Infinite Volume, Continuum Limit of Valence Approximation Hadron Masses

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ABSTRACT

We obtain estimates of several hadron mass ratios, for Wilson quarks in the valence (quenched) approximation, extrapolated to physical quark mass, infinite volume and zero lattice spacing.

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In the present article, we evaluate the pion, rho, proton and delta baryon masses using Wilson quarks in the valence (quenched) approximation for a range of different choices of quark mass, lattice volume, and lattice spacing. From these results we obtain estimates of the infinite volume continuum limits of eight different hadron mass ratios, evaluated at physical quark masses. Seven of these ratios differ from experiment by less than 6% which, in each case, is less than a factor of 1.5 multiplied by the corresponding statistical uncertainty. From the lattice gauge coupling constant, \( g_{\text{lat}} \), we determine the continuum coupling constant, \( g_{\text{cont}}^{(0)} \). Values of the rho mass in lattice units depend on \( g_{\text{cont}}^{(0)} \) as predicted by asymptotic scaling, for a \( \Lambda_{\text{cont}}^{(0)} \) within one standard deviation of the continuum limit value found in Ref. [1].

The motivation for this work is both to compare the valence approximation with experiment and to develop technology which will be useful in extrapolating results of the full theory to physical quark mass, infinite volume, and zero lattice spacing.

The calculations reported here were done on the GF11 parallel computer at IBM Research [2] and took approximately one year 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.

Hadron propagators were evaluated at \( \beta = 5.7 \) and \( k = 0.1400 - 0.1675 \) using 2349 configurations on a lattice \( 8^3 \times 32 \), 219 configurations on a lattice \( 16^3 \times 32 \) and 92 configurations on a lattice \( 24^3 \times 32 \). At \( \beta = 5.93 \) and \( k = 0.1543 - 0.1581 \), 217 configurations were used on a lattice \( 24^3 \times 36 \). At \( \beta = 6.17 \) and \( k = 0.1500 - 0.1532 \), 219 configurations were used on a lattice \( 30 \times 32^2 \times 40 \). Gauge configurations were generated by a version of the Cabbibo-Marinari-Okawa algorithm adapted for parallel computers [3]. The number of updating sweeps between successive configurations ranged from 1000 for the \( 8^3 \times 32 \) lattice at \( \beta \) of 5.7 to 6000 on the \( 30 \times 32^2 \times 40 \) lattice at \( \beta \) of 6.17. 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 \( \beta \) of 5.7 we used point sources and sinks in the hadron propagators. For all other lattices and \( \beta \), gaussian extended sources and both point
sinks and gaussian sinks were chosen. The mean squared radius of the gaussian source in all cases was 6 in lattice units. The mean squared radii of the gaussian sinks in lattice units were $3d^2/2$, for $d$ of 1 to 4. On the lattice $24^3 \times 32$ at $\beta$ of 5.7, 8 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. Random cube roots of 1 cause cross term cancellation both for meson and baryon propagators.

Each gauge configuration was first transformed to a completely fixed axial gauge and then to lattice Coulomb gauge. Since the axial gauge is uniquely defined and has no Gribov copies, the final Coulomb gauge transformation selects a uniquely specified Gribov copy which would not be changed by any gauge transformation of the original configuration.

Quark propagators were constructed using the conjugate gradient algorithm for the $8^3 \times 32$ lattice at $\beta$ of 5.7, using red-black preconditioned conjugate gradient for the other lattices at $\beta$ of 5.7 and 5.93, and using a red-black preconditioned minimum residual algorithm at $\beta$ of 6.17. For conjugate gradient, at the largest values of the hopping constant $k$, we found that red-black preconditioning decreased the computer time required for each inversion by very close to a factor of 3. At the largest $\beta$ the minimum residual algorithm gave an additional improvement by a factor of 2 over conjugate gradient. For each lattice and $\beta$, we found no configurations on which the inversion algorithm chosen failed to converge. The convergence criterion used in all cases was tuned to be 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 then determined by fits to hadron propagators constructed from the quark propagators. In all cases the pion mass was extracted by fitting propagator data for a point sink, on an interval of hyperplanes sufficiently far from the propagator’s source, to $Z\{exp(-mt) + exp[-m(N-t)]\}$ for hyperplane $t$ on a lattice with time-direction periodicity $N$. The best $Z$ and $m$ were found by minimizing the fit’s $\chi^2$ determined from the full statistical correlation matrix among the set of fitted hyperplanes. The range to be fit was first narrowed down by looking for an
approximate plateau in the large $t$ tail of graphs of the naive pion mass found by fitting only successive pairs of hyperplanes to $Z\{\exp(-mt) + \exp[-m(N - t)]\}$. The fitting program then chose an optimal fitting range within this region by trying all ranges including at least three hyperplanes and selecting the range yielding the smallest value of $\chi^2$ per degree of freedom. A corresponding procedure was used to determine the rho, nucleon and delta baryon masses for all values of $k$ on the lattice $8^3 \times 32$ and for all but the three largest values of $k$ on the other four lattices. For the nucleon and delta baryon the fitting function used was $Z\exp(-mt)$.

At the largest three $k$ values, the rho mass was found by simultaneously fitting the propagators for a point sink and for gaussian sinks with mean squared radius of $3d^2/2$, for $d$ of 1 and 2. The fitting function was taken to be $Z_d\{\exp(-mt) + \exp[-m(N - t)]\}$ with field strength renormalization constants $Z_0, Z_1, Z_2$, depending on the sink but mass $m$ independent of the sink. The optimal fitting parameters and fitting range were found by minimizing $\chi^2$ determined by the full correlation matrix among the complete set of fitted hyperplanes and sink sizes. Nucleon and delta baryon masses were determined similarly using the fitting function $Z_d\exp(-mt)$. Simultaneous fits to several sinks at once provides an unbiased resolution of the small differences between mass results obtained from fits to different individual sinks and give statistical uncertainties which are frequently smaller by a factor ranging from 0.85 to 0.9 than the smallest statistical uncertainty obtained by fitting a propagator for a single sink size.

The statistical errors for all fits were determined by the bootstrap method. Generating 100 bootstrap ensembles in all cases appeared to be sufficient to give stable values for statistical errors.

Comparing hadron masses in lattice units between the $8^3 \times 32$ and $16^3 \times 32$ lattices at $\beta$ 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 fixed $k$. Overall, the pion mass at fixed $k$ varied by less than $1.2 \pm 1.6$ % as the lattice size was changed. For the rho, nucleon and delta baryon, some differences were found comparing the $16^3 \times 32$ and $24^3 \times 32$ lattices. At $k$ of 0.16625, the nucleon mass fell by $4.4 \pm 1.7$ % from $16^3 \times 32$ to $24^3 \times 32$. 

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At $k$ of 0.1675, the rho fell by $3.4 \pm 1.4\%$, the nucleon fell by $4.6 \pm 2.2\%$ and the delta baryon fell by $4.7 \pm 2.6\%$ from $16^3 \times 32$ to $24^3 \times 32$. It appears quite likely that for the range of $k$, $\beta$ 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 $C\exp(-L/R)$, with a coefficient $R$ of the order of the radius of a the hadron’s wave function. At $\beta$ of 5.7 for the $k$ we considered, $R$ is thus typically 3 lattice units. Thus we expect that the differences we have found 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.

At the largest $k$ on each lattice, except $8^3 \times 32$, the ratio $m_\pi/m_\rho$ was close to 0.5. Thus to produce mass predictions for hadrons containing only ordinary quarks our data had to be extrapolated to still larger $k$. To do this we first determined the $k_{\text{crit}}$ at which $m_\pi$ becomes 0. As expected from a naive application of PCAC to Wilson fermions, we found $(m_\pi a)^2$ to be close to a linear function of $1/k$ over the entire range of $k$ considered on each lattice. Fits of $(m_\pi a)^2$ to linear functions of $1/k$ at the three highest $k$ on the lattices $16^3 \times 32$, $24^3 \times 32$, $24^3 \times 36$ and $30 \times 32^2 \times 40$ gave an averaged $\chi^2$ per degree of freedom of 1.20. These fits were then used to determine $k_{\text{crit}}$ for each lattice and $\beta$. Defining the quark mass in lattice units $m_qa$ to be $1/(2k) - 1/(2k_{\text{crit}})$, we found $m_\rho a$, $m_N a$ and $m_\Delta a$ to be nearly linear functions of $m_q a$ over the entire range of $k$ considered on each lattice. Figure 1 shows the nucleon mass $m_N$ and rho mass $m_\rho$ as functions of the quark mass $m_q$ in comparison to linear fits to the 3 smallest values of $m_q$. The hadron masses are shown in units of the physical value of $m_\rho$, given by $m_\rho$ evaluated at the “normal” quark mass $m_n$ which produces the physical value of $m_\pi/m_\rho$. The quark mass $m_q$ in Figure 1 is measured in units of the strange quark mass $m_s$, the determination of which will be discussed below. The fits shown in Figure 1 appear to be reasonably good and should form a fairly reliable method for extrapolations 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 $8^3 \times 32$.

A further test of our extrapolation method is given by a version of the Gell Mann-Okubo mass formula. For a rho composed of quarks with masses $m_1$ and $m_2$, 


Figure 1: For $16^3 \times 32$ at $\beta$ of 5.7, $m_N$ and $m_\rho$ in units of the physical $m_\rho$ as a function of the quark mass $m_q$ in units of $m_s$. 
assume, as suggested by Figure 1, that $m_\rho = \alpha_1 m_1 + \alpha_2 m_2 + \beta$. It is then easy to show we must have $\alpha_1 = \alpha_2$. Then the k-star, equivalent to 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 equivalent to a rho with $m_1 = m_2 = m_s$. By a further application of the linearity relation of Figure 1 we can then extrapolate the rho mass from the masses of k-star and phi. The extrapolated rho mass obtained in this way from observed k-star and phi masses lies below the observed rho mass by 0.53%. A similar extrapolation 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 nucleon mass found this way is 1.38% too large, and the delta baryon mass is 0.81% too large.

The relations discussed in the preceding paragraph, conversely, permit strange hadron masses to be constructed from the masses we have calculated for hadrons composed of a single species of heavy quark. Fitting the pseudoscalar kaon to the pion mass at a quark mass of $(m_s + m_n)/2$ gives the value for $m_s$ mentioned earlier. With $m_s$ and $m_n$ thus completely fixed, predictions for eight different hadron mass combinations, measured in units of the physical rho mass, follow from our data with no additional free parameters.

Finally, to obtain predictions for comparison with experiment we have extrapolated our results to 0 lattice spacing. For Wilson fermions we expect the leading lattice spacing dependence in mass ratios to be linear in $a$. A linear fit of our data for $m_N/m_\rho$ to the lattice spacing, measured in units of the physical rho mass, is shown in Figure 2. The vertical bar at 0 lattice spacing is the extrapolated prediction’s uncertainty, determined by the bootstrap method. The dot at 0 lattice spacing shows the observed physical value of $m_N/m_\rho$. The three data points in Figure 2 are for the lattices $16^3 \times 32$, $24^3 \times 36$ and $30 \times 32^2 \times 40$. The values of $\beta$ for these lattices were chosen so that the physical volume in each case is nearly the same. The lattice period $L$, measured in units of the physical rho mass, $m_\rho L$ is, respectively, $9.00 \pm 0.13$, $9.15 \pm 0.19$ and $8.76 \pm 0.13$.

Linear extrapolations to 0 lattice spacing for eight different hadron mass ratios, and the corresponding observed values, are shown in Table 1. Values of $\Lambda^{(0)}_{\text{ms}}$, found
Figure 2: $m_N/m_\rho$ as a function of the lattice spacing, $m_\rho a$, extrapolated to 0 lattice spacing.
following Ref. [1], give $\Lambda_{\text{ms}}^{(0)}/m_\rho$ which vary by only one standard deviation over the three lattices used for extrapolation. Thus the rho mass follows asymptotic scaling in $g_{\text{ms}}^{(0)}$. For the observed value of $\Lambda_{\text{ms}}^{(0)}$ we have inserted the calculated result of Ref. [1]. Seven of the eight predictions differ from experiment by less than 6% and less than 1.5 multiplied by the average of the upper and lower error bars.

The authors are grateful to Chi-Chai Huang, of Compunetix Inc., for his contributions to bringing GF11 up to full power and keeping it in operation during the course of this work.

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### Table 1: The continuum limits of hadron mass ratios in comparison to their observed values.

| ratio                                      | calculated          | observed |
|--------------------------------------------|---------------------|----------|
| $m_{K^{*}}/m_{\rho}$                       | 1.150 + 0.008       | 1.161    |
|                                            | - 0.012             |          |
| $m_{\Phi}/m_{\rho}$                        | 1.300 + 0.015       | 1.327    |
|                                            | - 0.024             |          |
| $m_{N}/m_{\rho}$                           | 1.284 + 0.071       | 1.222    |
|                                            | - 0.065             |          |
| $(m_{\Xi} + m_{\Sigma} - m_{N})/m_{\rho}$ | 1.869 + 0.030       | 2.046    |
|                                            | - 0.063             |          |
| $m_{\Delta}/m_{\rho}$                      | 1.627 + 0.051       | 1.604    |
|                                            | - 0.092             |          |
| $m_{\Sigma^{*}}/m_{\rho}$                 | 1.816 + 0.029       | 1.803    |
|                                            | - 0.074             |          |
| $m_{\Xi^{*}}/m_{\rho}$                     | 2.017 + 0.024       | 1.994    |
|                                            | - 0.078             |          |
| $m_{\Omega}/m_{\rho}$                      | 2.210 + 0.047       | 2.176    |
|                                            | - 0.068             |          |
| $\Lambda_{ms}^{(0)}/m_{\rho}$              | 0.3047 + 0.0050     | 0.305 + 0.018 |
|                                            | - 0.0109            | - 0.018  |