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The chiral condensate in a finite volume

Poul H. Damgaard^a and Hidenori Fukaya^{ab}

^a The Niels Bohr International Academy, The Niels Bohr Institute, Blegdamsvej 17 DK-2100 Copenhagen Ø Denmark
^b High Energy Accelerator Research Organization (KEK), Tsukuba 305-0801, Japan
E-mail: phdamg@nbi.dk, hfukaya@nbi.dk

ABSTRACT: Chiral perturbation theory at finite four-volume $V(=L^3T)$ is reconsidered with a view towards finding a computational scheme that can deal with any value of $M_{\pi}L$, where M_{π} is a generic Nambu-Goldstone mass. The momentum zero modes that cause the usual *p*-expansion to fail in the chiral limit are treated separately, and partly integrated out to all orders. In this way the theory remains infrared finite in the perturbative expansion, and the chiral limit can be considered at finite volume. We illustrate the technique by computing the quark condensate in a finite volume, smoothly connecting standard results in the *p*-regime for larger masses with those of the ϵ -regime for smaller masses. From the partially quenched theory we also obtain the spectral density of the Dirac operator, a smooth function from the microscopic region to the bulk region of the *p*-regime.

KEYWORDS: Chiral Lagrangians, Spontaneous Symmetry Breaking, Lattice QCD.



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1. Introduction

A number of studies have been devoted to the finite volume effects in low-energy QCD, or chiral perturbation theory (ChPT) [1]–[5]. The resulting finite-size scaling theory in ChPT has broad theoretical interest as it describes the critical behavior of dynamical symmetry breaking, and as such has corresponding applications in statistical physics as well. In lattice gauge theory it is certainly of great practical value to have analytical predictions for finite volumes available, as they can help in eliminating uncertainties due to the finite sizes used in numerical simulations [6].

To investigate the finite-size behavior of ChPT, essentially two perturbative approaches have been proposed so far [1]. One is the *p*-expansion, which has just the same form as the perturbative series in an infinite volume, only replacing momentum integrals by the discrete sums over momentum due to the quantization in units of 1/L (where L is the linear extent). If we denote by M_{π} the mass of a generic (pseudo) Nambu-Goldstone boson, this *p*-expansion is valid when $M_{\pi}L \gg 1$. It is well known what happens when one takes the chiral limit in a volume such that $M_{\pi}L$ crosses unity and gets even smaller [1, 2]: The propagators of the pseudo Nambu-Goldstone bosons blow up for one single momentum mode, the one of zero four-momentum. This invalidates the usual perturbative expansion, and a different technique is required. A solution to this problem was given in [1] in terms of a so-called ϵ -expansion. In this scheme the zero-momentum mode is, in a sense that becomes more clear below, integrated out exactly, while all the remaining momentum modes are treated perturbatively. Since the chiral Lagrangian involves an infinite series of terms, and since it is only the perturbative expansion that is jeopardized, "exact" integration here refers to the term that is leading order in the quark masses m.

The ϵ -expansion is thus perfectly suited for studying the extreme case where the quark mass m is so small that the pion Compton wave length overcomes the size of the volume, $M_{\pi}L \ll 1$. Since the zero-mode becomes dominant in this ϵ -regime, physical observables are mostly dependent on the leading low-energy constants: the infinite-volume chiral condensate Σ and the pion decay constant F, both in the chiral limit. The next-to-leading order terms (with coefficients L_i 's) at infinite volume are treated in perturbative fashion. This is similar to the p-regime expansion, but the ordering of terms is different. Also in this respect, the ϵ -regime provides an intriguing alternative to more conventional ChPT since different parts of the chiral theory are being probed to any given order. We note that the studies have now also been extended to Wilson ChPT where one has more terms which explicitly break the symmetry [7].

As the ϵ -regime deals with the extremely chiral limit where non-trivial finite-size scaling starts to appear (but still far from the symmetric phase since one keeps $L \gg 1/\Lambda_{\rm QCD}$), universality is at work. Perhaps the most important example of this is the equivalence of the zero-mode or vacuum part of the theory to chiral Random Matrix Theory (ChRMT) [8, 9]. Little is known in detail on how these universal phenomena cease and the ones depending on the dynamics specific to QCD appear when the quark mass increases and M_{π} becomes of order 1/L [10]. In particular, it is not known precisely how the spectral density of the Dirac operator, described by ChRMT in the low end matches on to the spectrum at larger scales, in the *p*-regime [11]–[13].

Recent developments in both computational facilities and algorithms have allowed simulations of full lattice QCD near the chiral limit, but no study has until now reached deep inside the ϵ -regime except at rather strong coupling. Although results have often compared favorably to the ϵ -expansion of ChPT, there may still be large systematic errors due to the condition $M_{\pi}L \ll 1$ not being well fulfilled (see, *e.g.*, ref. [14]). One might therefore ask whether it is possible to have a new approach which smoothly connects the *p*expansion and ϵ -expansion and which remains valid even in the region $M_{\pi}L \sim 1$. Recently, steps have been taken in that direction by means of a so-called mixed expansion [15, 16] (see also ref. [17]), where one treats the very light flavors with the counting rules of the ϵ -expansion, while heavier flavors are counted according to the *p*-expansion. The results turned out to be mixtures of the properties of the ϵ and *p* regimes: zero-mode fluctuations from the light sector in addition to 1-loop corrections from the heavier sector that include chiral logs and some of the L_i 's. But refs. [15, 16] treated the light and heavy flavors separately and did not attack directly the regime where $M_{\pi}L \sim 1$. Actually, two regimes at play here: one is the first obvious threshold when $M_{\pi} \sim 1/L$, the other is when $M_{\pi} \sim 1/L^2$, the scale of the ϵ -regime. The question is what happens in-between.

In this paper, we suggest a new perturbative approach where all the terms in the p-expansion are kept but the zero mode is treated in exactly same way as in the ϵ -expansion.¹ The expansion thus considers the zero momentum mode on a different footing from the rest, partially resumming terms to all orders. Before reaching the ϵ -regime this means that an infinite series of terms that are normally considered in the perturbative expansion are included to all orders. The result is a slightly re-ordered perturbation theory expansion that is free from perturbative infrared singularities in the chiral limit. As an example, we compute here a formula for the chiral condensate which smoothly connects the results of the p-regime [18] and the ϵ -regime. We will argue that our formula is reliable even in the intermediate region where we go from $M_{\pi} \sim 1/L$ to $M_{\pi} \sim 1/L^2$.

Using the partial quenching technique based on replicas, we can treat a general theory with valence flavors and physical sea quark flavors of masses which are non-degenerate. This allows us to take the discontinuity on the imaginary axis of the valence quarks, and thus obtain the corresponding spectral density of the Dirac operator. It is also given by a smooth formula that connects known results in the ϵ -regime [9] and p-regime [11, 12].

The rest of our paper is organized as follows. In section 2, we describe in detail our new perturbative method in ChPT. The chiral condensate to next-leading order is calculated in section 3. Taking the discontinuity on the imaginary axis, we obtain the spectral density of the Dirac operator in section 4. We show in section 5 that our results provide a smooth connection between the ϵ and p regimes. In section 6 we present some numerical examples which are useful when comparing with lattice QCD simulations. Conclusions and an outlook are given in section 7.

2. A chiral expansion at finite volume

Let us consider N_f -flavor chiral perturbation theory in a finite volume $(V = L^3 T)$,

$$\mathcal{L} = \frac{F^2}{4} \operatorname{Tr}[\partial_{\mu} U(x)^{\dagger} \partial_{\mu} U(x)] - \frac{\Sigma}{2} \operatorname{Tr}[\mathcal{M}^{\dagger} e^{-i\theta/N_f} U(x) + U(x)^{\dagger} e^{i\theta/N_f} \mathcal{M}] + \cdots, \quad (2.1)$$

where $U(x) \in SU(N_f)$ and θ denotes the vacuum angle. Here, Σ is the chiral condensate and F denotes the pion decay constant both in the chiral limit. There are of course nextto-leading order terms, indicated here by ellipses, with additional low-energy constants denoted by L_i 's, H_i 's and beyond.

In the partially quenched case, we use the replica method where the calculations are done within an $(N_f + N_v + (N - N_v))$ -flavor theory followed by the replica limit $N \rightarrow 0$ [19, 20]. The ordinary physical N_f -theory result can clearly be viewed either as one

¹We understand that F. Niedermayer (unpublished) has considered an analogous scheme in the context of the O(n) sigma model.

where $N = N_v = 0$, or, alternatively, one where $m_v = m_f$ with m_f denoting one of the physical quark masses.

From now on we consider sectors of fixed topology ν , obtained by Fourier transforming in θ in the usual way. This extends our integration from $SU(N + N_f)$ to $U(N + N_f)$ in the zero-momentum sector.

For the mass matrix, we consider a general diagonal case,

$$\mathcal{M} = \operatorname{diag}(\underbrace{m_v, m_v, \dots}_{N}, \underbrace{m_1, m_2, \dots}_{N_f}),$$
(2.2)

where we have $N = N_v + (N - N_v)$ replicated flavors and N_f physical flavors. Here N_v is the number of, in this case, degenerate valence quarks. What we do below can straightforwardly be generalized to non-degenerate valence quarks by just adding copies of each.

We start by factorizing the fields into the zero-momentum mode U and non-zero modes $\xi(x)$,

$$U(x) = U \exp(i\sqrt{2\xi(x)}/F), \qquad (2.3)$$

and expand perturbatively in $\xi(x)$ just as in the ϵ -regime [1]. But here we give the same counting rules for the fields and other parameters as in the *p*-regime:

$$\partial_{\mu} \sim \mathcal{O}(p), \quad \xi(x) \sim \mathcal{O}(p), \quad \mathcal{M} \sim \mathcal{O}(p^2), \quad T, L \sim \mathcal{O}(1/p),$$
(2.4)

in units of the cut-off $4\pi F$. The aim is to see if we can tune quark masses so that we go from mass scales $\mathcal{M} \sim \mathcal{O}(1/L^2)$ through $\mathcal{M} \sim \mathcal{O}(1/L^4)$ to zero. Here we of course assume that the linear sizes of the volume, L and T, are much larger than the inverse QCD scale $\Lambda_{\rm QCD}$ so that the effective theory is valid.

The above parametrization eq. (2.3) leads to a well-known Jacobian in the functional integral measure [3]. Although it is easily taken into account, its contribution is $\mathcal{O}(p^6)$ and beyond the accuracy with which we do actual calculations in this paper.

We now expand the Lagrangian in $\xi(x)$ according to the *p*-counting eq. (2.4), and write down the terms relevant to one-loop order for the chiral condensate,

$$\mathcal{L} = -\frac{\Sigma}{2} \operatorname{Tr} \left[\mathcal{M}^{\dagger} U + U^{\dagger} \mathcal{M} \right] + \frac{1}{2} \operatorname{Tr} (\partial_{\mu} \xi)^{2} + \frac{1}{2} \sum_{i} M_{ii}^{2} [\xi^{2}]_{ii} + \frac{\Sigma}{2F^{2}} \operatorname{Tr} [\mathcal{M}^{\dagger} (U-1)\xi^{2} + \xi^{2} (U^{\dagger} - 1)\mathcal{M}] - L_{6} \left(\frac{2\Sigma}{F^{2}} \operatorname{Tr} [\mathcal{M}^{\dagger} U + U^{\dagger} \mathcal{M}] \right)^{2} - L_{7} \left(\frac{2\Sigma}{F^{2}} \operatorname{Tr} [\mathcal{M}^{\dagger} U - U^{\dagger} \mathcal{M}] \right)^{2} - \frac{L_{8}}{2} \left(\frac{2\Sigma}{F^{2}} \right)^{2} \operatorname{Tr} [(\mathcal{M}^{\dagger} U + U^{\dagger} \mathcal{M})^{2} + (\mathcal{M}^{\dagger} U - U^{\dagger} \mathcal{M})^{2}] - H_{2} \left(\frac{2\Sigma}{F^{2}} \right)^{2} \operatorname{Tr} [\mathcal{M}^{\dagger} \mathcal{M}] + \cdots, \qquad (2.5)$$

where $M_{ij}^2 = (m_i + m)\Sigma/F$ and L_i 's are the usual higher-order low-energy constants of ChPT. Here we have added and subtracted a conventional mass term of the *p*-regime. We will treat the mass term of the first line in eq. (2.5) as part of the exact Gaussian integration that leads to the conventional massive propagator of the *p*-regime, while the remaining terms are treated in a perturbative expansion. We return to this point below. The contact term H_2 has no direct physical significance, but it is needed as a counterterm for the one-loop correction to the condensate [1]. All linear terms in ξ are absent due to

$$\int d^4x \,\xi(x) = 0.$$
 (2.6)

In eq. (2.5) the first line contains terms that in the usual *p*-expansion are of order p^2 (the first, a trivial constant in the usual infinite-volume *p*-expansion) and p^4 (the remaining two). In the ϵ -expansion the first two terms on the same line are of order ϵ^4 , while the third is of order ϵ^6 . In the last four lines we have written out explicitly those terms that are of order p^4 in the usual infinite-volume *p*-expansion (but trivial constants there). In the ϵ -counting these terms are of order ϵ^8 . Other terms involving the L_i 's will be of order p^6 in that same counting. However, as with the measure term, these terms will not contribute to the chiral condensate that we will compute below.

The one single term we have not yet discussed is that of

$$\Delta \mathcal{L} = \frac{\Sigma}{2F^2} \operatorname{Tr}[\mathcal{M}^{\dagger}(U-1)\xi^2 + \xi^2(U^{\dagger}-1)\mathcal{M}] . \qquad (2.7)$$

In the usual p-expansion a term of this type first occurs at order p^5 (because there will be three powers of ξ), and in the ϵ -expansion it is of order ϵ^6 . Here we treat any matrix elements of $\mathcal{M}^{\dagger}(U-1)$ (and its complex conjugate $(U^{\dagger}-1)\mathcal{M}$) as of $\mathcal{O}(p^3)$ for all values of \mathcal{M} . By performing the exact group integration over U, we can check that the combination $\mathcal{M}^{\dagger}(U-1)$ gives NLO contributions ($\leq \mathcal{O}(p^3)$) to the results. We illustrate this in section 5. In appendix B we describe an alternative method which expresses the magnitude of the contribution from the term in eq. (2.7) directly in terms of masses and the volume V, thus giving a precise counting of this term in terms of $p \sim 1/L$. This alternative method gives identical results, but is in practice more cumbersome than the scheme presented here.

By taking $\mathcal{M}^{\dagger}(U-1) \sim \mathcal{O}(p^3)$, one can thus, to this order, rewrite the Lagrangian

$$\mathcal{L} = -\frac{\Sigma}{2} \operatorname{Tr} \left[\mathcal{M}^{\dagger} U + U^{\dagger} \mathcal{M} \right] + \frac{1}{2} \operatorname{Tr} (\partial_{\mu} \xi)^{2} + \frac{1}{2} \sum_{i} M_{ii}^{2} [\xi^{2}]_{ii} + \frac{\Sigma}{2F^{2}} \operatorname{Tr} [\mathcal{M}^{\dagger} (U-1)\xi^{2} + \xi^{2} (U^{\dagger} - 1)\mathcal{M}] - L_{6} \left(\frac{2\Sigma}{F^{2}} \operatorname{Tr} [\mathcal{M}^{\dagger} U + U^{\dagger} \mathcal{M}] \right)^{2} - \frac{2L_{8} + H_{2}}{4} \left(\frac{2\Sigma}{F^{2}} \right)^{2} \operatorname{Tr} [(\mathcal{M}^{\dagger} U + U^{\dagger} \mathcal{M})^{2}], \quad (2.8)$$

where the second line is treated as an NLO interaction term and the contribution from the L_7 -term has been dropped.

It should be stressed at this point that adding and subtracting an ordinary p-regime mass term and then expanding the term (2.7) perturbatively has the effect of a complete re-ordering and partial resummation of the perturbative series. This resummation comes from the fact that when the chiral limit is taken and M_{π}^2 is no longer of order p^2 , but smaller, we still keep the full massive propagator. The error in doing this, rather than expanding the propagator to the needed order in M_{π}^2 , is however always of yet higher order and part of the unavoidable uncertainty in any fixed-order perturbative calculation. We always keep the full massive propagator in the expressions and plots we present below.

The Feynman rule for the ξ -propagator is thus obtained as usual, except that the zero-momentum modes are not included:

$$\langle \xi_{ij}(x)\xi_{kl}(y)\rangle_{\xi} = \delta_{il}\delta_{jk}\bar{\Delta}(x-y,M_{ij}^2) - \delta_{ij}\delta_{kl}\bar{G}(x-y,M_{ii}^2,M_{kk}^2), \qquad (2.9)$$

and the second term comes from the constraint $\text{Tr}\xi = 0$. The propagators $\bar{\Delta}$ and \bar{G} are given by,²

$$\bar{\Delta}(x, M^2) = \frac{1}{V} \sum_{p \neq 0} \frac{e^{ipx}}{p^2 + M^2},$$
(2.10)

$$\bar{G}(x, M_{ii}^2, M_{jj}^2) = \frac{1}{V} \sum_{p \neq 0} \frac{e^{ipx}}{(p^2 + M_{ii}^2)(p^2 + M_{jj}^2) \left(\sum_{f}^{N_f} \frac{1}{p^2 + M_{ff}^2}\right)},$$
(2.11)

where the summation is taken over the non-zero 4-momentum

$$p = 2\pi (n_t/T, n_x/L, n_y/L, n_z/L), \qquad (2.12)$$

with integer n_{μ} .

3. The chiral condensate

The chiral condensate of a valence flavor is obtained in the conventional manner by adding a source to the mass matrix; $\mathcal{M} \to \mathcal{M} + \mathcal{J}$ and differentiating the partition function $\mathcal{Z}(\mathcal{M} + \mathcal{J})$ with respect to \mathcal{J} . To leading order in our expansion this gives

$$\langle \bar{q}_v q_v \rangle_{\nu}^{LO} \equiv \left. \frac{1}{V} \frac{\partial}{\partial \mathcal{J}_{vv}} \ln \mathcal{Z}(\mathcal{M} + \mathcal{J}) \right|_{\mathcal{J}=0} = \frac{\Sigma}{2} \left\langle U_{vv} + U_{vv}^{\dagger} \right\rangle_U, \qquad (3.1)$$

where the zero-mode integral $\left\langle U_{vv} + U_{vv}^{\dagger} \right\rangle_U$ is computed non-perturbatively with respect to the zero-mode partition function

$$\mathcal{Z}_{LO}^{\nu} = \int_{\mathcal{U}(N+N_f)} dU \, (\det U)^{\nu} \exp\left[\frac{\Sigma}{2} \operatorname{Tr}\left(\mathcal{M}^{\dagger}U + U^{\dagger}\mathcal{M}\right)\right].$$
(3.2)

The analytical formula is known for the most general partially quenched case with nondegenerate physical N_f -flavors [21]. Some details are summarized in appendix A. Here we simply *define*

$$\hat{\Sigma}_{\nu}^{\mathrm{PQ}}(\mu_{v}, \{\mu_{\mathrm{sea}}\}) \equiv \frac{1}{2} \left\langle U_{vv} + U_{vv}^{\dagger} \right\rangle_{U}, \qquad (3.3)$$

²We do not consider the fully quenched theory in this paper. We thus have $N_f \neq 0$ in all that follows.

where $\mu_v = m_v \Sigma V$ and the set of the dynamical flavors are denoted by $\{\mu_{\text{sea}}\} = \{\mu_1, \mu_2, \ldots\}$ with $\mu_i = m_i \Sigma V$.

At next-to-leading order, it is convenient to first calculate the 1-loop perturbative correction due to the non-zero modes. This can be done by simply evaluating

$$\left\langle 1 - \int d^4x \frac{\Sigma}{2F^2} \operatorname{Tr}[(\mathcal{M} + \mathcal{J})^{\dagger} (U - 1)\xi^2 + \xi^2 (U^{\dagger} - 1)(\mathcal{M} + \mathcal{J})] \right\rangle_{\xi},$$
(3.4)

where $\langle \cdots \rangle_{\xi}$ denotes the integral over ξ , and then re-exponentiating it. The effective Lagrangian (with a scalar source \mathcal{J}) then reads

$$\mathcal{L}_{\text{eff}}(\mathcal{J}) = -\frac{\Sigma}{2} \sum_{i} Z_{i} \left[(\mathcal{M} + \mathcal{J})^{\dagger} U + U^{\dagger} (\mathcal{M} + \mathcal{J}) \right]_{ii} + \frac{1}{2} \text{Tr} (\partial_{\mu} \xi)^{2} + \frac{\Sigma}{F^{2}} \text{Tr} [(\mathcal{M} + \mathcal{J})(\xi^{2} - \langle \xi^{2} \rangle_{\xi})], \qquad (3.5)$$

where

$$Z_{i} \equiv 1 - \frac{1}{F^{2}} \left[\sum_{j} \bar{\Delta}(0, M_{ij}^{2}) - \bar{G}(0, M_{ii}^{2}, M_{ii}^{2}) - 16L_{6} \sum_{j} M_{jj}^{2} - 4(2L_{8} + H_{2})M_{ii}^{2} \right].$$
(3.6)

Both of the 1-loop integrations $\overline{\Delta}(0, M^2)$ and $\overline{G}(0, M^2, M^2)$ are UV divergent and their divergences are absorbed into the bare parameters L_6 , L_8 and H_2 . With an appropriate regularization such as dimensional regularization (see ref. [4] for a discussion of this issue) $\overline{\Delta}(0, M^2)$ is given by

$$\bar{\Delta}(0, M^2) = \frac{M^2}{16\pi^2} (\ln M^2 + c_1) + \bar{g}_1(M^2), \qquad (3.7)$$

where c_1 represents the conventional logarithmic divergence which is independent of Mand the volume [4]. The function \bar{g}_1 represents the finite size effects,

$$\bar{g}_1(M^2) \equiv \frac{1}{(4\pi)^2} \int_0^\infty \sum_{a\neq 0} \frac{dr}{r^2} \exp\left(-rM^2 - \frac{1}{4r} \sum_{\mu} (a_{\mu})^2\right) - \frac{1}{M^2 V},$$
(3.8)

and the sum is taken over a 4-dimensional vector $a_{\mu} = n_{\mu}L_{\mu}$ (L_{μ} being the lattice size in the μ -th direction) with integer n_{μ} . It is particularly important to note that the massless limit $M^2 \to 0$ of \bar{g}_1 is finite and given by $\bar{g}_1(0) = -\beta_1/\sqrt{V}$ where β_1 is the so-called shape coefficient [4]. This term dominates the NLO correction in the ϵ -regime. A detailed numerical treatment of $\bar{\Delta}(0, M^2)$ and its derivative is discussed in appendix C.

Expanding $\overline{G}(0, M^2, M^2)$ in M^2 (see appendix D), we get

$$\bar{G}(0, M^2, M^2) = \frac{2}{N_f} \bar{\Delta}(0, M^2) - \frac{1}{N_f^2} \sum_j \bar{\Delta}(0, M_{jj}^2) + \cdots, \qquad (3.9)$$

where the sum \sum_{j} is taken over physical flavors only. Since the $\mathcal{O}(M^4)$ terms indicated by ellipses are UV finite, the divergence in Z_i , eq. (3.6), is in total,

$$Z_i \sim -\frac{1}{16\pi^2 F^2} \left[\sum_j \frac{M_{ii}^2 + M_{jj}^2}{2} - \frac{2}{N_f} M_{ii}^2 + \frac{1}{N_f^2} \sum_j M_{jj}^2 \right] c_1,$$
(3.10)

which can be absorbed into redefinitions of L_6 , L_8 and H_2 ,

$$L_{6} = \frac{1}{(16\pi)^{2}} \left(\frac{1}{2} + \frac{1}{N_{f}^{2}} \right) c_{1} + L_{6}^{r}, \quad L_{8} = \frac{1}{(16\pi)^{2}} \left(\frac{N_{f}}{2} - \frac{2}{N_{f}} \right) c_{1} + L_{8}^{r},$$
$$H_{2} = \frac{2}{(16\pi)^{2}} \left(\frac{N_{f}}{2} - \frac{2}{N_{f}} \right) c_{1} + H_{2}^{r}, \tag{3.11}$$

where the renormalized constants are denoted by L_6^r , L_8^r and H_2^r . This renormalization is identical to that of the infinite volume case [1], as it should be.

To this order, the chiral condensate at fixed topology can thus be written

$$\langle \bar{q}_v q_v \rangle_{\nu} = \Sigma \frac{\mu'_v}{\mu_v} \hat{\Sigma}_{\nu}^{\mathrm{PQ}}(\mu'_v, \{\mu'_{\mathrm{sea}}\}), \qquad (3.12)$$

where $\mu'_v = Z_v m_v \Sigma V$ and $\{\mu'_{\text{sea}}\} = \{Z_1 m_1 \Sigma V, Z_2 m_2 \Sigma V, \ldots\}$. Note that the arguments of the function now include the chiral logarithms as explicitly seen in Z_i (see eq. (3.6)).

The expression in eq. (3.12) looks simple and compact. But in order to see the valence mass dependence, it is more convenient to decompose Z_v into two finite pieces,

$$Z_{v} = Z_{v}^{0} + \delta Z_{v}(m_{v}), \qquad (3.13)$$

$$Z_v^0 \equiv 1 - \frac{1}{F^2} \left[\sum_j \bar{\Delta}(0, M_{jj}^2/2) - \bar{G}(0, 0, 0) - 16L_6 \sum_j M_{jj}^2 \right],$$
(3.14)

$$\delta Z_{v}(m_{v}) \equiv -\frac{1}{F^{2}} \left[\sum_{j} (\bar{\Delta}(0, M_{jv}^{2}) - \bar{\Delta}(0, M_{jj}^{2}/2)) - (\bar{G}(0, M_{vv}^{2}, M_{vv}^{2}) - \bar{G}(0, 0, 0)) - 4(2L_{8} + H_{2})M_{vv}^{2} \right], \quad (3.15)$$

where only $\delta Z_v(m_v)$ has a valence mass dependence, and it vanishes in the limit $m_v \to 0$. Note that $\bar{G}(0,0,0)$ is infra-red finite (see appendix D).

With the above decomposition, the condensate can be expressed as

$$\langle \bar{q}_v q_v \rangle_{\nu} = \Sigma \left[Z_v^0 \, \hat{\Sigma}_{\nu}^{\mathrm{PQ}} (Z_v^0 \mu_v, \{\mu'_{\mathrm{sea}}\}) + \delta Z_v(m_v) \left(\hat{\Sigma}_{\nu}^{\mathrm{PQ}} (\mu_v, \{\mu_{\mathrm{sea}}\}) + \mu_v \frac{\partial}{\partial \mu_v} \hat{\Sigma}_{\nu}^{\mathrm{PQ}} (\mu_v, \{\mu_{\mathrm{sea}}\}) \right) + \cdots \right]$$

$$= \Sigma \left[Z_v^0 \, \hat{\Sigma}_{\nu}^{\mathrm{PQ}} (Z_v^0 \mu_v, \{\mu'_{\mathrm{sea}}\}) + \delta Z_v(m_v) \right] + \mathcal{O}(p^4) \,, \qquad (3.16)$$

where $\mu_v = m_v \Sigma V$. In the second line we have used the fact that $\delta Z_v(m_v) \sim \mathcal{O}(M_{vv}^2)$ does not contribute until $\hat{\Sigma}_{\nu}^{PQ}(\mu_v, \{\mu'_{sea}\})$ becomes close to $1 + \mathcal{O}(p^2)$. The explicit form will be given in section 6.

It is now clear that the chiral condensate near the chiral limit is dominated by zero modes, and hence expressed through combinations of Bessel functions as in the ϵ -regime. The argument $Z_v^0 m_v \Sigma V$, however, includes the chiral logarithm of the sea quarks in Z_v^0 . As the valence mass increases, $\hat{\Sigma}_v^{PQ}(\mu_v, \{\mu_{sea}\})$ approaches unity and the ordinary valence

quark chiral logarithm appears in $\delta Z_v(m_v)$. For yet larger values of m_v ,³ the term proportional to $2L_8^r + H_2^r$ becomes important. The unphysical quantity H_2^r depends on the regularization scheme, and the condensate is then not unambiguously defined, as is well known [22]. In such a region, one has to eliminate the H_2^r dependence to obtain unambiguous physical observables. An example would be to consider a difference between two topological sectors. As we will see in the next section, the spectral density is also free from this ambiguity.

4. The spectral density of the Dirac operator

In the previous discussion, we assumed that all quark masses were real and positive. As is well-known [9], by considering the expressions for imaginary valence quark masses, one can calculate all spectral correlation functions and individual eigenvalues distributions of the Dirac operator of the N_f -flavor theory. In this case partial quenching is simply used to extract a physical observable in the full theory. One expresses the valence quark condensate as a spectral sum over the Dirac eigenvalues $i\lambda_k$'s (λ_k is real),

$$\langle \bar{q}_v q_v \rangle |_{m_v} = \frac{1}{V} \sum_k \left\langle \frac{1}{m_v + i\lambda_k} \right\rangle.$$
(4.1)

Since every non-zero eigenvalue comes paired with one of opposite sign, the condensate satisfies

$$\langle \bar{q}_v q_v \rangle |_{m_v^*} = (\langle \bar{q}_v q_v \rangle |_{m_v})^*, \quad \langle \bar{q}_v q_v \rangle |_{-m_v} = -\langle \bar{q}_v q_v \rangle |_{m_v}, \tag{4.2}$$

where * denotes complex conjugation.

Using the above, the spectral density at fixed topology ν is given by

$$\rho_{\nu}(\lambda) \equiv \frac{1}{V} \sum_{k} \langle \delta(\lambda + \lambda_{k}) \rangle_{\nu}
= -\frac{1}{2\pi V} \sum_{k} \lim_{\epsilon \to 0} \left\langle \frac{1}{i(\lambda + \lambda_{k}) - \epsilon} - \frac{1}{i(\lambda + \lambda_{k}) + \epsilon} \right\rangle_{\nu}
= \lim_{\epsilon \to 0} \frac{1}{2\pi} (\langle \bar{q}_{v} q_{v} \rangle_{\nu}|_{m_{v} = i\lambda - \epsilon} - \langle \bar{q}_{v} q_{v} \rangle_{\nu}|_{m_{v} = i\lambda + \epsilon})
= \frac{\Sigma}{\pi} \left[Z_{v}^{0} \operatorname{Re} \hat{\Sigma}_{\nu}^{\mathrm{PQ}}(i\lambda \Sigma V Z_{v}^{0}, \{\mu_{\mathrm{sea}}^{\prime}\}) + \operatorname{Re}(\delta Z_{v}(i\lambda)) \right], \quad (4.3)$$

where we have neglected the $\delta(\lambda)$ term which represents the exactly zero eigenvalues due to the non-trivial topological charge ν . Similar expressions exist for all higher spectral correlation functions.

For the calculation of $\operatorname{Re}(\delta Z_v(i\lambda))$, we need the discontinuities of various functions. For the log-terms, for example, one obtains

$$\operatorname{Re}\ln(m + \sqrt{m_v^2})|_{m_v = i\lambda} = \frac{1}{2}\ln(m^2 + \lambda^2), \qquad (4.4)$$

$$\operatorname{Im}\ln(m + \sqrt{m_v^2})|_{m_v = i\lambda} = \arctan\frac{\lambda}{m},\tag{4.5}$$

³Because $m_v = \mu_v / (\Sigma L^4)$, such a term first appears at NNLO in the pure ϵ -expansion.

where m denotes a real and positive mass, for which the limit $m \to 0$ is well-defined. Some of the other functions occurring in eq. (4.3) need to be treated numerically, such as those in \bar{g}_1 . We collect some representations useful for numerical purposes in appendix C. Note that the term proportional to $2L_8 + H_2$ has disappeared upon taking the discontinuity across the imaginary valence quark axis.⁴

Next, using the properties of Bessel functions, one sees that the first term of eq. (4.3) reproduces the known form of the leading contribution to the microscopic spectral density in the ϵ -regime,

$$\operatorname{Re}\hat{\Sigma}_{\nu}^{\mathrm{PQ}}(i\zeta, \{\mu_{\mathrm{sea}}\}) = \pi\hat{\rho}_{\nu}^{\mathrm{mic}}(\zeta, \{\mu_{\mathrm{sea}}\}), \qquad (4.6)$$

where $\hat{\rho}_{\nu}^{\text{mic}}(\zeta, \{\mu_{\text{sea}}\})$ is given by [13]

$$\hat{\rho}_{\nu}^{\rm mic}(\zeta, \{\mu_{\rm sea}\}) \equiv (-1)^{2\nu+2[N_f/2]+1} \frac{|\zeta|}{2\prod_f^{N_f}(\zeta^2 + \mu_f^2)} \frac{\det \tilde{\mathcal{B}}}{\det \mathcal{A}}.$$
(4.7)

Here the $N_f \times N_f$ matrix \mathcal{A} and the $(N_f + 2) \times (N_f + 2)$ matrix $\tilde{\mathcal{B}}$ are defined by

$$\mathcal{A}_{ij} = \mu_i^{j-1} I_{\nu+j-1}(\mu_i) \tag{4.8}$$

$$\mathcal{B}_{1j} = \zeta^{j-2} J_{\nu+j-2}(\zeta), \qquad \qquad \mathcal{B}_{2j} = \zeta^{j-1} J_{\nu+j-1}(\zeta), \\ \tilde{\mathcal{B}}_{ij} = (-\mu_{i-2})^{j-1} I_{\nu+j-1}(\mu_{i-2}) \qquad \qquad (i \neq 1, 2).$$
(4.9)

The general formula for the spectral density can thus conveniently be written in a representation suitable for small eigenvalues that go into the "bulk" region,

$$\rho_{\nu}(\lambda) = \frac{\Sigma}{\pi} \left[\pi Z_{v}^{0} \, \hat{\rho}_{\nu}^{\mathrm{mic}}(Z_{v}^{0} \lambda \Sigma V, \{\mu_{\mathrm{sea}}^{\prime}\}) + \mathrm{Re}\left(\delta Z_{v}(i\lambda)\right) \right] \,. \tag{4.10}$$

5. From the *p*-regime to the ϵ -regime

In this section we explain how our formulae are consistent with known results in both ϵ and p regimes. We next consider the validity of our expressions in the intermediate region.

5.1 Checks in the *p*-regime and limit to the ϵ -regime

We first check that the expression derived in the previous section reproduces known results in the conventional perturbative *p*-expansion. The exact zero-mode integral above is expressed by complicated combinations of Bessel functions. But for large $m_i \Sigma V$, these Bessel functions can be expanded in $1/m_i \Sigma V$ (see, *e.g.*, ref. [23] for details),

$$\hat{\Sigma}_{\nu}^{\mathrm{PQ}}(\mu_{v}, \{\mu_{\mathrm{sea}}\}) = 1 - \sum_{j} \frac{1}{\mu_{v} + \mu_{j}} + \frac{4\nu^{2} - 1}{8\mu_{v}^{2}} + \mathcal{O}(p^{6}),$$
(5.1)

⁴This result may seem to contradict the fact that the condensate, conversely, should follow from a spectral sum involving $\rho(\lambda)$ as in eq. (4.1). The problem is that the spectral sum is UV divergent. It is this divergence that gives rise to an ambiguity such as indicated by the $2L_8 + H_2$ -term.

which, after summing over topology, gives

$$\hat{\Sigma}^{PQ}(\mu_v, \{\mu_{sea}\}) = 1 - \sum_j \frac{1}{\mu_v + \mu_j} + \frac{\langle \nu^2 \rangle}{2\mu_v^2} + \mathcal{O}(p^4)$$
$$= 1 - \sum_j \frac{1}{\mu_v + \mu_j} + \frac{1}{2\mu_v^2(\sum_f 1/\mu_f)} + \mathcal{O}(p^4), \quad (5.2)$$

where we have used

$$\langle \nu^2 \rangle = \frac{1}{\sum_f 1/\mu_f} + \cdots .$$
 (5.3)

in the chiral limit. Substituting eq. (5.2) into eq. (3.12), we reproduce the perturbative *p*-regime result,

$$\langle \bar{q}_v q_v \rangle = \Sigma \left[1 - \frac{1}{F^2} \left(\sum_j \Delta(0, M_{vj}^2) - G(0, M_{vv}^2, M_{vv}^2) \right) + \frac{1}{F^2} \left(16L_6 \sum_i M_{ii}^2 + 4(2L_8 + H_2) M_{vv}^2 \right) \right].$$
(5.4)

As is known from the matching between ϵ and p regimes, the zero-mode fluctuations which give rise to the second and third terms in eq. (5.2) are absorbed in the momentum sum in $\bar{\Delta}$ and \bar{G} so that we recover the usual propagators

$$\Delta(x, M^2) = \frac{1}{V} \sum_{p} \frac{e^{ipx}}{p^2 + M^2},$$
(5.5)

$$G(x, M_{ii}^2, M_{jj}^2) = \frac{1}{V} \sum_{p} \frac{e^{ipx}}{(p^2 + M_{ii}^2)(p^2 + M_{jj}^2) \left(\sum_{f}^{N_f} \frac{1}{p^2 + M_{ff}^2}\right)},$$
(5.6)

of the ordinary p-expansion.

The above expression agrees with known results that can be found in, *e.g.*, the work of Osborn et al. [12]. They derived a formula for the partially quenched case with N_f degenerate flavors of mass M_{sea}^2 in which case one can use

$$G(x, M_{vv}^2, M_{vv}^2) = \frac{1}{N_f} \left[\Delta(x, M_{vv}^2) + (M_{vv}^2 - M_{\text{sea}}^2) \partial_{M_{vv}^2} \Delta(x, M_{vv}^2) \right].$$
(5.7)

One can also check the ϵ -regime results at fixed topology ν are precisely reproduced just by reducing the quark masses in the formula eq. (3.16). One notes that in that limit,

$$Z_v^0 \to 1 + \frac{1}{F^2} \left(\frac{N_f^2 - 1}{N_f}\right) \frac{\beta_1}{\sqrt{V}}, \quad \delta Z_v(m_v) \to 0.$$
 (5.8)

The spectral density of the Dirac operator can easily be compared to known results in different limits as well. First of all, the Banks-Casher relation is trivially reproduced when we take the limit $V \to \infty$ before $m_i \to 0$,

$$\lim_{m_i \to 0} \lim_{V \to \infty} \rho_{\nu}(\lambda = 0) = \frac{\Sigma}{\pi},$$
(5.9)

after having used $\hat{\rho}_{\nu}^{\text{mic}}(\infty, \{\mu_{\text{sea}}\}) = 1/\pi, Z_v^0|_{V \to \infty, m_i \to 0} \to 1$, and $\delta Z_v(0) = 0$. In the same limit above, but for finite λ , one obtains

$$\lim_{m_i \to 0} \lim_{V \to \infty} \rho_{\nu}(\lambda) = \frac{\Sigma}{\pi} \left[1 + \operatorname{Re} \delta Z_{\nu}(i\lambda) |_{V \to \infty, m_i \to 0} \right]$$
$$= \frac{\Sigma}{\pi} \left[1 + \left(\frac{N_f^2 - 4}{N_f} \right) \frac{\Sigma}{32\pi F^4} |\lambda| \right], \tag{5.10}$$

which is the result of Smilga and Stern [11]. If one keeps the sea quark masses $m_i = m$ finite (and degenerate), one gets

$$\lim_{V \to \infty} \rho_{\nu}(\lambda) = \frac{\Sigma}{\pi} \left[Z_0^v |_{V \to \infty} + \operatorname{Re}\delta Z_v(i\lambda)|_{V \to \infty} \right]$$
$$= \frac{\Sigma}{\pi} \left[1 + \frac{\Sigma}{32\pi^2 N_f F^4} \left(2N_f^2 |\lambda| \arctan \frac{|\lambda|}{m} - 4\pi |\lambda| - N_f^2 m \ln \frac{\Sigma^2}{F^4} \frac{m^2 + \lambda^2}{\mu_{\mathrm{sub}}^4} - 4m \ln \frac{\Sigma}{F^2} \frac{|\lambda|}{\mu_{\mathrm{sub}}^2} \right) + \frac{32N_f L_6^r(\mu_{\mathrm{sub}}) \Sigma m}{F^4} \right], (5.11)$$

where μ_{sub} denotes the subtraction scale. This is consistent with the formula by Osborn et al. [12]. In the case of finite V and very small m_i and λ , the general result in the ϵ -regime [13],

$$\rho_{\nu}(\lambda) = \Sigma \hat{\rho}_{\nu}^{\text{mic}}(\lambda \Sigma V, \mu_{\text{sea}}), \qquad (5.12)$$

is easily recovered upon noting that to leading order we have $Z_v^0 = 1$.

5.2 Intermediate regime

As seen in the above discussion, our formulae for the condensate and the spectral density smoothly connect the results in the ϵ -regime with those of the *p*-regime. But we also need to know the precision in the intermediate region. The ϵ -regime assumes $M_{vv}L \ll 1$ while the *p*-regime counting requires $M_{vv}L \gg 1$. Our re-ordered perturbative expansion has removed this constraint. Instead, we make use of a non-trivial prescription for the fourth term in eq. (2.5) where we take $\mathcal{M}^{\dagger}(U-1)$ to be always small, specifically of $\mathcal{O}(p^3)$ or smaller.

One should note that non-zero mode's contributions are free from infra-red divergences by construction. This is also seen explicitly in the finite chiral limit of the finite-volume function $\bar{g}(M^2)$. For the non-zero modes, there is no need to distinguish the ϵ -regime from the *p*-regime. The smaller the quark masses, the better convergence of the nonzero mode expansion.

Therefore, the accuracy of our calculation needs to be assessed by considering the zeromode integrals. To show the general validity of the method, we need to confirm by explicit evaluation of the group integrals that the operator $\mathcal{M}^{\dagger}(U-1)$ consistently can be taken to be of $\mathcal{O}(p^3)$ or smaller. This in any combination of matrix elements, power and for an arbitrary choice of the mass matrix, including such as is needed for partial quenching.

However, for the calculation of the chiral condensate in this paper, we only need to check in eq. (3.1) that the U integral keeps the second term of NLO. Since $\langle \xi_{ij}^2 \rangle = \delta_{ij} \langle \xi_{ii}^2 \rangle$, it is in fact enough to confirm that $[\mathcal{M}^{\dagger}(U-1) + h.c.]_{ii} \sim \mathcal{O}(p^3)$ or

$$m_i \left(\frac{1}{2} \langle U_{ii} + U_{ii}^{\dagger} \rangle_U - 1\right) \sim \mathcal{O}(p^3), \tag{5.13}$$

for any *i*, which can be done directly by means of the exact group integration eq. (3.3). Without using the rather complicated exact expression, its asymptotic behavior is known [23] for $m_i \Sigma V \ll 1$ and $m_i \Sigma V \gg 1$, and this leads to

$$m_i \left(\frac{1}{2} \langle U_{ii} + U_{ii}^{\dagger} \rangle_U - 1\right) \to \begin{cases} \frac{\nu}{\Sigma V} & (m_i \Sigma V \to 0) \\ -\left(N_f - \frac{n_i}{2}\right) \frac{1}{\Sigma V} & (m_i \Sigma V \to \infty) \end{cases},$$
(5.14)

with the other masses m_j 's $(j \neq i)$ fixed, where n_i denotes the degeneracy of the mass m_i (Note that $n_i = 0$ in the partially quenched case). Since this function is everywhere regular for finite $m_i \Sigma V$, one expects that the two limiting cases above are smoothly connected and the function thus always kept small, here of $\mathcal{O}(1/V) \sim \mathcal{O}(p^4)$.⁵

In figure 1, we plot the function $m_i \Sigma \left(\langle U_{ii} + U_{ii}^{\dagger} \rangle_U / 2 - 1 \right)$ for various cases in a (2+1)flavor theory. Every curve shows a monotonous function connecting the two limits, thus
confirming that the $\mathcal{M}(U-1)\xi^2$ contribution to the condensate is always of order 1/V. We
provide an explicit analytical expression in an analogous U(1) toy model in appendix B.

6. A few examples

In this section, we present two explicit numerical examples. One is an $N_f = 2$ degenerate two-flavor theory and the other is an $N_f = 2 + 1$ theory including a strange quark whose mass is different from up and down quark masses. For the low-energy constants in both cases, we take the following phenomenologically reasonable values: $\Sigma^{1/3} = 250 \text{ MeV}, F =$ $90 \text{ MeV}, L_6^r(\mu_{\text{sub}} = 0.77 \text{ GeV}) = 0.05 \times 10^{-3} \text{ and } L_8^r(\mu_{\text{sub}} = 0.77 \text{ GeV}) = 0.5 \times 10^{-3} \text{ where}$ μ_{sub} denotes the subtraction scale.

6.1 degenerate $N_f = 2$

Let us first consider the two-flavor theory with degenerate up and down quark masses $m_u = m_d = m$. The factor $Z_v = Z_v^0 + \delta Z_v(m_v)$ is then explicitly given by

$$Z_{v}^{0} = 1 - \frac{1}{F^{2}} \left[\frac{M_{\pi}^{2}}{16\pi^{2}} \ln \frac{M_{\pi}^{2}}{2\mu_{\rm sub}^{2}} + 2\bar{g}_{1} \left(M_{\pi}^{2}/2 \right) + \frac{1}{2} \left\{ \frac{\beta_{1}}{\sqrt{V}} - M_{\pi}^{2} \left(\frac{1}{16\pi^{2}} \ln V^{1/2} \mu_{\rm sub}^{2} + \beta_{2} \right) \right\} - 32L_{6}^{r}(\mu_{\rm sub}) M_{\pi}^{2} \right], \quad (6.1)$$

⁵We note that $\mathcal{M}(U-1)$ contributes not as $\mathcal{O}(p^3)$ but even further suppressed, of $\mathcal{O}(p^4)$. This is due to the fact that we are here considering a one-point function.



Figure 1: The function $m_i \Sigma V \left(\langle U_{ii} + U_{ii}^{\dagger} \rangle_U / 2 - 1 \right)$ is plotted in various cases in 2+1 flavor theory: A. partially quenched theory $(m_i = m_v)$ with $m_{u,d}\Sigma V = 5, m_s\Sigma V = 40$ at $\nu = 0$ $(m_{u,d,s}$ denotes the quark mass of u, d, s flavors respectively.), B. The same as A but at $\nu = 2$, C. unquenched theory with $m_i = m_{u,d}$ at $\nu = 0$ where $m_s\Sigma V = 40$ is fixed. D. unquenched theory with $m_i = m_s$ at $\nu = 3$ where $m_{u,d}\Sigma V = 5$ is fixed. Every curve is kept at $\mathcal{O}(1)$ at any value of m_i , which confirms $\mathcal{M}(U-1)$ always can be considered as NLO to the calculation of the chiral condensate.

and

$$\delta Z_{v}(m_{v}) = -\frac{1}{F^{2}} \left[\frac{M_{\pi}^{2}}{16\pi^{2}} \left(1 + \frac{m_{v}}{m} \right) \ln \left(1 + \frac{m_{v}}{m} \right) + \frac{M_{\pi}^{2}}{16\pi^{2}} \frac{m_{v}}{m} \ln \frac{M_{\pi}^{2}}{2\mu_{sub}^{2}} \right. \\ \left. + 2\bar{g}_{1} \left(\frac{M_{\pi}^{2}}{2} \left(1 + \frac{m_{v}}{m} \right) \right) - 2\bar{g}_{1} \left(\frac{M_{\pi}^{2}}{2} \right) - \frac{1}{2} \left\{ \bar{g}_{1} \left(M_{\pi}^{2} \frac{m_{v}}{m} \right) + \frac{\beta_{1}}{\sqrt{V}} \right. \\ \left. - M_{\pi}^{2} \left(\frac{1}{16\pi^{2}} (\ln M_{\pi}^{2} \frac{m_{v}}{m} V^{1/2} + 1) - \bar{g}_{2} \left(M_{\pi}^{2} \frac{m_{v}}{m} \right) + \beta_{2} \right) \right. \\ \left. + M_{\pi}^{2} \frac{m_{v}}{m} \left(\frac{1}{16\pi^{2}} - \bar{g}_{2} \left(M_{\pi}^{2} \frac{m_{v}}{m} \right) + \frac{1}{8\pi^{2}} \ln \left(\frac{M_{\pi}^{2} m_{v}}{\mu_{sub}^{2} m} \right) \right) \right\} \\ \left. - 4 (2L_{8}^{r}(\mu_{sub}) + H_{2}^{r}(\mu_{sub})) M_{\pi}^{2} \frac{m_{v}}{m} \right],$$

$$(6.2)$$

where $M_{\pi}^2 = (m_u + m_d)\Sigma/F^2 = 2m\Sigma/F^2$. For the numerical implementation of \bar{g}_1 and \bar{g}_2 , see appendix C. Note that $\delta Z_v(m_v = 0) = 0$.

For the spectral density, we also need

$$\operatorname{Re}\delta Z_{v}(i\lambda) = -\frac{1}{F^{2}} \left[\frac{M_{\pi}^{2}}{16\pi^{2}} \left(\frac{1}{2} \ln \left(1 + \frac{\lambda^{2}}{m^{2}} \right) - \frac{\lambda}{m} \arctan \frac{\lambda}{m} \right) \right. \\ \left. + 2\operatorname{Re}\bar{g}_{1} \left(\frac{M_{\pi}^{2}}{2} \left(1 + \frac{i\lambda}{m} \right) \right) - 2\bar{g}_{1} \left(\frac{M_{\pi}^{2}}{2} \right) - \frac{1}{2} \left\{ \operatorname{Re}\bar{g}_{1} \left(M_{\pi}^{2} \frac{i\lambda}{m} \right) + \frac{\beta_{1}}{\sqrt{V}} \right\}$$

$$-M_{\pi}^{2} \left(\frac{1}{16\pi^{2}} (\ln M_{\pi}^{2} \frac{\lambda}{m} V^{1/2} + 1) - \operatorname{Re}\bar{g}_{2} \left(M_{\pi}^{2} \frac{i\lambda}{m} \right) + \beta_{2} \right)$$
$$+M_{\pi}^{2} \frac{\lambda}{m} \left(\operatorname{Im}\bar{g}_{2} \left(M_{\pi}^{2} \frac{i\lambda}{m} \right) - \frac{1}{16\pi} \right) \right\} \right].$$
(6.3)

As discussed above, the H_2 (and μ_{sub}) dependence has disappeared.

The non-perturbative expressions for the zero-mode integrals are given by [21]

$$\hat{\Sigma}_{\nu}^{\mathrm{PQ}}(\mu_{v},\mu) = -\frac{1}{(\mu^{2}-\mu_{v}^{2})^{2}} \\
+ \det \begin{pmatrix} \partial_{\mu_{v}}K_{\nu}(\mu_{v}) & I_{\nu}(\mu_{v}) & I_{\nu}(\mu) & \mu^{-1}I_{\nu-1}(\mu) \\ -\partial_{\mu_{v}}(\mu_{v}K_{\nu+1}(\mu_{v})) & \mu_{v}I_{\nu+1}(\mu_{v}) & \mu I_{\nu+1}(\mu) & I_{\nu}(\mu) \\ \partial_{\mu_{v}}(\mu_{v}^{2}K_{\nu+2}(\mu_{v})) & \mu_{v}^{2}I_{\nu+2}(\mu_{v}) & \mu^{2}I_{\nu+2}(\mu) & \mu I_{\nu+1}(\mu) \\ -\partial_{\mu_{v}}(\mu_{v}^{3}K_{\nu+3}(\mu_{v})) & \mu_{v}^{3}I_{\nu+3}(\mu_{v}) & \mu^{3}I_{\nu+3}(\mu) & \mu^{2}I_{\nu+2}(\mu) \end{pmatrix} \\
\times \frac{\det \begin{pmatrix} I_{\nu}(\mu) & \mu^{-1}I_{\nu-1}(\mu) \\ \mu I_{\nu+1}(\mu) & I_{\nu}(\mu) \end{pmatrix}}{\det \begin{pmatrix} I_{\nu}(\mu) & \mu^{-1}I_{\nu-1}(\mu) \\ \mu I_{\nu+1}(\mu) & I_{\nu}(\mu) \end{pmatrix}}, (6.4)$$

and

$$\hat{\rho}_{\nu}^{\mathrm{mic}}(\zeta,\mu) = (-1)^{2\nu+1} \frac{|\zeta|}{2(\mu^{2}+\zeta^{2})^{2}} \\
\det \begin{pmatrix} \zeta^{-1}J_{\nu-1}(\zeta) & J_{\nu}(\zeta) & I_{\nu}(\mu) & \mu^{-1}I_{\nu-1}(\mu) \\ J_{\nu}(\zeta) & \zeta J_{\nu+1}(\zeta) & -\mu I_{\nu+1}(\mu) & -I_{\nu}(\mu) \\ \zeta J_{\nu+1}(\zeta) & \zeta^{2}J_{\nu+2}(\zeta) & \mu^{2}I_{\nu+2}(\mu) & \mu I_{\nu+1}(\mu) \\ \zeta^{2}J_{\nu+2}(\zeta) & \zeta^{3}J_{\nu+3}(\zeta) - \mu^{3}I_{\nu+3}(\mu) - \mu^{2}I_{\nu+2}(\mu) \end{pmatrix} \\
\times \frac{\det \begin{pmatrix} I_{\nu}(\mu) & \mu^{-1}I_{\nu-1}(\mu) \\ \mu I_{\nu+1}(\mu) & I_{\nu}(\mu) \end{pmatrix}}{(6.5)}, \quad (6.5)$$

where $\mu_v = m_v \Sigma V$, $\mu = m \Sigma V$ and $\zeta = \lambda \Sigma V$.

Substituting the explicit expressions above into eq. (3.16) and (4.10), it is straightforward to compute numerically the chiral condensate and the spectral density of the Dirac operator. Using the numerical values listed in the beginning of this section, we plot the chiral condensate and the spectral density in figure 2 for the case of $m_u = m_d = 10 \text{ MeV}$, $L = T/2 = 2 \text{ fm}, \nu = 0$ and here taking just as an example $H_2^r(0.77 \text{GeV}) = 0.1 \times 10^{-3}$. One sees that the resulting thick line smoothly connects the one in the ϵ -regime (solid) with the one in the *p*-regime (dotted).⁶ It is clear that the effect of one-loop corrections to the spectral density of the Dirac operator in the *p*-expansion is relatively small when $N_f = 2$, in agreement with the prediction eq. (5.10) of Smilga and Stern [11].

It is useful to see what happens when we vary some parameters. In the larger volume (L = T/2 = 3 fm) shown in figure 3 the agreement between the three different expansions becomes visibly better around $ML \sim 2$ -3. The sea quark mass dependence is shown in

⁶Because we do not have *p*-regime predictions available at fixed topological charge ν , we always compare with *p*-regime expressions where topological sectors have been summed over. Of course, *p*-regime predictions at fixed topology will differ slightly from these, but the difference becomes insignificant at large volumes.



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Figure 2: The chiral condensate (top) and Dirac spectral density (bottom) for the case with $m_u = m_d = 10 \text{ MeV}, \ L = T/2 = 2 \text{ fm}$. The result of this paper is given by the thick line which smoothly connects the one in the ϵ -regime (solid) with the on of *p*-regime (dotted). Parameters have been chosen as $\Sigma^{1/3} = 250 \text{ MeV}, \ F = 90 \text{ MeV}, \ L_6^r(\mu_{\text{sub}} = 0.77 \text{GeV}) = 0.05 \times 10^{-3}, \ L_8^r(\mu_{\text{sub}} = 0.77 \text{GeV}) = 0.5 \times 10^{-3} \text{ and } H_2^r(\mu_{\text{sub}} = 0.77 \text{GeV}) = 0.1 \times 10^{-3}.$



Figure 3: The same plots as in figure 2, the condensate (left) and the spectral density (right) but with the larger volume size L = T/2 = 3 fm. The convergence of three expansions around $M_{vv}L \sim 2$ -3 or $\lambda \Sigma V \sim 10$ becomes better.



Figure 4: The condensate (left) and the spectral density (right) at fixed topology $\nu = 0$ for different sea quark masses at 2 MeV (solid), 10 MeV (dotted), 30 MeV (small dotted) are given. We again set L = T/2 = 2fm. The black filled circle in the left panel shows the physical points where $m_v = m_u = m_d$.



Figure 5: The topology ν dependence of the condensate (left) and the spectral density (right) at a fixed value of $m_u = 10$ MeV and L = T/2 = 2fm and $H_2^r(0.77 \text{GeV}) = 0.1 \times 10^{-3}$. The topology dependence becomes negligible around $M_{vv}L = 3$ -4.



Figure 6: The (full theory) condensate (left) where $m_v = m_u = m_d$ and the spectral density (right) at fixed $m_u = m_d = 10$ MeV, are given at $\theta = 0$. Due to the ambiguity of H_2^r , the condensate is not a well-defined quantity when M_{π} or $M_{vv} \neq 0$, while the spectral density is free from this ambiguity.

figure 4 where we show the plots for different sea quark masses at 2 MeV (solid), 10 MeV (dotted), and 30 MeV (small dotted). The black filled circle in the left part shows the physical points where $m_v = m_u = m_d$. In figure 5 the ν -dependence is presented at a fixed value of $m_u = 10$ MeV and L = T/2 = 2fm. The topology dependence disappears around $M_{vv}L = 3$ -4. The condensate of the physical theory with $m_v = m_u = m_d$ is plotted on the left part of figure 6 after summing of topology (See appendix A for the details). Of course, the condensate in the massive case is inherently ambiguous due to the presence of the coupling H_2 . On the other hand, the spectral density is free from this ambiguity. On the right part of figure 6 we plot the density after summing over topology at fixed $m_u = m_d = 10$ MeV. As has been observed before [24], the striking oscillations that are seen at sectors of fixed topological charge become smeared out upon summing over topology. In the massless limit the oscillations will reappear and the density approaches that of the $\nu = 0$ sector.

6.2 $N_f = 2 + 1$

Next, we consider the $N_f = 2 + 1$ theory where the strange quark mass is different from the up and down quark masses. Then $\bar{G}(x, M^2, M^2)$ becomes much more complicated, and we refer to the explicit expressions given in eqs. (D.15) and (D.16).

One obtains

$$Z_{v}^{0} = 1 - \frac{1}{F^{2}} \left[\frac{M_{ud}^{2}}{16\pi^{2}} \ln \frac{M_{ud}^{2}}{2\mu_{sub}^{2}} + 2\bar{g}_{1} \left(M_{ud}^{2}/2 \right) + \frac{M_{ss}^{2}}{32\pi^{2}} \ln \frac{M_{ss}^{2}}{2\mu_{sub}^{2}} + \bar{g}_{1} \left(M_{ss}^{2}/2 \right) \right. \\ \left. - \frac{1}{3} \left\{ -\frac{2(M_{ud}^{2} - M_{ss}^{2})^{2}}{(M_{ud}^{2} + 2M_{ss}^{2})^{2}} \left(\frac{M_{ud}^{2} + 2M_{ss}^{2}}{3 \times 16\pi^{2}} \ln \frac{M_{ud}^{2} + 2M_{ss}^{2}}{3\mu_{sub}^{2}} + \bar{g}_{1} \left(\frac{M_{ud}^{2} + 2M_{ss}^{2}}{3} \right) \right) \right. \\ \left. + \left(1 + \frac{2(M_{ud}^{2} - M_{ss}^{2})^{2}}{(M_{ud}^{2} + 2M_{ss}^{2})^{2}} \right) \left(-\frac{\beta_{1}}{\sqrt{V}} \right) - \frac{3M_{ud}^{2}M_{ss}^{2}}{M_{ud}^{2} + 2M_{ss}^{2}} \left(-\frac{1}{16\pi^{2}} \ln V^{1/2} \mu_{sub}^{2} - \beta_{2} \right) \right\} \\ \left. - 16L_{6}^{r}(\mu_{sub})(2M_{ud}^{2} + M_{ss}^{2}) \right], \tag{6.6}$$

and

$$\begin{split} \delta Z_{v}(m_{v}) &= -\frac{1}{F^{2}} \left[\frac{M_{ud}^{2}}{16\pi^{2}} \left(1 + \frac{m_{v}}{m_{u}} \right) \ln \left(1 + \frac{m_{v}}{m_{u}} \right) + \frac{M_{ud}^{2}}{16\pi^{2}} \frac{m_{v}}{m_{u}} \ln \frac{M_{ud}^{2}}{2\mu_{sub}^{2}} \right. \\ &+ 2\bar{g}_{1} \left(\frac{M_{ud}^{2}}{2} \left(1 + \frac{m_{v}}{m_{u}} \right) \right) - 2\bar{g}_{1} \left(\frac{M_{ud}^{2}}{2} \right) + \frac{M_{ss}^{2}}{32\pi^{2}} \left(1 + \frac{m_{v}}{m_{s}} \right) \ln \left(1 + \frac{m_{v}}{m_{s}} \right) \\ &+ \frac{M_{ss}^{2}}{32\pi^{2}} \frac{m_{v}}{m_{s}} \ln \frac{M_{ss}^{2}}{2\mu_{sub}^{2}} + \bar{g}_{1} \left(\frac{M_{ss}^{2}}{2} \left(1 + \frac{m_{v}}{m_{s}} \right) \right) - \bar{g}_{1} \left(\frac{M_{ss}^{2}}{2} \right) \\ &- \frac{1}{3} \left\{ -\frac{2(M_{ud}^{2} - M_{ss}^{2})^{2}}{(3M_{vv}^{2} - M_{ud}^{2} - 2M_{ss}^{2})^{2}} \left(\frac{M_{ud}^{2} + 2M_{ss}^{2}}{3 \times 16\pi^{2}} \ln \frac{M_{ud}^{2} + 2M_{ss}^{2}}{3\mu_{sub}^{2}} + \bar{g}_{1} \left(\frac{M_{ud}^{2} + 2M_{ss}^{2}}{3} \right) \right) \\ &+ \left(1 + \frac{2(M_{ud}^{2} - M_{ss}^{2})^{2}}{(3M_{vv}^{2} - M_{ud}^{2} - 2M_{ss}^{2})^{2}} \right) \left(\frac{M_{vv}^{2}}{16\pi^{2}} \ln \frac{M_{vv}^{2}}{\mu_{sub}^{2}} + \bar{g}_{1}(M_{vv}^{2}) \right) \\ &+ \frac{3(M_{vv}^{2} - M_{ud}^{2})(M_{vv}^{2} - M_{ss}^{2})^{2}}{3M_{vv}^{2} - M_{ud}^{2} - 2M_{ss}^{2}} \right) \left(\frac{1}{16\pi^{2}} \left(\ln \frac{M_{vv}^{2}}{\mu_{sub}^{2}} + \bar{g}_{1} \left(\frac{M_{ud}^{2} + 2M_{ss}^{2}}{3} \right) \right) \\ &+ \frac{2(M_{ud}^{2} - M_{ss}^{2})^{2}}{(M_{ud}^{2} + 2M_{ss}^{2})^{2}} \left(\frac{M_{ud}^{2} + 2M_{ss}^{2}}{3 \times 16\pi^{2}} \ln \frac{M_{ud}^{2} + 2M_{ss}^{2}}{3\mu_{sub}^{2}} + \bar{g}_{1} \left(\frac{M_{ud}^{2} + 2M_{ss}^{2}}{3} \right) \right) \\ &- \left(1 + \frac{2(M_{ud}^{2} - M_{ss}^{2})^{2}}{(M_{ud}^{2} + 2M_{ss}^{2})^{2}} \left(-\frac{\beta_{1}}{\sqrt{V}} \right) + \frac{3M_{ud}^{2}M_{ss}^{2}}{M_{ud}^{2} + 2M_{ss}^{2}} \left(-\frac{1}{16\pi^{2}} \ln V^{1/2}\mu_{sub}^{2} - \beta_{2} \right) \right) \right\} \\ &- 4(2L_{8}^{r}(\mu_{sub}) + H_{2}^{r}(\mu_{sub}))M_{vv}^{2} \right], \tag{6.7}$$

where its real part for the imaginary valence mass is taken as in the same way shown in the previous subsection. Here $M_{ud}^2 = (m_u + m_d)\Sigma/F^2$, $M_{ss}^2 = 2m_s\Sigma/F^2$, $M_{vv}^2 = 2m_v\Sigma/F^2$.

The non-perturbative zero-mode integrals are given by

$$\hat{\Sigma}_{\nu}^{\mathrm{PQ}}(\mu_{v}, \{\mu_{u}, \mu_{s}\}) = -\frac{1}{(\mu_{u}^{2} - \mu_{v}^{2})^{2}(\mu_{s}^{2} - \mu_{v}^{2})} \\
= \frac{\det \begin{pmatrix} \partial_{\mu_{v}}K_{\nu}(\mu_{v}) & I_{\nu}(\mu_{v}) & I_{\nu}(\mu_{u}) & \mu_{u}^{-1}I_{\nu-1}(\mu_{u}) & I_{\nu}(\mu_{s}) \\ -\partial_{\mu_{v}}(\mu_{v}K_{\nu+1}(\mu_{v})) & \mu_{v}I_{\nu+1}(\mu_{v}) & \mu_{u}I_{\nu+1}(\mu_{u}) & \mu_{s}I_{\nu+1}(\mu_{s}) \\ \partial_{\mu_{v}}(\mu_{v}^{2}K_{\nu+2}(\mu_{v})) & \mu_{v}^{2}I_{\nu+2}(\mu_{v}) & \mu_{u}^{2}I_{\nu+2}(\mu_{u}) & \mu_{u}I_{\nu+1}(\mu_{u}) & \mu_{s}^{2}I_{\nu+2}(\mu_{s}) \\ -\partial_{\mu_{v}}(\mu_{v}^{3}K_{\nu+3}(\mu_{v})) & \mu_{v}^{3}I_{\nu+3}(\mu_{v}) & \mu_{u}^{3}I_{\nu+3}(\mu_{u}) & \mu_{u}^{3}I_{\nu+3}(\mu_{u}) & \mu_{u}^{3}I_{\nu+3}(\mu_{u}) \\ \partial_{\mu_{v}}(\mu_{v}^{4}K_{\nu+4}(\mu_{v})) & \mu_{v}^{4}I_{\nu+4}(\mu_{v}) & \mu_{u}^{4}I_{\nu+4}(\mu_{u}) & \mu_{u}^{3}I_{\nu+3}(\mu_{u}) & \mu_{s}^{4}I_{\nu+4}(\mu_{s}) \end{pmatrix}} \\ \times \frac{\det \begin{pmatrix} I_{\nu}(\mu_{u}) & \mu_{u}^{-1}I_{\nu-1}(\mu_{u}) & I_{\nu}(\mu_{s}) \\ \mu_{u}I_{\nu+1}(\mu_{u}) & I_{\nu}(\mu_{u}) & \mu_{s}I_{\nu+3}(\mu_{s}) \end{pmatrix}}{\det \begin{pmatrix} I_{\nu}(\mu_{u}) & \mu_{u}^{2}I_{\nu+2}(\mu_{u}) & \mu_{s}^{3}I_{\nu+3}(\mu_{s}) \\ \mu_{u}^{3}I_{\nu+3}(\mu_{u}) & \mu_{u}^{2}I_{\nu+2}(\mu_{u}) & \mu_{s}^{3}I_{\nu+3}(\mu_{s}) \end{pmatrix}}.$$
(6.8)

where $\mu_u = m_{u,d} \Sigma V$ and $\mu_s = m_s \Sigma V$ and one can take the imaginary value of $\mu_v = i\zeta$ to obtain $\hat{\rho}_{\nu}^{\text{mic}}(\zeta, \{\mu_u, \mu_s\})$ in the same way as the 2-flavor case.

Substituting again the numerical values in the beginning of this section, we plot the chiral condensate and the spectral density in figure 7 for the case with $m_u = m_d = 10 \text{ MeV}$, $m_s = 110 \text{ MeV}$, L = T/2 = 2 fm, $\nu = 0$ and $H_2^r(0.77 \text{ GeV}) = 0.1 \times 10^{-3}$. Due to the large contribution from the chiral logarithm of strange quarks, both of the (normalized) condensate and spectral density shows a quite larger deviation from 1, which is the universal chiral limit when $V \to \infty$ with any number of flavors.



Figure 7: The condensate (top) and the Dirac spectral density (bottom) with $N_f = 2+1$ theory are given (solid curve). For the comparison, $N_f = 2$ plot is also presented (dotted). As the valence mass or the eigenvalue increases, both of them show larger deviation from 1 than the case with $N_f = 2$.

7. Conclusions

We have computed the quark condensate and the spectral density of the Dirac operator by means of the chiral Lagrangian in a finite volume. We have used a new perturbative method which keeps all the terms which appear in the conventional expansion in the *p*-regime but which treats zero-mode integral non-perturbatively in the same manner as in the ϵ -regime. The resulting perturbative series connects smoothly previous results in the *p*-regime with those of the ϵ -regime. Having analytical formulas available in the intermediate region may be of obvious value for lattice QCD simulations.

It would be interesting to investigate the present proposal for finite-volume chiral perturbation theory in greater detail. One should obviously consider using such a method to compute other finite-volume observables in chiral perturbation theory, such as two-point correlation functions.

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A. Non-perturbative zero-mode integrals

In this appendix, we briefly review how to perform the non-perturbative zero-mode integrals. We are interested in the most general partially quenched calculations for both practical purposes of comparisons to lattice data and for computing spectral correlation functions of the Dirac operator. Of course, results for the N_f -theory without separate valence quarks are trivially included in this.

For the evaluation of the zero-mode integrals it is convenient to use the graded formalism where partial quenching is achieved by adding additional bosonic and fermionic species. The zero-mode integral corresponding to the graded version of eq. (3.2) with n bosons and m fermions is known in closed analytical form for an arbitrary mass matrix [21],

$$\mathcal{Z}_{n,m}^{\nu}(\{\mu_i\}) = \frac{\det[\mu_i^{j-1}\mathcal{J}_{\nu+j-1}(\mu_i)]_{i,j=1,\dots,n+m}}{\prod_{j>i=1}^n (\mu_j^2 - \mu_i^2) \prod_{j>i=n+1}^{n+m} (\mu_j^2 - \mu_i^2)},$$
(A.1)

where $\mu_i = m_i \Sigma V$. Here \mathcal{J} 's are defined as $\mathcal{J}_{\nu+j-1}(\mu_i) \equiv (-1)^{j-1} K_{\nu+j-1}(\mu_i)$ for $i = 1, \ldots n$ and $\mathcal{J}_{\nu+j-1}(\mu_i) \equiv I_{\nu+j-1}(\mu_i)$ for $i = n+1, \ldots n+m$, where I_{ν} and K_{ν} are the modified Bessel functions. In this paper, we need the case with $(n,m) = (1, N_f + 1)$:

$$\mathcal{Z}_{1,1+N_{f}}^{\nu}(\mu_{b}|\mu_{v}, \{\mu_{\text{sea}}\}) = \frac{1}{\prod_{i=1}^{N_{f}}(\mu_{i}^{2} - \mu_{v}^{2})\prod_{j>k}^{N_{f}}(\mu_{j}^{2} - \mu_{k}^{2})} \times \det \begin{pmatrix} K_{\nu}(\mu_{b}) & I_{\nu}(\mu_{v}) & I_{\nu}(\mu_{1}) & I_{\nu}(\mu_{2}) & \cdots \\ -\mu_{b}K_{\nu+1}(\mu_{b}) & \mu_{v}I_{\nu+1}(\mu_{v}) & \mu_{1}I_{\nu+1}(\mu_{1}) & \mu_{2}I_{\nu+1}(\mu_{2}) & \cdots \\ \mu_{b}^{2}K_{\nu+2}(\mu_{b}) & \mu_{v}^{2}I_{\nu+2}(\mu_{v}) & \mu_{1}^{2}I_{\nu+2}(\mu_{1}) & \mu_{2}^{2}I_{\nu+2}(\mu_{2}) & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}$$
(A.2)

Here $\mu_b = m_b \Sigma V$, $\mu_v = m_v \Sigma V$ and $\mu_i = m_i \Sigma V$, where m_b , m_v and m_i denote the masses of the valence bosons, the valence quarks, and the physical sea quarks respectively. In the arguments, the set of sea flavors are denoted by $\{\mu_{\text{sea}}\} = \{m_1 \Sigma V, m_2 \Sigma V, \ldots\}$.

When some of the quark masses are degenerate, one simply uses l'Hopital's rule. For example, for $\mu_1 = \mu_2$ one has

$$\mathcal{Z}_{1,1+N_{f}}^{\nu}(\mu_{b}|\mu_{v}, \{\mu_{\text{sea}}\})|_{\mu_{1}=\mu_{2}} = \frac{1}{2\prod_{i=1}^{N_{f}}(\mu_{i}^{2}-\mu_{v}^{2})\prod_{j>k,j\geq3}^{N_{f}}(\mu_{j}^{2}-\mu_{k}^{2})} \\
\times \det \begin{pmatrix} K_{\nu}(\mu_{b}) & I_{\nu}(\mu_{v}) & I_{\nu}(\mu_{1}) & \mu_{1}^{-1}I_{\nu-1}(\mu_{1}) \cdots \\ -\mu_{b}K_{\nu+1}(\mu_{b}) & \mu_{v}I_{\nu+1}(\mu_{v}) & \mu_{1}I_{\nu+1}(\mu_{1}) & I_{\nu}(\mu_{1}) & \cdots \\ \mu_{b}^{2}K_{\nu+2}(\mu_{b}) & \mu_{v}^{2}I_{\nu+2}(\mu_{v}) & \mu_{1}^{2}I_{\nu+2}(\mu_{1}) & \mu_{1}I_{\nu+1}(\mu_{1}) & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix} . \quad (A.3)$$

Partially quenched observables are computed by differentiating eq. (A.2) with respect to suitable sources and subsequently taking the limit $\mu_b \to \mu_v$. For example, the zero-mode integral of eq. (3.3) is

$$\frac{1}{2} \langle U_{vv} + U_{vv}^{\dagger} \rangle_U = \hat{\Sigma}_{\nu}^{\mathrm{PQ}}(\mu_v, \{\mu_{\mathrm{sea}}\}) \equiv -\lim_{\mu_b \to \mu_v} \frac{\partial}{\partial \mu_b} \ln \mathcal{Z}_{1,1+N_f}^{\nu}(\mu_b | \mu_v, \{\mu_{\mathrm{sea}}\}).$$
(A.4)

To obtain the result in a $\theta = 0$ (or even $\theta \neq 0$) QCD vacuum, one could numerically sum over topology with the weight given by the partition function above;

$$\hat{\Sigma}_{\theta}^{\mathrm{PQ}}(\mu_{v}, \{\mu_{\mathrm{sea}}\}) = \frac{\sum_{\nu} e^{i\theta\nu} \hat{\Sigma}_{\nu}^{\mathrm{PQ}}(\mu_{v}, \{\mu_{\mathrm{sea}}\}) \mathcal{Z}_{0,N_{f}}^{\nu}}{\sum_{\nu} e^{i\theta\nu} \mathcal{Z}_{0,N_{f}}^{\nu}}, \qquad (A.5)$$

or use the analytic expressions known for the $N_f = 2, 3$ cases [25].

B. Doing the zero-mode integrals first: a U(1) toy model

The perturbative scheme presented in this paper relies on the operator

$$\frac{\Sigma}{2F^2} [\mathcal{M}^{\dagger}(U-1)\xi^2 + \xi^2(U^{\dagger}-1)\mathcal{M}],$$

being small, and more precisely of $\mathcal{O}(p^5)$ or smaller, for any value of the mass m as this mass is taken to zero at finite volume. The difficulty in giving a precise counting to this term lies of course in it being a combination of mass m, field $\xi(x)$ (both of which can be assigned clear countings) and the zero mode field U. It is therefore interesting that an alternative scheme exists, which gives identical results, but which assigns a definite magnitude to this term. This is achieved by first doing the zero mode integral exactly, and only subsequently performing the perturbative evaluations of the non-zero mode integrals.⁷ In the general $SU(N_f + N)$ case this becomes rather cumbersome in practice, but it has the advantage that all terms are explicitly ordered according to the expansion parameter 1/L. Here we

⁷We are grateful to M. Lüscher for suggesting this alternative method.

illustrate it for the case of a simple U(1) toy model at the topological sector with $\nu = 0$, where the zero-mode integrals are trivially performed.

We thus consider the U(1) "chiral Lagrangian"⁸

$$\mathcal{L} = \frac{F^2}{4} \partial_{\mu} U(x) \partial_{\mu} U^{\dagger}(x) - \frac{\Sigma}{2} [m^{\dagger} e^{i\theta} U(x) + \text{h.c.}] + \cdots, \qquad (B.1)$$

where $U(x) \in U(1)$. We separate into zero modes and non-zero modes,

$$U(x) = U e^{i\sqrt{2}\xi(x)/F} = e^{i\sqrt{2}\xi_0/F} e^{i\sqrt{2}\xi(x)/F},$$
 (B.2)

and do the analogue of fixing topology to $\nu = 0$ by integrating over θ . Expanding perturbatively in the non-zero modes $\xi(x)$, we get

$$\mathcal{L} = -\Sigma m \cos(\sqrt{2}\xi_0/F) \left(1 - \xi(x)^2/F^2\right) + \frac{1}{2}(\partial_\mu \xi(x))^2 + \cdots,$$
(B.3)

We now perform the zero-mode integration over ξ_0 exactly with respect to the term shown to get the partition function

$$\mathcal{Z} = \int [d\xi(x)] I_0 \left(m \Sigma V \left(1 - \frac{1}{VF^2} \int d^4 x \xi(x)^2 \right) \right) e^{-\frac{1}{2} \int d^4 x (\partial_\mu \xi)^2} + \cdots,$$
(B.4)

up to overall irrelevant factors.

Expanding the Bessel function using $I'_0(x) = I_1(x)$, and exponentiating the expanded term leads to the effective partition function

$$\mathcal{Z} = I_0(m\Sigma V) \int [d\xi(x)] e^{-\int d^4x [\frac{1}{2}(\partial_\mu \xi)^2 + \frac{1}{2}\tilde{m}_\pi^2 \xi(x)^2]} + \cdots, \qquad (B.5)$$

where an effective volume-dependent pion mass is defined by

$$\tilde{m}_{\pi}^2 \equiv \frac{2m\Sigma}{F^2} \frac{I_1(m\Sigma V)}{I_0(m\Sigma V)},\tag{B.6}$$

we note that, as expected, this effective pion mass approaches the standard tree-level pion mass expression in the limit where $m\Sigma V \to \infty$:

$$\tilde{m}_{\pi}^2 \to 2m\Sigma/F^2 = m_{\pi}^2 \qquad \text{as} \quad m\Sigma V \to \infty,$$
(B.7)

while in the opposite limit we find

$$\tilde{m}_{\pi}^2 \sim \frac{2m\Sigma}{F^2} \frac{1}{2}m\Sigma V = m_{\pi}^4 \frac{F^2 V}{4} \quad \text{as} \quad m\Sigma V \to 0,$$
(B.8)

Clearly, in the usual p-regime expansion this provides us with the standard massive propagator term, while in the chiral limit taken at finite volume V, there is no infrared

⁸Of course, in the real $N_f = 1$ theory chiral symmetry is broken explicitly by the anomaly, and this Lagrangian is therefore not relevant for describing the the $N_f = 1$ theory. We use it only as a simple toy model to illustrate in a very transparent way the effect of first integrating over the zero mode.

problem due to the momentum sums being taken over non-zero modes only. When $m\Sigma V$ becomes of order unity we recover the usual ϵ -regime expressions.

But here we are interested in seeing how our expansion looks if we add and subtract the standard mass term, as is done in the main part of this paper. We therefore do a trivial rewriting,

$$\mathcal{L} = \frac{1}{2} (\partial_{\mu} \xi(x))^2 + \frac{1}{2} \tilde{m}_{\pi}^2 \xi(x)^2 = \frac{1}{2} (\partial_{\mu} \xi(x))^2 + \frac{1}{2} m_{\pi}^2 \xi(x)^2 + \frac{1}{2} \delta m_{\pi}^2 \xi(x)^2,$$
(B.9)

where

$$\delta m_{\pi}^2 \equiv \tilde{m}_{\pi}^2 - m_{\pi}^2,$$
 (B.10)

Can we treat $\frac{1}{2}\delta m_{\pi}^2 \xi(x)^2$ as a perturbation? Near the usual *p*-regime where $m\Sigma V \to \infty$ we can use the asymptotic expansion of Bessel functions,

$$I_n(x) \sim \frac{e^x}{\sqrt{2\pi x}} \left(1 - \frac{4n^2 - 1}{8x} + \cdots \right),$$
 (B.11)

to see that

$$\delta m_{\pi}^2 = -\frac{1}{F^2 V} + \cdots,$$
 (B.12)

This is of $\mathcal{O}(p^4)$ as expected in this U(1) theory. When instead $m\Sigma V$ is of order unity, we get

$$\delta m_\pi^2 \sim -m_\pi^2,\tag{B.13}$$

which is also of $\mathcal{O}(p^4)$. The point here is that we know the full analytical expression

$$\delta m_{\pi}^2 = \frac{2m\Sigma}{F^2} \left[\frac{I_1(m\Sigma V)}{I_0(m\Sigma V)} - 1 \right], \qquad (B.14)$$

for all values of m and V, and it is easy to check that this function is of $\mathcal{O}(p^4)$ everywhere. The term $\delta m_{\pi}^2 \xi(x)^2$ is thus explicitly found to be of NLO and we can treat it perturbatively.

Of course, as already discussed in section 5, away from the conventional *p*-regime expansion, separating out $\delta m_{\pi}^2 \xi(x)^2$ and treating it perturbatively amounts to a re-ordering and partial resummation of terms in this expansion. This is because the propagator is taken to be the conventional massive one even when m_{π}^2 is no longer of $\mathcal{O}(p^2)$, but *smaller*. The difference between a calculation based on this propagator and one where the propagator has been expanded in m_{π}^2 up to the needed order is always of yet higher order, and thus only illustrates the inherent uncertainty in any fixed-order perturbative expansion.

C. Numerical evaluation of $\bar{\Delta}(0, M^2)$ and $\partial_{M^2}\bar{\Delta}(0, M^2)$

The definition of $\bar{g}_1(M^2)$ in eq. (3.8) and $\bar{g}_2(M^2) = -\partial_{M^2}\bar{g}_1(M^2)$, requires an infinite sum over the 4-vector $a_\mu = n_\mu L_\mu$ where $L_i = L$ (i = 1, 2, 3) and $L_4 = T$. In this appendix, we will suggest how to evaluate numerically $\bar{g}_1(M^2)$ and $\bar{g}_2(M^2)$. For ML > 1, the expansion [6],

$$\bar{g}_1(M^2) = \sum_{a \neq 0} \int \frac{d^4q}{(2\pi)^4} \frac{e^{-iqa}}{q^2 + M^2} - \frac{1}{M^2 V} = \sum_{a \neq 0} \frac{\sqrt{M^2}}{4\pi^2 |a|} K_1(\sqrt{M^2} |a|) - \frac{1}{M^2 V}, \quad (C.1)$$

in terms of modified Bessel functions is useful, while for ML < 1, the polynomial expression

$$\bar{g}_1(M^2) = -\frac{M^2}{16\pi^2} \ln(M^2 V^{1/2}) - \sum_{n=1}^{\infty} \frac{\beta_n}{(n-1)!} M^{2(n-1)} V^{(n-2)/2},$$
(C.2)

using the shape coefficients β_n 's [4] is appropriate. Here

$$\beta_n \equiv \left(\frac{-1}{4\pi}\right)^n \left(\alpha_n + \frac{2}{n(n-2)}\right) \quad (n \neq 2), \qquad \beta_2 \equiv \frac{\alpha_2 - \ln 4\pi + \gamma - 3/2}{16\pi^2}, \quad (C.3)$$
$$\alpha_n \equiv \int_0^1 dt \left\{ t^{n-3} \left(S\left(\frac{L^2}{V^{1/2}t}\right)^3 S\left(\frac{T^2}{V^{1/2}t}\right) - 1 \right) \right\}$$

$$+t^{-n-1}\left(S\left(\frac{V^{1/2}}{L^2t}\right)^3 S\left(\frac{V^{1/2}}{T^2t}\right) - 1\right)\right\},\tag{C.4}$$

$$S(x) \equiv \sum_{k=-\infty}^{\infty} \exp(-\pi k^2 x), \tag{C.5}$$

where $\gamma \sim 0.577215665$ is Euler's constant and the summation in S(x) is typically well approximated by a truncation to $|k| \leq 20$.

Since the modified Bessel function $K_{\nu}(x)$ is well-defined for the complex value of x, the both expressions above can be easily extended for the complex arguments using $(m + \sqrt{m_v^2})^{1/2}|_{m_v=i\lambda} = (m^2 + \lambda^2)^{1/4} e^{i \arctan(\lambda/m)/2}$, and the prescription given in eq. (4.4).

As shown in figure 8, ignoring the contribution from $|n_{\mu}| > 20$ in the summation in eq. (C.1), and n > 5 in the summation in eq. (C.2), both formulas agree in a rather long interval around ML = 1. We also find an excellent agreement between these two expansions for both $\operatorname{Re}\bar{g}_1(M^2)$ and $\operatorname{Re}\bar{g}_2(M^2)$ at imaginary values of M^2 , using the same truncation. It is in any case trivial to increase the accuracy by including more terms.

To summarize, we have used

$$\bar{g}_{1}(M^{2}) = \begin{cases} \bar{g}_{1}^{p}(M^{2}) \equiv \sum_{a \neq 0}^{|n_{i}| \leq 20} \frac{\sqrt{M^{2}}}{4\pi^{2}|a|} K_{1}(\sqrt{M^{2}}|a|) - \frac{1}{M^{2}V} & (|M|L > 1) \\ \\ \bar{g}_{1}^{\epsilon}(M^{2}) \equiv -\frac{M^{2}}{16\pi^{2}} \ln(M^{2}V^{1/2}) - \sum_{n=1}^{5} \frac{\beta_{n}}{(n-1)!} M^{2(n-1)} V^{(n-2)/2} & (|M|L \leq 1) \end{cases} , (C.6)$$

and similarly for their derivatives \bar{g}_2 . We plot $Re\bar{g}_1(M_0^2 + iM^2)$ and $Re\bar{g}_2(M_0^2 + iM^2)$ for various choices of fixed M_0 in figure 9.

Specifying the renormalization scale $\mu_{sub} = 0.77 \text{ GeV}$ of the low energy constants L_i 's, and the above prescription for \bar{g}_1 and \bar{g}_2 ,

$$\bar{\Delta}(0, M^2) = \frac{M^2}{16\pi^2} \ln \frac{M^2}{\mu_{\rm sub}^2} + \bar{g}_1(M^2), \qquad (C.7)$$



Figure 8: The plot of $\bar{g}_1(M^2)V^{1/2}$ (left part) and $\bar{g}_2(M^2)$ (right part) for T = 2L. The truncated sums in eq. (C.6) for $\bar{g}_{1,2}^p(M^2)$ (solid line) and $\bar{g}_{1,2}^\epsilon(M^2)$ (dotted) agree well around $ML \sim 1$. Note that $\bar{g}_1(M^2)V^{1/2}$ converges to $-\beta_1 = -0.08360$ in the chiral limit. Note also that $|\bar{g}_1(M^2)|$ attains its maximum at M = 0.



Figure 9: Plot of $\operatorname{Re}\bar{g}_1(M_0^2 + iM^2)V^{1/2}$ (left part) and $\operatorname{Re}\bar{g}_2(M_0^2 + iM^2)$ (right part) for T = 2L. for three fixed values of $M_0L = 0$ (solid), 0.05 (dotted) and 0.1 (small dotted).

$$\partial_{M^2}\bar{\Delta}(0,M^2) = \frac{1}{16\pi^2} \left(\ln \frac{M^2}{\mu_{\rm sub}^2} + 1 \right) - \bar{g}_2(M^2),$$
 (C.8)

can then be evaluated numerically. We note that in the small mass region the logarithmic contribution $\ln M^2$ is canceled by a similar one in \bar{g}_i and that both $\bar{\Delta}(0, M^2)$ and $\partial_{M^2}\bar{\Delta}(0, M^2)$ have no IR divergences in the limit $M^2 \to 0$.

D. Useful properties of $\overline{G}(x, M^2, M^2)$

We also need the 1-loop correction from off-diagonals part of ξ , $\bar{G}(0, M^2, M^2)$. It can, in principle, be expressed in terms of $\bar{\Delta}(0, M^2)$. In this appendix, we discuss the UV divergence of $\bar{G}(0, M^2, M^2)$ and rewrite it using $\bar{\Delta}(0, M^2)$ and $\partial_{M^2}\bar{\Delta}(0, M^2)$. Explicit examples for the degenerate case and non-degenerate $N_f = 2+1$ flavor theory will be given.

First let us consider the UV-divergent part of $\overline{\Delta}(0, M^2)$,

$$\bar{\Delta}(0, M^2) = \frac{1}{V} \sum_{p \neq 0} \frac{1}{p^2 + M^2}$$
$$= \frac{1}{V} \sum_{p \neq 0} \left(\frac{1}{p^2} - \frac{M^2}{p^4} \right) + \mathcal{O}(M^4).$$
(D.1)

Here the first term is quadratically divergent, the second term produces a logarithmic divergence, and the remaining $\mathcal{O}(M^4)$ terms are UV finite. As is well-known, the quadratic divergence is absent when we employ dimensional regularization.

By expanding in the mass, the UV-divergent part of $\overline{G}(0, M^2, M^2)$ can be written

$$\bar{G}(0, M^2, M^2) = \frac{1}{V} \sum_{p \neq 0} \frac{1}{(p^2 + M^2)^2 \left(\sum_{f}^{N_f} \frac{1}{p^2 + M_{ff}^2}\right)}$$

$$= \frac{1}{N_f V} \sum_{p \neq 0} \left(\frac{1}{p^2} - \frac{2M^2}{p^4} + \frac{1}{N_f} \sum_{f}^{N_f} \frac{M_{ff}^2}{p^4} + \mathcal{O}(M^4)\right)$$

$$= \frac{2}{N_f} \bar{\Delta}(0, M^2) - \frac{1}{N_f^2} \sum_{f}^{N_f} \bar{\Delta}(0, M_{ff}^2) + \mathcal{O}(M^4)$$

$$= \left(\frac{2}{N_f} M^2 - \frac{1}{N_f^2} \sum_{f}^{N_f} M_{ff}^2\right) \frac{c_1}{16\pi^2} + \cdots, \qquad (D.2)$$

where the logarithmic divergence of the last line is canceled by a renormalization of L_i 's as seen in section 3.

Although eq. (D.2) shows that $\bar{G}(0, M^2, M^2)$ inherits the UV properties of $\bar{\Delta}(0, M^2)$, the expansion is not useful when we want to see the finite part of $\bar{G}(0, M^2, M^2)$, since the omitted $\mathcal{O}(M^4)$ terms are the at the same order as the former two terms. In order to obtain a convenient rewriting, let us define a function

$$f(t) \equiv \frac{1}{N_f} \sum_{i}^{k} \frac{n_i}{t - M_{ii}^2},$$
 (D.3)

where k denotes the number of different quark masses and $n_i \ge 1$ is the degeneracy of the *i*-th mass satisfying $\sum_{i}^{k} n_i = N_f$. Here we have ordered the masses $M_{ii}^2 < M_{i+1 i+1}^2$ for any *i*. Noting f(t) is a monotonically decreasing function,

$$\frac{d}{dt}f(t) = -\frac{1}{N_f} \sum_{i}^{k} \frac{n_i}{(t - M_{ii}^2)^2} < 0,$$
(D.4)

and

$$\lim_{\epsilon \to 0} f(M_{ii}^2 + \epsilon) = \infty, \quad \lim_{\epsilon \to 0} f(M_{i+1\,i+1}^2 - \epsilon) = -\infty, \tag{D.5}$$

$$f(t) \neq 0$$
, for $t < M_{11}^2, M_{kk}^2 < t$, (D.6)

one can show that an equation f(t) = 0 has k - 1 different solutions (we denote them by $t = \overline{M}_{ii}^2$), each of them satisfying

$$M_{ii}^2 < \bar{M}_{ii}^2 < M_{i+1\,i+1}^2, \quad (1 \le i \le k-1).$$
(D.7)

We illustrate this in the plot figure 10.



Figure 10: Example of f(t) in eq. (D.3), where we have $N_f = 6$, k = 5, $n_i = 1 (i \neq 2)$, $n_2 = 2$, and $\{M_{ii}^2\} = \{0.1, 0.3, 0.5, 0.75, 0.9\}$. One can see f(t) = 0 has k - 1 = 4 solutions between the poles (plotted by the crosses).

Hence,

$$-f(-p^2) = \frac{\prod_i^{k-1}(p^2 + \bar{M}_{ii}^2)}{\prod_j^k(p^2 + M_{jj}^2)},$$
 (D.8)

and $\bar{G}(0,M^2,M^2)$ can thus alternatively be expressed as

$$\bar{G}(0, M^2, M^2) = \frac{1}{N_f V} \sum_{p \neq 0} \frac{\prod_j^k (p^2 + M_{jj}^2)}{(p^2 + M^2)^2 \prod_i^{k-1} (p^2 + \bar{M}_{ii}^2)}$$
$$= \frac{1}{N_f} \left[\sum_i^{k-1} A_i \bar{\Delta}(0, \bar{M}_{ii}^2) + B \bar{\Delta}(0, M^2) + C \,\partial_{M^2} \bar{\Delta}(0, M^2) \right], \quad (D.9)$$

where the coefficients A_i 's, B and C are given by the residue of

$$f_2(t) = \frac{\prod_j^k (-t + M_{jj}^2)}{(-t + M^2)^2 \prod_i^{k-1} (-t + \bar{M}_{ii}^2)},$$
 (D.10)

(or $-(-t + M^2)f_2(t)$ for C), at each pole. Note that C = 0 when M^2 is equal to any of the physical masses.

Noting that both $\bar{\Delta}(0, M^2)$ and $\partial_{M^2}\bar{\Delta}(0, M^2)$ are infra-red finite in the limit $M^2 \to 0$,

$$\bar{\Delta}(0, M^2)|_{M^2 \to 0} = -\frac{\beta_1}{\sqrt{V}},$$
 (D.11)

$$\partial_{M^2}\bar{\Delta}(0,M^2)|_{M^2\to 0} = -\frac{1}{16\pi^2}\ln V^{1/2} - \beta_2 + \frac{c_1}{16\pi^2},$$
 (D.12)

the chiral limit of $\overline{G}(0, M^2, M^2)$ is given by

$$\bar{G}(0,0,0) = \frac{1}{N_f} \left[\sum_{i}^{k-1} A_i |_{M^2 = 0} \bar{\Delta}(0, \bar{M}_{ii}^2) - B |_{M^2 = 0} \frac{\beta_1}{\sqrt{V}} - C |_{M^2 = 0} \left(\frac{1}{16\pi^2} \ln V^{1/2} + \beta_2 - \frac{c_1}{16\pi^2} \right) \right], \quad (D.13)$$

where UV divergence c_1 is absorbed into the renormalization of L_6 .

Here we give some useful examples. For the fully degenerate case, *i.e.*, equal masses $M_{ii}^2 = M_{\text{sea}}^2$ for all *i*, the above expression for \bar{G} is greatly simplified,

$$\bar{G}(0, M^2, M^2) = \frac{1}{N_f} \left[\bar{\Delta}(0, M^2) + (M^2 - M_{\text{sea}}^2) \partial_{M^2} \bar{\Delta}(0, M^2) \right], \quad (D.14)$$

in agreement with the result presented in ref. [12].

For an $N_f = 2 + 1$ flavor theory, the equation f(t) = 0 is easily solved and one obtains

$$\bar{G}(0, M^2, M^2) = \frac{1}{3} \left[A\bar{\Delta} \left(0, \frac{M_{ud}^2 + 2M_{ss}^2}{3} \right) + B\bar{\Delta}(0, M^2) + C \,\partial_{M^2}\bar{\Delta}(0, M^2) \right],$$
(D.15)

where $M_{ud}^2 = 2m_u\Sigma/F^2 = 2m_d\Sigma/F^2$, $M_{ss}^2 = 2m_s\Sigma/F^2$ and the coefficients are given by

$$A = -\frac{2(M_{ud}^2 - M_{ss}^2)^2}{(3M^2 - M_{ud}^2 - 2M_{ss}^2)^2}, \quad B = 1 + \frac{2(M_{ud}^2 - M_{ss}^2)^2}{(3M^2 - M_{ud}^2 - 2M_{ss}^2)^2},$$
$$C = \frac{3(M^2 - M_{ud}^2)(M^2 - M_{ss}^2)}{3M^2 - M_{ud}^2 - 2M_{ss}^2}.$$
(D.16)

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Erratum

Corrections in the equations

First we would like to correct some equations. Eq. (4.7) should be replaced by

$$\hat{\rho}_{\nu}^{mic}(\zeta, \{\mu_{sea}\}) \equiv \left| \frac{|\zeta|}{2 \prod_{f}^{N_{f}} (\zeta^{2} + \mu_{f}^{2})} \frac{\det \tilde{\mathcal{B}}}{\det \mathcal{A}} \right|.$$
(E.1)

In the same way, eq. (6.5) should be replaced by

$$\hat{\rho}_{\nu}^{mic}(\zeta,\mu) = \frac{|\zeta|}{2(\mu^{2}+\zeta^{2})^{2}} \\ \det \begin{pmatrix} \zeta^{-1}J_{\nu-1}(\zeta) & J_{\nu}(\zeta) & I_{\nu}(\mu) & \mu^{-1}I_{\nu-1}(\mu) \\ J_{\nu}(\zeta) & \zeta J_{\nu+1}(\zeta) & -\mu I_{\nu+1}(\mu) & -I_{\nu}(\mu) \\ \zeta J_{\nu+1}(\zeta) & \zeta^{2}J_{\nu+2}(\zeta) & \mu^{2}I_{\nu+2}(\mu) & \mu I_{\nu+1}(\mu) \\ \zeta^{2}J_{\nu+2}(\zeta) & \zeta^{3}J_{\nu+3}(\zeta) - \mu^{3}I_{\nu+3}(\mu) - \mu^{2}I_{\nu+2}(\mu) \end{pmatrix} \\ \times \frac{\det \begin{pmatrix} I_{\nu}(\mu) & \mu^{-1}I_{\nu-1}(\mu) \\ \mu I_{\nu+1}(\mu) & I_{\nu}(\mu) \end{pmatrix}}{\det \begin{pmatrix} I_{\nu}(\mu) & \mu^{-1}I_{\nu-1}(\mu) \\ \mu I_{\nu+1}(\mu) & I_{\nu}(\mu) \end{pmatrix}}.$$
(E.2)

Note that the difference in the above equations from the original ones is only in their sign.

There is another typo in eq. (6.8) which should be replaced by

$$\hat{\Sigma}_{\nu}^{PQ}(\mu_{v}, \{\mu_{u}, \mu_{s}\}) = -\frac{1}{(\mu_{u}^{2} - \mu_{v}^{2})^{2}(\mu_{s}^{2} - \mu_{v}^{2})} \\
det \begin{pmatrix} \partial_{\mu_{v}}K_{\nu}(\mu_{v}) & I_{\nu}(\mu_{v}) & I_{\nu}(\mu_{u}) & \mu_{u}^{-1}I_{\nu-1}(\mu_{u}) & I_{\nu}(\mu_{s}) \\
-\partial_{\mu_{v}}(\mu_{v}K_{\nu+1}(\mu_{v})) & \mu_{v}I_{\nu+1}(\mu_{v}) & \mu_{u}I_{\nu+1}(\mu_{u}) & I_{\nu}(\mu_{u}) & \mu_{s}I_{\nu+1}(\mu_{s}) \\
\partial_{\mu_{v}}(\mu_{v}^{2}K_{\nu+2}(\mu_{v})) & \mu_{v}^{2}I_{\nu+2}(\mu_{v}) & \mu_{u}^{2}I_{\nu+2}(\mu_{u}) & \mu_{u}I_{\nu+1}(\mu_{u}) & \mu_{s}^{2}I_{\nu+2}(\mu_{s}) \\
-\partial_{\mu_{v}}(\mu_{v}^{3}K_{\nu+3}(\mu_{v})) & \mu_{v}^{3}I_{\nu+3}(\mu_{v}) & \mu_{u}^{3}I_{\nu+3}(\mu_{u}) & \mu_{u}^{3}I_{\nu+3}(\mu_{u}) & \mu_{s}^{3}I_{\nu+3}(\mu_{s}) \\
\frac{\partial_{\mu_{v}}(\mu_{v}^{4}K_{\nu+4}(\mu_{v})) & \mu_{v}^{4}I_{\nu+4}(\mu_{v}) & \mu_{u}^{4}I_{\nu+4}(\mu_{u}) & \mu_{u}^{3}I_{\nu+3}(\mu_{u}) & \mu_{s}^{4}I_{\nu+4}(\mu_{s}) \end{pmatrix}}{\det \begin{pmatrix} I_{\nu}(\mu_{u}) & \mu_{u}^{-1}I_{\nu-1}(\mu_{u}) & I_{\nu}(\mu_{s}) \\
\mu_{u}I_{\nu+1}(\mu_{u}) & I_{\nu}(\mu_{u}) & \mu_{s}I_{\nu+1}(\mu_{s}) \\
\mu_{u}^{2}I_{\nu+2}(\mu_{u}) & \mu_{u}I_{\nu+1}(\mu_{u}) & \mu_{s}^{2}I_{\nu+2}(\mu_{s}) \end{pmatrix}}.$$
(E.3)

Additional comment on eq. (3.16)

In Eq. (3.16), we have shown that in the function $\hat{\Sigma}_{\nu}^{PQ}$ the valence argument $\mu'_{v} = Z_{v}m_{v}\Sigma V$ can be replaced by $Z_{v}^{0}m_{v}\Sigma V$ producing an additional term $\delta Z_{v}(m_{v})$. In the exactly same technique, one can replace the sea quark argument $\mu'_{i} = Z_{i}m_{i}\Sigma V$ by $Z_{i}^{0}m_{i}\Sigma V$. In this sea quark sector, no additional term appears. The difference between Z_{i} and Z_{i}^{0} in the above arguments is higher order and irrelevant to the analytic NLO formula but it would be more convenient to use the latter in the numerical studies since Z_{i}^{0} has no H_{2} dependence.