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 Kogut-Susskind quarks. By combining results for different lattice spacings, several volumes and five quark masses, we are able to take the light quark mass, infinite volume, continuum limit. When we use non-linear chiral extrapolations, we find that the nucleon to rho 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. This should be compared with the experimental value of 1.22. Our results indicate that the error due to quenching is less than about 5%.

The calculation of the light hadron spectrum is one of the main goals of lattice QCD. There have been many attempts to do so; however, one persistent problem has been an excessively large computed value for the nucleon to rho mass ratio. This has been true for calculations done with dynamical fermions, or in the quenched approximation [1], and for both the Wilson and Kogut-Susskind (staggered) methods of putting quarks on the lattice. [2]. To carry out a lattice calculation, it is necessary to use a finite volume box and a non-zero lattice spacing. In addition, because of the iterative algorithms used to calculate the quark propagators, it has been necessary to use quark masses larger than those of the up and down quarks. Thus, before attempting to compare the results of lattice calculations with the observed spectrum, one must take the infinite volume, zero lattice spacing, and light quark limits to remove systematic errors. We have carried out an extensive series of calculations with Kogut-Susskind quarks in the quenched approximation that provides us with good control over each of these extrapolations [3,4].

It is important to demonstrate that calculations with Wilson and staggered quarks have the same continuum limit. Butler *et al.* [5] calculated the spectrum with Wilson quarks in the quenched approximation. They used three lattice spacings, and extrapolated as indicated above. 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 some questions about how well they were able to control their extrapolations [6,4]. Quite recently, the CP-PACS collaboration has presented preliminary results from a more extensive Wilson quark calculation that should have good control of the extrapolations. This calculation is being carried out with four values of the gauge coupling on lattices with very large volumes. [7].

An additional motivation to improve the accuracy of calculations with the quenched approximation is recent work on improved actions [8]. Most such calculations are done within this approximation, so it is valuable to know what result they should approach in the $a \to 0$ limit.

Our quenched calculation with staggered quarks uses four lattice spacings. At two of the lattice spacings, we have multiple volumes to demonstrate control of finite-size effects [9]. Although we are able to use smaller quark masses than have been used for the Wilson quarks, we find that the mass extrapolation requires the most care. In Ref. [5], as in many spectrum calculations, a linear fit to the lightest three quark masses was used. We find deviations from linearity for our three lightest masses. More recent calculations with Wilson quarks have considered nonlinear chiral fits [10,6,7].

In Table I, we list the coupling, volume and size of each ensemble of lattices used in our calculation. The lattices were generated using a combination of overrelaxed and pseudo-heat bath sweeps in the ratio of 4 to 1, respectively. Each lattice is separated from the previous one by 200 combination sweeps, or a total of 800 overrelaxed and 200 pseudo-heat bath sweeps.

In order to calculate the hadron spectrum on the lattices, we used five quark masses for each ensemble, each a factor of two different from the next heavier or lighter.

(See the last column of Table I for the ranges.) We fix our lattices to Coulomb gauge and use wall sources. For a given source time, each site with all spatial coordinates even is set equal to one, all other sites are set to zero. 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 clearly correlated, so we block all those from each lattice 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. [9]. We have carried out detailed studies at gauge coupling $6/g^2 = 5.7$ using lattices with spatial dimensions $N_s = 8, 12, 16, 20, 24$, using the same five quark masses on all five lattices. At $6/g^2 = 5.85$, 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 rho 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 $6/g^2 = 6.15$. 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 rho is lighter on the smaller size. We expect somewhat larger finite size effects for the nucleon. For $6/g^2 = 5.85$ 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 $1/V$ [11], where V is the spatial lattice volume. For larger boxes, an eponential decay proportional to $\exp(-m_\pi L)$ is expected [12]. By the former consideration, the finite size effect for our 2.7 fm $6/g^2 = 6.15$ 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 ≈ 5. Thus, we expect finite size effects smaller than 1and even smaller effects for the two largest volumes at $\beta = 5.7$ and 5.85. More details regarding finite size effects for both Kogut-Susskind and Wilson quarks may be found in Ref. [2].

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. If our masses have large errors, or we fit over a sufficiently small range of quark mass, we may be able to fit the results to the simplest linear chiral form with good confidence level. Such extrapolations, however, may have little to do with the true low quark mass limit. Another complication arises from the quenched approximation. It is known that quenched chiral perturbation theory ($Q\chi PT$) [13] differs from the ordinary chiral perturbation theory (χPT) that applies to the real world.

Our lightest three masses cover a range of a factor of four, and, as indicated previously, cannot be fit to a linear function with even a marginally acceptable confidence level. (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 II). The term proportional to m_q appears at tree-level (in both χPT 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 χPT and $Q\chi PT$; while the more singular (at $m_q = 0$) terms proportional to $m_q^{1/2}$ and $m_q \log m_q$ arise only in $Q\chi PT$, and are due to η' loops [14]. However, we reject fits 1,2,3,4 and 10, which include an $m_q^{1/2}$ term, because the coefficient of $m_q^{1/2}$ 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 confidence level. As can be seen in the inset, several fits (2, 3, 4, 10) decrease sharply at small quark mass. However, $Q\chi PT$ predicts a sharp increase.

In addition, due to flavor breaking, the $m_q^{1/2}$ term is not really appropriate to quenched staggered fermions. It is actually the flavor singlet pion which appears [16] in $Q\chi PT$, and its mass is not proportional to $m_q^{1/2}$ at finite lattice spacing. Thus, we should use instead a term proportional to the mass of the non-Goldstone pion, commonly denoted m_{π_2}. 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 λ_1 and λ_2,

$$m'_N \equiv (m_N + \lambda_1 m_{\pi_2}) \frac{m_N^{\rm phys}}{m_N^{\rm phys} + \lambda_1 m_\pi^{\rm phys}} \qquad (1)$$

$$m'_\rho \equiv (m_\rho + \lambda_2 m_{\pi_2}) \frac{m_\rho^{\rm phys}}{m_\rho^{\rm phys} + \lambda_2 m_\pi^{\rm phys}}, \qquad (2)$$

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'_ρ to functions 8 and 12 (Table II) for various values of λ_1 and λ_2 obeying $0.0 \le \lambda_1 \le \lambda_2 \le 0.4$, which is the expected range of values from $Q\chi PT$ [14,15].

Table III contains the combined confidence level 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 confidence levels 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 enouraging that almost all the fit parameters are of the rough size (within a factor of 2) and sign predicted by $Q\chi PT$ [14,15]. The exception is the $m_q^{3/2}$ term in the ρ fits: its coefficient is more than an order of magnitude smaller than the size suggested in Ref. [14]. Such agreement is as good as could be expected, since the $Q\chi PT$ predictions are currently based either on rather arbitrary guesses of of parameters (*e.g.* in the ρ $m_q^{3/2}$ case) 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 λ 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 ??). 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 confidence levels: the highest of these is ~ 0.0001.

The final extrapolation is in the lattice spacing a. Although we expect $O(a^2)$ errors in general for the Kogut-Susskind action, flavor symmetry breaking gives $m_{\pi_2}^2 \approx Aa^2$ at $m_q = 0$ [17], which implies that m_{π_2} contributions to the nucleon and ρ could produce $O(a)$ terms in m_N/m_ρ. Since, however, we are attempting to *remove* the m_{π_2} dependence, we believe it is still reasonable to fit to the quadratic form $C + B(am_\rho)^2$ 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 ρ, which give the highest confidence levels in Table III. When we keep only the three weakest couplings (*i.e.*, omitting $\beta = 5.54$), the continuum extrapolation with these parameters has a good confidence level (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. A horizontal line gives the physical value of m_N/m_ρ. Extrapolating to the continuum limit we get 1.251 ± 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 III with confidence levels greater than 0.04. (The worst confidence level of the continuum extrapolation with these fits is 0.34). Fig. 3, shows the results of these extrapolations of m'_N/m'_ρ as a function of the confidence level of the continuum extrapolation. After averaging over all fits in Fig. 3, 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 confidence level: changing the cut to 0.005 or 0.06 (a cut greater than 0.06 would rule out all the ρ fits in Table III) 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 confidence levels 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_{π_2} dependence. Therefore, there may remain a small $O(a)$ term in m'_N/m'_ρ. To study this effect, we add a linear term in a to our central continuum exptrapolation fits above. (These are now contrained 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_{π_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 of including the strongest coupling point) and 0.010 (the effect of changing the cutoff on the confidence level). Combining them in quadrature with the 0.022 determined above, gives a total systematic error due to chiral and continuum extrapolations of 0.028.

To summarize, we have made a detailed study of the light quark spectrum in quenched QCD with Kogut-Susskind quarks. Concentrating on the long standing problem of the nucleon to the ρ mass ratio, we find that the chiral extrapolation is the most delicate issue. The simple linear chiral extrapolation is ruled out. Our results are reasonably well described by fits motivated by $Q\chi PT$. However the confidence levels of such fits are a slowly varying function of the parameters λ_1 and λ_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_ρ 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 σ level.

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FIG. 1. The nucleon mass *vs.* quark mass with $6/g^2 = 6.15$. Fits 2, 3, 4, 8, 9, 10 and 12, which all have confidence level > 0.45 are plotted.

FIG. 2. m_N/m_ρ at the physical quark mass *vs.* $(am_\rho)^2$. The individual points come from chiral fit 8 for the nucleon and 12 for the ρ, with the choice $\lambda_1 = 0.0$, $\lambda_2 = 0.1$. The horizontal line is drawn at the physical value. The solid straight line shows a linear (in $(am_\rho)^2$) extrapolation that only includes the three smallest lattice spacings. The dot-dashed straight line shows a linear extrapolation including 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 to avoid overlap, but they all represent extrapolations to $a = 0$.

FIG. 3. m'_N/m'_ρ extrapolated to $a = 0$ *vs.* the confidence level of the fit used for this extrapolation. Different points represent different choices for the chiral fits of the ρ and nucleon and different values of the parameters λ_1 and λ_2, as explained in the text. All extrapolations in a are quadratic and keep only the three weakest couplings. The combined confidence level over these couplings of each chiral fit included here is greater than 0.04.

TABLE I. Lattices used for quenched Kogut-Susskind calculations

$6/g^2$	size	#	am_q	aN_s (fm)
5.54	$16^3 \times 32$	200	0.02–0.32	4.96
5.7	$8^3 \times 48$	600	0.01–0.16	1.83
5.7	$12^3 \times 48$	400	0.01–0.16	2.75
5.7	$16^3 \times 48$	400	0.01–0.16	3.66
5.7	$20^3 \times 48$	200	0.01–0.16	4.58
5.7	$24^3 \times 48$	200	0.01–0.16	5.49
5.85	$12^3 \times 48$	200	0.01–0.16	1.76
5.85	$20^3 \times 48$	200	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 1:	$M + am_q^{1/2}$
Fit 2:	$M + am_q^{1/2} + bm_q$
Fit 3:	$M + am_q^{1/2} + bm_q + cm_q^{3/2}$
Fit 4:	$M + am_q^{1/2} + bm_q + cm_q^2$
Fit 5:	$M + am_q$
Fit 6:	$M + am_q + bm_q^{3/2}$
Fit 7:	$M + am_q + bm_q^2$
Fit 8:	$M + am_q + bm_q^{3/2} + cm_q^2$
Fit 9:	$M + am_q + bm_q \log m_q$
Fit 10:	$M + am_q^{1/2} + bm_q + cm_q \log m_q$
Fit 11:	$M + am_q + bm_q^2 \log m_q$
Fit 12:	$M + am_q + bm_q^2 + cm_q^2 \log m_q$

TABLE III. Combined confidence levels of chiral fit

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