Finite-Volume Partially-Quenched Two-Pion Amplitudes in the $I = 0$ Channel

C.-J.D. Lin$^a$, G. Martinelli$^b$, E. Pallante$^c$, C.T. Sachrajda$^a$, G. Villadoro$^b$

$^a$ School of Physics and Astronomy, Univ. of Southampton, Southampton, SO17 1BJ, UK.

$^b$ Dip. di Fisica, Univ. di Roma "La Sapienza" and INFN, Sezione di Roma, P.le A. Moro 2, I-00185 Rome, Italy.

$^c$ SISSA and INFN, Sezione di Trieste, Via Beirut 2-4, 34013, Trieste, Italy.

Abstract:

We present a study of the finite-volume two-pion matrix elements and correlation functions of the $I = 0$ scalar operator, in full and partially quenched QCD, at one-loop order in chiral perturbation theory. In partially quenched QCD, when the sea and valence light quark masses are not equal, the lack of unitarity leads to the same inconsistencies as in quenched QCD and the matrix elements cannot be determined. It is possible, however, to overcome this problem by requiring the masses of the valence and sea quarks to be equal for the $u$ and $d$ quarks while keeping the strange quark ($s$) quenched (or partially quenched), but only in the kinematic region where the two-pion energy is below the two-kaon threshold. Although our results are obtained at NLO in chiral perturbation theory, they are more general and are also valid for non-leptonic kaon decays (we also study the matrix elements of $(8, 1)$ operators, such as the QCD penguin operator $Q_6$). We point out that even in full QCD, where any problems caused by the lack of unitarity are clearly absent, there are practical difficulties in general, caused by the fact that finite-volume energy eigenstates are linear combination of two-pion, two-kaon and two-$\eta$ states. Our work implies that extracting $\Delta I = 1/2$, $K \rightarrow \pi\pi$ decay amplitudes from simulations with $m_s = m_{d,u}$ is not possible in partially quenched QCD (and is very difficult in full QCD).

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1 Introduction

Several methods have been proposed to compute non-leptonic kaon decay amplitudes in lattice QCD. In principle one could determine physical amplitudes, including the final state interaction (FSI) phase shifts, from matrix elements of the relevant operators of the effective Hamiltonian, computed on the lattice in full QCD, with realistic quark masses, in a finite volume [1, 2]. This programme requires, however, computer resources which are not available at present, and which will not be available in the foreseeable future. For this reason several strategies for the determination of the matrix elements at next-to-leading order (NLO) in the chiral expansion have been presented in the literature [3]-[6]. The general idea is to compute matrix elements at unphysical quark masses and for a range of energies and momenta for the mesons in order to determine all the low-energy constants required at NLO in Chiral Perturbation Theory (χPT). χPT at NLO can then be used to obtain the physical matrix elements.

A number of convenient choices have been suggested for the unphysical kinematics at which the matrix elements can be computed directly, and from which the complete set of couplings (low-energy constants) of the weak chiral Lagrangian at NLO in χPT can subsequently be determined. The original proposal was to compute the $K \to \pi\pi$ matrix elements with the kaon and one of the final state pions at rest, and to vary the momentum of the second pion (SPQR kinematics) [3]. Laiho and Soni (LS) on the other hand, propose to combine the $K \to 0, K \to \pi$ and $K \to \pi\pi$ amplitudes, with the two pions at rest [5, 6]. In this case one has to isolate only the contribution from the two-pion state with the smallest energy in the correlation functions. LS also argue that this method can be used in partially quenched two-flavour QCD (PQ2), provided that the mass of the “sea” quarks in the loops, $m_S$, is the same as the “valence” light quark mass, $m_V = m_u, d$ (the strange quark is quenched) [6].

In this paper we present a study of two-pion amplitudes in the $I=0$ channel and the corresponding correlation functions in a finite volume in partially quenched QCD. The results discussed below are important for recent attempts to develop new strategies for computing $K \to \pi\pi$ decay amplitudes using numerical simulations on the lattice. We also comment on subtleties in the evaluation of two-pion matrix elements in full QCD.

We have previously used χPT at NLO to study the determination of matrix elements with two-pion external states in quenched QCD both for $I=2$ final states (for which the difficulties discussed below are not present) [4] and for $I=0$ final states [7]. For $I=0$ final states, we had found that the absence of unitarity in quenched QCD means that the calculation of the amplitudes is not possible [7]. The LS proposal has prompted us to extend these studies to partially quenched theories. In this paper we confirm that the inconsistencies of the quenched theory, and in particular those resulting from the mixing of hadronic and ghost states, are also generally present in partially quenched QCD, unless the masses of the sea and valence quarks are degenerate. In PQ2, the masses of the sea and valence $u$ and $d$ quarks are indeed degenerate, the $\eta'$ is heavy and decouples from the low energy Lagrangian, nevertheless we show that the lack of unitarity prevents the extraction of “physical” amplitudes from finite volume correlation functions when the two-pion energy $W_\pi \geq W_{K}^{\min} \approx 2M_K$, where $W_{K}^{\min}$ is the smallest two-kaon energy in the finite volume, corresponding to the two-kaon threshold (throughout this paper we assume that $W_\pi$ is sufficiently small that inelasticity effects due to states with more than two mesons can be neglected). We illustrate this point with explicit calculations in χPT of the correlation function of the scalar operator $S$ with two pion fields (we had used the same example in our study of quenched QCD [7]). In addition we also consider $(8, 1)$ operators, such as the QCD penguin operator $Q_6$ whose matrix elements are important in the theoretical prediction for $\varepsilon'/\varepsilon$, and confirm the same features.

Our work clarifies the conditions necessary to evaluate matrix elements with two-pion external states, at NLO in χPT, in partially quenched QCD. In particular, in PQ2 the necessary condition $W_{\pi} < W_{K}^{\min}$ means that it is not possible to extract the $K \to \pi\pi$ matrix elements when $m_S = m_V = m_\pi$, where $m_\pi$ is the mass of the strange quark. Since these matrix elements are needed for the implementation of the LS proposal [6], we conclude that it cannot be applied in PQ2.

Our work also shows that, in spite of the difficulties mentioned above, the two-flavour partially quenched theory, PQ2, can still be useful at least at NLO in the chiral expansion. We show that a consistent extraction of the “physical” matrix elements is obtained if we work with $m_K > m_\pi$ ($m_\pi >$ ...
at an energy of the two-pion state in the finite volume, \(W_\pi\), which satisfies the Lellouch-Lüscher (LL) elasticity condition \(W_\pi < W_K^{min} \simeq 2M_K\). The consistency of PQ2 with this choice of the parameters opens new avenues for the calculation of the \(\Delta I = 1/2\) rule and \(\epsilon'/\epsilon\) amplitudes from \(K \to \pi\pi\) matrix elements following the proposal of refs. [3, 4]. For these transitions it would be very difficult in practice to determine the amplitudes from a full QCD three-flavour computation of the \(K \to \pi\pi\) matrix elements, with the mass of the strange quark different from the light quark masses. A two flavour unquenched calculation, although difficult, is nevertheless, feasible in the near future. With the required kinematical conditions however, one loses the practical advantage of using only pions at rest \(^1\). Below, we will also comment on some of the subtleties in the extraction of the \(K \to \pi\pi\) amplitude with \(m_K = m_\pi\) in full QCD.

We make the further important, if somewhat disappointing, observation. In ref. [8] it had been suggested that it is possible to obtain exact physical information about full QCD from three-flavour partially quenched QCD (PQ3), i.e. from unquenched simulations with three flavours at \(m_S \neq m_V\). The practical advantage of PQ3 is that it is computationally less expensive to vary, and in particular to reduce, the masses of the valence quarks. Having determined the low-energy constants of \(\chi PT\) in PQ3, one can then extrapolate to the physical point, \(m_S = m_\pi\). We have explicitly checked that for the cases at hand with two-pion final states (the matrix element of the scalar operator or kaon decay amplitudes) this suggestion does not work and one has the same difficulties as in PQ2: in infinite volume the amplitude is singular at threshold, there is mixing of hadronic and ghost states and the finite-volume correlation functions are plagued by terms which grow linearly or cubically with the volume thus making the extraction of physical amplitudes impossible. Moreover, even at fixed finite volume, the presence of terms which depend quadratically or cubically on the time distances prevents the reliable determination of the matrix element. Perhaps for some simple quantities, such as the leptonic decay constants of mesons or semileptonic form factors, the strategy proposed in [8] can be used. From the above considerations, we conclude that this is not true in general.

The plan for the remainder of this paper is as follows. In the following section we discuss the extraction of the matrix elements in full QCD. We show that although the theory is unitary, for the degenerate case \(m_s = m_d = m_u\) the fact that in a finite volume the energy eigenstates are linear combinations of two-pion, two-kaon and two-\(\eta\) states makes the extraction of two-pion matrix elements subtle and difficult. We then turn to partially quenched QCD for which the explicit results at NLO in \(\chi PT\) for both the scalar operator and for (8, 1) operators are presented in the appendix. In section 3 we study the implications of these results for the determination of two-pion matrix elements in partially quenched QCD. Section 4 contains our conclusions.

\section{Two-pion matrix elements in full QCD with \(m_K > m_\pi\) and \(m_K = m_\pi\)}

In this section we consider full QCD and present the finite volume correlation function of the scalar density operator \(S = \bar u u + \bar d d + \bar s s\)

\[ \langle 0| \pi^\pm_q(t_1)\pi^-_{q'}(t_2)S(0)|0\rangle, \]

at NLO in the chiral expansion. We take \(0 < t_2 \leq t_1\). \(\pi_q(t)\) is the Fourier transform of an interpolating operator for the pion \((\pi(t, \vec x))\)

\[ \pi_q(t) \equiv \int d^3x \ e^{-i\vec q \cdot \vec x} \pi(t, \vec x). \]

We only discuss correlation functions and amplitudes in the centre-of-mass frame of the two final-state mesons.

We focus only on those terms which concern the final state interactions (FSI). These are the terms which generate finite-volume corrections to the matrix element which decrease as powers of the volume and

\(^1\)Alternatively, one can work with \(m_K \neq W_\pi\) and additional ultraviolet power divergences have to be subtracted in the matrix element.
which give the shift in the two-meson energy [9]. The remaining terms are only subject to exponentially suppressed finite-volume corrections and are not relevant in this discussion. The complete expressions for the correlation functions at one-loop order in $\chi$PT can be found in ref. [7].

At one-loop order in chiral perturbation theory, for an arbitrary value of the two-pion energy, keeping only those terms which are relevant for the energy shifts and finite-volume corrections to the matrix elements, we find:

$$\langle 0 | \pi^+_q(t_1) \pi^-_q(t_2) S(0) | 0 \rangle = \frac{e^{-E_{t_1}} - e^{-E_{t_2}}}{2E} \left( -\frac{8}{f^2} \right) [1 + \text{I}_b(t_1, t_2)] , \quad (3)$$

where $E = \sqrt{q^2 + m^2}$ and $f$ is the pseudoscalar decay constant at lowest order in the chiral expansion. We write $I_b(t_1, t_2)$ in the form

$$I_b(t_1, t_2) = \frac{E^2}{2f^2} \frac{1}{L^3} \sum_{\vec{k}} \left( d_+(w) P(w) + c_+(w) P(w) + \frac{m^2}{6E^2 w^2} P(w) \right) + \ldots , \quad (4)$$

where the volume is a cube of size $L^3$, and

$$P(w) = 1 - \frac{e^{2(E-w)t_2}}{2(E-w)} , \quad w_i = \sqrt{\vec{k}^2 + m_i^2} ,$$

$$c_+(w) = \frac{2E^2 + Ew + w^2}{E^2 w^2} , \quad d_+(w) = 2c_+(w) - \frac{m^2}{2E^2 w^2} .$$

Evaluating the sum, we find

$$\langle 0 | \pi^+_q(t_1) \pi^-_q(t_2) S(0) | 0 \rangle = \frac{e^{-E_{t_1}} - e^{-E_{t_2}}}{2E} \left( -\frac{8}{f^2} \right) [1 + \text{Re}(A_{\infty}) + \mathcal{T}(t_2)] , \quad (5)$$

where $A_{\infty}$ is the infinite-volume one-loop correction to the amplitude [7] and

$$\mathcal{T}(t_2) = -\frac{E^2}{2f^2} \left\{ -\frac{\nu t_2}{E^2 L^3} \left( 4 - \frac{m^2}{2E^2} \right) - \frac{2\nu t_2}{E^2 L^3} \theta(E - m_K) - \frac{\nu t_2}{E^2 L^3} \frac{m^2}{6E^2} \theta(E - m_{\eta}) \right\} + \ldots , \quad (6)$$

$\nu = \sum_{\vec{k}: w=E}$ and only the terms which are proportional to $t_2$ are exhibited here.

The energy shift ($\Delta W$) can readily be extracted from the terms proportional to $t_2$. For $E < m_K < m_{\eta}$ only the first term on the right-hand side of eq. (6) contributes, giving

$$\Delta W = -\left( 2 - \frac{m^2}{4E^2} \right) \frac{\nu}{f^2 L^3} . \quad (7)$$

For energies such that $E > m_{\eta,K} = m_{\pi}$ on the other hand we find

$$\Delta W = -\left( 3 - \frac{m^2}{6E^2} \right) \frac{\nu}{f^2 L^3} . \quad (8)$$

The case $E < m_K < m_{\eta}$ was discussed in detail in ref. [7] and we refer the reader to this reference for details. We only remark that in this case only $P(w)$ in eq. (4) contains terms with vanishing denominators (and hence terms proportional to $t_2$). Since we were considering energies in the region $E < m_K < m_{\eta}$ in ref. [7], the terms proportional to $\theta(E - m_K)$ and $\theta(E - m_{\eta})$ were omitted in equation (23) of that paper, but here we also want to study the case $m_K = m_{\pi} = m_{\eta} \leq E$, for which $P(w_K)$ and $P(w_{\eta})$ also have vanishing denominators, so that the energy shift and the finite-volume corrections to the matrix element are modified. This result is in agreement with the Lüscher quantization condition [9], because the FSI do depend on whether we are above or below the two-kaon (and two-eta) threshold. The consistency can be readily checked by computing the one-loop expression of the relevant matrix element in infinite volume in Minkowski space:

$$\langle \pi^- (q) \pi^+ (-q) | S | 0 \rangle = -\frac{8}{f^2} [1 + A_{\infty}] = -\frac{8}{f^2} \left[ 1 + \frac{1}{(4\pi f)^2} (I_b + \ldots) \right] , \quad (9)$$

3
where

\[ I_b = (m_\pi^2 - 2s)A(m_\pi) - sA(m_K) - \frac{m_\pi^2}{3}A(m_\eta) + \ldots . \]  

(10)

In the above expressions, \( s = (p_{\pi^-} + p_{\pi^+})^2 \) is the square of the two-pion centre-of-mass energy and

\[ A(m) \equiv \sqrt{1 - 4\frac{m^2}{s}} \left( \log \left( \frac{1 + \sqrt{1 - 4\frac{m^2}{s}}}{1 - \sqrt{1 - 4\frac{m^2}{s}}} \right) - i\pi\theta \left( 1 - 4\frac{m^2}{s} \right) \right) . \]

(11)

When \( E < m_K < m_\eta \), the s-wave phase shift, which is obtained from the coefficient of the imaginary part of \( I_b \), is given by the first term of the r.h.s. of eq. (10) \(^2\):

\[ \delta(s) = \frac{2s - m_\pi^2}{16\pi f^2} \sqrt{1 - 4\frac{m_\pi^2}{s}} . \]

(12)

When \( E > m_K = m_\pi = m_\eta \) on the other hand, all the terms in eq. (10) contribute and we obtain

\[ \delta(s) = \frac{9s - 2m_\pi^2}{48\pi f^2} \sqrt{1 - 4\frac{m_\pi^2}{s}} . \]

(13)

From the result for the phase shift in eq. (13), we can extract the energy shift by using the Lüscher quantization formula \([9]\). The energy shift obtained in this way agrees of course with the result in eq. (8), obtained from a calculation of the correlation function in the finite volume.

For the degenerate case \( E > m_K = m_\pi = m_\eta \), the energy shifts discussed here correspond to finite-volume eigenstates which are two-meson \( SU(3) \) singlet states (\( S \) is an \( SU(3) \) singlet operator). A convenient procedure for the evaluation of the matrix element is to compute the correlation function of \( S \) with the \( SU(3) \) singlet two-meson operator \((\varphi \varphi)_1\),

\[ S - (\varphi \varphi)_1 \equiv \langle 0 | (\varphi_{t\bar{q}}^\dagger(t_1)\varphi_{t\bar{q}}(t_2))_1 S(0) | 0 \rangle , \]

(14)

where (for compactness of notation, in the following we suppress the labels \( t_{1,2} \) and \( \bar{q} \))

\[ (\varphi \varphi)_1 = \frac{1}{\sqrt{2}}KK + \frac{1}{2\sqrt{2}}\eta\eta + \frac{1}{2}\sqrt{\frac{3}{2}}\pi\pi , \]

(15)

and

\[ KK = \frac{1}{\sqrt{2}}(K^0K^0 + K^+K^-) , \quad \pi\pi = \frac{1}{\sqrt{3}}\left( \pi^0\pi^0 + \sqrt{2}\pi^+\pi^- \right) . \]

(16)

\((\varphi \varphi)_1\) creates or annihilates the \( SU(3) \) singlet state \(| 1 \rangle \), which is a combination of two-pion, two-kaon and two-\( \eta \) states with the same flavour structure as the corresponding operator

\[ | 1 \rangle = \frac{1}{\sqrt{2}}|KK\rangle + \frac{1}{2\sqrt{2}}|\eta\eta\rangle + \frac{1}{2}\sqrt{\frac{3}{2}}|\pi\pi\rangle , \]

\[ |KK\rangle = \frac{1}{\sqrt{2}}(|K^0K^0\rangle + |K^+K^-\rangle) , \quad |\pi\pi\rangle = \frac{1}{\sqrt{3}}\left( |\pi^0\pi^0\rangle + \sqrt{2}|\pi^+\pi^-\rangle \right) . \]

(17)

All the meson states are s-wave, \( I = 0 \) states. Similar expressions can be written for the octet and 27plet operators considered below. Computing in addition the \((\varphi \varphi)^\dagger - (\varphi \varphi)_1\) correlation function

\[ \langle 0 | (\varphi_{t\bar{q}}^\dagger(t_1)\varphi_{t\bar{q}}(t_2))_1 (\varphi_{t\bar{q}}^\dagger(-t_2)\varphi_{t\bar{q}}(-t_1))_1 | 0 \rangle , \]

(18)

\(^2\)For \( s \geq 4m_\pi^2 \), we have \( \text{Arg} \left[ \langle \pi^-(-\bar{q})\pi^+(\bar{q}) | S(0) \rangle \right] = \delta(s) \).
one obtains the finite volume matrix element $|\langle 1|S|0\rangle|_{FV}$ by dividing the correlation function (14) by the square root of the four-point function (18) at large time distances, following the procedure explained in ref. [7]

$$
|\langle 1|S|0\rangle|_{FV} = \frac{\langle 0|\{\phi_{t}^{+}(t_{1})\phi_{t}(t_{2})\}_{1}S(0)|0\rangle}{\sqrt{\langle 0|\{\phi_{t}^{+}(t_{1})\phi_{t}(t_{2})\}_{1}\{\phi_{t}^{+}(t_{2})\phi_{t}(-t_{1})\}_{1}|0\rangle}}.
$$

(19)

The $\pi\pi$ matrix element is then simply obtained by using the appropriate Clebsh-Gordan coefficient, $\langle \pi\pi|S|0\rangle = 2\sqrt{2/3}|\langle 1|S|0\rangle|_{FV}$.

For the sake of presentation, it was convenient to discuss the extraction of the matrix element using the ratio on the right-hand side of eq. (19), with the correlation function $S- (\varphi\varphi)_{1}$ in the numerator. Note however, that since $S$ is an $SU(3)$-singlet, we could equally well have used the correlation function $S- (\pi\pi)$.

In the case of (8, 1) or (8, 8) operators the simple procedure outlined above does not work because these operators have non-vanishing matrix elements between the kaon state, $|K^{0}\rangle$, and three different S-wave two-meson states with $I = 0$ and $I_{z} = 0$. The three states are the state $|1\rangle$ defined above and the octet and 27-plet states (created by the corresponding $(\varphi\varphi)_{8}$ and $(\varphi\varphi)_{27}$ operators)

$$
\begin{align*}
|8\rangle &= \frac{1}{\sqrt{5}}|KK\rangle + \frac{1}{\sqrt{5}}|\eta\eta\rangle - \sqrt{\frac{3}{5}}|\pi\pi\rangle, \\
|27\rangle &= -\sqrt{\frac{3}{10}}|KK\rangle + \frac{2\sqrt{7}}{40}|\eta\eta\rangle + \frac{1}{\sqrt{40}}|\pi\pi\rangle.
\end{align*}
$$

(20)

In a finite volume the three two-meson states (|1), |8) and |27) acquire different energies, and thus they appear in the correlation function with different exponentials in time. Thus, in order to obtain the matrix element $\langle \pi\pi|Q_{6}|K^{0}\rangle$, for example, one has to disentangle the different contributions, and extract all the matrix elements $\langle 1, 8, 27|Q_{6}|K^{0}\rangle$ and $\langle 1, 8, 27|1, 8, 27 \rangle$ by studying the $K^{0}-Q_{6}(\varphi\varphi)_{1}$, and the $(\varphi\varphi)_{1}-(\varphi\varphi)_{1}$ correlators. Then a suitable combination of $\langle 1, 8, 27|Q_{6}|K^{0}\rangle$ will give the required $\langle \pi\pi|Q_{6}|K^{0}\rangle$ amplitude. A further complication is that all the matrix elements should be computed at the same two-meson energy, which must be kept fixed in the infinite volume limit [1, 2]. Although possible in principle, the procedure appears to be very complicated to implement in practice.

### 3 Two-pion matrix elements in partially quenched QCD

In this section we discuss the evaluation of the same matrix elements, but now in partially quenched QCD. We consider the two cases: QCD with three sea-quark flavours for generic values of $m_{S}$, $m_{V}$ and $m_{s}$ (PQ3), and QCD with two light sea-quark flavours also with generic combinations of the quark masses (PQ2). These calculations correspond to theories with $SU(6)$ and $SU(5)$ graded Lie groups respectively. We have also studied the $SU(4)$ case, reaching the same physical conclusions, and for this reason this case will not be discussed explicitly.

PQ2 is partially quenched two-flavour QCD, with a mass $m_{S}$ for the sea quarks, a mass $m_{V}$ for the valence light quarks and a mass $m_{s}$ for the strange quark, which is always quenched. The rather lengthy formulae for $m_{S} \neq m_{V}$ are presented in the appendix for both the scalar operator and (8,1) operators. We explicitly confirm the expectations [6] that when the sea-quark mass is different from the valence-quark mass the problems are the same as in the quenched case [7]. The double poles induce terms which seem to grow linearly and cubically with the volume as well as ones which are quadratic or cubic in the time distance, see eq. (27). The extraction of the physical amplitude is therefore not possible, at least with our current level of understanding. In this respect we find that it is euphemistic to state that “the final state corrections can be significant” [6]; we simply do not know how to extract the infinite volume matrix element from the finite volume correlation function and the problem cannot be overcome by going to larger lattices. This pathology is not peculiar to PQ2 but is also present with the same symptoms in PQ3.
For $m_S = m_V$, for a generic energy $E$ and a generic strange quark mass $m_s$ we obtain in PQ2:

$$
(0|\pi^+_q(t_1)\pi^-_q(t_2)S^{pq}(0)|0) = \frac{e^{-Et_1}e^{-Et_2}}{2E}(\frac{-8}{t^2})[1 + I^{pq}_b(t_1, t_2)],
$$

(21)

where we choose $S^{pq} = \bar{u}u + \bar{d}d + \bar{s}s$ and the sum is only over the valence quarks,

$$
I^{pq}_b(t_1, t_2) = \frac{E^2}{2t^2}\sum_{\vec{q}}\left(d_+(w_\pi)P(w_\pi) + \frac{1}{2}c_+(w_K)P(w_K) + \frac{m^2_\pi}{4E^2w^2_\pi}P(w_\pi\pi)\right) + \ldots
$$

(22)

and $m^2_\pi = 2m^2_K - m^2_s$. When $m_K > m_{\pi}$ ($m_s > m_V = m_S$) and taking the two-pion energy such that $W_\pi < W^\text{min}_K$ (at this order in the chiral expansion this means $2E \leq 2m_K$), only the term proportional to $P(w_\pi)$ generates the energy shift and the finite volume power corrections, which are exactly the same as in the unquenched two-flavour theory. In this respect we agree with the conclusions of LS for $m_K = 2m_{\pi}$.

More generally, one has finite volume corrections under control and the validity of the LL formula, as in two-flavour full QCD, whenever $W_\pi < 2m_K$. Indeed, $W_\pi < 2m_K$ precisely the elasticity condition under which the LL formula applies. If we violate this condition however, then major difficulties arise. Consider for example the case $m_K = m_{\pi} = m_{3s}$: each of the three terms contributes to the energy-shift, and the final coefficient does not correspond to the correct result either in SU(2) or in SU(3). The reason for this is that the “quenched” states containing a strange quark now also contribute to the singular terms in the sum. The matrix elements now correspond to final states with a ghost component and therefore we are unable to extract the required two-pion amplitudes. In full QCD in sec. 2, we were able to use the SU(3) symmetry in the $m_u = m_d = m_s$ case to determine the $\pi\pi$-component in an SU(3)-singlet state. Here we are unable to carry out the analogous procedure. We note that one could avoid this difficulty by using a scalar operator which projects only onto two-pion states, such as $\bar{u}u + \bar{d}d$. In this case the problem of the mixing with intermediate states containing strange quarks does not arise. This feature, however, does not apply to the (8,1) or (8,8) operators of the weak effective Hamiltonian.

The problems above, which are related to the absence of unitarity in partially quenched theories, are also present in PQ3 when $W_\pi$ is above the threshold for any multi-hadron state containing “partially-quenched” quarks. Therefore in order to extract the $\Delta I = 1/2$ $K \to \pi\pi$ matrix elements with $m_u = m_d = m_s$ in PQ3, one is forced to work with the full QCD limit of the theory.

4 Conclusions

In this paper we study the extraction of matrix elements with two-pion final states from simulations in finite volumes in full and partially quenched QCD. In full QCD, not surprisingly, we confirm that the matrix elements can be determined in principle, up to exponentially small finite-volume corrections. We point out however, that even in this case, for three degenerate quark flavours there are considerable practical difficulties because the finite-volume energy eigenstates correspond to linear combinations of $\pi\pi$, $KK$ and $\eta\eta$ states. The determination of a matrix element with a two-pion final state with a fixed energy requires therefore the extraction of several finite-volume matrix elements at this energy. Each of these matrix elements will, in general, need to be computed from a simulation on a different volume.

For PQ2 we find that it is not possible to determine $K \to \pi\pi$ matrix elements in general, at least with our present level of understanding. For two-pion energies below the two-kaon threshold however, the theory is a consistent unquenched two-flavour one, the LL formula holds and it is possible to extract infinite volume physical amplitudes. Of course the value of the couplings of the effective weak chiral Lagrangian and the coefficients of the logarithms which appear at one loop are not those of full QCD. One may argue, however, that the contribution to these couplings due to the sea-strange quark loops are suppressed by the massive kaon propagators when $W_\pi << 2m_K$, since there are no singularities associated with the strange meson loops. If this is true, PQ2 can provide very useful physical information, although we are currently unable to estimate the systematic uncertainty. Given the apparent importance of unitarity in enabling the determination of physically meaningful results, we believe that it may be theoretically better to work with the unquenched two flavour theory rather than to weight the gauge
field configurations with fractional powers of the fermion determinant in order to mimic the three flavour theory. A study of this issue in chiral perturbation theory may be very useful to clarify the situation.

The disappointing news is that the sea and valence quark masses should be equal. It had been considered very useful to work with fixed sea-quark masses and to vary (and in particular to reduce) the valence ones, in order to calibrate the lattice spacing and to extrapolate the results to the physical point. In this respect, our results cast serious doubts on the applicability of PQ3 to the determination of matrix elements with two-meson (or in general, multi-hadron) external states. PQ3 may however, prove useful for the determination of some other quantities.

For PQ2 with the two-pion energy at or above the two-kaon threshold (more precisely for \( m_K \geq m_\pi \) (\( m_s \geq m_N = m_S \)), with \( W_\pi \geq W_K^{min} \)) with our present level of understanding it is not possible to extract the two-pion matrix elements. The difficulties are those already discussed for quenched QCD [7]. Unfortunately this implies that the proposal suggested by LS of combining \( K \to 0, K \to \pi \) and \( K \to \pi \pi \) amplitudes, with the two pions at rest, to determine the complete set of couplings of the weak chiral Lagrangian fails in PQ2. An ingredient in the LS proposal is the extraction of the two-pion matrix element with \( m_\pi = m_K \), which violates the consistency condition given above. Of course the LS proposal may work in full QCD, but requires care in the extraction of the \( K \to \pi \pi \) matrix element when \( m_K = m_\pi \). In this case the full two meson \( \to \) two meson correlation matrix must be studied, as explained in sec. 2.

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A Finite-volume correlation functions in partially quenched QCD

In this appendix we present the expressions for the correlation functions used in the extraction of two-pion matrix elements in partially quenched QCD, PQ2. The Euclidean partially quenched chiral Lagrangian in the supersymmetric formulation is [10]

\[
\mathcal{L}_\chi^{pq} = \frac{f^2}{8} \text{str} \left[ \left( \partial_\mu \Sigma^{pq} \right) \left( \partial_\mu \Sigma^{pq} \right) \right] - \frac{f^2}{8} \text{str} \left[ \Sigma^{pq} \chi + \chi \Sigma^{pq} \right] - m_\pi^2 \Phi_0^2 + \alpha (\partial_\mu \Phi_0)(\partial_\mu \Phi_0),
\]

(23)

where \( \Sigma^{pq} \) is the graded extension of the standard non-linear Goldstone field \( \Sigma \) in the full chiral perturbation theory. \( \Phi_0 \) is the super-\( \eta' \) field and \( \chi = 2B_0\mathcal{M}, \) where \( \mathcal{M} \) is the mass matrix and \( B_0 = -\langle 0|\bar{u}u + \bar{d}d|0\rangle/f^2. \)

The results reported here are obtained with the super-\( \eta' \) integrated out (the limit \( m_0 \to \infty \)), and are presented in terms of the following quantities:

\[
c(\pm)(w) = \frac{2}{3} \frac{E^2 \pm Ew + w^2}{E^2 w^2}; \quad c(0) = \frac{1}{3} E^2; \quad d(\pm)(w) = 2c(\pm)(w) - \frac{m_\pi^2}{2E^2 w^2};
\]

\[
w_S = \sqrt{k^2 + m_{Y_S}^2}; \quad m_{Y_S}^2 = B_0(m_u + m_S) \quad \text{and}
\]

\[
w_i = \sqrt{k^2 + m_i^2} \quad (\text{for } i \neq S), \quad \delta_s = (m_s^2 - m_{Y_S}^2), \quad B_{ij} = \frac{m_i^2 - m_j^2}{m_i^2 - m_j^2}.
\]

(24)

The finite volume scalar correlation function can be written in the following form (\( E = \sqrt{q^2 + m_\pi^2} \)):

\[
\langle 0|\pi^+(t_1)\pi^-_q(t_2)S^{pq}(0)|0\rangle = \frac{e^{-E_{t_1}} e^{-E_{t_2}}}{2E} \left( -\frac{8}{f^2} \right) \left[ 1 + P^{pq}_S + P^{pq}_u + P^{pq}_b(t_1, t_2) \right],
\]

(25)
where $I_{pq}^\pi$ and $I_{qq}^\pi$ are the contributions from the wave-function renormalization and tadpole diagram respectively. They give the infinite volume result up to exponentially suppressed corrections with the volume and are therefore not reported explicitly here.

$$I_{b}^{pq}(t_1, t_2) = -\frac{E^2}{2f^2} [A_{SS} + A_{KK} + A_{\pi\pi} + A_{0\pi} + A_{00}] ,$$

where

$$A_{SS} = \frac{1}{L^3} \sum_k \left\{ \frac{c_+(w_S)}{2(E-w_S)} - \frac{c_-(w_S)}{2(E+w_S)} - e^{2(E-w_S)t_2} \left( \frac{c_+(w_S)}{2(E-w_S)} + \frac{c_0(w_S)}{2w_S} \right) + e^{2Et_2-2w_S t_1} \left( \frac{c_0(w_S)}{2w_S} - \frac{c_-(w_S)}{2(w_S+E)} \right) \right\} ,$$

$$A_{KK} = \frac{1}{L^3} \sum_k \left\{ \frac{c_+(w_K)}{2(E-w_K)} - \frac{c_-(w_K)}{2(E+w_K)} - e^{2(E-w_K)t_2} \left( \frac{c_+(w_K)}{2(E-w_K)} + \frac{c_0(w_K)}{2w_K} \right) + e^{2Et_2-2w_K t_1} \left( \frac{c_0(w_K)}{2w_K} - \frac{c_-(w_K)}{2(w_K+E)} \right) \right\} ,$$

$$A_{\pi\pi} = \frac{1}{L^3} \sum_k \left\{ \frac{d_+(w_\pi) - c_+(w_\pi)}{2(E-w_\pi)} - \frac{d_-(w_\pi) - c_-(w_\pi)}{2(E+w_\pi)} - e^{2(E-w_\pi)t_2} \left( \frac{d_+(w_\pi)}{2(E-w_\pi)} + \frac{d_0(w_\pi)}{2w_\pi} \right) + e^{2Et_2-2w_\pi t_1} \left( \frac{d_0(w_\pi)}{2w_\pi} - \frac{d_-(w_\pi) - c_-(w_\pi)}{2(w_\pi+E)} \right) \right\} + \frac{1}{L^3} \sum_k \frac{m^2_\pi(2w^2 + w^2_\pi B_{K,K}^\pi)}{4E^2w^6_\pi} \left\{ \frac{1}{2(E-w_\pi)} - \frac{1}{2(E+w_\pi)} - e^{2(E-w_\pi)t_2} \left( \frac{1}{2(E-w_\pi)} + \frac{1}{2w_\pi} \right) \right\} + e^{2Et_2-2w_\pi t_1} \left( \frac{1}{2w_\pi} - \frac{1}{2(w_\pi+E)} \right) + \frac{1}{L^3} \sum_k \frac{m^2_\pi \delta^2}{E^3w^6_\pi} \left\{ \frac{1}{2(E-w_\pi)^2} + \frac{1}{2(E+w_\pi)^2} - e^{2(E-w_\pi)t_2} \left( \frac{1 - [2(E-w_\pi)]t_2}{2(E-w_\pi)^2} + \frac{1 + [2w_\pi]t_2}{2w_\pi} \right) 
- e^{2Et_2-2w_\pi t_1} \left( \frac{1 + [2w_\pi]t_1}{2w_\pi^2} - \frac{1 + [2(E+w_\pi)]t_1}{2(E+w_\pi)^2} \right) \right\} + \frac{1}{L^3} \sum_k \frac{m^2_\pi \delta^2}{E^2w^4_\pi} \left\{ \frac{1}{2(E-w_\pi)^3} - \frac{1}{2(E+w_\pi)^3} - e^{2(E-w_\pi)t_2} \left( \frac{1 - [2(E-w_\pi)]t_2 + [2(E-w_\pi)]^2 t^2_2/2}{2(E-w_\pi)^3} + \frac{1 + [2w_\pi]t_2 + [2w_\pi]^2 t^2_2/2}{2w_\pi^3} \right) 
+ e^{2Et_2-2w_\pi t_1} \left( \frac{1 + [2w_\pi]t_1 + [2w_\pi]^2 t^2_1/2}{2w_\pi^3} - \frac{1 + [2(E+w_\pi)]t_1 + [2(E+w_\pi)]^2 t^2_1/2}{2(E+w_\pi)^3} \right) \right\} ,$$

$$A_{0\pi} = \frac{1}{L^3} \sum_k \frac{m^2_\pi B_{K,K}^\pi}{2E^2w^2_\pi w_{ss}} \left\{ \frac{1}{2E-w_\pi - w_{ss}} - \frac{1}{2E+w_\pi + w_{ss}} - e^{2(E-w_\pi-w_{ss})t_2} \left( \frac{1}{2E-w_\pi - w_{ss}} + \frac{1}{w_\pi + w_{ss}} \right) 
+ e^{2Et_2-(w_\pi+w_{ss}) t_1} \left( \frac{1}{w_\pi + w_{ss}} - \frac{1}{w_{ss} + w_\pi + 2E} \right) \right\} ,$$

$$A_{00} = \frac{1}{L^3} \sum_k \frac{m^2_\pi B_{K,K}^\pi}{4E^2w^2_\pi w_{ss}^2} \left\{ \frac{1}{2(E+w_{ss})} - \frac{1}{2(E+w_\pi + w_{ss})} - e^{2(E-w_{ss})t_2} \left( \frac{1}{2(E-w_{ss})} + \frac{1}{2w_{ss}} \right) 
+ e^{2Et_2-2w_{ss} t_1} \left( \frac{1}{2w_{ss}} - \frac{1}{2(w_{ss} + E)} \right) \right\} .$$

Note that the presence of flavour-singlet double poles gives rise to terms proportional to powers of $t_1$ and
where the ellipses represent non-singular contributions, the sum runs over all mesons and

deﬁned in eq. (24).

The correlation function is given by

\[ \langle K(0) \bar{K}^0(t_K) | 0 \rangle = \frac{e^{-Et_1} e^{-Et_2} e^{m_K t_K}}{2E} \left( -\frac{8i}{f^3} \right) \left[ \tau(E, m_K, m_{\pi}) - \frac{E^2}{2f^2} \left( \sum_{l=\tau, \pi, KK,...} A_l + \ldots \right) \right], \]

where the ellipses represent non-singular contributions, the sum runs over all mesons and

\[ \tau(E, m_1, m_2) \equiv \frac{2E^2 + Em_1 - m_2^2}{2}. \]

To this order the relevant contributions to \( A_I \) can be written as

\[ A_I = \frac{1}{E^3} \sum_k \sum_{r=1}^{3} \frac{C_I^{(r)}}{(2E - w_i - w_j)^r} \left( 1 - e^{(2E - w_i - w_j)E} \sum_{n=0}^{r-1} (2E - w_i - w_j)^n \frac{t_n}{n!} \right) + \ldots, \]

where again only the terms containing poles have been kept. The only non-zero coefﬁcients are the following:

\[ C_{KK}^{(1)} = -\tau(w_K, m_K, m_K) c_+(w_K), \]
\[ C_{SS}^{(1)} = \tau(w_S, m_K, m_{\tau}) c_+(w_S), \]
\[ C_{\pi\pi}^{(1)} = \tau(w_\pi, m_K, m_{\pi}) (d_+(w_\pi) - c_+(w_\pi)) + \frac{m_{\pi}^2}{4E^2 w_{\pi}^5} \left( \delta_+^2 (w_\pi^2 - m_{\pi}^2) - m_{\pi} w_{\pi}^3 \delta_+ B_{\pi K} - 2w_{\pi}^4 \tau(w_\pi, m_\pi, m_{\pi}) B_{\pi K}^2 \right), \]
\[ C_{\pi\pi}^{(2)} = -\delta_+ m_{\pi}^2 \left( 2w_{\pi}^2 + w_{\pi} m_K - 2m_{\pi}^2 \right), \]
\[ C_{\tau}^{(3)} = \frac{\delta_+^2 \tau(w_\tau, m_K, m_{\pi}) m_{\pi}^2}{E^2 w_{\pi}^4}, \]
\[ C_{0}^{(1)} = -B_{\pi K} B_{\tau} \frac{m_{\pi}^2}{E^2 w_{\pi}^5} \tau \left( \frac{w_{\pi} + w_\tau}{2}, m_K, m_K \right) - \frac{m_{\pi}^2 m_K \delta_+^2 B_{\tau K}}{4E^2 w_{\pi}^5}, \]
\[ C_{0}^{(2)} = \frac{m_{\pi}^2 m_K \delta_+ B_{\tau K} (w_{\pi} - w_\tau)}{4E^2 w_{\pi} w_{\tau}^5}, \]
\[ C_{00}^{(1)} = -B_{\pi K}^2 \tau \left( w_{ss}, m_K, \sqrt{2m_K^2 - m_{\pi}^2} \right) \frac{m_{\pi}^2}{2E^2 w_{ss}^3}. \]

where the quantities on the right-hand side are deﬁned in eq. (24).

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