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Finite-volume correction to the pion decay constant in the ϵ-regime

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Abstract: In the chiral limit of QCD, the pion decay constant F can be extracted from lattice gauge theory by means of a coupling to isospin chemical potential. Here we compute the leading correction due to finite volume in the ϵ-expansion of chiral perturbation theory. A comparison is made to recent Monte Carlo data.

Keywords: Lattice QCD, Chiral Lagrangians.

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1. Introduction

Recently, much effort has gone into numerical lattice gauge theory computations in QCD very close to the chiral limit. Simulations have started to use chiral fermions for the dynamical quarks of masses close to the physical values [1 – 3]. It is thus becoming increasingly important to explore the analytical tools available for extracting physical observables in this region of almost massless quarks. Here we shall focus on one of the most important low-energy constants of QCD, the pion decay constant F. Because we consider the chiral limit, and because our purpose is to derive expressions useful for a comparison between finite-volume lattice gauge theory simulations and analytical predictions, we phrase our analysis in terms of the so-called ϵ-regime of QCD. Roughly speaking, we will here perform an expansion in $1/L$, where L is a typical length scale of the given four-volume V, *i.e.*, $L \equiv V^{1/4}$. This is a finite-volume scaling regime of almost-massless QCD.

To extract the pion decay constant F from lattice data one would like to focus on an observable that is particularly sensitive to the value of F. An example of such an observable has been given in ref. [4]. It is a two-point spectral correlation function of the Dirac operator when subjected to an (imaginary) isospin chemical potential μ. The advantage of this particular spectral function is that it focuses on a null-effect: when the isospin chemical potential vanishes, the two-point correlation function has a peak of zero width at coincident points. As soon as the imaginary isospin chemical potential is turned on, the width becomes finite. Since it depends only the scaling variable $\mu^2 F^2 V$, this gives a direct way to measure F from lattice data. The precise form of the spectral two-point function has been computed to leading order from chiral perturbation theory in the ϵ-regime for both the quenched theory and for QCD with two nearly massless quarks. More recently, it has been shown how these results can also be derived from a chiral Random Two-Matrix Theory [5]. The Random Matrix Theory approach has the advantage of being easily generalizable to any number of light quark flavors N_f, and also to the "partially quenched" situation in which the chemical potential is coupled only to valence quarks and not to the physical u and d quarks of QCD. In addition, it provides all spectral correlation

functions, of arbitrary order. In this way even individual eigenvalue distributions can be computed, so that one will be able to extract both the chiral condensate Σ and the pion decay constant F by a fit to the distribution of just one single Dirac operator eigenvalue. Any sector of fixed topological charge ν can be considered. An alternative using ordinary baryon chemical potential (which leads to a complex Dirac operator spectrum) has also been considered [6]. The equivalence between spectral correlation functions of arbitrarily high order computed from either the chiral Random Matrix Theories and the Chiral Lagrangian to leading order in the ϵ-regime has recently been shown by Basile and Akemann [7].

When comparing with lattice data it is crucial to be able to estimate the error due to restricting the analysis to leading order in the ϵ-expansion of chiral perturbation theory. Here we consider the first correction to the effective field theory at an external isospin chemical potential. Actually, the calculation is of more general validity, corresponding to any vector source $v_\mu = v_\mu^a T^a$ on $\mathrm{SU}(N)$ or $\mathrm{U}(N)$.

In the next section we briefly review the set-up of the ϵ-expansion in chiral perturbation theory. In section 3 we present the result of our calculation and make a comparison with preliminary lattice data. Section 4 contains our conclusions.

2. Chiral perturbation theory in the ϵ-regime of QCD

We are interested in QCD with two light flavors, but the calculation is easily done for an arbitrary number of light flavors N_f. We likewise consider isospin chemical in a more general sense: We couple all light quarks to a quark (baryon) charge operator $\mathbf{B}$. For two light flavors we have $\mathbf{B} = \mu\sigma^3$, where μ is isospin chemical potential and σ^3 is the third Pauli matrix. In the more general case we consider N_f to be even, and $\mathbf{B} = \mu\sigma^3 \otimes \mathbf{1}$. In fact, all that is important for the calculation that follows is the condition of vanishing trace, $\mathrm{Tr}\mathbf{B} = 0$. Even if we generalize to a vector source that is not traceless, the correction to the zero-mode integral is unchanged, and only the constant part of the action is modified. The calculation therefore also applies to, for example, ordinary baryon chemical potential.

In terms of Dirac operators we are thus dealing with two kinds,

$$\begin{aligned} D_+\psi_+^{(n)} &\equiv [\not{D}(A) + i\mu\gamma_0]\psi_+^{(n)} &&= i\lambda_+^{(n)}\psi_+^{(n)} \\ D_-\psi_-^{(n)} &\equiv [\not{D}(A) - i\mu\gamma_0]\psi_-^{(n)} &&= i\lambda_-^{(n)}\psi_-^{(n)} \end{aligned} \tag{2.1}$$

and correspondingly two sets of eigenvalues $\lambda_\pm^{(n)}$. Here $\not{D}(A)$ is the ordinary Dirac operator and $\psi_\pm^{(n)}$ denotes the eigenfunctions. The method for determining the pion decay constant F from these sets of eigenvalues has been explained in refs. [4, 5]. That analysis was restricted to the tree-level chiral Lagrangian in the ϵ-regime. In order to use it to compute F from a lattice simulation, one has to know the size of the leading correction. That is the subject of this investigation.

We are also interested in a situation where the theory under consideration has N_f light physical flavors that do *not* couple to isospin chemical potential, while N_v light valence quarks do couple to it. Computationally, this situation is of much interest since it means that the gauge field configurations that need to be used are ordinary ones, without any

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reference to isospin chemical potential. Only the smallest eigenvalues corresponding to valence quark Dirac operators of the kind (2.1) need to be computed anew.

Because we consider the chiral limit and assume that chiral symmetry is broken spontaneously, we phrase the analysis in terms of the effective theory of pseudo-Goldstone bosons, the chiral Lagrangian. In the ϵ-regime of QCD [8, 9] one performs an expansion around the zero momentum modes of the Goldstones, taking into account the non-zero momentum modes in a perturbative manner. Interestingly, the topological charge of gauge field configurations ν then plays a highly non-trivial role [10]. In a slightly confusing choice of terminology this is known as the ϵ-expansion of chiral perturbation theory.

Let us consider the $(N_f + N)$-flavor chiral Lagrangian,

$$\mathcal{L} = \frac{F^2}{4}\mathrm{Tr}\left[(\nabla_0 \mathrm{U}(x))^\dagger \nabla_0 \mathrm{U}(x) + \sum_{i=1}^{3}(\partial_i \mathrm{U}(x))^\dagger \partial_i \mathrm{U}(x)\right] - \frac{\Sigma}{2}\mathrm{Tr}\mathcal{M}(\mathrm{U}(x) + \mathrm{U}(x)^\dagger), \quad (2.2)$$

where

$$\nabla_0 \mathrm{U}(x) = \partial_0 \mathrm{U}(x) - i[\mathbf{B}, \mathrm{U}(x)]. \quad (2.3)$$

Here we assume that the mass matrix $\mathcal{M}$ is diagonal and all its elements are taken in the ϵ-regime; $\mathcal{M}\Sigma V \sim \mathcal{O}(1)$. The N additional replicated flavors can be used to obtain the pertinent expression for the partially quenched theory, after embedding N_v valence quarks into these N flavors and taking the replica limit $N \to 0$. We have singled out the zero-component of ∇_μ in order to keep the direct connection to isospin chemical potential. As explained in the introduction, this restriction is actually immaterial, and a more general traceless vector source will lead to identical results.

Separating the zero-mode from non-zero modes (denoted by U and $\xi(x)$ respectively),

$$\mathrm{U}(x) = U \exp(i\sqrt{2}\xi(x)/F), \quad (2.4)$$

the partition function in a sector with a fixed topological charge ν is written

$$\begin{aligned}\mathcal{Z}^\nu_{N_f+N} = &\int_{U(N_f+N)} dU (\det U)^\nu \exp\left[\frac{\Sigma V}{2}\mathrm{Tr}[\mathcal{M}U + \mathcal{M}U^\dagger] + \frac{F^2 V}{4}\mathrm{Tr}[U, \mathbf{B}][U^\dagger, \mathbf{B}]\right] \\ &\times \int_{U(N_f+N)} d\xi \exp\left[-\int d^4x \left(\frac{1}{2}\mathrm{Tr}[\partial_\mu \xi(x)\partial_\mu \xi(x)] + \frac{\Sigma}{2F^2}\mathrm{Tr}[\mathcal{M}(U + U^\dagger)\xi^2(x)]\right.\right. \\ &\left.\left. + \frac{1}{2}\mathrm{Tr}[(U^\dagger \mathbf{B} U)(\xi^2(x)\mathbf{B} - 2\xi(x)\mathbf{B}\xi(x) + \mathbf{B}\xi^2(x))] + \mathcal{L}_q(\xi)\right)\right]. \quad (2.5)\end{aligned}$$

Note that the integrals are performed over the $\mathrm{U}(N_f + N)$ group manifold. The additional kinetic term of the singlet non-zero modes is [11]

$$\mathcal{L}_q(\xi) = \frac{\alpha}{2N_c}(\partial_\mu \mathrm{Tr}\xi(x))^2 + \frac{m_0^2}{2N_c}(\mathrm{Tr}\xi(x))^2, \quad (2.6)$$

with additional constants α and m_0 that are needed when $N_f = 0$. Here N_c denotes the number of colors, and $1/N_c$ can be usefully thought of as an expansion parameter.

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The Lagrangian exhibited in (2.5) includes all terms of $\mathcal{O}(\epsilon^6)$ that have non-vanishing expectation values in the ϵ-expansion. In particular, kinetic terms of $\mathcal{O}(\epsilon^5)$ have not been displayed since they must be treated as corrections to the leading propagator matrix (which is of $\mathcal{O}(\epsilon^4)$[1]), and turn out to have vanishing expectation values. The counting rules are as follows: $\xi \sim 1/L \sim \epsilon$, $\mathcal{M} \sim \epsilon^4$, $\mathbf{B} \sim \epsilon^2$. The new scaling variable $F^2\mu^2 V$ is thus of order unity in this counting, just like $\mathcal{M}\Sigma V$.

The tree-level two-point correlation function of the ξ fields can be given compactly for any value of N_f, N_v and N [12]. In the ϵ-regime,

$$\langle \xi_{ij}(x)\xi_{kl}(y)\rangle \;=\; \delta_{il}\delta_{jk}\bar{\Delta}(x-y) - \delta_{ij}\delta_{kl}\bar{G}(x-y), \tag{2.7}$$

with $\bar{\Delta}(x)$ and $\bar{G}(x)$ defined by

$$\bar{\Delta}(x) \equiv \frac{1}{V}\sum_{p\neq 0}\frac{e^{ipx}}{p^2}, \tag{2.8}$$

$$\bar{G}(x) \equiv \begin{cases} \frac{1}{N_f}\bar{\Delta}(x) & (N_f \neq 0) \\ \frac{1}{V}\sum_{p\neq 0}\frac{e^{ipx}(m_0^2+\alpha p^2)/N_c}{p^4} & (N_f = 0). \end{cases}, \tag{2.9}$$

where the indices $i, j \cdots$ can be taken both in the valence and sea sectors.

Quenching artifacts appear in $\bar{G}(x)$ as double poles. One keeps track of the replica limit $N \to 0$ in the external indices of eq. (2.7). Recently, the chiral expansion with $\mu \neq 0$ has been considered in the p-regime by Splittorff and Verbaarschot [13]. In that case even the propagator matrix is μ-dependent. Here, to $\mathcal{O}(\epsilon^4)$ in the ϵ-expansion these μ-dependent terms do not contribute. In effect, the propagator we use to compute the one-loop correction below is insensitive to μ.

3. The leading finite-volume correction to F

With the set-up of the previous section it is now straightforward to compute the leading (one-loop) correction to F in the ϵ-regime. To this end, we compute the one-loop contribution to the partition function itself: We bring down the action S and saturate it to first non-trivial order in the fluctuation field $\xi(x)$. In this way we obtain the leading finite-volume corrections in the ϵ-regime. For the term involving the chiral condensate Σ this was done for the full theory in ref. [8], and for the quenched and partially quenched theories in refs. [14, 15]. Here we concentrate on the term $\mathrm{Tr}([\mathbf{B}, U][\mathbf{B}, U^\dagger])$.

The computation is now simple. Working in the replica formalism we can in one sweep compute the correction to F in the full theory, the quenched and the partially quenched theories.[2] We find

$$F \;\to\; F\left(1 - \frac{N_f}{F^2}\bar{\Delta}(0)\right) \tag{3.1}$$

[1] As is well known [14], the counting is more involved in the fully quenched theory due to the additional terms in $\mathcal{L}_q(\xi)$.

[2] Here the term "partially quenched" is used in the sense described above: We consider N_v valence quarks coupled to isospin chemical potential, while the N_f physical quarks do not couple to it.

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to this order. This calculation shows that $\mathcal{O}(\epsilon^2)$ effects can be absorbed in the redefinition of F in the LO Lagrangian, or the two-matrix theory, analogous to the case of the 1-loop correction to Σ [8, 14]. Another important observation is that the double-pole terms have canceled. There is simply no one-loop correction to F in the quenched limit, which can be viewed as $N_f \to 0$ above. In the partially quenched theory with both valence and sea quarks in the ϵ-regime the shift in F is as given in eq. (3.1); there is no difference with the full theory. An immediate consequence of this is that there is to this order no dependence on the poorly determined parameters m_0 and α in the quenched theory. This situation is reminiscent of what happens with current correlators in the ϵ-regime [16]. We can intuitively understand the equality between the full theory and the partially quenched theory (in the sense defined above) by noting that the pion loop responsible for the one-loop correction to this order is insensitive to the value of isospin chemical potential μ. It should therefore not matter whether the gauge field configurations have been generated with dynamical fermions associated with chemical potential or not.

As is well known, the integrated massless pion propagator $\bar{\Delta}(0)$ is ultraviolet divergent. In dimensional regularization it actually becomes finite in four dimensions, and it has been computed for various finite-volume geometries in ref. [17]. This can be parametrized in terms of the so-called "shape coefficient" β_1 which is a function of the four-geometry only, and which is readily computed for any shape following the discussion in [17]. The result is

$$F \;\to\; F_L = F\left(1 + N_f \frac{\beta_1}{F^2 L^2}\right) \tag{3.2}$$

where L is as previously defined. The appropriate finite-volume propagator has recently been computed by Splittorff and Verbaarschot in the p-regime [13] where μ is of same order as p. With the help of that expression one can find the matching between the ϵ and p regimes explicitly.

It is of interest to see the effect of this one-loop shift in F on presently available data [18]. The one calculation which has been performed to date took $N_f = 2$ and used a 12^4 volume at a lattice spacing where $aF \sim 0.07$. Using $\beta_1 = 0.1405$, the correction factor $F_L/F = 1.4$. This is uncomfortably large. The correction to the condensate is also large,

$$\Sigma \;\to\; \Sigma_L = \Sigma\left(1 + \frac{N_f^2 - 1}{N_f}\frac{\beta_1}{F^2 L^2}\right). \tag{3.3}$$

Because of the weak dependence on simulation volume, it is difficult to deal with the finite-volume corrections by simply pushing to large volume. (The simulations of ref. [2], the largest-scale $N_f = 2$ simulations done with fully chiral lattice fermions done to date, are only done at volumes which are about twice the size of those of [18].) Precision tests clearly require performing simulations at several volumes and observing behavior consistent with eqs. (3.2) and (3.3). Making the simulation volume asymmetric can help: for example, β_1 is reduced from 0.1405 to 0.0836 for a lattice of size $L^3 \times 2L$, as used by ref. [2] or -0.042 for size $L^3 \times 3L$. The effects of higher-order terms in the chiral expansion will also come in, as $1/V$ corrections [19]. Neither of the volumes of refs. [18] or [2] are particularly large by today's standards, but because of their extreme sensitivity to topology, these kind of

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ϵ-regime calculations require the use of lattice fermions with very good chiral properties. Of course, this problem becomes more acute for larger N_f. Here we have considered QCD with only light u and d quarks.

Finally, we should point out that the present calculation does not directly prove that the method proposed in ref. [4] can be applied at one-loop level by just performing the shifts (3.2) and (3.3). In principle, one would have to perform a full calculation of the needed susceptibility and resolvent in the graded or replicated chiral Lagrangian, and then go to the cut at imaginary mass [20]. We know of no indication that the result of such a calculation to one-loop order in the ϵ-regime should yield a result different from just performing the shifts (3.2) and (3.3), but to our knowledge it has not been shown explicitly. However, there is much circumstantial evidence in favor of this being the case. For instance, spectral sum rules [10] evaluated to one-loop accuracy are consistent with simply performing such a one-loop shift. This holds in the theory with finite chemical potential μ as well [21].

4. Conclusions

We have computed the one-loop correction to F in the ϵ-regime of QCD with a vector-like source that couples like (imaginary) isospin chemical potential. This correction is needed in order to quantify the finite-volume correction to the leading-order formula for F in the ϵ-regime based on the method described in ref. [4]. Lattice simulations which aim to predict low-energy constants from simulations in the $\epsilon-$regime will clearly need to be carefully designed to deal with these finite volume corrections.

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