A New Method for Determining F_π on the Lattice

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We derive the two-point spectral correlation function of the Dirac operator with a specific external source in the ϵ-regime of QCD. This correlation function has a unique and strong dependence on F_π, and thus provides an novel way to extract F_π from lattice simulations. We test the method in a quenched lattice simulation with staggered fermions.

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INTRODUCTION

One of the outstanding challenges to lattice gauge theory is the computation of physical observables that depend strongly on having very small quark masses in QCD. Here we exploit the fact that the low-lying spectrum of the Dirac operator in finite volume is particularly sensitive to the observables of spontaneously broken chiral symmetry. It is well established [1] that the chiral condensate $\Sigma = |\langle\bar\psi\psi\rangle|$ can be extracted from measurements of the low-energy Dirac spectrum. We carry this program one step further to determine the next low-energy constant, the pseudoscalar decay constant F_π, with similar high precision. We show that a certain spectral correlation function of the Dirac operator depends on F_π in a unique and quite spectacular way. Based on this dependence we propose and demonstrate a novel method for measuring F_π in lattice gauge theory simulations. The method is general for systems with spontaneous breaking of symmetries, and indeed the universal finite-volume scaling formulas have wide application in the context of condensed matter physics as well [2].

Conventionally, measurements of F_π on the lattice are carried out in the so-called p-regime using the 2-point function of the axial current. One then aims at lattices large enough that the Compton wavelength of the Goldstone bosons is much smaller than the lattice size while still performing an extrapolation to the chiral limit of very light u and d quarks [3]. The method we propose avoids such issues by going to the ϵ-regime.

The low-energy effective Lagrangian of the ϵ-regime in QCD [4, 5] is dominated by the zero-momentum modes of the pseudo-Goldstone bosons. In the absence of external sources, the leading term in the associated ϵ-expansion is proportional to the quark mass m. It has been supposed that F_π needs to be computed either from the tiny perturbative correction to the leading-order result for Σ [6, 7] or from an appropriate space-time correlation function [8]. Quenched Monte Carlo simulations have demonstrated that such a procedure is feasible, but numerically challenging [9].

Once external currents are included, the leading-order effective Lagrangian of the ϵ-regime depends not only on Σ, but also on F_π. We shall introduce an external vector source that can be interpreted either as an imaginary chemical potential for isospin [10, 11] or as twisted boundary conditions for the gauge potentials [7]. The advantage of an *imaginary* isospin chemical potential is twofold. First, the associated Dirac operator has a positive definite determinant and thus becomes amenable to numerical simulations. In addition, with an imaginary isospin potential, the Dirac operator is anti-Hermitian and thus its eigenvalue spectrum lies entirely on the imaginary axis.

For non-zero *baryon* chemical potential, the F_π-dependent spectral correlation functions in the ϵ-regime [12–14] can be used to glean information about chiral symmetry breaking [15]. However, the spectrum of the associated Dirac operator is complex, which makes the numerical determination of F_π more demanding. Quenched results in that direction have recently been presented [16].

We consider instead the correlation function

$$\rho(\lambda_1,\tilde\lambda_2;i\mu_{\rm iso}) \equiv \left\langle\sum_n\delta(\lambda_1-\lambda_n)\sum_m\delta(\tilde\lambda_2-\tilde\lambda_m)\right\rangle - \left\langle\sum_n\delta(\lambda_1-\lambda_n)\right\rangle\left\langle\sum_m\delta(\tilde\lambda_2-\tilde\lambda_m)\right\rangle \quad (1)$$

between the densities of eigenvalues $i\lambda_n$ of the anti-hermitian operator D_+, where

$$D_+\psi_n \equiv [\not{D}(A)+i\mu_{\rm iso}\gamma_0]\psi_n = i\lambda_n\psi_n, \quad (2)$$

and the eigenvalues $i\tilde\lambda_m$ of the likewise anti-hermitian operator D_-, defined by

$$D_-\tilde\psi_n \equiv [\not{D}(A)-i\mu_{\rm iso}\gamma_0]\tilde\psi_n = i\tilde\lambda_m\tilde\psi_n. \quad (3)$$

Here $\not{D}(A)$ is the Dirac operator associated with the gauge potential A_μ. Considering the operators D_+ and

D_- as acting on two separate flavors leads to a theory in which the u-quark has chemical potential $+i\mu_{\rm iso}$, while the d-quark has chemical potential $-i\mu_{\rm iso}$. Using the effective low energy theory for QCD in the ϵ-regime we will calculate the correlation function (1) in the microscopic limit where both $m\Sigma V$ and $\mu_{\rm iso}^2 F_\pi^2 V$ are held fixed as the four-volume V is taken to infinity. We can measure Σ very accurately from the distributions of the smallest eigenvalues of $\not{D}$ [17]. Then the spectral correlation function (1) for eigenvalues of the order $1/(\Sigma V)$ provides, as we shall see, a parameter-free determination of F_π in the chiral limit. Computationally, all that is required is the determination of a modest number (typically, the first 10-20 will suffice) of smallest eigenvalues of the Dirac operators $D_\pm$. As an additional check, one can verify that the dependence is through the combination $\mu_{\rm iso}^2 F_\pi^2 V$ only.

In this paper we will provide formulas and numerical results relevant to quenched QCD. Shortcomings of quenching are well known, and we use this approximation for illustrative purposes only. The case of dynamical quarks will be presented elsewhere.

THE CORRELATION FUNCTION IN THE ϵ-REGIME

The first step is to derive the quenched susceptibility, defined as

$$\chi(m_1,m_2;i\mu_{\rm iso}) \equiv \lim_{n\to 0}\frac{1}{n^2}\partial_{m_1}\partial_{m_2}\log Z_n(m_1,m_2;i\mu_{\rm iso}) \quad (4)$$

where the limit $n\to 0$ indicates use of the replica method [18]. In terms of the eigenvalues λ and $\tilde\lambda$ the susceptibility is

$$\chi(m_1,m_2;i\mu_{\rm iso}) = \left\langle \sum_n \frac{1}{i\lambda_n+m_1}\sum_m \frac{1}{i\tilde\lambda_m+m_2}\right\rangle - \left\langle\sum_n\frac{1}{i\lambda_n+m_1}\right\rangle\left\langle\sum_m\frac{1}{i\tilde\lambda_m+m_2}\right\rangle. \quad (5)$$

The spectral correlation function (1) then follows from the discontinuity across the imaginary axis of both m_1 and m_2,

$$\rho(\lambda_1,\tilde\lambda_2;i\mu_{\rm iso}) = \frac{1}{4\pi^2}{\rm Disc}\,\chi(m_1,m_2;i\mu_{\rm iso})\big|_{\substack{m_1=i\lambda_1\\ m_2=i\tilde\lambda_2}}. \quad (6)$$

The QCD partition function $Z_n(m_1,m_2;i\mu_{\rm iso})$ entering Eq. (4) contains $2n$ fermions, half of which have mass m_1 and chemical potential $i\mu_{\rm iso}$ while the other half have mass m_2 and chemical potential $-i\mu_{\rm iso}$. In the ϵ-regime the leading term in the partition function is [11]

$$Z_n(m_1,m_2;i\mu_{\rm iso}) = \int dU\,\det(U)^\nu e^{\frac{1}{4}VF_\pi^2\mu_{\rm iso}^2{\rm Tr}[U,B][U^\dagger,B]+\frac{1}{2}\Sigma V{\rm Tr}(M^\dagger U+MU^\dagger)} \quad (7)$$

at fixed gauge field topology ν. The integration is over the Haar measure of $U(2n)$, and we have defined

$$B=\begin{pmatrix}\mathbf{1} & 0\\ 0 & -\mathbf{1}\end{pmatrix} \quad\text{and}\quad M=\begin{pmatrix}m_1\mathbf{1} & 0\\ 0 & m_2\mathbf{1}\end{pmatrix}. \quad (8)$$

For $n=1$ the partition function (7) reduces to

$$Z_1(m_1,m_2;i\mu_{\rm iso}) = e^{-2VF_\pi^2\mu_{\rm iso}^2}\int_0^1 d\lambda\,\lambda\, e^{2VF_\pi^2\mu_{\rm iso}^2\lambda^2} I_\nu(\lambda m_1\Sigma V)I_\nu(\lambda m_2\Sigma V) \quad (9)$$

and from this all partition functions for $n\geq 2$ can be obtained [13] via

$$(m_1m_2)^{n(n-1)}Z_n(m_1,m_2;i\mu_{\rm iso}) = D_n\det\left[(m_1\partial_{m_1})^k(m_2\partial_{m_2})^l Z_1(m_1,m_2;i\mu_{\rm iso})\right]. \quad (10)$$

Here D_n is a normalization factor and $k,l=0,1,..,n-1$.

Recently it has been realized [19, 20] that to obtain the correct replica limit $n\to 0$ in Eq. (4) one can make use of the integrability relations satisfied by the partition functions. Equation (10) has the structure of a τ-function, implying that the Z_n satisfy the Toda lattice equation,

$$\frac{1}{4n^2V^4\Sigma^4}m_1\partial_{m_1}m_2\partial_{m_2}\log Z_n(m_1,m_2;i\mu_{\rm iso}) = (m_1m_2)^2\frac{Z_{n+1}(m_1,m_2;i\mu_{\rm iso})Z_{n-1}(m_1,m_2;i\mu_{\rm iso})}{[Z_n(m_1,m_2;i\mu_{\rm iso})]^2} \quad (11)$$

where D_n fixes the coefficient on the lhs [13]. Taking the $n\to 0$ limit of Eq. (11) and comparing to Eq. (4) we find

$$\frac{\chi(m_1,m_2;i\mu_{\rm iso})}{V^4\Sigma^4} = 4m_1m_2Z_1(m_1,m_2;i\mu_{\rm iso})Z_{-1}(m_1,m_2;i\mu_{\rm iso}). \quad (12)$$

The $n\to 0$ limit in Eq. (12) has naturally brought in the partition function with $n=-1$, i.e., one quark of bosonic statistics [20]. Like its fermionic analogue, the bosonic partition function is determined by the symmetries of the underlying QCD Lagrangian. In the bosonic case, moreover, one must take care to ensure convergence of the partition function. As the purely imaginary chemical potential does not affect the hermiticity of the Dirac operator this does not lead to additional constraints (as opposed to the case of a real chemical potential [13, 14]). The result for the bosonic partition function is

$$Z_{-1}(m_1,m_2;i\mu_{\rm iso}) = e^{2VF_\pi^2\mu_{\rm iso}^2}\times\int_1^\infty d\lambda\,\lambda\, e^{-2VF_\pi^2\mu_{\rm iso}^2\lambda^2}K_\nu(\lambda m_1\Sigma V)K_\nu(\lambda m_2\Sigma V). \quad (13)$$

The quenched susceptibility now follows from Eq. (12),

$$\frac{\chi(m_1,m_2;i\mu_{\rm iso})}{V^4\Sigma^4} = 4m_1m_2\int_0^1 d\lambda\,\lambda\, e^{2VF_\pi^2\mu_{\rm iso}^2\lambda^2} I_\nu(\lambda m_1\Sigma V)I_\nu(\lambda m_2\Sigma V) \times\int_1^\infty d\lambda\,\lambda\, e^{-2VF_\pi^2\mu_{\rm iso}^2\lambda^2} K_\nu(\lambda m_1\Sigma V)K_\nu(\lambda m_2\Sigma V). \quad (14)$$

Taking the discontinuity as in Eq. (6) we obtain the desired correlation function,

$$\rho(\xi_1,\tilde{\xi}_2;i\mu_{\rm iso}) = \xi_1\tilde{\xi}_2\int_0^1 d\lambda\,\lambda\, e^{2VF_\pi^2\mu_{\rm iso}^2\lambda^2} J_\nu(\lambda\xi_1)J_\nu(\lambda\tilde{\xi}_2) \quad (15)$$
$$\times\left[\frac{1}{4VF_\pi^2\mu_{\rm iso}^2}\exp\left(-\frac{\xi_1^2+\tilde{\xi}_2^2}{8VF_\pi^2\mu_{\rm iso}^2}\right) I_\nu\left(\frac{\xi_1\tilde{\xi}_2}{4VF_\pi^2\mu_{\rm iso}^2}\right) - \int_0^1 d\lambda\,\lambda\, e^{-2VF_\pi^2\mu_{\rm iso}^2\lambda^2} J_\nu(\lambda\xi_1)J_\nu(\lambda\tilde{\xi}_2)\right],$$

where we have defined the scaling variables $\xi_1 \equiv \lambda_1\Sigma V$ and $\tilde{\xi}_2 \equiv \tilde{\lambda}_2\Sigma V$. The spectacular change in this correlation function when $\mu_{\rm iso}$ is made non-zero can be seen in Fig. 1. A fit to Monte Carlo data with $\mu_{\rm iso} \neq 0$ using Eq. (15) will then readily produce a measurement of F_π.

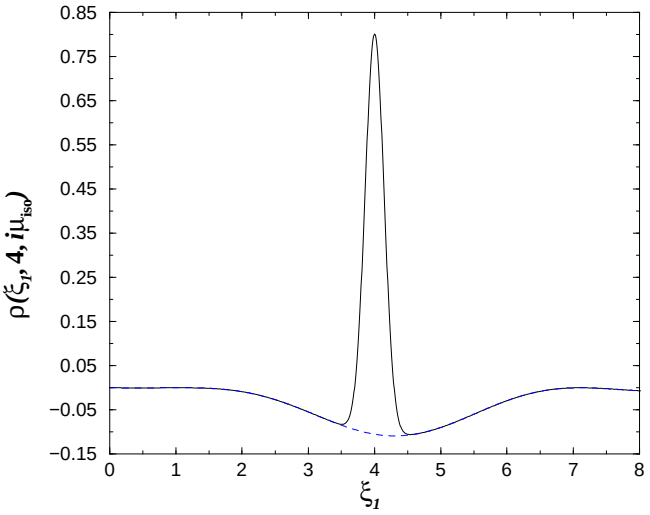

FIG. 1: The correlation function with one eigenvalue fixed at $\xi_2 = 4$, for $F_\pi\mu_{\rm iso}\sqrt{V} = 0.0717$ (full) and for $\mu_{\rm iso} = 0$ (dashed). The δ-function peak at $\xi_1 = \xi_2$ for $\mu_{\rm iso} = 0$ has not been shown.

The pronounced effect of $\mu_{\rm iso} \neq 0$ in the region where λ is close to $\tilde{\lambda}$ is not difficult to explain. For $\mu_{\rm iso} = 0$ both λ and $\tilde{\lambda}$ are eigenvalues of $\not{D}$, and this leads to a δ-function contribution to the correlation function stemming from the non-compact integral in the bosonic partition function (14), which diverges for $\mu_{\rm iso} = 0$ at $\lambda_1 = \tilde{\lambda}_2$. In this way we recover from Eq. (15) the known result [22],

$$\rho(\xi_1,\tilde{\xi}_2;i\mu_{\rm iso}=0) \quad (16)$$
$$= \delta(\xi_1-\tilde{\xi}_2)\frac{\xi_1}{2}[J_\nu^2(\xi_1) - J_{\nu+1}(\xi_1)J_{\nu-1}(\xi_1)]$$
$$-\frac{\xi_1\tilde{\xi}_2}{(\xi_1^2-\tilde{\xi}^2)^2}\left[\xi_1 J_{\nu+1}(\xi_1)J_\nu(\tilde{\xi}_2) - \tilde{\xi}_2 J_{\nu+1}(\tilde{\xi}_2)J_\nu(\xi_1)\right]^2.$$

The δ-function is not shown in the $\mu_{\rm iso} = 0$ curve in Fig. 1. When $\mu_{\rm iso}$ is non-zero, λ is an eigenvalue of D_+ while $\tilde{\lambda}$ is an eigenvalue of D_-; the effect of $\mu_{\rm iso}$ is therefore to smooth out the δ-function into a pronounced peak for λ near $\tilde{\lambda}$.

NUMERICAL SIMULATIONS

To test the method, we have performed simulations of quenched QCD using staggered fermions for $V = 8^4$ ($\mu_{\rm iso} = 0.01$) and $V = 12^4$ ($\mu_{\rm iso} = 0.002$). We have chosen to work with the standard Wilson plaquette action at $\beta = 5.7$ and with conventional, unimproved Dirac operators. In this way we are sure to have no ambiguities in the identification of the coset space of spontaneous chiral symmetry breaking, which here is $U(2n)$. The analysis presented above is based on the coset space $SU(2n)$. We can account for the extra $U(1)$ factor here by setting $\nu = 0$ in the formulas and comparing to numerical results *without* fixed topology (see for example the first paper of ref. [6]). Simulation at weaker coupling or the use of improved actions and Dirac operators will induce a crossover from $\nu = 0$ behavior to an explicit dependence on topological index [25], but it is not our purpose to explore that aspect here.

We include a chemical potential on the lattice in the standard way [23]. For an imaginary chemical potential this amounts to including a constant abelian gauge field with non-vanishing timelike component μ only. It leaves the hermiticity properties of the Dirac operator unchanged, allowing the computation of the lowest-lying eigenvalues with the Ritz variational algorithm [24].

When extracting physical observables we must keep in mind that the continuum theory describes 4 tastes of quark. In our simulation the staggered Dirac matrix is 4 times larger than that of a single continuum quark. The

statistical properties of the eigenvalue spectrum of that matrix behave as in a theory of one species in a volume four times as big. Therefore, to determine the values of F_π and Σ from the staggered eigenvalue spectrum we replace V in the analytical predictions by $4V$.

First we measure Σ. We can do that by fitting individual eigenvalue distributions to the analytical expressions [17]. It is a non-trivial prediction that k-point correlation functions of D_+ and D_- separately are independent of $\mu_{\rm iso}$ in the microscopic limit. This follows from Eq. (7) by taking B proportional to the unit matrix, and it ensures in particular that individual eigenvalue distributions are $\mu_{\rm iso}$-independent in this limit [21]. Alternatively, one can use the 2-point correlation functions of either D_+ or D_-. As follows from the argument above, these 2-point functions are $\mu_{\rm iso}$-independent, and they can provide independent determinations of Σ [26]. Using the latter approach for our 12^4 data, a best fit gives in lattice units the bare value $\Sigma = 0.0634(3)$ with $\chi^2/dof = 0.55$. This is consistent with what we find by fitting either individual eigenvalue distributions or the overall flat eigenvalue plateau. We can then determine F_π by a fit of the measured correlation function (1) to the analytical result (15). In Fig. 2 we show the data for $V = 8^4$ and compare them to the analytical curves using the best fit to F_π from the 12^4 data, as explained below. On $V = 8^4$ with $\beta = 5.7$ only the first few eigenvalues have distributions in agreement with the predictions of the ϵ-regime. For this reason we base our measured values of Σ and F_π on our 12^4 lattice simulations.

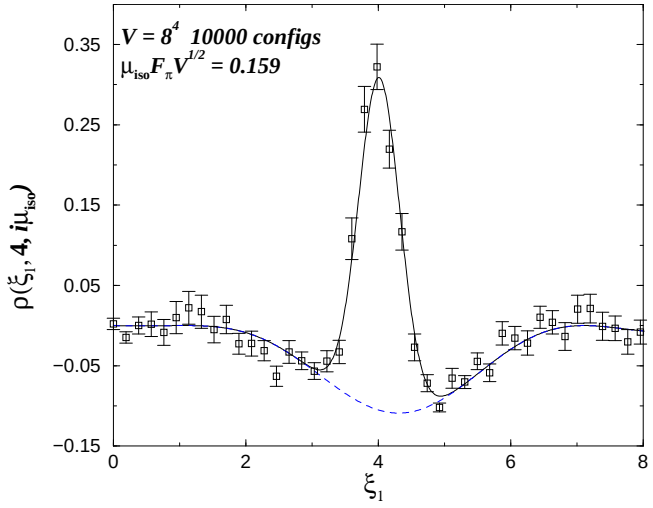

FIG. 2: The correlation function with fixed $\tilde{\xi}_2 = 4$ measured on our 8^4 lattice. The curves correspond to (15) with $F_\pi \mu_{\rm iso} \sqrt{V} = 0.159$ (full) and $\mu_{\rm iso} = 0$ (dashed).

Requiring that the eigenvalue $\tilde{\xi}_2$ fall within one bin around a fixed value (here $\tilde{\xi}_2 = 4$) means that a large fraction of the lattice configurations is obviously not used. In order to improve the statistics we consider the integrated correlation function

$$\rho_{\rm int}(x; i\mu_{\rm iso}) \equiv \int_{\tilde{\xi}_{\rm min}}^{\tilde{\xi}_{\rm max}} {\rm d}\tilde{\xi}\, \rho(x+\tilde{\xi}, \tilde{\xi}; i\mu_{\rm iso}). \qquad (17)$$

In Fig. 3 we show this integrated correlation function as measured on our 12^4 ensemble.

The best fit gives us $F_\pi = 0.1245(18)$ in bare lattice units with a $\chi^2/dof = 0.33$. This value is consistent with the result $F_\pi = 0.118(7)$ of ref. [27], which uses the same action and gauge coupling $\beta = 5.7$ (but of course a different method for extracting F_π).

It is well known that the unimproved staggered action leads to serious scaling violations. To quote a result in physical units would, at this value of β, require the use of improvement methods to reduce lattice artifacts. This is beyond the scope of this paper.

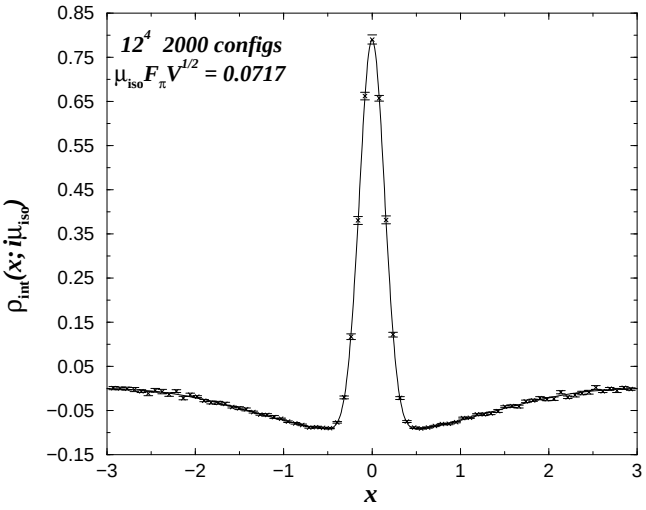

FIG. 3: The integrated correlation function (17) with $\tilde{\xi}_{\rm min} = 4$ and $\tilde{\xi}_{\rm max} = 43$. The value $F_\pi \mu_{\rm iso} \sqrt{V} = 0.0717$ is the best fit.

SUMMARY

We have proposed and tested a new method to measure F_π in lattice gauge theory simulations, using the pronounced F_π-dependence of a specific 2-point correlation function of the Dirac operator in the ϵ-regime.

We have performed quenched lattice simulations that demonstrate excellent agreement with our analytical predictions. Our study illustrates the ease with which this method can be implemented, and the high precision that can be achieved.

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of our numerical simulations were carried out on an SGI Origin 2800 computer operated by the High Performance Computing Unit of the Israel Inter-University Computation Center. Our computer code is based on the public lattice gauge theory code of the MILC Collaboration [28].

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