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Chiral interpolation in a finite volume

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A simulation of lattice QCD at (or even below) the physical pion mass is feasible on a small lattice size of ~ 2 fm. The results are, however, subject to large finite volume effects. In order to precisely understand the chiral behavior in a finite volume, we develop a new computational scheme to interpolate the conventional ε and p regimes within chiral perturbation theory. In this new scheme, we calculate the two-point function in the pseudoscalar channel, which is described by a set of Bessel functions in an infra-red finite way as in the ε regime, while chiral logarithmic effects are kept manifest as in the p regime. The new ChPT formula is compared to our 2+1-flavor lattice QCD data near the physical up and down quark mass, $m_{ud} \sim 3$ MeV on an $L \sim 1.8$ fm lattice. We extract the pion mass $= 99(4)$ MeV, from which we attempt a chiral "interpolation" of the observables to the physical point.

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PoS(Lattice 2011)101

1. Introduction

In the standard lattice QCD studies, one tries to keep the volume size L (or $V^{1/4}$) large so that the physics does not change very much from its infinite volume limit. Namely, denoting the generic pion mass by M, a dimensionless combination ML must be large. However, the numerical cost sharply grows in such a scaling limit, $M \to 0$ keeping a large value of ML.

In this work, we propose an alternative way: to investigate the chiral limit in a fixed sized box. With a fixed value of the lattice size, the numerical cost scales much mildly with M and even it saturates in the vicinity of the chiral limit since the lowest eigenvalue of the Dirac operator is no more controlled by $1/M$ but has a gap controlled by $1/V$. In fact, the JLQCD and TWQCD collaborations have been performing lattice QCD simulations near the chiral limit with dynamical overlap quarks [1, 2, 3].

The results are, of course, largely distorted from those in the infinite volume limit. It is, however, possible to analytically correct the finite size scaling using chiral perturbation theory (ChPT) [4, 5] since only the pion has a long correlation length near the chiral limit. If one has a good control of the pion physics, one can convert the data on a finite size lattice to those in the large volume limit, as long as the size of the system L is well above the inverse QCD scale $1/\Lambda_{\rm QCD}$.

In the very vicinity of the chiral limit, the ε expansion of ChPT [6] is useful as it treats the zero-momentum mode non-perturbatively, which gives the dominant contribution to the finite size effects. But the ε expansion is valid only in a small range $ML \ll 1$ (called the ε regime) and the formulas look very different from those in the conventional p regime. As we want to analyze the data both in and out of the ε regime in a uniform way, the use of the ε expansion is not very suitable.

Recently, a new perturbative approach of chiral expansion which interpolates the p and ε expansions is proposed [7] and the calculation is extended to the two-point functions by two of the authors [8]. This new scheme has no limitation on ML. The calculation is done by keeping both features of p and ε expansions: treating the zero-mode separately and exactly, while keeping all the terms that appear in the p expansion[1]. The results are expressed by a set of Bessel functions in an infra-red finite way as in the ε expansion, while the chiral logarithmic effects are kept manifest as in the p expansion.

Here we review the new perturbative scheme of ChPT and compare the formula with (preliminary) lattice QCD data. Our data at the lightest up and down quark mass $m_{ud} \sim 3$ MeV, indicate the pion mass less than its physical value. This means that in our finite size lattice, one can attempt a chiral "interpolation" of the observables to the physical point.

2. New chiral expansion

The difference between the two conventional p and ε expansions is in their parametrization of the chiral field (we denote $U(x) \in SU(N)$) and the counting rule for the mass term. In the p expansion, both of the zero mode and the non-zero momentum modes are equally and perturbatively

[1] Note that, at a given order of expansion, the ε expansion has less terms than the p expansion because it treats the mass term as one order smaller perturbation.

treated, and the mass term appears as a leading-order (LO) term in the Lagrangian. Namely,

$$p \text{ expansion} : U(x) = \exp\left(i\frac{\sqrt{2}\xi(x)}{F}\right), \quad M \sim \mathscr{O}(1/L), \tag{2.1}$$

where $\xi(x)$ denotes the generic pion field, and F is the (bare) pion decay constant. The counting rule is given in the units of the smallest non-zero momentum $1/L$.

In the ε regime, we treat the zero-mode separately and non-perturbatively, while the mass term is treated as a next-to-leading order (NLO) correction. Namely, we have

$$\varepsilon \text{ expansion} : U(x) = U_0 \exp\left(i\frac{\sqrt{2}\bar{\xi}(x)}{F}\right), \quad M \sim \mathscr{O}(1/L^2), \tag{2.2}$$

where U_0 denotes the zero-mode for which an exact group integration is performed over $SU(N)$ (or $U(N)$ in a fixed topological sector) manifold. Note that the zero-mode is absent in the perturbative mode $\bar{\xi}(x)$ (a condition $\int d^4x\, \bar{\xi}(x) = 0$ is imposed).

For our new computational scheme, which let us denote "i" (=interpolating) expansion, we have to keep the both features, non-perturbative treatment of the zero momentum mode, and the mass term kept at LO:

$$i \text{ expansion} : U(x) = U_0 \exp\left(i\frac{\sqrt{2}\bar{\xi}(x)}{F}\right), \quad M \sim \mathscr{O}(1/L). \tag{2.3}$$

In Refs.[7, 8], an additional counting rule is given for a certain combination of the quark mass matrix and the zero-mode : $\mathscr{M}(U_0 - 1) \sim \mathscr{O}(1/L^3)$, which helps to identify relevant/irrelevant diagrams. One can justify this new rule by a direct group integration (See Refs.[7, 8] for the details.).

With this new perturbative scheme, one can calculate correlation functions. As shown in Ref. [8], the calculation, which is a mixture of matrix integrals and perturbative ξ integrals, is fairly tedious but straightforward. In the end, one obtains a simple form for the calculation for the pseudoscalar correlator,

$$\int d^3x \langle P(\mathbf{x},t) P(0,0)\rangle = A\frac{\cosh(m_\pi^{\text{1-loop}}(t - T/2))}{\sinh(m_\pi^{\text{1-loop}} T/2)} + B, \tag{2.4}$$

where T denotes the temporal extent of the volume, and $m_\pi^{\text{1-loop}}$ denotes the pion mass which contains one-loop corrections including the finite size effects (from the non-zero modes), as well as Q dependence if the topology is fixed.

The coefficient A is a function of $m_\pi^{\text{1-loop}}$, the decay constant $f_\pi^{\text{1-loop}}$, and the chiral condensate Σ_{eff} while the constant B is a function of Σ_{eff} only (through a dimensionless combination $\mathscr{M}\Sigma_{\text{eff}}V$). These physical parameters include one-loop corrections from non-zero modes and thus the chiral logarithms as in the p regime. Σ_{eff} dependence is, however, embedded through the modified Bessel functions in an infra-red finite way, just as in the ε expansion.

In this new formula (2.4), the constant term B plays an essential role in the interpolation between the ε and p regimes: it precisely cancels an unphysical infra-red divergence in the first term in the massless limit, while it rapidly disappears in the large mass region. One can confirm that the ε expansion formula and that in the p expansion are interpolated as a smooth function of $m_\pi^{\text{1-loop}}$ by the new formula.

PoS(Lattice 2011)101

3. Preliminary lattice results

Let us compare the new ChPT formula with the lattice data generated by the JLQCD and TWQCD collaborations. Numerical simulations are performed with the Iwasaki gauge action at $\beta = 2.3$ including 2+1 flavors of dynamical overlap quarks on a $16^3 \times 48$ lattice. The lattice cutoff $1/a$ = 1.759(8)(5) GeV is determined from the Ω-baryon mass.

For the strange quark mass, we choose two different values but here we concentrate on the data at m_s = 0.080, which is closer to the physical value 0.081 determined from the kaon mass. With this fixed value of m_s, five values of up and down quark mass m_{ud} = 0.002, 0.015, 0.025, 0.035, and 0.050 are taken. The smallest value $m_{ud} = 0.002$ roughly corresponds to 3 MeV in the physical unit ($\overline{\mathrm{MS}}$ at 2 GeV), where the pions are in the ε regime while the kaons still remain in the p regime.

In the Hybrid Monte Carlo (HMC) updates, the global topological charge Q of the gauge field is fixed to its initial value by introducing extra (unphysical) Wilson fermions, which have a negative mass of cutoff order. In our main runs presented here, we set $Q = 0$.

For the computation of the pseudoscalar correlator, we use smeared sources with the form of a single exponential function. We observe that the smearing is effective even in the ε regime. To improve the statistical signal, the low-mode averaging technique is used: the low-mode part of the correlator is separately calculated by the 80 eigenmodes of the Dirac operator and averaged over different source points.

The auto-correlation time of the simulation is estimated by the history of the lowest Dirac eigenvalue, which turns out to be 6–24 trajectories depending on the simulation parameters. The statistical error is estimated by the jackknife method after binning data in every 100 trajectories.

Details of the numerical simulation will be reported elsewhere.

We attempt a two parameter ($m_\pi^{\text{1-loop}}$ and $f_\pi^{\text{1-loop}}$) fit with the fit function

$$f(t;\, m_\pi^{\text{1-loop}}, f_\pi^{\text{1-loop}}) \;=\; A(m_\pi^{\text{1-loop}}, f_\pi^{\text{1-loop}}, \Sigma_{\text{eff}})\frac{\cosh(m_\pi^{\text{1-loop}}(t-T/2))}{\sinh(m_\pi^{\text{1-loop}}T/2)} + B(\Sigma_{\text{eff}}), \tag{3.1}$$

taking $\Sigma_{\text{eff}} = 0.00204(07)$ from our recent result [3], as the input.

In order to determine the fitting range of t, we define the "local" mass and decay constant $m_\pi^{lc}(t)$ and $f_\pi^{lc}(t)$ at each time slice t, by the solutions of the equations

$$f(t;\, m_\pi^{lc}(t), f_\pi^{lc}(t)) \;=\; \text{lattice data at} \quad t, \tag{3.2}$$

$$f(t+1;\, m_\pi^{lc}(t), f_\pi^{lc}(t)) \;=\; \text{lattice data at} \quad t+1, \tag{3.3}$$

which can be numerically solved. The two equations are non-linear but we confirm that the solution for a given t is unique, at least in a range $m_\pi^{lc}(t), f_\pi^{lc}(t) < 2$GeV.

Figure 1 shows the local mass and decay constant plots for the lightest mass ($m_{ud} = 0.002$) data. We find a plateau for both of the mass and decay constant, from which we determine the fitting range as $t \geq 13$. For comparison, we also present a plot obtained with the conventional p expansion formula, which yields an unreasonable value $f_\pi^{lc} \sim 0.017$(30MeV). The zero-mode effect is thus shown to be essential near the chiral limit.

From the fit in the range $t \geq 13$, we obtain ($m_\pi^{\text{1-loop}}, f_\pi^{\text{1-loop}}$)= $(0.0566(24), 0.0711(30))$. We can further use ChPT to correct perturbative finite volume effects from the non-zero momentum

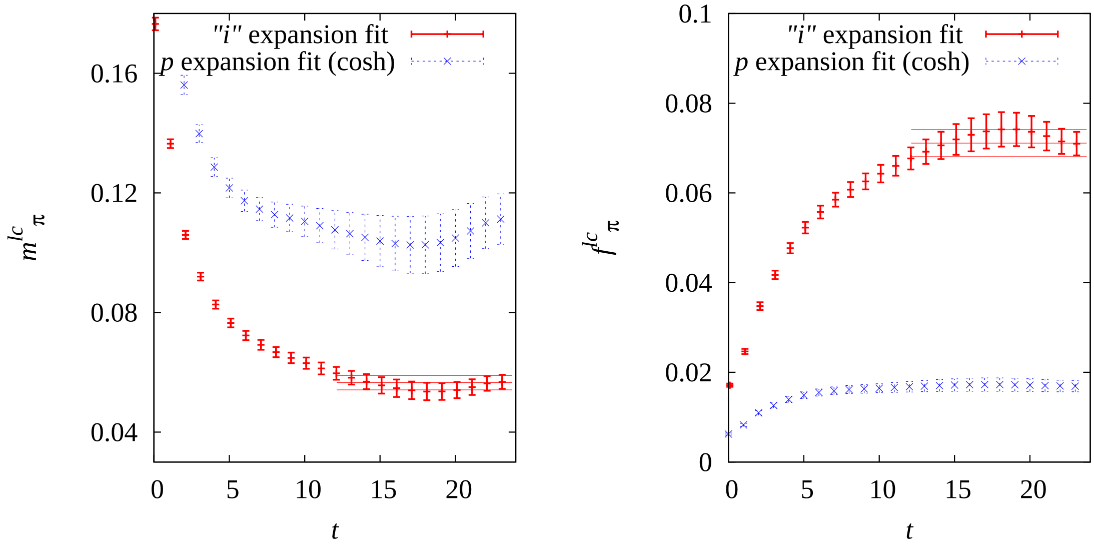

Figure 1: The “local” mass (left) and decay constant (right) of the pion at each time slice. The cross symbols show the conventional effective mass using the simple cosh form.

modes. After correcting these finite size effects with ChPT at one-loop, we obtain

$$m_\pi^{\text{1-loop}}|_{V\to\infty} = 0.0561(24)\ [98.7(4.2)\ \text{MeV}], \tag{3.4}$$

$$f_\pi^{\text{1-loop}}|_{V\to\infty} = 0.0724(30)\ [127.0(5.3)\ \text{MeV}], \tag{3.5}$$

at $m_{ud} = 0.002$. This result implies that the quark mass for our simulation in the ε regime is below the physical point.

We can repeat the same analysis also for the larger mass data in the p regime. However, we find that the results are different by only 1% from our previous p expansion analysis [9]. The zero-momentum mode effects in this region, $m_{ud} \geq 0.015$, are thus negligible.

Since $m_\pi^{\text{1-loop}}|_{V\to\infty}$ and $f_\pi^{\text{1-loop}}|_{V\to\infty}$ should have the conventional logarithmic m_{ud} dependence, we can “interpolate” the data to the physical value. Here we attempt the following two methods:

1. SU(3) ChPT 3-point ($m_{ud} = 0.002, 0.015, 0.025$) combined ($m_\pi$ and f_π simultaneously) fit with 4 free parameters (the chiral condensate Σ_0 and decay constant f_0 both in the $m_{ud} = 0$ limit, and the NLO low-energy constants $L^r_M \equiv 2L^r_6 + L^r_8$, and $L^r_F \equiv 2L^r_4 + L^r_5$).

2. linear 3-point fit for each of m_π and f_π.

The results are shown in Fig. 2. The physical point of f_π (open circle) is determined from the experimental input $m_\pi = 135$ MeV. Although the interpolated value is consistent with the experimental value, our data do not show the striking effect of the chiral logarithm. The lightest pion mass looks too low, by $\sim 7.5\%$ compared to the expected ChPT curve. The linear fit for the pion decay constant looks better. Similar result was also reported by RBC-UKQCD collaboration [10]. For comparison, our previous study in the p regime is also presented in Fig. 2 (dashed curves).

From the 4 parameter SU(3) fit, we extract the pion decay constant (at $m_s = 0.08$) as

$$f_\pi(\text{ at physical } m_{ud}) = 125(4)(^{+5}_{-0})\ \text{MeV}, \tag{3.6}$$

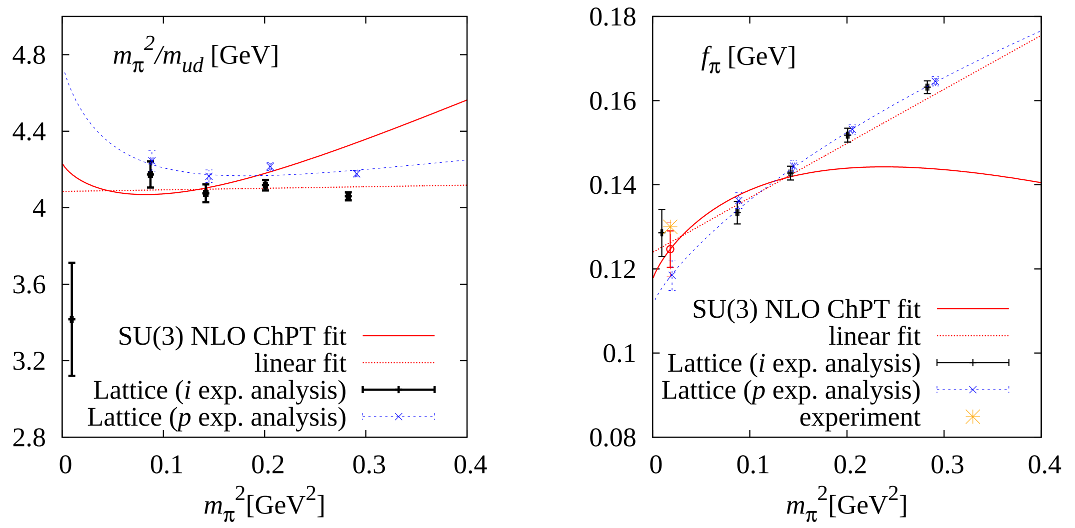

Figure 2: The chiral interpolation of the pion mass (left) and decay constant (right).

$$f_0(m_{ud}=0) = 117(5)(^{+8}_{-0}) \text{ MeV}, \tag{3.7}$$

where the first error is statistical and the second is systematic error from the choice of the interpolation function.

4. Convergence of the new formula

Our new ChPT formula is expected to be valid up to NNLO corrections. In order to estimate the systematic effects from the higher order contribution, we reanalyze our lattice data with another expression of the formula:

$$\int d^3x \langle P(\mathbf{x},t)P(0,0)\rangle = \left[\frac{A}{\sinh(m_\pi^{\text{1-loop}}T/2)} + B\right] \cosh(Z_m m_\pi^{\text{1-loop}}(t-T/2)),$$
$$Z_m = \sqrt{\frac{1}{1+B\sinh(m_\pi^{\text{1-loop}}T/2)/A}}, \tag{4.1}$$

where A and B are the same constants as those in (2.4). Noting that B rapidly disappears in the p regime, one can confirm that the formula (4.1) is equivalent to (2.4) upto NNLO corrections.

For the p regime data $m_{ud} \geq 0.015$, the change of the formula gives only 1% level differences. Namely, the formulas (2.4) and (4.1) are equally good and NNLO contribution is well under control.

However, for the lightest mass case $m_{ud} = 0.002$, we obtain $m_\pi^{\text{1-loop}} = 0.0636(32)$, which is 12% higher than the original analysis (0.0566(24)), while $f_\pi^{\text{1-loop}} = 0.0732(41)$ is consistent within the statistical error.

The significant difference of m_π in the ε-regime data only, may be explained as follows. Since we separately treat the zero mode and non-zero modes, our ChPT expansion for a general quantity has a form

$$O = O_{\text{LO+NLO}} + \delta O_{\text{NNLO}}(m_\pi^2, 1/V), \tag{4.2}$$

where the higher order correction term $\delta O_{\rm NNLO}(m_\pi^2, 1/V)$ has "mass-independent" contributions. For m_π, the LO+NLO contribution decreases for the lower quark mass while the correction term is kept finite, which means that the formula is less sensitive to m_π in the low mass region. This is not surprising since m_π is treated as an NLO quantity in the ε expansion. On the other hand, the determination of the decay constant f_π is stable as it has a finite chiral limit and treated as LO even in the ε expansion.

5. Summary

We have developed a new computational scheme in ChPT which interpolates the conventional ε and p regimes. The new formula for the pseudoscalar correlator allows us to analyze the lattice data both in the ε and p regimes equally and simultaneously.

Simulating the physical quark mass on the lattice is feasible within a reasonable computational cost if the volume is kept small. If we have a good control of the pion zero-mode within ChPT, we can precisely estimate the physical values in the large volume limit, and attempt a chiral interpolation to the physical point. In this work, we have demonstrated that the chiral interpolation indeed works for determination of the pion decay constant, while the pion mass seems to have a bad sensitivity to our scheme.

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PoS(Lattice 2011)101