Chiral and Continuum Extrapolation of Partially-Quenched Lattice Results

C. R. Allton \(^a\), W. Armour \(^a\), D. B. Leinweber \(^b\),
A. W. Thomas \(^c\), R. D. Young \(^c\)

\(^a\)Department of Physics, University of Wales Swansea, Swansea SA2 8PP, Wales, U.K.
\(^b\)CSSM and Department of Physics, University of Adelaide, Adelaide SA 5005, Australia
\(^c\)Jefferson Lab, 12000 Jefferson Ave., Newport News VA 23606, USA

Abstract

The vector meson mass is extracted from a large sample of partially quenched, two-flavor lattice QCD simulations. For the first time, discretisation, finite-volume and partial quenching artefacts are treated in a unified framework which is consistent with the low-energy behaviour of QCD. This analysis incorporates the leading infrared behaviour dictated by chiral effective field theory. As the two-pion decay channel cannot be described by a low-energy expansion alone, a highly-constrained model for the decay channel of the rho-meson is introduced. The latter is essential for extrapolating lattice results from the quark-mass regime where the rho is observed to be a physical bound state.

Recent developments in lattice QCD have enabled the first large-scale simulation of chiral, dynamical fermions [1]. While this accomplishment is a significant milestone in the progress towards an accurate description of physical QCD, the high demand on computing resources restricts practical calculations to an unphysical domain of simulation parameters. In particular, lattice QCD involves a discretised space-time of finite spatial extent, with input quark masses much larger than those in Nature. Each of these approximations requires special attention in the extraction of physical observables from Monte Carlo simulations. In this Letter we analyse a very large set of partially quenched data for the mass of the \(\rho\) meson. We show that a systematic analysis of this data enables us to remove the effects of partial quenching and to take both the continuum and infinite volume limits. The resulting data lies on a single, well defined curve which extrapolates to a value within \(\sim 1\%\) of the physical \(\rho\) mass. The contrast between the raw lattice data (note the scatter in Fig. 2) and the corrected data shown in Fig. 3 is striking.
Spontaneous chiral symmetry breaking in QCD dictates that, in the vicinity of the chiral limit, hadronic observables exhibit nonanalytic dependence on the quark mass [2]. This feature places tight constraints on the form of chiral extrapolations if they are to be consistent with the properties of low-energy QCD [3,4]. The most natural solution to this problem is to use effective field theory (EFT) to describe the quark-mass dependence of hadron properties. Considering a benchmark quantity, such as the nucleon mass, there is substantial phenomenological information on the quark-mass expansion near the chiral limit [5]. In the context of lattice simulations, where quark masses are significantly far from the chiral limit, the expansion is acutely sensitive to higher-order corrections. Fortunately, such issues can be alleviated by reformulating the EFT in the framework of finite-range regularisation (FRR) [6] — with demonstrated success in the efficient extrapolation [7] of lattice calculations of the nucleon mass [8].

Provided simulations are performed on a suitably large box, finite-volume corrections will be exponentially suppressed. Nevertheless, these leading corrections can be described by the same low-energy effective field theory used to understand the quark-mass variation [9]. Finite-volume corrections are dominated by the suppression of the infrared component of chiral loop diagrams — as observed in a recent study of volume dependence in lattice QCD [10] (using the quark-mass dependence described in Ref. [11]). Corrections of this type have previously been incorporated in quark-mass extrapolations [12,13,14]. They are essential in the case of the $p$-wave decay channels, such as $\rho \to \pi\pi$ [12] and $\Delta \to N\pi$ [13]. The modifications to EFT on a finite volume have been investigated for a range of observables — e.g., see Refs. [15,16,17,18,19].

Removal of discretisation artefacts from simulation results also represents an important step in the systematic extraction of continuum QCD physics. From a technical point of view, a great deal of effort has gone into action improvement [20] such that near-continuum results can be obtained at finite lattice spacing [21,22,23]. Residual discrepancies from the continuum can be incorporated as perturbative corrections in EFT [24,25,26,27], thereby providing a systematic approach to the continuum.

The generation of gauge field configurations with dynamical sea quarks is the most computationally demanding component of the calculation of standard observables. By comparison, the matrix inversion required to obtain quark propagators is relatively efficient. This enables the calculation of quark propagators over a range of quark masses for a fixed gauge field ensemble. Such calculations are referred to as partially quenched QCD (pQQCD), where the valence quark masses no longer match those simulated in the sea. Although an unphysical approximation, the connection to the physical theory in EFT has been demonstrated [28]. Most importantly, the partially quenched EFT does not require any new, unphysical parameters.
While EFT provides a systematic framework for the analysis of lattice results, the present analysis of the $\rho$ meson requires one to go beyond the scope of EFT. Near the chiral limit, the $\rho$ decays to two energetic pions. The pions contributing to the imaginary part of the $\rho$ mass cannot be considered soft, and therefore cannot be systematically incorporated into a low-energy counting scheme [29,30]. Because almost all the lattice simulation points in this analysis lie in the region $m_\pi > m_\rho/2$, it is evident that in the extrapolation to the chiral regime will encounter a threshold effect where the decay channel opens. To incorporate this physical threshold, we model the $\rho \to \pi\pi$ self-energy diagram constrained to reproduce the observed width at the physical pion mass. Including this contribution also provides a model of the finite volume corrections arising from the infrared component of the loop integral. In particular, we can also describe the lattice results in the region $m_\pi < m_\rho/2$, where the decay channel still has higher energy because of momentum discretisation.

In this Letter we present a global analysis of a very large set of sophisticated lattice simulation results. The aim is to produce an accurate determination of the (real part of the) $\rho$-meson mass in 2-flavour QCD, with the required input of the experimental width. For a complete account of the analysis procedure, the reader is referred to Ref. [31].

Partially-quenched lattice simulations are characterised by the distinction between the masses of quarks coupling to external sources and those associated with vacuum polarisation of the gauge field. Subsequently, the construction of effective field theories based on such simulations necessarily distinguishes the valence- and sea- quark composition of hadronic states. While the external legs of any $n$-point hadronic correlator are constructed of valence quarks only, internal (hadron) loop diagrams may comprise any mixture of sea and valence quarks. The mass of a particular vector meson state is therefore described by

$$M_{ijj}^a = M(a, m_i; m_j, m_k),$$

where the first two parameters of $M(a, m_i; m_j, m_k)$ specify the gauge field ensemble with lattice spacing $a$ and sea-quark mass $m_{\text{sea}} = m_i$. The masses of the valence quarks are given by $m_j$ and $m_k$. Similarly, $M_{ijj}^a$ is the mass of a pseudoscalar meson of equivalent quark composition.

The global parameterisation of the vector meson mass, dependent on quark masses, lattice spacing and physical volume, is written as

$$M_{ijj}^a = (\alpha_0 + X_2 a^2 + \alpha_2 m_{ijj}^a + \alpha_4 m_{ijj}^a)^2 + \Sigma_{\text{TOT}}^a(L).$$

The total loop correction to the $M_{ijj}^a$ meson, on a finite box of physical length $L = Na$, is described by

$$\Sigma_{\text{TOT}}^a(L) = \Sigma_{\pi\pi}^a(m_{ijj}^a, L) + \Sigma_{\pi\omega}^a(m_{ijj}^a, L) + \Sigma_{\eta\rho}^a(m_{ijj}^a, m_{ijj}^a, m_{ijj}^a, L).$$
Fig. 1. Left: Diagram providing the leading nonanalytic contribution to the chiral expansion of the $\rho$-meson mass (a) and its associated quark-flow (b). Middle: Two-pion contributions, (a), (c), to the $\rho$-meson self-energy and their associated quark flow diagrams in pQCD. While diagram (c) appears in quenched QCD, in pQCD (or full QCD) it is complemented by an infinite series of terms, the first two of which are depicted in diagrams (d) and (e). Right: The $\eta'$ contribution (a) and its associated quark flow diagrams in pQCD. While diagram (c) appears in quenched QCD, in pQCD (or full QCD) it is complemented by an infinite series of terms, the first two of which are depicted in diagrams (d) and (e).

The relevant loop corrections are depicted in Fig. 1. The corresponding loop integrals, in the $L \to \infty$ limit, are given by

$$\Sigma_{\pi\pi}^\rho(m_{\pi ij}^a) = -\frac{f_{\rho \pi \pi}^2}{24\pi^3} \int d^3k \frac{k^2 u_{\pi \pi}^2(k)}{\sqrt{k^2 + m_{\pi ij}^a} \left[ k^2 + m_{\pi ij}^a - \mu_\rho^2/4 \right]}, \quad (4)$$

$$\Sigma_{\pi\omega}^\rho(m_{\pi ij}^a) = -\frac{f_{\rho \pi \omega}^2}{12\pi^3 f_{\pi}^2} \int d^3k \frac{k^2 u_{\omega}^2(k)}{\sqrt{k^2 + m_{\pi ij}^a} \left[ \sqrt{k^2 + m_{\pi ij}^a} + (M_{\pi ij}^a - M_{\pi jj}^a) \right]}, \quad (5)$$

$$\Sigma_{\eta'\rho}^\rho(m_{\pi ij}^a, m_{\pi jj}^a, m_{\pi ii}^a) = \frac{f_{\rho \pi \omega}^2}{12\pi^3 f_{\pi}^2} \int d^3k \frac{k^2 u_{\omega}^2(k)}{(k^2 + m_{\pi ij}^a)^2} \left\{ \frac{(m_{\pi ij}^a - m_{\pi jj}^a)^2}{(k^2 + m_{\pi ij}^a)^2} + \frac{(m_{\pi ii}^a - m_{\pi jj}^a)^2}{(k^2 + m_{\pi jj}^a)^2} \right\}. \quad (6)$$

Symbols are summarised as: $f_\pi = 93$ MeV; physical $\rho$ and $\pi$ masses, $\mu_\rho = 0.770$ GeV and $\mu_\pi = 0.140$ GeV; $\rho \pi \pi$ coupling $f_{\rho \pi \pi} = 6.028$ [12]; $f_{\rho \pi \omega}^2 = \mu_\rho g_2^2$; $g_2$ (as introduced in Ref. [32]) is related to the $\omega \rho \pi$ coupling, $g_{\omega \rho \pi} = 16$ GeV$^{-1}$ [33], by $g_2 = g_{\omega \rho \pi} f_\pi/2 = 0.74$; $k = |\vec{k}|$; finite-range regularisation is implemented with a dipole form, $u(k) = (1 + k^2/\Lambda^2)^{-2}$, and the $\rho \pi \pi$ coupling is preserved at the physical threshold, $u_{\pi \pi}(k) = u(k)u^{-1}(\sqrt{\mu_\rho^2/4 - \mu_\pi^2})$. By demanding this physical threshold the infrared behaviour is no longer constrained and hence is not controlled by EFT. Therefore, such a model is essential to extrapolate lattice results from the regime $m_\pi > m_\rho/2$. 

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The leading finite-volume corrections are trivially incorporated by replacing
the continuum loop integrals in Eqs. (4,5,6) by a sum over discrete momenta
[12,13,14]
\[ \int d^3k \rightarrow \left(\frac{2\pi}{L}\right)^3 \sum \vec{k}, \] (7)
where \( \vec{k} = (2\pi/L) \vec{\ell} \) for \( \vec{\ell} \in \mathbb{Z}^3 \). This modification produces an infrared sup-
pression of the loop integrals, and is independent of the choice of ultra-violet
regularisation [16].

The bracketed term in Eq. (2) describes the residual variation of the vector
meson mass which is not contained in the one-loop Goldstone boson dia-
grams. The analytic variation of the quark-mass dependence is character ised by the
continuum parameters, \( \alpha_i \). At finite lattice spacing, all terms at order \( a \) and
\( a^2 \) must be treated consistently with the symmetry breaking patterns of the
prescribed fermion action [24]. This can potentially lead to more singular
chiral behaviour in the effective field theory at finite lattice spacing [26]. In
this study, the leading lattice spacing corrections to the terms analytic in the
quark mass are investigated.

The lattice simulation data considered in this analysis come from a large
sample of partially quenched simulation results from the CP-PACS Collabo-
ratio [8]. These simulations were performed using mean-field improved clover
fermions at four different couplings, \( \beta \). For each value of the coupling, four
different sea quark masses have been calculated, yielding a total of 16 inde-
pendent gauge field ensembles. On each ensemble, the quark propagator has
been evaluated for five values of the valence quark mass. For the vector mesons
constructed of degenerate valence quarks there are a total of 80 “data” points.
The lattice scale is set via the QCD Sommer scale \( r_0 = 0.49 \text{ fm} [34] \), enabling
all of these points to be shown in physical units — as in Fig. 2.

The form provided by Eq. (2) allows a universal fit to all these points with
just four free parameters (plus regulator scale). This is therefore a highly con-
strained fit to the large sample of simulation results. The best fit parameters
are displayed in Table 1. The \( \chi^2 \) indicates that Eq. (2) accurately describes
this large quantity of data. The regulator mass, \( \Lambda \), has also been optimised to
produce a best fit to the data, namely \( \Lambda = 655 \pm 35 \text{ MeV} \), with the bound de-
termined statistically from the 1-\( \sigma \) variation about the central fit. Studying the
variation of the fit over this domain introduces a small additional uncertainty
to the extrapolated result which is listed below in the error estimate.

Variations of Eq. (2) have also been investigated. Scaling corrections to the parameters $\alpha_2$ and $\alpha_4$ yield coefficients which are consistent with zero. Linear corrections in the lattice spacing, taking the form of a term $X_1a$, are observed to be small and hence do not improve on the fit with $X_1 = 0$. Extending to higher analytic order in the quark mass expansion, by a term $\alpha_6m_\pi^6$, reduces the stability of the fit, indicating that the data are consistent with $\alpha_6 = 0$ — see Ref. [31] for a complete account of these effects. The systematic error quoted below covers the range found with all of these variations.

The fit parameters shown in Table 1 allow one to shift the simulation results to the infinite-volume, continuum limit and to remove the effects of partial quenching — hence restoring unitarity in the quark masses. Complete details of the procedure are outlined in Ref. [31]. The results are displayed in Fig. 3, where we observe a remarkable result. The tremendous spread of data seen in Fig. 2 is dramatically reduced, with all 80 points now lying very accurately on a universal curve.

The curve through Fig. 3 displays the determined variation of the $\rho$-meson mass with pion mass. This curve also presents an extrapolation to the physical point, allowing extraction of the physical $\rho$-meson mass

$$M_\rho = 778(4)_{-6}^{+16}(8)\text{ MeV},$$

where the first error is statistical, the second is systematic and the third from the determination of $\Lambda$ [31]. This result is in excellent agreement with the
Fig. 3. The same 80 lattice data points as in Fig. 2, after correction to restore the infinite-volume, continuum and quark-mass unitarity limits. The central curve displays the best-fit from the global analysis. The dashed curves show the bounds on the FRR scale, $0.620 < \Lambda < 0.690$ GeV.

The systematic uncertainty arises from the choice of fitting function, as outlined above, and also from the choice of finite-range regulator. In addition to the presented dipole form, the analysis has been repeated with monopole and Gaussian regulators. The central values of the extrapolated result with the monopole and Gaussian forms differs by $+3$ and $-6$ MeV, respectively, from the dipole result. Each regularisation scheme produces a different model of the $\rho \to \pi \pi$ vertex. This suggests that the model-dependence of this contribution is small, once constrained to produce the correct width at the physical point.

This extrapolation of the lattice results also offers an estimate of the vector meson mass in the chiral limit, $M^0_\rho$. The central value of the preferred fit gives a value 775 MeV, with errors similar to those quoted above for the vector mass at the physical point. These errors are from extrapolation of lattice results only, whereas for phenomenological purposes the physical point provides a further constraint. We therefore report the correlated difference between the physical and chiral limit value

$$M_\rho - M^0_\rho = 3.7(2)^{+4}_{-3}(8) \text{ MeV}.$$  

Interestingly, the chiral limit value of $M_\rho$ is very similar to that of the physical value. This feature is observed in the reduction in slope of the extrapolation curve in Figure 3 as the chiral limit is approached. The underlying physics giving rise to this reduced slope is the presence of substantial spectral strength in the low-energy two-pion channel below the rho-meson mass [35]. This sug-
gests a small sigma term for the $\rho$ in comparison with the nucleon, where the curvature is enhanced near the chiral limit [7].

This analysis demonstrates the ability to treat all lattice artifacts within a unified framework. Both scaling violations and finite-volume discrepancies can be removed through the procedure outlined. The number of simulation points can be increased dramatically by including partially quenched results. This in turn permits a highly constrained fit to produce an accurate extrapolation to the physical point. With minimal input, namely the $\rho\pi\pi$ and $\omega\rho\pi$ coupling constants, the real part of the $\rho$-meson mass has been accurately determined in two-flavour QCD\(^1\). The final result for the pion mass variation, as described by the universal curve in Fig. 3, sets a benchmark for the continuum, infinite-volume limit of the $\rho$ meson in two-flavour QCD.

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\(^1\) This is two-flavour QCD with the $q\bar{q}$ force normalised to the physical value at a length scale $r_0 = 0.49\text{ fm}$. 
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