LU TP 15-53
November 2015

PROCEEDINGS OF SCIENCE

ChPT meets lattice: finite volume and partial quenching for masses, decay constants and VEVs at NNLO

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We discuss finite volume effects and partial quenching for Chiral Perturbation Theory in the mesonic sector. The effects are computed in terms of analytical expressions for masses, decay constants and vacuum expectation values (VEVs) to two-loop order. Numerical examples are presented for a number of interesting and relevant cases. All numerical programs are publically available, the prospects of a combination of these studies with lattice gauge theory computations are discussed briefly.

To be published in the proceedings of:
The 8th International Workshop on Chiral Dynamics
29 June 2015 - 03 July 2015
Pisa, Italy

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1. Introduction: Chiral Perturbation Theory and unphysical artefacts

Chiral Perturbation Theory (ChPT) [1, 2, 3] is the effective field theory for QCD when looking at physics in the low-energy limit. Unphysical effects and artefacts as needed in lattice gauge theory can be systematically included in this framework. Calculations in Lattice Gauge Theory can highly benefit when ChPT-guided extrapolations are employed to keep these effects - such as unphysical valence and/or sea quark masses, the finite lattice spacing, the finite lattice size and lattice artefacts, due to the choice of action, under control.

The talk discusses progress for two of these effects inside the ChPT framework: the finite size and the unphysical masses [4, 5]. To simplify the use for the lattice community, we provide fully flexible and unrestricted access to our numerical programs via the CHIRON [6] program collection. This can be downloaded from [7]. The analytical expressions can be downloaded from [8].

It is inevitably the nature of any numerical lattice calculation that it is performed in a finite volume. In order to perform a proper matching between a lattice QCD calculation and ChPT, good control over the additional quantum corrections to physical quantities which emerge due to the finiteness of the volume is required. Then, infinite volume ChPT can serve as a reliable validity check for the lattice calculation, or low-energy constants (LECs) can be properly extracted from the lattice result. Conceptually, in our work, a finite volume (FV) is introduced that restricts the size of the Euclidean 3-dimensional space. The "time" dimension is assumed to be infinitely extended. This treatment clearly breaks Lorentz invariance. Dealing with the effects of all of this in ChPT at two-loop order is quite involved. We discuss first shortly finite volume loop integrals, Sect. 2, then our results for standard ChPT in finite volume [4] in Sect. 3. The largest part is devoted to the partially quenched case, Sect. 4. We present a few numerical results as well as the checks performed. Finally, we point out the recent extension to QCD-like theories.

Introductions to ChPT can be found in the talks by Ecker [9] and Bernard [10] at this conference. A more extensive introduction aimed at lattice theorists is [11].

2. Finite volume integrals

Two different methods for the numerical evaluation of FV integrals have been suggested at one-loop order [12, 13, 14, 15]. The integrals over momentum components in finite size direction are really discrete sums. Using the Poisson summation theorem the sum can be turned into a sum over integrals again. The advantage of doing this is that the infinite volume expression can easily be removed from this. The separation of the infinite volume (IV) and FV part of an integral leaves a sum of integrals as the structure to be calculated numerically. Depending on the preferred method, either the summation or the integration can be eliminated. The actual evaluation routines then have to solve only a summation over modified Bessel functions [12, 13, 14] or a numerical integration over Jacobi theta functions [15]. This is strictly true for the one-propagator cases, for two or more propagators additional numerical integrations over Feynman parameters might be necessary. Note that since the finite volume breaks Lorentz invariance extra structures can appear in the integrals.

The extension of both methods to the general two-loop sunset integral can be found in [16]. Expressions for all the integrals needed in this work can be found there. They are also available in

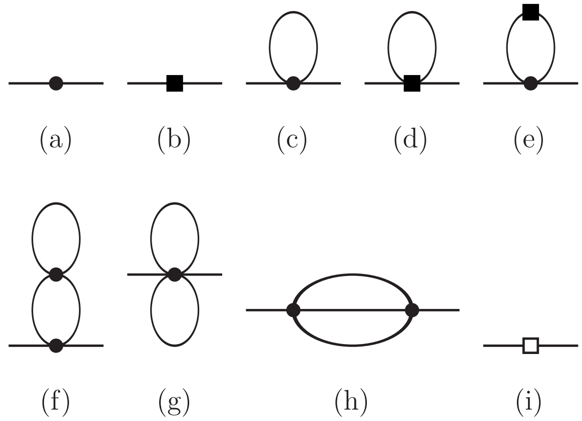


Figure 1: The Feynman diagrams needed for the mass calculation. A dot indicates a vertex of order p^2, a filled box a vertex of order p^4 and an open box a vertex of order p^6.

the program package CHIRON [6, 7]. The precise definitions for the Minkowski versions we use in our work discussed here can be found in [4, 5].

3. Finite volume for standard ChPT

The calculation at finite volume is very much like the calculations in infinite volume but one has to keep in mind the extra terms and extra structures in the loop-integrals. The diagrams that need to be evaluated are depicted in Fig. 1.

For numerical inputs we use

$$\begin{aligned} F_\pi &= 92.2 \text{ MeV},\ m_\pi = 134.9764 \text{ MeV}, \mu = 770 \text{ MeV},\ m_K = 494.53 \text{ MeV}, \\ m_\eta &= 547.30 \text{ MeV},\ \bar{l}_1 = -0.4,\ \bar{l}_2 = 4.3,\ \bar{l}_3 = 3.0\ \bar{l} = 4.3\,. \end{aligned} \tag{3.1}$$

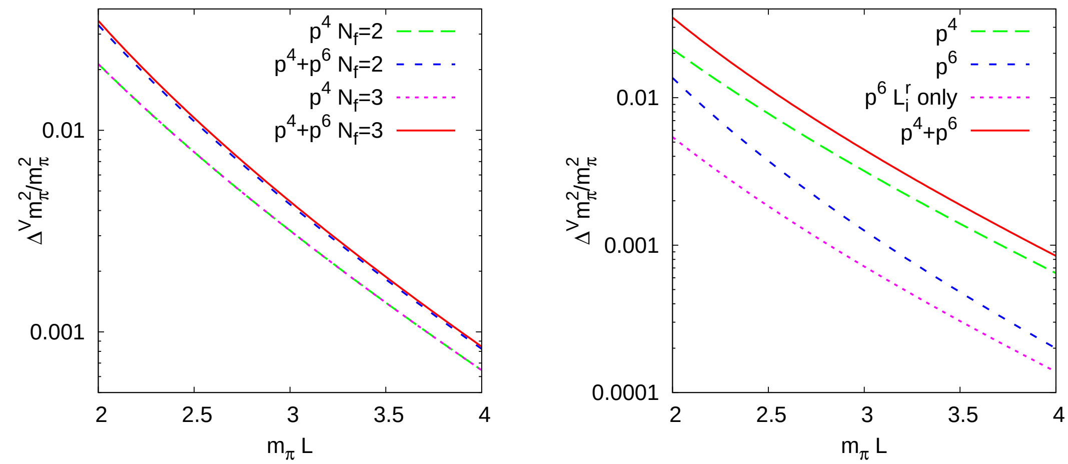
For the three flavour LECs (L_i^r) we use the values of the recent fit to continuum data [17].

The analytical result for the finite volume correction to the pion mass for the two flavour case agrees with the one-loop result of [14] and as far as we were able to check with the two-loop result of [18]. The infinite volume result agrees with [19, 20]. For the three flavour case we agree for all masses with the infinite volume result [21] and the one-loop finite volume results [15].

Numerical results for the pion mass are shown in Fig. 2. We have varied L but kept all other inputs constant as given in (3.1). The two and three flavour results are numerically in good agreement showing that as expected the kaon and eta effects are small.

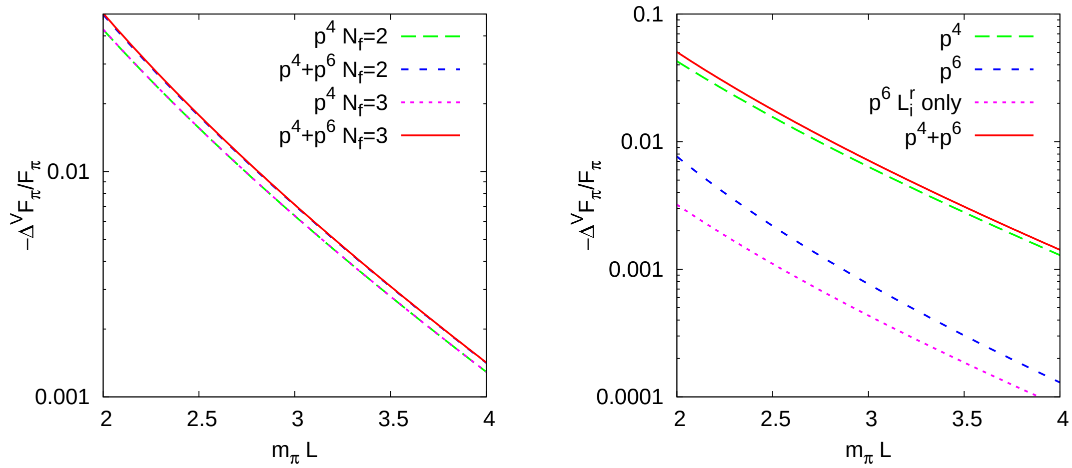
The decay constants can be calculated in a similar fashion. We reproduced the known infinite volume two-loop results as well as the one-loop results. We have a small disagreement with the partial two-loop results in [22]. Numerical results for the pion decay constants are shown in Fig. 3.

Some examples using the same LECs as above but varying input kaon and pion masses with a calculated consistent value for F_π and m_η are shown in Fig. 4. The method of calculating consistent values is explained in [4].



(a) (b)

Figure 2: The relative finite volume corrections to the pion mass squared with varying L. The other inputs are given in the main text. (a) Comparison of the two- and three-flavour results. (b) The three-flavour case also showing the L_i^r dependent part.



(a) (b)

Figure 3: The finite volume corrections to the pion decay constant as a function of L. The other inputs can be found in the text. Plotted is $-(F_\pi^V - F_\pi)/F_\pi$. (a) Comparison of the two- and three-flavour results. (b) The corrections for the three-flavour case showing the L_i^r dependent part separately.

4. Finite volume results for partially quenched three flavour ChPT

4.1 Partial quenching

In the partially quenched case, we give different masses to the valence and sea quarks. Valence quarks have flavour lines which connect to the external fields. Sea quarks, on the other hand, appear only in closed loops. The distinction is crucial for comparison to partially quenched lattice calculations. For the sea quarks, a (functional) fermion determinant appears in the generating

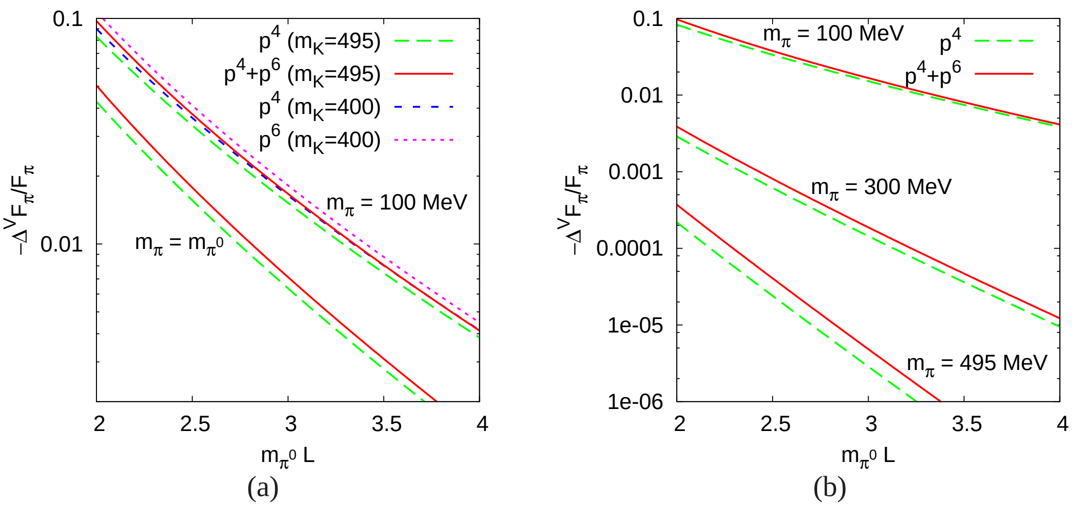


Figure 4: The finite volume corrections to the pion decay constant for a number of mass cases. Plotted is the quantity $-(F_\pi^V - F_\pi)/F_\pi$. (a) Physical case and $(m_\pi, m_K) = (100, 495)$ and $(100, 400)$ MeV. (b) $m_K =$ 495 MeV and $m_\pi = 100, 300, 495$ MeV. The size L is given in units of the physical π^0 mass.

functional

$$Z = \int D[\psi\bar{\psi}A] \exp\left(-S_G - \int [\bar{\psi}(\not{D} + m)\psi]\right) = \int D[A] \exp(-S_G) \det(\not{D} + m) \tag{4.1}$$

when integrating over the anti-commuting fermionic Grassmann fields. Hence, the exponential containing the gauge field action S_G is modified by a factor containing the fermion mass m.[1] The (Monte-Carlo) evaluation of the determinant is computationally very expensive, it is much cheaper to vary the valence quark mass only. Then, the produced gauge field configurations do not need to be changed in the lattice computation, but only the mass scale that is used to calculate the operator expectation value.

An important issue for a partially quenched ChPT (PQChPT) calculation is the question how to prevent quark fields in the valence sector from contributing according to equation (4.1) to the determinant. One way is given by a construction, due to Morel [23], that involves bosonic spin-$1/2$ fields. By fixing the mass matrix $\tilde{m}$ of these "ghost" fields to the one used in the valence sector, the unwanted contribution cancels exactly from the determinant as can be seen from

$$\begin{aligned} Z &= \int D[\psi\bar{\psi}\tilde{\psi}\bar{\tilde{\psi}}A] \exp\left(-S_G - \int [\bar{\psi}(\not{D} + m)\psi + \bar{\tilde{\psi}}(\not{D} + \tilde{m})\tilde{\psi}]\right) \\ &= \int D[A] \exp(-S_G) \frac{\det(\not{D} + m)}{\det(\not{D} + \tilde{m})} \end{aligned} \tag{4.2}$$

with $\tilde{\psi}$ denoting the bosonic Dirac field. This method, also called the supersymmetric formulation of PQChPT, has the advantage that the partial quenching is completely performed by the construction of the Goldstone manifold and the Lagrangian. Given that, the Feynman-diagrammatic calculation then simply follows the ordinary rules of Field Theory. It should be noted though on the side

[1] The equations also hold for several fermions, arranged in a column vector ψ, and a mass matrix m.

that this does not change the fact that the partially quenched theory is no longer a proper Quantum Field Theory in the strict sense: The supersymmetric formulation allows rewriting partially quenched theory in terms of a local Lagrangian for a statistical mechanical model - in violation of the spin-statistics theorem.

The chiral group in the supersymmetric framework is formally extended to the graded

$$G = SU(n_{\text{val}} + n_{\text{sea}}|n_{\text{val}})_L \times SU(n_{\text{val}} + n_{\text{sea}}|n_{\text{val}})_R \tag{4.3}$$

for the case of n_{val} valence and n_{sea} quarks. G is then spontaneously broken to the diagonal subgroup $SU(n_{\text{val}} + n_{\text{sea}}|n_{\text{val}})_V$. We have done our calculations in the flavour basis rather than in the meson basis. We thus use fields ϕ_{ab} corresponding to the flavour content of $q_a\bar{q}_b$. The mixing of the neutral eigenstates and the integrating out of the singlet degree of freedom is taken care of by using a more complicated propagator. It is possible to use the same method also in standard ChPT.

The corresponding Goldstone manifold is then parametrized by fields with generic structure

$$\Phi = \begin{pmatrix} \left[\; q_V\bar{q}_V \;\right] & \left[\; q_V\bar{q}_S \;\right] & \left[\; q_V\bar{q}_B \;\right] \\ \\ \left[\; q_S\bar{q}_V \;\right] & \left[\; q_S\bar{q}_S \;\right] & \left[\; q_S\bar{q}_B \;\right] \\ \\ \left[\; q_B\bar{q}_V \;\right] & \left[\; q_B\bar{q}_S \;\right] & \left[\; q_B\bar{q}_B \;\right] \end{pmatrix} \tag{4.4}$$

where V denotes valence, S denotes sea and B denotes the bosonic ghost quarks. Note that the meson fields containing one single ghost quark only will themselves obey fermionic, i. e. anticommuting, statistics.

The structure of the Lagrangian is similar to standard ChPT for a generic number of flavours. The lowest order Lagrangian is

$$\mathscr{L}_2 = \frac{F_0^2}{4}\langle u_\mu u^\mu + \chi_+\rangle\,. \tag{4.5}$$

At one-loop, the terms relevant to our work are given by

$$\begin{aligned}\mathscr{L}_4 \;=\; & \hat{L}_0\langle u^\mu u^\nu u_\mu u_\nu\rangle + \hat{L}_1\langle u^\mu u_\mu\rangle^2 + \hat{L}_2\langle u^\mu u^\nu\rangle\langle u_\mu u_\nu\rangle + \hat{L}_3\langle (u^\mu u_\mu)^2\rangle \\ & + \hat{L}_4\langle u^\mu u_\mu\rangle\langle\chi_+\rangle + \hat{L}_5\langle u^\mu u_\mu \chi_+\rangle + \hat{L}_6\langle\chi_+\rangle^2 + \hat{L}_7\langle\chi_-\rangle^2 + \frac{\hat{L}_8}{2}\langle\chi_+^2 + \chi_-^2\rangle + \ldots\,.\end{aligned} \tag{4.6}$$

The generalized Goldstone manifold is parametrized as

$$u \equiv \exp\left(i\Phi/(\sqrt{2}\hat{F})\right) \tag{4.7}$$

similar to the exponential representation in standard ChPT. For three physical flavours, it is a 9×9 matrix with fermionic parts. We have furthermore introduced

$$\begin{aligned} u_\mu \;&=\; i\left\{u^\dagger(\partial_\mu - ir_\mu)u - u(\partial_\mu - il_\mu)u^\dagger\right\}, \\ \chi_\pm \;&=\; u^\dagger \chi u^\dagger \pm u\chi^\dagger u\,. \end{aligned} \tag{4.8}$$

The matrix χ is for this work restricted to

$$\chi = 2B_0\,\text{diag}(m_1, \ldots, m_9) \tag{4.9}$$

with m_i the quark mass of quark i and B_0 a LEC. We have here $m_1 = m_7, m_2 = m_8, m_3 = m_9$ as the valence masses and m_4, m_5, m_6 as the sea quark masses. Ordinary traces have been replaced by supertraces, denoted by $\langle\ \rangle$, defined in terms of the ordinary ones by

$$\mathrm{Str}\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \mathrm{Tr}A - \mathrm{Tr}D\,. \tag{4.10}$$

B and C denote the fermionic blocks in the matrix. The supersinglet Φ_0, generalizing the η', is integrated out to account for the axial anomaly as in standard ChPT, implying the additional condition

$$\langle\Phi\rangle = \mathrm{Str}\,(\Phi) = 0\,. \tag{4.11}$$

However, as mentioned above, we will work in the flavour basis enforcing the constraint (4.11) via the propagator.

A calculation in PQChPT has to be performed using a larger set of operators since no further reduction by means of Cayley-Hamilton relations can be performed. The three-flavour PQChPT Lagrangian (equation (4.6)) thus has 11 LECs for PQChPT.

An additional comment is that the divergences for PQChPT are directly related to those for n_{sea}-flavour ChPT [24] when all traces are replaced by supertraces. This can be argued using the formal equivalence of the equations of motion used or via the replica trick [25].

This method was used in the pioneering work for actual calculations in partially quenched ChPT [26]. More details can be found in [27, 28]. In those references you can also find a detailed derivation of the double poles that appear in the propagators for neutral particles.

4.2 Quark flow

An alternative method to do (partially) quenched calculations in ChPT is to use the quark flow method introduced in [29]. It basically consists of working in the flavour basis and keeping all flavour lines. The removal of the singlet degree of freedom is now done via extra terms in the neutral propagator. In the end one checks which flavour lines are connected to external fields or operators and those are given the corresponding valence quark flavour. The remaining ones are to be summed over the sea quark flavours. This was generalized to the two-loop diagrams in our calculation.

4.3 Results

The analytical calculations were performed using both methods, supersymmetric and quark flow, with results in full agreement. We also reproduced the known infinite volume results [30, 31, 32] and the one-loop finite volume expressions [33, 34]. The expressions for the different mass cases reduce to each other and to the unquenched case when taking the relevant mass limits.

For the LECs we use the results of the L_i^r of the recent fit [17] and we set the additional LEC $L_0^r = 0$. The scale is set to $\mu = 0.77$ GeV and the lattice size L we choose as that $ML = 2$ for $M = 0.13$ GeV. For the lowest order pion decay constant we use $F_0 = 87.7$ MeV. The lowest order kaon mass we fix to 450 MeV.

As an example we plot the pion mass for a number of cases where we keep the lowest order (valence) pion mass at 130 MeV but vary the sea quark masses to get a sea pion mass varying from

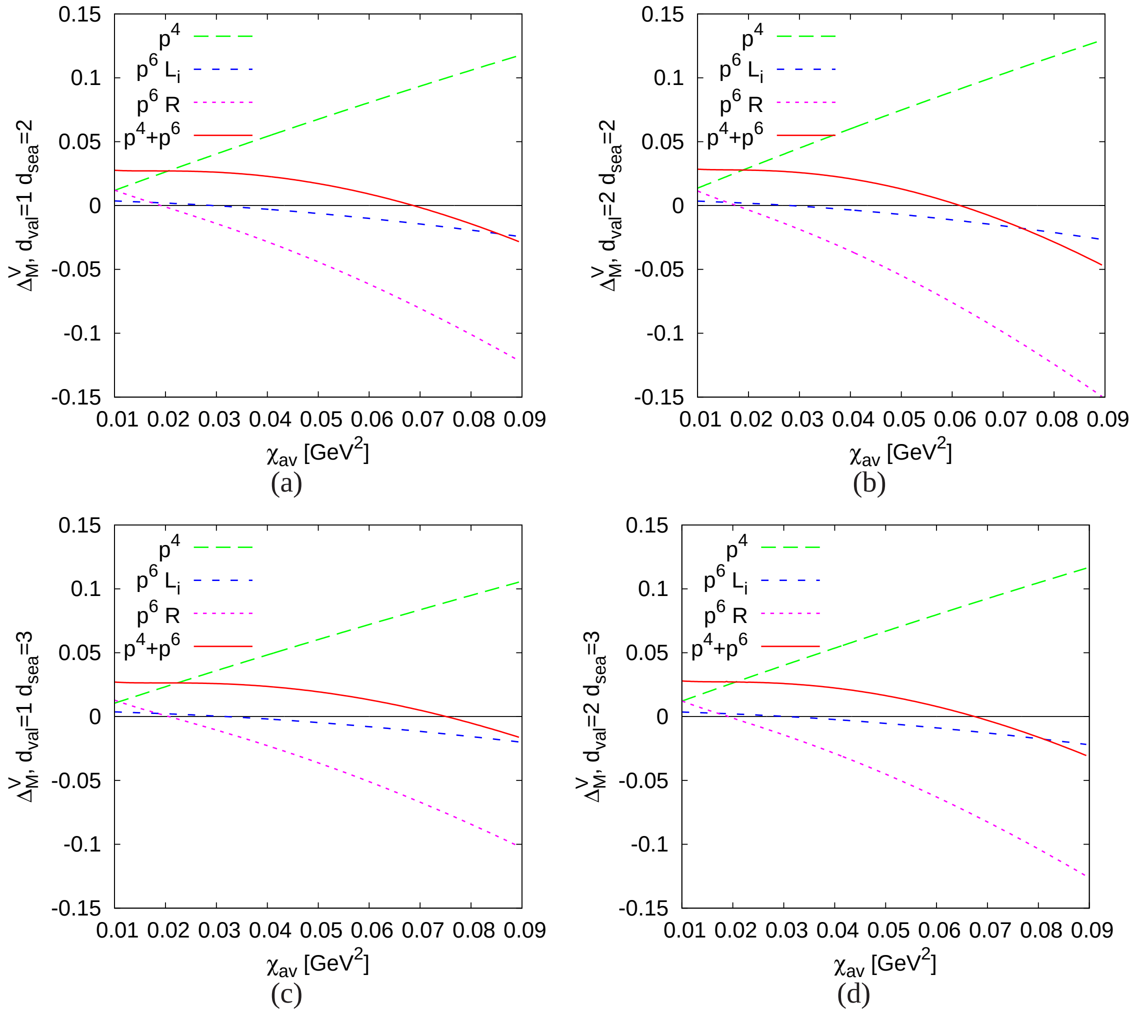


Figure 5: The corrections for the pion mass relative to the lowest order mass as a function of the average up and down sea quark mass via $\chi_{\rm av}$. When isospin breaking is included the ration of up to down quark mass is chosen to be 1/2. (a) The isospin limit in sea and valence, (b) Isospin breaking in the valence sector only. (c) Isospin breaking in the sea sector only. (d) Isospin breaking in both sectors.

100 to 300 MeV. The sea strange quark is fixed at a mass slight above the valence sea mass. The variation with the sea pion mass squared $\chi_{\rm av}$ is shown in Fig. 5. We show the cases for up-down mass equal for both sea and valence, different for valence only, different for sea only and both different. The cancellation between the up-down mass differences between sea and valence effects is accidental. It does not happen for the decay constant. The four different cases are compared in Fig. 6.

The same cases for the pion decay constant are shown in Fig. 7. The cancellation which happened for the masses is not present here. Figures for a number of other cases can be found in the paper.

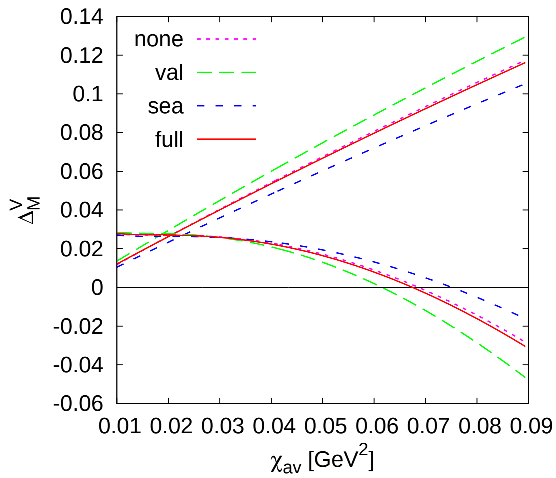


Figure 6: Comparing the finite volume correction for the meson masses for the cases with no isospin breaking (none), only in the valence sector (val), only in the sea sector (sea) and in both (full) for the meson mass squared. The upper curves are the p^4, the bottom the $p^4 + p^6$ results.

5. Update: QCD-like theories

The finite volume corrections for masses, decay constants and the quark-antiquark vacuum expectation value in the effective field theory for QCD-like theories have been recently calculated as well. The extension to the partially quenched case was done in the same work [35]. This work can be seen as an extension of our work in ChPT discussed above and of the unquenched infinite volume results of [36].

Acknowledgments

We thank the organizers for a very pleasant and well-run conference. This work is supported in part by the Swedish Research Council grants 621-2011-5080 and 621-2013-4287.

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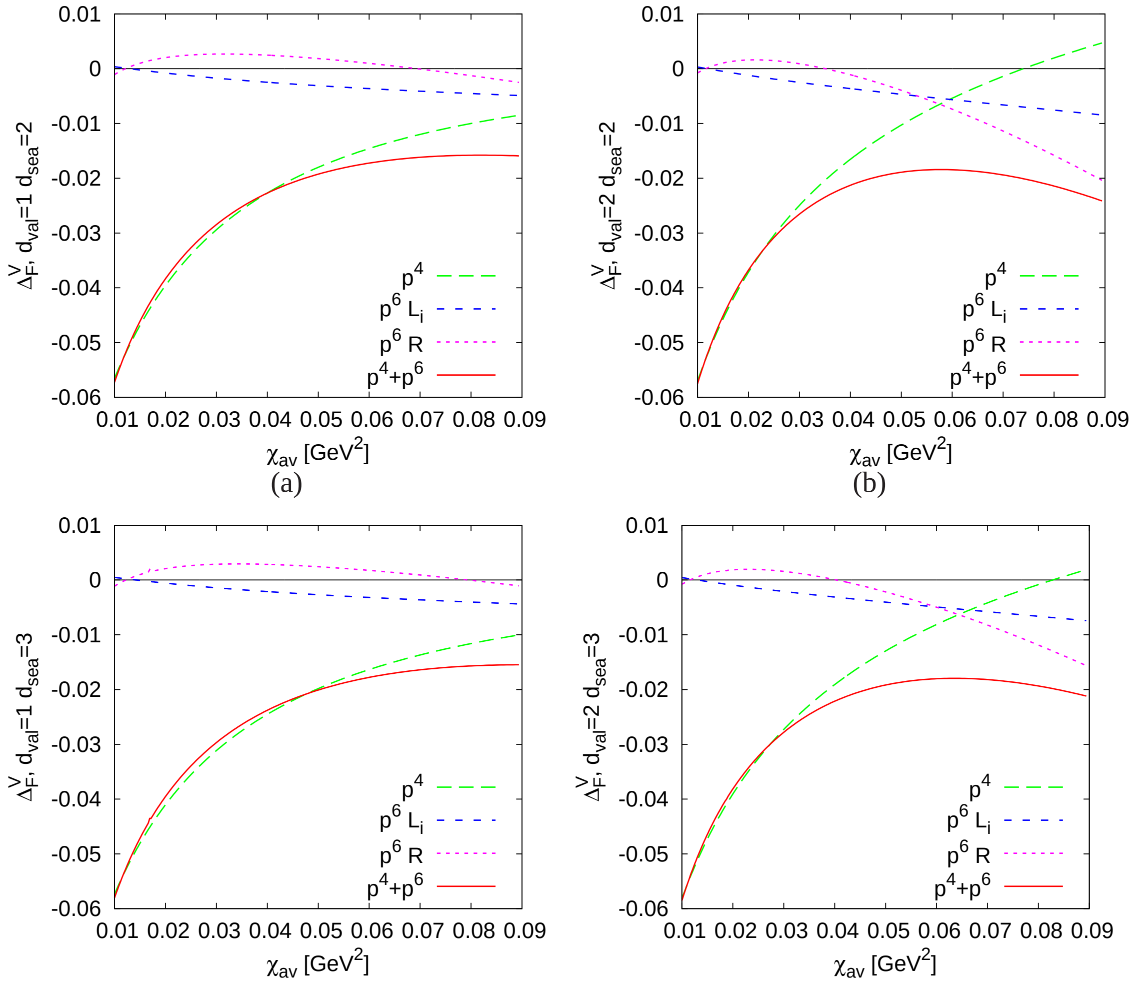

(a) (b) (c) (d)

Figure 7: The corrections for the pion decay constant relative to its lowest order value as a function of the average up and down sea quark mass via χ_{av}. (a) The isospin limit. (b) Isospin breaking in the valence sector. (c) Isospin breaking in the sea sector. (d) Isospin breaking in both sectors.

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