Quantum Chromodynamics at $6/g^2 = 5.60$

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We have carried out a simulation of quantum chromodynamics using the hybrid-molecular-dynamics algorithm with two flavors of Kogut-Susskind quarks. We have used Kogut-Susskind and Wilson valence quarks to calculate the hadron mass spectrum. Among our extensive results we discuss baryon hyperfine splitting, the nucleon-to-ρ mass ratio, the scalar-to-tensor-glueball mass ratio, and the quantization and susceptibility of the topological charge. We have used a gauge coupling of $6/g^2=5.60$, and quark masses $am_q=0.025$ and 0.01, in generating gauge configurations on 12^4, $12^3\times 24$, and 16^4 lattices.

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The calculation of the mass spectrum of quantum chromodynamics is one of the major objectives of lattice gauge theory. However, to achieve it will require a prodigious effort due to technical difficulties with dynamical fermions and the need to use large lattices in order to eliminate finite-size effects and to extrapolate results to the continuum limit. Recent improvements in calculational techniques and increases in computer power are leading to significant incremental improvements in these calculations. In this Letter we present results from our recent efforts in this direction. A more detailed description of this work will be given elsewhere.[1,2]

We have generated gauge configurations using two flavors of Kogut-Susskind quarks, and calculated hadron masses on these configurations with both Kogut-Susskind and Wilson valence quarks in order to test universality. Representative examples of our spectroscopy results are given in Table I.[3] Our lattice spacing and quark masses are too large to expect quantitative agreement with experiment; however, in our hadron spectrum calculations we see significant improvements over earlier results obtained with dynamical quarks at larger lattice spacings. In particular, the nucleon-to-ρ mass ratio and the breaking of flavor symmetry in the masses of the Kogut-Susskind pions has decreased. The splitting of the Δ and proton masses in the Wilson spectroscopy has increased over that found in quenched calculations. The spectrum results with Wilson and Kogut-Susskind valence quarks are in rough agreement, but, as one would expect, there is no value of the hopping parameter κ for which the Wilson spectroscopy exactly matches the Kogut-Susskind spectroscopy.

In addition to measuring the meson/baryon spectrum, we have studied the glueball spectrum including the effects of dynamical quarks. We have measured the propagators for glueballs of spins 0, 1, 2 and several spin-parity assignments; however, the only states for which we can make reasonable mass measurements are

TABLE I. Representative spectroscopy results. The columns labeled $L=12$ and $L=16$ contain results for these spatial dimensions with a quark mass $am_q=0.01$. The column labeled $am_q=0.025$ contains results for this quark mass and the spatial dimension $L=12$. Results are shown for the π, the ρ, and the nucleon N, for both Kogut-Susskind (KS) and Wilson (W) quarks. For the latter the superscript indicates the value of κ. The quoted errors are the statistical errors only, for a fit with a single distance range. Results are also given for the 0^{++} and 2^{++} glueballs and the string tension σ. All values are in units of the lattice spacing.

Particle	$L=12$	$L=16$	$am_q=0.025$
π_{KS}	0.2663(30)	0.2661(12)	0.4150(17)
ρ_{KS}	0.544(7)	0.519(6)	0.631(7)
N_{KS}	0.848(11)	0.770(8)	0.982(9)
$\pi_{\mathrm{W}}^{0.1585}$	0.344(7)	0.319(7)	0.375(4)
$\pi_{\mathrm{W}}^{0.1600}$	0.233(6)	0.21(1)	0.281(5)
$\rho_{\mathrm{W}}^{0.1585}$	0.46(2)	0.442(7)	0.50(1)
$N_{\mathrm{W}}^{0.1585}$	0.78(2)	0.698(6)	0.79(2)
$m_{0^{++}}$	0.84(6)	0.86(8)	0.85(6)
$m_{2^{++}}$	1.17(6)	1.50(16)	1.34(8)
$\sigma^{1/2}$	0.215(4)	0.247(8)	0.239(5)

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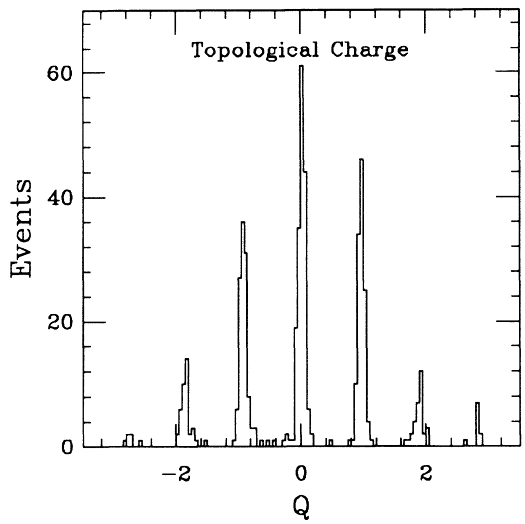

FIG. 1. Histogram of the raw topological charge distribution on a 12^4 lattice at $am_q = 0.01$.

the 0^{++} and 2^{++} glueballs. In addition, we have measured the Wilson-Polyakov line which enables us to estimate the string tension σ. Results for these quantities are given in Table I.

The nontrivial topological structure of QCD plays a crucial role in the resolution of the U(1) problem (the absence of a light isosinglet pseudoscalar meson and the failure of naive current-algebra predictions for the η decays), in chiral-symmetry breaking, and in hadron structure. For this reason we have attempted to measure the topological charge Q and from it the topological susceptibility $\chi = \langle Q^2 \rangle / V$, where V is the space-time volume of the lattice (in lattice units) for the gauge configurations. We have used the cooling method of Teper[4] to extract the topological charge for each configuration. Since, on the lattice, these charges are not necessarily integers, we force each to the nearest integer value. In Fig. 1 we see that the lattice topological charges do tend to occur with near integer values.

We have used the hybrid-molecular-dynamics algorithm[5,6] with two flavors of Kogut-Susskind quarks to equilibrate 12^4, $12^3 \times 24$, and 16^4 lattices at a gauge coupling of $6/g^2 = 5.60$. For the 12^4 lattices we used quark masses of 0.025 and 0.01 in lattice units, while for the larger lattices we used a quark mass of 0.01. We generated 5000 hybrid-molecular-dynamics time units at each value of the quark mass for the 12^4 lattices, 1280 time units for the 16^4 lattices, and 1000 for the $12^3 \times 24$ lattices, after equilibration runs for each lattice and quark mass. We obtained an additional 1670 trajectories for the 12^4 lattices at $am_q = 0.01$ with increased conjugate gradient accuracy. Every tenth lattice was saved for hadron and glueball spectrum calculations. All of the lattices were doubled, and the 12^4 lattices quadrupled for the calculation of hadron masses. We computed Wilson spectroscopy at three values of the hopping parameter $\kappa = 0.1565$, 0.1585, and 0.1600, at both values of the dynamic mass. Our relatively high statistics allowed us to make some studies of systematic errors.

We calculated hadron propagators on the equilibrated lattices using both point and wall sources. For the latter we fixed the gauge and used a source spread uniformly over one time slice. We extracted masses from the hadron propagators by using data from adjacent time slices to calculate effective masses and by making correlated fits to the propagators. In both of these procedures we took into account correlations among successive lattices by blocking the data and studying the dependence of our error estimates on block size. We have confidence in our correlated fits only if the effective mass reaches a plateau when plotted as a function of the time separation of the source and sink. For the pion and nucleon such a plateau is reached for both the Kogut-Susskind and Wilson quarks. However, the ρ effective masses fail to reach a convincing plateau with either species of quarks, so our results for this particle should be treated cautiously.

We doubled and in some cases quadrupled our lattices for the spectrum calculations. Our statistics are good enough that we can see the effects of doubling at the few percent level. We believe that our results indicate that doubling of lattices should be avoided.

We have made a number of tests of potential systematic errors, but much more work in this direction would have been desirable. By repeating the spectrum calculations for quark mass 0.01 on 16^4 lattices, we saw that the results for the 12^4 lattices had significant finite-size effects. They were observed primarily in the baryon masses, as is seen in Table I. In our production runs we used a step size of 0.01 in numerically integrating the molecular-dynamics equations. Tests with other step sizes indicated that errors from this source were under reasonable control, but these tests were not of sufficient precision to allow us to observe the dt^2 variation of errors expected on theoretical grounds.

We did not expect that the gauge coupling $6/g^2 = 5.60$ would put us in the continuum limit, and there is ample evidence that it did not. With Kogut-Susskind quarks there are two pointlike operators that can create pions. We refer to the one that in the chiral-symmetry limit would be an exact Goldstone boson as the π, and to the other, which behaves more nearly like an ordinary meson, as the π_2. The pion masses obtained from these operators need only agree in the scaling limit. In Fig. 2 we plot the ratio m_{π_2}/m_π as a function of m_π measured in lattice units. We include in the figure data from an earlier Kogut-Susskind spectrum study[7] on a $10^3 \times 24$ lattice with lattice spacing approximately 1.33 times larger than in the present calculation and quark masses 0.05 and 0.025. We see from Fig. 2 that m_{π_2}/m_π is significantly smaller in the present study, but that we still have a considerable way to go before flavor symmetry is restored. For the Wilson spectroscopy the mass splitting between the Δ and proton is too small, as is the ρ-pion mass split-

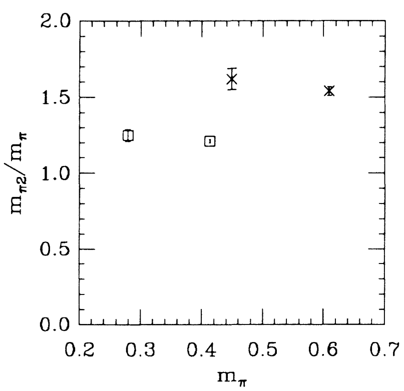

FIG. 2. Ratios of two KS pion masses. The squares are the results of this simulation at $am_q = 0.025$ and 0.01. The crosses are from a previous simulation at larger lattice spacing with $am_q = 0.05$ and 0.025.

ting. In Fig. 3 we plot these splittings, normalized by the center of mass of the multiplets, versus each other. We only use data for $\kappa = 0.1585$ and 0.1600 from the 16^4 lattices in this figure, since the smaller lattices suffer from finite-size effects. We have also included results from quenched simulations by the APE Collaboration.[8] The figure shows that while the baryon hyperfine splitting is less than the experimental value, its fractional deviation is smaller than that for the meson hyperfine splitting. Furthermore, the Δ-proton splitting is larger than has been obtained in quenched calculations.

In Fig. 4 we present an Edinburgh plot which includes our new data with both Kogut-Susskind and Wilson valence quarks, and the older, larger-lattice-spacing Kogut-Susskind results for quark masses of 0.05 and 0.025. Note that the large-lattice-spacing points have large nucleon-to-ρ mass ratios. As we mentioned previously, there is a significant shift in the nucleon mass in going from the 12^4 to 16^4 lattice for $am_q = 0.01$, which causes the drop in the nucleon-to-ρ mass ratio between these two points. This figure has a similar qualitative appearance to the Edinburgh plot for quenched calculations with values of $6/g^2$ below 6.0. The nucleon-to-ρ mass ratio is too large, but it appears to be moving in the right direction.

For our calculations of the glueball spectrum we have employed blocked "fuzzy" wave functions[9] to enhance the overlap between the chosen wave functions and the lowest-lying glueball states. As in the quenched case, these wave functions give a dramatic improvement in the signal/noise ratio as is shown in Fig. 5, where we plot the propagator for the 0^{++} wave functions based on a simple plaquette, at various levels of blocking for the 12^4 lattice at quark mass 0.01.

Our glueball measurements are limited by statistics. The best we have been able to do, even on the 12^4 lattice, has been to measure the effective mass for a zero spatial momentum propagator from a temporal separation 1 to a

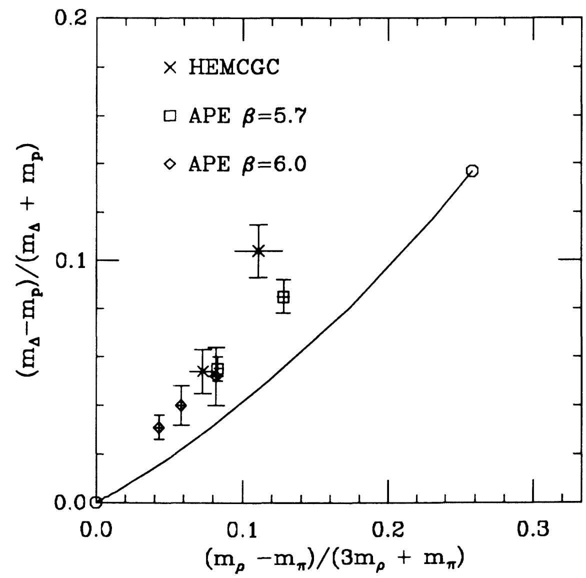

FIG. 3. Baryon and meson hyperfine splittings. The two circles show the expected values of hyperfine splitting in the limit of infinite quark mass and from experiment. The line interpolating between them is a simple quark model. The crosses are our results for $\kappa = 0.1585$ and 0.1600, while the squares and diamonds are results of quenched calculations of the APE Collaboration (Ref. 8).

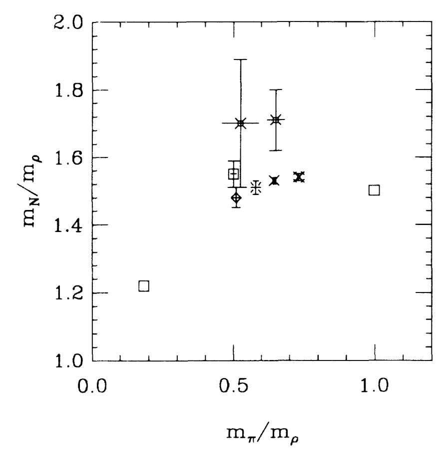

FIG. 4. Edinburgh plot of our results. The simple cross is the Kogut-Susskind point with $am_q = 0.025$, the square the Kogut-Susskind point with $am_q = 0.01$ and $L = 12$, and the diamond the Kogut-Susskind point with $am_q = 0.01$ and $L = 16$. The decorated cross is the Wilson point with dynamical quark mass $am_q = 0.01$ and Wilson hopping parameter $\kappa = 0.1585$, while the burst is the Wilson point with $am_q = 0.01$ and $\kappa = 0.1600$. The two points with the decorated square are results from a previous simulation at larger lattice spacing. The two squares without error bars are the heavy-quark limit and the real world value. The error bars plotted on the Kogut-Susskind ratios here include an estimate of the systematic error obtained from the scatter of the three runs with $am_q = 0.01$ and $L = 12$.

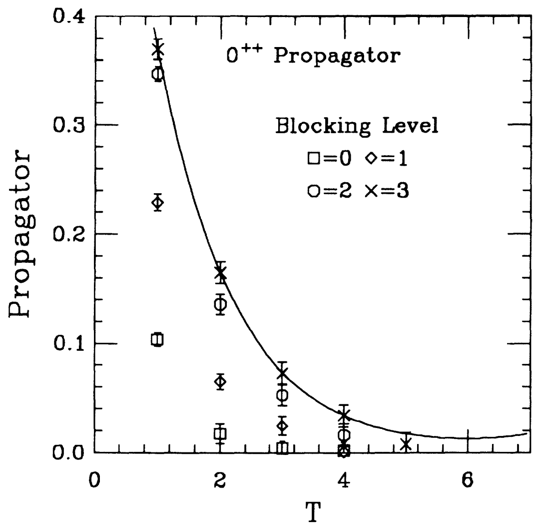

FIG. 5. The 0^{++} propagators for different blocking levels with wave functions based on the simple plaquette, for a 12^4 lattice with $am_q=0.01$. The fit is by the form

$$0.8298\{\exp(-0.8080t)+\exp[-0.8080(12-t)]\},$$

which fits the points $t=1$ and $t=2$ of the blocking level 3 propagator exactly.

temporal separation 2. A fit is shown in Fig. 5. Such estimates give only upper bounds to the glueball masses. The $12^3\times24$ and 16^4 results are limited by statistics. Since there is some evidence that these quantities are particularly sensitive to long-time correlations in the system, the errors could well be underestimated, even though the data have been binned to reduce the effects of time correlations.

The measured values for the topological susceptibility χ at $am_q=0.01$ are $6.5(1.2)\times10^{-5}$, $7.7(1.4)\times10^{-5}$, and $6.7(1.0)\times10^{-5}$ for the 12^4, $12^3\times24$, and 16^4 lattices, respectively. The agreement of our results on different sized lattices is surprisingly good given that this quantity has long-time fluctuations which make our error estimates suspect. At $am_q=0.025$ on the 12^4 lattices we find $\chi=9.4(1.0)\times10^{-5}$. The mass dependence of χ is in poor agreement with the $\chi\sim m_q$ behavior expected in this the chirally broken phase.[10] However, it is clearly in even worse agreement with the $\chi\sim m_q^2$ behavior expected in the chirally symmetric, deconfined phase. There are a number of possible explanations for this poor agreement including an underestimation of the statistical fluctuations, finite-size–finite-lattice-spacing effects, or an inadequacy in the definition of the topological charge on the lattice. Since even the 12^4 data at $am_q=0.01$ show evidence for statistical fluctuations whose time constant is comparable with the length of the run, we suspect that the first of these effects may be the most important.

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