Finite size effects on $M_\pi$ in QCD from Chiral Perturbation Theory∗†‡

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We present a determination of the shift $M_\pi(L) - M_\pi$ due to the finite spatial box size $L$ by means of $N_f = 2$ Chiral Perturbation Theory and Lüscher’s formula. The range of applicability of the chiral prediction is discussed.

1. INTRODUCTION

Finite size effects are important systematic effects in the Monte Carlo treatment of lattice field theories [1]. They become particularly large when the spectrum contains light particles as it happens for QCD with light quark masses. Fortunately, chiral symmetry allows to investigate this region analytically by chiral perturbation theory (CHPT) [2,3,4]. In fact, through the detour of the chiral Lagrangian, information about infinite volume QCD may be obtained from finite volume simulations with box size $L$ [5]. An important restriction is that $F_\pi L \gg 1$, $M_\pi/(4\pi F_\pi) \ll 1$ (1) has to be satisfied, since the chiral theory is a low-energy (long distance) expansion. In addition, one has to distinguish whether $L$ is large compared to the Compton wave length of the pion or not [4]. We shall here restrict ourselves to the former case but investigate what eq. (1) means quantitatively, by considering more than the leading order (LO) in the chiral expansion.

More specifically, we study the pion mass, $M_\pi(L)$, defined as an eigenvalue of the QCD Hamiltonian in an $L \times L \times L$ box (periodic boundary conditions), as it is extracted on a Euclidean lattice for sufficiently large time. The goal is to calculate the shift $M_\pi(L) - M_\pi$ with $M_\pi = M_\pi(L = \infty)$.

2. LÜSCHER FORMULA

The formula that we will use [6],

$$M_\pi(L) - M_\pi = \frac{3}{16\pi^2 M_\pi L} \times \left( \int_{-\infty}^{\infty} dy e^{-\sqrt{M_\pi^2 + y^2} L} F(iy) + O(e^{-ML}) \right),$$

relates the finite volume mass shift to the $\pi-\pi$ forward scattering amplitude $F$ in infinite volume. The subleading term involves $\bar{M} > \sqrt{3/2} M_\pi$. An additive piece referring to the 3-particle vertex present in the original formula [6] does not contribute, because of parity conservation in QCD. Since eq. (2) builds on the unitarity of the theory, it holds only in full QCD, while a generalization to the quenched approximation seems impossible.

![Figure 1. Integration contour in the complex $\nu$ plane where $\nu$ is the crossing variable in the (Minkowski space) forward scattering amplitude.](image-url)
A particular virtue of the Lüscher formula is an economic one: inserting on the r.h.s. the one-loop expression in CHPT for \( F \) in infinite volume and integrating along the contour depicted in Fig. 1, one gets the asymptotic part of a formula which, otherwise, would have required a two-loop computation in a finite volume.

3. INPUT FROM CHIRAL PT

The simple \( a, b \rightarrow c, d \) forward kinematics

\[
\begin{align*}
    s(\nu) &= (p^{(a)} + p^{(c)})^2 = 2M_{\pi}^2 + 2M_{\pi}\nu \\
    t(\nu) &= (p^{(a)} - p^{(c)})^2 = 0 \\
    u(\nu) &= 4M_{\pi}^2 - s = 2M_{\pi}^2 - 2M_{\pi}\nu
\end{align*}
\]

with the cross section

\[
\nu = \frac{p^{(a)}p^{(b)}}{M_{\pi}} = \frac{s}{2M_{\pi}} - M_{\pi}
\]

means that the forward scattering amplitude, after summing over isospin, reads

\[
F(\nu) = A(s(\nu), 0, u(\nu)) + A(u(\nu), 0, s(\nu)) + 3A(0, s(\nu), u(\nu))
\]

where the isospin-invariant \( \pi-\pi \) scattering amplitude \( A(s, t, u) \) as defined in (3) enters.

We now use the expression for \( A \) at either leading or next-to-leading order \( \langle 0 \rangle \), construct \( F(\nu) \) via eq. (3), and insert the result into eq. (2). At LO, this procedure has already been used in (2).

4. MASS SHIFTS AT LO/NLO

The LO chiral expression for the amplitude \( A \)

\[
A(s, t, u)|_{\text{LO}} = (s - M_{\pi}^2)/F_{\pi}
\]

depends only on \( s \), and henceforth the forward amplitude eq. (6) is a constant and the relative shift

\[
\frac{M_{\pi}(L) - M_{\pi}}{M_{\pi}} \big|_{\text{LO}} = \frac{3}{8\pi^2} \frac{M_{\pi}^2}{F_{\pi}^2} K_1(M_{\pi}L) \sim \frac{3}{4(2\pi)^{3/2}} \frac{M_{\pi}^2}{F_{\pi}^2} e^{-M_{\pi}L}
\]

follows in closed form. As noticed by Gasser and Leutwyler, this expression agrees with their one-loop result \( \langle 0 \rangle \) for \( M_{\pi}(L) \), when the non-leading terms \( O(e^{-M_{\pi}L}) \) are dropped in the latter (here, \( \overline{M} = \sqrt{2M_{\pi}} \)). In addition, at that order of CHPT, one can check explicitly that the non-leading terms get very small around \( M_{\pi}L \sim 4 \).

We now investigate, whether the subleading chiral corrections in \( A \) lead to a sizeable modification of the LO mass shift eq. (7). At NLO the chiral expression for the scattering amplitude is more involved than eq. (6) \( \langle 0 \rangle \), and we evaluated the integral in eq. (2) numerically. The low-energy constants which are needed at NLO are taken from \( \langle 0 \rangle \), and – for the time being – the influence of their uncertainties is not investigated.

It is instructive to first look at the integrand \( I(y) = \exp(-\sqrt{M_{\pi}^2 + y^2} L) F(iy) \) in eq. (2). In Fig. 2 we plot it, with \( F \) constructed via LO and NLO CHPT, respectively. Since the calculation is based on CHPT and the integration variable \( y \) has the dimension of a mass, either the integrand tends to zero sufficiently fast beyond \( O(100) \) MeV or the calculation cannot be trusted.

The two integrands are close to each other when the pion is light and the box size sufficiently large. However, in the whole range of \( L \) and \( M_{\pi} \) studied in the graphs, the relative difference is substantial. The reason is that at NLO \( F(iy) \) contains contributions which grow quite strongly with \( y \). To suppress these, a large \( L \) in the kinematic factor \( \exp(-\sqrt{M_{\pi}^2 + y^2} L) \) is needed. Indeed, one roughly needs \( F_{\pi}L \geq 3 \) and \( M_{\pi}F_{\pi} \leq 4 \).

![Figure 2. The integrand \( I(y) \) at LO (dotted) and NLO (full line).](image-url)
if one requires $I_{\text{NLO}}$ to differ only by a few percent from $I_{\text{LO}}$.

Note that in the graphs in Fig. 2 also values of $M_\pi L$ appear which are too small for the asymptotic formula eq. (3) to apply. We do this in order to check which value of $L$ is needed for a precise prediction for the integrand from CHPT. In addition, it is an attempt to shed some light on the general question, what the condition $F_\pi L \gg 1$ in eq. (1) means numerically. This question is relevant also for applications of CHPT in the regime $M_\pi L \ll 1$, where eq. (2) has no basis but where other expansions (SS) are applicable.

The relative mass shift $R = (M_\pi(L) - M_\pi)/M_\pi$ is plotted in Fig. 3. One observes that for $M_\pi L = 4$ and $L = 1.5 \text{ fm}$ the predicted mass shift is significantly below 1% and decreases further when $L$ is increased. Even though the difference between LO and NLO is not so small, we expect this to hold beyond NLO, on the basis of our preliminary numerical study of NNLO effects.

Larger mass shifts are predicted for a pion mass of e.g. 200 MeV, and box sizes below 2.5 fm. In this region, one would then like to correct lattice MC results for such effects, but it seems that the mass shifts of NLO CHPT may only be trusted within around 20% (of the very shift).

We did not study $L < 1.5 \text{ fm}$, since in this region, the “distortion of the pion wave function” due to finite $L$ may be large (SS), and we expect that higher order CHPT contributions will at most describe the onset of such effects.

In summary, it appears that CHPT may be applied to find out the region of parameters where the finite size effects are small and negligible compared to other errors of lattice QCD. We do, however, find that in the region where a correction for finite size effects is necessary, a LO CHPT result is not sufficient to apply this correction with confidence. In order to really assess the precision of the NLO prediction, it will be interesting to include yet one more order in the scattering amplitude (SS), but then the uncertainties in the needed low-energy constants have to be investigated in detail. Such work is in progress.

REFERENCES
1. M. Fukugita, N. Ishizuka, H. Mino, M. Okawa and A. Ukawa, Phys. Rev. D 47, 4739 (1993).
2. J. Gasser and H. Leutwyler, Annals Phys. 158, 142 (1984).
3. J. Gasser and H. Leutwyler, Phys. Lett. B 184 (1987) 83.
4. H. Neuberger, Phys. Rev. Lett. 60, 889 (1988); H. Neuberger, Nucl. Phys. B 300, 180 (1988); P. Hasenfratz and H. Leutwyler, Nucl. Phys. B 343 (1990) 241; F.C. Hansen, Nucl. Phys. B 345 (1990) 685.
5. A. Hasenfratz et al., Nucl. Phys. B 356 (1991) 332; P.H. Damgaard, M.C. Diamantini, P. Hernandez and K. Jansen, Nucl. Phys. B 629 (2002) 445 [hep-lat/0112016].
6. M. Lüscher, Commun. Math. Phys. 104, 177 (1986).
7. G. Colangelo, J. Gasser and H. Leutwyler, Nucl. Phys. B 603, 125 (2001) [hep-ph/0103088].