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Chiral symmetry restoration, the eigenvalue density of the Dirac operator, and the axial U(1) anomaly at finite temperature

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We reconsider constraints on the eigenvalue density of the Dirac operator in the chiral-symmetric phase of two-flavor QCD at finite temperature. To avoid possible ultraviolet divergences, we work on a lattice, employing the overlap Dirac operator, which ensures the exact "chiral" symmetry at finite lattice spacings. Studying multipoint correlation functions in various channels and taking their thermodynamical limit (and then taking the chiral limit), we obtain stronger constraints than those found in the previous studies: both the eigenvalue density at the origin and its first and second derivatives vanish in the chiral limit of two-flavor QCD. In addition, we show that the axial U(1) anomaly becomes invisible in susceptibilities of scalar and pseudoscalar mesons, suggesting that the second-order chiral phase transition with the $O(4)$ scaling is not realized in two-flavor QCD. Possible lattice artifacts when the nonchiral lattice Dirac operator is employed are briefly discussed.

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I. INTRODUCTION

The QCD Lagrangian with N_f massless quarks is invariant under $\mathrm{SU}(N_f)_L \times \mathrm{SU}(N_f)_R \times \mathrm{U}(1)_V \times \mathrm{U}(1)_A$ chiral rotations. This symmetry, however, is broken in two different ways: the $\mathrm{SU}(N_f)_L \times \mathrm{SU}(N_f)_R$ part is spontaneously broken to $\mathrm{SU}(N_f)_V$ in the QCD vacuum, while the $\mathrm{U}(1)_A$ part is broken explicitly at the quantum level by the anomaly.

At a finite temperature T, it is widely believed that the $\mathrm{SU}(N_f)_L \times \mathrm{SU}(N_f)_R$ chiral symmetry is recovered above the (critical) temperature $T_c \sim 150$ MeV, and plenty of evidence has been reported in the first-principle calculations of lattice QCD. For the $\mathrm{U}(1)_A$ part, however, it remains an open question *if, how* (*much*), *and when* the symmetry is restored. We only know that the $\mathrm{U}(1)_A$ symmetry should be recovered in the $T \to \infty$ limit, where fermions eventually decouple as the lowest Matsubara frequency goes to infinity, so that the anomaly term cannot survive.

In particular, the question of whether the $\mathrm{U}(1)_A$ symmetry is restored near T_c is of phenomenological importance. For simplicity, let us consider the $N_f = 2$ case. As Pisarski and Wilczek [1] have discussed, the order of the phase transition may depend on the fate of the $\mathrm{U}(1)_A$ symmetry: if it remains to be broken at T_c, the chiral phase transition can be second-order, while it is likely to be first-order when the $\mathrm{U}(1)_A$ symmetry is also restored. Furthermore, the particle spectrum with the presence or absence of the $\mathrm{U}(1)_A$ symmetry is quite different [2]. A connection between the restoration of $\mathrm{U}(1)_A$ symmetry and the gap in the eigenvalue density of the Dirac operator near the origin is also suggested [3].

In principle, the fate of the $\mathrm{U}(1)_A$ symmetry and related issues can be investigated by numerical lattice QCD simulations [4,5]. Such studies are, however, still not easy, since both chiral and thermodynamical (the infinite volume) limits are required. Currently, four simulations with different quark actions are ongoing, but they have reported different results. Two of them [6,7] have reported that the eigenvalue density of the Dirac operator has no gap at the origin and its quark-mass scaling is consistent with the broken $\mathrm{U}(1)_A$ scenario. Another group [8] has also reported no gap at the origin but they have found that small eigenmodes, which mainly contribute to $\mathrm{U}(1)_A$-breaking correlation functions, are localized and uncorrelated, suggesting that their contribution to the correlation functions is negligible. A simulation with overlap quarks [9], however, has reported the existence of a gap in the Dirac eigenvalue density and a degeneracy of pion and eta (-prime) meson correlators, which suggests the recovery of $\mathrm{U}(1)_A$ symmetry.

In this paper, we address these problems again on a lattice, but using an analytic method. For simplicity, we concentrate on the $N_f = 2$ case in this paper. We employ the overlap Dirac operator [10,11], which ensures the exact $\mathrm{SU}(2)_L \times \mathrm{SU}(2)_R$ symmetry [12] through the Ginsparg-Wilson relation [13], but the $\mathrm{U}(1)_A$ symmetry is (correctly) broken by the fermionic measure [14]. By using the spectral decomposition of the multipoint correlation functions, and assuming the restoration of the $\mathrm{SU}(2)_L \times \mathrm{SU}(2)_R$ symmetry, we investigate if there are new constraints on the Dirac eigenvalue density in addition to the manifest one implied by the well-known Banks-Casher relation [15]. We also investigate whether the effect of the $\mathrm{U}(1)_A$ symmetry breaking disappears above T_c.

Since similar analytical investigations have been made in previous studies, let us here revisit them and make clear what is new in this paper. The first analysis based only on QCD was done by Cohen [16]. Assuming an absence of the zero-mode's contribution, they concluded that all the *disconnected* contributions of the two-point functions in the $SU(2)_L \times SU(2)_R$-symmetric phase disappear in the chiral limit. This means that the pion, sigma, delta, and eta(-prime) meson correlators are all identical, realizing the $U(1)_A$ symmetry. In this work, we include the zero-mode contribution explicitly to check whether or not this conclusion survives.

In fact, Lee and Hatsuda [17] (see also a related work by Evans *et al.* [18]) claimed that the zero-mode's contribution does not vanish but keeps the disconnected contribution of the scalar channel nonzero:

$$\begin{aligned}&\lim_{m\to 0}(\langle \bar{q}(x)q(x)\bar{q}(y)q(y)\rangle - \langle \bar{q}(x)T^3q(x)\bar{q}(y)T^3q(y)\rangle)\\ &\quad = \lim_{m\to 0}\frac{\int d[A]_{\nu=\pm 1}e^{-S_{YM}}\det'[\not{D}+m]^2\times 4\bar{\phi}_0^A(x)\phi_0^A(x)\bar{\phi}_0^A(y)\phi_0^A(y)}{Z} + O(m),\end{aligned} \tag{1}$$

where q denotes the quark field and T^3 is the third generator of SU(2). On the rhs, Z is the partition function of QCD, $d[A]_{\nu=\pm 1}$ denotes the gauge field integrals with a fixed topological charge $\nu = \pm 1$, S_{YM} denotes the gauge part of the action, $\det'[\not{D}+m] = \det[\not{D}+m]/m$ is the (continuum) fermion determinant with the quark mass m from which the zero-mode contribution is subtracted, and ϕ_0^A is an eigenfunction for the zero-mode at a given configuration A.

The thermodynamical limit of Eq. (1) is, however, nontrivial and subtle, as was pointed out by Cohen [3]. In fact, we find that the rhs of Eq. (1) is at least an $O(1/V)$ quantity. Integrating Eq. (1) over x and then taking an average over y, (which should be grater than the original lhs), one immediately obtains

$$\frac{1}{V}\int d^4y\int d^4x[\text{lhs of Eq.(1)}] = C\frac{4N_\phi^2}{V}\to 0, \qquad V\to\infty, \tag{2}$$

since both $N_\phi = \int d^4x\bar{\phi}_0^A(x)\phi_0^A(x)$ and $C = \lim_{m\to 0}(Z_1 + Z_{-1})/m^2Z$ (where $Z_{\pm 1}$ denotes the partition function in the topological sector of $\nu = \pm 1$) are finite. In fact, our work will show that not only Eq. (1) but also any contributions from zero-modes of the Dirac operator are in general $O(1/V)$ quantities, and thus disappear in the large-volume limit. It is not difficult to intuitively understand our result. In the large-volume limit that $V\to\infty$, the number of the fermion modes contributing to the denominator Z increases (it is natural to assume it to be proportional to V), while that of the numerator, where the bulk $O(V)$ contributions are canceled, is fixed to be $O(1)$.

Two years later, Cohen [3] discussed a constraint on the eigenvalue density of the QCD Dirac operator in the chiral limit. Relating the scalar one-point function and pseudoscalar two-point functions in the chiral-symmetric phase, he concluded that the eigenvalue density near zero,

$$\rho(\lambda)\sim|\lambda|^\alpha, \tag{3}$$

must have $\alpha > 1$. In this paper, we examine up to four-point correlation functions in more various channels, and obtain a stronger constraint: $\alpha > 2$. In the case of integer α, we believe that our constraint that α is equal to or larger than 3 should be the *strongest*, since we know of a theory which has both $\alpha = 3$ and unbroken $SU(2)_L\times SU(2)_R$ [and also $U(1)_A$] chiral symmetries: two-flavor massless free quarks.

Although we perform no numerical analysis in our study, we would like to discuss possible artifacts in lattice QCD simulations. In our analysis, the fully recovered $SU(2)_L\times SU(2)_R$ symmetry is crucial. We discuss possible modifications to our conclusions due to discretization effects if a nonchiral quark action is employed in numerical simulations. We also comment on finite-volume effects.

Our paper is organized as follows. In Sec. II, we explain our setup, what we observe, and what we assume. The constraints on the eigenvalue density with integer power at the origin are given in Sec. III. In Sec. IV, we address a question on the fate of the $U(1)_A$ symmetry. In Sec. V, we discuss possible systematic effects which may arise in lattice QCD simulations. Section VI is devoted to a case where the eigenvalue density has a fractional power at the origin. A conclusion and discussion are given in Sec. VII. Some useful formula and detailed calculations are collected in two appendices.

II. LATTICE SETUP

A. Spectral decomposition of the overlap fermion

We consider N_f-flavor lattice QCD in a finite volume V, with the (anti)periodic boundary condition in space(time).

The quark part of the action is given by

$$\begin{aligned}S_F &= a^4\sum_x[\bar{\psi}D(A)\psi + m\bar{\psi}F(D(A))\psi](x),\\ F(D) &= 1-\frac{Ra}{2}D,\end{aligned} \tag{4}$$

where $\psi = (\psi_1, \psi_2, \dots \psi_{N_f})^T$ denotes the set of N_f fermion fields with the degenerate mass m, a is the lattice spacing, and $D(A)$ is the overlap Dirac operator [10,11] for a given gauge field A,

$$D(A) = \frac{1}{Ra}\left(1+\frac{D_W(A)-1/Ra}{\sqrt{(D_W(A)-1/Ra)^\dagger(D_W(A)-1/Ra)}}\right). \tag{5}$$

Here $D_W(A)$ denotes the Wilson-Dirac operator for the same gauge configuration A, and R is an arbitrary constant. We have omitted the identity matrix $\mathbf{1}_{N_f\times N_f}$ for the flavor indices for simplicity.

It is well-known that the overlap Dirac operator satisfies the γ_5 hermiticity, $D(A)^\dagger = \gamma_5 D(A)\gamma_5$, and the Ginsparg-Wilson (GW) relation [13],

$$D(A)\gamma_5 + \gamma_5 D(A) = aD(A)R\gamma_5 D(A). \tag{6}$$

With this relation, the action (4) in the $m \to 0$ limit is exactly symmetric [12] under the *lattice* chiral rotation,

$$\delta_a \psi(x) = i\theta T_a \gamma_5[(1 - RaD(A))\psi](x), \tag{7}$$

$$\delta_a \bar{\psi}(x) = i\theta \bar{\psi}(x) T_a \gamma_5, \tag{8}$$

where θ is an infinitesimal real parameter, T_a denotes the generator of SU(N_f) for $a = 1, 2, \ldots N_f^2 - 1$, and $T_0(= \mathbf{1}_{N_f\times N_f})$ denotes that for U$(1)_A$.

We now consider eigenvalues and eigenfunctions of $D(A)$: $D(A)\phi_n^A = \lambda_n^A \phi_n^A$. The GW relation implies that

$$\lambda_n^A + \bar{\lambda}_n^A = aR\bar{\lambda}_n^A \lambda_n^A, \tag{9}$$

where λ_n^A and its complex conjugate $\bar{\lambda}_n^A$ are in general complex numbers and therefore $(\phi_n^A)^\dagger D(A)^\dagger = (\phi_n^A)^\dagger \bar{\lambda}_n^A$. Moreover, from the GW relation (6) and its consequence (9) we have

$$D(A)\gamma_5\phi_n^A = -\frac{\lambda_n^A}{1 - Ra\lambda_n^A}\gamma_5\phi_n^A = \bar{\lambda}_n^A \gamma_5 \phi_n^A. \tag{10}$$

Since $(\bar{\lambda}_n^A - \lambda_m^A)(\phi_n^A, \gamma_5\phi_m^A) = 0$, eigenfunctions with complex eigenvalues can be orthonormalized as $(\phi_n^A, \phi_m^A) = (\gamma_5\phi_n^A, \gamma_5\phi_m^A) = \delta_{nm}$, and $(\phi_n^A, \gamma_5\phi_m^A) = 0$. Here an inner product is defined as $(f, g) \equiv a^4\sum_x f^\dagger(x)g(x)$. For the real eigenvalues $\lambda_k^A = 0$ and $\lambda_K^A = 2/(Ra)$, their eigenfunctions can be chiral eigenstates, since $D(A)$ and γ_5 commute for these real modes. In the following, let us denote the number of the left(right)-handed zero eigenmodes as $N_L(N_R)$ and that of the left(right)-handed $\lambda_K^A = 2/Ra$ (doubler) eigenmodes as $n_L(n_R)$.

Thus the propagator of the massive overlap fermion (for each flavor) can be expressed in terms of these eigenvalues and eigenfunctions as

$$\begin{aligned} S_A(x,y) = &\sum_{\{n|\mathrm{Im}\lambda_n^A>0\}}\left[\frac{\phi_n^A(x)\phi_n^A(y)^\dagger}{f_m\lambda_n^A + m} + \frac{\gamma_5\phi_n^A(x)\phi_n^A(y)^\dagger\gamma_5}{f_m\bar{\lambda}_n^A + m}\right] \\ &+ \sum_{k=1}^{N_{R+L}^A}\frac{\phi_k^A(x)\phi_k^A(y)^\dagger}{m} + \sum_{K=1}^{n_{R+L}^A}\frac{\phi_K^A(x)\phi_K^A(y)^\dagger}{2/(Ra)}, \end{aligned} \tag{11}$$

where $f_m = 1 - Rma/2$, $N_{R+L}^A = N_R^A + N_L^A$ is the total number of zero-modes, and $n_{R+L}^A = n_R^A + n_L^A$ is the total number of doubler modes.

A measure for a given gauge field A can be also written in terms of eigenvalues as

$$\begin{aligned} P_m(A) = &e^{-S_{YM}(A)} m^{N_f N_{R+L}^A} (\Lambda_R)^{N_f n_{R+L}^A} \\ &\times \prod_{\mathrm{Im}\lambda_n>0} (Z_m^2 \bar{\lambda}_n^A \lambda_n^A + m^2)^{N_f}, \end{aligned} \tag{12}$$

where $S_{YM}(A)$ is the gauge part of the action (whose explicit form is not needed in this work), $\Lambda_R = 2/(Ra)$, and $Z_m^2 = 1 - m^2/\Lambda_R^2$. Note that for even N_f, $P_m(A)$ is positive definite and an even function of m.

It is important to note that all quantities which consist of $S_A(x, y)$ and $P_m(A)$ are finite at $V < \infty$, $m \neq 0$ and $a \neq 0$. We then carefully take the $V \to \infty$ and $m \to 0$ limits without worrying about possible ultraviolet (UV) divergences, until we eventually take the continuum limit.

B. Chiral Ward-Takahashi identities on the lattice

Now let us study the quantum aspects of the symmetry, performing the functional integral of an operator $\mathcal{O}$ over the quark fields,

$$\langle \mathcal{O} \rangle_F \equiv \int d\psi d\bar{\psi}\, \mathcal{O} e^{-S_F}. \tag{13}$$

The global lattice chiral rotation (7) gives the integrated Ward-Takahashi identity (WTI),

$$\langle (\delta_{a0}J_0 - \delta_a S_F)\mathcal{O} + \delta_a \mathcal{O}\rangle_F = 0, \tag{14}$$

where J_0 is the contribution from the chiral anomaly, or the Jacobian of the measure,

$$\begin{aligned} J_0 &= -2iN_f a^4 \sum_x \sum_{N=n,k,K} \phi_N^A(x)^\dagger \gamma_5 \left(1 - \frac{R}{2}aD\right)\phi_N^A(x) \\ &= -2iN_f \times Q(A), \end{aligned} \tag{15}$$

where $Q(A) = N_R^A - N_L^A$ is the index of the overlap Dirac operator [14], which gives an appropriate definition of the topological charge for the given gauge configuration A.

In this paper, we consider the (volume integrals of) scalar and pseudoscalar density operators

$$S_a = a^4 \sum_x [\bar{\psi} T_a (F(D(A))\psi](x), \tag{16}$$

$$P_a = a^4 \sum_x [\bar{\psi} T_a i\gamma_5 (F(D(A))\psi](x), \tag{17}$$

and their correlations. These two operators are transformed as

$$\delta_b S_a = 2\sum_c d_{ab}^c P_c, \qquad \delta_b P_a = -2\sum_c d_{ab}^c S_c, \tag{18}$$

where $\{T_a, T_b\} = 2\sum_c d_{ab}^c T_c$. In particular, in the $N_f = 2$ case, we have

$$\delta_b S_a = 2\delta_{ab} P_0, \qquad \delta_b P_a = -2\delta_{ab} S_0 \quad (\text{for } a, b = 1, 2, 3), \tag{19}$$

$$\delta_0 S_a = \delta_a S_0 = 2P_a, \qquad \delta_0 P_a = \delta_a P_0 = -2S_a \quad (\text{for } a = 0, 1, 2, 3), \tag{20}$$

where we have adopted the normalization $(T^a)^2 = 1_{2\times 2}$ without summation on a. It is now obvious that our mass term in the action (4) can be simply expressed by mS_0, and its transformation is $\delta_a S_F = 2mP_a$.

C. Basic properties and assumptions

In this subsection, we explicitly give the basic properties and assumptions used in this paper.

If the $SU(2)_L \times SU(2)_R$ chiral symmetry is restored at $T > T_c$, we should have

$$\lim_{m\to 0} \lim_{V\to\infty} \langle \delta_a \mathcal{O} \rangle_m = 0 \quad (\text{for } a \neq 0) \tag{21}$$

for an arbitrary operator $\mathcal{O}$, where an average over gauge fields is defined by

$$\langle \mathcal{O}(A) \rangle_m = \frac{1}{Z} \int \mathcal{D}A P_m(A) \mathcal{O}(A), \qquad Z = \int \mathcal{D}A P_m(A). \tag{22}$$

Here we have included the subscript m to remind the readers of the m dependence.

In the following analysis, we will normalize the operator $\mathcal{O}$ (by multiplying $1/V^k$ with an integer k) so that $\lim_{V\to\infty} \langle \delta_a \mathcal{O} \rangle$ is well-defined. Note that $P_m(A)$ is positive for even N_f, and $\int \mathcal{D}A P_m(A)/Z = 1$.

In our analysis, we assume that the vacuum expectation values of the m-independent observable $\mathcal{O}(A)$ is an analytic function of m^2 if the chiral symmetry is restored. Therefore if $\mathcal{O}(A)$ is m-independent and positive for all A, and is shown to satisfy

$$\lim_{m\to 0} \frac{1}{m^k} \langle \mathcal{O}(A)^{l_0} \rangle_m = 0 \tag{23}$$

with a non-negative integer k and a positive integer l_0, we can write

$$\langle \mathcal{O}(A)^{l_0} \rangle_m = m^{2([k/2]+1)} \int \mathcal{D}A \hat{P}(m^2, A) \mathcal{O}(A)^{l_0}, \tag{24}$$

where $[c]$ is the largest integer not larger than c, $\hat{P}(0, A) \neq 0$ for $^{\exists}A$ and $\int \mathcal{D}A \hat{P}(m^2, A) \mathcal{O}(A)^{l_0}$ is non-negative and assumed to be finite in the large-volume limit. In other words, the leading m dependence arises from the contribution of configurations which satisfy $\hat{P}(0, A) \neq 0$.

Under the above assumption, it is easy to see that

$$\begin{aligned}\langle \mathcal{O}(A)^{l} \rangle_m &= m^{2([k/2]+1)} \int \mathcal{D}A \hat{P}(m^2, A) \mathcal{O}(A)^{l} \\ &= O(m^{2([k/2]+1)})\end{aligned} \tag{25}$$

for an arbitrary positive integer l, as long as $\int \mathcal{D}A \hat{P}(m^2, A) \mathcal{O}(A)^{l}$ is finite, since $\mathcal{O}(A)^{l_0}$ and $\mathcal{O}(A)^{l}$ are both positive and therefore share the same support in the configuration space.

More generally, if a set of non-negative m-independent functions $\mathcal{O}_i(A)$ satisfies $\langle \mathcal{O}_i(A) \rangle_m = O(m^{2n_i})$ with non-negative integers n_i $(i = 1, 2, 3, \ldots k)$, it is easy to see that

$$\left\langle \prod_i^k \mathcal{O}_i(A) \right\rangle_m = O(m^{2n_{\max}}), \tag{26}$$

where $n_{\max} = \max(n_1, n_2, \ldots, n_k)$.

If a non-negative $\mathcal{O}_0$ and an arbitrary operator $\mathcal{O}_1$ are m-independent and satisfy

$$\langle \mathcal{O}_0 \rangle_m = O(m^{2n_0}), \qquad \langle \mathcal{O}_1 \rangle_m = O(m^{2n_1}), \tag{27}$$

we then have

$$\begin{aligned}\langle \mathcal{O}_0 \mathcal{O}_1 \rangle_m &= m^{2n_0} \int \mathcal{D}\mathcal{A}\, \mathcal{O}_0(A) \mathcal{O}_1(A) \{\hat{P}_+(m^2, A) \\ &\quad + \hat{P}_-(m^2, A)\} \\ &= O(m^{2n_0}),\end{aligned} \tag{28}$$

irrespective of values of n_0 and n_1, where $\hat{P}(m^2, A) = \hat{P}_+(m^2, A) + \hat{P}_-(m^2, A)$ and

$$\mathcal{O}_1(A) P(m^2, A) = \begin{cases} \mathcal{O}_1(A) P_+(m^2, A), & \mathcal{O}_1(A) > 0, \\ \mathcal{O}_1(A) P_-(m^2, A), & \mathcal{O}_1(A) < 0, \\ 0, & \mathcal{O}_1(A) = 0. \end{cases} \tag{29}$$

As will be seen later, we have

$$\lim_{m\to 0} \lim_{V\to\infty} \frac{1}{mV} \langle N^A_{R+L} \rangle_m = 0 \tag{30}$$

as a constraint from the chiral symmetry restoration. This leads to

$$\lim_{V\to\infty} \frac{1}{V} \langle N^A_{R+L} \rangle_m = O(m^2). \tag{31}$$

This condition is, however, much weaker than the naive expectation that the configuration A, which gives $N^A_{R+L} = O(V)$, has the weight $P_m(A) \propto m^{N_f O(V)}$ and therefore is much more suppressed in the large-volume limit. We do not assume such a highly suppressed weight $P_m(A)$ in this paper. As will be shown later, however, we can further prove that

$$\lim_{V\to\infty} \frac{1}{V} \langle N^A_{R+L} \rangle_m = 0 \tag{32}$$

for small enough m, using our weaker assumption, Eq. (24).

Note that analyticity in m^2 for physical observables and its consequence (24) do not hold at $T < T_c$, where the chiral symmetry is spontaneously broken. For example, the topological charge $Q(A)$ is expected to satisfy

$$\lim_{V\to\infty}\frac{1}{V}\langle Q(A)^2\rangle_m = \frac{m\Sigma}{N_f} + O(m^2), \tag{33}$$

where Σ is the chiral condensate. The odd power of m reflects the nonanalyticity of the QCD partition function at $m = 0$.

In the following analysis, the thermodynamical limit of the eigenvalue density for a given configuration A,

$$\rho^A(\lambda) = \lim_{V\to\infty}\frac{1}{V}\sum_{n(\mathrm{Im}\lambda_n^A>0)}\delta(\lambda - \sqrt{\bar{\lambda}_n^A\lambda_n^A}), \tag{34}$$

plays a crucial role. Since the temperature of the system is fully controlled by $P_m(A)$, the eigenvalue density $\rho^A(\lambda)$ itself is not sensitive to the temperature.[1] It is also notable that $\int_0^{\Lambda_R} d\lambda\rho(\lambda)$ is finite on the lattice. Therefore, $\rho^A(\lambda)$ is positive semidefinite for arbitrary choices of λ and A.[2]

Although the original eigenvalue spectrum at finite V is a sum of delta functions, we expect that such a spiky feature is smeared out in the thermodynamical limit, and that $\rho^A(\lambda)$ becomes a smooth function. We here further assume that $\rho^A(\lambda)$ can be analytically expanded around $\lambda = 0$[3]:

$$\rho^A(\lambda) = \sum_{n=0}^{\infty}\rho_n^A\frac{\lambda^n}{n!}. \tag{35}$$

An arbitrarily small convergence radius of this expansion, denoted by ϵ, works well for our later discussion where we take the massless limit. As is well-known and will be seen later, the Banks-Casher relation [15], $\lim_{m\to 0}\langle\rho_0^A\rangle_m \neq 0$, implies the spontaneous breaking of the chiral symmetry.

III. CONSTRAINTS FROM THE $SU(2)_L \times SU(2)_R$ RESTORATION

In the following analysis, we concentrate on the case with $N_f = 2$. In this section, we derive the constraints on the eigenvalue density of the Dirac operator in the $SU(2)_L \times SU(2)_R$ chiral-symmetric phase at finite temperature.

A. WTIs for scalar and pseudoscalar operators

Let us consider a product of the scalar and pseudoscalar operators defined in Eqs. (16) and (17),

$$\mathcal{O}_{n_1,n_2,n_3,n_4} = P_a^{n_1}S_a^{n_2}P_0^{n_3}S_0^{n_4}, \tag{36}$$

where a represents a nonsinglet index ($a = 1, 2, 3$). Here and in the following, a summation over a is not taken, and we explicitly use "0" for the singlet operators.

Nontrivial WTIs are obtained from the set

$$\mathcal{O}_a^{(N)} \equiv \left\{\mathcal{O}_{n_1,n_2,n_3,n_4}|n_1 + n_2 = \text{odd}, n_1 + n_3 = \text{odd}, \sum_i n_i = N\right\}, \tag{37}$$

which requires the operator to be a nonsinglet and parity-odd. More explicitly, we have at $T > T_c$

$$\lim_{m\to 0}\lim_{V\to\infty}\frac{1}{V^k}\langle\delta_a\mathcal{O}_{n_1,n_2,n_3,n_4}\rangle_m = 0 \quad \text{for } \mathcal{O}_{n_1,n_2,n_3,n_4} \in \mathcal{O}_a^{(N)}, \tag{38}$$

where

$$\delta_a\mathcal{O}_{n_1,n_2,n_3,n_4} = -2n_1\mathcal{O}_{n_1-1,n_2,n_3,n_4+1} + 2n_2\mathcal{O}_{n_1,n_2-1,n_3+1,n_4} - 2n_3\mathcal{O}_{n_1,n_2+1,n_3-1,n_4} + 2n_4\mathcal{O}_{n_1+1,n_2,n_3,n_4-1}. \tag{39}$$

Note that the fermion integrals are performed before the gauge integrals: $\langle\mathcal{O}\rangle_m = \langle\langle\mathcal{O}\rangle_F\rangle_m$, but we have omitted $\langle\cdots\rangle_F$ for notational simplicity. Here the minimum power k which makes the $V\to\infty$ limit finite depends on the choice of $\mathcal{O}_{n_1,n_2,n_3,n_4}$. For further details, such as a relation of n_1, n_2, n_3, and n_4 to k, see Appendix A 5.

B. Constraints at $N = 1$

At $N = 1$, there is only one operator, $\mathcal{O}_{1000} = P_a$ in $\mathcal{O}_a^{(N=1)}$, which gives

$$\delta^a P_a = -2S_0. \tag{40}$$

Using the decomposition in Eq. (11), and the normalization conditions $(\phi_n^A, \phi_m^A) = (\gamma_5\phi_n^A, \gamma_5\phi_m^A) = \delta_{nm}$, the thermodynamical limit of the functional integral for S_0 is expressed as

$$\begin{aligned}\lim_{V\to\infty}\frac{1}{V}\langle -S_0\rangle_m &= \lim_{V\to\infty}\frac{N_f}{V}\left\langle\frac{N_{R+L}^A}{m} + \sum_{n(\mathrm{Im}\lambda_n^A>0)}\frac{2m}{Z_m^2\bar{\lambda}_n^A\lambda_n^A + m^2}\times\left(1 - \frac{\bar{\lambda}_n^A\lambda_n^A}{\Lambda_R^2}\right)\right\rangle_m \\ &= \lim_{V\to\infty}\frac{N_f}{mV}\langle N_{R+L}^A\rangle_m + N_f\langle I_1\rangle_m,\end{aligned} \tag{41}$$

where

$$I_1 = m\int_0^{\Lambda_R} d\lambda\rho^A(\lambda)\frac{2g_0(\lambda^2)}{Z_m^2\lambda^2 + m^2}, \qquad g_0(x) = 1 - \frac{x}{\Lambda_R^2}. \tag{42}$$

In the chiral limit $m\to 0$, only the vicinity of $\lambda = 0$ contributes to the integral, since

[1]The gauge configuration average $\langle\rho^A(\lambda)\rangle_m$ does, of course, depend on the temperature.

[2]Strictly speaking, $\rho^A(\lambda)$ has a logarithmic divergence in the continuum limit, which can be absorbed by multiplying the quark mass m.

[3]More precisely, we here assume that configurations which do not have the expansion (35) are measure-zero in the path integral with $P_m(A)$. This assumption excludes a possibility that $\langle\rho^A(\lambda)\rangle_m$ has a fractional power such that $\langle\rho^A(\lambda)\rangle_m \sim \lambda^\gamma$ with noninteger γ at small λ. We consider the fractional case later in Sec. VI.

$$\int_{\epsilon}^{\Lambda_R} d\lambda \rho^A(\lambda) \frac{2g_0(\lambda^2)}{Z_m^2\lambda^2 + m^2} \tag{43}$$

is finite for arbitrarily small but positive ϵ, and thus, does not contribute to I_1 in the limit. Expanding $\rho^A(\lambda)$ for $\lambda < \epsilon$, [see Eq. (35)], it is not difficult to obtain (see Appendix A 3)

$$I_1 = m\int_0^{\epsilon} d\lambda \rho_0^A \frac{2g_0(\lambda^2)}{Z_m^2\lambda^2 + m^2} + O(m) = \pi\rho_0^A + O(m). \tag{44}$$

As an exercise, let us consider the $T < T_c$ case, where the chiral symmetry is spontaneously broken. Assuming that $\lim_{V\to\infty}\langle N^A_{R+L}\rangle_m/V \to 0$,[4] the famous Banks-Casher relation [15] is reproduced:

$$\lim_{m\to 0}\lim_{V\to\infty}\frac{1}{N_f V}\langle -S_0\rangle_m = \pi\lim_{m\to 0}\langle\rho_0^A\rangle_m (= \pi\lim_{m\to 0}\langle\rho^A(0)\rangle_m) \neq 0. \tag{45}$$

On the other hand, in the chiral-symmetric phase $T > T_c$, we require

$$\begin{aligned}\lim_{m\to 0}\lim_{V\to\infty}\frac{1}{V}\langle -S_0\rangle_m &= \lim_{m\to 0}\lim_{V\to\infty}\frac{N_f}{mV}\langle N^A_{R+L}\rangle_m + N_f\lim_{m\to 0}\langle I_1\rangle_m \\ &= 0.\end{aligned} \tag{46}$$

Since both N^A_{R+L} and I_1 are positive, it is equivalent to separately require the following two constraints:

$$\lim_{V\to\infty}\frac{N_f}{V}\langle N^A_{R+L}\rangle_m = O(m^2), \qquad \langle\rho_0^A\rangle_m = O(m^2). \tag{47}$$

Using Eqs. (26) and (28), $\langle\rho_0^A\rangle_m = O(m^2)$ implies $\langle I_1^2\rangle_m = O(m^2)$, which will be useful in the analysis below.

C. Contribution from zero-modes at general N

Before extending our analysis to higher N, let us discuss the fate of the zero-mode contribution at general N. For this purpose we consider an operator $\mathcal{O}_{1,0,0,N-1} \in \mathcal{O}_a^{(N)}$, whose nonsinglet chiral WTI requires

$$\lim_{m\to 0}\lim_{V\to\infty}(-\langle\mathcal{O}_{0,0,0,N}\rangle_m + (N-1)\langle\mathcal{O}_{2,0,0,N-2}\rangle_m) = 0. \tag{48}$$

Its dominant contribution at large volume is

$$-\frac{1}{V^N}\langle(S_0)^N\rangle_m = -N_f^N\left\langle\left\{(-1)\left(\frac{N^A_{R+L}}{mV} + I_1\right)\right\}^N\right\rangle_m + O(V^{-1}), \tag{49}$$

and, therefore, from the positivity of N^A_{R+L} and I_1,

$$\lim_{V\to\infty}\frac{\langle(N^A_{R+L})^N\rangle_m}{V^N} = \begin{cases} O(m^{N+2}) & (\text{for even } N), \\ O(m^{N+1}) & (\text{for odd } N). \end{cases} \tag{50}$$

Since this holds for arbitrary N, and N^A_{R+L} does not explicitly depend on m, we conclude that

$$\lim_{V\to\infty}\frac{\langle N^A_{R+L}\rangle_m}{V} = 0 \tag{51}$$

at small but nonzero m.

This result implies that any zero-mode's contributions to an arbitrary local operator is *measure-zero* in the thermodynamical limit, as we have already seen (for example, in Sec. I) [17]. Therefore, we hereafter set $\lim_{V\to\infty}\langle N^A_{R+L}\rangle_m/V = 0$ even at small but nonzero m.

D. Constraints at $N = 2$

We next consider the $N = 2$ case. In this case, two WTIs from $\mathcal{O}_{1001}$ and $\mathcal{O}_{0110} \in \mathcal{O}_a^{(N=1)}$ require that the so-called (nonsinglet) chiral susceptibilities,

$$\chi^{\sigma-\pi} = \frac{1}{V^2}\langle S_0^2 - P_a^2\rangle_m, \quad \chi^{\eta-\delta} = \frac{1}{V}\langle P_0^2 - S_a^2\rangle_m, \tag{52}$$

vanish in the $V\to\infty$ and $m\to 0$ limits at $T > T_c$. The first one, $\chi^{\sigma-\pi}$, has already been examined in the previous subsection.

In a similar way to the $N = 1$ case, $\chi^{\eta-\delta}$ can be expressed in terms of eigenvalues as

$$\lim_{V\to\infty}\chi^{\eta-\delta} = \lim_{V\to\infty}\left\langle -\frac{N_f^2}{m^2 V}Q(A)^2\right\rangle_m + N_f\left\langle\left(\frac{I_1}{m} + I_2\right)\right\rangle_m, \tag{53}$$

where I_2 is defined by

$$\begin{aligned} I_2 &= 2\int_0^{\Lambda_R} d\lambda\rho^A(\lambda)\frac{m^2 g_0^2(\lambda^2) - \lambda^2 g_0(\lambda^2)}{(Z_m^2\lambda^2 + m^2)^2} \\ &= \left(\frac{2}{\epsilon} + \frac{2\epsilon}{\Lambda_R^2}\right)\rho_0^A + \left(2 + \frac{\epsilon^2}{\Lambda_R^2} - \log\frac{\epsilon^2}{m^2}\right)\rho_1^A + O(1). \end{aligned} \tag{54}$$

Noting that

$$\begin{aligned}\frac{I_1}{m} + I_2 = 2mI_3 &= 4m^2\int_0^{\epsilon} d\lambda\rho^A(\lambda)\frac{g_0^2(\lambda^2)}{(Z_m^2\lambda^2 + m^2)^2} \\ &= \rho_0^A\frac{\pi}{m} + 2\rho_1^A + O(m)\end{aligned} \tag{55}$$

for an arbitrarily small (positive) parameter ϵ, and expanding $\rho^A(\lambda)$ around $\lambda = 0$, we obtain a condition in the chiral limit that

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[4] In chiral perturbation theory, one can confirm that $\langle|Q(A)|\rangle_m/V$ is an $O(1/\sqrt{V})$ quantity (even when m is finite). Since the minimum of N^A_{R+L} is equal to $|Q(A)|$ in the topological sector of $Q(A)$, it is natural to assume that $\langle N^A_{R+L}\rangle_m/V$ is also $O(1/\sqrt{V})$. Moreover, using the fact that there is no massless pole in the nonsinglet scalar correlator $\langle S_a S_a\rangle$ in the chiral limit, one can show that $\langle N^A_{R+L}\rangle_m/V = O(m^2)$.

$$\lim_{m\to 0}\lim_{V\to\infty}\chi^{\eta-\delta} = N_f\lim_{m\to 0}\left[-\lim_{V\to\infty}\frac{N_f\langle Q(A)^2\rangle_m}{m^2V} + \frac{\pi}{m}\langle\rho_0^A\rangle_m + 2\langle\rho_1^A\rangle_m + O(m)\right]. \quad (56)$$

Since we already know that $\langle\rho_0^A\rangle_m = O(m^2)$, this condition leads to

$$\lim_{V\to\infty}\frac{N_f\langle Q(A)^2\rangle_m}{m^2V} = 2\langle\rho_1^A\rangle_m + O(m^2). \quad (57)$$

Note that there should be no $O(m)$ term in Eq. (57) according to the analyticity in m^2. Therefore the $O(m)$ term can not be cancelled in Eq. (56) at nonzero m.

E. Constraints at $N = 3$

From the WTIs at $N = 3$, except the one considered in Sec. III C, the four quantities

$$\chi_1 = \frac{\langle\mathcal{O}_{0201}\rangle_m}{V^2} = N_f^2\langle I_1I_2\rangle_m + O(1/V),$$
$$\chi_2 = \frac{\langle\mathcal{O}_{1110}\rangle_m}{V} = -N_f\left\langle N_f\frac{Q(A)^2}{m^3V} - 2I_3\right\rangle_m + O(1/V),$$
$$\chi_3 = \frac{\langle\mathcal{O}_{0021}\rangle_m}{V^2} = -N_f^2\left\langle I_1\left(\frac{I_1}{m} - \frac{N_fQ(A)^2}{m^2V}\right)\right\rangle_m + O(1/V),$$
$$\chi_4 = \frac{\langle\mathcal{O}_{2001}\rangle_m}{V^2} = -\frac{N_f^2}{m}\langle I_1^2\rangle_m + O(1/V), \quad (58)$$

should vanish after taking the $V\to\infty$ and $m\to 0$ limits. Here I_3 (and its asymptotic form near the chiral limit) is given by

$$I_3 = 2m\int_0^\epsilon d\lambda\rho^A(\lambda)\frac{g_0^2(\lambda^2)}{(Z_m^2\lambda^2+m^2)^2} = \left(\frac{\pi}{2m^2} - \frac{3\pi}{4\Lambda_R^2}\right)\rho_0^A + \frac{\rho_1^A}{m} + \frac{\pi}{4}\rho_2^A + O(m). \quad (59)$$

Substituting the explicit form of I_1 and I_2, the result (47) in the previous subsection and our assumptions in Eqs. (26) and (28) give

$$\langle I_1I_2\rangle_m = O(m), \qquad \langle(I_1)^2\rangle_m = O(m^2), \quad (60)$$

so that χ_1 and χ_4 automatically vanish in the $V\to\infty$ and $m\to 0$ limits. Using the same assumptions and the result (57) the following relations can also be shown:

$$\frac{\langle Q(A)^2I_1\rangle_m}{m^2V} = \pi\frac{\langle Q(A)^2\rho_0^A\rangle_m}{m^2V} + O(m), \quad (61)$$

$$N_f\frac{\langle Q(A)^2\rangle_m}{m^3V} = 2\frac{\langle\rho_1^A\rangle_m}{m} + O(m). \quad (62)$$

The two remaining nontrivial conditions are

$$\lim_{m\to 0}\lim_{V\to\infty}\chi_2 = -\pi N_f\lim_{m\to 0}\left[\frac{\langle\rho_0^A\rangle_m}{m^2} + \frac{\langle\rho_2^A\rangle_m}{2}\right] = 0, \quad (63)$$

$$\lim_{m\to 0}\lim_{V\to\infty}\chi_3 = \pi N_f^3\lim_{m\to 0}\lim_{V\to\infty}\frac{\langle Q(A)^2\rho_0^A\rangle_m}{m^2V} = 0. \quad (64)$$

From the first condition, we obtain a constraint:

$$\langle\rho_0^A\rangle_m = -m^2\frac{\langle\rho_2^A\rangle_m}{2} + O(m^4). \quad (65)$$

Moreover, since $\langle\rho_0^A\rangle_m$ is positive [which is required by the positivity of $\langle\rho^A(0)\rangle_m$], $\langle\rho_2^A\rangle_m$ must be negative for small m.

The condition for χ_3 leads to

$$\lim_{V\to\infty}\frac{\langle Q(A)^2\rho_0^A\rangle_m}{m^2V} = O(m^2). \quad (66)$$

This condition does not necessarily give a stronger constraint than $\langle Q(A)^2\rangle_m = O(m^2V)$ and $\langle\rho_0^A\rangle_m = O(m^2)$, since it only requires that a set of gauge configurations that satisfies both $Q(A)^2 \neq 0$ and $\rho_0^A \neq 0$ has a weight $m^4\hat{P}(A, m^2) + O(m^6)$.

F. Constraints at $N = 4$

The eight WTIs at $N = 4$ give seven independent constraints:

$$\langle\mathcal{O}_{4000} - \mathcal{O}_{0004}\rangle_m \to 0, \qquad \langle\mathcal{O}_{4000} - 3\mathcal{O}_{2002}\rangle_m \to 0,$$
$$\langle\mathcal{O}_{0400} - \mathcal{O}_{0040}\rangle_m \to 0, \qquad \langle\mathcal{O}_{0400} - 3\mathcal{O}_{0220}\rangle_m \to 0,$$
$$\langle\mathcal{O}_{2020} - \mathcal{O}_{0202}\rangle_m \to 0, \qquad \langle\mathcal{O}_{2200} - \mathcal{O}_{0022}\rangle_m \to 0,$$
$$\langle 2\mathcal{O}_{1111} - \mathcal{O}_{0202} + \mathcal{O}_{0022}\rangle_m \to 0, \quad (67)$$

where the $V\to\infty$ and $m\to 0$ limits are abbreviated by the arrows. The $O(V^4)$ contribution from S_0^4 in the first equation has already been considered.

At $O(V^3)$, there are three conditions:

$$\lim_{V\to\infty}\frac{1}{V^3}\langle P_a^2S_0^2\rangle_m = N_f^3\frac{\langle I_1^3\rangle_m}{m} \to 0, \quad (68)$$

$$\lim_{V\to\infty}\frac{1}{V^3}\langle S_a^2S_0^2\rangle_m = -N_f^3\langle I_1^2I_2\rangle_m \to 0, \quad (69)$$

$$\lim_{V\to\infty}\frac{1}{V^3}\langle P_0^2S_0^2\rangle_m = N_f^3\left\langle I_1^2\left\{\frac{I_1}{m} - \frac{N_fQ(A)^2}{m^2V}\right\}\right\rangle_m \to 0. \quad (70)$$

It is not difficult to confirm that all of them are automatically satisfied, since

$$\langle I_1^n\rangle_m = \langle\{\pi\rho_0^A + O(m)\}^n\rangle_m = O(m^2) \quad (71)$$

for any integer $n \geq 2$ from $\langle\rho_0^A\rangle_m = O(m^2)$, and

$$\frac{\langle I_1^2Q(A)^2\rangle_m}{m^2V} = \frac{\langle\{\pi\rho_0^A + O(m)\}^2Q(A)^2\rangle_m}{m^2V} = O(m^2) \quad (72)$$

from Eq. (66) together with the assumption (28) for remaining cross terms. Namely, these three give no additional constraint.

At $O(V^2)$ we have

$$\frac{1}{V^2}\langle S_a^4 - P_0^4\rangle_m \to 0, \qquad \frac{1}{V^2}\langle S_a^4 - 3S_a^2P_0^2\rangle_m \to 0,$$
$$\frac{1}{V^2}\langle P_a^2(P_0^2 - S_a^2) - 2P_aS_aP_0S_0\rangle_m \to 0. \tag{73}$$

After a little algebra using the formulas in Appendices A 2 and A 5, the first condition becomes

$$3N_f^2\langle (I_2 + I_1/m)(I_2 - I_1/m)\rangle_m + \frac{6N_f^3}{m^3V}\langle Q(A)^2I_1\rangle_m - \frac{N_f^4}{m^4V^2}\langle Q(A)^4\rangle_m \to 0. \tag{74}$$

Using

$$I_2 - \frac{I_1}{m} = \rho_0^A\left(-\tfrac{\pi}{m} + \tfrac{4}{\epsilon} + \tfrac{4\epsilon}{\Lambda_R^2}\right) + \rho_1^A\left(2 + \tfrac{2\epsilon^2}{\Lambda_R^2} - 4\log\tfrac{\epsilon}{m}\right) + O(1), \tag{75}$$

Eq. (55) and $\langle (\rho_0^A)^n\rangle_m = O(m^2)$, we can show that the first term in Eq. (74) is at most logarithmically divergent in the limit $m \to 0$. Note that the second term is also logarithmically divergent due to cross contributions from the $O(m)$ terms in I_1 (Appendix A 3) and Eq. (57). Therefore, in order to satisfy Eq. (74), the last term should not be power divergent and should at least fulfill

$$\lim_{V\to\infty}\frac{1}{V^2}\langle Q(A)^4\rangle_m = O(m^4), \tag{76}$$

which leads to

$$\lim_{V\to\infty}\frac{1}{V^k}\langle Q(A)^{2k}\rangle_m = O(m^4) \tag{77}$$

for an arbitrary positive integer k. Combining this with Eq. (57), we obtain a constraint on the spectral density,

$$\langle \rho_1^A\rangle_m = O(m^2), \tag{78}$$

so that Eq. (74) now becomes

$$-3N_f^2\frac{\pi^2}{m^2}\langle (\rho_0^A)^2\rangle_m - \frac{N_f^4}{m^4V^2}\langle Q(A)^4\rangle_m \to 0. \tag{79}$$

Since both terms are negative semidefinite, this WTI requires

$$\langle (\rho_0^A)^k\rangle_m = O(m^4), \qquad \lim_{V\to\infty}\frac{1}{V^l}\langle Q(A)^{2l}\rangle_m = O(m^6) \tag{80}$$

for arbitrary positive integers k and l. The first condition also gives

$$\langle \rho_2^A\rangle_m = O(m^2) \tag{81}$$

from Eq. (65).

The last constraint, Eq. (81), can be obtained through a different argument. From Eq. (78), the eigenvalue density near the chiral limit becomes

$$\langle \rho^A(\lambda)\rangle_m = \langle \rho_2^A\rangle_m\frac{\lambda^2}{2} + O(\lambda^3) + O(m^2). \tag{82}$$

The positivity of $\langle \rho^A(\lambda)\rangle_m$ implies $\langle \rho_2^A\rangle_m \geq 0$ near $m = 0$, but this contradicts the positivity of $\langle \rho_0^A\rangle_m$ in Eq. (65) unless $\langle \rho_2^A\rangle_m = O(m^2)$, and thus $\langle \rho_0^A\rangle_m = O(m^4)$.

It is now easy to see that the second and third conditions in Eq. (73) are automatically satisfied: the second one gives

$$6N_f^2m\langle I_2I_3\rangle_m - \frac{3N_f^3}{m^2V}\langle I_2Q(A)^2\rangle_m = O(m^2) + O(m^4), \tag{83}$$

while the third one is evaluated as

$$6N_f^2\langle I_1I_3\rangle_m - \frac{3N_f^3}{m^3V}\langle I_1Q(A)^2\rangle_m = O(m^2) + O(m^3). \tag{84}$$

G. Special constraints at general N

In this subsection, we consider a special type of operator: $\mathcal{O}_{0,1,(4k-1),0} \in \mathcal{O}_a^{(N=4k)}$ at a general positive integer k, whose nonsinglet WTI gives the condition

$$\lim_{m\to 0}\langle (4k-1)S_a^2P_0^{4k-2} - P_0^{4k}\rangle_m = 0. \tag{85}$$

At the leading order of V (V^{2k} in this case), the above condition corresponds to

$$-(4k-1)\frac{N_f}{V^{2k-1}}\langle I_2P_0^{4k-2}\rangle_m - \frac{1}{V^{2k}}\langle P_0^{4k}\rangle_m \to 0 \tag{86}$$

in the chiral limit. From the results in Appendices A 2 and A 5,

$$\frac{\langle P_0^{4k}\rangle_F}{V^{2k}} = \sum_{n=0}^{2k} {}_{4k}C_{2n}(2n-1)!!\left(\frac{-N_f^2Q(A)^2}{m^2V}\right)^{2k-n}\left(\frac{N_fI_1}{m}\right)^n + O(V^{-1}), \tag{87}$$

where we have used the definition $(-1)!! = 1$. The nonsinglet WTI is expressed by

$$-(4k-1)\sum_{n=0}^{2k-1} {}_{4k-2}C_{2n}(2n-1)!!\left\langle\left(\frac{-N_f^2Q(A)^2}{m^2V}\right)^{2k-1-n}\times\left(\frac{N_fI_1}{m}\right)^n N_fI_2\right\rangle_m - \sum_{n=0}^{2k} {}_{4k}C_{2n}(2n-1)!!\times\left\langle\left(\frac{-N_f^2Q(A)^2}{m^2V}\right)^{2k-n}\left(\frac{N_fI_1}{m}\right)^n\right\rangle_m \to 0. \tag{88}$$

From the above condition(s), we would like to inductively prove that

$$\frac{\langle Q^{2l}\rangle_m}{V^l} = O(m^{4k+2}), \qquad \langle (\rho_0^A)^l\rangle_m = O(m^{2k+2}) \tag{89}$$

holds for arbitrary positive integers l and k.

Suppose

$$\frac{\langle Q^{2l}\rangle_m}{V^l} = O(m^{4k-2}), \qquad \langle(\rho_0^A)^l\rangle_m = O(m^{2k}) \quad (90)$$

is obtained from the WTI at $N = 4k - 4$ (this is true for $k = 2$). The constraint above is then reduced to

$$-\Bigg\langle (4k-1)!!\left(\frac{N_f I_1}{m}\right)^{2k-1} N_f(I_2 + I_1/m) + \left(\frac{-N_f^2 Q(A)^2}{m^2 V}\right)^{2k} + (4k-1) \times \left(\frac{-N_f^2 Q(A)^2}{m^2 V}\right)^{2k-1} N_f(I_2 + 2kI_1/m)\Bigg\rangle_m \to 0, \quad (91)$$

where only those terms with $n = 0,\ 2k-1$ in the first summation and $n = 0,\ 1,\ 2k$ in the second summation remain. While the first and third terms are finite and linearly divergent in the $m \to 0$ limit, the second term is seen to be quadratically divergent from Eq. (90) as

$$-\frac{N_f^{4k}}{m^{4k}}\frac{\langle Q(A)^{4k}\rangle_m}{V^{2k}} = O(m^{-2}). \quad (92)$$

In order for the WTI to be satisfied, the quadratic divergence should be absent, so that $\langle Q(A)^{2l}/V^l\rangle_m = O(m^{4k})$ for an arbitrary positive integer l, thanks to Eq. (25).

Using this result the third term disappears faster than the others and the WTI becomes

$$-(4k-1)!!N_f^{2k-1}\frac{\langle(\pi\rho_0^A)^{2k}\rangle_m}{m^{2k}} - \frac{N_f^{4k}}{m^{4k}}\frac{\langle Q(A)^{4k}\rangle_m}{V^{2k}} \to 0. \quad (93)$$

Note here that both terms are negative semidefinite and therefore each term *must vanish* in the chiral limit. This completes the proof for Eq. (89).

Since k can be arbitrarily large, we now have another stronger constraint on the zero-mode's contribution,

$$\lim_{V\to\infty}\frac{\langle Q(A)^2\rangle_m}{V} = 0, \quad (94)$$

and on that of the spectral density,

$$\langle\rho_0^A\rangle_m = 0, \quad (95)$$

which hold even at small but nonzero m.

H. Short summary of the constraints

Here we summarize the constraints obtained in this section. For the eigenvalue density, we have

$$\langle\rho_0^A\rangle_m = 0, \quad \langle\rho_1^A\rangle_m = O(m^2), \quad \langle\rho_2^A\rangle_m = O(m^2), \quad (96)$$

at a small but nonzero m. Namely, the eigenvalue density must have the form

$$\lim_{m\to 0}\langle\rho^A(\lambda)\rangle_m = \langle\rho_3^A\rangle_0\frac{\lambda^3}{3!} + O(\lambda^4). \quad (97)$$

We believe that this new condition is not only stronger than those found in previous works, but that it is also the *strongest*, since we know that the $N_f = 2$ massless free quark theory has $\langle\rho_3^A\rangle_0 \neq 0$, keeping the exact chiral $SU(2)_L \times SU(2)_R$ [and $U(1)_A$] symmetry. Therefore, it is very likely that we will not find any additional information from $N \geq 5$ correlation functions.

For the discrete zero-modes, we have obtained

$$\lim_{V\to\infty}\frac{1}{V^k}\langle(N_{R+L}^A)^k\rangle_m = 0, \quad \lim_{V\to\infty}\frac{1}{V^k}\langle Q(A)^{2k}\rangle_m = 0, \quad (98)$$

for an arbitrary positive integer k at a small but nonzero m. These zero-modes give no contribution to the correlation functions we are considering.

IV. FATE OF THE $U(1)_A$ ANOMALY

In this section, we discuss how the constraints in the $SU(2)_L \times SU(2)_R$-symmetric phase, obtained in the previous section, affect the $U(1)_A$-breaking correlators. Here we consider a set of (pseudoscalar singlet) operators,

$$\mathcal{O}_0^{(N)} \equiv \Big\{\mathcal{O}_{n_1,n_2,n_3,n_4} | n_1 + n_2 = \text{even}, n_1 + n_3 = \text{odd}, \sum_i n_i = N\Big\}, \quad (99)$$

and its chiral $U(1)_A$ rotation,

$$\delta_0\mathcal{O}_{n_1,n_2,n_3,n_4} = -2n_1\mathcal{O}_{n_1-1,n_2+1,n_3,n_4} + 2n_2\mathcal{O}_{n_1+1,n_2-1,n_3,n_4} - 2n_3\mathcal{O}_{n_1,n_2,n_3-1,n_4+1} + 2n_4\mathcal{O}_{n_1,n_2,n_3+1,n_4-1}. \quad (100)$$

For later convenience, let us also define a set of (scalar singlet) operators,

$$\mathcal{O}^{(N)} \equiv \Big\{\mathcal{O}_{n_1,n_2,n_3,n_4} | n_1 + n_2 = \text{even}, n_1 + n_3 = \text{even}, \sum_i n_i = N\Big\}. \quad (101)$$

As QCD keeps the vector-like $SU(2)_V$ symmetry and the parity symmetry, any operator with a nonzero expectation value must be a member of $\mathcal{O}^{(N)}$. Note that we have already introduced the set of pseudoscalar nonsinglet operators $\mathcal{O}_a^{(N)}$ in Eq. (37).

Since the $U(1)_A$ transformation is anomalous, the expectation value of the variation $\langle\delta_0\mathcal{O}\rangle_m$ is nonzero [as shown by the WTI; see Eq. (15)],

$$\lim_{m\to 0}\langle\delta_0\mathcal{O}\rangle_m = 2iN_f\lim_{m\to 0}\langle Q(A)\mathcal{O}\rangle_m, \quad (102)$$

and the $U(1)_A$ symmetry is broken.

It is, however, still possible to have zeros on both sides of Eq. (102). If this is the case, the $U(1)_A$ anomaly is invisible. In fact, we show below that the constraints obtained in the previous section are strong enough to suppress the variation $\langle\delta_0\mathcal{O}\rangle_m$ for $\mathcal{O}\in\mathcal{O}_0^{(N)}$ to be zero in the large-volume $V\to\infty$ and chiral $m\to 0$ limits. Namely, the $\mathrm{U}(1)_A$ symmetry must be restored, at least, for the operator set $\mathcal{O}_0^{(N)}$.

A. Odd-N case

For the odd-N cases, we can show a relation for the number of operators $|\mathcal{O}_a^{(N)}| = |\mathcal{O}_0^{(N)}| = |\mathcal{O}^{(N)}|$, where $|\mathcal{A}|$ denotes the number of independent operators in $\mathcal{A}$. See Appendix B for the details.

As the exact chiral $\mathrm{SU}(2)_L\times\mathrm{SU}(2)_R$ symmetry requires $|\mathcal{O}_a^{(N)}|$-independent WTIs in the chiral limit to be zero,

$$\lim_{m\to 0}\langle\delta_a\mathcal{O}_i\rangle_m = \lim_{m\to 0}\sum_{j=1}^{|\mathcal{O}^{(N)}|} M_{ij}\langle\mathcal{O}_j\rangle_m = 0, \qquad \mathcal{O}_i\in\mathcal{O}_a^{(N)},\qquad \mathcal{O}_j\in\mathcal{O}^{(N)}, \tag{103}$$

where the matrix M is specified by the WTI that one considers. Since the chiral transformation keeps the independence of the operator, it can be proved that $\det M\neq 0$,[5] and the WTI requires

$$\lim_{m\to 0}\langle\mathcal{O}_i\rangle_m = 0 \quad \text{for any } \mathcal{O}_i\in\mathcal{O}^{(N)}, \tag{104}$$

or equivalently, that there is no operator in $\mathcal{O}^{(N)}$, $\delta_a\mathcal{O}_a^{(N)}$, and $\delta_0\mathcal{O}_0^{(N)}$ which has a nonzero expectation value in the $\mathrm{SU}(2)_L\times\mathrm{SU}(2)_R$-symmetric phase.

Since the $\mathrm{U}(1)_A$ variation of any operator in $\mathcal{O}_0^{(N)}$ is an element of $\mathcal{O}^{(N)}$, we can conclude that

$$\lim_{m\to 0}\langle\delta_0\mathcal{O}\rangle_m = 0 \quad \text{for any } \mathcal{O}\in\mathcal{O}_0^{(N)}. \tag{105}$$

Without referring to any specific constraints obtained in the previous section, we can thus show that the $\mathrm{U}(1)_A$ breaking is invisible for these operators.

B. $N = 2$, 4, and 6

For even N, the situation is not so simple as for the odd N's (see Appendix B for the details). We need to examine the WTIs explicitly.

At $N = 2$, there remains one nontrivial susceptibility, but one can immediately show that it should vanish:

$$\chi^{\pi-\eta} = \frac{1}{V}\langle P_a^2 - P_0^2\rangle_m = \lim_{V\to\infty}\frac{N_f^2}{m^2V}\langle Q(A)^2\rangle_m = 0, \tag{106}$$

for small but nonzero m, thanks to Eq. (94). Noting that $P_a^2 - P_0^2 = (P_a^2 - S_0^2) + (S_0^2 - S_a^2) + (S_a^2 - P_0^2)$, we can also show that

$$\chi^{\delta-\sigma} = \frac{1}{V^2}\langle S_a^2 - S_0^2\rangle_m = O(1/V) + O(m^2). \tag{107}$$

Since the lhs of Eq. (107) is the (double) volume average of the lhs of Eq. (1), this provides another proof that the $\mathrm{U}(1)_A$-breaking effect in Ref. [17] cannot survive in the thermodynamical limit.

At $N = 4$, there are two nontrivial susceptibilities:

$$\chi_5 = \langle\mathcal{O}_{0022} - \mathcal{O}_{2002}\rangle_m, \quad \chi_6 = \langle\mathcal{O}_{0022} - \mathcal{O}_{0220}\rangle_m. \tag{108}$$

Neglecting N_{R+L}^A/V and $Q(A)^2/V$ terms and using the constraint on I_1 obtained in the previous section, both of them disappear as

$$\lim_{m\to 0}\lim_{V\to\infty}\frac{\chi_5}{V^3} = -\lim_{m\to 0}\lim_{V\to\infty}N_f^3\left\langle\frac{N_fQ(A)^2}{m^2V}\left(\frac{N_{R+L}^A}{mV} + I_1\right)^2\right\rangle_m = 0, \tag{109}$$

$$\begin{aligned}\lim_{m\to 0}\lim_{V\to\infty}\frac{\chi_6}{V^3} &= \lim_{m\to 0}\lim_{V\to\infty}\frac{N_f^3}{m}\left\langle\left(\frac{N_{R+L}^A}{mV} + I_1\right)^2 \times\left(\frac{N_{R+L}^A}{mV} + I_1 - \frac{N_fQ(A)^2}{mV}\right)\right\rangle_m \\ &= \lim_{m\to 0}\frac{N_f^3}{m}\langle I_1^3\rangle_m = 0.\end{aligned} \tag{110}$$

At $N = 6$, we have four nontrivial susceptibilities:

$$\chi_7 = \langle\mathcal{O}_{0024} - \mathcal{O}_{2004}\rangle_m, \quad \chi_8 = \langle\mathcal{O}_{2040} - \mathcal{O}_{0204}\rangle_m, \tag{111}$$

$$\chi_9 = \langle\mathcal{O}_{0420} - \mathcal{O}_{0042}\rangle_m, \quad \chi_{10} = \langle\mathcal{O}_{0042} - \mathcal{O}_{0024}\rangle_m. \tag{112}$$

In the large-volume limit, they behave as

$$\lim_{V\to\infty}\frac{\chi_7}{V^5} = 0, \tag{113}$$

$$\lim_{V\to\infty}\frac{\chi_8}{V^5} = N_f^5\langle I_2 I_1^4\rangle_m = O(m^4), \tag{114}$$

$$\lim_{V\to\infty}\frac{\chi_9}{V^4} = -\frac{N_f^4}{m^2}\langle I_1^4\rangle_m = O(m^2), \tag{115}$$

$$\lim_{V\to\infty}\frac{\chi_{10}}{V^5} = -\frac{N_f^5}{m}\langle I_1^5\rangle_m = O(m^4), \tag{116}$$

all of which vanish after the chiral limit is taken.

We thus conclude that the $\mathrm{U}(1)_A$ symmetry breaking is not viable for at least $N\leq 6$.

C. General even N

In order to consider the general N case, let us look at the rhs of Eq. (102). Namely, if we can show that

$$\lim_{m\to 0}\lim_{V\to\infty}\frac{1}{V^k}\langle Q(A)\mathcal{O}\rangle_m = 0 \tag{117}$$

[5] If $\det M = 0$, we can construct a chiral-invariant operator from a linear combination of operators in $\mathcal{O}_a^{(N)}$. Since all operators in $\mathcal{O}_a^{(N)}$ have odd numbers of the index a, however, no chiral-invariant operator should exist in $\mathcal{O}_a^{(N)}$.

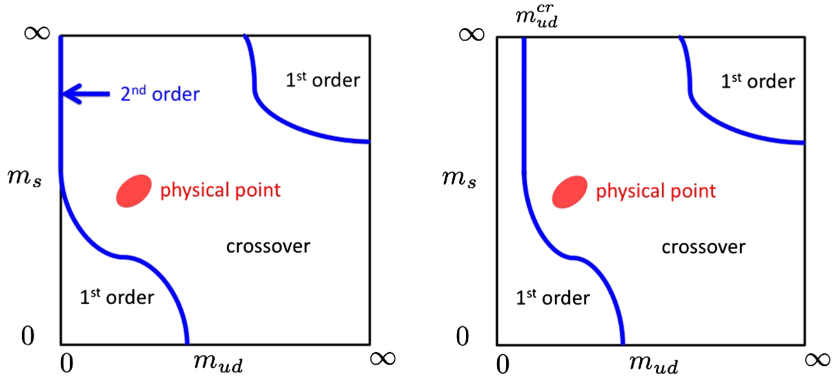

FIG. 1 (color online). Possible phase diagrams including the strange quark. Left: A conventional diagram with the second-order scenario in the $m_s \to \infty$ limit. Right: A possible diagram with the first-order scenario where the critical curve is smoothly connected to the small m_s region.

with some appropriate power of k, we can prove that the lhs of Eq. (102) also vanishes. In the analysis below, we divide $\mathcal{O}_0^N$ into two classes: one with $(n_1, n_2, n_3) = (\text{even}, \text{even}, \text{odd})$, and another with $(n_1, n_2, n_3) = (\text{odd}, \text{odd}, \text{even})$.

For the former class, or more explicitly in the case of $(n_1, n_2, n_3) = (2k_1, 2k_2, 2k_3 + 1)$, the leading contribution in $\delta_0 \mathcal{O}_{n_1,n_2,n_3,n_4}$ comes from $-n_3 \mathcal{O}_{n_1,n_2,n_3-1,n_4+1}$, whose leading contribution in V has $O(V^k)$ with $k = k_1 + k_2 + k_3 + n_4 + 1$ (see Appendix A 5). Therefore, we have

$$\frac{iN_f}{V^k}\langle Q(A)\mathcal{O}_{n_1,n_2,n_3,n_4}\rangle_m \simeq N_f^{k+1} n_3 (2k_1-1)!!(2k_2-1)!!(2k_3-1)!! \times \left\langle N_f \frac{Q^2}{mV}\left(\frac{I_1}{m}\right)^{k_1+k_3}(-I_2)^{k_2}(-I_1)^{n_4}\right\rangle_m \tag{118}$$

in the large-volume limit, where zero-mode contributions are neglected except for the first term. According to the property (98) and the assumption (28), the rhs indeed vanishes in the $V \to \infty$ limit at small but nonzero m. In the case with $(n_1, n_2, n_3) = (\text{odd}, \text{odd}, \text{even})$, a similar analysis gives the same conclusion.

We conclude that, for the class of operators we have considered in this paper, the $U(1)_A$-breaking effects are invisible in the thermodynamical limit.

D. Possible phase diagrams including the strange quark

Although we have so far only discussed the $N_f = 2$ case, it is interesting to consider possible phase diagrams including the dynamical strange quark. (In this subsection, let us denote the up and down quark mass by m_{ud} and the strange quark mass by m_s.)

Assuming that the $U(1)_A$ symmetry is still broken above the critical temperature, a phase diagram like the left panel of Fig. 1 is often shown in the literature. The quenched limit ($m_{ud} = m_s = \infty$) and the SU(3)-symmetric chiral limit ($m_{ud} = m_s = 0$) are both expected to be in the first-order transition regions, while the physical point is located in the middle crossover region. The critical curve around the SU(3) limit has an endpoint at a finite value of m_s, from which a second-order transition line [with $O(4)$ scaling [1]] is extended to the $N_f = 2$ ($m_s = \infty$) limit.

Our new results may suggest a different diagram. Since the $U(1)_A$ anomaly effects are invisible, the chiral phase transition could be first-order. Then, as shown in the right panel of Fig. 1, one should have a critical value of the up and down quark mass (let us denote this by m_{ud}^{cr}) from which the critical curve may be extended to the finite m_s region and even connected to the curve around the first-order transition region near $m_s = 0$.

Since our study is limited to the $N_f = 2$ case only, the above scenario is just one example of many possible diagrams. As pointed out in Refs. [19–21], the second-order transition is also possible. But even in this case, its $U(2)_L \otimes U(2)_R/U(2)_V$ universality class is different from the conventional $O(4)$ class.

Our simple analysis in the $N_f = 2$ theory thus suggests a richer structure in the QCD phase diagram. It is particularly interesting for lattice QCD studies to investigate the existence of m_{ud}^{cr}, which may also be the boundary of the region where Eq. (98) holds.[6]

V. POSSIBLE ARTIFACTS IN LATTICE QCD

In the previous sections, we have investigated the symmetry restoration for $T > T_c$, fully relying on the exact chiral $SU(2)_L \times SU(2)_R$ symmetry and taking the thermodynamical limit $V \to \infty$. However, numerical lattice QCD simulations must be performed on a finite volume, sometimes employing fermion actions which explicitly break the chiral symmetry. In this section, we would like to briefly address possible systematic effects of not having these two key properties.

First, we discuss the explicit breaking of the chiral $SU(2)_L \times SU(2)_R$ symmetry. In order to characterize its violation, let us introduce a *mass* parameter m_{break}. Since m_{break}

[6] Namely, the number of the exact zero-modes could be an order parameter.

should disappear in the continuum limit, it is natural to assume $m_{\mathrm{break}} \sim \Lambda_{\mathrm{QCD}}^2 a$, where Λ_{QCD} is the QCD scale. At finite temperature T, we also have a possibility of $m_{\mathrm{break}} \sim T^2 a$ or $m_{\mathrm{break}} \sim \Lambda_{\mathrm{QCD}} T a$. But it is unlikely that the lattice artifacts grow with T, since they are naively expected to be milder in the weakly coupled region at higher temperature. We also neglect the possibility of $m_{\mathrm{break}} \sim T_c^2 a$ since T_c is not essentially different from Λ_{QCD}.

If one employs improved Wilson-type actions or staggered-type actions, it may be reduced to $O(a^2)$: $m_{\mathrm{break}} \sim \Lambda_{\mathrm{QCD}}^3 a^2$. For the domain-wall fermion action, as an approximation of the overlap fermion action, the suppression of the discretization effects could be stronger. In this case, the so-called residual mass, m_{res}, is a good estimate for m_{break}. For this reason, we have introduced a rather abstract parameter, m_{break}, to treat the conditions with different actions in a uniform manner.

Now the discussion is simple. By losing the required exact chiral symmetry, every result in the previous sections should be, in principle, modified by the effects of m_{break} unless some special cancellation mechanism occurs. The condition $\langle \rho_0^A \rangle_m = 0$ may be the only exception, as it is a *definition* of the symmetry restoration.

Namely, instead of Eqs. (97), we should have

$$\langle \rho^A(\lambda) \rangle_m = \alpha m_{\mathrm{break}} \Lambda_{\mathrm{QCD}} \lambda + \beta m_{\mathrm{break}} \lambda^2 + (\langle \rho_3^A \rangle_0 + \gamma m_{\mathrm{break}}/\Lambda_{\mathrm{QCD}}) \frac{\lambda^3}{3!} + \cdots, \qquad (119)$$

where $\alpha, \beta, \gamma, \ldots$ are unknown dimensionless $O(1)$ coefficients. Similarly, $\langle N_{R+L} \rangle_m / V$, $\langle Q(A)^2 \rangle_m / V$, $\chi^{\pi-\eta}$, and so on should not be zero, but rather $O(m_{\mathrm{break}})$. Note that there is no reason for the $\mathrm{U}(1)_A$ symmetry to get restored as long as the chiral symmetry is explicitly broken by the quark action at finite lattice spacings.

Next, let us discuss the finite-volume effects. Even in the continuum limit, it is possible to obtain different results from what we have shown in this paper. It is good to remember that Eq. (1) is an example of the $\mathrm{U}(1)_A$ breaking in the continuum theory as a finite-volume effect. The recovery of the $\mathrm{U}(1)_A$ symmetry is not as strong as the other symmetries—under which the Lagrangian is strictly constrained—but rather is a consequence from QCD dynamics, which is manifest only in the thermodynamical limit.

Above the critical temperature, the long-range physics of the system would be characterized by the correlation length ξ, or the inverse of some screening mass, which diverges at T_c if the phase transition is of second order while remaining finite for the first-order transition.

It is then natural to assume that a lattice QCD simulation has finite-volume effects as functions of $\xi/V^{1/4}$. It is also important to note that, unlike the truly local quantity, whose finite-volume effects are exponential $\sim \exp(-V^{1/4}/\xi)$, the susceptibilities considered in this paper are volume-averaged quantities, so that any finite-volume effect is expected to be a power function of $\xi/V^{1/4}$. A careful estimate for the thermodynamical limit is thus required, in particular, for temperatures near T_c, where ξ could become larger.

VI. EIGENVALUE DENSITY WITH FRACTIONAL POWER

So far, we have assumed that $\rho^A(\lambda)$ is analytic around $\lambda = 0$, and have used the expansion in Eq. (35). In this section, let us extend our analysis to a nonanalytic case where

$$\rho^A(\lambda) = c^A \lambda^\gamma, \qquad (120)$$

with a fractional power γ for $\lambda < \epsilon$, where c^A is an A-dependent constant. Since $\lim_{m\to 0} \langle \rho^A(0) \rangle_m = 0$ in the $\mathrm{SU}(2)_L \times \mathrm{SU}(2)_R$-symmetric phase, γ should be positive as long as $\langle c^A \rangle_m = O(1)$. It is still true in this case that only the vicinity of $\lambda = 0$ contributes to the WTIs. We thus can neglect additional terms with higher-order fractional powers, even if they exist in the bulk region of $\lambda \geq \epsilon$.

In this case, I_1, I_2, and I_3 are expressed as

$$I_1 = c^A [m^\gamma (d_1 + O(m^2)) + m(e_1 + O(m^2))], \qquad (121)$$

$$\frac{I_1}{m} + I_2 = 2m I_3 = c^A [m^{\gamma-1}(d_2 + O(m^2)) + m^2 (e_2 + O(m^2)]), \qquad (122)$$

where the d_i's and e_i's are given by

$$d_1 = \pi \sec\left(\frac{\gamma\pi}{2}\right), \qquad d_2 = (1-\gamma)\pi \sec\left(\frac{\gamma\pi}{2}\right), \qquad (123)$$

and

$$e_1 = \int_\epsilon^{\Lambda_R} d\lambda \rho^A(\lambda) \frac{2 g_0(\lambda^2)}{Z_m^2 \lambda^2 + m^2} + \epsilon^{\gamma-1} \frac{\Gamma(\frac{\gamma-1}{2}) - \frac{\epsilon^2}{\Lambda_R^2} \frac{\Gamma(\frac{\gamma+1}{2})^2}{\Gamma(\frac{\gamma+3}{2})}}{\Gamma(\frac{\gamma+1}{2})}, \qquad (124)$$

$$e_2 = \int_\epsilon^{\Lambda_R} d\lambda \rho^A(\lambda) \frac{4 g_0^2(\lambda^2)}{(Z_m^2 \lambda^2 + m^2)^2} + \epsilon^{\gamma-3} \frac{(\gamma+3)\Gamma(\frac{\gamma-1}{2})}{2(\gamma-3)\Gamma(\frac{\gamma+5}{2})} \times \left[(\gamma+1)(\gamma-1) - 2\frac{\epsilon^2}{\Lambda_R^2}(\gamma+1)(\gamma-3) + \frac{\epsilon^4}{\Lambda_R^4}(\gamma-1)(\gamma-3)\right], \qquad (125)$$

with the UV cutoff Λ_R and the IR cutoff ϵ. Note that the d_i's and e_i's are all finite.

A. $0 < \gamma < 1$

We first consider the case with $\gamma < 1$. With the above expressions for the I_i's, let us reexamine the WTIs given in the previous sections.

For $\langle S_0^N \rangle_m / V^N$ with an arbitrary N, the WTI requires

$$\lim_{m\to 0} \lim_{V\to\infty} \left\langle \left\{ \frac{N_{R+L}^A}{mV} + I_1 \right\}^N \right\rangle_m = 0, \tag{126}$$

where the positivity of each term implies

$$\lim_{V\to\infty} \frac{\langle N_{R+L}^A \rangle_m}{V} = 0 \tag{127}$$

at small m, and

$$\lim_{m\to 0} m^{N\gamma} d_1^N \langle (c^A)^N \rangle_m = 0, \tag{128}$$

which is automatically satisfied for positive γ.

At $N = 2$, we have

$$\left\langle \frac{I_1}{m} + I_2 - \frac{N_f Q(A)^2}{m^2 V} \right\rangle_m = d_2 m^{\gamma-1} \langle c^A \rangle_m - \frac{N_f \langle Q(A)^2 \rangle_m}{m^2 V} \to 0. \tag{129}$$

Taking into account the fact that both c^A and Q^2 are mass-independent and their expectation value should be written as an even power of mass, both terms in Eq. (129) should vanish separately, which leads to

$$\langle c^A \rangle_m = O(m^2), \qquad \frac{\langle Q(A)^2 \rangle_m}{V} = O(m^4). \tag{130}$$

At $N = 3$, it is not difficult to see that all the nontrivial conditions are automatically satisfied with the above constraints.

At $N = 4$ there remains one nontrivial WTI:

$$\langle 6mI_3(I_2 - I_1/m) \rangle_m + \frac{6N_f \langle I_1 Q(A)^2 \rangle_m}{m^3 V} - \frac{N_f^2 \langle Q(A)^4 \rangle_m}{m^4 V^2} \to 0. \tag{131}$$

Since the first two terms vanish in the chiral limit, we obtain a new constraint that

$$\lim_{V\to\infty} \frac{\langle Q(A)^2 \rangle_m}{V} = O(m^6). \tag{132}$$

Let us finally consider the WTI from $\mathcal{O}_a^{N=4k} = \mathcal{O}_{0,1,(4k-1),0}$, as before. In a way very similar to that in Sec. III G, we can show that

$$\lim_{V\to\infty} \frac{\langle Q(A)^2 \rangle_m}{V} = 0, \tag{133}$$

$$\langle c^A \rangle_m = 0, \tag{134}$$

even at nonzero m. This means that the Dirac eigenvalue density with a fractional power, Eq. (120), is incompatible with the $SU(2)_L \times SU(2)_R$ chiral symmetry restoration for $0 < \gamma < 1$.

B. $1 < \gamma < 2$

Next, let us consider $1 < \gamma < 2$. Our strategy is the same as in the previous subsection, except that the leading term is not $O(m^\gamma)$, but rather is $O(m)$ in I_1.

Up to $N = 4$, one can easily confirm that most of the conditions are automatically satisfied for $1 < \gamma < 2$, keeping the constraints on the zero-mode contribution [Eqs. (127) and (133)] unchanged. The only nontrivial WTI appears at $N = 3$:

$$\lim_{V\to\infty} \frac{\langle \mathcal{O}_{1110} \rangle_m}{V} = 2N_f \langle I_3 \rangle_m = 2N_f d_3 m^{\gamma-2} \langle c^A \rangle_m + O(m) = 0, \tag{135}$$

which leads to a constraint,

$$\langle c^A \rangle_m = O(m^2). \tag{136}$$

Namely, the fractional power $\gamma < 2$ cannot survive in the chiral limit.

C. $2 < \gamma < 3$

In this case, all the conditions from the WTIs are automatically satisfied up to $N = 6$ as long as Eqs. (127) and (133) are satisfied. We thus have no constraint on $\langle c^A \rangle$.

However, it is important to note that excluding $\gamma \leq 2$ in the chiral limit is enough to achieve all of the $U(1)_A$-symmetric identities in Sec. IV. As discussed in Sec. IV C, the zero-mode's contribution plays a more important role than bulk contributions from nonzero modes.

VII. SUMMARY AND DISCUSSION

In this paper, we have investigated the eigenvalue density $\rho^A(\lambda)$ of the Dirac operator in the chiral $SU(2)_L \times SU(2)_R$-symmetric phase at finite temperature. In order to avoid possible ultraviolet divergences, we have worked analytically on a lattice, employing the overlap Dirac operator, which ensures the exact chiral symmetry at finite lattice spacings.

From the various WTIs of the scalar and pseudoscalar operators, we have shown that a behavior such as $\langle \rho^A(\lambda) \rangle_m \propto \lambda^\gamma$ for small λ cannot survive in the chiral limit for $\gamma \leq 2$. If $\langle \rho^A(\lambda) \rangle_m$ is analytical around $\lambda = 0$, this means that it should start with a cubic term, as is the case with the free quark theory. Moreover, we have found a strong suppression on the zero-mode's contributions in the thermodynamical limit. As shown in Eq. (98), they disappear even with a small but finite m. It is worth mentioning that the use of the overlap fermion is crucial for obtaining the results in this paper since only this fermion formulation can preserve the exact chiral symmetry with a nonperturbative cutoff, which makes our arguments more rigorous.

The obtained constraints on the Dirac spectrum are strong enough for all of the $U(1)_A$-breaking effects among correlation functions of scalar and pseudoscalar operators considered in this paper to vanish in the limits of $V \to \infty$ and $m \to 0$. Namely, there is no remnant of the $U(1)_A$ anomaly above the critical temperature, at least in these correlation functions.

This does not contradict the apparently opposite results about the $U(1)_A$ restoration in previous works. As we have shown in Sec. I, their $U(1)_A$-breaking parts cannot survive in the thermodynamical limit ($V \to \infty$), but they could be finite on a finite box, which may be a part of the difficulties of numerical lattice QCD simulations.

We only use a part of the chiral Ward-Takahashi identities to derive the constraints in this paper, which are therefore necessary conditions to be fulfilled if the chiral symmetry is restored. Our results strongly rely on analyticity in m^2 for m-independent observables and its consequence (24). If our results are shown to be incorrect by some numerical simulations, these assumptions must also be violated in the simulations.

One of the most important consequence of our study is that, since the $U(1)_A$ anomaly effect disappears in scalar and pseudoscalar sectors at T_c, the chiral phase transition for two-flavor QCD is likely to be of first order [1] or of second order in the $U(2)_L \otimes U(2)_R/U(2)_V$ universality class [19–21], contrary to the expectation that the chiral phase transition of two-flavor QCD belongs to the $O(4)$ universality class.

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APPENDIX A: USEFUL FORMULAS

1. Quark contractions for the (pseudo) scalar operator

Here we give a contraction formula for the (pseudo) scalar operators when we integrate out the fermion fields:

$$\begin{aligned}
\langle S_0\rangle_F &= -N_f \mathrm{tr}\tilde{S}_A, \qquad \langle P_0\rangle_F = -iN_f \mathrm{tr}\gamma_5\tilde{S}_A,\\
\langle S_a^2\rangle_F &= -N_f \mathrm{tr}\tilde{S}_A^2, \qquad \langle P_a^2\rangle_F = N_f \mathrm{tr}(\gamma_5\tilde{S}_A)^2,\\
\langle S_0^2\rangle_F &= -N_f \mathrm{tr}\tilde{S}_A^2 + (N_f\mathrm{tr}\tilde{S}_A)^2,\\
\langle P_0^2\rangle_F &= N_f \mathrm{tr}(\gamma_5\tilde{S}_A)^2 - (N_f\mathrm{tr}\gamma_5\tilde{S}_A)^2,\\
\langle S_0P_0\rangle_F &= -iN_f\mathrm{tr}\gamma_5\tilde{S}_A^2 + iN_f^2\mathrm{tr}\tilde{S}_A\mathrm{tr}\gamma_5\tilde{S}_A,\\
\langle S_aP_a\rangle_F &= -iN_f\mathrm{tr}\gamma_5\tilde{S}_A^2,
\end{aligned} \tag{A1}$$

where $\tilde{S}_A(x,y) \equiv F(D)S_A(x,y)$.

2. Trace of fermion propagators

Here we give useful formulas for the trace of fermion propagators in a form of the eigenvalue decomposition.

Let us first define S_A^n as

$$\begin{aligned}
\tilde{S}_A^n &\equiv \int d^4x_1 d^4x_2 \dots d^4x_n \tilde{S}_A(x_1,x_2)\tilde{S}_A(x_2,x_3)\dots\tilde{S}_A(x_n,x_1)\\
&= \int \prod_{i=1}^{n} d^4x_i \tilde{S}_A(x_i,x_{i+1}), \qquad (x_{n+1}=x_1).
\end{aligned} \tag{A2}$$

Inserting the eigenvalue decomposition for the fermion propagator (11), we obtain

$$\frac{1}{V}\mathrm{tr}\tilde{S}_A = \frac{N_{R+L}^A}{mV} + I_1, \qquad \frac{1}{V}\mathrm{tr}\tilde{S}_A^2 = \frac{N_{R+L}^A}{m^2V} + I_2, \tag{A3}$$

$$\begin{aligned}
\frac{1}{V}\mathrm{tr}(\gamma_5\tilde{S}_A)^2 &= \frac{N_{R+L}^A}{m^2V} + \frac{I_1}{m},\\
\frac{1}{V}\mathrm{tr}\gamma_5\tilde{S}_A\gamma_5\tilde{S}_A^2 &= \frac{N_{R+L}^A}{m^3V} + I_3,
\end{aligned} \tag{A4}$$

$$\frac{1}{\sqrt{V}}\mathrm{tr}\gamma_5\tilde{S}_A = \frac{Q(A)}{m\sqrt{V}}, \qquad \frac{1}{\sqrt{V}}\mathrm{tr}\gamma_5\tilde{S}_A^2 = \frac{Q(A)}{m^2\sqrt{V}}, \tag{A5}$$

where I_i ($i = 1, 2, 3$) are expressed in terms of the eigenvalue density in the large-volume limit as

$$I_{2k-1} = m\int_0^{\Lambda_R} d\lambda \rho^A(\lambda)\frac{2g_0^k(\lambda^2)}{(Z_m^2\lambda^2+m^2)^k}, \tag{A6}$$

$$g_0(\lambda^2) = 1 - \frac{\lambda^2}{\Lambda_R^2}, \qquad Z_m^2 = 1 - \frac{m^2}{\Lambda_R^2}, \tag{A7}$$

$$I_2 = -\frac{I_1}{m} + 2mI_3. \tag{A8}$$

3. Various integrals of eigenvalue density

The above I_i's are evaluated by expanding the eigenvalue density as Eq. (35). In evaluating I_{2k-1} it may be better to rewrite $I_{2k-1} = I_{2k-1}^{\epsilon} + O(m)$, where

$$I_{2k-1}^{\epsilon} = \frac{m_R}{Z_m^{2k-1}}\int_0^{\epsilon} d\lambda \rho^A(\lambda)\frac{2g_0^k(\lambda^2)}{(\lambda^2+m_R^2)^k} \tag{A9}$$

by using $m_R = m/Z_m$. The expansion is given by

$$I^{\epsilon}_{2k-1} = \sum_{n=0}^{\infty} \rho^A_n I^{(n)}_{2k-1}, \tag{A10}$$

with the expansion coefficient

$$I^{(n)}_{2k-1} = \frac{1}{Z_m^{2k-1}} \int_0^{\epsilon} d\lambda \frac{\lambda^n}{n!} \frac{2m_R g_0^k(\lambda^2)}{(\lambda^2 + m_R^2)^k}. \tag{A11}$$

At $n > 2k-1$ the leading term in m is given by

$$I^{(n)\text{leading}}_{2k-1} = 2m_R \int_0^{\epsilon} \frac{\lambda^{n-2k}}{n!}\left(1 - \frac{\lambda^2}{\Lambda_R^2}\right)^k. \tag{A12}$$

The explicit form of the coefficient is given as follows for a few k and n:

$$I_1^{(0)} = \frac{2}{Z_m}\left[\left(1 + \frac{m_R^2}{\Lambda_R^2}\right)\tan^{-1}\left(\frac{\epsilon}{m_R}\right) - \frac{m_R\epsilon}{\Lambda_R^2}\right], \tag{A13}$$

$$I_1^{(1)} = \frac{m_R}{Z_m}\left[\left(1 + \frac{m_R^2}{\Lambda_R^2}\right)\log\left(\frac{\epsilon^2}{m_R^2} + 1\right) - \frac{\epsilon^2}{\Lambda_R^2}\right], \tag{A14}$$

$$I_1^{(2)} = \frac{m_R}{Z_m}\left[\epsilon\left(1 + \frac{3m_R^2 - \epsilon^2}{3\Lambda_R^2}\right) - m_R\left(1 + \frac{m_R^2}{\Lambda_R^2}\right)\tan^{-1}\left(\frac{\epsilon}{m_R}\right)\right], \tag{A15}$$

$$I_3^{(0)} = \frac{1}{Z_m^3 m_R^2}\left[\left(1 - 3\frac{m_R^2}{\Lambda_R^2}\right)\left(1 + \frac{m_R^2}{\Lambda_R^2}\right)\tan^{-1}\left(\frac{\epsilon}{m_R}\right) + \frac{m_R\epsilon}{m_R^2 + \epsilon^2}\left(1 + \frac{m_R^2}{\Lambda_R^2}\right)^2 + \frac{2m_R^3\epsilon}{\Lambda_R^4}\right], \tag{A16}$$

$$I_3^{(1)} = \frac{m_R}{Z_m^3}\left[\frac{\epsilon^2}{m_R^2(\epsilon^2 + m_R^2)}\left(1 + \frac{m_R^2}{\Lambda_R^2}\right)^2 + \frac{\epsilon^2}{\Lambda_R^4} + \frac{2}{\Lambda_R^2}\left(1 + \frac{m_R^2}{\Lambda_R^2}\right)\log\left(\frac{m_R^2}{\epsilon^2 + m_R^2}\right)\right], \tag{A17}$$

$$I_3^{(2)} = \frac{1}{2Z_m^3}\left[\left(1 + \frac{m_R^2}{\Lambda_R^2}\right)\left(1 + 5\frac{m_R^2}{\Lambda_R^2}\right)\tan^{-1}\left(\frac{\epsilon}{m_R}\right) + \frac{2m_R\epsilon^3}{3\Lambda_R^4} - \frac{m_R\epsilon}{\Lambda_R^2}\left(1 + \frac{m_R^2}{\Lambda_R^2}\right)\left(4 + \frac{\Lambda_R^2 + m_R^2}{\epsilon^2 + m_R^2}\right)\right], \tag{A18}$$

$$I_3^{(3)} = \frac{m_R}{6Z_m^3}\left[\left(1 + \frac{m_R^2}{\Lambda_R^2}\right)\left(1 + 3\frac{m_R^2}{\Lambda_R^2}\right)\log\left(\frac{\epsilon^2}{m_R^2} + 1\right) + \frac{\epsilon^4}{2\Lambda_R^4} - \frac{\epsilon^2}{\Lambda_R^2}\left(1 + \frac{m_R^2}{\Lambda_R^2}\right)\left(2 + \frac{\Lambda_R^2 + m_R^2}{\epsilon^2 + m_R^2}\right)\right]. \tag{A19}$$

According to the equality the coefficient for I_2 is given by

$$I_2^{(0)} = \frac{2\epsilon\left(\frac{(\Lambda_R^2 + m_R^2)^2}{\epsilon^2 + m_R^2} + 2m_R^2 + \Lambda_R^2\right) - 6m_R(\Lambda_R^2 + m_R^2)\tan^{-1}(\frac{\epsilon}{m_R})}{\Lambda_R^4 Z_m^2}, \tag{A20}$$

$$I_2^{(1)} = \frac{\epsilon^2\left(\frac{2(\Lambda_R^2 + m_R^2)^2}{\epsilon^2 + m_R^2} + 2m_R^2 + \Lambda_R^2\right) - (\Lambda_R^2 + 4m_R^2)(\Lambda_R^2 + m_R^2)\log\left(\frac{\epsilon^2}{m_R^2} + 1\right)}{\Lambda_R^4 Z_m^2}, \tag{A21}$$

$$I_2^{(2)} = \frac{1}{3\Lambda_R^4 Z_m^2}\left[3m_R(\Lambda_R^2 + m_R^2)(2\Lambda_R^2 + 5m_R^2)\tan^{-1}\left(\frac{\epsilon}{m_R}\right) - \epsilon\left(3(\Lambda_R^2 + m_R^2)\left\{\Lambda_R^2 + 4m_R^2 + m_R^2\frac{\Lambda_R^2 + m_R^2}{\epsilon^2 + m_R^2}\right\} - \epsilon^2(\Lambda_R^2 + 2m_R^2)\right)\right]. \tag{A22}$$

4. Integrals of eigenvalue density with fractional power

If we consider the fractional power for the eigenvalue density with $\gamma > 0$, the eigenvalue integral

$$I^{(\gamma)}_{2k-1} = \frac{m_R}{Z_m^{2k-1}} \int_0^{\epsilon} d\lambda \lambda^{\gamma} \frac{2g_0^k(\lambda^2)}{(\lambda^2 + m_R^2)^k} \tag{A23}$$

is given in terms of the hypergeometric function as

$$I_1^{(\gamma)} = \frac{2\epsilon^{\gamma+1}\left((\gamma + 3)_2F_1\left(1, \frac{\gamma+1}{2}; \frac{\gamma+3}{2}; -\frac{\epsilon^2}{m_R^2}\right) - \frac{\epsilon^2}{\Lambda_R^2}(\gamma + 1)_2F_1\left(1, \frac{\gamma+3}{2}; \frac{\gamma+5}{2}; -\frac{\epsilon^2}{m_R^2}\right)\right)}{(\gamma + 1)(\gamma + 3)Z_m m_R}, \tag{A24}$$

$$I_3^{(\gamma)} = \frac{\epsilon^{\gamma+1}}{m_R^3 Z_m^3}\left[\frac{m_R^2}{\epsilon^2+m_R^2} g_0(\epsilon^2)^2 - \frac{\gamma-1}{\gamma+1}{}_2F_1\left(1, \frac{\gamma+1}{2}; \frac{\gamma+3}{2}; -\frac{\epsilon^2}{m_R^2}\right) - \frac{2\epsilon^2}{\Lambda_R^2}\frac{\gamma+1}{\gamma+3}{}_2F_1\left(1, \frac{\gamma+3}{2}; \frac{\gamma+5}{2}; -\frac{\epsilon^2}{m_R^2}\right) - \frac{\epsilon^4}{\Lambda_R^4}\frac{\gamma+3}{\gamma+5}{}_2F_1\left(1, \frac{\gamma+5}{2}; \frac{\gamma+7}{2}; -\frac{\epsilon^2}{m_R^2}\right)\right], \tag{A25}$$

where ${}_2F_1$ is the Gaussian hypergeometric function given by

$${}_2F_1(\alpha, \beta, \gamma; z) = \frac{\Gamma(\gamma)}{\Gamma(\alpha)\Gamma(\beta)}\sum_{n=1}^{\infty}\frac{\Gamma(\alpha+n)\Gamma(\beta+n)}{\Gamma(\gamma+n)}\frac{z^n}{n!}. \tag{A26}$$

Performing an expansion for $m_R/\epsilon \ll 1$ we have

$$I_1^{(\gamma)} = \frac{m_R}{\epsilon}\frac{\epsilon^{\gamma}\left(\Gamma(\frac{\gamma-1}{2}) - \frac{\epsilon^2}{\Lambda_R^2}\frac{\Gamma(\frac{\gamma+1}{2})^2}{\Gamma(\frac{\gamma+3}{2})}\right)}{Z_m\Gamma(\frac{\gamma+1}{2})} + O\left(\left(\frac{m_R}{\epsilon}\right)^3\right) + \left(\frac{m_R}{\epsilon}\right)^{\gamma}\left[\frac{2\epsilon^{\gamma}\Gamma(\frac{1}{2}-\frac{\gamma}{2})\Gamma(\frac{\gamma}{2}+\frac{3}{2})}{(1+\gamma)Z_m} + O\left(\left(\frac{m_R}{\epsilon}\right)^2\right)\right], \tag{A27}$$

$$I_3^{(\gamma)} = \frac{(\gamma+3)\epsilon^{\gamma-2}\Gamma(\frac{\gamma-1}{2})(\frac{m_R}{\epsilon})}{4(\gamma-3)Z_m^3\Gamma(\frac{\gamma+5}{2})}\left[(\gamma+1)(\gamma-1) - \frac{2\epsilon^2}{\Lambda_R^2}(\gamma+1)(\gamma-3) + \frac{\epsilon^4}{\Lambda_R^4}(\gamma-1)(\gamma-3)\right] + O\left(\left(\frac{m_R}{\epsilon}\right)^2\right) + \left(\frac{m_R}{\epsilon}\right)^{\gamma-2}\left[\frac{(1-\gamma)\epsilon^{\gamma-2}\Gamma(\frac{1-\gamma}{2})\Gamma(\frac{1+\gamma}{2})}{2Z_m^3} + O\left(\left(\frac{m_R}{\epsilon}\right)^2\right)\right]. \tag{A28}$$

5. General correlation functions in the large-volume limit

Here we consider the leading volume scaling of the general correlation functions made of S_a's and P_a's.

At the given order $N = 2(k_1+k_2+k_3)+n_4$, there are two types of parity-even and chiral-symmetric operators:

$$\mathcal{O}_1^N = \mathcal{O}_{2k_1,2k_2,2k_3,n_4}, \qquad \mathcal{O}_2^N = \mathcal{O}_{2k_1+1,2k_2+1,2k_3+1,n_4-3}. \tag{A29}$$

For $\mathcal{O}_1^N$, the integration over the fermion fields in the large-volume limit is given by

$$\langle\mathcal{O}_1^N\rangle_F \simeq \langle P_a^{2k_1}\rangle_F\langle S_a^{2k_2}\rangle_F\langle P_0^{2k_3}\rangle_F\langle S_0\rangle_F^{n_4} \sim \langle P_a^2\rangle_F^{k_1}\langle S_a^2\rangle_F^{k_2}\langle P_0^2\rangle_F^{k_3}\langle S_0\rangle_F^{n_4}, \tag{A30}$$

where each $\langle\mathcal{O}\rangle_F$ gives an $O(V)$ contribution. An overall constant coming from combinatorial factors is omitted here and hereafter. Therefore the leading contribution is $O(V^{k_1+k_2+k_3+n_4})$ for $\mathcal{O}_1^N$.

Similarly, we have

$$\langle\mathcal{O}_2^N\rangle_F \sim \langle P_aS_a\rangle_F\langle P_a^2\rangle_F^{k_1}\langle S_a^2\rangle_F^{k_2}\langle P_0^{2k_3+1}\rangle_F\langle S_0\rangle_F^{n_4-3}, \tag{A31}$$

where

$$\langle P_0^{2k_3+1}\rangle_F \sim \langle P_0\rangle_F\langle P_0^{2k_3}\rangle_F \sim \langle P_0\rangle_F\langle P_0^2\rangle_F^{k_3}. \tag{A32}$$

Since $\langle P_aS_a\rangle_F$ and $\langle P_0\rangle_F$ are proportional to $Q(A)$ and are therefore $O(\sqrt{V})$, the leading volume dependence of $\mathcal{O}_2^N$ is $O(V^{k_1+k_2+k_3+n_4-2})$.

APPENDIX B: STRUCTURE OF WARD-TAKAHASHI IDENTITIES FOR SCALAR AND PSEUDOSCALAR OPERATORS

In this appendix, we summarize the general structures of WTIs among the scalar and pseudoscalar operators, $\mathcal{O}_{n_1,n_2,n_3,n_4} = P_a^{n_1}S_a^{n_2}P_0^{n_3}S_0^{n_4}$.

In this paper, we study the relation between three operator sets:

$$\mathcal{O}_a^{(N)} \equiv \left\{\mathcal{O}_{n_1,n_2,n_3,n_4}|n_1+n_2 = \text{odd}, n_1+n_3 = \text{odd}, \sum_i n_i = N\right\}, \tag{B1}$$

$$\mathcal{O}_0^{(N)} \equiv \left\{\mathcal{O}_{n_1,n_2,n_3,n_4}|n_1+n_2 = \text{even}, n_1+n_3 = \text{odd}, \sum_i n_i = N\right\}, \tag{B2}$$

$$\mathcal{O}^{(N)} \equiv \Big\{\mathcal{O}_{n_1,n_2,n_3,n_4} | n_1 + n_2 = \text{even}, n_1 + n_3 = \text{even}, \sum_i n_i = N\Big\}. \tag{B3}$$

Note that only the $\mathcal{O}^{(N)}$ can have a nonzero expectation value in QCD with two degenerate quarks.

Since

$$\begin{aligned} \delta_a \mathcal{O}_a^{(N)} &\equiv \{\delta_a \mathcal{O} | \mathcal{O} \in \mathcal{O}_a^{(N)}\} \in \mathcal{O}^{(N)}, \\ \delta_0 \mathcal{O}_0^{(N)} &\equiv \{\delta_0 \mathcal{O} | \mathcal{O} \in \mathcal{O}_0^{(N)}\} \in \mathcal{O}^{(N)}, \end{aligned} \tag{B4}$$

the goal of this paper is to understand constraints from the $SU(2)_L \times SU(2)_R$ symmetry restoration, $\langle \delta_a \mathcal{O}_a^{(N)} \rangle = 0$, and to examine whether $\delta_0 \mathcal{O}_0^{(N)}$ can have a nonzero expectation value, which would mean that the $U(1)_A$ is still broken. For simplicity, hereafter we denote $n = (n_1 n_2 n_3 n_4)$ instead of $\mathcal{O}_{n_1,n_2,n_3,n_4}$ to represent an operator.

1. WTIs at odd N

As shown in Sec. IV, we can show that $\langle \delta_0 \mathcal{O}_0^{(N)} \rangle = 0$ if $\langle \delta_a \mathcal{O}_a^{(N)} \rangle = 0$ when N is odd. This follows from the fact that $|\mathcal{O}_a^{(N)}| = |\mathcal{O}_0^{(N)}| = |\mathcal{O}^{(N)}|$, where $|\mathcal{O}|$ means a number of independent operators in $\mathcal{O}$. Here we give a proof for this equality for general odd $N = 2k + 1$.

At $k = 0$, we have only one operator for each set: $n_A = (1000)$ for $\mathcal{O}_a^{(N)}$, $n_B = (0010)$ for $\mathcal{O}_0^{(N)}$, and $n_C = (0001)$ for $\mathcal{O}^{(N)}$. Thus, $|\mathcal{O}_a^{(N)}| = |\mathcal{O}_0^{(N)}| = |\mathcal{O}^{(N)}| = 1$ for $k = 0$.

At $k = 1$, we can create the operators by adding to the above $n_X (X = A, B, C)$ a pair of the *same* operators, namely, adding 2 to one element of n_X. Since each n_X has four elements, we have four operators for each set. We should, however, note that there is one additional type of operator for each set: $\bar{n}_A = (0111) \in \mathcal{O}_a^{(N)}$, $\bar{n}_B = (1101) \in \mathcal{O}_0^{(N)}$, and $\bar{n}_C = (1110) \in \mathcal{O}^{(N)}$. Therefore, $|\mathcal{O}_a^{(N)}| = |\mathcal{O}_0^{(N)}| = |\mathcal{O}^{(N)}| = 5$ in total. For example, we have (1002), (1020), (1200), (3000), and (0111) in $\mathcal{O}_a^{(N)}$.

In fact, every operator at higher k can be generated by adding 2 to one element of n_X k times or adding 2 to one element of $\bar{n}_X$ $k - 1$ times. A number of independent operators at a given k, therefore, is obtained by selecting k (or $k - 1$) numbers from 1, 2, 3, 4, which is ${}_{k+3}C_3$ (${}_{k+2}C_3$). In total, we have

$${}_{k+3}C_3 + {}_{k+2}C_3 = \frac{(k+2)(k+1)(2k+3)}{3!} \tag{B5}$$

for each set. This completes the proof for $|\mathcal{O}_a^{(N)}| = |\mathcal{O}_0^{(N)}| = |\mathcal{O}^{(N)}|$ at an arbitrary odd number N.

2. WTIs at even N

We next consider the case with $N = 2k$. We have $n_A (n_B) = 0110(0011)$ and $\bar{n}_A (\bar{n}_B) = 1001(1100)$ at $k = 1$ for $\mathcal{O}_a^{(N)}$ ($\mathcal{O}_0^{(N)}$), while $n_C = 0000$ at $k = 0$ and $\bar{n}_C = 1111$ at $k = 2$ for $\mathcal{O}^{(N)}$. As before, it is easy to count a number of independent operators for each case. There are $2 \times ({}_{k+2}C_3)$ operators for $\mathcal{O}_a^{(N)}$ and $\mathcal{O}_0^{(N)}$, while there are ${}_{k+3}C_3 + {}_{k+1}C_3$ for $\mathcal{O}^{(N)}$. From this, it is easy to see that

$$\begin{aligned} |\mathcal{O}^{(N)}| - |\mathcal{O}_{a,0}^{(N)}| &= {}_{k+3}C_3 + {}_{k+1}C_3 - 2 \times ({}_{k+2}C_3) \\ &= (k+1) > 0, \end{aligned} \tag{B6}$$

which means that $|\mathcal{O}^{(N)}| > |\mathcal{O}_a^{(N)}| = |\mathcal{O}_0^{(N)}|$ at $N = 2k$. Therefore, $\delta_a \mathcal{O}_0^{(N)} = 0$ is not equivalent to $\delta_0 \mathcal{O}_0^{(N)} = 0$.

3. Explicit WTIs at small $N = 2k$

a. $k = 1$

In this case, the two nonsinglet WTIs are given by

$$(0020) - (0200) = 0, \qquad (2000) - (0002) = 0, \tag{B7}$$

while the singlet ones give

$$\delta^0(0011) = (0020) - (0002), \tag{B8}$$

$$\begin{aligned} \delta^0(1100) &= (2000) - (0200) = (0002) - (0020) \\ &= -\delta^0(0011). \end{aligned} \tag{B9}$$

Therefore, one nontrivial $U(1)_A$ rotation can remain. For simplicity, we omit the bracket of $\langle (n_1 n_2 n_3 n_4) \rangle$ here.

b. $k = 2$

In this case, eight nonsinglet WTIs read

$$\begin{aligned} (2020) - (2200) - 2(1111) &= 0, \\ (4000) - 3(2002) &= 0, \end{aligned} \tag{B10}$$

$$\begin{aligned} (2200) - (0202) + 2(1111) &= 0, \\ 3(0220) - (0400) &= 0, \end{aligned} \tag{B11}$$

$$\begin{aligned} (2020) - (0022) - 2(1111) &= 0, \\ (0040) - 3(0220) &= 0, \end{aligned} \tag{B12}$$

$$\begin{aligned} (0022) - (0202) + 2(1111) &= 0, \\ 3(2002) - (0004) &= 0, \end{aligned} \tag{B13}$$

which can be reduced to

$$\begin{aligned} (4000) &= (0004) = 3(2002), \\ (0400) &= (0040) = 3(0220), \end{aligned} \tag{B14}$$

$$\begin{aligned} &(2020) = (0202), \qquad (2200) = (0022), \\ &2(1111) = (0202) - (0022). \end{aligned} \tag{B15}$$

Note that these are symmetric under $n_1 \leftrightarrow n_4$, $n_2 \leftrightarrow n_3$.

Using the above conditions, we have two independent quantities,

$$(0022) - (2002), \qquad (0022) - (0220), \tag{B16}$$

with which to examine the $U(1)_A$ chiral symmetry.

c. $k = 3$

We have 20 WTIs from the nonsinglet chiral symmetry:

$$\begin{aligned}(4020) - (4200) - 4(3111) &= 0,\\ (6000) - 5(4002) &= 0,\end{aligned} \tag{B17}$$

$$\begin{aligned}(2400) - (0402) + 4(1311) &= 0,\\ (0600) - 5(0420) &= 0,\end{aligned} \tag{B18}$$

$$\begin{aligned}3(2220) - (2400) - 2(1311) &= 0,\\ (4200) - 3(2202) + 2(3111) &= 0,\end{aligned} \tag{B19}$$

$$\begin{aligned}(2040) - 3(2220) - 2(1131) &= 0,\\ (4020) - 3(2022) - 2(3111) &= 0,\end{aligned} \tag{B20}$$

plus equations derived from the above by $n_1 \leftrightarrow n_4$, $n_2 \leftrightarrow n_3$, and

$$\begin{aligned}(2022) - (2202) - 2(1113) + 2(3111) &= 0,\\ 3(4002) - 3(2004) &= 0,\end{aligned} \tag{B21}$$

$$\begin{aligned}(2220) - (0222) + 2(1131) - 2(1311) &= 0,\\ 3(0240) - 3(0420) &= 0.\end{aligned} \tag{B22}$$

The above conditions are summarized as

$$\begin{aligned}
&(4002) = (2004), \qquad (0240) = (0420),\\
&(4020) = (0204), \qquad (4200) = (0024),\\
&(2400) = (0042), \qquad (0402) = (2040),\\
&(6000) = (0006) = 5(2004),\\
&(0600) = (0060) = 5(0420),\\
&6(2220) = 6(0222) = (0042) + (2040),\\
&6(2202) = 6(2022) = (0204) + (0024),\\
&4(3111) = 4(1113) = (0204) - (0024),\\
&4(1311) = 4(1131) = (2040) - (0042).
\end{aligned} \tag{B23}$$

In this case, there remain four nontrivial chiral $U(1)_A$ rotations:

$$\begin{aligned}&(0024) - (2004), \qquad (2040) - (0204),\\ &(0420) - (0042), \qquad (0042) - (0024).\end{aligned} \tag{B24}$$

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