark mass $m_{\rm ref} = 0.005$ in order to cancel the quadratic UV divergence, which is denoted by

$$\frac{\Sigma_{\rm sub.}(m,T)}{m} = \left[\frac{\Sigma(m,T)}{m} - \frac{\langle|Q(A)|\rangle}{m^2V}\right] - \left[\frac{\Sigma(m_{\rm ref},T)}{m_{\rm ref}} - \frac{\langle|Q(A)|\rangle|_{m=m_{\rm ref}}}{m_{\rm ref}^2 V}\right]. \tag{14}$$

Note in the discussion above we have used the notation in the continuum theory but the corresponding lattice expression can be given by the eigenvalues of the massive overlap Dirac operator $H_m = \gamma_5[(1-m)D_{\rm ov} + m]$ [9]. The precise chiral symmetry is, however, essential in the decomposition[13]. Our goal of this work is to quantify how much the $U(1)_A$ breaking contributes to the signal of the chiral susceptibility in lattice QCD with exactly chiral symmetric Dirac operator.

3. Numerical results

We simulate $N_f = 2$ QCD with a lattice spacing fixed at $1/a = 2.6$ GeV. We employ the Symanzik gauge action with $\beta = 4.30$ and Möbius domain-wall fermions [14] for configuration generations with the residual mass less than 1 MeV. The quark mass is taken in a range $[3, 30]$ MeV, which covers a point below the physical up and down quark mass and we have six different temperatures obtained by changing the temporal lattice size L_t from 8 to 18, which corresponds to [147–330] MeV. Our main lattice size is 32 or 2.4 fm but for lower temperatures we extend to 40($\sim$ 3fm) or 48($\sim$ 3.6fm) to study the finite volume systematics. As will be discussed below, the pseudo-critical temperature is estimated to be $T_c \sim 165$ MeV (at the physical point) and the lowest simulated temperature on $L_t = 18$(147 MeV) lattices correspond to $0.9T_c$.

In order to reduce the lattice artifact due to the violation of the Ginsparg-Wilson relation [10], we use the reweighting technique to replace the Möbius domain-wall fermion determinant by that of the overlap fermion action, in which the sign function for the low modes of the kernel Dirac operator are taken exactly. The residual mass is reduced to 0.001 MeV with this procedure. We also increase the simulation points by the same reweighting technique but with different quark mass. With the mass reweighting, we obtain the results down to $m = 0.0002$ or 1/5 physical point mass.

In this work, the observables are computed with the spectral decomposition or the summation over the eigenvalues. The cutoff of the summation at 30–40-th lowest modes, which corresponds to 150–300 MeV, gives a good saturation and consistency with direct inversion of Möbius domain-wall Dirac operator as far as $T \leq 260$ MeV. At T =330 MeV, the convergence is marginal and we do not employ the low-mode approximation.

In Fig. 2 the connected (top panel) and disconnected (bottom) chiral susceptibilities are plotted as a function of the quark mass at 6 simulated temperatures. The open solid symbols are the lattice data, while the filled dashed symbols are $U(1)_A$ breaking part. We can see that the $U(1)_A$ breaking contribution dominates the signals. Specifically the axial $U(1)$ susceptiblity dominates the connected part of the chiral susceptibility and the topological susceptibility divided by the quark mass squared is respobsible for the signal of the disconnected chiral susceptibility. This is the case even for the lower temperature around 147 MeV in pentagons and lower quark masses obtained by the reweighting and larger volumes. However, this $U(1)_A$ dominance becomes less obvious with noisier signals for light quark mass points at lower temperatures. This behavior is shown in the top panel of Fig. 3 where the T dependence of the disconnected susceptibility is presented. Fitting data to a quadratic function, we can estimate the position of the peak at each quark mass. The chiral extrapolation of the susceptibility peak is shown in the bottom panel of Fig. 3. The preliminary estimate for the (pseudo-) critical temperature is $T_c \sim 165$ MeV at the physical point, and $T_c \sim 153$ MeV in the chiral limit.

4. Summary

We simulate $N_f = 2$ QCD at high temperatures. The chiral condensate and susceptibility are related not only to the standard $SU(2)_L \times SU(2)_R$ chiral symmetry but also to the anomalous $U(1)_A$ symmetry. In the spectral decomposition of the Dirac operator with exact chiral symmetry on a lattice, we can separate the purely $U(1)_A$ breaking effect. We have found that the connected part is dominated by the axial $U(1)$ susceptibility, and the disconnected part is governed by the topological susceptibility. But for lower T, the deviation becomes sizable. Our results suggest that the axial $U(1)$ anomaly may play more important role in the QCD phase diagram [15] than expected.

We thank L. Glozman and Y. Sumino for useful discussions. For the numerical simulation we have used the QCD software packages Grid [16, 18] for configuration generations and Bridge++ [17, 19] for measurements. Numerical simulations were performed on Oakforest-PACS and Wisteria/BDEC-01 at JCAHPC under a support of the HPCI System Research Projects (Project IDs: hp170061, hp180061, hp190090, and hp200086, hp210104, hp220093, hp230070) as well as Multidisciplinary Cooperative Research Program in CCS, University of Tsukuba (Project IDs: xg17i032, xg18i023 and wo22i038) and Fugaku computer provided by the RIKEN Center for Computational Science under a support of the HPCI System Research Projects (Project IDs: hp200130, hp210165, hp210231, hp220279, hp230323). This work was (partly) achieved through the use of SQUID at the Cybermedia Center, Osaka University. We used Japan Lattice Data Grid (JLDG) [20] for storing a part of the numerical data generated for this work. This work is supported in part by the Japanese Grant-in-Aid for Scientific Research (No. JP26247043, JP18H01216, JP18H04484, JP18H05236, JP22H01219) and by Joint Institute for Computational Fundamental Science (JICFuS).

References

[1] T. Bhattacharya *et al.* [HotQCD Collaboration], "QCD Phase Transition with Chiral Quarks and Physical Quark Masses," Phys. Rev. Lett. **113**, no.8, 082001 (2014)

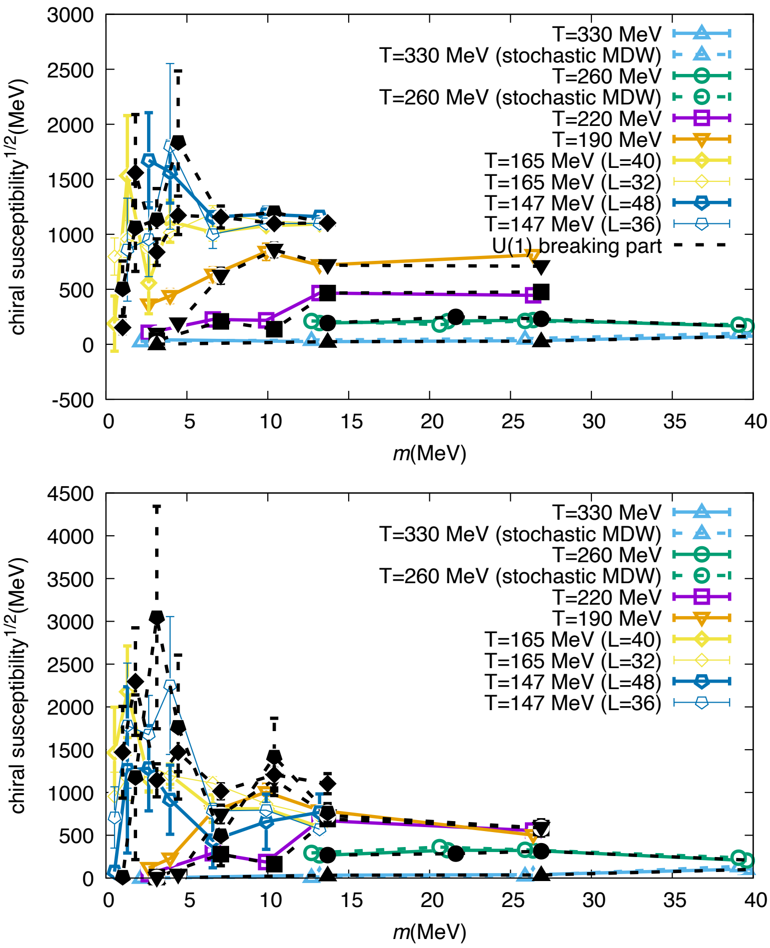

Figure 2: The connected (top panel) and disconnected (bottom) susceptibilities are plotted as a function of the quark mass at 6 different temperatures. Compared to the total contribution in open solid symbols, the axial $U(1)$ anomaly part in dashed filled are dominant. But this $U(1)_A$ dominance becomes unclear and noisier for light quark mass points at lower temperatures.

doi:10.1103/PhysRevLett.113.082001 [arXiv:1402.5175 [hep-lat]].

[2] C. Bonati, M. D'Elia, M. Mariti, M. Mesiti, F. Negro and F. Sanfilippo, "Curvature of the chiral pseudocritical line in QCD: Continuum extrapolated results," Phys. Rev. D **92**, no.5, 054503 (2015) doi:10.1103/PhysRevD.92.054503.

[3] B. B. Brandt, A. Francis, H. B. Meyer, O. Philipsen, D. Robaina and H. Wittig, "On the strength of the $U_A(1)$ anomaly at the chiral phase transition in $N_f = 2$ QCD," JHEP **12**, 158 (2016) doi:10.1007/JHEP12(2016)158 [arXiv:1608.06882 [hep-lat]].

[4] Y. Taniguchi *et al.* [WHOT-QCD Collaboration], "Exploring $N_f = 2{+}1$ QCD thermodynamics from the gradient flow," Phys. Rev. D **96**, no.1, 014509 (2017) [erratum: Phys. Rev. D **99**, no.5, 059904 (2019)] doi:10.1103/PhysRevD.96.014509 [arXiv:1609.01417 [hep-lat]].

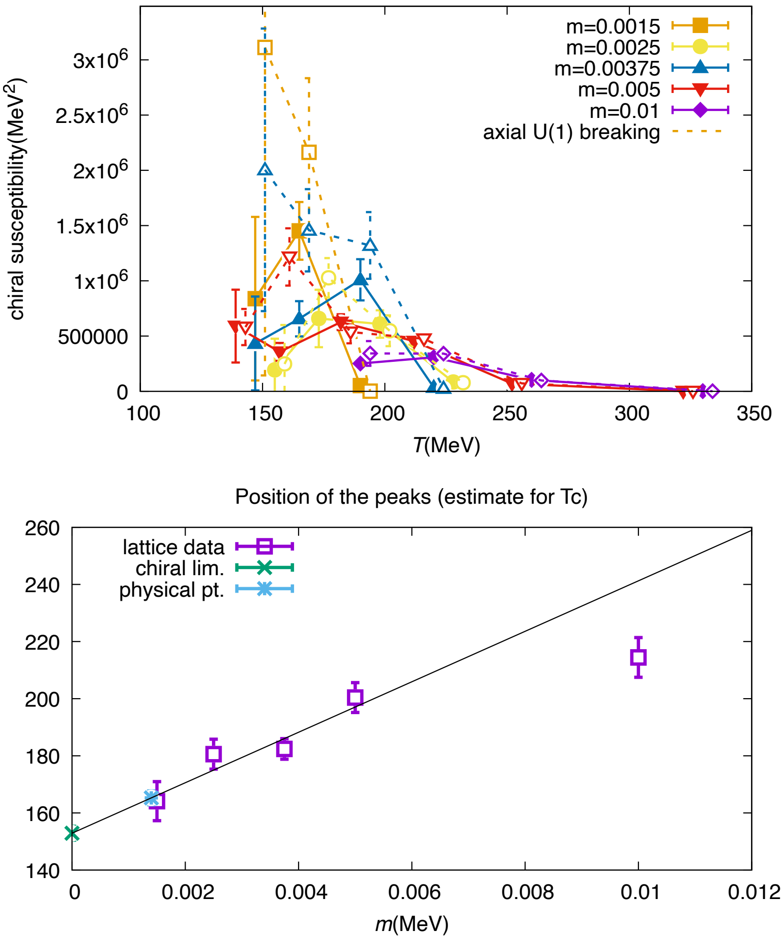

Figure 3: Top: T dependence of the disconnected susceptibility at 5 different quark masses. Bottom: The chiral extrapolation of the peak position of the disconnected susceptibility gives an estimate for the (pseudo-) critical temperature. Bottom: Our estimate for T_c from the quark mass dependence of the peak position of the disconnected susceptibility.

[5] H. T. Ding *et al.* [HotQCD Collaboration], "Chiral Phase Transition Temperature in 2 + 1-Flavor QCD," Phys. Rev. Lett. **123**, no.6, 062002 (2019) doi:10.1103/PhysRevLett.123.062002 [arXiv:1903.04801 [hep-lat]].

[6] C. G. Callan, Jr., R. F. Dashen and D. J. Gross, "Toward a Theory of the Strong Interactions," Phys. Rev. D **17**, 2717 (1978) doi:10.1103/PhysRevD.17.2717

[7] D. Diakonov and V. Y. Petrov, "CHIRAL CONDENSATE IN THE INSTANTON VACUUM," Phys. Lett. B **147**, 351-356 (1984) doi:10.1016/0370-2693(84)90132-1

[8] H. Neuberger, "Exactly massless quarks on the lattice," Phys. Lett. B **417**, 141 (1998) doi:10.1016/S0370-2693(97)01368-3 [hep-lat/9707022].

[9] S. Aoki, H. Fukaya and Y. Taniguchi, "Chiral symmetry restoration, eigenvalue density of

Dirac operator and axial U(1) anomaly at finite temperature," Phys. Rev. D **86**, 114512 (2012) doi:10.1103/PhysRevD.86.114512 [arXiv:1209.2061 [hep-lat]].

[10] G. Cossu *et al.* [JLQCD Collaboration], "Violation of chirality of the Möbius domain-wall Dirac operator from the eigenmodes," Phys. Rev. D **93**, no. 3, 034507 (2016) doi:10.1103/PhysRevD.93.034507 [arXiv:1510.07395 [hep-lat]].

[11] A. Tomiya *et al.* [JLQCD Collaboration] "Evidence of effective axial U(1) symmetry restoration at high temperature QCD," Phys. Rev. D **96**, no. 3, 034509 (2017) Addendum: [Phys. Rev. D **96**, no. 7, 079902 (2017)] doi:10.1103/PhysRevD.96.034509, 10.1103/PhysRevD.96.079902 [arXiv:1612.01908 [hep-lat]].

[12] S. Aoki *et al.* [JLQCD], "Study of the axial $U(1)$ anomaly at high temperature with lattice chiral fermions," Phys. Rev. D **103**, no.7, 074506 (2021) doi:10.1103/PhysRevD.103.074506 [arXiv:2011.01499 [hep-lat]].

[13] A. Gómez Nicola and J. Ruiz De Elvira, "Chiral and $U(1)_A$ restoration for the scalar and pseudoscalar meson nonets," Phys. Rev. D **98**, no.1, 014020 (2018) doi:10.1103/PhysRevD.98.014020 [arXiv:1803.08517 [hep-ph]].

[14] R. C. Brower, H. Neff and K. Orginos, "Mobius fermions," Nucl. Phys. Proc. Suppl. **153**, 191 (2006) doi:10.1016/j.nuclphysbps.2006.01.047 [hep-lat/0511031]; "The Möbius domain wall fermion algorithm," Comput. Phys. Commun. **220**, 1 (2017) doi:10.1016/j.cpc.2017.01.024 [arXiv:1206.5214 [hep-lat]].

[15] R. D. Pisarski and F. Wilczek, "Remarks on the Chiral Phase Transition in Chromodynamics," Phys. Rev. D **29**, 338 (1984) doi:10.1103/PhysRevD.29.338.

[16] P. Boyle, A. Yamaguchi, G. Cossu and A. Portelli, "Grid: A next generation data parallel C++ QCD library," doi:https://doi.org/10.22323/1.251.0023 [arXiv:1512.03487 [hep-lat]].

[17] S. Ueda, S. Aoki, T. Aoyama, K. Kanaya, H. Matsufuru, S. Motoki, Y. Namekawa, H. Nemura, Y. Taniguchi and N. Ukita, "Development of an object oriented lattice QCD code 'Bridge++'," J. Phys. Conf. Ser. **523**, 012046 (2014) doi:10.1088/1742-6596/523/1/012046

[18] N. Meyer, P. Georg, S. Solbrig and T. Wettig, "Grid on QPACE 4," PoS **LATTICE2021**, 068 (2022) doi:10.22323/1.396.0068 [arXiv:2112.01852 [hep-lat]].

[19] Y. Akahoshi, S. Aoki, T. Aoyama, I. Kanamori, K. Kanaya, H. Matsufuru, Y. Namekawa, H. Nemura and Y. Taniguchi, "General purpose lattice QCD code set Bridge++ 2.0 for high performance computing," J. Phys. Conf. Ser. **2207**, no.1, 012053 (2022) doi:10.1088/1742-6596/2207/1/012053 [arXiv:2111.04457 [hep-lat]].

[20] T. Amagasa, S. Aoki, Y. Aoki, T. Aoyama, T. Doi, K. Fukumura, N. Ishii, K. I. Ishikawa, H. Jitsumoto and H. Kamano, *et al.* "Sharing lattice QCD data over a widely distributed file system," J. Phys. Conf. Ser. **664**, no.4, 042058 (2015) doi:10.1088/1742-6596/664/4/042058

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