## Hadron Masses in QCD with Two Flavors of Dynamical Fermions at $\beta = 5.7$

Frank R. Brown, Frank P. Butler, Hong Chen, Norman H. Christ, Zhihua Dong, Wendy Schaffer,

Leo I. Unger, and Alessandro Vaccarino

Department of Physics, Columbia University, New York, New York 10027

(Received 10 April 1991)

A hadron mass calculation is reported using two flavors of dynamical, staggered fermions with masses of ma = 0.01, 0.015, 0.02, and 0.025 on a  $16^3 \times 32$  lattice. The masses of hadrons containing valence quarks with ma = 0.004, 0.07, 0.1, 0.14, and 0.25 were also computed to study the limit  $ma \rightarrow 0$  and the strange particle spectrum. For ma = 0.01, the mass ratio  $m_N/m_\rho = 1.527(11)$  is 25% larger than experiment while the results  $f_\pi/m_\rho = 0.14(1)$  and  $(m_k^2 - m_\pi^2)/(m_k^\pi - m_\rho)m_\rho = 2.25(3)$  agree somewhat better.

PACS numbers: 12.38.Gc

Lattice gauge theory simulations should permit the numerical computation of low-energy hadronic physics directly from the underlying theory of quantum chromodynamics (QCD). Successful calculation of known masses and matrix elements of low-lying hadron states would provide an essential demonstration of the correctness of lattice techniques and important underpinning for new lattice QCD predictions of thermodynamic properties of the QCD vacuum or not yet measured weak matrix elements.

Most recent large-scale lattice QCD calculations of known hadronic masses and matrix elements try to explore and extend the available range of lattice volumes, lattice spacings, and quark masses in an attempt to control the associated errors. To date this program has not been entirely successful with one of the most accessible hadronic mass ratios,  $m_N/m_\rho$ , typically coming out 25% too high [1].

In this paper we describe a series of lattice QCD calculations [2] that were carried out in about 9 months on the 256-node Columbia parallel supercomputer at a sustained speed of 6.4 Gflops [3]. The dynamical effects of two degenerate flavors of staggered fermions are incorporated using the hybrid-molecular-dynamics R algorithm [4]. We work on a  $16^3 \times 32$  lattice (we equilibrate the full  $16^3 \times 32$  lattice without "doubling") where the longer time dimension allows a more precise fitting of the hadron propagators' exponential time dependence. In addition to using a variety of masses for our two dynamical fermion flavors, with mass labeled  $m_{sea}$ , we also compute the masses for states which contain one or more "quenched" species of quarks that do not enter the fermion determinant and have mass  $m_{\text{val}}$ . Table I lists the masses, molecular-dynamics time step sizes ( $\Delta \tau$ ), and simulation times  $(\tau)$  for the calculations reported here. The quantities  $\Delta \tau$  and  $\tau$  are defined according to Ref. [4]. We used a conjugate gradient stopping condition of  $(R^2/S^2)^{1/2} < 1.1 \times 10^{-5}$  in the evolution and  $2.2 \times 10^{-6}$ for the hadron propagators in the notation of Refs. [5,6].

To compute the hadron propagators, we use three extended spatial sources each corresponding to a different color direction. For each source, the sites with even spatial coordinates on a specific time slice are assigned to the same orthornormal color vector in Coulomb gauge. The sink is completely local and formed from the conventional hadron operators [7]. The boundary conditions are periodic in the space and antiperiodic in the time directions for both the evolution and hadron propagator calculations.

Two methods, effective mass and fitting, are used to extract hadron masses from the propagators. A one-state model with two parameters is used for the pion and a two-state model with four parameters for the others.

The effective mass  $m_{\rm eff}(t)$  comes from propagators with time separation  $t, t+1, \ldots, t+n$ , where n=1 for the pseudoscalar mesons and n=3 for the other states. The results for the  $\rho$  with  $m_{\rm sea}a = 0.01$  are shown in Fig. 1. A nice plateau for  $t \ge 2$  can be seen from which it is relatively easy to deduce  $m_{\rho}$ . The fitted mass  $m_{\rm fit}(t_{\rm min})$  is determined from propagators with separation  $t_{\rm min}$  to  $N_t/2$ by minimizing  $\chi^2$  computed using the full covariance matrix [5]. We quote this fitted mass as our result. For  $m_{\rm sea}a = 0.01$  we use  $t_{\rm min} = 9$  for the pseudoscalar fits and  $t_{\rm min} = 6$  for the others, while for  $m_{\rm sea}a > 0.01$  we use the corresponding values  $t_{\rm min} = 14$  and 11. With these fitting ranges we obtain values of  $\chi^2/(\text{degree of freedom}) \le 2$ .

TABLE I. Combinations of sea quark and valence quark masses with the corresponding times steps  $\Delta \tau$  and the ranges of molecular-dynamics time used in the calculation.

$m_{\rm sea}a$	$m_{\rm val}a$	τ range
$0.01 \ (\Delta \tau = 0.0078)$	0.01	1050-2700
	0.004	250-2700
$0.015 (\Delta \tau = 0.0078)$	0.015	250-3010
	0.07	1880-3010
	0.1	250-1750
$0.02 (\Delta \tau = 0.01)$	0.02	250-1425
	0.07	250-1425
	0.1	250-1425
$0.025 (\Delta \tau = 0.01)$	0.025	530-2830
	0.1	1480-2830
	0.14	530-1480
	0.25	200-500



FIG. 1. Four-parameter effective-mass plot of  $\rho$  at ma = 0.01 from data with  $\tau$  between 1050 and 2700. The upper points represent the state with opposite parity in the same channel.

The errors are computed with the jackknife technique using blocks of 30 time units and taking autocorrelation into account. Only statistical errors are quoted.

The nucleon,  $\rho$ , and  $\pi$  masses obtained for the four choices  $m_{u,d}a = 0.01$ , 0.015, 0.02, and 0.025 are shown in Fig. 2 and given in Table II. For these results  $m_{u,d}$  $= m_{val} = m_{sea}$ . As can be seen, our large space-time volume, considerable statistics, smaller lattice spacing, and inclusion of dynamical quarks have not lowered the high value of  $m_N/m_\rho$  [1,6].

Since our smallest quark mass  $m_{u,d}a = 0.01$  gives a  $\pi$ which is too massive, it is natural to attempt to extrapolate  $m_{u,d}$  down to the physical value. Unfortunately, this is made difficult by the nonlinear variation of  $m_N$ ,  $m_\rho$ , and  $m_{\pi}^2$  with quark mass shown in Fig. 2. Although the effect is only  $\approx 2\sigma$  for  $m_N$  and  $m_\rho$ , it is more significant for  $m_{\pi}^2$  where we have the additional constraint that  $m_{\pi}(m_{u,d}=0)=0$ . While  $m_{u,d}a=0.015$ , 0.02, and 0.025 lie nicely on a line passing through the origin, the  $m_{u,d}=0.01$  point lies significantly above this line. If the linearity of 0.015, 0.02, and 0.025 is coincidental and the quark mass  $m_{u,d}a=0.015$  is too large for  $m_{\pi}$  to show linear quark-mass dependence, then we cannot extrapolate  $m_{u,d} \rightarrow 0$ .

On the other hand, it is possible that the 0.01 point is misleading either because the errors have been underestimated or because this lightest pion mass is being disproportionately distorted by the finite lattice volume. Without this 0.01 point, a linear fit of  $m_{\pi}^2$ ,  $m_{\rho}$ ,  $m_N$ , and  $\langle \bar{\chi} \chi \rangle$  to the three mass values 0.015, 0.02, and 0.025 yields

$$m_{\pi}^{2}a^{2} = -0.011(3) + 6.48(14)m_{u,d}a \quad (\chi^{2} = 4.2),$$
  

$$m_{\rho}a = 0.31(2) + 9.7(8)m_{u,d}a \quad (\chi^{2} = 0.06),$$
  

$$m_{N}a = 0.47(3) + 14.9(1.1)m_{u,d}a \quad (\chi^{2} = 2.6),$$
  

$$\langle \bar{\chi}\chi \rangle a^{3} = 0.0085(4) + 1.99(2)m_{u,d}a \quad (\chi^{2} = 1.1).$$

These results can be used to determine the pion decay constant  $f_{\pi}$ . We use the approximate PCAC (partial con-



FIG. 2. The nucleon mass (diamonds),  $\rho$  mass (circles), and  $\pi$  mass squared (squares) as a function of  $m_{u,d}$ . The numerical values are given in Table II.

servation of axial-vector current) relation [8]

$$f_{\pi} = \left(\frac{3m_{u,d}\langle \bar{\chi}\chi(m_{u,d}=0)\rangle}{2m_{\pi}^2}\right)^{1/2}$$
(1)

and obtain  $f_{\pi}a = 0.044(1)$  or the dimensionless ratios  $f_{\pi}/m_{\rho} = 0.14(1)$  and  $f_{\pi}/m_{N} = 0.095(6)$ , where the  $m_{u,d} \rightarrow 0$  values of  $m_{N}$  and  $m_{\rho}$  are used [9]. We can compare these ratios to the experimental values 0.1212(2) and 0.0992(1), respectively, obtained using the measured value  $f_{\pi} = 93.15(11)$  MeV.

In a consistent calculation the quark masses that enter the fermion determinant  $(m_{sea})$  and those that appear in the hadron propagators  $(m_{val})$  must be the same. Nevertheless, it is often convenient to distinguish them. Our results for all values of  $m_{val}$  and  $m_{sea}$  are combined in Fig. 3. Here we plot the hadron masses (or masses squared) versus the total mass  $m_{tot}$  of all the valence quarks used to form the state. The gross features of this figure can be summarized in a strikingly simple fashion: The mass (or mass squared) is approximately a linear function of  $m_{tot}$ with intercept and slope nearly independent of  $m_{sea}$ . Of course significant deviations from this simple universal behavior are evident on the 5% level.

TABLE II. Masses and  $\bar{\chi}\chi$  expectation value computed for the four values of  $m_{u,d} = m_{val} = m_{sea}$  used. The states  $\pi(2)$  and  $\rho(2)$  are flavor partners of the  $\pi$  and  $\rho$ . The lack of flavor degeneracy is the result of finite-lattice-spacing effects.

	$m_{u,d}a$						
	0.01	0.015	0.02	0.025			
m <sub>π</sub> a	0.252(3)	0.293(2)	0.349(2)	0.388(1)			
$m_{\pi(2)}a$	0.295(3)	0.333(3)	0.389(3)	0.436(3)			
m₀a	0.454(4)	0.455(8)	0.501(7)	0.551(4)			
$m_{a(2)}a$	0.457(7)	0.453(7)	0.502(9)	0.553(5)			
mNa	0.692(6)	0.685(10)	0.781(10)	0.839(6)			
$\langle \bar{\gamma} \gamma \rangle a^3$	0.0277(3)	0.0385(1)	0.0483(2)	0.0584(1)			
$m_N/m_\rho$	1.527(11)	1.506(13)	1.560(19)	1.522(10)			



FIG. 3. Plot of nucleon masses (upper band),  $1^{-}$  vector meson masses (middle band), and squares of pseudoscalar meson masses (lower band) as a function of the total mass of their valence quarks. The dynamical quark masses used are distinguished by symbols as shown in the key.

Let us now examine these  $m_{val} \neq m_{sea}$  results in more detail. Most easy to interpret are the  $m_{sea} = 0.01$ ,  $m_{val} = 0.004$  calculations. Here we attempt to study smallquark-mass behavior by using small  $m_{val}$ . Of greatest interest is the ratio  $m_N/m_\rho = 1.506(46)$  obtained with the lighter  $m_{val}a = 0.004$  quarks. We can further compare this to the same ratio computed above for  $m_{val}a = m_{sea}a$ = 0.01 using the same ensemble of gauge configurations with the results

$$\frac{m_N/m_\rho(m_{\rm val}a=0.01)}{m_N/m_\rho(m_{\rm val}a=0.004)} = 1.013(24).$$
(2)

Thus, within our fixed  $16^3$  volume we see no significant change in this ratio as the valence quark mass is decreased from 0.01 to 0.004.

We can use the above results to compute the mass spectrum of the strange mesons and baryons in the (plausible) approximation where the strange quark is omitted from the fermion determinant. The linearity in  $m_{\rm val}$ shown in Fig. 3 guarantees that the results will be consistent with the Gell-Mann-Okubo mass formula and can be viewed as justifying octet dominance.

Let us discuss the strange mesons first. Our calculation gives the masses of the pseudoscalar and vector states K and K<sup>\*</sup> without further approximation. The simulation of the  $\phi$  and nonstrange  $\omega$  require the inclusion of intermediate gluon graphs which we have not done. (These are graphs in which the source and sink can be disconnected by cutting only gluon lines.) However, the near degeneracy of the  $\rho$  and  $\omega$  and the narrow width of the  $\phi$  are conventionally interpreted as demonstrating that the intermediate gluon graphs (which would split the vector meson octet and singlet) are small compared to SU(3)-breaking effects (i.e.,  $m_s - m_{u,d}$ ) so that the  $\omega - \phi$ states are distinguished principally by their strange quark content. The approximation of neglecting intermediate gluon graphs implies  $m_{\rho} = m_{\omega}$  and allows us to interpret

TABLE III. A comparison of the values that we obtain for ratios of SU(3)-breaking mass differences with experiment. Here  $\delta_{AB}$  represents the difference of the masses of the particles A and B in lattice units while  $\delta_{AB}^2$  is the corresponding difference of the squares of the masses. The strange states were computed using a valence strange quark with the mass  $m_s$  given in the second column.

	$m_{\rm sea}a$						
	msa	0.015	0.02	0.025	Expt.		
$\delta_{K\pi}^2/\delta_{K^*}m_{\rho}$	0.07	2.24(3)	2.15(2)		2.388(3)		
$\delta_{K\pi}^2/\delta_{K}*m_{\rho}$	0.1	2.41(1)	2.29(1)	2.18(2)	2.388(3)		
$\delta_{K\pi}^2/\delta_{K*}m_N$	0.1	1.60(2)	1.47(2)	1.43(2)	1.953(1)		
800/8K*	0.1	1.94(1)	1.92(1)	1.91(1)	2.033(2)		
$\delta_{\tilde{\Xi}N}/\delta_{\Lambda N}$	0.1	1.96(3)	1.98(3)	1.94(2)	2.146(1)		
$\delta_{\Lambda N}/\delta_{K^{*}\rho}$	0.1	1.07(4)	0.99(4)	1.07(3)	1.431(1)		

our vector meson with two strange quarks as the  $\phi$ . We show our predictions for the SU(3) violating differences between the masses of these states in Table III for  $m_{u,d} = 0.015, 0.02$ , and 0.025 as well as the corresponding experimental values.

The results for strange baryons are more ambiguous. In terms of the valence quarks, the  $\Lambda^0$  and  $\Sigma^0$  are distinguished by the symmetry of the (u,d) quark pair—the state is antisymmetric for the  $\Sigma^0$  and symmetric for the  $\Lambda^0$ . The conventional local nucleon operator which we use [7],  $u_{\alpha}d_{\beta}s_{\gamma}\epsilon^{\alpha\beta\gamma}$  with  $\alpha$ ,  $\beta$ , and  $\gamma$  color indices, contains both combinations [10] and so is expected to couple to both states. Thus we will assume that the mass we extract for the baryon containing one strange quark is that of the lighter  $\Lambda^0$ . However, given the small mass difference between the  $\Lambda^0$  and the  $\Sigma^0$ , it is not clear that our temporal range  $0 \le t \le 16$  is sufficient to eliminate or even recognize a significant  $\Sigma^0$  admixture.

The problem of interpreting the two-strange-quark,  $\Xi$ like state is more severe. For the physical  $\Xi$ , Fermi statistics requires the two strange quarks to be in an antisymmetric state like the *u* and *d* quarks in the  $\Sigma^0$ . However, with the four species of staggered fermions that are present in our propagator, it is likely that our state,  $\tilde{\Xi}$ , contains two distinct species of strange quarks in an unphysical, symmetric state, which, in analogy with  $m_{\Sigma^0} > m_{\Lambda^0}$ , one might expect to be lighter than the physical  $\Xi$ . Thus we expect discrepancies on the order of  $(m_{\Sigma^0} - m_{\Lambda^0})/(m_{\Lambda^0} - m_N) \approx 50\%$  in comparing our SU(3)breaking mass differences with those for the correct experimental states. For completeness, we also give these numbers in Table III.

Given the linearity shown in Fig. 3, it is natural to present our results in terms of ratios of differences in order to avoid introducing strong dependence on the new parameter  $m_s$  [2]. In all but the first row of Table III we use the value  $m_s a = 0.1$  which was chosen to give the  $\Xi$ nucleon splitting about right for the case  $m_{sea} a = 0.025$ . For  $m_s a = 0.1$ ,  $m_{u,d} a = 0.025$ , we have  $(m_{\Xi} - m_N)/m_N$  =0.458(14) compared to the measured value of 0.4039(1). Varying  $m_s a$  among 0.07, 0.1, and 0.14 changes the numbers in Table III by less than 2 standard deviations except for the ratio  $(m_K^2 - m_\pi^2)/(m_{K^*} - m_\rho)m_\rho$ . For that case we give both the  $m_s a$  =0.07 and 0.1 results.

It is interesting to speculate about the cause of the large ratio  $m_N/m_{\rho} = 1.5$ . Optimistically, one might suppose that either  $m_{\rho}$  is too light or  $m_N$  too heavy. Heuristic arguments can be advanced for each possibility. The nucleon, containing three quarks, may have its mass disproportionately increased by finite-volume effects. On the other hand, the failure to allow the decay  $\rho \rightarrow \pi\pi$  caused by  $m_{\pi} \ge m_{\rho}/2$  could artificially lower the mass of the  $\rho$ .

However, the notion that  $\Gamma_{\rho} = 150$  MeV should have an important effect on the  $\rho$  mass conflicts with the conventional explanation of the  $m_{\omega} - m_{\rho} = 14$  MeV degeneracy and the small ratio  $\Gamma_{\phi \to \pi\pi\pi}/\Gamma_{\omega \to \pi\pi\pi} = 1.1 \times 10^{-2}$ , which assumes that intermediate gluon graphs can be neglected. This assumption should also imply that  $\Gamma_{\rho}$  can be neglected since  $\Gamma_{\rho} \approx \Gamma_{\rho} - \Gamma_{\omega}$  and the latter difference is also due to intermediate gluon graphs.

The work reported here does not support the notion that either  $m_{\rho}$  or  $m_N$  is computed more accurately than the other. Our results for  $f_{\pi}/m_N$  suggest that the nucleon mass may be more successfully calculated, while the more accurate ratio  $(m_K^2 - m_{\pi}^2)/(m_{K^*} - m_{\rho})m_{\rho}$  given in Table III favors the interpretation that  $m_{\rho}$  may be less affected by systematic errors.

The most sensible interpretation of our results is that their  $\approx 25\%$  agreement with experiment can be quantitatively anticipated from the discrepancy from linear  $m_{u,d}$ behavior seen in Fig. 2. This indicates systematic errors coming from the extrapolation of  $m_{u,d}$  down to physical values that are on this same 25% level. Thus we view our results as a successful calculation of the ratios  $m_N/m_\rho$ ,  $f_{\pi}/m_{\rho}$ , and  $(m_K^2 - m_{\pi}^2)/(m_{K^*} - m_{\rho})m_{\rho}$  with small statistical but  $\approx 25\%$  systematic errors.

We would like to thank M. S. Gao and P. F. Hsieh for their significant contributions to the design of the hardware and the software environment in which this calculation was carried out, S. Gottlieb, G. Kilcup, S. Sharpe, and A. Soni for helpful discussions of physics issues, and, especially, R. Mawhinney for ideas and advice. This research was supported in part by the U.S. Department of Energy.

- For recent reviews see R. Gupta, Nucl. Phys. B (Proc. Suppl.) 17, 70 (1990); T. DeGrand, University of Colorado Report No. COL-HEP-238 [in *Lattice 90*, Proceedings of the 1990 Symposium on Lattice Field Theory, Tallahassee, Florida, October 1990, edited by U. Heller *et al.* [Nucl. Phys. B (Proc. Suppl.)].
- [2] A preliminary version of these results appears in H. Chen, Columbia University Report No. CU-TP-497 [in Lattice 90, Proceedings of the 1990 Symposium on Lattice Field Theory, Tallahassee, Florida, October 1990 (Ref. [1])].
- [3] A. Vaccarino, Nucl. Phys. B (Proc. Suppl.) 17, 421 (1990); N. H. Christ, Nucl. Phys. B (Proc. Suppl.) 17, 267 (1990).
- [4] S. Gottlieb et al., Phys. Rev. D 35, 2531 (1987).
- [5] S. Gottlieb et al., Phys. Rev. D 38, 2245 (1988).
- [6] K. M. Bitar *et al.*, Phys. Rev. Lett. **65**, 2106 (1990);
   Phys. Rev. D **42**, 3794 (1990).
- [7] K. C. Bowler, Nucl. Phys. B284, 299 (1987).
- [8] G. W. Kilcup and S. R. Sharpe, Nucl. Phys. B283, 493 (1987).
- [9] For earlier quenched results see R. Gupta *et al.*, Phys. Rev. D 36, 2813 (1987); L. Maiani, Nucl. Phys. B (Proc. Suppl.) 9, 193 (1989).
- [10] M. F. L. Golterman, Nucl. Phys. B273, 663 (1986).