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Finite-size Scaling of Meson Propagators

P.H. Damgaard[a1], M.C. Diamantini[a2], P. Hernández[a3], K. Jansen[b,]

[a] Theory Division, CERN, 1211 Geneva 23, Switzerland
[b] NIC/DESY Zeuthen, Platanenallee 6, D-15738 Zeuthen, Germany

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Abstract

Using quenched chiral perturbation theory we compute meson correlation functions at finite volume and fixed gauge field topology. We also present the corresponding analytical predictions for the unquenched theory at fixed gauge field topology. These results can be used to measure the low-energy parameters of the chiral Langrangian from lattice simulations in volumes much smaller than one pion Compton wavelength.

[1] On leave from Niels Bohr Institute, Blegdamsvej 17, DK-2100 Copenhagen, Denmark.
[2] Swiss National Science Foundation fellow.
[3] On leave from Dept. de Física Teórica, Universidad de Valencia.

1 Introduction

It is becoming increasingly clear that the study of strongly coupled gauge theories in unphysical settings, such as finite volume or fixed gauge field topology, can be extremely fruitful. From the point of view of lattice simulations, the restriction to finite volume is of course ideal. It was realized long ago that it can be advantageous to consider the propagation of the pseudo-Goldstone bosons inside volumes too small to even contain one Compton wavelength $1/m_\pi$ of these light degrees of freedom [1, 2]. This idea was explored in depth in the chiral Lagrangian framework of full QCD [3, 4], as well as in a class of sigma models [5]. Already at that time numerical simulations successfully reproduced these predictions for sigma models [6, 7].

In the meantime lattice simulations of QCD with very light quarks are beginning to become feasible. If one restricts oneself to the same regime of finite size $L \equiv V^{1/4}$, where $m_\pi \ll 1/L$, it was noted by Leutwyler and Smilga that gauge field topology now plays a much more important role than in the infinite-volume theory [8]. This fact can be an advantage also in numerical simulations. If one has very definite and different predictions in the various sectors of fixed topological charge ν, it means that one can perform a whole series of independent fits to lattice data, and not just one.

It is thus of interest to combine finite volume with fixed gauge field topology, and to consider QCD correlation functions in such a situation. A systematic framework for analysing QCD in the regime $m_\pi \ll 1/L \ll 4\pi F$, the so-called ϵ-expansion [1], turns out to generalize easily to sectors of fixed topology. In this paper we shall describe our computation of finite-volume meson correlation functions in the quenched analogue of this ϵ-expansion. We shall also provide new results for the unquenched theory in the same finite-volume regime, but restricted to fixed topology. The completely quenched theory is well-known to be special. Eliminating the fermion determinant renders the theory non-unitary. Still, it is obviously of great interest to understand this truncation of the real theory in view of lattice simulations. Here we shall adopt the point of view that the quenched theory can be given some meaning close to the full theory, over a certain range of scales. The difficulties of the finite-volume quenched theory in the chiral limit at the quark level show up again in the effective field theory description, and there is no way around this fact.

Our paper is organized as follows. In section 2 we discuss the two different ways in which to do quenched chiral perturbation theory, the supersymmetric method, and the replica method. Section 3 discusses two different regimes of chiral perturbation theory at finite volume, yielding two different perturbation series known as the p- and ϵ-expansions. We point out the peculiarities of the counting of orders in these two expansions when going to the quenched theory, and explain why sectors of fixed gauge field topology can be particularly useful in the quenched case. In section 4 we recalculate the leading order correction to the quenched chiral condensate in the ϵ-expansion, and show that it gives the same result as computed earlier in the replica formalism in [9]. Section 5 contains the results of our quenched calculation of mesonic correlation functions at fixed topology, to leading order in the ϵ-expansion. We illustrate our results for typical values of lattice parameters, and point out how these results can be used to determine the low-energy parameters of the chiral Lagrangian such as the pion mass m_π and the pion decay constant F. We also present various checks on our calculations, such as consistency with exact Ward identities. In section 6 we present the results of the analogous calculations for full QCD with N_f light quark flavours at fixed gauge field topology. Section 7 contains our conclusions, and in two appendices we collect various technical details relevant to our calculations.

2 Supersymmetry and Replicas

There are two different, yet equivalent, methods for performing quenched chiral perturbation theory. The standard one is based on a chiral Lagrangian extended to a supergroup [10], and the other on the replica method [11]. In the former, internal quark loops are cancelled by a mechanism similar to the cancellation of vacuum diagrams in space-time supersymmetric field theories. In the latter, quark loops are removed by setting the number of quarks equal to zero. The equivalence of the two methods in chiral perturbation theory follows quite easily once one sees the two different sets of Feynman rules. In both cases quenching simply corresponds to removing the fermion determinant in the original theory.

Let us begin at the quark level. Because we shall be interested in computing quantities that include quarks on external lines, we denote by N_v the number of such "valence quarks". In the supersymmetric formulation we include appropriate sources J for these valence quarks (for simplicity restricted to quark bilinears here), but cancel their contributions, at vanishing sources, by quarks of wrong statistics. The generating functional is thus

$$Z_{Susy}[J] \;=\; \int [dA_\mu] \frac{\det(i\not{D} - m_v + J)}{\det(i\not{D} - m_v)^{N_v}} e^{-S[A]} \;, \tag{2.1}$$

where the determinant in the numerator is over N_v fields. The resulting theory is not space-time supersymmetric, because there are no superpartners of the gluons, but internal quark loops are cancelled by their ghost partners.

In the replica method we embed the N_v valence quarks in a theory with N quarks in total (all of which are of ordinary fermionic statistics). At that stage the generating functional reads

$$Z_{Replica}[J] \;=\; \int [dA_\mu] \det(i\not{D} - m_v + J) \det(i\not{D} - m_v)^{N-N_v} e^{-S[A]} \;, \tag{2.2}$$

where the first determinant is taken over N_v fields. The dependence on N is parametric, and the limit $N \to 0$ can be taken:

$$Z_{Replica}[J] \;=\; \int [dA_\mu] \frac{\det(i\not{D} - m_v + J)}{\det(i\not{D} - m_v)^{N_v}} e^{-S[A]} \;. \tag{2.3}$$

It is not just that the two methods succeed in removing the quark determinant in the partition function. The two *generating functionals* (2.1) and (2.3) are simply identical. Passing to the effective field theory description, the equivalence is thus guaranteed from the very beginning. This can easily be verified at the perturbative level of the chiral Lagrangian with the same sources [11]. It is also clear that it trivially generalizes to the partially quenched case.

We assume that in the quenched theories so constructed, the chiral flavour symmetry is spontaneously broken to the diagonal subgroup. The low energy degrees of freedom are the corresponding Goldstone bosons, the dynamics of which can be described by a chiral Lagrangian. In the replica method, the symmetry breaking pattern is as in QCD $SU(N)_L \times SU(N)_R \to SU(N)_{L+R}$, while in the supersymmetric case we have naively a graded flavour symmetry of the breaking pattern $SU(N_v|N_v)_L \times SU(N_v|N_v)_R \to SU(N_v|N_v)_{L+R}$. One new feature common to both methods comes from the fact that in contrast with the full theory the flavour singlet cannot be integrated out: it is a degree of freedom that does not decouple. This is well-known in the supersymmetric formulation, and it is even more easily understood in the replica formalism. There is simply no replica limit $N \to 0$ of

a theory with $SU(N)$ symmetry, and the trace part must be allowed to fluctuate.[4]

Although the perturbative series obtained by the two methods coincide, we need to go beyond perturbation theory here, as we shall be treating the zero momentum modes of the Goldstone bosons exactly. Then a very precise definition of the supersymmetric Haar measure in the supersymmetric formulation, different from the one employed in formal perturbative expansions, is required. This has been explained in detail in refs. [12, 13] (see also the recent discussion [14]). To obtain the precise Haar measure over which to integrate, a more careful analysis of the flavour symmetries with bosonic and fermionic quark species is required. The outcome is that one should replace the naive supersymmetric generalization $U(N_v|N_v)$ by $Gl(N_v|N_v)$, or rather what in the mathematics literature is called the maximally symmetric Riemannian submanifold [12] of this supergroup (for simplicity of notation we will not make this distinction in what follows, and will just denote it by $Gl(N_v|N_v)$). It basically amounts to choosing well-defined integration paths for the fields involved; in particular assuring that the action is bounded from below in all bosonic directions. The replica method is in principle much easier since no supergroup is needed at all, and one is working with an ordinary chiral Lagrangian throughout. The perturbative Feynman rules are simpler, but at the non-perturbative level it is not known how to go beyond series expansions in general [15] (an exception is QCD_3, where the expansion terminates [16] and it thus gives the exact result [17]). So while equivalence is trivial in perturbation theory, it is highly non-trivial at the non-perturbative level. By doing all computations both ways, we thus get important cross-checks on our results.

3 Regimes of (Quenched) Chiral Perturbation Theory

Let us consider QCD in a toroidal volume V of average length scale $L = V^{1/4}$. We assume that the volume is large with respect to the QCD scale. As in an infinite volume the lightest degrees of freedom are the Goldstone bosons of chiral symmetry breaking. They are describable in terms of a chiral Lagrangian given by an expansion in powers of the pion momentum $p = 2\pi n/L$ and mass m_π over the cutoff of the effective theory, $\Lambda \simeq 4\pi F$. This is the standard chiral expansion, in which both quantities p and m_π are taken to be of the same order. At leading order, the chiral Lagrangian in a θ vaccuum is usually writen as

$$\mathcal{L}^{(2)} = \frac{F^2}{4}\mathrm{Tr}\left(\partial_\mu U \partial_\mu U^\dagger\right) - \frac{\Sigma}{2}\mathrm{Tr}\left(\mathcal{M}e^{i\theta/N_f}U + e^{-i\theta/N_f}U^\dagger\mathcal{M}^\dagger\right) + O\left(\frac{p}{\Lambda}\right)^4 , \tag{3.4}$$

where Σ and F are the infinite volume quark condensate and pion decay constant, both in the chiral limit. $\mathcal{M}$ is the quark mass matrix that for simplicity we will take as proportional to the identity, $\mathcal{M} = mI$. Furthermore, $U = e^{i\sqrt{2}\xi/F}$ is an element of $SU(N_f)$. In the chiral expansion U is expanded around the classical solution $U = 1 + i\sqrt{2}\xi/F + ...$ Consider the quadratic term in the action in momentum space

$$\mathcal{S}^{(2)} = \frac{V}{2}(p^2 + m_\pi^2)\mathrm{Tr}[\xi_p^2] . \tag{3.5}$$

It provides a gaussian damping factor that limits the fluctuations of $Tr[\xi_p^2]$ to be

$$O\left(\frac{1}{V(p^2+m_\pi^2)}\right) \sim O\left(\frac{1}{Vm_\pi^2}\right) .$$

[4] There is no corresponding problem with partial quenching, i.e. taking the replica limit $N \to 0$ of a partially quenched theory of flavour group $SU(N_f + N)$, with $N_f \geq 2$. Then the m_0-term is not required to define the theory, and it can be decoupled.

When the linear size L is much larger than the Compton wavelength of the pions $1/m_\pi$, the system hardly feels the finite volume, and the typical momentum scale is thus $p \sim m_\pi$. So for $m_\pi \gg 1/L$, the fluctuations are much smaller than $1/L^2$ and the expansion around the classical solution is an expansion in powers of a quantity much smaller than $1/(LF)^2 \ll 1$. As the size of the box or the quark mass becomes smaller, finite size effects start to become important, but provided $m_\pi L \geq 1$, ordinary perturbation theory is still applicable. In the boundary of this regime, when $m_\pi L \sim 1$, the expansion of the field $U(x)$ around the classical solution and the expansion in powers of momenta of the Lagrangian itself become the same expansion in powers of $1/FL$. This is the so-called *p-expansion* [1] in which

$$\frac{|\xi_p|}{F} \sim \frac{m_\pi}{\Lambda} \sim \frac{p}{\Lambda} \sim \frac{1}{LF} .$$

If the chiral limit is approached further in such a way that the Compton wavelength of the pion is larger than the box size ($L > 1/m_\pi$), the conventional p-expansion eventually breaks down due to propagation of pions with zero momenta [1]. Indeed, according to eq. (3.5), when $m_\pi L^2 \sim 1$ (in units of the cut-off, i.e. $m_\pi L^2 F = (2m\Sigma V)^{1/2} \sim 1$) the fluctuations of the zero modes, ξ_0^2, are of $O(1)$ and the perturbative expansion for these modes breaks down. But the non-zero modes still have fluctuations that are

$$O\left(\frac{1}{Vp^2}\right) < O\left(\frac{1}{L^2}\right)$$

and they are still perturbative. A convenient expansion for this regime is the so-called *ϵ-expansion*, in which [1]

$$\frac{m_\pi}{\Lambda} \sim \frac{p^2}{\Lambda^2} \sim \frac{1}{L^2F^2} \sim \epsilon^2 .$$

The zero modes of the pion can be isolated by factorizing $U(x)$ into a constant collective field U_0 and the pion fluctuations $\xi(x)$:

$$U(x) = U_0 \exp i\frac{\sqrt{2}\xi(x)}{F} . \tag{3.6}$$

The difficulty in this regime comes from the fact that the integral over U_0 needs to be done exactly, while ordinary chiral perturbation theory applies to the non-zero mode integration, since $\xi_p^2 \sim O(\epsilon^2)$. To leading order, the partition function is [5]

$$\mathcal{Z}(\theta, \mathcal{M}) = \int_{SU(N_f)} d\xi dU_0 \exp\left[\frac{1}{2}\int d^4x \,\mathrm{Tr}\,(\partial_\mu \xi \partial_\mu \xi) + \frac{m\Sigma V}{2}\mathrm{Tr}\left(e^{i\theta/N_f}U_0 + e^{-i\theta/N_f}U_0^\dagger\right)\right].$$

If $FL \gg 1$, the p- and ϵ-expansions should match in the range of quark masses such that $m_\pi L \sim 1$. In this regime $m\Sigma V \sim (FL)^2(m_\pi L)^2 \gg 1$, so the results in the ϵ-expansion should reproduce those of the p-expansion in the limit of large $m\Sigma V$.

It is also interesting to consider averages in sectors of fixed topology [8]. Fourier-transforming in θ, we get, to the same order:

$$\mathcal{Z}_\nu(\mathcal{M}) = \int_{SU(N_f)} d\xi \int_{U(N_f)} dU_0 \,(\det U_0)^\nu \exp\left[\frac{1}{2}\int d^4x \,\mathrm{Tr}\,(\partial_\mu \xi \partial_\mu \xi) + \frac{m\Sigma V}{2}\mathrm{Tr}\left(U_0 + U_0^\dagger\right)\right].$$

The ϵ- and p-expansions can be defined in the same way in this truncation of the theory.

[5] The measure contains additional terms of order ϵ^2 and higher [3] due to the change of variables to coordinates $\xi(x)$. These terms are not needed to the order at which we will be working.

3.1 Quenched Chiral Perturbation Theory

In the supersymmetric formulation of the quenched theory, assuming the pattern of chiral symmetry breaking of the previous section, the low-energy behaviour of the theory can be described by the supersymmetric chiral Lagrangian,

$$\mathcal{L}^{(2)} = \frac{F^2}{4}\mathrm{Str}\left(\partial_\mu U^{-1}\partial_\mu U\right) - \frac{m\Sigma}{2}\mathrm{Str}\Big(U_\theta U + U^{-1}U_\theta^{-1}\Big) + \frac{m_0^2}{2N_c}\Phi_0^2 + \frac{\alpha}{2N_c}\partial_\mu\Phi_0(x)\partial^\mu\Phi_0(x)\ , \quad (3.7)$$

where Str denotes the supertrace, $\Phi_0 \equiv \frac{F}{\sqrt{2}}\mathrm{Str}[-i\log(U)]$ and $U_\theta \equiv \exp(i\theta/N_v)I_{N_v} + \tilde{I}_{N_v}$. Here, I_{N_v} is the identity matrix in the fermion–fermion block of "physical" Goldstone bosons and zero otherwise, while $\tilde{I}_{N_v}$ is the identity in the boson–boson block and zero elsewhere. As explained in the previous section, the integral over the Goldstone fields is over a submanifold of $Gl(N_v|N_v)$. An important difference with the full theory is the unavoidable presence of the singlet field, which cannot be decoupled in this case. Actually, the chiral expansion signals the breakdown of the perturbative series if the singlet mass m_0 becomes comparable to or larger than the cutoff scale in the effective theory $\Lambda \sim 4\pi F$. To see this, let us consider the case of $N_v = 1$ in the context of the supersymmetric method. Using the parametrization of the Goldstone submanifold of $Gl(1|1)$ from ref. [13],

$$U(x) = \begin{pmatrix} e^{i\phi(x)\frac{\sqrt{2}}{F}} & 0 \\ 0 & e^{s(x)\frac{\sqrt{2}}{F}} \end{pmatrix} \exp\begin{pmatrix} 0 & \gamma(x)\frac{\sqrt{2}}{F} \\ \beta(x)\frac{\sqrt{2}}{F} & 0 \end{pmatrix}\ ,$$

where $\phi(x)$ and $s(x)$ are the real bosonic fields, and $\gamma(x)$ and $\beta(x)$ are the fermionic ones, we consider the usual p-expansion about the classical vacuum $U = 1$. The action expanded to quadratic order is

$$\begin{aligned}\mathcal{S}^{(2)} &= \int d^4x \left\{ \frac{1}{2}\left(\phi\left(-\partial^2 + \frac{2\Sigma m}{F^2}\right)\phi + s\left(-\partial^2 + \frac{2\Sigma m}{F^2}\right)s + (\phi + is)\left(\frac{m_0^2 - \alpha\partial^2}{N_c}\right)(\phi + is)\right)\right. \\ &+ \left.\gamma\left(-\partial^2 + \frac{2\Sigma m}{F^2}\right)\beta\right\}. \end{aligned} \quad (3.8)$$

where $m_\pi^2 F^2 = 2m\Sigma$. In contrast to the naive choice of $U(1|1)$ as the coset of chiral symmetry breaking, the gaussian integrals are absolutely convergent for all momenta such that $(m_0^2 + \alpha p^2)/N_c < p^2 + m_\pi^2$ and to any finite order in $(m_0^2 + \alpha p^2)/N_c$ even if this condition is not satisfied. It is only then that we are able to make meaningful statements about the magnitude of fluctuations.

Using the properly normalized measure we get to this order:

$$\mathcal{Z} = \frac{\det(-\partial^2 + m_\pi^2)}{\det(-\partial^2 + m_\pi^2)^{1/2}\det(-\partial^2 + m_\pi^2)^{1/2}} = 1\ , \quad (3.9)$$

and $\mathcal{Z}$ is thus independent of m_0^2 in the absence of sources. This explains, to this order, the puzzle of how the effective partition function apparently could depend on one new parameter m_0, when, in the absence of sources, it should equal unity by construction. Only when we include external sources for the quarks can a dependence on m_0 appear; in particular individual propagators will depend on m_0. It follows that m_0 must have at its origin gluonic dynamics, which is probed by appropriate quark sources. This picture is in nice agreement with what is found at the level of the zero modes, see below.

The fluctuations of the Fourier modes of s and ϕ are seen to be

$$\langle\phi_p^2\rangle = \frac{(1 - \alpha/N_c)p^2 + m_\pi^2 - m_0^2/N_c}{V(p^2 + m_\pi^2)^2}, \qquad \langle s_p^2\rangle = \frac{(1 + \alpha/N_c)p^2 + m_\pi^2 + m_0^2/N_c}{V(p^2 + m_\pi^2)^2}\ . \quad (3.10)$$

Clearly if m_0^2/N_c is larger than the chiral scales p^2 or m_π^2, the fluctuations of the fields are controlled by this parameter and the perturbative expansion breaks down for all modes (i.e. zero and non-zero) when $m_0^2/N_c \geq F^2$ [6]. This is an artefact of the quenched approximation, related to the fact that the singlet cannot be integrated out. Defining $\epsilon'^2 = (m_0^2)/(N_c F^2)$ and $\epsilon^2 = 1/(FL)^2$, in the regime of the p-expansion we have

$$\frac{1}{(FL)^2} \sim \frac{m_\pi^2}{\Lambda^2} \sim O(\epsilon^2), \qquad \frac{\phi_p^2}{F^2} \sim O(\epsilon^2 - \epsilon'^2), \qquad \frac{s_p^2}{F^2} \sim O(\epsilon^2 + \epsilon'^2) \ . \tag{3.11}$$

In the case of the zero modes, eqs. (3.10) imply that the series breaks down when $m_\pi^2/\Lambda^2 \leq \epsilon'\epsilon^2$. For $\epsilon' > \epsilon^2$ this will happen before zero modes need to be treated separately in the unquenched theory. This is, however, not the case if we only consider averages in sectors of fixed topology at finite ν. Using left and right invariance of the super-Haar measure, the factorization into zero modes and non-zero modes goes through as in the unquenched case eq. (3.6), and the partition function restricted to fixed topology ν is to the order we need it

$$\begin{aligned} \mathcal{Z}_\nu(\mathcal{M}) \ = \ & \frac{1}{\sqrt{2\pi\langle\nu^2\rangle}} e^{-\nu^2/2\langle\nu^2\rangle} \int_{Gl(N_f|N_f)} dU_0 d\xi \, (\mathrm{Sdet} U_0)^\nu \exp\left[\frac{m\Sigma V}{2}\mathrm{Str}\Big(U_0 + U_0^{-1}\Big)\right. \\ & \left. + \int d^4x \left(-\frac{1}{2}\mathrm{Str}\,(\partial_\mu\xi\partial_\mu\xi) - \frac{m_0^2}{2N_c}\mathrm{Str}(\xi)^2 - \frac{\alpha}{2N_c}\,(\partial_\mu \mathrm{Str}[\xi])^2 \right) + ... \right] , \end{aligned}$$

where Sdet is the superdeterminant. The distribution of winding numbers is Gaussian with mean

$$\langle\nu^2\rangle \ = \ \frac{F^2 m_0^2 V}{2N_c} \ , \tag{3.12}$$

a relation that will play a crucial role when we match results in the ϵ-regime with those of the p-expansion regime. The otherwise menacing Φ_0 has disappeared in the zero-mode sector at fixed topology, leaving as its only trace the average distribution of topological charges. As a result of this, the usual ϵ-regime, where

$$\frac{1}{(FL)^2} \sim \frac{m_\pi}{\Lambda} \sim O(\epsilon^2) \ , \tag{3.13}$$

can be approached. This result may seem puzzling, as it indicates that a more chiral regime can be reached in sectors of fixed gauge field topology, whereas after summing over topology we find that the double-pole term of the quenched propagator blows up at a scale much before the regime of the ϵ-expansion is reached. In fact this is correct, and the resolution is found by noting that also the quenched ϵ-expansion in sectors of fixed topology eventually fails, when $|\nu| \to \infty$. In the sum over topology, the dominant contributions are those around $|\nu| \sim Fm_0\sqrt{V}$, and for topological charges that large, the ϵ-expansion breaks down even in sectors of fixed topology. In other words, the sickness that we found in the direct analysis for $m_\pi^2/\Lambda^2 < \epsilon'\epsilon^2$ reappears in this case when summing over topology. Actually this problem of the perturbative expansion close to the chiral limit is probably unresolvable, since it is also found at the quark level: in a background gauge field with topological charge ν, the contribution of the topological zero modes to any quark propagator is $|\nu|/mV$. Using eq. (3.12) the average over topology implies that this contribution becomes of order $Fm_0/(m\sqrt{V})$, which is of $O(1)$ when $m \sim \epsilon'\epsilon^2$. Concerning the non-zero modes, the perturbative expansion remains a simultaneous expansion in ϵ and ϵ' also at fixed topology. We will be working to lowest non-trivial order in *both* expansion parameters.

[6] We assume the parameter $\alpha \sim 1$.

Let us now summarize the relevant Feynman rules. We have already displayed the usual supersymmetric version of the Lagrangian and the propagators for the bosonic fields in eq. (3.10) for the $N_v = 1$ case. The propagator for the fermionic fields γ and β is, after a simple rescaling, read off from eq. (3.8) to be simply a conventional bosonic propagator. These rules differ by some signs from the usual ones based on $U(1|1)$ [10]. These differences are irrelevant in perturbation theory. The generalization to $N_v > 1$ follows similarly [10], with a few sign changes. Let us introduce some convenient notation and define

$$\Delta(x) \equiv \frac{1}{V}\sum_p \frac{e^{ipx}}{p^2+m_\pi^2} \quad , \qquad \bar{\Delta}(x) \equiv \frac{1}{V}\sum_p{}' \frac{e^{ipx}}{p^2} \ , \tag{3.14}$$

where a prime on the sum indicates that zero momentum is excluded. We will also need the corresponding expressions for the peculiar double-pole term. Let

$$G(x) \equiv \frac{1}{V}\sum_p \frac{e^{ipx}}{(p^2+m_\pi^2)^2} \quad \text{and} \qquad \bar{G}(x) \equiv \frac{1}{V}\sum_p{}' \frac{e^{ipx}}{p^4} \ . \tag{3.15}$$

One notes that

$$\int d^4x \ \bar{\Delta}(x) = \int d^4x \ \bar{G}(x) = 0 \ , \tag{3.16}$$

properties that greatly facilitate comparison with integrated Ward identities in the ϵ-expansion. There is also the relation

$$\Delta(x) = \frac{1}{m_\pi^2 V} + \bar{\Delta}(x) - m_\pi^2 \bar{G}(x) + \dots \ , \tag{3.17}$$

so that both $\bar{\Delta}(x)$ and $\bar{G}(x)$ immediately follow from Taylor expanding the finite-volume massive pion propagator $\Delta(x)$.

In the replica formulation [11], all of the above discussion also applies. The action is that of eq. (3.7) after replacing Str by Tr everywhere, and after changing the group manifold to $U(N)$. The m_0 term actually serves to interpolate between $SU(N)$ and $U(N)$: when $m_0 \to \infty$ we go from $U(N)$ to $SU(N)$, but then there can be no replica limit. The way the m_0 term serves to allow a replica limit becomes particularly transparent when one looks at the Feynman rules: in a quark basis the propagator of the off-diagonal mesons will have the usual form of $\Delta(x)$, while the diagonal combination has a propagator (with E being a $N \times N$ matrix with unity in every entry):

$$\mathcal{G}_{ij}(x) = \frac{1}{V}\sum_p \left[\frac{\delta_{ij}}{(p^2+m_\pi^2)} - E_{ij} \frac{(m_0^2+\alpha p^2)/N_c}{(p^2+m_\pi^2)^2 \mathcal{F}(p^2)} \right] e^{ipx} \ . \tag{3.18}$$

Here

$$\mathcal{F}(p^2) \equiv 1 + \frac{m_0^2+\alpha p^2}{N_c}\left(\frac{N}{p^2+m_\pi^2}\right) \ . \tag{3.19}$$

For any finite N we can take the limit $m_0 \to \infty$, in which case the double pole in the last term is cancelled. We then get the ordinary propagator with a factor of $1/N$ in front, combining with the first term to give the usual diagonal propagator in the quark basis. The singularity at $N = 0$ is regularized by keeping a finite m_0. The replica limit $N \to 0$ is then taken only at the end of the calculation, keeping m_0 finite.

4 The Chiral Condensate

The leading order result for the chiral condensate in a finite volume and fixed topological sector was computed from the fully and partially quenched chiral Lagrangian in ref. [13]. For full QCD the first

correction to this result follows directly from the calculation of Gasser and Leutwyler [1]. It is also of interest to find this first correction in the fully quenched theory, and this was recently done using the replica method [9]. In this section we show how the same result is obtained from the supersymmetric method.

Let us consider the simplest case of $N_v = 1$, because the result clearly does not depend on N_v. For the group $Gl(1|1)$, the chiral condensate in a sector with fixed topology can be defined as:

$$\Sigma_\nu(m) \;=\; \frac{1}{V}\frac{\partial}{\partial J}\ln \mathcal{Z}_\nu(\mathcal{M}_J)\mid_{J=0} \;\; . \tag{4.20}$$

where $\mathcal{M}_J = \mathrm{diag}(m+j, m)$. At leading order in the ϵ-expansion one finds [13, 18]

$$\frac{\Sigma_\nu(\mu)}{\Sigma} \;=\; \mu\left(I_\nu(\mu)K_\nu(\mu) + I_{\nu+1}(\mu)K_{\nu-1}(\mu)\right) + \frac{\nu}{\mu} \;, \tag{4.21}$$

where $I_\nu(\mu), K_\nu(\mu)$ are modified Bessel functions, and $\mu = m\Sigma V$.

To derive the first correction to this result in the ϵ-expansion it is convenient to first calculate the 1-loop improvement of the action due to the fluctuations of the non-zero momentum modes. To $O(\epsilon^2)$ the contribution from the measure does not affect the result, and to that order we simply evaluate

$$\left\langle 1 - \frac{\Sigma}{2F^2}\mathrm{Str}\left[\mathcal{M}_J\left(U_0 + U_0^{-1}\right)\int d^4x\,\xi^2(x)\right]\right\rangle \;\; .$$

Performing the integral over ξ to leading order, and then re-exponentiating the correction, we obtain

$$\mathcal{Z}_\nu(\mathcal{M}_J) \;=\; \int_{Gl(1|1)} dU_0\,(\mathrm{Sdet}U_0)^\nu \exp\left[\frac{\Sigma_{eff}V}{2}\mathrm{Str}\left(\mathcal{M}_J\left(U_0 + U_0^{-1}\right)\right)\right] \;\; . \tag{4.22}$$

Then the effective coefficient determining the strength of the condensate at finite volume is

$$\Sigma_{eff}(V) \;\equiv\; \Sigma\left(1 + \frac{1}{N_c F^2}(m_0^2\bar{G}(0) + \alpha\bar{\Delta}(0))\right) \;, \tag{4.23}$$

were $\bar{G}, \bar{\Delta}$ are defined in eqs. (3.14-3.15). The m_0^2 and α terms are what remains from the partial cancellation of the fermionic propagator and the bosonic ones. The partition function is then the same as the one at leading order with the change $\Sigma \to \Sigma_{eff}(V)$.

It is now easy to calculate the condensate to one loop, by differentiating eq. (4.22) as in eq. (4.20) to get

$$\begin{aligned}\Sigma_\nu^{1-\mathrm{loop}}(\mu) \;&=\; \Sigma_\nu(\mu')\frac{\mu'}{\mu} \\ &=\; \Sigma_\nu(\mu) + 2\frac{1}{N_c F^2}(m_0^2\bar{G}(0) + \alpha\bar{\Delta}(0))\mu I_\nu(\mu)K_\nu(\mu) + \ldots \quad ,\end{aligned} \tag{4.24}$$

where

$$\mu' \;\equiv\; m\Sigma_{eff}V \;=\; \mu\left(1 + \frac{1}{N_c F^2}(m_0^2\bar{G}(0) + \alpha\bar{\Delta}(0))\right). \tag{4.25}$$

One peculiarity of the quenched approximation is that the $O(\epsilon^2)$ correction to the condensate is ultraviolet divergent even in dimensional regularization because of the double pole propagator [19, 20]. We find [5]

$$\bar{G}(0) \;=\; \beta_2 + \frac{1}{8\pi^2}\left(\ln(L/L_0) - c_1\right) \;\; , \quad \bar{\Delta}(0) \;=\; -\frac{\beta_1}{L^2}, \tag{4.26}$$

where β_1 and β_2 are two of the universal "shape coefficients". It depends on the shape of the box, and the precise value can, for any given volume, be computed from the general expression given in ref. [5]. In dimensional regularization the constant c_1 reads

$$c_1 \;=\; \frac{1}{d-4} - \frac{1}{2}\left(\Gamma'(1) + 1 + \ln(4\pi)\right) + O(d-4) \;, \tag{4.27}$$

and $1/L_0$ is the ultraviolet subtraction point. The divergent term in c_1 matches precisely the 1-loop counterterm needed for the condensate in the infinite-volume theory [20]. Below we present the numerical results corresponding to the subtractions that are required by the $\overline{MS}$ scheme.

Note that the one-loop contribution contains a quenched finite-volume logarithm [9], which reflects the infrared sickness of the quenched approximation. It is the finite-volume counterpart of the usual logarithmic chiral divergence in infinite-volume quenched chiral perturbation theory. The analysis is clearly restricted to domains where this divergence does not yet overwhelm the tree-level result.

Several methods have been proposed and implemented to calculate the coupling Σ by finite-size scaling techniques. One method is to take the discontinuity of the chiral condensate (4.24) across the imaginary μ-axis to get the spectral density of the Dirac operator eigenvalues in this regime [13]. Since the density depends on the parameter Σ, the leading tree-level expression for the density can be used to extract Σ in this way [21]. Alternatively, the condensate may also be computed directly on the lattice [22, 23, 24, 25] and one can then fit its finite size and quark-mass dependence to the prediction in eq. (4.24). Both methods have been shown to work well in extracting Σ by neglecting the contributions of eq. (4.24). With sufficiently high statistics, one could also aim at a determination of the pion decay constant F [1, 9] from these corrections. In the quenched case the problem is that it brings in two new unknowns: m_0 and α. To estimate the typical size of the correction, we can compare the 1-loop-improved chiral condensate at two different volumes, after subtracting the trivial topological zero mode contributions and keeping $\mu = m\Sigma V$ fixed. In this way we do not have to address the issue of the L_0 scale dependence[7]:

$$\frac{\Sigma^{1-loop}_{\nu,L_1}(\mu) - |\nu|/\mu}{\Sigma^{1-loop}_{\nu,L_2}(\mu) - |\nu|/\mu} \;=\; 1 + \frac{1}{4\pi^2}\frac{1}{N_c F^2}\frac{\mu I_\nu(\mu) K_\nu(\mu)}{\Sigma_\nu(\mu) - |\nu|/\mu}\left(m_0^2 \ln\left(\frac{L_1}{L_2}\right) - \alpha\beta_1\left(\frac{1}{L_1^2} - \frac{1}{L_2^2}\right)\right) \;. \tag{4.28}$$

As an example, for the smallest and largest lattice volumes considered in [23] in the $\nu = 1$ sector, the second term in eq. (4.28) is around 15% for $m_0 \sim 600$ MeV. Although the statistical errors in [26] are larger than this, this is not clearly beyond hope in more precise studies.

5 Quenched Correlation Functions

Meson correlation functions can be computed systematically in the ϵ-expansion. Here we present the results of the $O(\epsilon^2)$ calculation for scalar and pseudoscalar correlation functions in the quenched theory. We have performed all computations in both the supersymmetric and replica formulations, checking that the final results are identical. We begin with the flavour-singlet combinations involving

$$S^0(x) \;\equiv\; \bar\psi(x) I_{N_v} \psi(x) \;, \qquad P^0(x) \;\equiv\; \bar\psi(x) i\gamma_5 I_{N_v} \psi(x) \;, \tag{5.29}$$

where I_{N_v} is the flavour projector onto the physical quark sector or that of the N_v valence quarks. For simplicity we consider $N_v = 1$ for the singlet case. To compute these correlation functions, we make

[7] In the direct computation of the quark condensate UV divergences appear at the quark level which must be subtracted before comparing to eq. (4.28) [23].

use of the correspondence between local sources added at the quark level

$$\mathcal{L}_{QCD} \;\rightarrow\; \mathcal{L}_{QCD} + s(x)S^0(x) + p(x)P^0(x) \;, \tag{5.30}$$

and the substitution

$$\mathcal{M} \;\rightarrow\; \chi(x) = \mathcal{M} + s(x)I_{N_v} + ip(x)I_{N_v} \tag{5.31}$$

in the effective theory. Two functional derivatives of the generating functional with respect to $s(x)$ and $p(x)$ thus give us the scalar and the pseudoscalar 2-point functions, respectively, to the desired order. In the supersymmetric formulation we follow the procedure outlined in section 2, and thus add the sources in the fermion–fermion block only. Using the two sets of Feynman rules for the fluctuation fields $\xi(x)$, we find, to order ϵ^2:

$$\langle S^0(x)S^0(0)\rangle \;=\; C_S^0 + \frac{\Sigma^2}{2F^2}\left[\frac{1}{N_c}\left(m_0^2\bar{G}(x) + \alpha\bar{\Delta}(x)\right)a_- - \bar{\Delta}(x)\frac{a_+ + a_- - 4}{2}\right] \tag{5.32}$$

$$\langle P^0(x)P^0(0)\rangle \;=\; C_P^0 - \frac{\Sigma^2}{2F^2}\left[\frac{1}{N_c}\left(m_0^2\bar{G}(x) + \alpha\bar{\Delta}(x)\right)a_+ - \bar{\Delta}(x)\frac{a_+ + a_- + 4}{2}\right] \;, \tag{5.33}$$

with

$$a_\pm \;=\; \langle (U_{11} \pm U_{11}^{-1})^2\rangle \;. \tag{5.34}$$

The constant terms are given by the same expectation values of eq.(5.34)

$$C_S^0 \;=\; \frac{\Sigma_{eff}^2}{4}a_+^{1-loop} \;, \qquad C_P^0 \;=\; -\frac{\Sigma_{eff}^2}{4}a_-^{1-loop} \;, \tag{5.35}$$

but now evaluated with respect to the one-loop-improved action (4.22), and Σ_{eff} is as defined in eq. (4.23). In this way we obtain these constant terms to the required order ϵ^2.

These expressions are valid in both formulations. As a first check, we note that when $U \rightarrow 1$ the x-dependent part of $\langle S^0(x)S^0(0)\rangle$ vanishes: there is no tree-level scalar propagation in the quenched theory. But there *should* be tree-level propagation of the quenched pseudoscalar singlet, and indeed in this limit the x-dependent part of $\langle P^0(x)P^0(0)\rangle$ approaches

$$\frac{2\Sigma^2}{F^2}\left[\left(1 - \frac{\alpha}{N_c}\right)\bar{\Delta}(x) - \frac{m_0^2}{N_c}\bar{G}(x)\right] \tag{5.36}$$

which is simply the massless singlet propagator (cf. eq. (3.18)). We shall make a more detailed comparison, also including the zero-momentum modes, below.

To evaluate the remaining group integrals in closed form, we can make use of the exact results obtained in the supersymmetric formulation [13]. For a source $\mu_J \equiv \mu + J$ in the fermion–fermion slot, the generating function becomes

$$\mathcal{Z}_\nu[J] \;=\; \frac{1}{2}\mu_J\left(I_{\nu+1}(\mu_J) + I_{\nu-1}(\mu_J)\right)K_\nu(\mu) + \frac{1}{2}\mu I_\nu(\mu_J)\left(K_{\nu+1}(\mu) + K_{\nu-1}(\mu)\right) \;. \tag{5.37}$$

Using the fact that $Z_\nu[0] = 1$ (which here is a consequence of two Wronskian identities for the Bessel functions), this gives us the expectation value

$$\left\langle (U_{11} + (U^{-1})_{11})^2\right\rangle \;=\; 4\frac{\delta^2}{\delta J^2}Z_\nu[J]\Big|_{J=0}$$

$$= \quad 4\left[I_\nu(\mu)K_\nu(\mu) - I_{\nu+1}(\mu)K_{\nu-1}(\mu) + 1 + \frac{\nu(\nu-1)}{\mu^2}\right] \ . \tag{5.38}$$

It is quite simple to find the remaining matrix element by means of the explicit parametrization:

$$\begin{aligned}\left\langle U_{11}(U^{-1})_{11}\right\rangle &= \langle 1+\gamma\beta\rangle \\ &= 1 + 2\int_0^{2\pi}\frac{d\theta}{2\pi}\int_0^\infty ds d\gamma d\beta\ \gamma\beta e^{\nu(i\theta-s)}e^{\mu(\cos(\theta)-\cosh(s))} \\ &= 1 + 2I_\nu(\mu)K_\nu(\mu)\ . \end{aligned} \tag{5.39}$$

These expectation values suffice to compute the correlation functions in eqs. (5.32) and (5.33). Rewriting the final answer in terms of the tree-level chiral condensate eq. (4.21) and its derivative

$$\frac{\Sigma'_\nu(\mu)}{\Sigma} \ = \ I_\nu(\mu)K_\nu(\mu) - I_{\nu+1}(\mu)K_{\nu-1}(\mu) - \frac{\nu}{\mu^2}\ , \tag{5.40}$$

we find:

$$a_+ = 4\left[\frac{\Sigma'_\nu(\mu)}{\Sigma} + 1 + \frac{\nu^2}{\mu^2}\right]\ , a_- = 4\left[-\frac{1}{\mu}\frac{\Sigma_\nu(\mu)}{\Sigma} + \frac{\nu^2}{\mu^2}\right], \tag{5.41}$$

while the constants to the same order are:

$$\begin{aligned} C_S^0 &= \Sigma_{eff}^2\left[\frac{\Sigma'_\nu(\mu')}{\Sigma_{eff}} + 1 + \frac{\nu^2}{\mu'^2}\right] \ = \ \Sigma^2\left[\frac{\Sigma_\nu^{1-loop\ '}(\mu)}{\Sigma} + \left(\frac{\Sigma_{eff}}{\Sigma}\right)^2 + \frac{\nu^2}{\mu^2}\right] \\ C_P^0 &= \Sigma_{eff}^2\left[\frac{1}{\mu'}\frac{\Sigma_\nu(\mu')}{\Sigma_{eff}} - \frac{\nu^2}{\mu'^2}\right] \ = \ \Sigma^2\left[\frac{1}{\mu}\frac{\Sigma_\nu^{1-loop}(\mu)}{\Sigma} - \frac{\nu^2}{\mu^2}\right]\ , \end{aligned} \tag{5.42}$$

where μ' and Σ_{eff} are defined in eqs. (4.25) and (4.23), respectively.

Using the relation

$$\frac{\Sigma'_\nu(\mu)}{\Sigma} + \frac{1}{\mu}\frac{\Sigma_\nu(\mu)}{\Sigma} \ \to \ 0 \qquad \text{as} \ \ \mu \ \to \ 0\ , \tag{5.43}$$

it is easy to show that in the sum of the scalar and pseudoscalar correlation functions, the poles in the quark mass due to the zero modes cancel, and the sum has then a well-defined massless limit even at finite volume for $\nu \neq 0$. The case $\nu = 0$ is special: there is then an additional infrared singularity due to the distribution of the smallest non-zero Dirac operator eigenvalue. However, the infrared divergence for $\mu \to 0$ in that case is only logarithmic.

It is instructive to see, analytically, how the p- and ϵ-expansions match one another when $m_\pi L \sim 1$ (with $FL \gg 1$). We have already noted above that the x-dependent part of the $\langle P^0(x)P^0(0)\rangle$ correlation function to $O(\epsilon^2)$ approaches the tree-level propagator of a massless flavour singlet. Now that we have the constant part of this correlation function evaluated explicitly, we can see how this constant part precisely serves, to leading order, to restore the full massive propagator of the p-expansion. To see the matching we need to sum over topology first, because this is how the p-expansion is usually done. After performing this sum over topology, using relation (3.12) as well as the Gell-Mann–Oakes–Renner relation, we get, to leading order:

$$\begin{aligned}\langle P^0(x)P^0(0)\rangle &\sim \Sigma^2\left(\frac{1}{\mu} - \frac{\langle\nu^2\rangle}{\mu^2}\right) + \frac{2\Sigma^2}{F^2}\left[\left(1-\frac{\alpha}{N_c}\right)\bar{\Delta}(x) - \frac{m_0^2}{N_c}\bar{G}(x)\right] \\ &= \frac{2\Sigma^2}{F^2}\left[\frac{1}{m_\pi^2 V} - \frac{m_0^2}{N_c}\frac{1}{m_\pi^4 V} + \left(1-\frac{\alpha}{N_c}\right)\bar{\Delta}(x) - \frac{m_0^2}{N_c}\bar{G}(x)\right]\end{aligned}$$

$$= \frac{2\Sigma^2}{F^2}\left[\Delta(x) - \frac{\alpha}{N_c}\sum_p \frac{p^2 e^{ipx}}{(p^2+m_\pi^2)^2} - \frac{m_0^2}{N_c}G(x) + O(m_\pi^2)\right]$$
$$= \frac{2\Sigma^2}{F^2}\mathcal{G}(x) + O(m_\pi^2)\ . \tag{5.44}$$

As in the case of the one-loop correction to the chiral condensate [9], the sum over topology precisely restores the m_0-dependence needed for the ϵ- and p-expansions to match.

For comparisons with lattice gauge theory data, it is convenient to recast the above results in terms of the space-integrated correlators in the (euclidean) time direction, here labelled by t:

$$\mathcal{P}^i(t) = \int d^3x \langle P^i(x) P^i(0)\rangle \quad , \quad \mathcal{S}^i(t) = \int d^3x \langle S^i(x) S^i(0)\rangle. \tag{5.45}$$

For this purpose we need the projections onto zero momentum of both the usual massless propagator and the double-pole term. They both follow immediately from Taylor-expanding the massive pion propagator in powers of m_π. From

$$\int d^3x\ \Delta(x) \ = \ \frac{\cosh(m_\pi(T/2-t))}{2m_\pi \sinh(m_\pi T/2)}\ , \tag{5.46}$$

and eq. (3.17), we find

$$\int d^3x\ \Delta(x) \ = \ \frac{1}{Tm_\pi^2} + \frac{T}{2}\left[\left(\tau-\frac{1}{2}\right)^2 - \frac{1}{12}\right] + \frac{T^3}{24}\left[\tau^2(\tau-1)^2 - \frac{1}{30}\right] m_\pi^2 + \ldots, \tag{5.47}$$

which makes it convenient to define [5]

$$h_1(\tau) \ = \ \frac{1}{T}\int d^3x\ \bar{\Delta}(x) \ = \ \frac{1}{2}\left[(\tau-\frac{1}{2})^2 - \frac{1}{12}\right] \tag{5.48}$$
$$h_2(\tau) \ = \ -\frac{1}{T^3}\int d^3x\ \bar{G}(x) \ = \ \frac{1}{24}\left[\tau^2(\tau-1)^2 - \frac{1}{30}\right]\ . \tag{5.49}$$

Here T is the extent in the temporal direction, and $\tau = t/T$. These 2nd and 4th order polynomials replace the exponentially decaying correlations in the regime of the ϵ-expansion.

Figures 1 show the result for $\mathcal{P}^0(t)$ and $\mathcal{S}^0(t)$ in this ϵ regime, for three values of the topological charge $\nu = 0, 1, 2$, and a quark mass $m = 3$ MeV in a typical lattice of $V = 16^3 32$ at $a^{-1} = 2$ GeV. In these plots, and in those of the next sections, we have used the values $m_0 = 600$ MeV and $\alpha = 0.6$. For Σ we take as indicative the value (270 MeV)^3 at the commonly used renormalization scale $L_0 = (4\pi F)^{-1}$.

We should stress that in these predictions, and in any other predictions given in this paper, the contributions from higher excited states with the same quantum numbers are neglected. These higher states clearly do contribute to the correlation functions at short time separations, but they are exponentially suppressed at large t. Therefore our predictions should only fit the measured correlation functions for sufficiently large time separation between the sources.

5.1 Flavoured Correlation Functions

The computation of mesonic correlation functions in non-singlet channels is a little more difficult, because we need the exact evaluation of the group integral over zero momentum modes for $N_v > 1$. Here we restrict ourselves to the simplest case of $N_v = 2$.

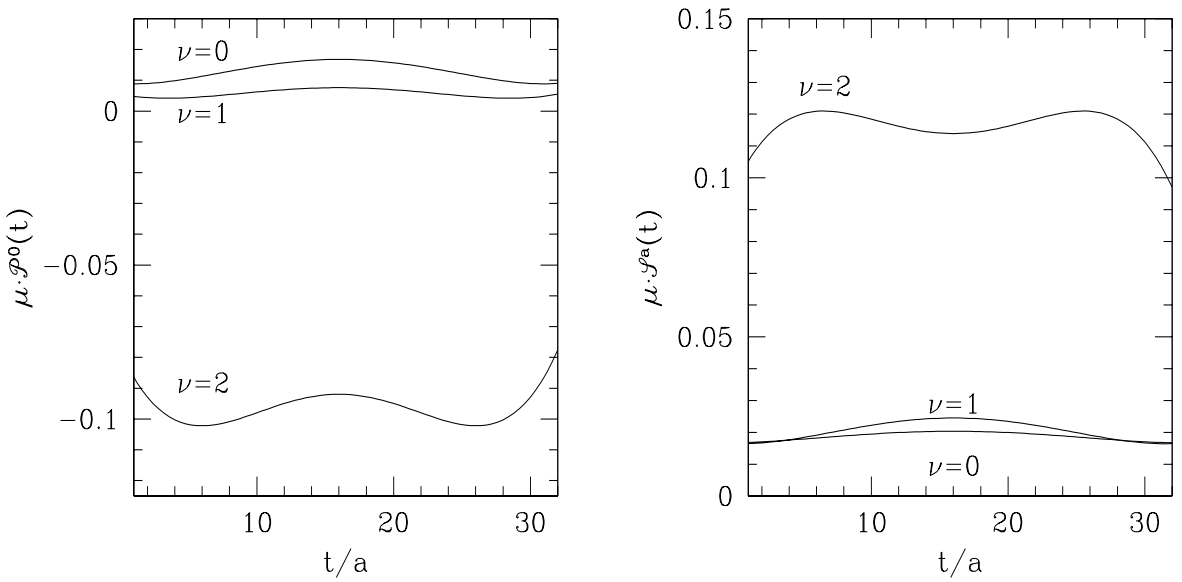

Figure 1: $\mu\mathcal{P}^0(t)$ (left) and $\mu\mathcal{S}^0(t)$ (right) in a lattice of $V = L^3T = 16^3 32$ and $a^{-1} \simeq 2$ GeV. The quark mass is $m = 3$ MeV and the three curves correspond to $\nu = 0, 1$ and 2.

Let us denote the quark bilinears as follows:

$$S^a(x) \equiv \bar{\psi}(x) t^a I_{N_v} \psi(x) \quad , \qquad P^a(x) \equiv \bar{\psi}(x) t^a i\gamma_5 I_{N_v} \psi(x) \ , \tag{5.50}$$

where in this case $t^a = \tau^a/2$, and the τ^a's are the usual Pauli matrices. The corresponding two-point functions are $\langle S^a(x) S^a(0)\rangle$ and $\langle P^a(x) P^a(0)\rangle$, for a=1-3. Here we present some details of the calculation of the correlators for $a = 1$.

The appropriate flavoured sources $s^a(x)$ and $p^a(x)$ are obtained by lettting

$$\mathcal{L}_{QCD} \ \rightarrow \ \mathcal{L}_{QCD} + s^a(x) S^a(x) + p^a(x) P^a(x) \tag{5.51}$$

at the quark level. This translates into

$$\mathcal{M} \ \rightarrow \ \chi(x) = \mathcal{M} + s^a(x) t^a I_{N_v} + i p^a(x) t^a I_{N_v} \tag{5.52}$$

in the effective theory. Two functional derivatives with respect to these sources then give us the desired correlation functions. To order ϵ^2, we find:

$$\langle S^1(x) S^1(0)\rangle = C_S^1 + \frac{\Sigma^2}{2F^2}\left[\frac{1}{N_c}\left(m_0^2 \bar{G}(x) + \alpha \bar{\Delta}(x)\right) c_- - \bar{\Delta}(x) b_-\right] \tag{5.53}$$

$$\langle P^1(x) P^1(0)\rangle = C_P^1 - \frac{\Sigma^2}{2F^2}\left[\frac{1}{N_c}\left(m_0^2 \bar{G}(x) + \alpha \bar{\Delta}(x)\right) c_+ - \bar{\Delta}(x) b_+\right] \ , \tag{5.54}$$

where, after using some of the identities provided in Appendix A, one finds

$$c_\pm = \frac{1}{4}\left\langle (U_{12} + U_{21} \pm (U^{-1})_{12} \pm (U^{-1})_{21})^2 \right\rangle \tag{5.55}$$

$$b_\pm = \frac{1}{2}\left\langle U_{11} U_{22} + (U^{-1})_{11} (U^{-1})_{22} \right\rangle \pm 1 \ . \tag{5.56}$$

The constant terms will also be evaluated to $O(\epsilon^2)$. Since they are flavour-symmetric, we can simply take the constant part of

$$\frac{1}{3}\frac{\delta^2}{\delta s^a(x)\delta s^a(0)}\mathcal{Z}_\nu[J]$$

and similarly for C_P^a. Using the $SU(2)$ completeness relation

$$t^a_{ij}t^a_{kl} \;=\; \frac{1}{2}\left[\delta_{il}\delta_{jk} - \frac{1}{2}\delta_{ij}\delta_{kl}\right] \;, \tag{5.57}$$

we then get

$$\begin{aligned} C_S^a \;&=\; \frac{\Sigma_{eff}^2}{24}\left\langle \frac{1}{2}\left((U_{11}+(U^{-1})_{11})^2 + (U_{22}+(U^{-1})_{22})^2\right) + 2(U_{12}+(U^{-1})_{12})(U_{21}+(U^{-1})_{21}) \right. \\ &\quad \left. - (U_{11}+(U^{-1})_{11})(U_{22}+(U^{-1})_{22})\right\rangle \\ C_P^a \;&=\; -\frac{\Sigma_{eff}^2}{24}\left\langle \frac{1}{2}\left((U_{11}-(U^{-1})_{11})^2 + (U_{22}-(U^{-1})_{22})^2\right) + 2(U_{12}-(U^{-1})_{12})(U_{21}-(U^{-1})_{21}) \right. \\ &\quad \left. - (U_{11}-(U^{-1})_{11})(U_{22}-(U^{-1})_{22})\right\rangle \;. \end{aligned} \tag{5.58}$$

Here the expectation values are again to be computed with respect to the one-loop-improved action eq. (4.22) so as to reach $O(\epsilon^2)$ accuracy.

In order to calculate the various integrals over the zero-momentum modes explicitly, we make use of the fact that they can all be related to an expectation value already computed in eq. (5.38), and

$$\left\langle (U_{11}+(U^{-1})_{11})(U_{22}+(U^{-1})_{22})\right\rangle \;, \tag{5.59}$$

which was evaluated explicitly for the zero-momentum mode integral with $N_v = 2$ in ref. [27]. The idea of how to get the other integrals from these two is simple, and most easily explained in the replica formalism. There it is particularly clear that the quantity $\det(\mathcal{M})^{-\nu}\mathcal{Z}_\nu$ is a function of the eigenvalues of $\mathcal{M}\mathcal{M}^\dagger$ only. This means that all quadratic expectation values, after appropriate manipulations, can be related directly to the expectation value of eq.(5.59), and that of eq. (5.38).

Using a variety of 2×2 matrix sources J, we have collected a list with the results of explicit evaluations of all needed zero-momentum mode integrals. For the reader interested in the technical details, see Appendix A. Here we simply present the final results:

$$\begin{aligned} b_+ \;&=\; 2\left(1+\frac{\nu^2}{\mu^2}\right) \;, \qquad b_- = 2\frac{\nu^2}{\mu^2} \\ c_+ \;&=\; 2\frac{\Sigma'_\nu(\mu)}{\Sigma} \;, \qquad c_- = -2\frac{1}{\mu}\frac{\Sigma_\nu(\mu)}{\Sigma} \end{aligned} \tag{5.60}$$

and

$$C_S^a = \frac{1}{2}\Sigma\Sigma_\nu^{1-loop\;\prime}(\mu) \;, \qquad C_P^a = \frac{1}{2\mu}\Sigma\Sigma_\nu^{1-loop}(\mu) \;. \tag{5.61}$$

As a non-trivial check on the calculation, we have also evaluated the correlators corresponding to $a = 2$ and 3. In the latter case the intermediate details are very different, but the final results coincide in both cases with the ones above for $a = 1$, as expected.

In the sum of the two flavoured correlation functions, our expressions simplify. We find (no sum on a):

$$\langle S^a(x)S^a(0)\rangle \;+\; \langle P^a(x)P^a(0)\rangle \;=\; \frac{1}{2}\Sigma\left[\Sigma_\nu^{1-loop\;\prime}(\mu)+\frac{1}{\mu}\Sigma_\nu^{1-loop}(\mu)\right] + \frac{\Sigma^2}{F^2}\left[\bar{\Delta}(x)-\left(\frac{\Sigma_\nu(\mu)}{\Sigma}+\frac{1}{\mu}\frac{\Sigma_\nu(\mu)}{\Sigma}\right)\frac{1}{N_c}\left(m_0^2\bar{G}(x)+\alpha\bar{\Delta}(x)\right)\right]\;. \tag{5.62}$$

As in the flavour-singlet case, the sum remains finite in the $\mu\to 0$ limit for $\nu\neq 0$, on account of eq. (5.43).

Here we can also check analytically that the ϵ- and p-expansions join on to each other. This is because the $\langle P^a(x)P^b(0)\rangle$ correlation function we have computed should simply reproduce the tree-level pion propagation of the p-expansion to $O(\epsilon^2)$. Indeed, we find, to lowest order (no sum on a):

$$\begin{aligned}\langle P^a(x)P^a(0)\rangle &\sim \left[\frac{\Sigma^2}{2\mu}+\frac{\Sigma^2}{F^2}\bar{\Delta}(x)\right]\\ &= \frac{\Sigma^2}{F^2}\left[\frac{1}{m_\pi^2 V}+\bar{\Delta}(x)\right]\\ &= \frac{\Sigma^2}{F^2}\Delta(x)+O(m_\pi^2)\;,\end{aligned} \tag{5.63}$$

which is precisely the tree-level result of the p-expansion. The constant again provides the term needed to restore the pion zero-mode term in the propagator.

Again it is convenient to reformulate these results in terms of projections onto zero momentum. The relevant definitions have already been given above, and in Figure 2 we show $\mathcal{P}^a(t)$ for $\nu=0,1,2$ and various quark masses within the ϵ regime. As expected, the effect of the zero modes are dominant in this regime, inducing a large dependence on the topological charge. The same effect is observed for the scalar correlator in Fig. 3. Note that this correlation function is negative for $\nu=1,2$. This feature was first noted by the authors of [31] for larger quark masses in the p-expansion regime (ie. not at fixed topology). As explained above, it is possible to cancel the poles induced by the topological zero modes by considering the sum of the scalar and pseudoscalar propagators. This is shown in Figures 4. The only divergence in the $\mu\to 0$ limit is then restricted to the $\nu=0$ sector and it is only logarithmic.

As far as we are aware, there are at present no lattice data for any of these correlation functions in quenched QCD at fixed topology and in the appropriate quark mass range. Very recently, there has been a study of pseudoscalar correlation functions in the $N_f=2$ Schwinger model at fixed topology [28], and distinct signatures of topology were actually found there. But, unfortunately, neither the present calculation for quenched QCD nor the one presented in section 6 for full QCD at fixed topology can directly be compared with these two-dimensional results. It has also recently been suggested to study QCD at fixed topology, but at volumes so large that correlations are still exponential in the masses [29].

5.2 Ward Identities at Fixed Topology

Ward identities associated with the chiral rotation of the physical (valence in the replica context) quarks provide useful cross-checks on the above results. For the singlet chiral transformation, the relation is

$$\langle(\partial_\mu A_\mu^0(x)-2mP^0(x)-2iN_v\omega(x))\mathcal{O}(0)\rangle \;=\; -\langle\delta\mathcal{O}(0)\rangle\delta(x), \tag{5.64}$$

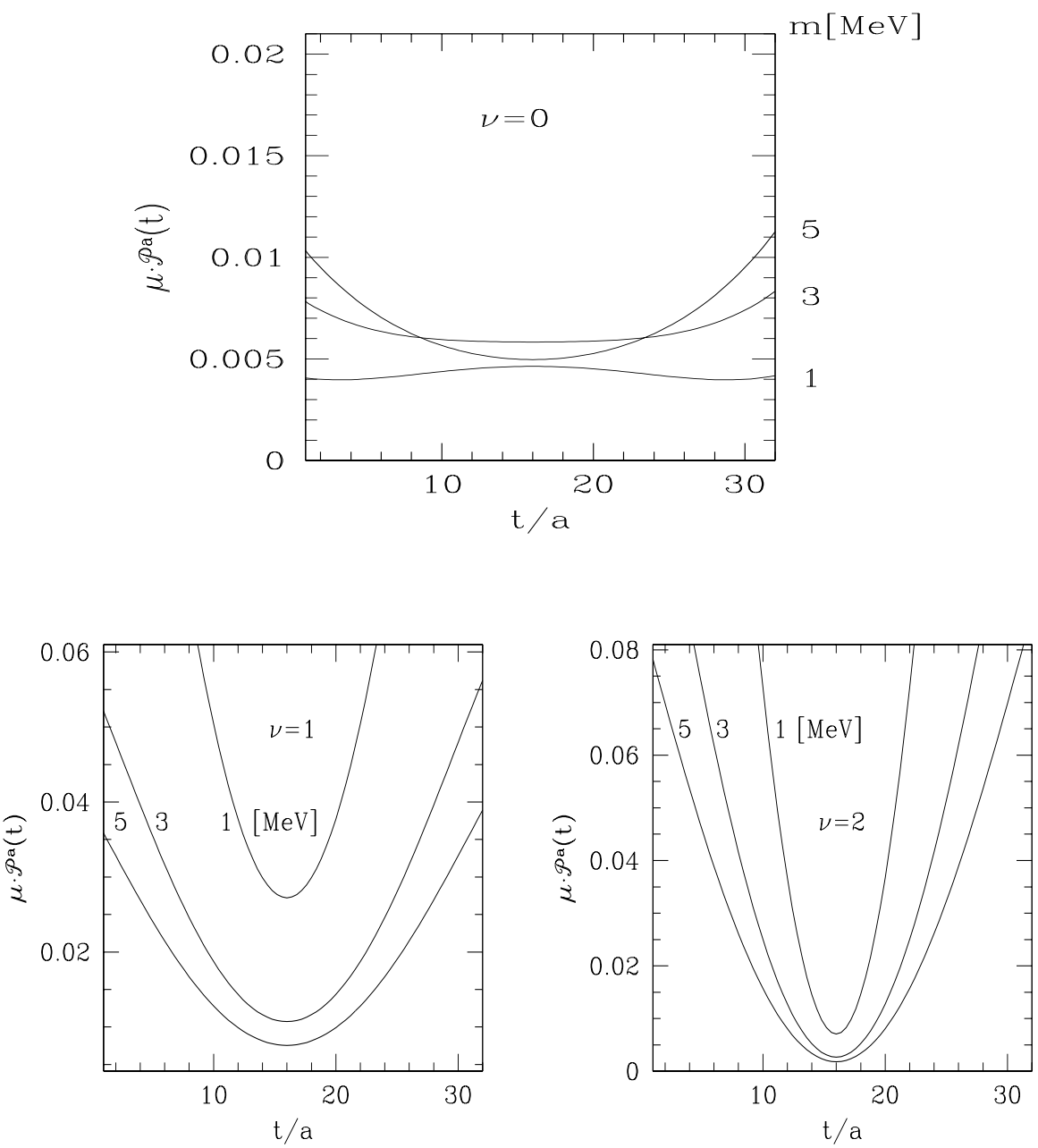

Figure 2: $\mu\mathcal{P}^a(t)$ for quark masses $m = 1, 3$ and 5 MeV and $\nu = 0$ (upper), 1 (down left), 2 (down right). The lattice volume is $V = L^3T = 16^3 32$ and $a^{-1} \simeq 2$ GeV.

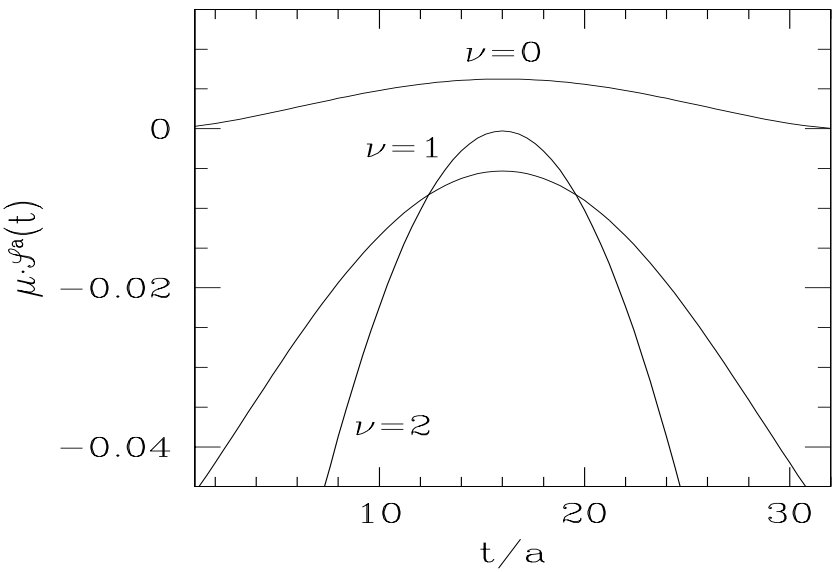

Figure 3: $\mu\mathcal{S}^a(t)$ for a quark mass $m = 3$ MeV and $\nu = 0, 1, 2$. The lattice volume is $V = L^3T = 16^3 32$ and $a^{-1} \simeq 2$ GeV.

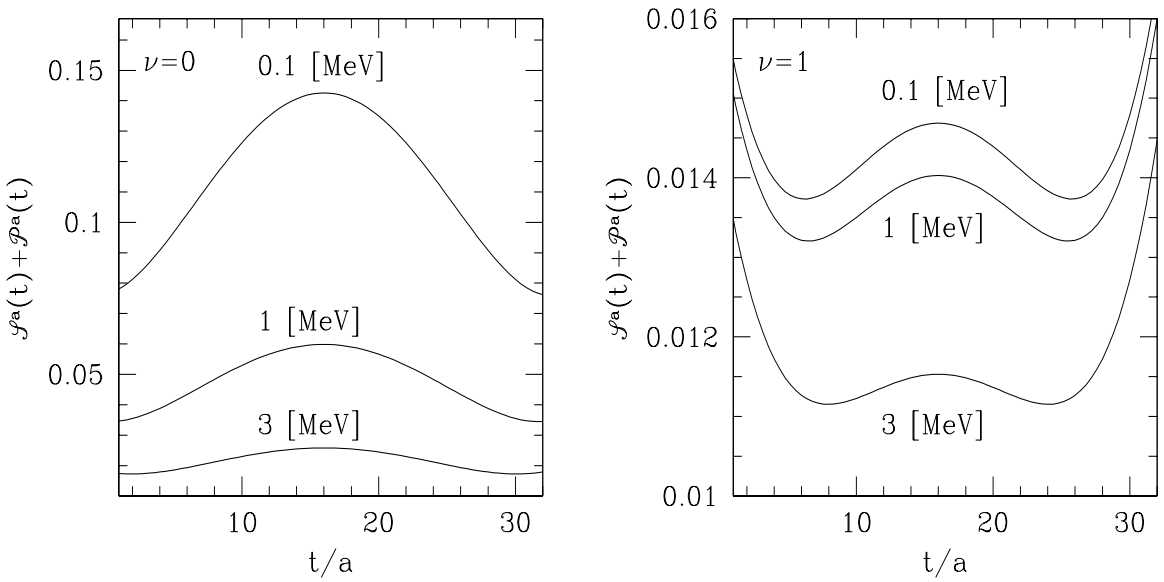

Figure 4: $\mathcal{P}^a(t) + \mathcal{S}^a(t)$ for quark masses $m = 0.1, 1$ and 3 MeV and $\nu = 0$ and 1. The lattice volume is $V = L^3T = 16^3 32$ and $a^{-1} \simeq 2$ GeV.

where $A^0_\mu = \bar{\psi} I_{N_v} \gamma_\mu \gamma_5 \psi$. The operator

$$\omega(x) \;=\; \frac{1}{16\pi^2} Tr F_{\mu\nu} \tilde{F}_{\mu\nu} \tag{5.65}$$

is the topological charge density, $\mathcal{O}(x)$ is any local operator and $\delta\mathcal{O}(x)$ is its variation under an infinitesimal singlet chiral rotation at point x. The identity of eq. (5.64) is normally considered in the full theory, after summing over all topological sectors. But it is exact, and in fact simpler, also in sectors of fixed topology. We also remark that although all effects of quark loops disappear in the quenched theory, the above identity reflects the consequences of a chiral rotation in part of the theory only (i.e. in the valence sector). It would reduce to a triviality if we were to rotate all fields simultaneously.

If we combine the Ward identity for $\mathcal{O}(x) = P^0(x)$ and $\mathcal{O}(x) = \omega(x)$, and integrate over space-time, we can eliminate $\langle \omega(x) P^0(0) \rangle$ to get at fixed topology

$$\int d^4x \; \langle P^0(x) P^0(0) \rangle \;=\; -\frac{\nu^2}{m^2 V} - \frac{\langle S^0 \rangle}{mV} \; . \tag{5.66}$$

where S^0 is defined in eq. (5.29) and we have here used $N_v = 1$. Inserting eq. (5.33) and taking into account eq. (3.16), we get, to $O(\epsilon^2)$:

$$C^0_P \;=\; \frac{\Sigma^{1-loop}_\nu(\mu)}{mV} - \frac{\nu^2}{(mV)^2} \; , \tag{5.67}$$

which coincides precisely with our result in eq. (5.42). Actually, at fixed gauge field topology, $\langle \omega(x) P^0(0) \rangle$ can be computed directly using eq. (A.17) of Appendix A:

$$\frac{1}{\Sigma} \langle P^0(0) \rangle \;=\; \frac{i\nu}{\mu} \; . \tag{5.68}$$

Inserting this into the identity of $\mathcal{O}(x) = P^0(x)$ gives precisely the same relation as (5.67).

Similarly, the general Ward identity for a flavour non-singlet chiral rotation is

$$\langle (\partial_\mu A^a_\mu(x) - 2m P^a(x)) \mathcal{O}(0) \rangle \;=\; -\langle \delta^a \mathcal{O}(0) \rangle \delta(x) \; , \tag{5.69}$$

where $\delta^a \mathcal{O}(x)$ is the variation of $\mathcal{O}$ under an infitesimal chiral rotation at x in the flavour direction a. Combining the identities thus obtained for $\mathcal{O}(x) = P^a(x)$ and $\mathcal{O}(x) = \partial_\mu A^a_\mu(x)$, and subsequently integrating over space-time we arrive at the relation, to order ϵ^2 (no sum on a):

$$\int d^4x \; \langle P^a(x) P^a(0) \rangle \;=\; -\frac{1}{4} \frac{\langle S^0 \rangle}{mV} \;=\; \frac{1}{2} \frac{\Sigma^{1-loop}_\nu(\mu)}{m} + \ldots \; , \tag{5.70}$$

which also agrees with the constant term C^a_P of eq. (5.61), computed to the same order. Note that S^0 in eq. (5.70) is the one corresponding to $N_v = 2$.

Although not Ward identities as such, a series of relations that follow from spectral representations of the involved correlation functions can also give useful checks on our results. Such relations were derived in ref. [30], using the language of lattice overlap fermions, but they can easily be transcribed into continuum language. In the quenched case a particularly interesting relation gives a sum rule for the flavoured scalar correlation function. In our normalization, with no sum on a,

$$\int d^4x \; \langle S^a(x) S^a(0) \rangle \;=\; -\frac{1}{2V} \frac{\partial}{\partial m} \langle S^0 \rangle \;=\; \frac{1}{2} \frac{\partial}{\partial m} \Sigma^{1-loop}_\nu(\mu) + \ldots \; , \tag{5.71}$$

which agrees with our value of the constant C_S^a in eq. (5.61). The authors of ref. [30] have also derived some general relations for the $m \to 0$ limit of the finite volume correlation functions we have considered here. For $N_v = 2$ they are in our normalization (again no sum on a):

$$\int d^4x \ \left[\langle P^0(x)P^0(0)\rangle - 4\langle S^a(x)S^a(0)\rangle\right] \ \sim \ \frac{4|\nu|}{m^2V} - \frac{4\nu^2}{m^2V} \tag{5.72}$$

$$\int d^4x \ \left[\langle P^a(x)P^a(0)\rangle - \langle S^a(x)S^a(0)\rangle\right] \ \sim \ \frac{|\nu|}{m^2V} \tag{5.73}$$

as $m \to 0$. We have not computed $\langle P^0(x)P^0(0)\rangle$ explicitly for $N_v = 2$, but to check eq. (5.72) we need only the constant part of this $N_v = 2$ correlator. It is fixed by the Ward identity of eq. (5.64) to be

$$N_v \left[\frac{\Sigma_\nu(\mu)}{mV} - \frac{N_v\nu^2}{(mV)^2}\right]$$

to lowest order. Plugging this in, and using the relation eq. (5.71), which we have just confirmed, we find that eq. (5.72) is indeed satisfied. Similarly, eq. (5.73) is easily seen to be satisfied by taking the $m \to 0$ limit of our exact finite-volume expressions.

6 Full QCD at Fixed Topology

Eventually lattice computations with light quarks will be pushed beyond the quenched limit. It is therefore useful to know the corresponding analytical expressions for finite-volume meson propagators also in full QCD. The ϵ-expansion of the chiral Lagrangian is much simpler in this case, as all effects of the flavour singlet term can be ignored. More precisely, we obtain the relevant chiral Lagrangian by taking the limit $m_0 \to \infty$ of the replica chiral Lagrangian. This enforces $\mathrm{Tr}\xi(x) = 0$, and the singlet field decouples. The relevant expansion was carried through to order ϵ^4 in ref. [3], probably beyond the realistic accuracy of lattice simulations in the near future. It is of interest to find also the corresponding analytical expressions in sectors of fixed gauge field topology. Such expressions cannot immediately be inferred from ref. [3], as all results are listed in a manner valid only for flavour group $SU(N_f)$[8]. We first list the correlation functions up to order ϵ^2 in the full theory with summation over topological charges, which agree with the results of ref. [3] to this order[9]:

$$\begin{aligned}
\langle S^0(x)S^0(0)\rangle &= C_S^0 - \frac{\Sigma^2}{2F^2}\left[\left\langle \mathrm{Tr}[(U-U^\dagger)^2]\right\rangle - \frac{1}{N_f}\left\langle (\mathrm{Tr}(U-U^\dagger))^2\right\rangle\right]\bar{\Delta}(x) \\
\langle P^0(x)P^0(0)\rangle &= C_P^0 + \frac{\Sigma^2}{2F^2}\left[\left\langle \mathrm{Tr}[(U+U^\dagger)^2]\right\rangle - \frac{1}{N_f}\left\langle (\mathrm{Tr}(U+U^\dagger))^2\right\rangle\right]\bar{\Delta}(x) \\
\langle S^a(x)S^b(0)\rangle &= \frac{\delta^{ab}}{N_f^2-1}\left\{C_S - \frac{\Sigma^2}{4F^2}\left[\left(\frac{N_f^2+1}{N_f^2}\right)\left\langle (\mathrm{Tr}(U))^2 + (\mathrm{Tr}(U^\dagger))^2\right\rangle\right.\right. \\
&\quad \left.\left. -\frac{2}{N_f}\left\langle \mathrm{Tr}(U^2) + \mathrm{Tr}(U^{\dagger 2})\right\rangle - 2N_f^2 + 4 - \frac{2}{N_f^2}\left\langle \mathrm{Tr}(U)\mathrm{Tr}(U^\dagger)\right\rangle\right]\bar{\Delta}(x)\right\} \\
\langle P^a(x)P^b(0)\rangle &= \frac{\delta^{ab}}{N_f^2-1}\left\{C_P + \frac{\Sigma^2}{4F^2}\left[\left(\frac{N_f^2+1}{N_f^2}\right)\left\langle (\mathrm{Tr}(U))^2 + (\mathrm{Tr}(U^\dagger))^2\right\rangle\right.\right.
\end{aligned}$$

[8] In particular, the author of ref. [3] has implicitly used the identity $\langle \mathrm{Tr}(U)\rangle = \langle \mathrm{Tr}(U^\dagger)\rangle$, which holds only after summing over topological charges. Also, other identities specific to the group $SU(N_f)$ have been employed prior to the listing of results in ref. [3].

[9] Our notation is the same as in the previous sections.

$$-\frac{2}{N_f}\left\langle \mathrm{Tr}(U^2)+\mathrm{Tr}(U^{\dagger 2})\right\rangle + 2N_f^2 - 4 + \frac{2}{N_f^2}\left\langle \mathrm{Tr}(U)\mathrm{Tr}(U^\dagger)\right\rangle\Bigg]\bar{\Delta}(x)\Bigg\} \quad . (6.74)$$

To the order at which we are working, we need the $O(\epsilon^2)$ contributions to the constant terms. As in the quenched theory, these are entirely given by the one-loop correction to the chiral condensate, which here reads [1]

$$\frac{\Sigma_{eff}(V)}{\Sigma} = 1 + \frac{N_f^2-1}{N_f}\frac{1}{F^2}\frac{\beta_1(L_i/L)}{L^2} + \ldots \tag{6.75}$$

Here $\beta_1(L_i/L)$ is another of the universal shape coefficients [2, 5]. To order ϵ^2 the constant terms are given by

$$\begin{aligned}
C_S^0 &= \frac{\Sigma_{eff}^2}{4}\left\langle (\mathrm{Tr}(U+U^\dagger))^2\right\rangle \\
C_P^0 &= -\frac{\Sigma_{eff}^2}{4}\left\langle (\mathrm{Tr}(U-U^\dagger))^2\right\rangle \\
C_S &= \frac{\Sigma_{eff}^2}{8}\left[\left\langle \mathrm{Tr}[(U+U^\dagger)^2]\right\rangle - \frac{1}{N_f}\left\langle (\mathrm{Tr}(U+U^\dagger))^2\right\rangle\right] \\
C_P &= -\frac{\Sigma_{eff}^2}{8}\left[\left\langle \mathrm{Tr}[(U-U^\dagger)^2]\right\rangle - \frac{1}{N_f}\left\langle (\mathrm{Tr}(U-U^\dagger))^2\right\rangle\right] \quad ,
\end{aligned} \tag{6.76}$$

where the expectation values are taken with respect to the one-loop improved action (simply let $\Sigma \to \Sigma_{eff}$ in the tree level action). As a check on these results, we note that upon substituting $U \to 1$ the coefficients of $\Delta(x)$ vanish for the first three correlators. Indeed, there should be no tree level propagation of non-zero modes in any of these correlation functions[10]. A similar substitution in the last (flavoured, pseudoscalar) correlation function yields the coefficient Σ^2/F^2, corresponding to tree level propagation of the non-zero-momentum modes in this channel.

Next, to project down on sectors of fixed topological charge ν we again integrate over θ as in section 3, simultaneously extending the group integration from $SU(N_f)$ to $U(N_f)$ for the zero-momentum modes. Thus only the integration over the zero-momentum modes is affected by this projection, and the fluctuation part is precisely as in ref. [3]. In particular, the fluctuations $\xi^a(x)$ still belong to the adjoint representation of $SU(N_f)$. The above expressions then remain valid in sectors of fixed topological charge, once expectation values over the zero-momentum modes are interpreted as being with respect to the measure of

$$\mathcal{Z}_\nu = \int_{U(N_f)} dU\ (\det U)^\nu \exp\left[\frac{1}{2}\mu\mathrm{Tr}(U+U^\dagger)\right] \quad . \tag{6.77}$$

One obvious benefit of going to sectors of fixed topological charge is that all pertinent expectation values can be evaluated explicitly for any N_f. In order to do so, we first invoke the identities (see Appendix A for a derivation)

$$\begin{aligned}
\left\langle \mathrm{Tr}(U^2)\right\rangle &= N_f - \frac{2(N_f+\nu)}{\mu}\left\langle \mathrm{Tr}(U)\right\rangle \\
\left\langle \mathrm{Tr}(U^{\dagger 2})\right\rangle &= N_f + \frac{2(\nu-N_f)}{\mu}\left\langle \mathrm{Tr}(U^\dagger)\right\rangle
\end{aligned}$$

[10] In contrast to the quenched case, where we do have flavour-singlet propagation at tree level.

$$\langle \mathrm{Tr}(U) \rangle \;=\; \left\langle \mathrm{Tr}(U^\dagger) \right\rangle - \frac{2N_f\nu}{\mu} \;. \tag{6.78}$$

Let us define

$$\frac{\Sigma_\nu(\mu)}{\Sigma} \;\equiv\; \frac{1}{N_f}\frac{\partial}{\partial\mu} \ln \mathcal{Z}_\nu \;, \tag{6.79}$$

for a theory with N_f quarks of equal mass. The partition function Z_ν is known explicitly in all generality [32, 8]. Up to an irrelevant overall factor the integration of eq. (6.77) gives

$$\mathcal{Z}_\nu(\{\mu_i\}) = \det[\mu_i^{j-1} I_{\nu+j-1}(\mu_i)] / \prod_{i>j}^{N_f} (\mu_i^2 - \mu_j^2) \;, \tag{6.80}$$

where $I_n(x)$ is the modified Bessel function, and the determinant in the numerator is over a matrix of size $N_f \times N_f$ (the indices i and j denote the matrix elements). In practice one may be mostly interested in the equal-mass case, where this expression simplifies considerably. Up to an irrelevant overall factor,

$$\mathcal{Z}_\nu(\{\mu\}) = \det[I_{\nu+j-i}(\mu)] \;, \tag{6.81}$$

where again the determinant is taken over a matrix of size $N_f \times N_f$. Then $\Sigma_\nu(\mu)$ is known explicitly in terms of modified Bessel functions for all N_f. Next, using

$$\frac{\Sigma_\nu(\mu)}{\Sigma} \;=\; \frac{1}{2N_f} \left\langle \mathrm{Tr}(U + U^\dagger) \right\rangle \tag{6.82}$$

and the last of the identities (6.78), we obtain

$$\begin{aligned} \langle \mathrm{Tr}(U) \rangle &= N_f \left(\frac{\Sigma_\nu(\mu)}{\Sigma} - \frac{\nu}{\mu} \right) \\ \left\langle \mathrm{Tr}(U^\dagger) \right\rangle &= N_f \left(\frac{\Sigma_\nu(\mu)}{\Sigma} + \frac{\nu}{\mu} \right) \;. \end{aligned} \tag{6.83}$$

Upon substituting eq. (6.83), the first two identities of eq. (6.78) as well as eq. (B.19) in eq. (6.74), we finally get

$$\begin{aligned} \langle S^0(x) S^0(0) \rangle &= C_S^{0(\nu)} + \frac{2\Sigma^2}{F^2}(N_f^2 - 1)\frac{1}{\mu}\frac{\Sigma_\nu(\mu)}{\Sigma}\bar{\Delta}(x) \\ \langle P^0(x) P^0(0) \rangle &= C_P^{0(\nu)} + \frac{2\Sigma^2}{F^2} N_f \left[1 - \frac{N_f}{\mu}\frac{\Sigma_\nu(\mu)}{\Sigma} - \frac{1}{N_f}\frac{\Sigma_\nu'(\mu)}{\Sigma} - \left(\frac{\Sigma_\nu(\mu)}{\Sigma}\right)^2 + \frac{\nu^2}{\mu^2} \right] \bar{\Delta}(x) \\ \langle S^a(x) S^b(0) \rangle &= \frac{\delta^{ab}}{N_f^2 - 1} \left\{ C_S^{(\nu)} - \frac{\Sigma^2}{4F^2} \left[2N_f \left(\frac{\Sigma_\nu'(\mu)}{\Sigma} + N_f \left(\frac{\Sigma_\nu(\mu)}{\Sigma}\right)^2 - N_f \right) \right.\right. \\ &\quad \left.\left. + (2N_f^2 - 4)\frac{\nu^2}{\mu^2} + \left(\frac{6N_f^2 - 4}{N_f} \right) \frac{1}{\mu}\frac{\Sigma_\nu(\mu)}{\Sigma} \right] \bar{\Delta}(x) \right\} \\ \langle P^a(x) P^b(0) \rangle &= \frac{\delta^{ab}}{N_f^2 - 1} \left\{ C_P^{(\nu)} + \frac{\Sigma^2}{4F^2} \left[2(N_f^2 + 2) \left[\left(\frac{\Sigma_\nu(\mu)}{\Sigma}\right)^2 + \frac{1}{N_f}\frac{\Sigma_\nu'(\mu)}{\Sigma} \right] \right.\right. \\ &\quad \left.\left. + 2N_f^2 - 8 + \frac{6N_f}{\mu}\frac{\Sigma_\nu(\mu)}{\Sigma} - \frac{8\nu^2}{\mu^2} \right] \bar{\Delta}(x) \right\} \;. \end{aligned} \tag{6.84}$$

As a check of these expressions we can take the limit $\mu \to \infty$. For any finite ν, this freezes the zero-mode integral at $U = 1$, and we indeed find that the coefficients of the $\Delta(x)$ terms in the first three

equations of eq. (6.84) vanish in that limit. Similarly, the last coefficient approaches the required coefficient Σ^2/F^2 for reproducing the tree-level propagation of non-zero-momentum modes of the flavoured Goldstone bosons.

The explicit expressions for the constant terms in eq. (6.84) are

$$\begin{aligned}
C_S^{0(\nu)} &= \Sigma^2 N_f \left[\frac{\Sigma_\nu^{1-loop\ \prime}(\mu)}{\Sigma} + N_f \left(\frac{\Sigma_\nu^{1-loop}(\mu)}{\Sigma} \right)^2 \right] \\
C_P^{0(\nu)} &= \Sigma^2 N_f \left[\frac{1}{\mu} \frac{\Sigma_\nu^{1-loop}(\mu)}{\Sigma} - \frac{\nu^2 N_f}{\mu^2} \right] \\
C_S^{(\nu)} &= \frac{\Sigma^2 N_f}{2} \left[\left(\frac{\Sigma_{eff}}{\Sigma} \right)^2 - \frac{1}{N_f} \frac{\Sigma_\nu^{1-loop\ \prime}(\mu)}{\Sigma} - \frac{N_f}{\mu} \frac{\Sigma_\nu^{1-loop}(\mu)}{\Sigma_\nu} - \left(\frac{\Sigma_\nu^{1-loop}(\mu)}{\Sigma_\nu} \right)^2 + \frac{\nu^2}{\mu^2} \right] \\
C_P^{(\nu)} &= (N_f^2 - 1) \frac{1}{2\mu} \Sigma \Sigma_\nu^{1-loop}(\mu) \ . \qquad (6.85)
\end{aligned}$$

One notices that these QCD correlation functions at fixed topology need not be positive-definite. In the quenched theory the negative correlations had an immediate interpretation in terms of unitarity violation caused by eliminating the fermion determinant. Here, the origin of unitarity violation is only the restriction to fixed gauge field topology, and this peculiarity should disappear once we sum over ν. Consider the main culprit, the constant part $C_P^{0(\nu)}$ of the $\langle P^0(x) P^0(0) \rangle$ correlation function. For any given N_f we will have

$$C_P^{0(\nu)} < 0 \qquad (6.86)$$

for sufficiently large ν. But when we sum over topology with the correct weight this does not occur. Consider the large-μ limit, where calculations can be made very explicitly. The distribution of winding numbers is then Gaussian [8], with average [33]

$$\langle \nu^2 \rangle \ = \ m \Sigma V / N_f \ = \ \mu / N_f \ . \qquad (6.87)$$

In this large-μ limit we can average over topology explicitly, keeping the leading order in $1/\mu$:

$$\begin{aligned}
\langle C_P^{0(\nu)} \rangle &= \Sigma^2 N_f \left\langle \frac{1}{\mu} \frac{\Sigma_\nu(\mu)}{\Sigma} - \frac{\nu^2 N_f}{\mu^2} \right\rangle \\
&\sim \Sigma^2 N_f \left[\frac{1}{\mu} - \frac{\langle \nu^2 \rangle N_f}{\mu^2} \right] \\
&= 0 \ . \qquad (6.88)
\end{aligned}$$

To this order, negativity is precisely just avoided. This is consistent with the expression of eq. (6.76), where, after taking the limit $U \to 1$, we also find zero.

As in the quenched theory, some of the above results have nice explanations in terms of general Ward identities, which are formally the same as in the quenched theory, with the obvious replacement $N_v \to N_f$. Thus, from eq. (5.64), by combining again the identities corresponding to $\mathcal{O}(x) = P^0(x)$ and $\mathcal{O}(x) = \omega(x)$ we obtain to order ϵ^2, after integrating over space-time:

$$C_P^{0(\nu)} \ = \ \Sigma^2 N_f \left[\frac{1}{\mu} \frac{\Sigma_\nu^{1-loop}(\mu)}{\Sigma} - \frac{\nu^2 N_f}{\mu^2} \right] \ , \qquad (6.89)$$

which precisely matches what we found by explicit computations in eq. (6.85). Similarly, the identity for a non-singlet chiral flavour rotation of eq. (5.69) requires

$$C_P^{(\nu)} \;=\; (N_f^2-1)\frac{1}{2\mu}\Sigma\Sigma_\nu^{1-loop}(\mu)\;, \tag{6.90}$$

to $\mathcal{O}(\epsilon^2)$ which again agrees precisely with the result of the explicit computation in eq. (6.85).

Finally, we can also verify the Ward identity of eq. (5.64) for $\mathcal{O}(x) = P^0(x)$ directly. Using the last of the identities of eq. (6.78) we find, to this order in the ϵ-expansion:

$$\frac{1}{\Sigma}\left\langle\bar\psi(x)i\gamma_5\psi(x)\right\rangle = -\frac{i}{2}\left\langle \mathrm{Tr}(U-U^\dagger)\right\rangle = \frac{i\nu N_f}{\mu}\;. \tag{6.91}$$

Then the Ward identity eq. (5.64), after integrating over space-time, is seen to be identical to eq. (6.89), and hence also verified by our explicit calculations.

There is no simple analogy of the quenched relation eq. (5.71), but the other relations of ref. [30] for $N_f = 2$ written in our normalization in eqs. (5.72) and (5.73) should be satisfied. One first has to compute the chiral condensate in the $N_f = 2$ theory from eq. (6.79), and also find its first derivative. Next, plugging in $N_f = 2$ in eq. (6.85), and taking the $\mu \to 0$ limit, we find complete agreement. The cancellations required for this to happen are rather non-trivial, and hence constitute one more independent check on the calculation.

7 Conclusions

There are two very different regimes in which one can take the chiral limit of finite-volume QCD. The one that is normally considered is the one in which the volume is required to always exceed by far the Compton wavelength of all excitations, including the pseudo-Goldstone bosons that eventually become ultra-light. In this regime, there are still finite-volume effects, but they are exponentially small. This regime can be studied by lattice gauge theory simulations, but as the quark masses are decreased, it becomes increasingly difficult to provide the enormous volumes that are needed. This is where the usual p-expansion of chiral perturbation theory is relevant. For instance, if one wishes to measure the pion mass, the straightforward procedure is to ensure *a posteriori* that the linear extent of the lattice L by far exceeds the inverse pion mass $1/m_\pi$, and then fit the Monte Carlo data to the usual zero-momentum projection of the pseudoscalar correlation function of eq. (5.46). Here we are advocating another procedure, which is much less costly in terms of computer resources close to the chiral limit. Instead of insisting on the large-volume condition $L \gg 1/m_\pi$, one can go to any lattice size, and even go to the opposite regime $L \ll 1/m_\pi$. In this regime another chiral perturbation theory, that of the ϵ-expansion, is relevant. If one measures the same pseudoscalar correlation function in this regime, there is a modified formula that describes the correlation function. It depends on the same parameters of the chiral Lagrangian as in the infinite-volume case, and therefore it can just as well be used to determine these parameters. In particular, to lowest order it depends on the infinite-volume chiral condensate Σ, the pion decay constant F, and the quark mass m. By the Gell-Mann–Oakes–Renner relation, with corrections if required, this directly provides the pion mass m_π. In this way the pion mass can be determined from a correlation function in a volume so small that not one single pion Compton wavelength can fit inside.

In this paper we have discussed the new analytical formulae that arise in this regime of the ϵ-expansion. In particular, we have derived the scalar and pseudoscalar correlation functions for quenched QCD in

sectors of fixed topological charge ν, and for full QCD with N_f light flavours, also in sectors of fixed topology. Simultaneously we have discussed various aspects of the quenched ϵ-expansion, especially its limitations, and the reason why it is particularly advantageous to consider the chiral limit of the quenched theory in sectors of fixed topology. We hope also to have made it apparent that the alternative replica formulation of quenched chiral perturbation theory can be very useful.

As is well known, quenched QCD is a troubled theory, and in the end one should not consider our predictions for the quenched theory as more than a testing-ground for full QCD. In particular, we have found that the quenched finite-volume logarithms of the ϵ-expansion do appear also in the scalar and pseudoscalar correlation functions. Here we have simply assumed that the quenched theory nevertheless can be defined over a certain range of scales. Our formulae can then be directly compared with results of quenched computer simulations.

The predictions of Hansen [3] for full QCD, and our results here for full QCD in sectors of fixed topology, stand on a different footing. In full QCD the chiral ϵ-expansion does not suffer from any of the pathologies of the quenched analogy. This is of course as expected, since in this case the theory is well-defined. Also here the analytical predictions can dramatically simplify certain aspects of Monte Carlo simulations, since they allow for a determination of the infinite-volume parameters of low-energy QCD from volumes much smaller than normally thought to be required. It will be interesting to see also these predictions of full QCD confronted with lattice gauge theory.

8 Acknowledgement

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A Quenched Integrals over Zero-Momentum Modes

In this appendix we give the technical details on how to derive all the $Gl(2|2)$ group integrals needed for the calculation of the flavoured correlation functions in section 5.1. We have already outlined the idea in the main text. Here we also show how at this level one can switch between the supersymmetric and replica formulations.

First a simple observation, most easily explained in the replica formulation. Since $\det \mathcal{M}^{-\nu} \mathcal{Z}_\nu$ is a function of $\mathcal{M}\mathcal{M}^\dagger$ only, there exist a series of identities among zero-momentum mode expectation values. For example, all expectation values that can be obtained including $\mathcal{M}$ sources such that both $\det \mathcal{M}$ and $\mathcal{M}\mathcal{M}^\dagger$ remain invariant, are identical. This gives us the first useful identity. Let $\chi = \Sigma V(\mathcal{M} + J)$, with $\mathcal{M}$ diagonal. Two sources introduced by either[11]

$$J \;=\; \frac{1}{\Sigma V} \begin{pmatrix} 0 & j \\ 0 & 0 \end{pmatrix} \tag{A.1}$$

or

$$J \;=\; \frac{1}{\Sigma V} \begin{pmatrix} 0 & ij \\ 0 & 0 \end{pmatrix} \;, \tag{A.2}$$

[11] In the supersymmetric formalism the sources are added in the fermion–fermion block only. In the replica formalism they are added in the upper left-hand corner, and the matrix is then supplemented by $N - N_v = N - 2$ additional mass-degenerate entries.

share the same $\det\chi$ and $\chi\chi^\dagger$. This immediately leads to one useful identity, which is needed in section 5.1:

$$\left\langle U_{21}^2 + (U^{-1})_{12}^2 \right\rangle \;=\; 0 \;. \tag{A.3}$$

Next we note that for a source matrix

$$J \;=\; \frac{1}{\Sigma V}\begin{pmatrix} j_1 & 0 \\ 0 & j_2 \end{pmatrix} \;, \tag{A.4}$$

we obtain the expectation value of eq. (5.59) after differentiating with respect to j_1 and j_2. What was evaluated explicitly in ref. [27] was rather the susceptibility

$$\begin{aligned} \chi_\nu(\mu) \;&\equiv\; \frac{\delta^2}{\delta j_1 \delta j_2} \ln \mathcal{Z}_\nu \Big|_{j_1=j_2=0} \\ &=\; -\mu^2 \Big(K_\nu(\mu)^2 - K_{\nu+1}(\mu)K_{\nu-1}(\mu)\Big)\Big(I_\nu(\mu)^2 - I_{\nu+1}(\mu)I_{\nu-1}(\mu)\Big) \;. \end{aligned} \tag{A.5}$$

We therefore have, after substituting $\Sigma_\nu(\mu)$ from eq. (4.21):

$$\begin{aligned} \frac{\delta^2}{\delta j_1 \delta j_2}\mathcal{Z}_\nu\Big|_{j_1=j_2=0} \;&=\; \frac{1}{4}\left\langle (U_{11}+U_{11}^{-1})(U_{22}+U_{22}^{-1})\right\rangle \\ &=\; \chi_\nu(\mu) + \left(\frac{\Sigma_\nu(\mu)}{\Sigma}\right)^2 \\ &=\; 1 + \frac{\nu^2}{\mu^2} \;, \end{aligned} \tag{A.6}$$

where in the last line the remarkable simplification is due to a series of Bessel function identities.

To see how we can use this result, and that of eq. (5.38), to evaluate all needed expectation values, let us, as an example, consider a source matrix of the form

$$J \;=\; \frac{1}{\Sigma V}\begin{pmatrix} 0 & j \\ 0 & 0 \end{pmatrix} \;. \tag{A.7}$$

This provides us with the expectation value

$$\left\langle (U_{21} + (U^{-1})_{12})^2 \right\rangle \;=\; 4\,\frac{\delta^2}{\delta j^2}\mathcal{Z}_\nu\Big|_{j=0} \;. \tag{A.8}$$

To evaluate it, we note that the square roots of the eigenvalues of the corresponding matrix $\chi\chi^\dagger$ with $\chi \equiv \mathcal{M} + J$ are

$$\begin{aligned} m_1 \;&=\; \frac{1}{\sqrt{2}}\left(2\mu^2 + j^2 + (j^4 + 4m^2j^2)^{1/2}\right)^{1/2} \\ m_2 \;&=\; \frac{1}{\sqrt{2}}\left(2\mu^2 + j^2 - (j^4 + 4m^2j^2)^{1/2}\right)^{1/2} \;, \end{aligned} \tag{A.9}$$

and, in the replica formalism, $N - N_v = N - 2$ additional degenerate eigenvalues μ. By the chain rule, and using that $(\det\chi)^{-\nu}Z_\nu$ clearly is a *symmetric* function of the eigenvalues $m_{1,2}$, we get

$$\frac{\partial^2}{\partial j^2}\mathcal{Z}_\nu\Big|_{j=0} \;\to\; \frac{1}{2\mu}\,\frac{\partial}{\partial m_1}\mathcal{Z}_\nu\Big|_{m_1=m_2=\mu} + \frac{1}{2}\,\frac{\partial^2}{\partial m_1^2}\mathcal{Z}_\nu\Big|_{m_1=m_2=\mu} - \frac{1}{2}\,\frac{\partial^2}{\partial m_1 \partial m_2}\mathcal{Z}_\nu\Big|_{m_1=m_2=\mu} \;, \tag{A.10}$$

where on the right-hand side Z_ν is the partition function of diagonal sources

$$\mathcal{M} + J \;=\; \frac{1}{\Sigma V}\begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} \;. \tag{A.11}$$

Performing the required differentiations, and substituting eq. (5.38) and eq. (5.40), we find the compact expression

$$\left\langle (U_{21} + (U^{-1})_{12})^2 \right\rangle = 2\left[\frac{1}{\mu}\frac{\Sigma_\nu(\mu)}{\Sigma} + \frac{\Sigma'_\nu(\mu)}{\Sigma}\right] \;. \tag{A.12}$$

Next, consider a purely imaginary source matrix such as

$$J \;=\; \frac{1}{\Sigma V}\begin{pmatrix} ij_1 & 0 \\ 0 & ij_2 \end{pmatrix} \;. \tag{A.13}$$

With $\chi = \Sigma V(\mathcal{M} + J)$, the eigenvalues of $\chi\chi^\dagger$ are either $\mu^2 + j_1^2, \mu^2 + j_2^2$ (in the supersymmetric formulation), or $\mu^2 + j_1^2, \mu^2 + j_2^2, \{\mu^2\}$ (in the replica method). In the latter formulation there are $N - N_v$ degenerate eigenvalues in the last set. In both cases we have

$$\det(\chi) \;=\; \left(1 + \frac{ij_1}{\mu}\right)\left(1 + \frac{ij_2}{\mu}\right) \tag{A.14}$$

in the quenched limit. Now consider

$$\frac{\partial^2}{\partial j_1 \partial j_2}\left[(\det\chi)^{-\nu}\mathcal{Z}_\nu\right]_{j_1=j_2=0} \;=\; -\frac{\nu^2}{\mu^2} - \frac{2i\nu}{\mu}\frac{\partial}{\partial j_1}\mathcal{Z}_\nu\Big|_{j_1=j_2=0} + \frac{\partial^2}{\partial j_1 \partial j_2}\mathcal{Z}_\nu\Big|_{j_1=j_2=0} \;. \tag{A.15}$$

Here the right-hand side actually vanishes, as follows from switching to the square roots of the eigenvalues of $\chi\chi^\dagger$. We thus have

$$\frac{\partial^2}{\partial j_1 \partial j_2}\mathcal{Z}_\nu\Big|_{j_1=j_2=0} \;=\; \frac{\nu^2}{\mu^2} + \frac{2i\nu}{\mu}\frac{\partial}{\partial j_1}\mathcal{Z}_\nu\Big|_{j_1=j_2=0} \;. \tag{A.16}$$

To evaluate the remaining single derivative, we can proceed analogously, using

$$0 \;=\; \frac{\partial}{\partial j_1}\left[(\det\chi)^{-\nu}\mathcal{Z}_\nu\right]_{j_1=j_2=0} \;=\; -\frac{i\nu}{\mu} + \frac{\partial}{\partial j_1}\mathcal{Z}_\nu\Big|_{j_1=j_2=0} \;. \tag{A.17}$$

Putting everything together, we finally have

$$\begin{aligned}\left\langle (U_{11} - (U^{-1})_{11})(U_{22} - (U^{-1})_{22}) \right\rangle \;&=\; -4\,\frac{\partial^2}{\partial j_1 \partial j_2}\mathcal{Z}_\nu\Big|_{j_1=j_2=0} \\ &=\; \frac{4\nu^2}{\mu^2} \;.\end{aligned} \tag{A.18}$$

These, and those given in section 5, are all the expectation values we need for evaluating the flavoured correlation functions.

B $U(N)$ Group Integral Identities

In section 6 we used some identities for group integrals over $U(N_f)$ of the zero-mode action eq. (6.77). These identities, and others needed if one wishes to go beyond leading order, can be viewed as Schwinger–Dyson equations on that particular group manifold. Here we outline how to derive such identities.

To begin, we introduce the notion of left- and right-handed differentiation on the group. Let t^a be the generators of the algebra $u(N_f)$ in a given representation. Differentiation on group elements of $U(N_f)$ in the same representation can be defined by either

$$F(Ue^{i\epsilon_a t^a}) \;=\; F(U) + \epsilon_a \nabla^a_R F(U) + \dots \;, \tag{B.1}$$

for right-handed differentiation, or

$$F(e^{i\epsilon_a t^a}U) \;=\; F(U) + \epsilon_a \nabla^a_L F(U) + \dots \;, \tag{B.2}$$

for left-handed differentiation. The latter is probably the most intuitive to work with, and we will use it in what follows. For simplicity of notation we omit the subscript L from now on. One immediately sees that an explicit representation of ∇^a is

$$\nabla^a \;=\; i(t^a U)_{ij}\frac{\partial}{\partial U_{ij}} \;. \tag{B.3}$$

By hermitian conjugation, or by invoking unitarity, one finds the way ∇^a acts on hermitian conjugates. For example,

$$\nabla^a U^\dagger \;=\; -\,iU^\dagger t^a \;. \tag{B.4}$$

The derivative in eq. (B.3) satisfies the Leibniz rule

$$\nabla^a(FG) \;=\; (\nabla^a F)G + F(\nabla^a G) \;, \tag{B.5}$$

and the Lie algebra

$$[\nabla^a, \nabla^b] \;=\; f^{abc}\nabla^c \;, \tag{B.6}$$

where f^{abc} are the structure constants.

Left-invariance of the Haar measure on U(N_f) implies that

$$\int dU\; \nabla^a F(U) \;=\; 0 \;, \tag{B.7}$$

which, in conjunction with the Leibniz rule, leads to a simple rule for partial integration.

Let us now focus on the zero-mode theory of (6.77). Schwinger–Dyson equations of this theory are obtained by applying the rule (B.7) through an insertion of a set of functions of U in the group integral. As an example, consider

$$0 \;=\; \int dU\; \mathrm{Tr}[t^a \nabla^a (F(U)(\det U)^\nu e^{S(U)})] \;, \tag{B.8}$$

where

$$S(U) \;\equiv\; \frac{\mu}{2}\mathrm{Tr}(U + U^\dagger) \;. \tag{B.9}$$

We normalize the generators by $\mathrm{Tr}(t^a t^b) = \frac{1}{2}\delta^{ab}$, and we also need the $U(N_f)$ completeness relation $t^a_{ij} t^a_{kl} = \frac{1}{2}\delta_{il}\delta_{jk}$ in that normalization. Choosing $F(U) = U$ in (B.8) leads to the identity

$$\left\langle \mathrm{Tr}(U^2) \right\rangle \;=\; N_f - \frac{2(N_f+\nu)}{\mu} \left\langle \mathrm{Tr}(U) \right\rangle \;, \tag{B.10}$$

which was used repeatedly in section 6. Because the integration measure in (B.8) is not real when $\nu \neq 0$, the analogous identity for the hermitian conjugate does not follow trivially from this. Rather, from choosing $F(U) = U^\dagger$ in (B.8) one finds

$$\left\langle \mathrm{Tr}((U^\dagger)^2) \right\rangle \;=\; N_f + \frac{2(\nu - N_f)}{\mu} \left\langle \mathrm{Tr}(U^\dagger) \right\rangle \;. \tag{B.11}$$

As a consistency check we note that it can also be obtained from eq. (B.10) by taking the hermitian conjugate while simultaneously letting $\nu \to -\nu$. Next, by considering an identity such as

$$0 \;=\; \int dU \; \nabla^0 [\mathrm{Tr}(U - U^\dagger)(\det U)^\nu e^{S(U)}] \;, \tag{B.12}$$

one finds

$$\frac{\mu}{2} \left\langle [\mathrm{Tr}(U - U^\dagger)]^2 \right\rangle \;=\; -\left\langle \mathrm{Tr}(U + U^\dagger) \right\rangle - \nu N_f \left\langle \mathrm{Tr}(U - U^\dagger) \right\rangle \;. \tag{B.13}$$

In order to simplify the last term, one can consider the identity obtained from

$$0 \;=\; \int dU \; \nabla^0 [(\det U)^\nu e^{S(U)}] \;, \tag{B.14}$$

which gives

$$\left\langle \mathrm{Tr}(U - U^\dagger) \right\rangle \;=\; -\frac{2N_f \nu}{\mu} \;. \tag{B.15}$$

Inserting this into eq. (B.13) gives

$$\frac{\mu}{2} \left\langle [\mathrm{Tr}(U - U^\dagger)]^2 \right\rangle \;=\; -2N_f \frac{\Sigma_\nu(\mu)}{\Sigma} + \frac{2\nu^2 N_f^2}{\mu} \;, \tag{B.16}$$

with $\Sigma_\nu(\mu)$ as defined in eq. (6.79). We also need to extract individual terms on the left-hand side. Let $\mathcal{Z}_\nu$ be as defined in eq. (6.77). Then the relation

$$\frac{1}{4} \left\langle [\mathrm{Tr}(U + U^\dagger)]^2 \right\rangle \;=\; \frac{1}{\mathcal{Z}_\nu} \frac{\partial^2}{\partial \mu^2} \mathcal{Z}_\nu \tag{B.17}$$

gives

$$\left\langle [\mathrm{Tr}(U + U^\dagger)]^2 \right\rangle \;=\; 4N_f \left[\frac{\Sigma'_\nu(\mu)}{\Sigma} + N_f \left(\frac{\Sigma_\nu(\mu)}{\Sigma} \right)^2 \right] \;. \tag{B.18}$$

Adding and subtracting (B.16) and (B.18) finally provides the needed identities:

$$\begin{aligned} \left\langle \mathrm{Tr}(U)\mathrm{Tr}(U^\dagger) \right\rangle \;&=\; N_f \left[\frac{\Sigma'_\nu(\mu)}{\Sigma} + N_f \left(\frac{\Sigma_\nu(\mu)}{\Sigma} \right)^2 + \frac{1}{\mu} \frac{\Sigma_\nu(\mu)}{\Sigma} - \frac{\nu^2 N_f}{\mu^2} \right] \\ \left\langle (\mathrm{Tr}(U))^2 + (\mathrm{Tr}(U^\dagger))^2 \right\rangle \;&=\; 2N_f \left[\frac{\Sigma'_\nu(\mu)}{\Sigma} + N_f \left(\frac{\Sigma_\nu(\mu)}{\Sigma} \right)^2 + \frac{\nu^2 N_f}{\mu^2} - \frac{1}{\mu} \frac{\Sigma_\nu(\mu)}{\Sigma} \right] \;. \end{aligned} \tag{B.19}$$

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