

## Finite volume scaling of pseudo Nambu-Goldstone bosons in QCD

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F. Bernardoni,<sup>a</sup> P. H. Damgaard,<sup>b</sup> H. Fukaya<sup>bc</sup> and P. Hernández<sup>a</sup>

<sup>a</sup>*Dpto. Física Teórica-UV and IFIC-CSIC, Edificio Institutos Investigación,  
Apt. 22085, E-46071 Valencia, Spain*

<sup>b</sup>*The Niels Bohr Institute, The Niels Bohr International Academy,  
Blegdamsvej 17 DK-2100 Copenhagen Ø Denmark*

<sup>c</sup>*High Energy Accelerator Research Organization (KEK),  
Tsukuba 305-0801, Japan*

*E-mail: fabio.bernardoni@ific.uv.es, phdamg@nbi.dk, hfukaya@nbi.dk,  
pilar.hernandez@ific.uv.es*

**ABSTRACT:** We consider chiral perturbation theory in a finite volume and in a mixed regime of quark masses. We take  $N_l$  light quarks near the chiral limit, in the so-called  $\epsilon$ -regime, while the remaining  $N_h$  quarks are heavier and in the standard  $p$ -regime. We compute in this new mixed regime the finite-size scaling of the light meson correlators in the scalar, pseudoscalar, vector and axial vector channels. Using the replica method, we easily extend our results to the partially quenched theory. With the help of our results, lattice QCD simulations with 2+1 flavors can safely investigate pion physics with very light up and down quark masses even in the region where the pion's correlation length overcomes the size of the space-time lattice.

**KEYWORDS:** Lattice QCD, Chiral Lagrangians.

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**1. Introduction**

It is now becoming feasible to simulate Quantum Chromodynamics (QCD) near the chiral limit in lattice gauge theory. Deeper theoretical understanding of chiral symmetry on the lattice, development of very efficient algorithms, and a constant progress in the computational resources have allowed a reduction of the dynamical quark masses almost to the physical point of the  $u$  and  $d$  quarks. As the quark masses approach zero, however, one has to be increasingly careful about finite-volume effects since the correlation lengths of the pions, the pseudo-Nambu-Goldstone bosons, diverge in that limit.

Such an infrared effect due to finite volume can be systematically treated within the framework of the low-energy effective theory. Due to the mass gap between the lightest particles, the pseudo-Nambu-Goldstone bosons that are generically referred to as “pions”, and the other hadrons, the heavier particles have an entirely different sensitivity to the finite volume. The euclidean partition function of QCD receives contributions from the full spectrum, but if the chiral limit is taken at finite volume these higher states give

exponentially suppressed contributions. In this way, by varying the volume, one can tune to as high accuracy as one wants by including only those degrees of freedom that are associated with the pseudo-Nambu-Goldstone bosons. In QCD, one is interested in a situation where two of the quarks (the  $u$  and the  $d$ ) are extremely light, while a third (the  $s$ ) is closer to the QCD scale  $\Lambda_{\text{QCD}}$ , but still light on the scale of the ultraviolet cut-off  $4\pi F$  (where  $F$  is the pion decay constant) in the effective low-energy theory.

It is therefore important to investigate how the finite volume can affect low-energy dynamics within the pion *effective* theory, chiral perturbation theory (ChPT) [1]–[5]. An extreme finite-volume situation is reached in the so-called  $\epsilon$ -regime where the pion correlation length  $1/m_\pi$  exceeds the size  $L, T$  of the 4-dimensional space-time volume  $V = TL^3$ ,

$$\frac{1}{\Lambda_{\text{QCD}}} \ll L, T \ll \frac{1}{m_\pi}. \quad (1.1)$$

The lower bound is to ensure validity of the effective chiral theory, the coupling constants of which are the same as those at infinite volume.

A systematic expansion exists in the  $\epsilon$ -regime, where all zero-momentum modes of the pseudo-Nambu-Goldstone bosons have to be treated exactly. An appropriate power-counting in this regime is

$$\sqrt{m_q} \sim m_\pi \sim p^2 \sim 1/L^2 \sim 1/T^2 \sim \epsilon^2, \quad (1.2)$$

in units of the cut-off of the theory. With this counting, the operators in the Chiral Lagrangian have different weights than in the ordinary ChPT at infinite volume, known as the  $p$ -expansion. There is therefore a re-ordering of the perturbative expansion: in many cases, the infinite-volume chiral condensate  $\Sigma$  and the pion decay constant  $F$  (both in the massless limit), play a more prominent role than in the conventional large volume regime, since next-to-leading order corrections are calculable in terms of these leading-order couplings alone. This opens up the possibility of extracting some of these low-energy constants from lattice QCD in new ways [1]–[5].

With non-degenerate quark masses one can define an  $\epsilon$ -regime and a  $p$ -regime for each of the now mass-split pseudo-Nambu-Goldstone bosons. In particular, one can also consider a *mixed* regime in which some pseudo-Nambu-Goldstones obey the condition for the  $\epsilon$ -regime, while others fall into the  $p$ -regime [6]. For the latter, the counting rules are the usual ones of chiral perturbation theory,

$$m_q \sim m_\pi^2 \sim p^2 \sim 1/L^2 \sim 1/T^2 \sim \epsilon^2. \quad (1.3)$$

A typical situation could be  $u$  and  $d$  quarks so light that the physical pions are in the  $\epsilon$ -regime, but the strange quark mass is such that the physical kaons are in the  $p$ -regime. Further possibilities open up when one considers partially quenched theories. In those cases one can imagine situations in which all physical  $u, d$  and  $s$  quarks are in the  $p$ -regime, while valence quarks corresponding to all or some of these are taken closer towards the chiral limit, and thus end up in the  $\epsilon$ -regime. Such situations could perhaps be realized in the context of mixed-action lattice simulations where dynamical configurations are generated

with physical quarks that are in the  $p$ -regime and can be well treated by, say, ordinary Wilson fermion actions. Valence quarks, which are taken to the chiral limit, could then be of, say, overlap type. Another situation could be the use of overlap quarks that are all or partly in the  $p$ -regime, while also overlap valence quarks are taken to the  $\epsilon$ -regime.

It is our belief that all these possibilities must be and will be explored in future lattice gauge theory studies. The present paper gives an analytical formalism for studying correlation functions of pseudo-Nambu-Goldstone bosons in that setting. Apart from quark masses, the two remaining limitations are the approach to the continuum limit, and the finite volume. In the present framework the finite volume  $V \gg 1/\Lambda_{\text{QCD}}^4$  is used as a tunable parameter with which to extract physical observables. The *only* extrapolation needed will thus be the one associated with taking the continuum scaling limit. With the new analytical formulas for partially quenched correlation functions available one can extract far more information for a given number of lattice configurations. In addition, with the mixed-regime predictions we also provide here one is effectively covering the full SU(3) flavor sector of QCD at low energy. The extent to which the  $s$  quark at the physical point is light enough to provide a good description in terms of chiral dynamics remains to be tested in detail on the lattice.

One important feature of the  $\epsilon$ -regime is the strong sensitivity to the topology of the gauge fields, a direct consequence of the finite volume. A crucial ingredient in making the  $\epsilon$ -regime so useful for lattice gauge theory computations is the fact that the zero-momentum integrals can be performed analytically at fixed topology, typically in terms of Bessel functions. With different detailed predictions for each sector of topological charge there is a wealth of analytical results that can be used to confront numerical lattice data.

These analytical predictions are non-perturbative in the gauge theory coupling. Remarkably, some of the leading-order  $\epsilon$ -regime results were first derived on the basis of chiral Random Matrix Theory [7]. It is particularly simple to derive analytical expressions for Dirac operator eigenvalues in that formulation [8], and it is well understood how to go between the two formulations [9]. These features all carry over into the mixed regime.

The computation of meson correlators in the  $\epsilon$ -regime was first performed in [3] and extended to both quenched and unquenched QCD at fixed topology a few years ago [10]–[12]. The effect of a coupling to isospin chemical potential has also been considered [13]. Partially quenched ChPT (PQChPT) in the  $\epsilon$ -regime was done for the chiral condensate itself in [14]. Recently, partially quenched space-time correlation functions were computed in several channels (pseudoscalar, scalar, and the left-current) of meson correlators [15, 6]. Also, the first computation of three-point correlation functions relevant for weak decays in the  $\epsilon$ -regime was done in [16]. Some of these studies have led to determinations of the leading order low-energy coefficients  $\Sigma$  and  $F^1$  at various sectors of fixed topology in quenched lattice simulations (see, e.g., [18]–[28]), as well as the low-energy couplings of the  $\Delta S = 1$  Hamiltonian from three-point functions [29, 30]. Difficulties associated with the quenched approximation have been discussed in [10, 12]. Recently, several groups have successfully extended this to full QCD in or close to the  $\epsilon$ -regime. This has been done both

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<sup>1</sup>See, e.g. ref. [17] for a recent summary of results.

on the basis of Dirac operator eigenvalues and space-time correlation functions [31]–[40].

In this paper, we present the results for various meson correlators in the mixed regime of ChPT where  $N_l$  light quarks are in the  $\epsilon$ -regime while  $N_h = N_f - N_l$  quarks remain relatively heavy and belong to the standard  $p$ -regime. We have used two different methods to treat this regime. The first uses the same mixed-regime perturbative expansion that was introduced in [6]. As a check, we have also used a new perturbative approach which has the advantage that it provides a smooth interpolation between the  $\epsilon$ -regime and the  $p$ -regime. The expected matching between the mixed regime and the standard  $\epsilon$ -regime is trivial to check in that formalism. The two methods should agree to all orders, and we have checked explicitly that they do agree at least up next-to-leading order in the mixed-regime power counting.

We treat the most general non-degenerate case where the required non-perturbative zero-mode integrals are performed according to ref. [15]. The two-point functions of the light sector, for the pseudoscalar, scalar, axial, vector channels, are then computed. They can be used to extract the leading low-energy constants  $\Sigma$  and  $F$ . Because we work at next-to-leading order, there is also explicit dependence on some of the  $L_i$ 's. In principle these low-energy constants can be determined from fits to varying quark masses in the heavier sector, as will become clear below. The pseudoscalar and scalar channels for the disconnected diagrams are also given. We easily extend our results to the partially (and fully) quenched theory by applying the replica method. One can confirm that our formulae reduce to all previously derived limiting cases of both the degenerate  $N_f$ -flavor theories and the fully quenched theory. There are new isospin-breaking effects when the  $u$  and  $d$  quark masses are split, and the existence of these terms can be used to extract additional information from the correlators. The new more general expressions should be helpful for future lattice gauge theory simulations that aim at approaching the chiral limit.

We start in section 2 by reviewing the mixed-regime perturbative expansion of [6]. The results for the two-point functions at next-to-leading order are presented in section 3. An alternative new approach is also briefly described there. The calculations are completed in section 4 by explicitly performing the zero-mode integrals for the full, the partially quenched, and the fully quenched theories. As a check on our results, we note the complete agreement between our two approaches and the correct matching between the mixed and pure  $\epsilon$  regimes is then also explicitly confirmed. In section 5, we give an explicit example for  $N_f = 2+1$  theory presenting the pseudoscalar and axial vector correlators. Conclusions and an outlook for the future are presented in section 6.

## 2. Chiral perturbation theory in the mixed-regime

In this section we review the perturbative expansion of the chiral Lagrangian that was introduced in [6] to treat the mixed regime. It incorporates features of both  $\epsilon$  and  $p$  expansions, allowing for the simultaneous presence of quarks with masses corresponding to these two regimes. The existence of such a mixed expansion will be useful for lattice simulations at the physical points of the three lightest quark flavors  $u, d$  and  $s$ , or, more modestly, simulations where only associated valence quarks are taken to that limit.

Let us consider an  $N_f$ -flavor theory in a finite volume  $V = L^3T$ ,

$$\mathcal{L} = \frac{F^2}{4} \text{Tr}[\partial_\mu U(x)^\dagger \partial_\mu U(x)] - \frac{\Sigma}{2} \text{Tr}[\mathcal{M}^\dagger U(x) U_\theta + U_\theta^\dagger U(x)^\dagger \mathcal{M}] + \dots, \quad (2.1)$$

where  $U(x) \in \text{SU}(N_f)$  and  $U_\theta = \exp(i\theta/N_f)\mathbf{I}$ . Here  $\theta$  is a QCD vacuum angle, introduced here only in order to be able to project on fixed gauge field topology by doing a Fourier transform in  $\theta$ . As usual,  $\Sigma$  denotes the infinite-volume chiral condensate in the massless limit, and  $F$  is similarly the pion decay constant in the chiral limit. Note that there are next-to-leading order terms, indicated here by ellipses, each of which correspond to additional low-energy constants denoted by, in the  $\text{SU}(3)$  case,  $L_i$ .

For the mass matrix  $\mathcal{M} = \text{diag}(m_1, m_2 \dots)$ , we consider the most general non-degenerate case, where we have  $N_l$  light quark masses in the  $\epsilon$ -regime:

$$\mathcal{M}_{l_i l_i} \equiv m_{l_i} \sim \mathcal{O}(1/V), \quad (2.2)$$

while the other  $N_h = N_f - N_l$  quarks are heavier:

$$\mathcal{M}_{h_i h_i} \equiv m_{h_i} \sim \mathcal{O}(1/V^{1/2}), \quad (2.3)$$

in units of the cut-off of the theory. Here and in the following, we put a subscript  $l$  for the light sector and  $h$  for the heavier sector and denote the mass matrices in those sectors by:

$$\mathcal{M}_l \equiv \mathbf{P}_l \mathcal{M} \mathbf{P}_l \quad \mathcal{M}_h \equiv \mathbf{P}_h \mathcal{M} \mathbf{P}_h, \quad (2.4)$$

where  $\mathbf{P}_l, \mathbf{P}_h$  are projectors on the *light* and *heavier* sectors respectively. The working assumption is of course always that chiral perturbation theory is meaningful even for the heavier sector.

In ref. [6] an expansion was proposed according to the following counting rules:

$$p_\mu \sim \mathcal{O}(\epsilon), \quad L, T \sim \mathcal{O}(1/\epsilon), \quad \mathcal{M}_{ll} \sim \mathcal{O}(\epsilon^4), \quad \mathcal{M}_{hh} \sim \mathcal{O}(\epsilon^2). \quad (2.5)$$

An inspection of the pion propagator shows that the zero modes of the Nambu-Goldstone fields associated with the generators in  $\text{SU}(N_l)$  need to be treated non-perturbatively. All the remaining zero-modes are perturbative when  $N_l, N_h \neq 0$ . Some subtleties appear however in the partially-quenched case where all the light quarks are quenched, that is the replica limit  $N_l \rightarrow 0$ .<sup>2</sup> In this case, it is easy to see that the Goldstone field associated to the generator  $T_\eta$ ,

$$T_\eta = \begin{pmatrix} \frac{1}{2N_l} \mathbf{I}_l & 0 \\ 0 & -\frac{1}{2N_h} \mathbf{I}_h \end{pmatrix}, \quad (2.6)$$

gets massless in the replica limit  $N_l = 0$ . Here  $\mathbf{I}_{l/h}$  are the identity matrices in the light and heavier sectors. Note that  $T_\eta$  looks ill-defined when  $N_l = 0$  but keeping  $N_l$  finite until the very end of the calculation, one sees that the replica limit  $N_l \rightarrow 0$  can be safely taken.

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<sup>2</sup>As usual the fully-quenched case  $N_l + N_h = 0$  requires the presence of the singlet to be well-defined, but as long as  $N_l + N_h \neq 0$  the singlet decouples.

To treat all cases on the same footing, we therefore consider the following parametrization:<sup>3</sup>

$$U(x) = \exp\left(\frac{2i\xi(x)}{F}\right) \begin{pmatrix} U_0 & 0 \\ 0 & \mathbf{I}_h \end{pmatrix} \exp(i\eta T_\eta), \quad (2.7)$$

where  $U_0 \in \text{SU}(N_l)$  is a constant matrix,  $\eta$  is the zero-mode of the Nambu-Goldstone field associated with the  $T_\eta$  generator. The  $\xi$  fields contain the non-zero modes corresponding to all Nambu-Goldstone fields, and also all zero modes of those degrees of freedom that are not treated separately. They therefore satisfy the constraints

$$\int d^4x \text{Tr}[T_a \xi(x)] = \int d^4x \text{Tr}[T_\eta \xi(x)] = 0, \quad (2.8)$$

where  $T_a$  is a generator of the subgroup  $\text{SU}(N_l)$ . Note that the zero-mode of the  $T_\eta$  generator is not included in the  $\xi$  field (it is projected out by the second constraint in eq. (2.8)), and included explicitly in the last term of eq. (2.7).

We are interested in computing the correlation functions in sectors of fixed topology. Following the same derivation in [6] we rewrite

$$U(x)U_\theta = U(x) \begin{pmatrix} e^{\frac{i\theta}{2N_l} \mathbf{I}_l} & 0 \\ 0 & e^{\frac{i\theta}{2N_h} \mathbf{I}_h} \end{pmatrix} = \exp\left(\frac{2i\xi(x)}{F}\right) \begin{pmatrix} \bar{U}_0 & 0 \\ 0 & e^{-i\frac{\bar{\eta}}{N_h} \mathbf{I}_h} \end{pmatrix}, \quad (2.9)$$

where we have defined

$$\bar{\eta} \equiv \frac{\eta - \theta}{2} \quad \bar{\theta} \equiv \frac{\eta + \theta}{2} \quad (2.10)$$

and  $\bar{U}_0 \in U(N_l)$  with  $\det \bar{U}_0 = e^{i\bar{\theta}} \det(U_0) = e^{i\bar{\theta}}$ . The partition functional in sectors of fixed topology can then be written as:

$$\mathcal{Z}_\nu \simeq \int [d\xi] [d\bar{\eta}] \int_{U(N_l)} [d\bar{U}_0] J(\xi) \det(\bar{U}_0)^\nu \exp\left(-\int d^4x \mathcal{L}(\xi, \bar{\eta}, \bar{U}_0)\right), \quad (2.11)$$

where as in the standard  $\epsilon$ -regime, the projection on fixed topology results in the enlargement of the zero-mode integration from  $\text{SU}(N_l)$  to  $U(N_l)$ .  $J(\xi)$  is the Jacobian of the change of variables of eq. (2.7). According to the power-counting of eq. (2.5), it can be shown that a consistent power-counting for the fields  $\xi$  is:

$$\xi \sim \mathcal{O}(\epsilon), \quad (2.12)$$

therefore both the Lagrangian and the Jacobian can be perturbatively expanded in powers of  $\xi$ . At next-to-leading order we find [3, 6]:

$$J(\xi) = 1 - \frac{4}{3F^2V} \int d^4x \sum_{a \in \text{SU}(N_l) \cup T_\eta} \text{Tr}[T_a^2 \xi^2 - (T_a \xi)^2](x) + \mathcal{O}(\epsilon^4). \quad (2.13)$$

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<sup>3</sup>In reference [6] a different parametrization was considered for the case when some or all of the light quarks are dynamical. In that case the  $\eta$  zero-mode is also perturbative and can be included in  $\xi$ . It turns out that the parametrization of eq. (2.7) simplifies the calculations and allows one to consider the full and partially quenched cases on the same footing. Therefore we consider only eq. (2.7) in the present paper. We have checked that both give the same result in the full case.

The Lagrangian can also be obtained as an expansion in  $\epsilon$ :

$$\mathcal{L} = \mathcal{L}^{(4)} + \mathcal{L}^{(6)} + \dots, \quad (2.14)$$

with terms up to  $\mathcal{O}(\epsilon^4)$ , up to  $\mathcal{O}(\epsilon^6)$ , etc. Concerning the integration over the variable  $\bar{\eta}$ , we can perform a saddle-point approximation following the derivation of [6]. The leading-order Lagrangian is found to be:

$$\mathcal{L}^{(4)} \equiv \text{Tr} [\partial_\mu \xi \partial_\mu \xi] - \frac{\Sigma}{2} \text{Tr} [\mathcal{M}_l (\bar{U}_0 + \bar{U}_0^\dagger)] + \frac{2\Sigma}{F^2} \text{Tr} \left[ \mathcal{M}_h \left( \xi - \frac{F}{2} \frac{\bar{\eta}}{N_h} \mathbf{P}_h \right)^2 \right] + i \frac{\nu}{V} \bar{\eta}. \quad (2.15)$$

This quadratic form implies also a power-counting of  $\bar{\eta} \sim \epsilon$ . According to this rule, the last term in eq. (2.15) could be treated as a perturbation. This is true as long as  $\nu \sim \mathcal{O}(\epsilon^0)$ , as is usually the case in the  $\epsilon$ -regime. However, in the partially-quenched case  $N_l = 0$ , the distribution of topological charge is controlled by the heavy quarks only. Indeed the  $\nu$  dependence of the leading-order partition function is found to be

$$Z_\nu^{\text{LO}} \propto \exp \left( -\frac{\nu^2}{VF^2} \sum_h \frac{1}{M_{hh}^2} \right) \int_{U(N_l)} [d\bar{U}_0] \det(\bar{U}_0)^\nu \exp \left( \frac{\Sigma}{2} \text{Tr} [\mathcal{M}_l (\bar{U}_0 + \bar{U}_0^\dagger)] \right), \quad (2.16)$$

which in the case  $N_l = 0$  implies:

$$\langle \nu^2 \rangle = \frac{1}{2} VF^2 \frac{1}{\sum_h \frac{1}{M_{hh}^2}} \sim \epsilon^{-2}, \quad (2.17)$$

a scaling that makes the last term in eq. (2.15) of  $\mathcal{O}(\epsilon^4)$ , and therefore of leading-order. In order to recover the results at  $\theta = 0$  by averaging over topology, it is therefore necessary to keep the last term in eq. (2.15) in the leading-order Lagrangian, or equivalently assume that  $\nu \sim \epsilon^{-1}$ . This is not necessary however as long as  $N_l > 0$ , since the distribution of topological charge in that case is controlled by the light quarks.

It is straightforward to derive the propagator for the  $\xi$  fields in the light or mixed sectors from eq. (2.15), validating the power-counting of eq. (2.12) and ensuring that the replica limit  $N_l = 0$  is well-defined:

$$\langle \xi_{l_1 l_2}(x) \xi_{l_3 l_4}(y) \rangle = \frac{1}{2} \left[ \delta_{l_1 l_4} \delta_{l_2 l_3} \bar{\Delta}(x-y, 0) - \delta_{l_1 l_2} \delta_{l_3 l_4} \bar{G}(x-y, 0, 0) \right], \quad (2.18)$$

$$\langle \xi_{l_1 h_1}(x) \xi_{h_2 l_2}(y) \rangle = \frac{1}{2} \delta_{l_1 l_2} \delta_{h_1 h_2} \Delta \left( x-y, \frac{M_{h_1 h_1}^2}{2} \right) \quad (2.19)$$

$$\langle \xi_{l_1 l_2}(x) \xi_{h_1 h_2}(y) \rangle = -\frac{1}{2} \delta_{l_1 l_2} \delta_{h_1 h_2} \bar{G}(x-y, 0, M_{h_1 h_1}^2), \quad (2.20)$$

while in the heavy sector there always appear the combination:

$$\begin{aligned} \left\langle \left( \xi_{h_1 h_2}(x) - \frac{F\bar{\eta}}{2N_h} \delta_{h_1 h_2} \right) \left( \xi_{h_3 h_4}(y) - \frac{F\bar{\eta}}{2N_h} \delta_{h_3 h_4} \right) \right\rangle = \\ \frac{1}{2} \left[ \delta_{h_1 h_4} \delta_{h_2 h_3} \Delta(x-y, M_{h_1 h_2}^2) - \delta_{h_1 h_2} \delta_{h_3 h_4} (\bar{G}(x-y, M_{h_1 h_1}^2, M_{h_3 h_3}^2) \right. \\ \left. + G_0(M_{h_1 h_1}^2, M_{h_3 h_3}^2)) \right], \quad (2.21) \end{aligned}$$



where

$$\bar{\Delta}(x, M^2) \equiv \frac{1}{V} \sum_{p \neq 0} \frac{e^{ipx}}{p^2 + M^2}, \quad \Delta(x, M^2) \equiv \bar{\Delta}(x, M^2) + \frac{1}{VM^2} \quad (2.22)$$

$$\bar{G}(x, M_1^2, M_2^2) \equiv \frac{1}{V} \sum_{p \neq 0} \frac{e^{ipx}}{(p^2 + M_1^2)(p^2 + M_2^2) \left( \frac{N_l}{p^2} + \sum_h^{N_h} \frac{1}{p^2 + M_{hh}^2} \right)} \quad (2.23)$$

$$G_0(M_1^2, M_2^2) \equiv \frac{2\nu^2}{V^2 F^2} \left( \frac{1}{M_1^2 M_2^2} \right), \quad (2.24)$$

and

$$M_{hh'}^2 \equiv (m_h + m_{h'}) \frac{\Sigma}{F^2}, \quad (2.25)$$

is the mass of the meson fields made of the heavier quarks. The summation  $\sum_{p \neq 0}$  is taken over the 4-momentum

$$p = 2\pi(n_t/T, n_x/L, n_y/L, n_z/L), \quad (2.26)$$

with integers  $n_i$ 's. Note that the term  $G_0$  is formally of higher order if  $\nu \sim \mathcal{O}(1)$ .

In this work, one encounters  $\bar{G}(x, M_1^2, M_2^2)$  with  $M_1 = M_2 = 0$  only, both in full and partially quenched theory.<sup>4</sup> In the full theory,  $\bar{G}(x, 0, 0)$  can in principle be rewritten in terms of  $\bar{\Delta}$ 's, as one would have expected on general grounds. In the case of  $N_l = 2$  and  $N_h = 1$ , which is the phenomenologically most interesting case, for example,

$$\bar{G}(x, 0, 0) = \frac{1}{V} \sum_{p \neq 0} \frac{e^{ipx}}{p^4 \left( \frac{2}{p^2} + \frac{1}{p^2 + M_{hh}^2} \right)} = \frac{1}{2} \bar{\Delta}(x, 0) - \frac{1}{6} \bar{\Delta} \left( x, \frac{2}{3} M_{hh}^2 \right). \quad (2.27)$$

But we keep using the notation of  $\bar{G}(x, 0, 0)$  for simplicity in both the general case with  $N_l + N_h$  flavors and the partially quenched case, where a double pole appears.

Correlation functions are obtained by inserting appropriate source operators in the above partition function and taking suitable functional derivatives [3]. The  $U(N_l)$  integral over zero modes  $\bar{U}_0$  is then done exactly, while the  $\xi, \bar{\eta}$  integrals are treated perturbatively. We return to the zero-mode integrations in section 4. Here we will be working at next-to-leading order in the perturbative expansion and therefore up to the  $\mathcal{L}^{(6)}$  term in the Lagrangian contributes:

$$\begin{aligned} \mathcal{L}^{(6)} = & \frac{2}{3F^2} \text{Tr} [(\partial_\mu \xi(x) \xi(x))^2 - (\partial_\mu \xi(x))^2 \xi^2(x)] - \frac{2\Sigma}{3F^4} \text{Tr} [\mathcal{M}_h \xi^4(x)] \\ & + \frac{\Sigma}{F^2} \text{Tr} \left[ \mathcal{M}_l \left( \xi^2(x) \bar{U}_0 + \bar{U}_0^\dagger \xi^2(x) \right) \right] + \frac{16\Sigma^2 L_4}{F^4} \text{Tr} [\mathcal{M}_h] \text{Tr} [\partial_\mu \xi(x) \partial_\mu \xi(x)] \\ & - 16 \frac{\Sigma L_6}{F^4} \text{Tr} [\mathcal{M}_h] \text{Tr} \left[ \mathcal{M}_l \left( \bar{U}_0 + \bar{U}_0^\dagger \right) \right] + \dots \end{aligned} \quad (2.28)$$

where the ellipses indicate terms of the same order that involve only  $\xi_{hl}$  or  $\xi_{hh}$  and do not contribute to the observables where valence quarks are only in the light sector, as we will be considering in this paper.

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<sup>4</sup>The fully quenched case needs special care; it will be discussed later.

### 3. Two-point correlation functions

Correlation functions are obtained by inserting appropriate source operators in the above partition function and taking suitable functional derivatives [3]. Since we consider the fully non-degenerate theory, we have to treat all possible  $N_f \times N_f$  bilinear quark operators separately. We therefore define

$$\begin{aligned} P^{ij}(x) &= i\bar{q}_i(x)\gamma_5 q_j(x), & S^{ij}(x) &= \bar{q}_i(x)q_j(x), \\ A_\mu^{ij}(x) &= i\bar{q}_i(x)\gamma_5\gamma_\mu q_j(x), & V_\mu^{ij}(x) &= i\bar{q}_i(x)\gamma_\mu q_j(x). \end{aligned} \quad (3.1)$$

The corresponding operators in ChPT are to the leading order given by

$$P^{ij}(x) = -i\frac{\Sigma}{2} \left( [U(x)U_\theta]_{ij} - [U_\theta^\dagger U^\dagger(x)]_{ji} \right), \quad (3.2)$$

$$S^{ij}(x) = \frac{\Sigma}{2} \left( [U(x)U_\theta]_{ij} + [U_\theta^\dagger U^\dagger(x)]_{ji} \right), \quad (3.3)$$

$$A_\mu^{ij}(x) = i\frac{F^2}{2} [\partial_\mu U(x)U^\dagger(x) - \partial_\mu U^\dagger(x)U(x)]_{ij}, \quad (3.4)$$

$$V_\mu^{ij}(x) = i\frac{F^2}{2} [\partial_\mu U(x)U^\dagger(x) + \partial_\mu U^\dagger(x)U(x)]_{ij}. \quad (3.5)$$

The conventional irreducible representations are obtained by appropriate combinations of  $i$ 's and  $j$ 's. The charged pion-type meson operator and the neutral one are, for example, given by (we simply denote 1 for the up quark and 2 for the down quark)

$$P^{\pi^\pm}(x) = \frac{1}{2}(P^{12}(x) + P^{21}(x)), \quad \text{and} \quad P^{\pi^0}(x) = \frac{1}{2}(P^{11}(x) - P^{22}(x)). \quad (3.6)$$

In the following, we use indices  $v$  and  $v'$  in order to specify the valence sector which in this paper is always taken to be in the  $\epsilon$ -regime.

In figures 1 and 2 we show the Feynman diagrams resulting from the  $\xi$  integration that contribute to the current and scalar propagators at next-to-leading order in the  $\epsilon$ -expansion. The scalar correlators start at  $\mathcal{O}(\epsilon^0)$ , while the first contribution to the currents is  $\mathcal{O}(\epsilon^2)$ . Note that disconnected diagrams contribute because they are connected through the zero-mode integrations. We also assume here that the operators are separated from each other and the usual contact terms are not included.

For the practical purpose of comparing to lattice QCD simulations, we will present results in the non-singlet irreducible representation, or "charged-pion" type correlation functions, with the zero-momentum projection (integration over 3-dimensional space), namely,

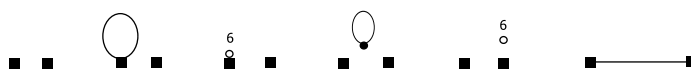
$$\mathcal{P}_{vv'}^c(t) \equiv \frac{1}{4} \int d^3x \langle (P^{vv'}(x) + P^{v'v}(x))(P^{vv'}(0) + P^{v'v}(0)) \rangle_{U,\xi}, \quad (3.7)$$

$$\mathcal{S}_{vv'}^c(t) \equiv \frac{1}{4} \int d^3x \langle (S^{vv'}(x) + S^{v'v}(x))(S^{vv'}(0) + S^{v'v}(0)) \rangle_{U,\xi}, \quad (3.8)$$

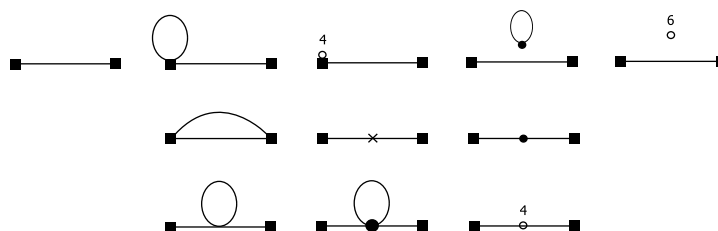
$$\mathcal{A}_{vv'}^c(t) \equiv \frac{1}{4} \int d^3x \langle (A_0^{vv'}(x) + A_0^{v'v}(x))(A_0^{vv'}(0) + A_0^{v'v}(0)) \rangle_{U,\xi}, \quad (3.9)$$

$$\mathcal{V}_{vv'}^c(t) \equiv \frac{1}{4} \int d^3x \langle (V_0^{vv'}(x) + V_0^{v'v}(x))(V_0^{vv'}(0) + V_0^{v'v}(0)) \rangle_{U,\xi}, \quad (3.10)$$

where we assume  $v \neq v'$ .



**Figure 1:** Diagrams contributing to the scalar and pseudoscalar connected correlators. The lines are  $\xi$  propagators. Squares indicate the scalar and pseudoscalar operators. The filled dots indicate a mass insertion from the Lagrangian. Empty dots indicate the insertion of an operator coming from the NLO Lagrangian, and they are also labeled with the subindex of the associated coupling constant,  $L_i$ .



**Figure 2:** Diagrams contributing to the vector and axial correlators. The lines are  $\xi$  propagators. Squares indicate the vector or axial vector operators. The filled dots indicate a mass insertion. A cross indicate a contribution from the Jacobian. Empty dots indicate the insertion of an operator coming from the NLO Lagrangian, and they are also labeled with the subindex of the associated coupling constant,  $L_i$ .

We also present the "disconnected" contributions for the scalar and pseudoscalars,

$$\mathcal{P}_{vv'}^d(t) \equiv \int d^3x \langle P^{vv}(x) P^{v'v'}(0) \rangle_{U,\xi}, \quad (3.11)$$

$$\mathcal{S}_{vv'}^d(t) \equiv \int d^3x \langle S^{vv}(x) S^{v'v'}(0) \rangle_{U,\xi}, \quad (3.12)$$

which are useful to estimate the finite size contributions from the chiral fields to the  $\eta'$  meson correlators.

To simplify the  $t$ -dependence of our expressions, let us define

$$h_1(t/T) \equiv \frac{1}{T} \int d^3x \bar{\Delta}(x, 0) = \frac{1}{2} \left( \frac{t}{T} - \frac{1}{2} \right)^2 - \frac{1}{24}, \quad (3.13)$$

and

$$r(t) \equiv \int d^3x \bar{G}(x, 0, 0). \quad (3.14)$$

Note that the latter still depends on the  $N_h$  heavier quark masses. In the appendix A, we list how to perform the zero-momentum projection of various combination of  $\bar{\Delta}(x, M^2)$ 's.

Defining also

$$\frac{\tilde{\Sigma}}{\Sigma} \equiv 1 - \frac{1}{F^2} \left[ N_l \bar{\Delta}(0, 0) + \sum_h^{N_h} \Delta(0, M_{hh}^2/2) - \bar{G}(0, 0, 0) - 16L_6 \sum_h^{N_h} M_{hh}^2 \right], \quad (3.15)$$

$$\frac{\tilde{F}}{F} \equiv 1 - \frac{1}{2F^2} \left[ N_l \bar{\Delta}(0, 0) + \sum_h^{N_h} \Delta(0, M_{hh}^2/2) - 8L_4 \sum_h^{N_h} M_{hh}^2 \right], \quad (3.16)$$

and

$$\mu_l \equiv m_l \Sigma V, \quad (3.17)$$

the results for the pseudoscalar and scalar non-singlet (connected) correlators can be written as

$$\mathcal{P}_{vv'}^c(t) = -L^3 \frac{\tilde{\Sigma}^2}{4} \left[ \mathcal{K}_-^{0(N_l)} \right]_{\text{NLO}} + \frac{\Sigma^2}{2F^2} \left[ \mathcal{K}_+^{1(N_l)} Th_1 \left( \frac{t}{T} \right) - \mathcal{K}_+^{0(N_l)} r(t) \right], \quad (3.18)$$

$$\mathcal{S}_{vv'}^c(t) = L^3 \frac{\tilde{\Sigma}^2}{4} \left[ \mathcal{K}_+^{0(N_l)} \right]_{\text{NLO}} + \frac{\Sigma^2}{2F^2} \left[ \mathcal{K}_-^{1(N_l)} Th_1 \left( \frac{t}{T} \right) + \mathcal{K}_-^{0(N_l)} r(t) \right], \quad (3.19)$$

and their disconnected correlators are given by

$$\mathcal{P}_{vv'}^d(t) = -L^3 \tilde{\Sigma}^2 \left[ \mathcal{K}_-^{2(N_l)} \right]_{\text{NLO}} + \frac{2\Sigma^2}{F^2} \left[ \mathcal{K}^{3(N_l)} Th_1 \left( \frac{t}{T} \right) - \mathcal{K}_+^{2(N_l)} r(t) \right], \quad (3.20)$$

$$\mathcal{S}_{vv'}^d(t) = L^3 \tilde{\Sigma}^2 \left[ \mathcal{K}_+^{2(N_l)} \right]_{\text{NLO}} - \frac{2\Sigma^2}{F^2} \left[ \mathcal{K}^{3(N_l)} Th_1 \left( \frac{t}{T} \right) - \mathcal{K}_-^{2(N_l)} r(t) \right], \quad (3.21)$$

The  $\mathcal{K}$  functions represent the zero-mode integrals over  $U(N_l)$  and they depend only on the light quark masses (to simplify the notation we denote  $\bar{U}_0$  by  $U$  in this section):

$$\mathcal{K}_{\pm}^{0(N_l)}(\{\mu_l\}) = \frac{1}{4} \langle (U_{vv'} + U_{v'v} \pm U_{v'v}^\dagger \pm U_{vv'}^\dagger)^2 \rangle_{U(N_l)}, \quad (3.22)$$

$$\mathcal{K}_{\pm}^{1(N_l)}(\{\mu_l\}) = 1 \pm \frac{1}{2} \langle U_{vv} U_{v'v'} + U_{vv}^{\dagger} U_{v'v'}^{\dagger} \rangle_{U(N_l)} \pm \frac{1}{4} \langle U_{vv'}^2 + U_{v'v}^2 + h.c. \rangle_{U(N_l)}, \quad (3.23)$$

$$\mathcal{K}_{\pm}^{2(N_l)}(\{\mu_l\}) = \frac{1}{4} \langle (U_{vv} \pm U_{vv}^{\dagger})(U_{v'v'} \pm U_{v'v'}^{\dagger}) \rangle_{U(N_l)}, \quad (3.24)$$

$$\mathcal{K}^{3(N_l)}(\{\mu_l\}) = \frac{1}{4} \langle U_{vv'} U_{v'v} + U_{v'v}^{\dagger} U_{vv'}^{\dagger} \rangle_{U(N_l)}, \quad (3.25)$$

where averages are over zero modes:

$$\langle (\dots) \rangle_{U(N_l)} \equiv \int_{U(N_l)} dU (\dots) (\det U)^{\nu} e^{\frac{\Sigma V}{2} \text{Tr}[\mathcal{M}_l U + U^{\dagger} \mathcal{M}_l^{\dagger}]}. \quad (3.26)$$

The label  $\square_{\text{NLO}}$  implies that the integral must be computed with  $\tilde{\Sigma}$  instead of  $\Sigma$ . We will present the explicit results for these integrals in section 4.

For the axial and vector (connected) current correlators we obtain:

$$\begin{aligned} \mathcal{A}_{vv'}^c(t) &= -\frac{\tilde{F}^2}{2T} \left[ \mathcal{J}_+^{0(N_l)} \right]_{\text{NLO}} + \frac{T}{2V} \left[ N_l k_{00} + \sum_h^{N_h} k_{00}^s (M_{hh}^2/2) \right] \mathcal{J}_-^{0(N_l)} \\ &\quad - \frac{\Sigma}{4} \left( \mathcal{J}_+^{1(N_l)} + \frac{2N_l}{\Sigma V} \left( \mathcal{J}_+^{0(N_l)} - \mathcal{J}_-^{0(N_l)} \right) \right) Th_1 \left( \frac{t}{T} \right), \end{aligned} \quad (3.27)$$

$$\begin{aligned} \mathcal{V}_{vv'}^c(t) &= -\frac{\tilde{F}^2}{2T} \left[ \mathcal{J}_-^{0(N_l)} \right]_{\text{NLO}} + \frac{T}{2V} \left[ N_l k_{00} + \sum_h^{N_h} k_{00}^s (M_{hh}^2/2) \right] \mathcal{J}_+^{0(N_l)} \\ &\quad - \frac{\Sigma}{4} \left( \mathcal{J}_-^{1(N_l)} + \frac{2N_l}{\Sigma V} \left( \mathcal{J}_-^{0(N_l)} - \mathcal{J}_+^{0(N_l)} \right) \right) Th_1 \left( \frac{t}{T} \right), \end{aligned} \quad (3.28)$$

where we have defined

$$\frac{T^2}{V} k_{00}^s(M^2) \equiv T \frac{d}{dT} \Delta(0, M^2) \quad \frac{T^2}{V} k_{00} \equiv T \frac{d}{dT} \bar{\Delta}(0, 0), \quad (3.29)$$

and the  $\mathcal{J}$  functions are given by:

$$\mathcal{S}_v^{(N_l)}(\{\mu_l\}) \equiv \frac{1}{2} \langle U_{vv} + U_{vv}^{\dagger} \rangle_{U(N_l)}, \quad (3.30)$$

$$\mathcal{J}_{\pm}^{0(N_l)}(\{\mu_l\}) \equiv 1 \pm \frac{\langle U_{vv'} U_{vv'}^{\dagger} + U_{vv} U_{v'v'}^{\dagger} + h.c. \rangle_{U(N_l)}}{2}, \quad (3.31)$$

$$\begin{aligned} \mathcal{J}_{\pm}^{1(N_l)}(\{\mu_l\}) &\equiv \left( (2m_{v'} \pm m_v) \mathcal{S}_v^{(N_l)} \right. \\ &\quad \left. \pm \frac{\langle U_{vv}^{\dagger} (U \mathcal{M}_l U)_{v'v'} + U_{v'v}^{\dagger} (U \mathcal{M}_l U)_{vv'} + h.c. \rangle_{U(N_f)}}{2} \right) \pm (v \leftrightarrow v') \end{aligned} \quad (3.32)$$

We stress that all the heavier mass dependence is explicit in the results of eqs. (3.18)–(3.19), (3.20)–(3.21) and (3.27)–(3.28) since the zero-mode integrals involve the light sector only. We also note that these results agree with those obtained for the special case of the left-handed current two-point function obtained in [6].

Next, we need to discuss the ultraviolet divergences of  $\Delta(0, M^2)$ 's and similar ones associated with  $\bar{G}$ 's. The explicit form in finite volume is given by [4],

$$\Delta(0, M^2) = \frac{M^2}{16\pi^2} (\ln M^2 + c_1) + g_1(M^2), \quad (3.33)$$

where  $c_1$  represents the logarithmic divergence which is independent of  $M$  and the volume, and  $g_1$  denotes the finite volume correction [4]. The numerical evaluation of  $g_1$  is discussed in section 5.

Since  $F$  and  $m_i \Sigma$  are not renormalized at infinite volume, the logarithmic divergence  $c_1$  must be absorbed in a renormalization of  $L_i$ 's. The mass-independent shift in

$$L_4 \rightarrow L_4 + \frac{1}{(16\pi)^2} c_1, \quad L_6 \rightarrow L_6 + \frac{1}{(16\pi)^2} \left( \frac{1}{2} + \frac{1}{N_f^2} \right) c_1 \quad (3.34)$$

is enough to give finite results in the above correlators. This shift is exactly the same as at infinite volume [1].

Note that the formally divergent expressions other than  $\bar{\Delta}(0, M^2)$  (for non-zero  $M$ ),

$$\bar{\Delta}(0, 0) = -\frac{\beta_1}{V^{1/2}}, \quad (3.35)$$

$$k_{00}^s(M^2) = \sum_{\mathbf{q}=(p_1,p_2,p_3)} \frac{-1}{4 \sinh^2(\sqrt{|\mathbf{q}|^2 + M^2 T/2})},$$

$$k_{00} = \sum_{\mathbf{q}=(p_1,p_2,p_3) \neq 0} \frac{-1}{4 \sinh^2(|\mathbf{q}|T/2)} + \frac{1}{12}, \quad (3.36)$$

become finite after dimensional regularization.

Finally we note that the dependence on the heavier quark masses is as expected on general grounds (see also the discussion in [6]). Indeed, up to exponentially suppressed finite-volume corrections in  $M_{hh}L$ , the correlators above coincide with those in the  $\epsilon$ -regime for  $N_l$  light quarks as if there were no heavier quarks whatsoever. The only remnant of the heavier quarks is seen in the modified low-energy couplings  $\Sigma$  and  $F$ , i.e. by the terms that depend on  $M_{hh}$  in  $\tilde{\Sigma}$  and  $\tilde{F}$ . This is as usual in chiral perturbation theory.

### 3.1 An alternative mixed-regime expansion

As a check on our results, we have performed the same calculation by means of an alternative method where the parametrization of fields is as in the standard  $\epsilon$ -regime. The counting rule we use, however, is the same as the one in the standard  $p$ -regime for the heavy flavors. All zero modes in the full  $SU(N_f)$  group are then treated non-perturbatively. Such a parametrization has the advantage that the matching to the  $\epsilon$  regime is smooth by construction.

The result of this alternative scheme leads to definitions of  $\tilde{\Sigma}$  and  $\tilde{F}$  which are identical to eqs. (3.15) and (3.16) except for the replacements  $\Delta \rightarrow \bar{\Delta}$  and  $G \rightarrow \bar{G}$ . Similarly, all other results presented above are reproduced with the only difference that now all zero-mode integrals are performed over the whole  $U(N_f)$  group and therefore depend on all the quark masses, including the heavier ones.

In contrast to the results presented in eqs. (3.18)–(3.21) and (3.27)–(3.28), in this alternative approach one can take the limit  $M_{hh} \rightarrow 0$  smoothly. The results then coincide with those fully in the  $\epsilon$ -regime. Indeed, our results in that limit agree with partially quenched scalar and pseudoscalar correlators for non-degenerate masses that can be found

in ref. [15]. The left-handed current correlator can be found in [6], and our present results also reproduce that special case.

The reason that the matching limit is smooth in this parametrization is because the zero-momentum modes of the massive mesons are resummed, while in the expansion of section 2, they are treated perturbatively. The two results should therefore coincide when the zero-mode integrals of the  $U(N_f)$ -theory are expanded to the appropriate order in  $1/\mu_h \sim \mathcal{O}(\epsilon^2)$ . In the next section we will show that this is indeed the case. This provides a rather non-trivial consistency check on our results, and it confirms that the expected matching between  $\epsilon$  and mixed regimes actually holds.

#### 4. Non-perturbative zero-mode integrals

In this section, we complete the calculations of the correlators by giving explicitly the zero-mode integrals defined in eqs. (3.22)–(3.25) and (3.30)–(3.32), in the full (unquenched), the partially quenched, and the fully quenched theories. Here we present the results of general partially quenched calculations. As is well-known, the results for the full theory can be viewed as special cases, obtained by equating the valence quark masses to those of the sea quarks. The essential ingredient is the functional [42],

$$\mathcal{Z}_{n,m}^\nu(\{\mu_i\}) = \frac{\det[\mu_i^{j-1} \mathcal{J}_{\nu+j-1}(\mu_i)]_{i,j=1,\dots,n+m}}{\prod_{j>i=1}^n (\mu_j^2 - \mu_i^2) \prod_{j>i=n+1}^{n+m} (\mu_j^2 - \mu_i^2)}, \quad (4.1)$$

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  $i = 1, \dots, n$  and  $\mathcal{J}_{\nu+j-1}(\mu_i) \equiv I_{\nu+j-1}(\mu_i)$  for  $i = n+1, \dots, n+m$ , where  $I_\nu$  and  $K_\nu$  are the modified Bessel functions.  $m = N_v + N_l$  denotes the number of (light) quarks, from which  $N_v$  valence quarks are quenched by the  $n = N_v$  bosonic quark contents. Since we are interested in mesonic two-point functions, we need  $n = N_v = 2$  at most.

From this functional, by taking appropriate derivatives with respect to the parameters  $\mu_i$ , one can derive all the required integrals, both in the full as in the partially-quenched limits. The technical steps of our calculation have followed those of ref. [15] and in this section we simply show the final results. Details of how this can be used to compute all relevant group integrals are presented in appendix B. An important relation can be derived from Ward-Takahashi identities (see appendix C) that holds for the full, partially-quenched and quenched cases:

$$\mathcal{J}_\pm^{1(N_l)} = 2(m_v \pm m_{v'}) (\mathcal{S}_v^{(N_l)} \pm \mathcal{S}_{v'}^{(N_l)}) \mp \frac{2N_l}{\Sigma V} (\mathcal{J}_+^{0(N_l)} - \mathcal{J}_-^{0(N_l)}). \quad (4.2)$$

As building blocks, let us define two quantities,

$$\frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma} \equiv - \lim_{\mu_b \rightarrow \mu_v} \frac{\partial}{\partial \mu_b} \ln \mathcal{Z}_{1,1+N_l}^\nu(\mu_b | \mu_v, \{\mu_s\}), \quad (4.3)$$

$$D_\nu^{\text{PQ}}(\mu_{v1}, \mu_{v2}, \{\mu_s\}) \equiv \lim_{\mu_{b1} \rightarrow \mu_{v1}, \mu_{b2} \rightarrow \mu_{v2}} \frac{\partial_{\mu_{v1}} \partial_{\mu_{v2}} \mathcal{Z}_{2,2+N_l}^\nu(\mu_{b1}, \mu_{b2} | \mu_{v1}, \mu_{v2}, \{\mu_s\})}{\mathcal{Z}_{N_l}^\nu(\{\mu_s\})}. \quad (4.4)$$

where the sea quark mass dependence is denoted by  $\{\mu_s\} = \{\mu_{l_1}, \dots, \mu_{l_{N_l}}\}$ .

Let us also give their analogous expressions in the unquenched theory (we need only the case where the valence mass is equal to one of the light sector,  $m_v = m_l$  in the  $\epsilon$ -regime.),

$$\frac{\Sigma_\nu^{\text{full}}(\mu_l, \{\mu_s\})}{\Sigma} \equiv \frac{\partial}{\partial \mu_l} \ln \mathcal{Z}_{N_l}^\nu(\{\mu_s\}) = \lim_{\mu_v \rightarrow \mu_l} \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma}, \quad (4.5)$$

$$D_\nu^{\text{full}}(\mu_{l1}, \mu_{l2}, \{\mu_s\}) \equiv \frac{\partial_{\mu_{l1}} \partial_{\mu_{l2}} \mathcal{Z}_{N_l}^\nu(\{\mu_s\})}{\mathcal{Z}_{N_l}^\nu(\{\mu_s\})} = \lim_{\mu_{v_i} \rightarrow \mu_{l_i}} D_\nu^{\text{PQ}}(\mu_{v1}, \mu_{v2}, \{\mu_s\}), \quad (4.6)$$

and the fully quenched limits,

$$\lim_{\{\mu_s\} \rightarrow \infty} \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma} = \frac{\Sigma_\nu^{\text{FQ}}(\mu_v)}{\Sigma}, \quad (4.7)$$

$$\lim_{\{\mu_s\} \rightarrow \infty} D_\nu^{\text{PQ}}(\mu_{v1}, \mu_{v2}, \{\mu_s\}) = 1 + \frac{\nu^2}{\mu_{v1} \mu_{v2}}. \quad (4.8)$$

#### 4.1 Explicit results

With the above expressions, one can calculate all the non-perturbative integrals we need to evaluate  $\mathcal{J}_\pm$  etc. Further details can be found in appendix B.

##### 1. Full (unquenched) theory

We start by listing the results for the full (unquenched) theory, where the valence masses are equal to those of the sea quarks ( $m_v = m_l$  and  $m_{v'} = m_{l'}$ ).

$$\mathcal{S}_l^{(N_l)}(\mu_l, \{\mu_s\}) = \frac{\Sigma_\nu^{\text{full}}(\mu_l, \{\mu_s\})}{\Sigma}, \quad (4.9)$$

$$\mathcal{K}_\pm^{0(N_l)}(\mu_l, \mu_{l'}, \{\mu_s\}) = \frac{\pm 2}{\mu_l \mp \mu_{l'}} \left( \frac{\Sigma_\nu^{\text{full}}(\mu_l, \{\mu_s\})}{\Sigma} \mp \frac{\Sigma_\nu^{\text{full}}(\mu_{l'}, \{\mu_s\})}{\Sigma} \right), \quad (4.10)$$

$$\mathcal{K}_\pm^{1(N_l)}(\mu_l, \mu_{l'}, \{\mu_s\}) = 1 \pm \left( D_\nu^{\text{full}}(\mu_l, \mu_{l'}, \{\mu_s\}) + \frac{\nu^2}{\mu_l \mu_{l'}} \right), \quad (4.11)$$

$$\mathcal{K}_+^{2(N_l)}(\mu_l, \mu_{l'}, \{\mu_s\}) = D_\nu^{\text{full}}(\mu_l, \mu_{l'}, \{\mu_s\}), \quad (4.12)$$

$$\mathcal{K}_-^{2(N_l)}(\mu_l, \mu_{l'}, \{\mu_s\}) = \frac{\nu^2}{\mu_l \mu_{l'}}, \quad (4.13)$$

$$\mathcal{K}^{3(N_l)}(\mu_l, \mu_{l'}, \{\mu_s\}) = \frac{1}{\mu_l^2 - \mu_{l'}^2} \left( \mu_{l'} \frac{\Sigma_\nu^{\text{full}}(\mu_l, \{\mu_s\})}{\Sigma} - \mu_l \frac{\Sigma_\nu^{\text{full}}(\mu_{l'}, \{\mu_s\})}{\Sigma} \right), \quad (4.14)$$

$$\mathcal{J}_\pm^{0(N_l)}(\mu_l, \mu_{l'}, \{\mu_s\}) = 1 \pm \left( D_\nu^{\text{full}}(\mu_l, \mu_{l'}, \{\mu_s\}) - \frac{\nu^2}{\mu_l \mu_{l'}} \right), \quad (4.15)$$

$$\begin{aligned} \mathcal{J}_\pm^{1(N_l)}(\mu_l, \mu_{l'}, \{\mu_s\}) &= 2(m_l \pm m_{l'}) \left( \frac{\Sigma_\nu^{\text{full}}(\mu_l, \{\mu_s\})}{\Sigma} \pm \frac{\Sigma_\nu^{\text{full}}(\mu_{l'}, \{\mu_s\})}{\Sigma} \right) \\ &\mp \frac{2N_l}{\Sigma V} \left( \mathcal{J}_+^{0(N_l)} - \mathcal{J}_-^{0(N_l)} \right), \end{aligned} \quad (4.16)$$

where  $\{\mu_s\} = \{\mu_{l_1}, \mu_{l_2}, \dots, \mu_{l_{N_l}}\}$ .



## 2. Partially quenched theory ( $N_l \neq 0$ )

The partially quenched results where the valence masses are different from the sea quark masses, are obtained analogously for the case  $N_l \neq 0$ ,

$$\mathcal{S}_v^{(N_l)}(\mu_v, \{\mu_s\}) = \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma}, \quad (4.17)$$

$$\mathcal{K}_\pm^{0(N_l)}(\mu_v, \mu_{v'}, \{\mu_s\}) = \frac{\pm 2}{\mu_v \mp \mu_{v'}} \left( \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma} \mp \frac{\Sigma_\nu^{\text{PQ}}(\mu_{v'}, \{\mu_s\})}{\Sigma} \right), \quad (4.18)$$

$$\mathcal{K}_\pm^{1(N_l)}(\mu_v, \mu_{v'}, \{\mu_s\}) = 1 \pm \left( D_\nu^{\text{PQ}}(\mu_v, \mu_{v'}, \{\mu_s\}) + \frac{\nu^2}{\mu_v \mu_{v'}} \right), \quad (4.19)$$

$$\mathcal{K}_+^{2(N_l)}(\mu_v, \mu_{v'}, \{\mu_s\}) = D_\nu^{\text{PQ}}(\mu_v, \mu_{v'}, \{\mu_s\}), \quad (4.20)$$

$$\mathcal{K}_-^{2(N_l)}(\mu_v, \mu_{v'}, \{\mu_s\}) = \frac{\nu^2}{\mu_v \mu_{v'}}, \quad (4.21)$$

$$\mathcal{K}^{3(N_l)}(\mu_v, \mu_{v'}, \{\mu_s\}) = \frac{1}{\mu_v^2 - \mu_{v'}^2} \left( \mu_{v'} \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma} - \mu_v \frac{\Sigma_\nu^{\text{PQ}}(\mu_{v'}, \{\mu_s\})}{\Sigma} \right), \quad (4.22)$$

$$\mathcal{J}_\pm^{0(N_l)}(\mu_v, \mu_{v'}, \{\mu_s\}) = 1 \pm \left( D_\nu^{\text{PQ}}(\mu_v, \mu_{v'}, \{\mu_s\}) - \frac{\nu^2}{\mu_v \mu_{v'}} \right), \quad (4.23)$$

$$\begin{aligned} \mathcal{J}_\pm^{1(N_l)}(\mu_v, \mu_{v'}, \{\mu_s\}) &= 2(m_v \pm m_{v'}) \left( \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma} \pm \frac{\Sigma_\nu^{\text{PQ}}(\mu_{v'}, \{\mu_s\})}{\Sigma} \right) \\ &\mp \frac{2N_l}{\Sigma V} (\mathcal{J}_+^0 - \mathcal{J}_-^0). \end{aligned} \quad (4.24)$$

## 3. Partially quenched theory ( $N_l = 0$ )

In the case with  $N_l = 0$ , one needs the *fully quenched* integral over  $\bar{U}_0$ :

$$\mathcal{S}_v^{(0)}(\mu_v) = \frac{\Sigma_\nu^{\text{FQ}}(\mu_v)}{\Sigma}, \quad (4.25)$$

$$\mathcal{K}_\pm^{0(0)}(\mu_v, \mu_{v'}) = \frac{\pm 2}{\mu_v \mp \mu_{v'}} \left( \frac{\Sigma_\nu^{\text{FQ}}(\mu_v)}{\Sigma} \mp \frac{\Sigma_\nu^{\text{FQ}}(\mu_{v'})}{\Sigma} \right), \quad (4.26)$$

$$\frac{\mathcal{K}_+^{1(0)}(\mu_v, \mu_{v'})}{2} = \mathcal{K}_+^{2(0)}(\mu_v, \mu_{v'}) = 1 + \frac{\nu^2}{\mu_v \mu_{v'}}, \quad (4.27)$$

$$\frac{\mathcal{K}_-^{1(0)}(\mu_v, \mu_{v'})}{2} = \mathcal{K}_-^{2(0)}(\mu_v, \mu_{v'}) = \frac{\nu^2}{\mu_v \mu_{v'}}, \quad (4.28)$$

$$\mathcal{K}^{3(0)}(\mu_v, \mu_{v'}) = \frac{1}{\mu_v^2 - \mu_{v'}^2} \left( \mu_{v'} \frac{\Sigma_\nu^{\text{FQ}}(\mu_v)}{\Sigma} - \mu_v \frac{\Sigma_\nu^{\text{FQ}}(\mu_{v'})}{\Sigma} \right), \quad (4.29)$$

$$\mathcal{J}_+^{0(0)}(\mu_v, \mu_{v'}) = 2,$$

$$\mathcal{J}_-^{0(0)}(\mu_v, \mu_{v'}) = 0. \quad (4.30)$$

$$\mathcal{J}_\pm^{1(0)}(\mu_v, \mu_{v'}) = 2(m_v \pm m_{v'}) \left( \frac{\Sigma_\nu^{\text{FQ}}(\mu_v)}{\Sigma} \pm \frac{\Sigma_\nu^{\text{FQ}}(\mu_{v'})}{\Sigma} \right). \quad (4.31)$$

#### 4. Fully quenched theory ( $N_l = N_h = 0$ )

When  $N_l = N_h = 0$  or the theory is fully quenched, the zero-mode integrals we use are the same as the partially quenched case with  $N_l = 0$  above. But we need further to include the singlet degree of freedom for the non-zero modes, with additional low-energy constants  $\alpha$  and  $m_0^2$  as quenched artifacts [43, 44, 11, 12]. This results in the modification of  $r(t)$  to

$$r(t) = \frac{1}{N_c} \left( -\frac{m_0^2 T^3}{24} \left[ \left( \frac{t}{T} \right)^2 \left( \frac{t}{T} - 1 \right)^2 - \frac{1}{30} \right] + \alpha T h_1(t) \right), \quad (4.32)$$

where  $N_c$  denotes the number of colors. See e.g. ref. [11] for details.

Using the unitarity condition given in ref. [15], we have checked that all of the above expressions precisely reproduce the known results for degenerate  $N_l \neq 0$  flavors (setting  $N_h = 0$ ), and the quenched results (the  $N_l = N_h = 0$  limit), obtained earlier [11, 12].

#### 4.2 Equivalence of the two mixed-regime expansions

The apparent difference between results obtained in the two mixed-regime expansions considered in section 3 arises from the contribution of the zero-momentum modes of the heavy mesons. They are computed perturbatively in the first case and resummed in the second. In order for the two results to agree, an additional expansion in  $1/\mu_h \sim \epsilon^2$  of the zero-mode integrals for  $U(N_f)$  must of course be performed so that only terms at subleading order in the  $\epsilon$  expansion are consistently kept in the correlators. Performing this expansion one finds:<sup>5</sup>

$$\begin{aligned} \mathcal{J}_\pm^{0(N_f)}(\{\mu_l\}, \{\mu_h\}) &= \mathcal{J}_\pm^{0(N_l)}(\{\tilde{\mu}_l\}) \left( 1 - \sum_h \frac{1}{\mu_h} \right) + \sum_h \frac{1}{\mu_h} \mathcal{J}_\mp^{0(N_l)}(\{\mu_l\}), \\ \mathcal{J}_\pm^{1(N_f)}(\{\mu_l\}, \{\mu_h\}) &= \mathcal{J}_\pm^{1(N_l)}(\{\mu_l\}) + \mathcal{O}\left(\frac{1}{\mu_h}\right), \\ \mathcal{K}_\pm^{0(N_f)}(\{\mu_l\}, \{\mu_h\}) &= \mathcal{K}_\pm^{0(N_l)}(\{\tilde{\mu}_l\}) \left( 1 - \sum_h \frac{2}{\mu_h} \right) + \mathcal{O}\left(\frac{1}{\mu_h}\right)^2, \\ \mathcal{K}_\pm^{n(N_f)}(\{\mu_l\}, \{\mu_h\}) &= \mathcal{K}_\pm^{n(N_l)}(\{\mu_l\}) + \mathcal{O}\left(\frac{1}{\mu_h}\right), \quad n = 1, 2, 3. \end{aligned} \quad (4.33)$$

We have here denoted

$$\tilde{\mu}_i \equiv \mu_i \left( 1 - \sum_h \frac{1}{\mu_h} \right). \quad (4.34)$$

Using these expansions the results from the two different schemes agree.

As another non-trivial check in the opposite direction, one can also confirm that a fully perturbative approach as in the  $p$ -regime, where all of  $N_f = N_l + N_h$  flavors are perturbatively treated, is consistent with our results in an unrealistic limit  $FL \gg 1$  while  $M_\pi L < 1$  kept.

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<sup>5</sup>We have checked these expansions in several special cases with a rather small number of flavors.

## 5. Useful examples for 2+1 flavor theory

In this section we give some explicit examples that are useful when comparing with lattice QCD simulations. Here we consider the 2+1 flavor theory where the up and down quark masses are degenerate,  $m_u = m_d$  and different from the strange quark mass  $m_s$ . We choose the low-energy constants to be the phenomenologically reasonable values  $F = 90\text{MeV}$ ,  $\Sigma^{1/3} = 250\text{MeV}$ ,  $L_4^r(0.77\text{GeV}) = 0.1 \times 10^{-3}$  and  $L_6^r(0.77\text{GeV}) = 0.05 \times 10^{-3}$ .

For the calculation of  $g_1(M^2)$ , we use an expansion in the modified Bessel function [45],

$$g_1(M^2) = \sum_{\substack{|n_i| \leq n_{\max} \\ a \neq 0}} \frac{M}{4\pi^2 |a|} K_1(M|a|), \quad (5.1)$$

where the summation is taken over 4-dimensional vector  $a_\mu = (n_0T, n_1L, n_2L, n_3L)$  with integers  $n_i$ 's. Truncation above at  $n_{\max} = 5$  already shows a good convergence when  $M > 200 \text{ MeV}$  and  $L = T/2 = 2 \text{ fm}$ , for example.

In this theory, and for the cases we will consider, one can express  $\bar{G}(x, 0, 0)$  in terms of  $\bar{\Delta}(x, M^2)$ :

$$\bar{G}(x, 0, 0) = \frac{1}{3} [A\bar{\Delta}(x, M_\eta^2) + B\bar{\Delta}(x, 0) + C \partial_{M^2}\bar{\Delta}(x, 0)], \quad (5.2)$$

and, therefore,

$$\begin{aligned} r(t) &= \int d^3x \bar{G}(x, 0, 0) \\ &= \frac{1}{3} \left[ A \left( \frac{\cosh(M_\eta(t - T/2))}{2M_\eta \sinh(M_\eta T/2)} - \frac{1}{M_\eta^2 T} \right) + BT h_1(t/T) + CT^3 h_2(t/T) \right] \\ &= \frac{1}{3} \left[ BT h_1(t/T) + CT^3 h_2(t/T) - \frac{A}{M_\eta^2 T} + \mathcal{O}(e^{-M_\eta t}) \right]. \end{aligned} \quad (5.3)$$

where

$$h_2(t/T) \equiv \frac{1}{24} \left[ \left( \frac{t}{T} \right)^2 \left( \frac{t}{T} - 1 \right)^2 - \frac{1}{30} \right]. \quad (5.4)$$

and  $A, B, C, M_\eta$  are functions of the p-regime masses only. The term proportional to  $C$  only appears in the case with  $N_l = 0$ . With this set up, one obtains

$$\bar{\Delta}(0, 0) = -\frac{\beta_1}{\sqrt{V}}, \quad \partial_{M^2}\bar{\Delta}(0, M^2)|_{M^2=0} = -\frac{1}{16\pi^2} \ln \mu_{\text{sub}}^2 V^{1/2} - \beta_2, \quad (5.5)$$

where  $\beta_1$  and  $\beta_2$  are the usual shape coefficients and  $\mu_{\text{sub}}$  ( $=0.77\text{GeV}$  in this section) is the subtraction scale.

With this input, one can now calculate meson correlators on the basis of our expressions. In the following, we will give two examples where in both we let the volume size be given by  $L = 2 \text{ fm}$ . One is the case where the physical up and down quarks are in the  $\epsilon$ -regime, i.e.,  $N_l = 2$  and  $N_h = 1$ . The other is the case with rather heavy sea quark masses, i.e.,  $N_h = 3$ , but the valence quarks are taken to the  $\epsilon$ -regime.

As seen below, the 1-loop corrections to the condensate and decay constant are considerable even in the limit  $V \rightarrow \infty$  because of large strange quark mass. Recently, it has been argued that  $N_f=2+1$  flavor ChPT at NLO may have difficulty in fitting lattice QCD data [46, 47]. It is clearly important to check whether NNLO contributions are essential for analyzing such lattice results at the physical  $s$ -quark mass, or if the strange quark is simply out of the region where ChPT provides a useful expansion. If the latter case is true, one would need to integrate the strange quark out and use an "effective"  $N_f = 2$  ChPT. In this paper, we do not wish to address this issue and hence just give the NLO formulae for the  $N_f=2+1$  theory. Even in the  $N_f = 2$  theory one may be interested in keeping the  $u$  and  $d$  quarks in the  $p$ -regime, while taking the valence quarks masses to the  $\epsilon$ -regime. Our formulas given in this paper easily extend to that case, but we do not display them here.

### 5.1 The case with $N_l = 2, N_h = 1$

Let us first choose  $m_u = m_d = 2\text{MeV}$ ,  $m_s = 110\text{MeV}$ , where the physical pions are certainly in the  $\epsilon$ -regime in a volume as small as  $L = 2\text{fm}$ .

In this case, the coefficients of eq. (5.3) are

$$A = -\frac{1}{2}, \quad B = \frac{3}{2}, \quad C = 0, \quad r(t) = \frac{1}{2}Th_1(t/T) + \frac{1}{6M_\eta^2 T}, \quad (5.6)$$

where  $M_\eta^2 = \frac{2}{3}M_{ss}^2 = \frac{4m_s\Sigma}{3F^2}$ . The 1-loop corrections to the condensate and decay constant are then given by

$$\begin{aligned} \frac{\tilde{\Sigma}}{\Sigma} &= 1 - \frac{1}{F^2} \left[ -\frac{3\beta_1}{2\sqrt{V}} + \frac{M_K^2}{16\pi^2} \ln \frac{M_K^2}{\mu_{\text{sub}}^2} + \frac{M_\eta^2}{96\pi^2} \ln \frac{M_\eta^2}{\mu_{\text{sub}}^2} - \frac{1}{6M_\eta^2 V} - 32L_6^r(\mu_{\text{sub}})M_K^2 \right], \\ \frac{\tilde{F}}{F} &= 1 - \frac{1}{2F^2} \left[ -\frac{2\beta_1}{\sqrt{V}} + \frac{M_K^2}{16\pi^2} \ln \frac{M_K^2}{\mu_{\text{sub}}^2} - 16L_4^r(\mu_{\text{sub}})M_K^2 \right], \end{aligned} \quad (5.7)$$

where  $M_K^2 = m_s\Sigma/F^2$ , and we have neglected exponentially small  $g_1(M_K^2)$  and  $g_1(M_\eta^2)$  ( $< (1\text{MeV})^2$ ). One can ignore  $k_{00}^s(M_K^2)$ , too.  $\mu_{\text{sub}} = 770\text{MeV}$  is what we have taken as the subtraction scale. In the case with  $L = T/2 = 2\text{fm}$  (where  $\beta_1 = 0.0836$ ), one obtains  $\tilde{\Sigma} = 1.3\Sigma$  and  $\tilde{F} = 1.2F$ , respectively.

For the zero-mode integral, we use the partition function

$$\begin{aligned} \mathcal{Z}_{1,1+(N_l=2)}^\nu(\mu_b|\mu_v, \mu) &= \frac{1}{2(\mu^2 - \mu_v^2)^2} \\ &\times \det \begin{pmatrix} K_\nu(\mu_b) & I_\nu(\mu_v) & I_\nu(\mu) & \mu^{-1}I_{\nu-1}(\mu) \\ -\mu_b K_{\nu+1}(\mu_b) & \mu_v I_{\nu+1}(\mu_v) & \mu I_{\nu+1}(\mu) & I_\nu(\mu) \\ \mu_b^2 K_{\nu+2}(\mu_b) & \mu_v^2 I_{\nu+2}(\mu_v) & \mu^2 I_{\nu+2}(\mu) & \mu I_{\nu+1}(\mu) \\ -\mu_b^3 K_{\nu+3}(\mu_b) & \mu_v^3 I_{\nu+3}(\mu_v) & \mu^3 I_{\nu+3}(\mu) & \mu^2 I_{\nu+2}(\mu) \end{pmatrix}, \end{aligned} \quad (5.8)$$

where  $\mu = m_u\Sigma V = m_d\Sigma V$ .

When the valence masses are degenerate, we use

$$\mathcal{K}_+^0 = 2 \frac{\partial_{\mu_v} \Sigma_\nu^{\text{PQ}}(\mu_v, \mu)}{\Sigma}, \quad \mathcal{K}_-^0 = -2 \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \mu)}{\mu_v \Sigma},$$

$$\begin{aligned}\mathcal{K}_\pm^1 &= 1 \pm \left( D_\nu^{\text{PQ}}(\mu_v, \mu_v, \mu) + \frac{\nu^2}{\mu_v^2} \right), & \mathcal{J}_\pm^0 &= 1 \pm \left( D_\nu^{\text{PQ}}(\mu_v, \mu_v, \mu) - \frac{\nu^2}{\mu_v^2} \right), \\ \mathcal{J}_+^1 &= 8m_v \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \mu)}{\Sigma} - \frac{4}{\Sigma V} (\mathcal{J}_+^0 - \mathcal{J}_-^0).\end{aligned}\tag{5.9}$$

We now present the explicit form of the correlators for the pseudoscalar and axial vector channels with  $m_v = m_{v'}$ ,

$$\begin{aligned}\mathcal{P}_{vv'}^c(t) &= L^3 \left( \frac{\tilde{\Sigma}^2 \Sigma_\nu^{\text{PQ}}(\tilde{\mu}_v, \tilde{\mu})}{2\tilde{\mu}_v \Sigma} - \frac{\Sigma^2}{6F^2 M_\eta^2 V} \frac{\partial_{\mu_v} \Sigma_\nu^{\text{PQ}}(\mu_v, \mu)}{\Sigma} \right) \\ &\quad + \frac{\Sigma^2}{2F^2} \left( 1 + D_\nu^{\text{PQ}}(\mu_v, \mu_v, \mu) + \frac{\nu^2}{\mu_v^2} - \frac{\partial_{\mu_v} \Sigma_\nu^{\text{PQ}}(\mu_v, \mu)}{\Sigma} \right) Th_1(t/T),\end{aligned}\tag{5.10}$$

$$\begin{aligned}\mathcal{A}_{vv'}^c(t) &= -\frac{\tilde{F}^2}{2T} \left( 1 + D_\nu^{\text{PQ}}(\tilde{\mu}_v, \tilde{\mu}_v, \tilde{\mu}) - \frac{\nu^2}{\tilde{\mu}_v^2} \right) + \frac{Tk_{00}}{V} \left( 1 - D_\nu^{\text{PQ}}(\mu_v, \mu_v, \mu) + \frac{\nu^2}{\mu_v^2} \right) \\ &\quad - \frac{2\mu_v \Sigma_\nu^{\text{PQ}}(\mu_v, \mu)}{V \Sigma} Th_1(t/T),\end{aligned}\tag{5.11}$$

where  $\tilde{\mu}_i = m_i \tilde{\Sigma} V$ . We plot these correlators in figures 3 and 4 using  $k_{00} = 0.08331$  for this case.

## 5.2 $N_l = 0, N_h = 3$

As the second example, let us consider the case with  $m_u = m_d = 30$  MeV,  $m_s = 110$  MeV while the valence quark masses are taken to be very light,  $m_v = \mathcal{O}(1)$  MeV. In this case, all the sea quarks are in the  $p$ -regime and we therefore have  $N_l = 0$  and  $N_h = 3$ . In this case, we have

$$A = -\frac{2(M_{ud}^2 - M_{ss}^2)^2}{(M_{ud}^2 + 2M_{ss}^2)^2}, \quad B = 1 + \frac{2(M_{ud}^2 - M_{ss}^2)^2}{(M_{ud}^2 + 2M_{ss}^2)^2}, \quad C = -3\frac{M_{ud}^2 M_{ss}^2}{M_{ud}^2 + 2M_{ss}^2},\tag{5.12}$$

while  $M_\eta^2 = (M_{ud}^2 + 2M_{ss}^2)/3$ , where  $M_{ud}^2 = (m_u + m_d)\Sigma/F^2$ ,  $M_{ss}^2 = 2m_s\Sigma/F^2$ . Note that a double pole contribution now appears in  $r(t)$  as a partial quenching artifact since  $C \neq 0$ .

The 1-loop corrections to the condensate and decay constant in this case are

$$\begin{aligned}\frac{\tilde{\Sigma}}{\Sigma} &= 1 - \frac{1}{F^2} \left[ \frac{2M_\pi^2}{16\pi^2} \ln \frac{M_\pi^2}{\mu_{\text{sub}}^2} + 2g_1(M_\pi^2) + \frac{M_K^2}{16\pi^2} \ln \frac{M_K^2}{\mu_{\text{sub}}^2} \right. \\ &\quad \left. - \frac{A}{3} \left( \frac{M_\eta^2}{16\pi^2} \ln \frac{M_\eta^2}{\mu_{\text{sub}}^2} - \frac{1}{M_\eta^2 V} \right) + B \frac{\beta_1}{3\sqrt{V}} + \frac{C}{3} \left( \frac{\ln \mu_{\text{sub}}^2 V^{1/2}}{16\pi^2} + \beta_2 \right) \right. \\ &\quad \left. - 32L_6^r(\mu_{\text{sub}})(M_\pi^2 + M_K^2) \right], \\ \frac{\tilde{F}}{F} &= 1 - \frac{1}{2F^2} \left[ \frac{2M_\pi^2}{16\pi^2} \ln \frac{M_\pi^2}{\mu_{\text{sub}}^2} + 2g_1(M_\pi^2) + \frac{M_K^2}{16\pi^2} \ln \frac{M_K^2}{\mu_{\text{sub}}^2} - 16L_4^r(\mu_{\text{sub}})(M_\pi^2 + M_K^2) \right],\end{aligned}\tag{5.13}$$

where  $M_\pi^2 = (m_u + m_d)\Sigma/F^2$  denotes the pion mass. Again we set  $\mu_{\text{sub}} = 770$  MeV. In this case, the corrections are uncomfortably large:  $\tilde{\Sigma} = 1.5\Sigma$  and  $\tilde{F} = 1.2F$ .

The zero-mode partition function for  $N_l = 0$  is given by

$$\mathcal{Z}_{1,1+(N_l=0)}^\nu(\mu_b|\mu_v) = \det \begin{pmatrix} K_\nu(\mu_b) & I_\nu(\mu_v) \\ -\mu_b K_{\nu+1}(\mu_b) & \mu_v I_{\nu+1}(\mu_v) \end{pmatrix}. \quad (5.14)$$

When the valence masses are degenerate, we use

$$\begin{aligned} \mathcal{K}_+^0 &= 2 \frac{\partial_{\mu_v} \Sigma_\nu^{\text{FQ}}(\mu_v)}{\Sigma}, & \mathcal{K}_-^0 &= -2 \frac{\Sigma_\nu^{\text{FQ}}(\mu_v)}{\mu_v \Sigma}, & \mathcal{K}_+^1 &= 2 + 2 \frac{\nu^2}{\mu_v^2}, \\ \mathcal{J}_+^0 &= 2, & \mathcal{J}_-^0 &= 0, & \mathcal{J}_+^1 &= 8m_v \frac{\Sigma_\nu^{\text{FQ}}(\mu_v)}{\Sigma}. \end{aligned} \quad (5.15)$$

Here we present the correlators for the pseudoscalar and axial vector channels ( $m_v = m_{v'}$ ),

$$\begin{aligned} \mathcal{P}_{vv'}^c(t) &= L^3 \left( \frac{\tilde{\Sigma}^2 \Sigma_\nu^{\text{FQ}}(\tilde{\mu}_v)}{2\tilde{\mu}_v \Sigma} + \frac{A\Sigma^2}{3F^2 M_\eta^2 V} \frac{\partial_{\mu_v} \Sigma_\nu^{\text{FQ}}(\mu_v)}{\Sigma} \right) \\ &\quad + \frac{\Sigma^2}{2F^2} \left( 2 + 2 \frac{\nu^2}{\mu_v^2} - \frac{2B}{3} \frac{\partial_{\mu_v} \Sigma_\nu^{\text{FQ}}(\mu_v)}{\Sigma} \right) Th_1(t/T) \\ &\quad - \frac{\Sigma^2}{2F^2} \left( \frac{2C}{3} \frac{\partial_{\mu_v} \Sigma_\nu^{\text{FQ}}(\mu_v)}{\Sigma} \right) T^3 h_2(t/T), \end{aligned} \quad (5.16)$$

$$\mathcal{A}_{vv'}^c(t) = -\frac{\tilde{F}^2}{T} - \frac{2\mu_v \Sigma_\nu^{\text{FQ}}(\mu_v)}{V \Sigma} Th_1(t/T), \quad (5.17)$$

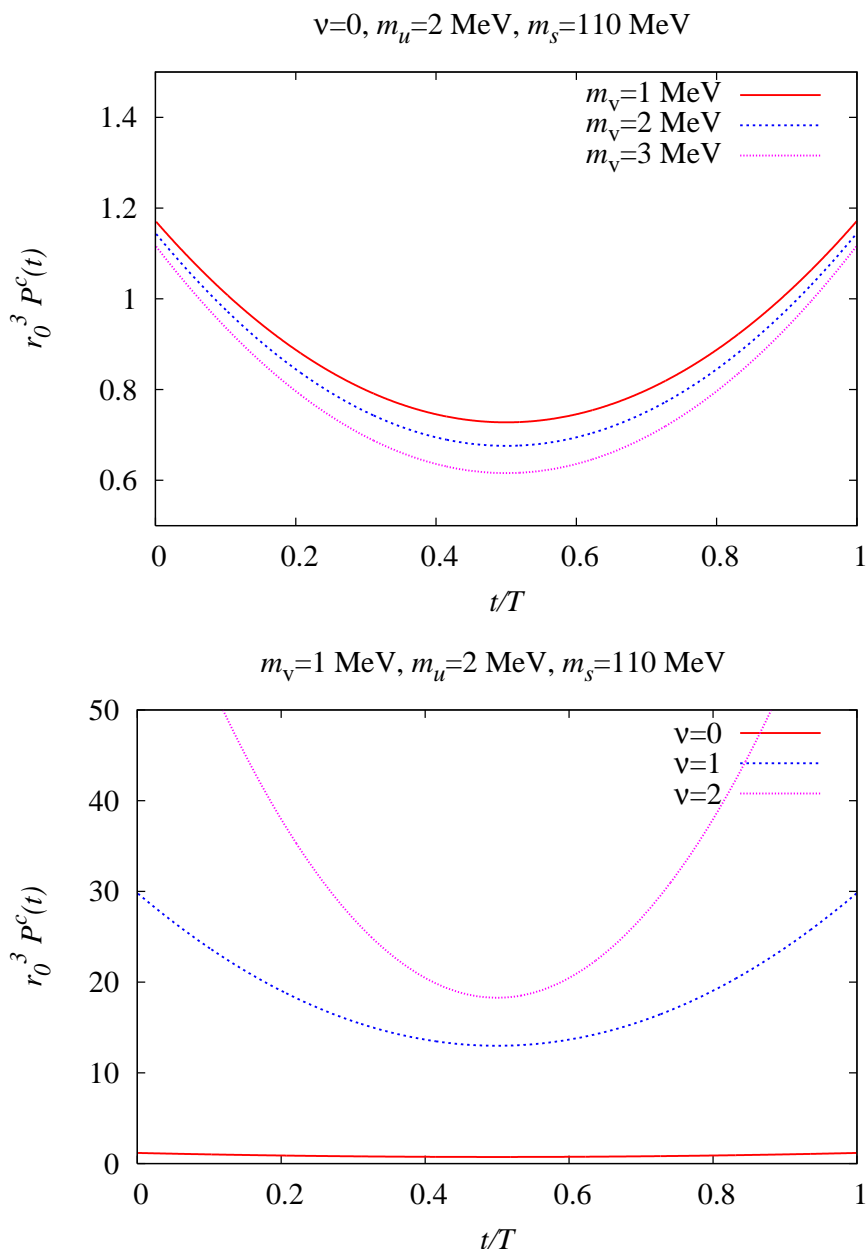
where  $\tilde{\mu}_i = m_i \tilde{\Sigma} V$ . We plot these correlators in figures 5 and 6.

## 6. Conclusions

We have developed a new scheme of calculations for chiral perturbation theory with non-degenerate quark masses in finite volume. With our new counting rules separating  $N_l$  light quarks in the  $\epsilon$ -regime and the other  $N_h$  quarks in the  $p$ -regime, we have calculated the meson correlators in various channels: pseudoscalar, scalar, vector and axial vector. We have also calculated the disconnected contributions for the pseudoscalar and scalar channels.

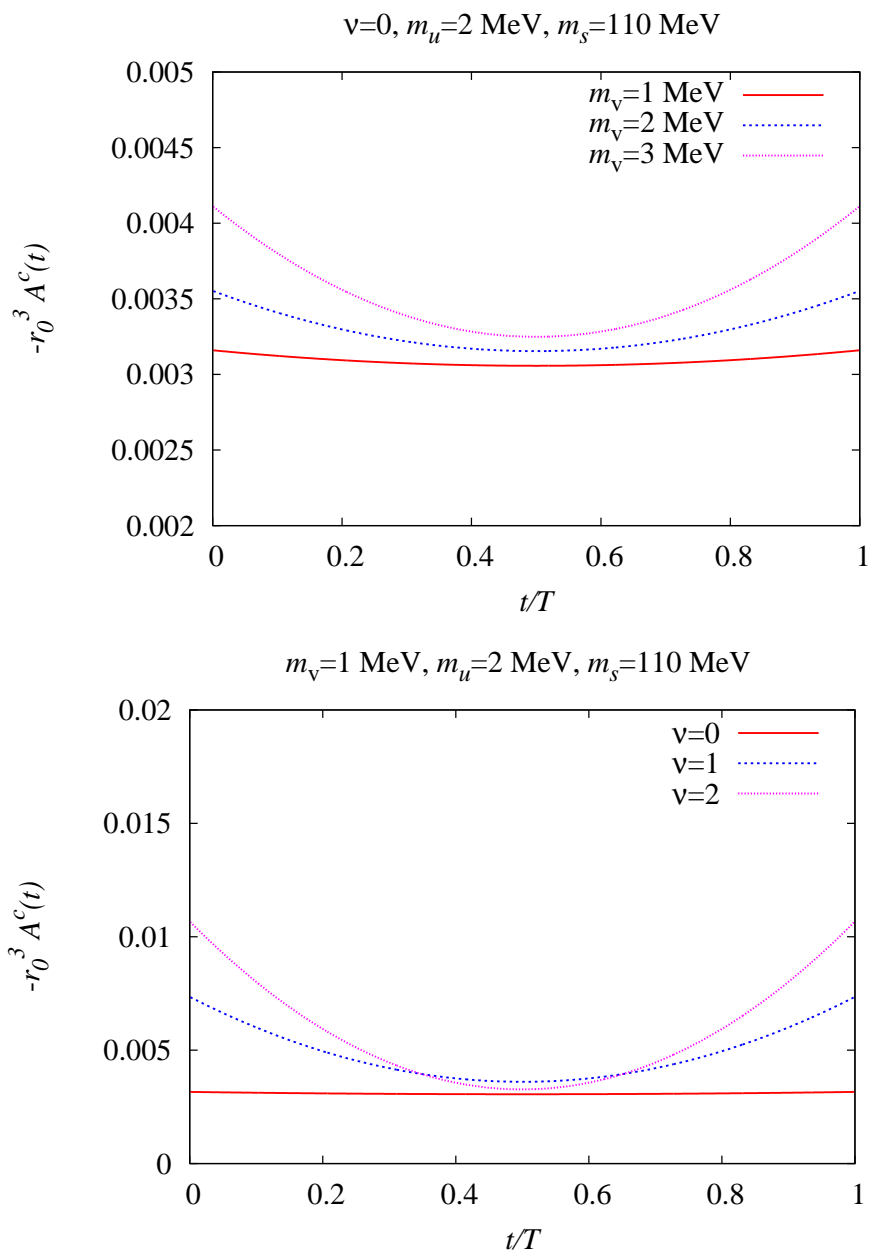
With the help of the replica method, we have also extended our study to the partially quenched case. Our results are shown to be consistent with all earlier work in the literature, both in the quenched and full QCD limit, with degenerate valence quarks.

Our results can be compared to lattice QCD simulation with 2+1 flavors where the up and down quark masses are very light, but the volume is such that the theory is in the  $\epsilon$ -regime with respect to the corresponding pseudo Nambu-Goldstone bosons. The two-point functions are useful to determine the leading low-energy constants, the chiral condensate  $\Sigma$ , and the pion decay constant  $F$  in the chiral limit. As we have demonstrated, the formulae may also be used to extract the numerical values of higher-order low energy constants  $L_4$  and  $L_6$ . This work can be extended to other observables in the case where one valence



**Figure 3:** The pseudoscalar correlators with  $m_\nu = 1-3 \text{ MeV}$ ,  $m_u = m_d = 2 \text{ MeV}$  and  $m_s = 110 \text{ MeV}$  in a sector of trivial topology,  $\nu = 0$  (top) and in sectors of  $\nu = 0-2$  for fixed  $m_\nu = 1 \text{ MeV}$  (bottom). We set  $L = T/2 = 2 \text{ fm}$  and the correlators are normalized by the Sommer scale  $r_0 = 0.49 \text{ fm}$  [48].

quark is heavy, i.e. the chiral dynamics of kaons. With the new partially quenched chiral perturbation theory in this mixed regime one has an excellent analytical tool with which to explore future lattice simulations with nearly massless  $u$  and  $d$  quarks. It would be most interesting to investigate by analytic means also the region between the two regimes, where



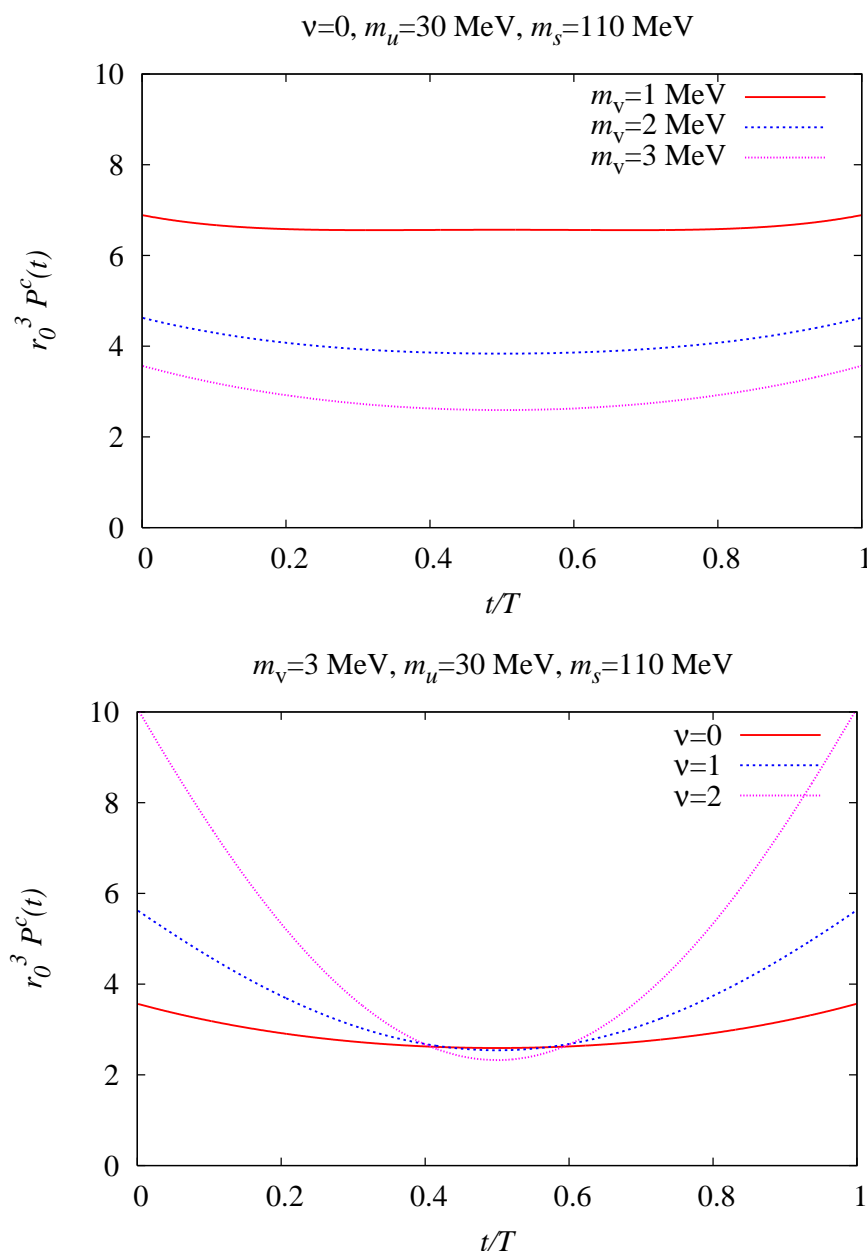
**Figure 4:** The axial correlators for same parameter values as in figure 3.

$m_\pi L \sim 1$ .

### Acknowledgments

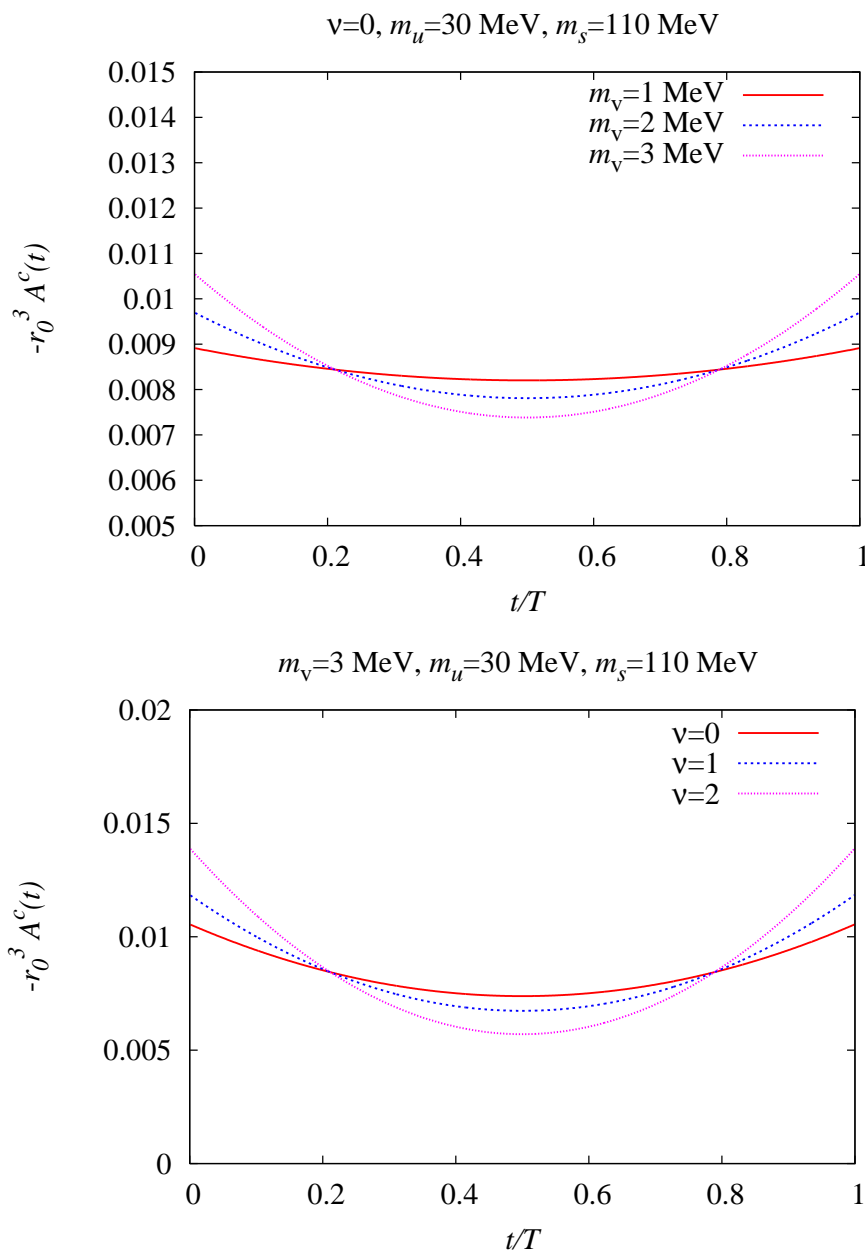
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**Figure 5:** The pseudoscalar correlators with  $m_\nu = 1-3 \text{ MeV}$ ,  $m_u = m_d = 30 \text{ MeV}$  and  $m_s = 110 \text{ MeV}$  in a sector of trivial topology,  $\nu = 0$  (top) and in sectors of  $\nu = 0-2$  for fixed  $m_\nu = 3 \text{ MeV}$  (bottom).

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**Figure 6:** The axial correlators for the same parameter values as in figure 5.

work was completed.

### A. Space-integrals involving propagators

In this appendix, we list several useful formulae for zero-momentum projection (or, equivalently, 3-dimensional space integrals) of functions expressed by  $\bar{\Delta}(x, M^2)$ .

A useful identity is

$$\sum_n \frac{g\left(\frac{2\pi n}{L}\right) e^{i\frac{2\pi n}{L}x}}{\left(\frac{2\pi n}{L}\right)^2 + M^2} = \frac{L}{4M} \frac{1}{\sinh\left(\frac{ML}{2}\right)} \left[ g(iM)e^{-M(x-L/2)} + g(-iM)e^{M(x-L/2)} \right], \quad (\text{A.1})$$

which holds for an arbitrary regular function  $g(p)$ . The zero-mode projection of  $\bar{\Delta}(x, M^2)$ , for example, can be easily derived by setting  $g = 1$ ;

$$\int d^3x \bar{\Delta}(x, M^2) = \frac{1}{2M} \frac{\cosh(M(t-T/2))}{\sinh(MT/2)} - \frac{1}{M^2T}. \quad (\text{A.2})$$

We are particularly interested in the massless limit:

$$\int d^3x \bar{\Delta}(x, 0) = \frac{T}{2} \left( \frac{t}{T} - \frac{1}{2} \right)^2 - \frac{T}{24} \equiv Th_1(t/T). \quad (\text{A.3})$$

It follows its second time derivative is given by

$$\int d^3x \partial_0^2 \bar{\Delta}(x, M^2) = \frac{M}{2} \frac{\cosh(M(t-T/2))}{\sinh(MT/2)}, \quad (\text{A.4})$$

$$\int d^3x \partial_0^2 \bar{\Delta}(x, 0) = \frac{1}{T}. \quad (\text{A.5})$$

In this paper, we have also needed the following integral involving two  $\bar{\Delta}$ 's

$$\int d^3x \int d^4z \partial_0 \bar{\Delta}(z-x, 0) \partial_0 \bar{\Delta}(z, 0) = Th_1(t/T), \quad (\text{A.6})$$

and the more non-trivial integral

$$\begin{aligned} & \int d^3x (\partial_0 \bar{\Delta}(x, M^2) \partial_0 \bar{\Delta}(x, M^2) - \bar{\Delta}(x, M^2) \partial_0^2 \bar{\Delta}(x, M^2)) \\ &= \frac{T}{V} \left( k_{00}^s(M^2) + \frac{1}{M^2T^2} \right) + \frac{1}{V} \left( \frac{\cosh(M(t-T/2))}{2M \sinh(MT/2)} - \frac{1}{M^2T} \right), \end{aligned} \quad (\text{A.7})$$

where

$$k_{00}^s(M^2) \equiv \sum_{\mathbf{q}=(p_1, p_2, p_3)} \frac{-1}{4 \sinh^2(\sqrt{|\mathbf{q}|^2 + M^2}T/2)}. \quad (\text{A.8})$$

The chiral limit of eq. (A.7) is given by

$$\int d^3x (\partial_0 \bar{\Delta}(x, 0) \partial_0 \bar{\Delta}(x, 0) - \bar{\Delta}(x, 0) \partial_0^2 \bar{\Delta}(x, 0)) = \frac{T}{V} k_{00} + \frac{T}{V} h_1(t/T), \quad (\text{A.9})$$

where

$$k_{00} \equiv \sum_{\mathbf{q}=(p_1, p_2, p_3) \neq 0} \frac{-1}{4 \sinh^2(|\mathbf{q}|T/2)} + \frac{1}{12}, \quad (\text{A.10})$$

becomes now a constant depending only on the shape of the box [4].

## B. Summary of zero-mode group integrals

Here we summarize the most essential zero-mode group integrals which are needed in the general partially quenched case, see also ref. [15] for additional details.

The zero-mode contribution to the partition function with  $n$  bosons and  $m$  fermions is known as seen in eq. (4.1). In this paper, we need the case with  $(n, m) = (1, N + 1)$  ( $N$  is the number of physical quarks):

$$\mathcal{Z}_{1,1+N}^\nu(\mu_b|\mu_v, \{\mu_s\}) = \frac{1}{\prod_{s1=1}^N(\mu_{s1}^2 - \mu_v^2) \prod_{s2>s3}^N(\mu_{s2}^2 - \mu_{s3}^2)} \quad (\text{B.1})$$

$$\times \det \begin{pmatrix} K_\nu(\mu_b) & I_\nu(\mu_v) & I_\nu(\mu_{s1}) & I_\nu(\mu_{s2}) & \cdots \\ -\mu_b K_{\nu+1}(\mu_b) & \mu_v I_{\nu+1}(\mu_v) & \mu_{s1} I_{\nu+1}(\mu_{s1}) & \mu_{s2} I_{\nu+1}(\mu_{s2}) & \cdots \\ \mu_b^2 K_{\nu+2}(\mu_b) & \mu_v^2 I_{\nu+2}(\mu_v) & \mu_{s1}^2 I_{\nu+2}(\mu_{s1}) & \mu_{s2}^2 I_{\nu+2}(\mu_{s2}) & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix},$$

and  $(n, m) = (2, N + 2)$ :

$$\mathcal{Z}_{2,2+N}^\nu(\mu_{b1}, \mu_{b2}|\mu_{v1}, \mu_{v2}, \{\mu_s\}) = \quad (\text{B.2})$$

$$\frac{1}{(\mu_{b2}^2 - \mu_{b1}^2)(\mu_{v2}^2 - \mu_{v1}^2) \prod_{s1=1}^N(\mu_{s1}^2 - \mu_{v2}^2)(\mu_{s1}^2 - \mu_{v1}^2) \prod_{s2>s3}^N(\mu_{s2}^2 - \mu_{s3}^2)}$$

$$\times \det \begin{pmatrix} K_\nu(\mu_{b1}) & K_\nu(\mu_{b2}) & I_\nu(\mu_{v1}) & I_\nu(\mu_{v2}) & \cdots \\ -\mu_{b1} K_{\nu+1}(\mu_{b1}) & -\mu_{b2} K_{\nu+1}(\mu_{b2}) & \mu_{v1} I_{\nu+1}(\mu_{v1}) & \mu_{v2} I_{\nu+1}(\mu_{v2}) & \cdots \\ \mu_{b1}^2 K_{\nu+2}(\mu_{b1}) & \mu_{b2}^2 K_{\nu+2}(\mu_{b2}) & \mu_{v1}^2 I_{\nu+2}(\mu_{v1}) & \mu_{v2}^2 I_{\nu+2}(\mu_{v2}) & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{pmatrix}.$$

Here  $\mu_b = m_b \Sigma V$ ,  $\mu_v = m_v \Sigma V$ , where  $m_b$ ,  $m_v$ , denote the masses of the valence bosons, the valence quarks respectively. Partially quenched observables can be computed by differentiating eq. (B.1) or (B.2) with respect to suitable sources and subsequently taking the limit  $\mu_b \rightarrow \mu_v$ .

As building blocks, we use two quantities defined in eqs. (4.3) and (4.4),

$$\frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma} \quad \text{and} \quad D_\nu^{\text{PQ}}(\mu_{v1}, \mu_{v2}, \{\mu_s\}). \quad (\text{B.3})$$

Note that in the degenerate limit  $\mu_{v1} = \mu_{v2} = \mu_v$ ,

$$D_\nu^{\text{PQ}}(\mu_v, \mu_v, \{\mu_s\}) = - \lim_{\mu_b \rightarrow \mu_v} \frac{\partial}{\partial \mu_b} \frac{\partial}{\partial \mu_v} \frac{\mathcal{Z}_{1,1+N}^\nu(\mu_b|\mu_v, \{\mu_s\})}{\mathcal{Z}_{0,N}^\nu(\{\mu_s\})} \equiv - \frac{\Delta \Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma}. \quad (\text{B.4})$$

The needed formulae for one valence index are

$$\frac{1}{2} \langle (U_{vv} + U_{vv}^\dagger) \rangle_U = \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma}, \quad (\text{B.5})$$

$$\frac{1}{4} \langle (U_{vv} + U_{vv}^\dagger)^2 \rangle_U = \frac{\partial_{\mu_v} \Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma} - \frac{\Delta \Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma}, \quad (\text{B.6})$$

$$\frac{1}{2} \langle (U_{vv} - U_{vv}^\dagger) \rangle_U = -\frac{\nu}{\mu_v}, \quad (\text{B.7})$$

$$\frac{1}{4}\langle(U_{vv} - U_{vv}^\dagger)^2\rangle_U = -\frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\mu_v \Sigma} + \frac{\nu^2}{\mu_v^2}, \quad (\text{B.8})$$

$$\begin{aligned} \langle U_{vv} U_{vv}^\dagger \rangle_U &= \frac{1}{4}\langle(U_{vv} + U_{vv}^\dagger)^2\rangle_U - \frac{1}{4}\langle(U_{vv} - U_{vv}^\dagger)^2\rangle_U \\ &= \frac{\partial_{\mu_v} \Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma} - \frac{\Delta \Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma} + \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\mu_v \Sigma} - \frac{\nu^2}{\mu_v^2}. \end{aligned} \quad (\text{B.9})$$

For two valence indices,

$$\frac{1}{4}\langle(U_{vv} + U_{vv}^\dagger)(U_{v'v'} + U_{v'v'}^\dagger)\rangle_U = D_\nu^{\text{PQ}}(\mu_v, \mu_{v'}, \{\mu_s\}), \quad (\text{B.10})$$

$$\frac{1}{4}\langle(U_{vv} - U_{vv}^\dagger)(U_{v'v'} - U_{v'v'}^\dagger)\rangle_U = \frac{\nu^2}{\mu_v \mu_{v'}}, \quad (\text{B.11})$$

$$\langle U_{vv} U_{v'v'} \rangle_U + \langle U_{vv}^\dagger U_{v'v'}^\dagger \rangle_U = 2D_\nu^{\text{PQ}}(\mu_v, \mu_{v'}, \{\mu_s\}) + \frac{2\nu^2}{\mu_v \mu_{v'}}. \quad (\text{B.12})$$

Similarly,

$$\begin{aligned} \frac{1}{4}\langle(U_{vv'} \pm U_{v'v}^\dagger)^2\rangle_U &= \frac{1}{4}\langle(U_{v'v} \pm U_{vv'}^\dagger)^2\rangle_U \\ &= \frac{\pm 1}{2}\langle U_{vv'} U_{v'v}^\dagger \rangle_U = \frac{\pm 1}{2}\langle U_{v'v} U_{vv'}^\dagger \rangle_U \\ &= \frac{\pm 1}{\mu_v^2 - \mu_{v'}^2} \left( \mu_v \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma} - \mu_{v'} \frac{\Sigma_\nu^{\text{PQ}}(\mu_{v'}, \{\mu_s\})}{\Sigma} \right), \\ \frac{1}{4}\langle U_{vv'}^2 + (U_{v'v}^\dagger)^2 \rangle_U &= 0, \end{aligned} \quad (\text{B.13})$$

as well as

$$\begin{aligned} \frac{1}{4}\langle(U_{vv'} \pm U_{v'v}^\dagger)(U_{v'v} \pm U_{vv'}^\dagger)\rangle_U &= \frac{1}{\mu_v^2 - \mu_{v'}^2} \left( \mu_{v'} \frac{\Sigma_\nu^{\text{PQ}}(\mu_v, \{\mu_s\})}{\Sigma} - \mu_v \frac{\Sigma_\nu^{\text{PQ}}(\mu_{v'}, \{\mu_s\})}{\Sigma} \right), \\ \langle U_{vv'} U_{v'v}^\dagger + U_{v'v} U_{vv'}^\dagger \rangle_U &= 0. \end{aligned} \quad (\text{B.14})$$

were also derived in ref. [15].

### C. Some Ward-Takahashi identities at fixed topology

For the computation of vector and axial vector correlation functions we needed a set of zero-mode expectation values involving three zero-mode fields  $U$ . These can be reduced to known integrals by means of exact identities on the group manifold of  $U(N)$ . Such relations correspond to Schwinger-Dyson equations on the group manifold and encode, in physics terms, Ward-Takahashi Identities (WTI) of spontaneous chiral symmetry breaking in a sector of fixed topological charge  $\nu$ . The derivation below follows the method described in detail in appendix B of ref. [11].

Let  $t^a$  denote generators of  $U(N)$  in a chosen representation, here the fundamental. In addition, let  $\epsilon_a$  be infinitesimal parameters. We introduce left-handed differentiation  $\nabla^a$  on the group by means of

$$F(e^{i\epsilon_a t^a} U) = F(U) + \epsilon_a \nabla^a F(U) + \dots \quad (\text{C.1})$$

The derivatives  $\nabla^a$  give rise to a standard Leibniz rule, and left-invariance of the Haar measure on  $U(N)$  ensures that

$$\int dU \nabla^a F(U) = 0. \quad (\text{C.2})$$

Choosing different functions  $F(U)$  this simple identity generates an infinity of exact relations on the coset of symmetry breaking for the zero-mode fields. For the present purposes we can choose, e.g.,

$$F(U) \equiv \text{Tr}[M_1 U] \text{Tr}[U^\dagger M_2] P(U), \quad (\text{C.3})$$

where  $M_1$  and  $M_2$  are arbitrary  $N \times N$  matrices, and the Boltzmann weight  $P(U)$  is defined in the obvious way:

$$P(U) \equiv (\det U)^\nu \exp \left[ \frac{\Sigma V}{2} \text{tr}(\mathcal{M} U + U^\dagger \mathcal{M}) \right]. \quad (\text{C.4})$$

Different choices of the matrices  $M_1$  and  $M_2$  lead to identities that are useful in connection with the vector and axial vector correlators. For example,  $(M_1)_{ij} = \delta_{iv} t_{v'j}^a$  and  $(M_2)_{ij} = \delta_{iv} \delta_{vj}$  (and the similar choice with indices  $v$  and  $v'$  swapped) gives, after use of the  $U(N)$  completeness relation (with a sum over  $a$ )  $(t^a)_{ij} (t^a)_{kl} = \frac{1}{2} \delta_{il} \delta_{jk}$ ,

$$\langle U_{vv}^\dagger (U \mathcal{M} U)_{v'v'} \rangle_U = \left\langle \mathcal{M}_{v'v'} U_{vv}^\dagger - \frac{2}{\Sigma V} (N + \nu) U_{vv}^\dagger U_{v'v'} \right\rangle_U, \quad (\text{C.5})$$

where we used  $\mathcal{M}^\dagger = \mathcal{M}$ , and the hermitian conjugate relation (Note  $(\det U)^\nu = (\det U^\dagger)^{-\nu}$ ),

$$\langle U_{vv} (U^\dagger \mathcal{M} U^\dagger)_{v'v'} \rangle_U = \left\langle \mathcal{M}_{v'v'} U_{vv} - \frac{2}{\Sigma V} (N - \nu) U_{vv} U_{v'v'}^\dagger \right\rangle_U. \quad (\text{C.6})$$

Another choice,  $(M_1)_{ij} = \delta_{iv} t_{v'j}^a$  and  $(M_2)_{ij} = \delta_{iv} \delta_{v'j}$  gives

$$\langle U_{v'v}^\dagger (U \mathcal{M} U)_{v'v} \rangle_U = -\frac{2}{\Sigma V} (N + \nu) \langle U_{v'v}^\dagger U_{v'v} \rangle_U = 0. \quad (\text{C.7})$$

See the appendix B for the last equality to zero. The hermitian conjugate is also vanishes,

$$\langle U_{v'v} (U^\dagger \mathcal{M} U^\dagger)_{v'v} \rangle_U = 0. \quad (\text{C.8})$$

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