Continuum Limit of Lattice QCD with Staggered Quarks in the Quenched Approximation — A Critical Role for the Chiral Extrapolation

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We calculate the light quark spectrum of lattice QCD in the quenched approximation using staggered quarks. We take the light quark mass, infinite volume, continuum limit. With non-linear chiral extrapolations, we find that the nucleon to ρ mass ratio is $m_N/m_\rho = 1.254 \pm 0.018 \pm 0.028$, where the errors are statistical and systematic (within the quenched approximation), respectively. Since the experimental value is 1.22, our results indicate that the error due to quenching is $\leq 5\%$.

12.38.Gc, 14.20.-c, 14.40.-n

The calculation of the light hadron spectrum is one of the main goals of lattice QCD. However, the computed hadron mass ratios have persistently been too large. This has been true for calculations done with dynamical fermions, or in the quenched approximation, and for both the Wilson and staggered methods of putting quarks on the lattice. In such calculations, one must use a finite-volume box and a non-zero lattice spacing. In addition, because of the iterative algorithms used to calculate the quark propagators, quark masses larger than those of the up and down quarks are necessary. Thus, before comparing with experiment, one must take the infinite volume, zero lattice spacing, and light quark limits to remove systematic errors. Our extensive series of calculations with staggered quarks in the quenched approximation provides good control over each of these extrapolations. Here we present a new analysis of the chiral extrapolation fully consistent with quenched chiral perturbation theory.

It is important to demonstrate that calculations with Wilson and staggered quarks have the same continuum limit. Butler et al. calculated the quenched Wilson quark spectrum using three lattice spacings. Their results had a statistical accuracy of 5-6%, and they claimed good agreement with the real world for a number of hadron mass ratios. However, there are concerns about how well they were able to control their extrapolations. Recently, the CP-PACS collaboration has presented preliminary results with Wilson quarks, using four values of the gauge coupling on large lattices.

In Table I, we list the coupling, volume and size of each or our ensembles of lattices. (Computational details are found in Ref.). We used five quark masses for each ensemble, each a factor of two different from the next heavier or lighter. To increase our statistics, we calculated propagators from every eighth time slice, so we have four to eight sets of hadron propagators per lattice (depending on $N_t$). These propagators are correlated, so they are blocked together for further analysis.

Now let us turn to the sources of systematic errors. The initial motivation for these calculations was to understand finite volume effects. We have carried out detailed studies at gauge coupling $g^2 = 5.7$ using lattices with spatial dimensions $N_s = 8, 12, 16, 20, 24$, with the same five quark masses on all five lattices. At $g^2 = 5.85$, we use three sizes, $N_s = 12, 20$ and 24. The last column of Table I contains the box size in fm based on a scale set by the ρ mass extrapolated to the physical quark mass. In each case, the smallest size is 1.8 fm, considerably smaller than the 2.7 fm size for $g^2 = 6.15$. We expect that in a small volume the mass will increase as the hadron becomes squeezed by the box, and that this effect increases for smaller quark masses. For the ρ there is very little evidence for finite size effects. Comparing the smallest and largest sizes for the three lightest quark masses, the largest difference is $2.5 \pm 1.3\%$ and the ρ is lighter on the smaller size. We expect somewhat larger finite size effects for the nucleon. For $g^2 = 5.85$ we find a $3.2 \pm 1.1\%$ effect for the lightest quark mass; however, at $5.7$ for the corresponding quark mass the effect is only $1.0 \pm 1.2\%$. For small box sizes, there is evidence that finite-size effects fall like $1/V$ where $V$ is the spatial lattice volume. For larger boxes, an exponential decay proportional to $\exp(-m_\rho L)$ is expected. By the former consideration, the finite size effect for our 2.7 fm $g^2 = 6.15$ lattice should be smaller by...
a factor of \((2.7/1.8)^3 \approx 3.4\). By the latter, there should be a decrease by a factor of \(\approx 5\). Thus, we expect finite size effects smaller than 1% for \(6/g^2 = 6.15\), and even smaller effects for the two largest volumes at \(6/g^2 = 5.7\) and 5.85.

The chiral extrapolation requires the most care and controls the final error. It is based on a small mass expansion, but since we cannot generate accurate results for small quark masses, we are forced to use intermediate and heavy quark masses. In this mass region the contribution of the higher order terms in the chiral expansion can be significant, and the extrapolation to the physical light quark masses has to be performed very carefully. Another complication arises from the quenched approximation. Quenched chiral perturbation theory \((Q\chi PT)\) differs from the ordinary chiral perturbation theory \((\chi PT)\) that applies to the real world.

Our lightest three masses cover a range of a factor of four, and cannot be fit to a linear function with even a marginally acceptable confidence level (CL). (The chiral fits are done using the full covariance matrix of the hadron masses for different quark masses.) We began by trying a dozen different fitting forms (Table I). The term proportional to \(m_q\) appears at tree-level (in both \(\chi PT\) and \(Q\chi PT\)) and is therefore expected to be the most important correction to the chiral limit for a “reasonable” range of masses. The other \(m_q\) dependent terms should be thought of as one-loop corrections: \(m_q^{3/2}, m_q^2\), and \(m_q^2 \log m_q\) are standard terms which appear in both \(\chi PT\) and \(Q\chi PT\); while the more singular (at \(m_q = 0\)) terms proportional to \(\sqrt{m_q}\) and \(m_q \log m_q\) arise only in \(Q\chi PT\), and are due to \(\eta'\) loops \([12]\). However, we reject fits 1, 2, 3, 4, and 10, which include an \(\sqrt{m_q}\) term, because the coefficient of \(\sqrt{m_q}\) found by the fits is opposite in sign to what is expected from \(Q\chi PT\). In Fig. 1, we show seven fits for the nucleon at \(6/g^2 = 6.15\) that have good CL. As can be seen in the inset, several fits (2, 3, 4, 10) decrease sharply at small quark mass. However, a \(\sqrt{m_q}\) term with the sign implied by \(Q\chi PT\) would cause a sharp increase.

In addition, due to flavor breaking, the \(\sqrt{m_q}\) term is not really appropriate to quenched staggered quarks. It is actually the flavor singlet pion that appears \([12]\) in \(Q\chi PT\), and its mass is not proportional to \(\sqrt{m_q}\) at finite lattice spacing. Thus, we should use instead a term proportional to the mass of the non-Goldstone pion, commonly denoted \(m_{\pi}\). Since \(Q\chi PT\) gives us only a rough idea of the values of the proportionality constants, we consider a range of values. In practice, we define, for fixed \(\lambda_1\) and \(\lambda_2\),

\[
m_N' \equiv (m_N + \lambda_1 m_{\pi}) \frac{m_N^{\text{phys}}}{m_N^{\text{phys}} + \lambda_1 m_{\pi}^{\text{phys}}} \tag{1}
\]

\[
m_{\rho}' \equiv (m_{\rho} + \lambda_2 m_{\pi}) \frac{m_{\rho}^{\text{phys}}}{m_{\rho}^{\text{phys}} + \lambda_2 m_{\pi}^{\text{phys}}} \tag{2}
\]

where “phys” stands for the physical values and the other quantities are values computed at given quark mass and lattice spacing. We then fit \(m_N'\) and \(m_{\rho}'\) to functions 8 and 12 (Table I) for various values of \(\lambda_1\) and \(\lambda_2\) obeying \(0.0 \leq \lambda_1 \leq \lambda_2 \leq 0.4\), which is the expected range of values from \(Q\chi PT\) \([12,14]\).

Table II contains the combined CL of these chiral fits for our five lattices with the weakest couplings and largest volumes: \(N_s = 32\) at \(6/g^2 = 6.15\), and \(N_s = 20\) and 24 at \(6/g^2 = 5.7\) and 5.85. Although many of these fits are marginally acceptable, none of the CL are very good. This may be due to the fact that \(Q\chi PT\) to order \(m_q^2\) would require all the terms that appear in either Fit 8 or 12; while we are limited to a maximum of 4 fit parameters since we have only 5 masses at our disposal. It is nevertheless encouraging that almost all the fit parameters are of the rough size (within a factor of 2) and sign predicted by \(Q\chi PT\) \([12]\). The exception is the \(m_{\pi}^{3/2}\) term in the \(\rho\) fits: its coefficient is more than an order of magnitude smaller than the size suggested in \([12]\). Such agreement is as good as could be expected, since the \(Q\chi PT\) predictions are currently based either on rather arbitrary guesses of parameters (e.g. the \(m_{\pi}^{3/2}\) case for the \(\rho\)) or on parameter estimates taken from real-world (i.e., not quenched) data and determined only up to large errors. As expected, the linear term in \(m_q\) is dominant; all other terms give small corrections except at the largest values of the quark mass. The fit parameters are relatively stable: As the fit (8 or 12) or \(\lambda\) values are changed, the parameters change by at most \(\pm 25\%\) from their average values, while the masses extrapolated to the chiral limit are considerably more stable (see Table IV). The range of results for the acceptable fits gives us an estimate of the chiral extrapolation error. All the other fit functions in Table II are either inconsistent with \(Q\chi PT\) or have very low CL: the highest of these is \(\approx 0.0001\).

The final extrapolation is in the lattice spacing \(a\). Although we expect \(O(a^2)\) errors in general for the staggered action, flavor symmetry breaking gives \(m_{\pi}^2 \approx Aa^2\) at \(m_q = 0\) \([15]\), which implies that \(m_{\pi}\) contributions to the nucleon and \(\rho\) could produce \(O(a)\) terms in \(m_N/m_{\rho}\). Since, however, we are attempting to remove the \(m_{\pi}\) dependence, we believe it is still reasonable to fit to the quadratic form \(C + B(m_{\rho})^2\) for our central values. In Fig. 2, we show the lattice spacing extrapolation based on chiral fit 8 with \(\lambda_1 = 0.0\) for the nucleon and fit 12 with \(\lambda_2 = 0.1\) for the \(\rho\), which give the highest CL. For the \(\pi\) chiral extrapolation, which is needed to determine the physical light quark mass, we use the form \(m_{\pi}^2 = am_q + bm_q^2 + cm_q^3 + dm_q \ln m_q\). When we keep only the three weakest couplings, the continuum extrapolation with these parameters has a good CL (0.74) and gives a result which is close to the overall average of the continuum extrapolations of all the chiral fits. For each of the two intermediate couplings, we plot the two largest
volumes, but only the largest volume was included in the fit to the $a$ dependence. Extrapolating to the continuum limit we get $1.251 \pm 0.018$.

To obtain our central value, we look at all (quadratic) continuum extrapolations of the three weakest couplings coming from any of the chiral fits in Table 11 with CL greater than 0.04. (The continuum extrapolations all have CL $> 0.34$.) Figure 8 shows the results of these extrapolations of $m_N/m_\rho$ as a function of the CL of the continuum extrapolation. After averaging over all fits in Fig. 8, we obtain $m_N/m_\rho = 1.254 \pm 0.018 \pm 0.022$, where the last error is the standard deviation over the fits, which we take as a combination of chiral extrapolation and continuum extrapolation errors. The result is rather insensitive to the cut on chiral CL: changing the cut to 0.005 or 0.06 (a cut greater than 0.06 would rule out all the $\rho$ fits in Table 11) changes the central value by 0.010 or 0.008, respectively.

To explore further the error in the continuum extrapolation, we then include the strongest coupling point and repeat the analysis. Averaging over all fits with chiral and continuum CL greater than 0.04 gives 1.248$\pm 0.016 \pm 0.008$. We then change the continuum extrapolation to include the higher power $(am_\rho)^4$, as well as $(am_\rho)^2$. By averaging as before, we obtain $1.266 \pm 0.020 \pm 0.021$.

Because the true values of $\lambda_{1,2}$ are not known, we cannot definitively subtract off the $m_{\pi^2}$ dependence. Therefore, there may remain a small $O(a)$ term in $m_N/m_\rho$. To study this effect, we add a linear term in $a$ to our central continuum extrapolation fits above. (These are now constrained fits.) The coefficient of the linear term is always consistent with 0, with the errors giving a bound on its magnitude of the size expected from a small residual $m_{\pi^2}$ contribution. Averaging the extrapolated values of $m_N/m_\rho$ gives $1.269 \pm 0.096 \pm 0.016$.

These considerations lead us to include additional errors of 0.015 (the effect changing the continuum extrapolation) and 0.010 (the effect of changing the cutoff on the CL). Combining them in quadrature with the 0.022 determined above, gives a total systematic error due to chiral and continuum extrapolations of 0.028.

In summary, the chiral extrapolation is the most delicate issue in our computation of the nucleon to the $\rho$ mass ratio. The simple linear chiral extrapolation is ruled out. Our results are reasonably well described by fits motivated by $Q\chi PT$. However, the CL of such fits is a slowly varying function of the parameters $\lambda_1$ and $\lambda_2$, which therefore are not determined in our procedure. Instead, we average over reasonable ranges of these parameters. Fortunately, the continuum values of $m_N/m_\rho$ produced are not strongly dependent on the parameters. Taking into account the variance over the fits, we obtain $m_N/m_\rho = 1.254 \pm 0.018 \pm 0.028$. Comparison with the observed value of 1.22 indicates that the effects of quenching are less than about 5% at the 1 $\sigma$ level.

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FIG. 1. The nucleon mass vs. quark mass with $6/g^2 = 6.15$. We plot fits 12, 8, 9, 10, 3, 4 and 2 (listed in order of decreasing chiral limit), all of which have CL greater than 0.45.

FIG. 2. $m_N/m_\rho$ at the physical quark mass vs. $(am_\rho)^2$. The points come from fit 8 for the nucleon and 12 for the $\rho$, with $\lambda_1 = 0.0$, $\lambda_2 = 0.1$. The horizontal line indicates the physical value. The solid straight line shows a linear (in $(am_\rho)^2$) extrapolation that includes only the three smallest lattice spacings; the dot-dashed straight line, all four lattice spacings. The curve is a higher order fit to all four spacings. The extrapolated values near $am_\rho = 0$ have been spread horizontally for clarity.

FIG. 3. $m_N'/m_\rho'$ extrapolated to $a = 0$ vs. the CL of the fit used for this extrapolation. The points represent different choices for the chiral fits of the $\rho$ and nucleon and different values of the parameters $\lambda_1$ and $\lambda_2$. All extrapolations in $a$ are quadratic and keep only the three weakest couplings. The combined CL over these couplings of each chiral fit included here is greater than 0.04.

TABLE I. Lattices used for spectrum calculation

| $6/g^2$ | size          | #  | $am_q$ | $aN_s$ (fm) |
|---------|---------------|----|--------|-------------|
| 5.54    | $16^3 \times 32$ | 205 | 0.02–0.32 | 4.96        |
| 5.7     | $8^3 \times 48$   | 605 | 0.01–0.16 | 1.83        |
| 5.7     | $12^3 \times 48$  | 405 | 0.01–0.16 | 2.75        |
| 5.7     | $16^3 \times 48$  | 405 | 0.01–0.16 | 3.66        |
| 5.7     | $20^3 \times 48$  | 205 | 0.01–0.16 | 4.58        |
| 5.7     | $24^3 \times 48$  | 199 | 0.01–0.16 | 5.49        |
| 5.85    | $12^3 \times 48$  | 205 | 0.01–0.16 | 1.76        |
| 5.85    | $20^3 \times 48$  | 205 | 0.01–0.16 | 2.93        |
| 5.85    | $24^3 \times 48$  | 200 | 0.01–0.16 | 3.52        |
| 6.15    | $32^3 \times 64$ | 115 | 0.005–0.08 | 2.65        |

TABLE II. Our fitting functions

| Fit | Function                      |
|-----|-------------------------------|
| 1   | $M + am_q^{3/2}$              |
| 2   | $M + am_q^{3/2} + bm_q$       |
| 3   | $M + am_q^{3/2} + bm_q + cm_q^{3/2}$ |
| 4   | $M + am_q^{3/2} + bm_q + cm_q^2$ |
| 5   | $M + am_q$                    |
| 6   | $M + am_q + bm_q^{3/2}$       |
| 7   | $M + am_q + bm_q^2$           |
| 8   | $M + am_q + bm_q^{3/2} + cm_q^2$ |
| 9   | $M + am_q + bm_q + cm_q \log m_q$ |
| 10  | $M + am_q^{3/2} + bm_q + cm_q \log m_q$ |
| 11  | $M + am_q + bm_q^2 \log m_q$  |
| 12  | $M + am_q + bm_q^2 \log m_q + cm_q \log m_q$ |
### TABLE III. Combined CL of chiral fits

| Fit  | $\lambda = 0.0$ | $\lambda = 0.1$ | $\lambda = 0.2$ | $\lambda = 0.3$ | $\lambda = 0.4$ |
|------|----------------|----------------|----------------|----------------|----------------|
|      | Nucleon Jackknife fits |          |          |          |          |
| 8    | 0.186          | 0.140        | 0.103        | 0.075        | 0.054         |
| 12   | 0.086          | 0.050        | 0.028        | 0.015        | 0.008         |
|      | Rho Jackknife fits |        |          |          |          |
| 8    | 0.048          | 0.041        | 0.035        | 0.031        | 0.028         |
| 12   | 0.059          | 0.060        | 0.054        | 0.046        | 0.037         |

### TABLE IV. Dependence of nucleon and $\rho$ masses on chiral fit at $6/g^2 = 6.15$. $\tilde{m}_N \equiv m_N + \lambda_1 m_{\pi^2}$ extrapolated to $m_u = 0$. $\langle m_N \rangle \equiv \tilde{m}_N - \lambda_1 m_{\pi^2}$, where $m_{\pi^2}$ is separately extrapolated to $m_u = 0$ with the same fit. Similarly for $\rho$.

| Fit  | $\lambda_1 = 0.0$ | $\lambda_1 = 0.2$ | $\lambda_1 = 0.4$ |
|------|-----------------|-----------------|-----------------|
| $\tilde{m}_N$ | 8 | 0.404(6) | 0.427(5) | 0.450(5) |
| $\langle m_N \rangle$ | 8 | 0.404(6) | 0.407(5) | 0.410(5) |
| $\tilde{m}_N$ | 12 | 0.409(5) | 0.433(5) | 0.457(5) |
| $\langle m_N \rangle$ | 12 | 0.409(5) | 0.413(5) | 0.417(5) |
| $\tilde{m}_\rho$ | 8 | 0.320(4) | 0.343(4) | 0.366(4) |
| $\langle m_\rho \rangle$ | 8 | 0.320(4) | 0.323(4) | 0.326(4) |
| $\tilde{m}_\rho$ | 12 | 0.319(3) | 0.343(3) | 0.367(3) |
| $\langle m_\rho \rangle$ | 12 | 0.319(3) | 0.323(3) | 0.327(3) |