Hadron Mass Predictions of the Valence Approximation to Lattice QCD

F. Butler, H. Chen, J. Sexton,[a] A. Vaccarino, and D. Weingarten
IBM Watson Research Center, P.O. Box 218, Yorktown Heights, New York 10598
(Received 22 December 1992)

We evaluate the infinite-volume, continuum limits of eight hadron mass ratios predicted by lattice QCD with Wilson quarks in the valence (quenched) approximation. Each predicted ratio differs from the corresponding observed value by less than 6%.

PACS numbers: 12.38.Gc, 14.20.−c, 14.40.−n

A key goal of the lattice formulation of QCD is to reproduce the masses of the low-lying baryons and mesons. Lattice QCD mass predictions for the real world are supposed to be obtained from masses calculated with finite lattice spacing and finite lattice volume by taking the limits of zero spacing and infinite volume. In addition, since the algorithms used for hadron mass calculations become progressively slower for small quark masses, results are presently found with quark masses much larger than the expected values of the up and down quark masses. Predictions for the masses of hadrons containing up and down quarks then require a further extrapolation to small quark mass. We report here mass predictions combining all three extrapolations for Wilson quarks in the valence (quenched) approximation. This approximation may be viewed as replacing the momentum and frequency dependent color dielectric constant arising from quark-antiquark vacuum polarization with its zero-momentum, zero-frequency limit and might be expected to be fairly reliable for low-lying baryon and meson masses [1].

To our knowledge there have been no previous systematic attempts to extrapolate hadron masses to physical quark mass, zero lattice spacing, and infinite volume. For a review of lattice QCD mass calculations see Ref. [2].

Our main result consists of a prediction of eight different hadron mass ratios. Each of the predicted ratios differs from experiment by less than 6%. In each case, the error is less than a factor of 1.6 multiplied by the corresponding statistical uncertainty. We believe it is reasonable to take these results as quantitative confirmation of the mass predictions both of QCD and of the valence approximation. It seems unlikely to us that the valence approximation would agree with experiment for eight different mass ratios yet differ significantly from QCD's predictions including the full effect of quark-antiquark vacuum polarization.

Following Refs. [3, 4], we also determine the continuum (modified minimal subtraction) coupling constant, $g^{(0)}_{\overline{\rm MS}}$, from the lattice coupling constant, $g_{\rm lat}$, and from $g^{(0)}_{\overline{\rm MS}}$ determine $\Lambda^{(0)}_{\overline{\rm MS}}$. Two independent calculations of $\Lambda^{(0)}_{\overline{\rm MS}}$, done by rather different methods [3, 5] lie within the 4% statistical uncertainty of our continuum, infinite-volume result for $\Lambda^{(0)}_{\overline{\rm MS}}$. The values we obtain for the rho mass at finite lattice spacing, measured in units of inverse lattice spacing, depend on $g^{(0)}_{\overline{\rm MS}}$ and $\Lambda^{(0)}_{\overline{\rm MS}}$ as predicted by asymptotic scaling. This result tends to support the reliability of our extrapolation of masses to the continuum limit.

In addition to comparing the valence approximation to QCD with experiment, a goal of the present work is to develop technology which might be useful in extrapolating results of the full theory to physical quark mass, infinite volume, and zero lattice spacing.

The calculations described here were done on the GF11 parallel computer at IBM Research Center [6] and took approximately 1 yr to complete. GF11 was used in configurations ranging from 384 to 480 processors, with sustained speeds ranging from 5 Gflops to 7 Gflops. With the present set of improved algorithms and 480 processors, these calculations could be repeated in less than 4 months.

Table I lists the lattice sizes and parameter values for which hadron propagators were evaluated. We chose periodic boundary conditions in all directions for both gauge fields and quark fields. Gauge configuations were generated using a version of the Cabbibo-Marinari-Okawa algorithm, with the number of sweeps skipped between configurations and total count of configurations as given in the table. A variety of correlation tests showed all of the configurations on which propagators were evaluated were statistically independent.

For the $8^3 \times 32$ lattice at β of 5.7 we used point sources and sinks in the quark propagators. For all other lattices and β, each gauge configuration was transformed to lattice Coulomb gauge and quark propagators were then found for Gaussian extended sources and for point sinks and four different sizes of Gaussian sinks [7]. The mean squared radius of the Gaussian source in all cases was

TABLE I. Configurations analyzed.

Lattice	β	k	Skip	Count
$8^3 \times 32$	5.7	0.1400–0.1650	1000	2349
$16^3 \times 32$	5.7	0.1400–0.1550	2000	47
		0.1600–0.1675	2000	219
$24^3 \times 32$	5.7	0.1600–0.1675	4000	92
$24^3 \times 36$	5.93	0.1543–0.1581	4000	217
$30 \times 32^2 \times 40$	6.17	0.1500–0.1532	6000	219

6, in lattice units. The mean squared radii of the Gaussian sinks ranged from 1.5 to 24, in lattice units. On the lattice $24^3 \times 32$ at β of 5.7, eight independent Gaussian sources were placed on the source hyperplane, each multiplied by a random cube root of 1 to cancel cross terms between the propagation of different sources for both baryon and meson propagators.

Quark propagators were constructed using the conjugate gradient algorithm for the $8^3 \times 32$ lattice at β of 5.7, using a red-black preconditioned conjugate gradient for the other lattices at β of 5.7 and 5.93, and using a red-black preconditioned minimum residual algorithm at β of 6.17 [8]. At the largest hopping constant values at β of 5.7 and 5.93, preconditioning the conjugate gradient algorithm increased its speed by a factor of 3, and at the largest hopping constant values at β of 6.17, the change from conjugate gradient to the minimum residual algorithm yielded an additional factor of 2 in speed. The convergence criterion used in all cases was equivalent to the requirement that effective pion, rho, nucleon, and delta masses evaluated between successive pairs of time slices must be within 0.2% of their values obtained on propagators run to machine precision.

Hadron masses were determined by fits to hadron propagators constructed from the quark propagators. The pion mass for all values of the hopping constant k, and the rho, nucleon, and delta masses for all but the three largest values of k at each β, were obtained from the propagators for a point sink. At the largest three k values, the rho, nucleon, and delta baryon masses were found by simultaneously fitting a single mass value to the propagators for a point sink and for Gaussian sinks with mean squared radius of 1.5 and 6. The statistical errors for all fits were determined by the bootstrap method [9]. A more detailed discussion of our fits and error analysis will be given elsewhere [10].

Comparing hadron masses in lattice units between the $8^3 \times 32$ and $16^3 \times 32$ lattices at β of 5.7 for k up to 0.1650 showed no statistically significant differences. Comparing $16^3 \times 32$ and $24^3 \times 32$ for k up to 0.1675 showed no statistically significant differences in the pion mass. For the rho, nucleon, and delta, marginally significant differences were found at the largest k. Percentage changes in mass going from $16^3 \times 32$ to $24^3 \times 32$ are given in Table II. Although some of the changes shown in Table II take smaller values if we use different procedures to determine hadron masses from hadron propagators, none become larger [10]. Thus a conservative interpretation of the changes in Table II is to view them primarily as upper bounds on volume dependence. It appears quite likely that for the range of k, β, and lattice volume we have examined, the errors in valence approximation hadron masses due to calculation in a finite volume L^3 are bounded by an expression of the form $Ce^{-L/R}$, with a coefficient R of the order of the radius of a hadron's wave function. At β of 5.7 for the k we considered, R is thus typically 3 lattice units. We therefore expect that the differences between masses on a 16^3 volume and those on a 24^3 volume are nearly equal to the differences between 16^3 and true infinite volume limiting values.

TABLE II. Changes in mass from a lattice $16^3 \times 32$ to a lattice $24^3 \times 32$ at β of 5.7.

Particle	k	Change
Pion	All	$< 1.2\pm1.6\%$
Rho	0.1675	$-3.4\pm1.4\%$
Nucleon	0.16625	$-4.4\pm1.7\%$
	0.1675	$-4.6\pm2.2\%$
Delta	0.1675	$-4.7\pm2.6\%$

At the largest k on each lattice, except $8^3 \times 32$, the ratio m_π/m_ρ is close to 0.5. For the lattice $8^3 \times 32$, this ratio is 0.691. These values of m_π/m_ρ are significantly above the experimentally observed value of 0.179 for charge averaged m_π and m_ρ. To produce mass predictions for hadrons containing only light quarks our data has to be extrapolated to larger k or, equivalently, to smaller quark mass. We did not calculate hadron masses directly at larger k both because the algorithms we used to find quark propagators became too slow and because the statistical errors we found in trial calculations became too large.

For each lattice except $8^3 \times 32$, we extrapolated hadron mass values down to small quark mass. To do this we first determined the $k_{\rm crit}$ at which m_π becomes 0. As expected from a naive application of PCAC, $(m_\pi a)^2$ turned out to be roughly a linear function of $1/k$ over the entire range of k considered on each lattice, and for the three largest k on each lattice, $(m_\pi a)^2$ fit a linear function of $1/k$ quite well. From these fits we then found $k_{\rm crit}$ for each lattice and β. Defining the quark mass in lattice units, $m_q a$, to be $1/2k - 1/2k_{\rm crit}$, we found $m_\rho a$, $m_N a$, and $m_\Delta a$ to be roughly linear functions of $m_q a$ over the entire range of k considered on each lattice and quite close to linear functions at the three smallest m_q (corresponding to the three largest k). Figure 1 shows m_π^2, m_ρ, m_N, and m_Δ, for the lattice $30 \times 32^2 \times 40$ at β of 6.17, as functions of m_q. The lines in Fig. 1 are fits to each data set at the three smallest values of m_q. For convenience, we show all hadron masses in units of the physical rho mass, $m_\rho(m_n)$, given by m_ρ evaluated at the "normal" quark mass m_n which produces the physical value of m_π/m_ρ. The quark mass m_q in Fig. 1 is shown in units of the strange quark mass m_s, the determination of which will be discussed below. The fits shown in Fig. 1 appear to be reasonably good and provide, we believe, a reliable method for extrapolating hadron masses down to light quark masses. Fits comparable to those shown were obtained for the nucleon, rho, and delta baryon on all the lattices we considered except $8^3 \times 32$.

Using a version of the Gell-Mann-Okubo mass formula, the accuracy of linear extrapolation in quark mass can

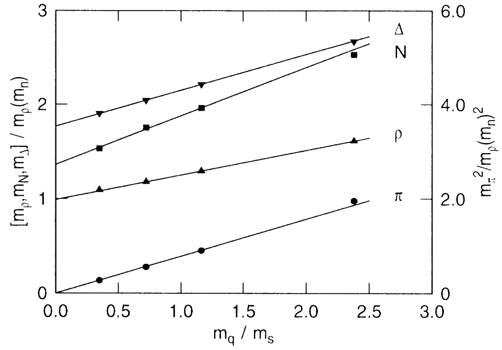

FIG. 1. For a $30 \times 32^2 \times 40$ lattice at β of 6.17, m_π^2, m_ρ, m_N, and m_Δ, in units of the physical rho mass $m_\rho(m_n)$, as functions of the quark mass m_q, in units of the strange quark mass m_s. The symbol at each point is larger than the error bars.

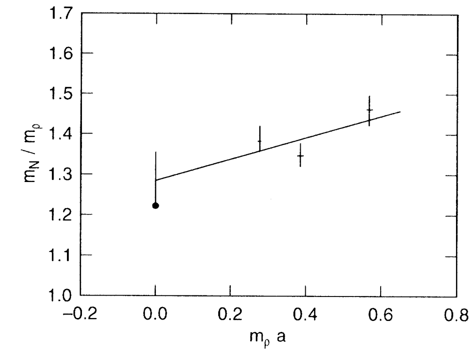

FIG. 2. m_N/m_ρ as a function of the lattice spacing a, in units of $1/m_\rho$. The straight line is an extraploation to zero lattice spacing, the error bar at zero lattice spacing is the uncertainty in the extrapolated ratio, and the point at zero lattice spacing is the observed value.

be checked with observed hadron masses. For a rho composed of a quark with mass m_1 and an antiquark with mass m_2, Fig. 1 suggests $m_\rho = \alpha_1 m_1 + \alpha_2 m_2 + \beta$. Charge conjugation invariance then gives $\alpha_1 = \alpha_2$. It follows that the k star, which is a rho with $m_1 = m_s$ and $m_2 = m_n$, will have the same mass as a rho composed of a single type of quark with $m_1 = m_2 = (m_s + m_n)/2$. In the valence approximation the phi is a rho with $m_1 = m_2 = m_s$. The linear relation $m_\rho = \alpha(m_1 + m_2) + \beta$ then permits the rho mass to be extrapolated from the masses of k star and phi. The extrapolated rho mass obtained from observed k star and phi masses lies below the observed rho mass by 0.53%. Similar extrapolations can be made to determine the nucleon mass from the observed masses of its strange partners and to determine the delta baryon mass from its strange partners. The extrapolated nucleon mass is larger than experiment by 1.38%, and the extrapolated delta baryon mass is large by 0.81%.

The relations discussed in the preceding paragraph can also be used to determine the masses of hadrons composed of both strange and normal quarks from the masses we have calculated for hadrons composed of a single species of heavy quark. Fitting the kaon to the pion mass at a quark mass of $(m_s + m_n)/2$ gives the value for m_s mentioned above. With m_s and m_n thus determined, the ratios of eight different hadron mass combinations to the physical rho mass follow from our data with no additional free parameters.

These ratios we extrapolated to zero lattice spacing with the physical lattice volume nearly held fixed. For Wilson fermions the leading lattice spacing dependence in mass ratios is expected to be linear in a. Figure 2 shows a linear fit of our data for m_N/m_ρ to the rho mass, at physical quark mass, measured in lattice units, $m_\rho a$. The horizontal axis may also be interpreted as the lattice spacing a measured in units of $1/m_\rho$. The vertical bar at $m_\rho a$ of 0 is the extrapolated prediction's uncertainty, determined by the bootstrap method. The dot at $m_\rho a$ of 0 is the experimental value of m_N/m_ρ. The three data points in Fig. 2 are for the lattices $16^3 \times 32$, $24^3 \times 36$, and $30 \times 32^2 \times 40$. The values of β for these lattices were chosen so that the physical volume in each case is nearly the same. For lattice period L, the quantity $m_\rho L$ is, respectively, 9.08 ± 0.13, 9.24 ± 0.19, and, averaged over three directions, 8.67 ± 0.12.

The continuum ratios we found in finite volume were then extrapolated to infinite volume. This was done by using the differences between mass ratios found on the lattice $16^3 \times 32$, at β of 5.7, and mass ratios found on the lattice $24^3 \times 32$, at β of 5.7, as finite lattice spacing approximations to the differences between continuum mass ratios in a box with period having $m_\rho L$ of 9 and continuum mass ratios in infinite volume. The error in this procedure can be estimated to be about 1% as follows. All of the finite volume extrapolated zero lattice spacing mass ratios which we obtained were within 20% of their values on the lattice $16^3 \times 32$ at β of 5.7. Moreover, as we argued earlier, the changes in masses we found, at β of 5.7, between $16^3 \times 32$ and $24^3 \times 32$ should be nearly the same as corresponding changes between $16^3 \times 32$ and inifinite volume. Combining these two pieces of information, we expect that with a relative error of 20% or less, the changes we found in mass ratios between $16^3 \times 32$ and $24^3 \times 32$ at β of 5.7 should be the same as the changes between continuum mass ratios in a box with period having $m_\rho L$ of 9 and corresponding continuum ratios in infinite volume. Since the changes we found in mass ratios, extrapolated to physical quark mass, between $16^3 \times 32$ and $24^3 \times 32$ are all less than 5%, the overall error in using these differences as estimates of corresponding continuum differences between $m_\rho L$ of 9 and infinite volume should be of the order of 20% of 5%, which is 1%.

Eight different hadron mass ratios, extrapolated to zero lattice spacing with $m_\rho L$ fixed at 9, and then extrapolated to infinite volume are shown in Table III. All eight infinite volume continuum predictions differ from

TABLE III. Calculated values of hadron mass ratios at physical quark masses, extrapolated to zero lattice spacing in finite volume, then corrected to infinite volume, compared with observed values, and with calculations of Refs. [3, 5] for $\Lambda^{(0)}_{\overline{\rm MS}}/m_\rho$. The mass difference Δm is $m_\Xi + m_\Sigma - m_N$.

Ratio	Finite volume	Infinite volume	Observed
m_{K^*}/m_ρ	1.149±0.010	1.167±0.016	1.164
m_Φ/m_ρ	1.297±0.019	1.333±0.032	1.327
m_N/m_ρ	1.285±0.070	1.219±0.105	1.222
$\Delta m/m_\rho$	1.867±0.046	1.930±0.073	2.047
m_Δ/m_ρ	1.628±0.075	1.595±0.111	1.604
m_{Σ^*}/m_ρ	1.813±0.051	1.821±0.075	1.803
m_{Ξ^*}/m_ρ	2.013±0.052	2.063±0.067	1.996
m_Ω/m_ρ	2.206±0.058	2.298±0.098	2.177
$\Lambda^{(0)}_{\overline{\rm MS}}/m_\rho$	0.305±0.008	0.319±0.012	0.305 ± 0.018
			0.320 ± 0.007

experiment by less than 6% and less than 1.6 standard deviations. The central values of the infinite volume ratios shown in Table III are marginally closer to experiment than the finite volume ratios. We believe the main significance of the infinite volume numbers shown in Table III, however, is that their error bars include the uncertainty in estimating infinite volume ratios from finite volume. Variations of our mass fitting procedure which decrease some of the volume dependence shown in Table II do not produce statistically significant changes in the numbers shown in Table III. The errors on all quantities in this table were found by the bootstrap method.

Of the eight hadron mass ratios in Table III, the values of m_Φ/m_ρ, m_N/m_ρ, $(m_\Xi + m_\Sigma - m_N)/m_\rho$, m_Δ/m_ρ, and m_Ω/m_ρ may be viewed as entirely independent predictions. The predicted values of m_{K^*}/m_ρ, m_{Σ^*}/m_ρ, and m_{Ξ^*}/m_ρ, on the other hand, are the infinite volume, continuum limits of ratios obtained by combining linear fits to hadron masses as a function of quark mass with our version of the Gell-Mann-Okubo mass formula. The agreement of these values with experiment may be viewed as confirmation of our prediction that low-lying hadron masses depend linearly on quark mass.

Values of $\Lambda^{(0)}_{\overline{\rm MS}}$, determined following Ref. [3], give $\Lambda^{(0)}_{\overline{\rm MS}}/m_\rho$ which vary by only 1 standard deviation over the three lattices used for extrapolation. Thus the rho mass follows asymptotic scaling in $g^{(0)}_{\overline{\rm MS}}$. The continuum and infinite volume continuum limits of $\Lambda^{(0)}_{\overline{\rm MS}}/m_\rho$ are shown in Table III. For the observed value of $\Lambda^{(0)}_{\overline{\rm MS}}/m_\rho$ we have inserted the calculated results of Refs. [3, 5].

The authors are grateful to Mike Cassera and Dave George for their work in putting GF11 into operation, to Chi Chai Huang, of Compunetix Inc., for his contributions to bringing GF11 up to full power and to its continued maintenance, and to Ed Nowicki and Molly Elliot for their work on GF11's disk software.

[a] Permanent address: Department of Mathematics, Trinity College, Dublin 2, Ireland.

[1] D. H. Weingarten, Phys. Lett. **109B**, 57 (1982); Nucl. Phys., **B215** [**FS7**], 1 (1983).
[2] D. Toussaint, Nucl. Phys. B (Proc. Suppl.) **26**, 3 (1992).
[3] A. X. El-Khadra, G. H. Hockney, A. S. Kronfeld, and P. B. Mackenzie, Phys. Rev. Lett. **69**, 729 (1992).
[4] G. P. Lepage and P. B. Mackenzie, Report No. Fermilab-Pub-91/353-T (to be published).
[5] G. S. Bali and K. Schilling, in *Lattice 92–Proceedings of the 1992 Symposium on Lattice Field Theory* (North-Holland, Amsterdam, 1993).
[6] D. Weingarten, Nucl. Phys. B (Proc. Suppl.) **17**, 272 (1990).
[7] L. Griffiths, C. Michael, and P. Rakow, Phys. Lett. **129B**, 351 (1983); P. Bacilieri *et al.*, Nucl. Phys. **B317**, 509 (1989).
[8] Y. Oyanagi, Comput. Phys. Commun. **42**, 333 (1986); T. DeGrand, Comput. Phys. Commun. **52**, 161 (1988); T. DeGrand, P. Rossi, Comput. Phys. Commun. **60**, 211 (1990).
[9] B. Efron, *The Jacknife, the Bootstrap and Other Resampling Plans* (Society for Industrial and Applied Mathematics, Philadelphia, 1982).
[10] F. Butler, H. Chen, J. Sexton, A. Vaccarino, and D. Weingarten (to be published).