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Hadron Mass Extraction from Lattice QCD

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The extraction of quantities from lattice QCD calculations at realistic quark masses is of considerable importance. Whilst physical quark masses are some way off, the recent advances in the calculation of hadron masses within full QCD now invite improved extrapolation methods. We show that, provided the correct chiral behaviour of QCD is respected in the extrapolation to realistic quark masses, one can indeed obtain a fairly reliable determination of masses, the sigma commutator and the J parameter. We summarise these findings by presenting the nonanalytic behaviour of nucleon and rho masses in the standard Edinburgh plot.

1. INTRODUCTION

There are well-known difficulties associated with making dynamical fermion lattice QCD calculations at light quark masses. There is the need however, to relate quantities calculated on the lattice with physical observables, hence results are required at physical quark masses. These two mutually exclusive restrictions on the field have motivated the necessity for extrapolation from the region in which calculations are able to be performed — that is, the region of unphysically heavy quarks — to lighter masses, including the physical quark masses. In this paper we discuss the construction and application of an extrapolation method for masses [1,2] that respects the correct chiral behaviour of QCD and also allows the extraction of other quantities [2,3]. This approach is not limited to the case of masses in dynamical fermion lattice QCD calculations. Other successes of this approach may be found, for example, in the extrapolation of baryon charge radii [4], magnetic moments [5], structure functions [6,7] and quenched QCD data [8].

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1.1. Goldstone Boson Loops

It is accepted that Goldstone Boson loops play an important role in all hadronic properties — their role is in one sense the basis of Chiral Perturbation Theory (χPT). Lattice QCD calculations, as an ab initio approach to calculating quantities in QCD, implicitly includes these loop contributions. It has become clear recently, with calculations appearing at lighter quark masses [9,10], that the naïve linear extrapolation methods are not reproducing the data. In particular in [10] it was stated

> "The existence of curvature [at small quark masses] is observed, necessitating a cubic Ansatz for extrapolation to the chiral limit."

The following section reviews how the inclusion of chiral physics allows reliable extrapolations of lattice QCD calculations [1,2]. Section 3 reports new results for the Edinburgh plot.

2. EXTRAPOLATION METHODS

In QCD chiral symmetry is dynamically broken, and the pion is almost a Goldstone boson. It plays a significant role in the self-energy contributions to the N and Δ, because of the strong coupling to the baryons. Chiral symmetry requires that, in the region where perturbations around light quarks makes sense, the mass of the nucleon has the form

$$m_N(m_\pi) = m_N^{(0)} + \alpha m_\pi^2 + \beta m_\pi^3 + \gamma m_\pi^4 \ln m_\pi + \dots , \qquad (1)$$

where $m_N^{(0)}$, α, β and γ are functions of the strong coupling constant. In particular the values of the coefficients of the non-analytic (in quark mass) terms — recall that $m_\pi^2 \propto m_q$ — are known exactly from χPT. However it is only recent results from the lattice that have indicated any need of higher order terms beyond that of a linear extrapolation in quark mass (or m_π^2).

2.1. Chirally Motivated Form

An attempt at having a chirally motivated form for extrapolating masses has been

$$m_N(m_\pi) = m_0 + \tilde{\alpha} m_\pi^2 + \tilde{\beta} m_\pi^3 , \qquad (2)$$

where m_0, $\tilde{\alpha}$ and $\tilde{\beta}$ are fit parameters. Naïvely this is a good choice. It reflects the known non-analyticity from χPT and still reproduces the lattice results. The problem with this method is associated with the choice of $\tilde{\beta}$. The value of the coefficient of the cubic term is known explicitly in χPT. So a functional form, motivated by chiral symmetry, should preserve the known value of $\tilde{\beta}$. Optimising $\tilde{\beta}$ via a best fit to existing lattice data provides -0.55 GeV^{-2}. However, the result from χPT is -5.6 GeV^{-2}. That the coefficient is so small is not surprising. The functional form attempts to reproduce the lattice data over a large range of m_π^2, where the data is predominantly linear — as can be seen in Fig. 1. However χPT is an expansion about the massless quark limit and would not be expected to be applicable (or even convergent) at such large quark masses.

2.2. Current Calculation

It has been found [1,2] that by retaining the contributions to the self-energy of the hadron mass that vary the most rapidly with m_π near the chiral limit, a successful extrapolation method may be formed. This methodology includes the most important non-analytic structure in the hadron mass near the chiral limit with *exactly* the correct coefficients. The pion mass dependence of the masses of the N, Δ and ρ are:

$$m_N = a_0 + a_2 m_\pi^2 + \sigma_{NN\pi}(\Lambda_N, m_\pi) + \sigma_{N\Delta\pi}(\Lambda_N, m_\pi) \qquad (3)$$

$$m_\Delta = b_0 + b_2 m_\pi^2 + \sigma_{\Delta\Delta\pi}(\Lambda_\Delta, m_\pi) + \sigma_{\Delta N\pi}(\Lambda_\Delta, m_\pi) \qquad (4)$$

$$m_\rho = c_0 + c_2 m_\pi^2 + \sigma_{\rho\omega\pi}(\Lambda_\rho, m_\pi) + \sigma_{\rho\pi\pi}(\Lambda_\rho, m_\pi) \qquad (5)$$

where σ_{ABC} indicates the contribution from the $A \to BC \to A$ self-energy process. The expressions for these self-energy contributions for the N and Δ may be found in [1]. The two significant processes for the ρ are the $\rho \to \omega\pi$ and $\rho \to \pi\pi$ self-energies and they are presented in [2].

An additional level of detail explicitly included in these extrapolation methods is the inclusion of the decay channels (in the case of the Δ the process $\Delta \to N\pi$). This process is not included in other methods, and yet is a vitally important and physically based consideration. However, because of the finite nature of the lattice, decays are not always possible. The finite periodic volume of the lattice restricts the available momenta to discrete values

$$k_\mu = \frac{2\pi n_\mu}{a L_\mu}, \quad \text{with} \quad -\frac{L_\mu}{2} < n_\mu \le \frac{L_\mu}{2} \qquad (6)$$

where L_μ and a are the lattice size and spacing in the μ direction, respectively.

Figure 1 indicates the expected behaviour of the masses of the N, Δ and ρ using Eqs. (3), (4) and (5), with the physical masses being 0.940, 1.173, 0.713 GeV respectively.[3] We also present an error analysis of the fitting for the particular case of the ρ meson in Fig. 2. The shaded region is bounded below by an increase of 1σ in the χ^2 per degree of freedom of the fit, and above by a physical constraint in our approach. It is clear that whilst the central value of the extrapolation gives an acceptable value for the physical mass, the uncertainties are large. A Gedanken experiment performed in [2] suggests that a ten-fold increase in the number of configurations at the lowest pion mass data point ($m_\pi^2 \sim 0.1$ GeV^2)

[3] The excellent agreement with the experimental mass of the nucleon is coincidental.

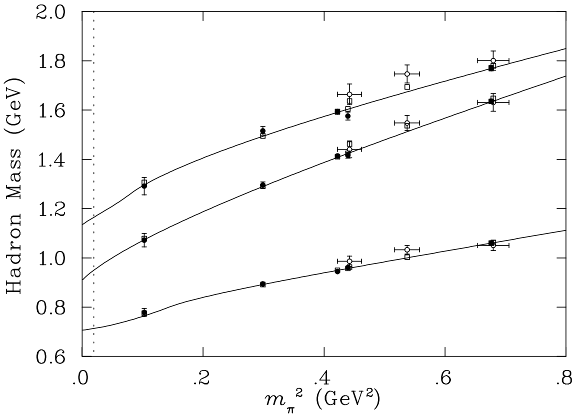

Figure 1. Two-flavour, dynamical fermion lattice QCD data for the Δ, N and vector meson (ρ) mass data from UKQCD [9] (open circles) and CP-PACS [10] (filled circles). The solid lines are the continuum limit, infinite volume predictions of Eqs. (4), (3) and (5). The squares (barely discernable from the data) are the predicted masses on a lattice of the same dimensions as the data at that pion mass.

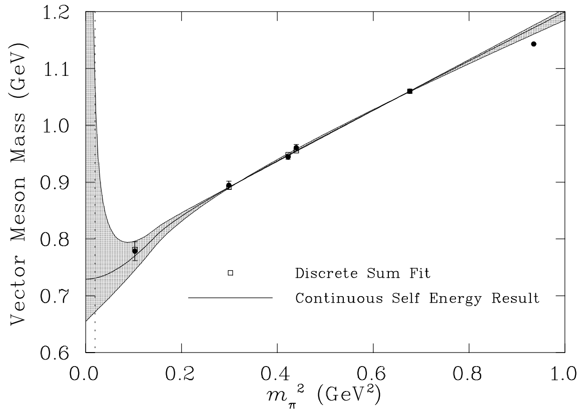

Figure 2. Analysis of the lattice data for the vector meson (ρ) mass calculated by CP-PACS [10] as a function of m_π^2. The shaded area is bounded below by a 1σ error bar. The upper bound is limited by a physical constraint discussed in [2].

would reduce the uncertainty in the extrapolated value to the 5% level.

3. OTHER QUANTITIES

The advantage of calculating the mass of the hadrons in the manner described above is that the form allows the direct extraction of other properties of the hadron that depend upon the quark mass dependence of the hadron mass.

3.1. The Sigma Commutator

The sigma commutator is a direct source of information about chiral symmetry breaking within QCD [11]. As such it is a quantity of considerable importance to extract from lattice QCD calculations. The form of the commutator is

$$\sigma_N = \bar{m}\langle N|\bar{u}u + \bar{d}d|N\rangle \quad (7)$$

$$= \bar{m}\frac{\partial m_N}{\partial \bar{m}}\,, \quad (8)$$

where $\bar{m}$ is the average mass of the *up* and *down* quarks.

σ_N is not directly accessible via experiment, however world data suggests a value of 45 ± 8 MeV [12]. Early attempts at evaluating Eq. (8) found results in the range 15 to 25 MeV, and the attention soon changed to evaluating the matrix element, Eq. (7), directly. In quenched calculations the results were in the 40–60 MeV range, but a two flavour dynamical fermion calculation by the SESAM collaboration [13] found a value of 18 ± 5 MeV. The difficulties associated with these approaches are two-fold. Firstly, the scale independent quantity of σ_N must be constructed from the renormalisation depended quantities $\bar{m}$ and $\langle N|\bar{u}u+\bar{d}d|N\rangle$. Additionally there still is the need to extrapolate the quantities to the physical pion mass.

Our recent work showed that provided the extrapolation method is under control the evaluation of σ_N at $m_\pi = 140$ MeV, is a straightforward calculation. The important advantage of this approach is that one need only work with renormalisation group invariant quantities.

We discussed previously how a chirally motivated form, Eq. (2), will not reproduce the lattice data if the coefficient of the m_π^3 term is the value required by χPT. However we also showed that allowing this coefficient to be a fit parameter results in a value that is wrong by almost an order of magnitude. This becomes even more significant in the case of the sigma commutator. The required derivative promotes this coefficient to greater significance *and* the sign of the terms acts to reduce the value of σ_N. However this is not an issue with the extrapolation forms discussed above. The sign and magnitude of the cubic term is exactly that predicted by χPT, but the effects are countered by higher order terms — resulting in a prediction for the value of σ_N that included the correct chiral physics. We find [3] that the value of the sigma commutator is approximately 45 MeV.

3.2. The J Parameter

This dimensionless parameter was proposed as a quantitative measure, independent of the need for extrapolation — an ideal lattice observable [14]. It has the form

$$J = m_\rho \left. \frac{dm_\rho}{dm_\pi^2} \right|_{m_\rho/m_\pi = 1.8} \tag{9}$$

$$\simeq m_{K^*} \frac{m_{K^*} - m_\rho}{m_K^2 - m_\pi^2}, \tag{10}$$

which, by substituting the experimental mass values, yields the value [14]

$J = 0.48(2)$,

In Fig. 3 we present the value of the J parameter as obtained from Eqs. (5) and (9). The detailed slope of the curve is parameter dependent, however the presence of the cusp is model independent. The cusp is a result of the two pion cut in the rho spectral function and has been ignored in previous attempts at evaluating the J parameter. We find a value for the J parameter of 45(7) in good agreement with the experimental value. We note, however, that if the point of evaluation corresponded to $m_\pi^2 \sim 0.15$ GeV^2 the J parameter would have been around 50% larger.

3.3. Edinburgh Plot

The baryon and meson masses on the lattice are all determined modulo the lattice spacing – a

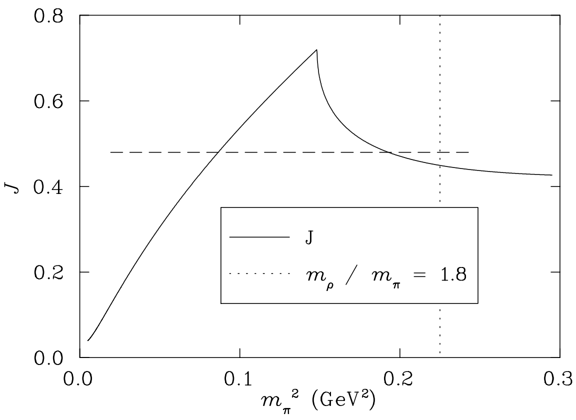

Figure 3. The solid curve is a plot of the value of the J-parameter as a function of m_π^2 obtained from Eq. (9) and the best fit to the lattice results. The vertical dotted line shows the point at which the J-parameter is evaluated ($m_\rho/m_\pi = 1.8$). The horizontal line displays the experimental value (0.48) plotted between the physical values of m_π^2 and m_K^2.

scale that must be determined from some piece of data external to the lattice. One method of removing this scale is by plotting a ratio of masses — the Edinburgh plot. In Fig. 4 we present a prediction for the infinite volume, continuum limit extrapolation of the lattice data previously presented. The two points known explicitly are indicated by open stars on the plot. The first known point is ratio of the physical masses of the π, ρ and N. The second point is the heavy quark limit, when the masses of the hadrons become proportional to the constituent quarks. The effect of the opening of the decay channel of the rho is visible at $m_\pi/m_\rho = 0.5$. The effects induced, and the expected behaviour on the finite sized lattice will be presented in a future work [15].

4. SUMMARY

The importance of including the correct chiral behaviour in extrapolation methods is becoming more important as dynamical lattice QCD re-

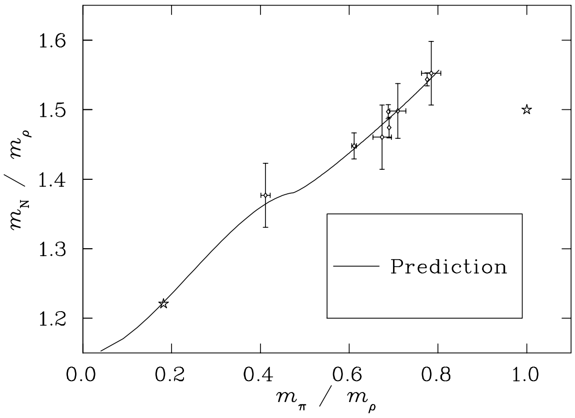

Figure 4. Edinburgh plot for CP-PACS (filled symbols) and UKQCD (open symbols) results. The stars represent the known limiting cases, at the physical and heavy quark limits respectively. The solid line is the infinite volume, continuum limit behaviour predicted by our functional forms for the extrapolation of the N and ρ masses.

sults appear at lighter quark masses. The successes of the approach outlined above include not only predictions for the physical masses of the hadrons investigated, but other quantities successfully reproduced. These other successes include the sigma commutator and the J parameter — both of which have been a thorn in the side of dynamical fermion calculations. It is through the inclusion of the dominant chiral physics, the recognition that decay channels are important, and the understanding of some of the finite size lattice artifacts that we have been able to successfully extrapolate the Edinburgh plot to the known physical limit.

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