Progress Report

In this attachment, we review research that we have carried out at the NSF Centers during the last year, and present a set of figures that illustrate some of this work.

Generation of gauge configurations with improved gauge and quark actions: The Table at the end of the attachment entitled *Impact of the Asqtad Gauge Configurations* shows the current status of our three flavor gauge configuration sets with lattice spacings $a \approx 0.15$, 0.12, 0.09 and 0.06 fm. Ensembles marked with an N are available from the NERSC Gauge Connection archive and those marked with an R are still in progress. During the past year we completed the most ambitious run we have carried out to date, that with $a \approx 0.09$ fm and light quark mass $m_l = 0.1\,m_s$. The time history of this run is shown in Fig. 2 below. Note the major increase in progress when one of the streams was shifted to the PSC Cray XT3. This ensemble will anchor our extrapolations to the physical value of m_l. We have made major progress on our run at $a \approx 0.06$ fm and $m_l = 0.4 m_s$ on $48^3 \times 144$ lattices. As of July 6, 2006 we had saved 297 equilibrated configurations, following our practice of saving one configuration every five molecular dynamics time steps. We expect to complete this ensemble on the Brookhaven National Laboratory's QCDOC during the next twelve months. In addition, we have begun to equilibrate a $48^3 \times 144$ lattice with $a \approx 0.06$ fm and $m_l = 0.2\,m_s$, and expect to complete this process and start archiving equilibrated configurations by October 1, 2006. The $a \approx 0.06$ fm configurations will have lattice artifacts that are smaller than those of the $a \approx 0.09$ fm ones by a factor of nearly 2.6. They will therefore enable us to significantly reduce errors in the extrapolation of physical quantities to the continuum limit. We have completed the generation five ensembles with lattice spacing $a \approx 0.15$ fm and light quark masses $m_l = 1.0\,m_s$, $0.6\,m_s$, $0.4\,m_s$, $0.2\,m_s$ and $0.1\,m_s$ begun last year. These configurations are helping us estimate the size of the finite lattice artifacts in physical quantities. As is the case with all our configurations, the new ones are being made available to other physicists for use in their research. In the attachment titled *Impact of the Asqtad Gauge Configurations*, we set out the wide range of topics which our configurations are currently being used to study, and list the papers that have arisen from this work.

Physics of light pseudoscalars: During the past year, we have refined our computations of leptonic decay constants, quark masses, and low energy constants, first published in Refs. [1, 2]. The previous calculation was based on the analysis of π and K mesons on all the coarse ($a \approx 0.12$ fm) configurations with $am_s = 0.05$ and on the fine ($a \approx 0.09$ fm) configurations with $m_l = 0.4\,m_s$ and $m_l = 0.2\,m_s$. We now have a complete ensemble on the fine configurations with $m_l = 0.1\,m_s$ and a partial ensemble at the "super fine" ($a \approx 0.06$ fm) lattice spacing with $m_l = 0.4\,m_s$. In addition we have analyzed these quantities on the coarser configurations with $a \approx 0.15$ fm and $a \approx 0.18$ fm.

For each set of sea quark masses we have lattice data for a wide range of valence quark masses; in other words the data is "partially quenched." We then fit, simultaneously, masses and decay constants at multiple lattice spacings to the form required by SχPT [3], which takes into account discretization errors up to $\mathcal{O}(a^2)$. Good fits are possible including all but the coarsest configurations ($a \approx 0.18$ fm), where the $\mathcal{O}(a^4)$ effects are clearly too large to be neglected. The fact that both finer and coarser configurations than those included in Ref. [1] can be fit with the same SχPT forms gives us added confidence that the systematic effects of discretization errors are well understood. From such fits we can extrapolate fit parameters to the continuum and set valence and sea quark masses equal to obtain full QCD results.

Figure 3 shows fits to the kaon and pion masses as a function of light quark mass. Extrapolating fit parameters to the continuum gives the dashed red line. Requiring that the π and K take on their physical masses $m_{\hat{\pi}}$ and $m_{\hat{K}}$ (in the absence of electromagnetism and averaged over isospin) determines, up to overall normalization, the physical values of the strange quark mass m_s and the average of the up and down masses, $\hat{m}$. Extrapolating the light valence mass in the kaon further until the K^+ mass is reached then gives the up quark mass m_u. We obtain (still preliminary):

$$\begin{aligned}
m_s/\hat{m} &= 27.2(0)(4)(0)(0) \\
m_u/m_d &= 0.42(0)(1)(0)(4) \\
m_s^{\overline{\rm MS}} &= 90(0)(5)(4)(0)\ \text{MeV} \\
\hat{m}^{\overline{\rm MS}} &= 3.3(0)(2)(2)(0)\ \text{MeV}
\end{aligned}$$

$$\begin{aligned} m_u^{\overline{\mathrm{MS}}} &= 2.0(0)(1)(1)(1)\ \mathrm{MeV} \\ m_d^{\overline{\mathrm{MS}}} &= 4.6(0)(2)(2)(1)\ \mathrm{MeV} \end{aligned}$$

where the errors are statistical (rounded down to 0), lattice systematics, perturbation theory, and an estimate of the effects of electromagnetism, which have not been included in the simulation. The masses are evaluated at scale 2 GeV. The result for m_u/m_d rules out, at the 10σ level, the possibility of $m_u = 0$. This puts to rest a long standing proposal [4] that the up quark could be massless. A massless up quark might have solved the Strong CP Puzzle [5]. Alternative solutions are now more likely: *e. g.* , the axion [6], a possible component of Dark Matter.

To obtain the above values of quark masses in MeV, the matching factor for the lattice to continuum mass is needed. In Refs. [1, 2], the one-loop perturbative evaluation of the mass renormalization constant [2, 7] was used. The two-loop value has recently been calculated [8], and it in fact differs quite significantly ($\approx 12\%$ higher) from the one-loop result. This is the main reason that the quark mass values quoted above are larger than those in Refs. [1, 2]. For example, $m_s^{\overline{\mathrm{MS}}}$ has increased by 14 MeV; 11 MeV of that are due to perturbation theory, and the remaining 3 MeV comes from the new running. Since the two-loop term is so large, it becomes very important to evaluate the renormalization non-perturbatively in order to check that the corrections from still higher orders are under control. We propose such a computation for the coming year.

Figure 4 shows similar SχPT fits for the decay constant f_π, which governs the decay of the π to a muon (or electron) and neutrino. Such fits give (also preliminary)

$$\begin{aligned} f_\pi &= 128.6 \pm 0.4 \pm 3.0\ \mathrm{MeV} \\ f_K &= 155.3 \pm 0.4 \pm 3.1\ \mathrm{MeV} \\ f_K/f_\pi &= 1.208(2)(^{+\ 7}_{-14}) \end{aligned}$$

where the first error is statistical and the second is systematic.

Our result for f_π is consistent with the value [9] 130.7 ± 0.4MeV, which comes from an experimental determination of the decay rate coupled with the accurately known CKM matrix element, V_{ud}, that gives the strength of the weak interaction in the decay. For f_K (or more precisely the ratio f_K/f_π), our errors are small enough that our result can be used to provide a competitive determination of the corresponding CKM element, V_{us}. Following Marciano [10], we find $|V_{us}| = 0.2223(^{+26}_{-14})$. The Particle Data Book [9] quotes $0.2200(26)$ for V_{us}; while newer experiments [11] give $0.2262(23)$.

At the moment, our configurations with the smallest discretization errors (the super fine, with $a \approx 0.06$ fm and $m_l = 0.4m_s$) does not have much influence on the final results for decay constants. That is because: (1) the run is only half finished and the statistical errors are significantly greater than those for the other configurations, and (2) the light sea quark mass m_l is among the largest of those included in the fit, so its effect on the chiral extrapolation is limited. Note in particular that the f_π data from this (blue "fancy diamonds" in Fig. 4) are further from the continuum, full QCD (red) line, than the lowest mass fine points (black squares). The situation will improve as this run is completed and as the super fine simulations at lighter mass ($m_l = 0.2m_s$ and $m_l = 0.1m_s$) are added over the coming one to two years. Once those ensembles are included, we expect this method to reduce the uncertainty in V_{us} significantly, providing an important constraint on the Standard Model.

The current data set already allows us to substantially improve the evaluation of chiral low energy constants in Ref. [1]. The improvement comes largely from the light mass $m_l = 0.1m_s$ fine ensemble, completed over the last year, as well as additional coarse runs with lighter, and hence more chiral, strange sea quark masses (the 0.03/0.03 and 0.01/0.03 runs). Our preliminary new results are

$$\begin{aligned} 2L_6 - L_4 &= 0.5(1)(2) \\ 2L_8 - L_5 &= -0.1(1)(1) \\ L_4 &= 0.1(2)(2) \\ L_5 &= 2.0(3)(2) \end{aligned}$$

in units of 10^{-3}, at chiral scale m_η. These are consistent with, but have significantly smaller errors than, the phenomenological values, summarized for example by Pich [12]. The errors on these parameters have been reduced by 20 to 100% from our previously published numbers, and should continue to go down as the new runs become available over the next one to two years. Figure 5 shows the impact our published numbers have already had on determinations of the pion scattering lengths; it will be very interesting to see how the determinations are affected by our updated results.

Weak decays of particles containing heavy quarks: During the past year we and our Fermilab collaborators have extended our calculations of the weak decays of particles containing heavy quarks in essential ways.

Last year we used the $a \approx 0.12$ fm gauge configurations to predict the leptonic decay constants of the D^+ and D_s mesons. We found $f_{D^+} = 201 \pm 3 \pm 6 \pm 9 \pm 13$ MeV and $f_{D_s} = 249 \pm 3 \pm 11 \pm 10$ MeV, where the uncertainties are statistical and a sequence of systematic errors [13]. Several lattice uncertainties cancel in the ratio of the decay constants, so it is useful to define the quantity $R_{d/s} = \sqrt{m_{D^+}} f_{D^+} / \sqrt{m_{D_s}} f_{D_s}$. Our prediction for it was $R_{d/s} = 0.786 \pm 0.042$ [13]. Since then, an experiment by the CLEO-c Collaboration found $f_{D^+} = 223 \pm 16^{+7}_{-9}$ MeV [14], and one by the BaBar Collaboration gave $f_{D_s} = 279 \pm 17 \pm 6 \pm 19$ MeV [15]. Taking the ratio of decay constants from these experiments gives $R_{d/s} = 0.779 \pm 0.093$ [14, 15] in nice agreement the lattice result. The experimental results for the individual decay constants agree with the lattice predictions within errors, but it is clear that errors need to be reduced for both. Additional experimental data is being collected, and during the past year we have extended our calculations of the decay constants to the $a \approx 0.15$ and 0.09 fm configurations, which should substantially reduce our errors in extrapolations to the continuum limit. We will present results from this calculation at the Lattice 2006 meeting.

We have nearly completed a computation of the leptonic decay constants of the B and B_s mesons on the $a \approx 0.15$, 0.12 and 0.09 fm configurations, and will present first results for these important quantities at Lattice 2006. Our new results for B decays will be compared with those from the HPQCD Collaboration, which also employ our configurations, but use a different technique for the b quark called NRQCD [16].

We have also used our $a \approx 0.12$ fm configurations to calculate the form factors for the semileptonic decay $D \to Kl\nu$ [17]. Our prediction was first confirmed experimentally by the Focus Collaboration [18], and more recently by the Belle Collaboration with more precise data [19]. We show our results and the Belle data in Fig. 6. We are in the process of extending this calculation to the $a \approx 0.09$ fm ensembles. As noted in the proposal, the calculation of form factors for the semileptonic decays of B mesons, as well as the study of $B^0 - \bar{B}^0$ and $B^0_s - \bar{B}^0_s$ mixing are among our major goals for the coming year. Work on these projects has begun on the $a \approx 0.12$ fm configurations, and preliminary results will be presented at Lattice 2006.

Hadron mass spectrum with the improved action: Calculation of the masses of the lightest hadrons remains an essential test of lattice QCD, and computations of the masses of excited hadrons have the potential to clarify long standing questions in the quark model of hadrons and to help clarify the existence or nonexistence of exotic hadrons. We have been computing the masses of the simplest hadrons on all of our improved three flavor configurations. With several quark masses and lattice spacings to work with, we can make extrapolations to the physical light quark mass and to the continuum limit. Figure 7 shows a comparison of several of the lightest hadrons with experiment, as well as splittings of $\bar{c}c$ and $\bar{b}b$ mesons calculated by the HPQCD and Fermilab Lattice Collaborations using our configurations.

The masses of two baryons made of light quarks, the nucleon and Ω^-, are “gold plated” quantities, meaning that they can be accurately measured and are theoretically clean. Among other things, this requires that they be well below strong interaction decay thresholds. These lattice masses, extrapolated to the continuum and physical quark masses, are an important test of our lattice methods. The Ω^- mass also tests our determination of the strange quark mass. Figure 8 shows nucleon masses from our simulations, and a continuum extrapolation. The solid curves are chiral perturbation theory with various assumptions, and the cluster of points at the left are the experimental value and the various chiral extrapolations. The inset shows how the chiral extrapolations compare to the experimental value of 938 MeV. Figure 9 shows Ω^- masses, with a continuum and chiral extrapolation. Since the Ω^- mass has no chiral logs involving m_π, the chiral extrapolation for this quantity is much simpler than for most other particles.

With Kogut-Susskind quarks there are many different pions, corresponding to different combinations of the four internal flavors of quarks. While they are degenerate in the continuum limit, at nonzero lattice spacing their mass differences are easily resolved. They have been studied in detail on the $a \approx 0.12$ and 0.09 fm ensembles, and on our $a \approx 0.06$ fm, $m_l = 0.4 m_s$ run now in progress. These splittings are important input for including the “taste symmetry breaking” effects in chiral perturbation theory. They also provide a good test of whether the taste symmetry is restored in the expected way as the lattice spacing shrinks. Figure 10 shows the splittings among these pions at three different lattice spacings: $a \approx 0.12$, 0.09 and 0.06 fm with $m_l = 0.4\,m_s$. The splittings are plotted as a function of $a^2\alpha_s^2$, where a is the lattice spacing and α_s the strong coupling constant. We expect the splittings to be linear in this quantity.

The P-wave scalar mesons a_0 and f_0 decay typically to two lighter S-wave pseudoscalar mesons, including pions, kaons, and the eta meson. At the nearly physical quark masses in our simulations, these two-body channels are lighter than the pure quark-antiquark states. Thus, standard methods to observe them in two-point correlators must take into account the two-body states. Fortunately, chiral perturbation theory provides a credible model for the two-body contributions. But, perhaps the most important reason for studying these channels with the staggered fermion action is that the effects of taste-symmetry breaking are very apparent [20], so, we must use staggered chiral perturbation theory to model their contributions. The model is highly non-trivial. Thus, a study of the spectroscopy in these channels becomes a test of the methodology. Using previously generated ensembles at 0.12 fm, we have completed a study of the scalar meson decay channels for the a_0 and f_0 and confirm predictions of staggered chiral perturbation theory for these channels [21].

High temperature QCD with three flavors of quarks: We have completed our study of the equation of state at zero baryon chemical potential with three flavors of Asqtad staggered quarks at lattice resolutions of $N_t = 4$ and 6. Final results will be presented at the Lattice 2006 conference at the end of July, and a journal article is in preparation [22]. This is the first study at this resolution with an improved action and a realistic set of quarks. Our results for $N_t = 6$ and $m_l = 0.1\,m_s$ are shown in Fig. 11. Our principal result is an accurate determination of the energy density at temperatures up to twice the crossover temperature T_c.

We have begun a study of the equation of state at nonzero baryon chemical potential, using the Taylor expansion method of the Bielefeld-Swansea group [23]. This method is expected to give a reliable extrapolation to the experimentally relevant regime. For this study we are reusing our existing archive of configurations. The code was brought into production this Spring, and we will report preliminary results for $N_t = 4$ at the Lattice 2006 conference.

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Figures Illustrating Recent Progress

Comparison of Lattice Results with Experiment

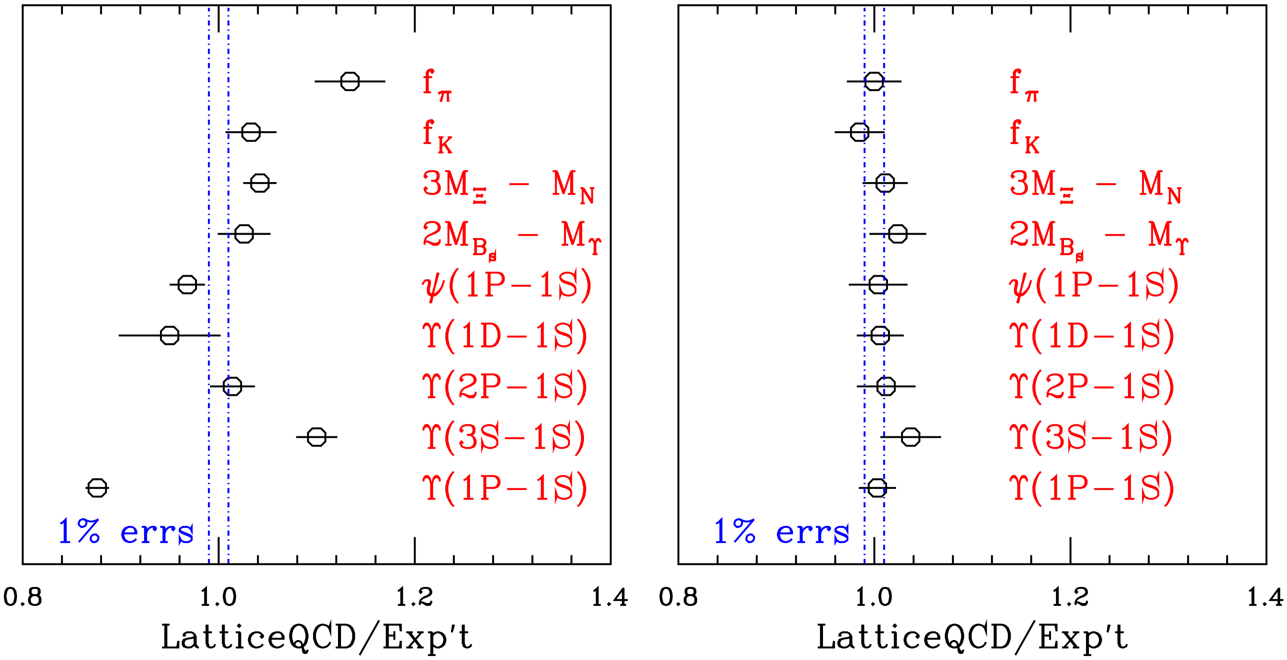


Figure 1: The ratio of several quantities calculated with the Asqtad gauge configurations to their experimental values [24]. The panel on the left shows results from the quenched approximation in which the vacuum polarization due to the quarks is neglected, and that on the right from full QCD. Some of these quantities involve only light valence quarks, while others have *s*, *c* or *b* valence quarks. This work is a joint effort of the MILC Collaboration, and of the Fermilab Lattice, HPQCD, and UKQCD Collaborations, which are also using our configurations.

Time History of the Gauge Ensemble $\mathbf{a \approx 0.09}$ fm and $\mathbf{m_l = 0.1 m_s}$

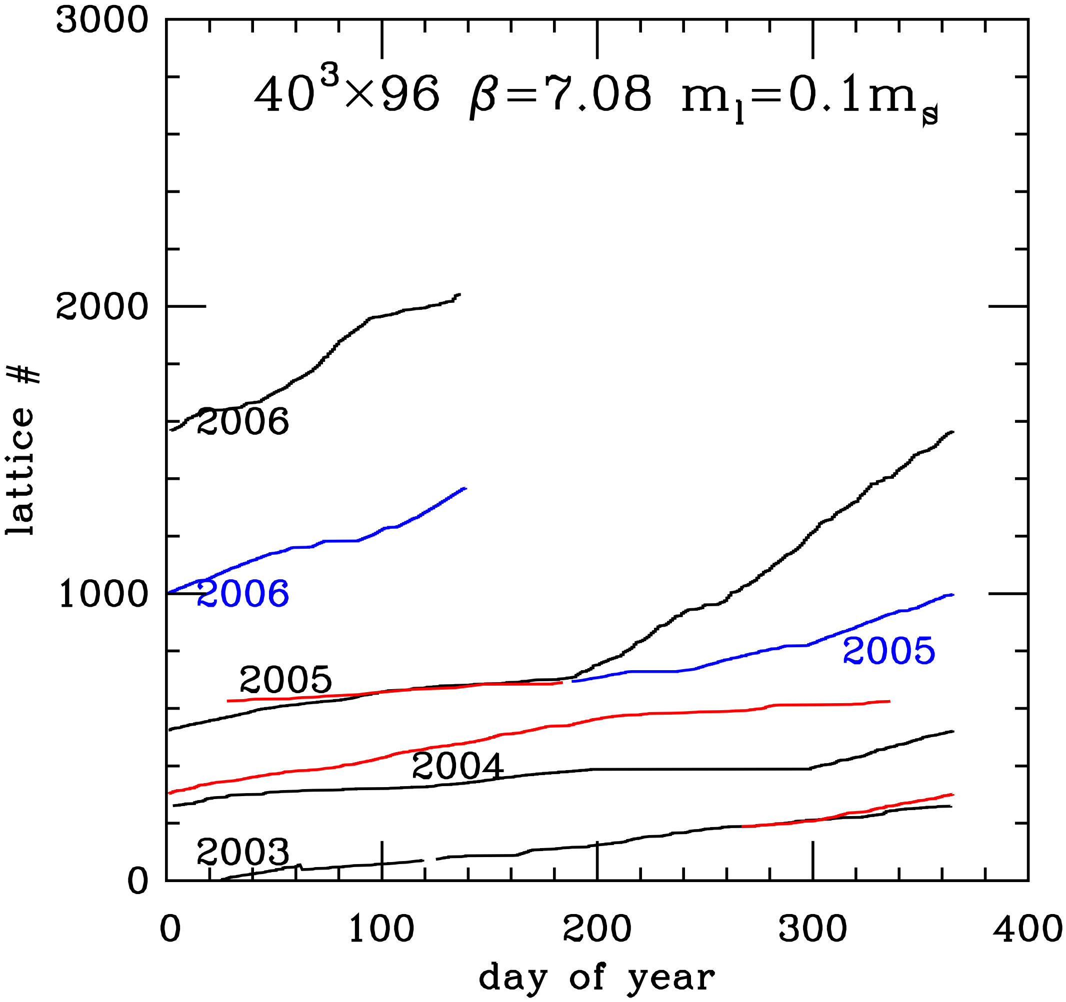


Figure 2: The history of progress in generating configurations on a $40^3 \times 96$ lattice with $a \approx 0.09$ fm and $m_l = 0.1 m_s$. The run was started in early 2003. After equilibration it was split into two streams. The stream in black was run on the PSC TCS1 until mid-2005 when it was moved to the PSC Cray XT3. Note the large improvement in the rate of lattice generation on the XT3. The red stream was run on the NCSA Tungsten cluster and at NERSC. In mid-2005, this stream was moved to the QCDOC at Brookhaven National Lab (blue line).

Pseudoscalar Meson Masses

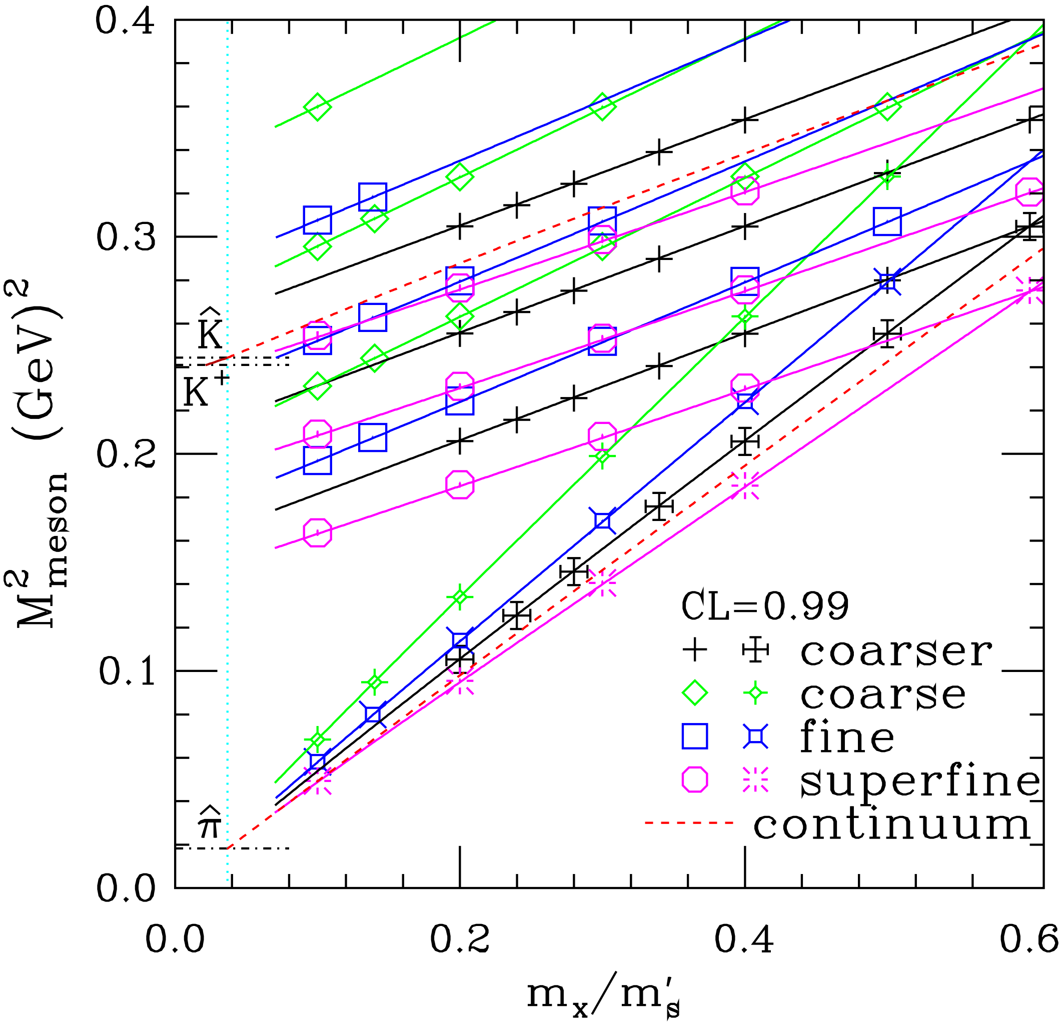


Figure 3: Squared meson masses as a function of light valence mass (m_x) divided by the simulation value of the strange quark mass, m_s'. We show results from four lattices: $a \approx 0.15$ fm ("coarser") with sea quark masses $0.00484, 0.0484$; $a \approx 0.12$ fm ("coarse"), with sea masses $0.005, 0.05$; $a \approx 0.09$ fm ("fine"), with sea masses $0.0031, 0.031$; and $a \approx 0.06$ fm ("super fine"), with sea masses $0.0072, 0.018$. Three sets of kaon points, with various heavier valence quark mass (m_y) near the strange mass are plotted for each lattice. Pion points have $m_x = m_y$. The statistical errors in the points are not visible on this scale. The dashed red lines give the continuum-extrapolated fit, and the cyan vertical dotted line shows the physical $\hat{m}/m_s$ obtained. Extending the red kaon line (short dark red continuation) until it intersects the K^+ value then gives m_u/m_s', from which we find $m_u/\hat{m}$ or m_u/m_d.

Leptonic Decay Constant of the Pion

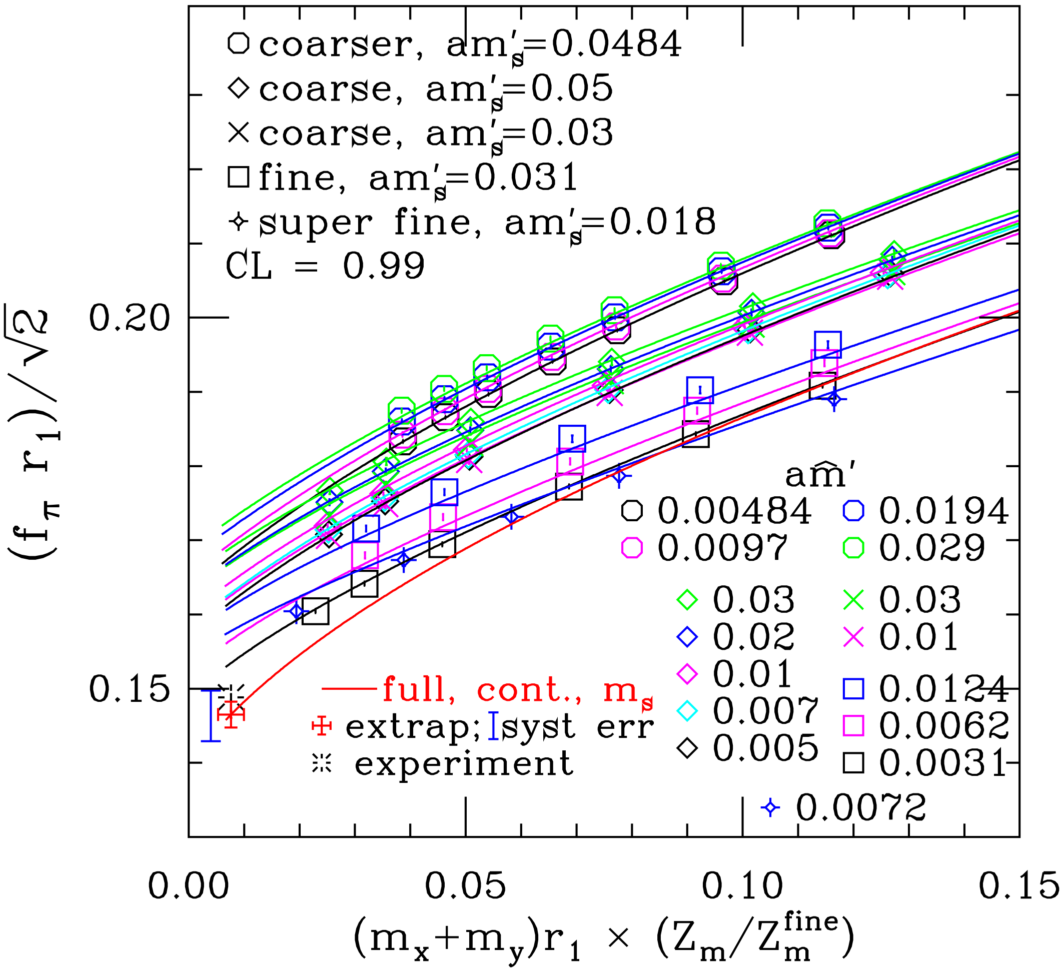


Figure 4: Pion decay constants *vs.* quark mass, in units of the scale r_1 form the static quark potential. The mass renormalization the lattices (relative the fine lattices) has been included so that data from all may be presented on the same plot. Lines through the data points come from a SχPT fit to the entire data set for decay constants and masses. The red line represents the fit function in “full QCD” (valence and sea masses set equal) after extrapolation of parameters to the continuum, and with strange sea quark fixed at its physical mass. The red plus shows our extrapolated value of f_π, in agreement with experiment (black burst) within systematic errors (blue bar).

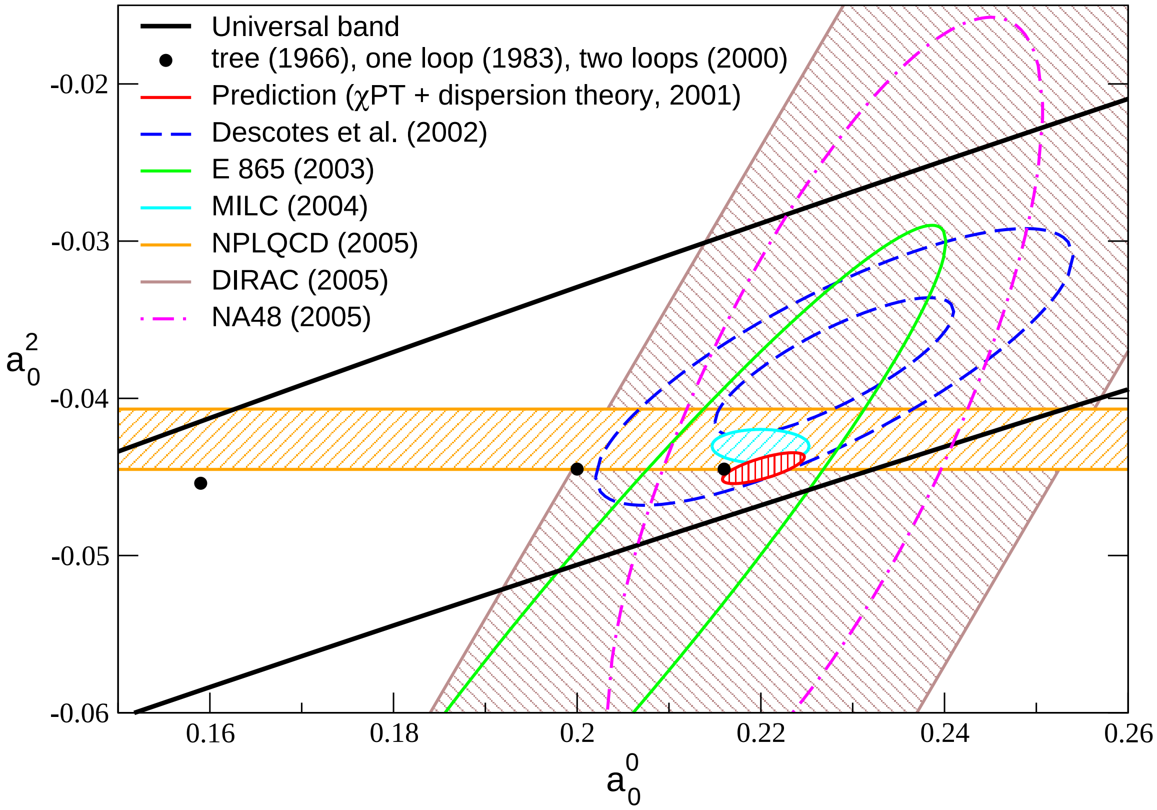


Figure 5: Various determinations of the pion scattering lengths a_0^2 and a_0^0. The previously published MILC results give the light blue horizontal ellipse. We thank G. Collangelo for providing us with this plot.

Semileptonic Form Factor of the D Meson

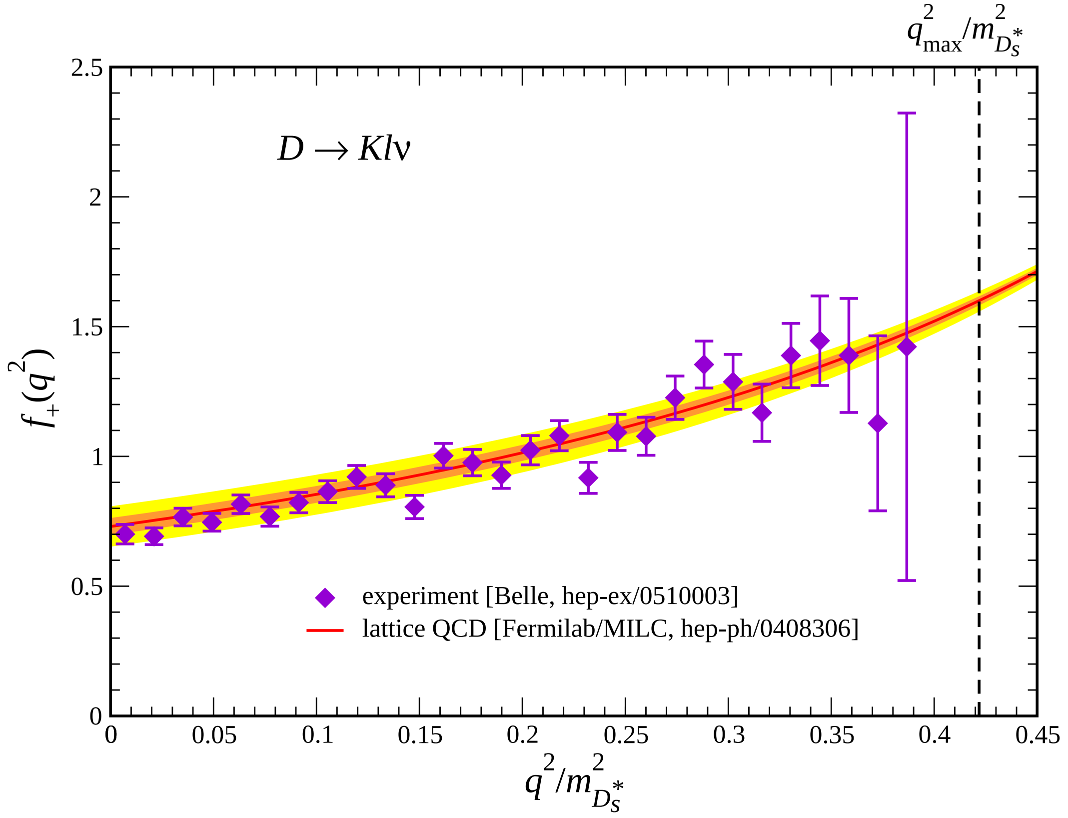
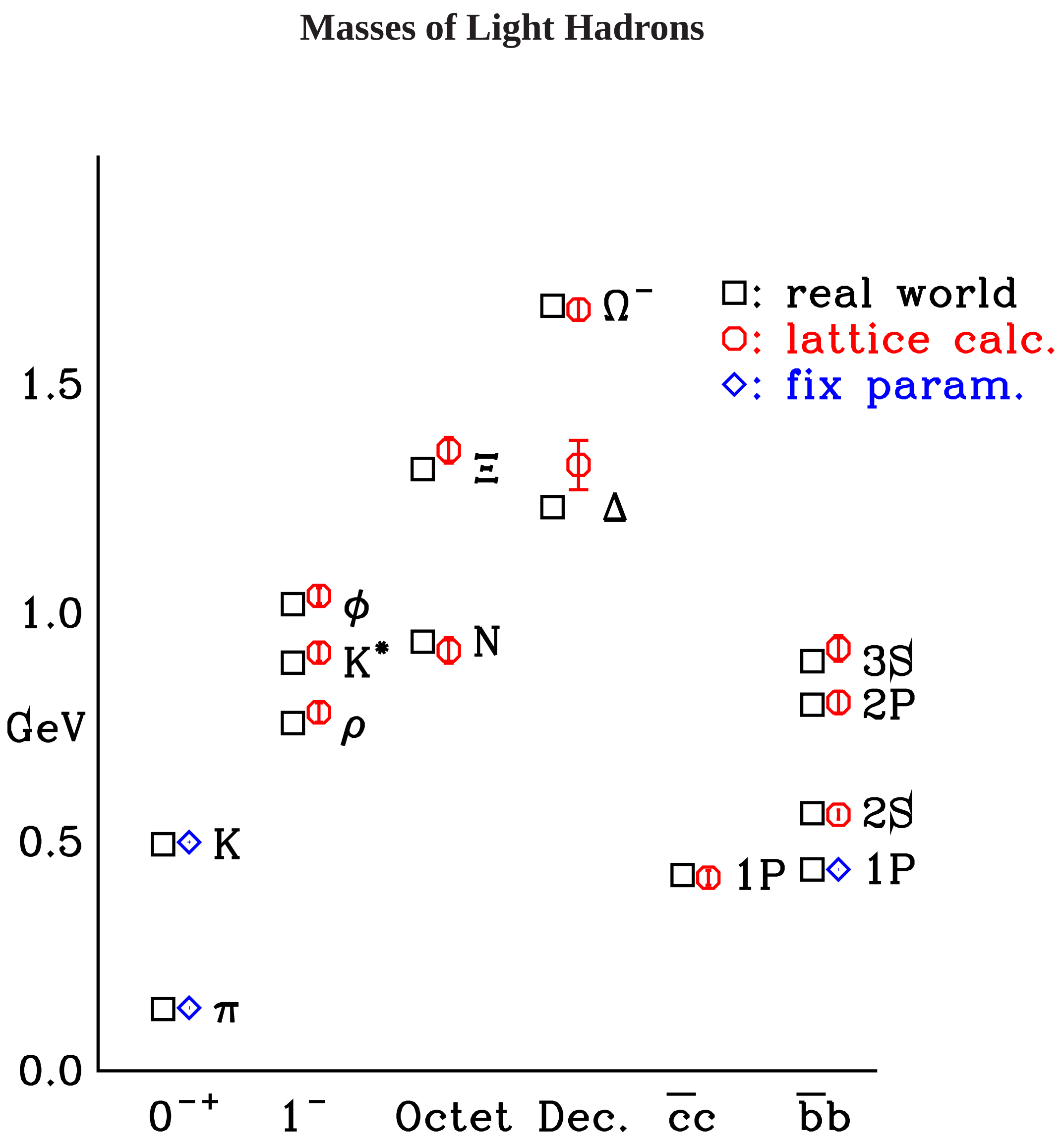


Figure 6: The semileptonic form factor $f_+(q^2)$ for the decay of a D meson into a K meson, a lepton,and a neutrino, as a function of the momentum transfer to the leptons q^2. The orange curve is our lattice prediction, and the blue points are the experimental results of the Belle Collaboration.



Masses of Light Hadrons

Figure 7: Comparison of lattice and experimental values for a variety of hadron masses and splittings. The known π and K masses are used to fix the light quark masses. The $\bar{c}c$ and $\bar{b}b$ (Υ) masses are shown as splittings relative to the $1S$ ground state. The Υ $1S-1P$ splitting is used to determine the lattice spacing.

Mass of the Nucleon

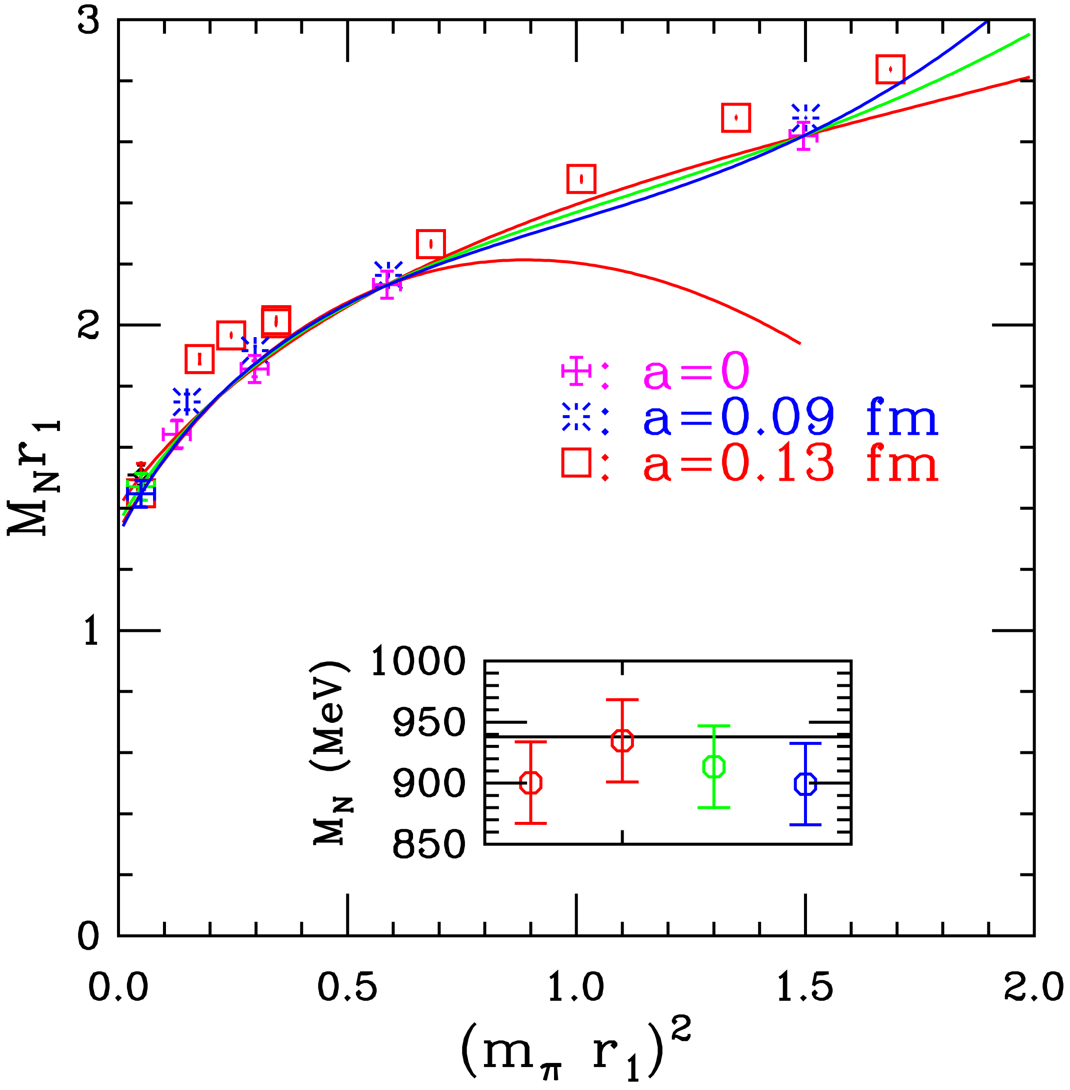


Figure 8: This figure shows the nucleon mass from our simulations, and an extrapolation of our results to the continuum limit. The solid curves are chiral perturbation theory with various assumptions, and the cluster of points at the left are the experimental value and the various chiral extrapolations. The inset shows how the chiral extrapolations compare to the experimental value of 938 MeV.

Mass of the Ω^-

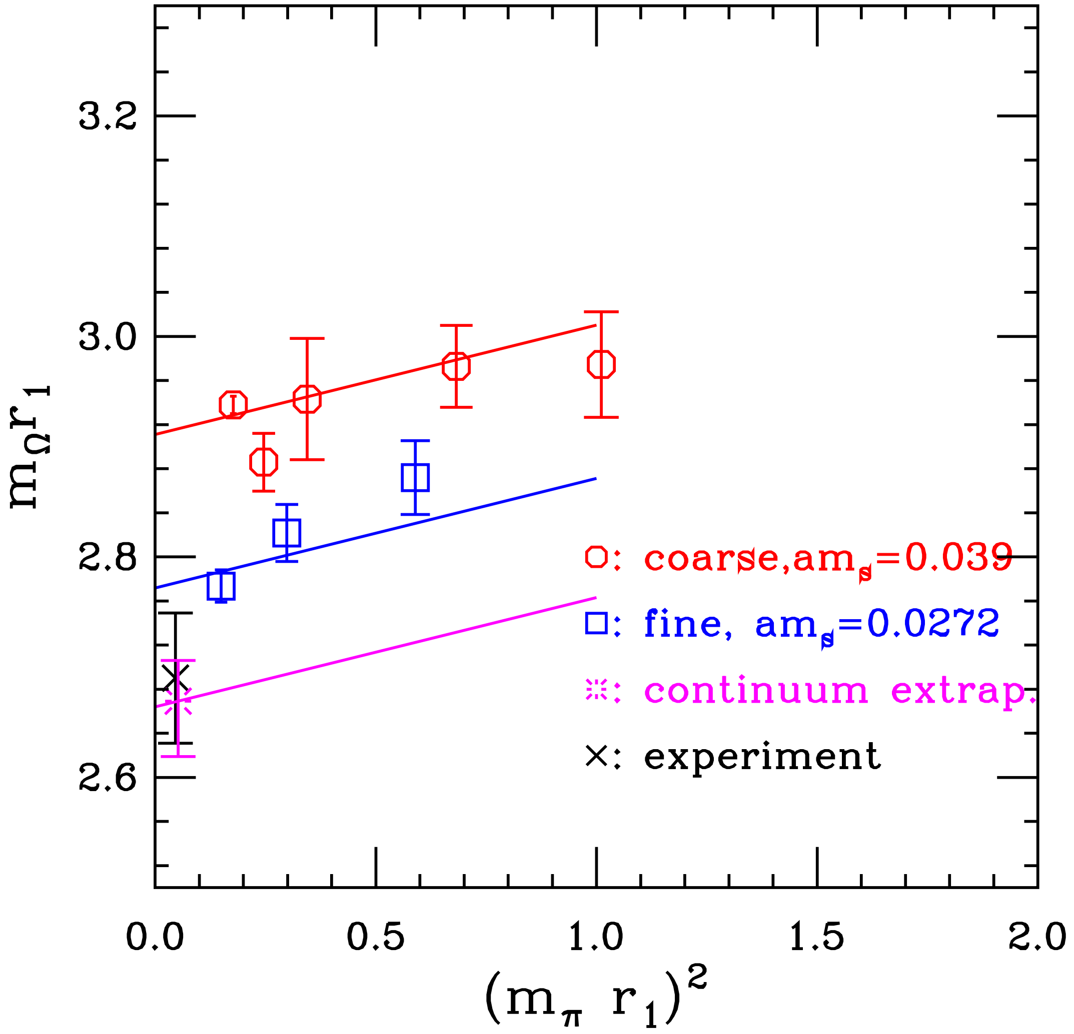


Figure 9: The mass of the Ω^- as a function of the square of the pion mass in units of r_1. The red octagons are data from the coarse ($a \approx 0.12$ fm configurations, and the red line the extrapolation of these points to the physical value of m_l. The blue squares and blue line are the data and chiral extrapolation for the fine ($a \approx 0.09$ fm configurations). The magenta line shows the continuum and chiral extrapolations, and the black cross is the experimental value.. Since the Ω^- mass has no chiral logs involving m_π, the chiral extrapolation for this particle is much simpler than for most others, so its mass can be determined with high accuracy on the lattice. This calculation serves as an important check on our determination of the strange quark mass.

Taste Splittings of the Pion

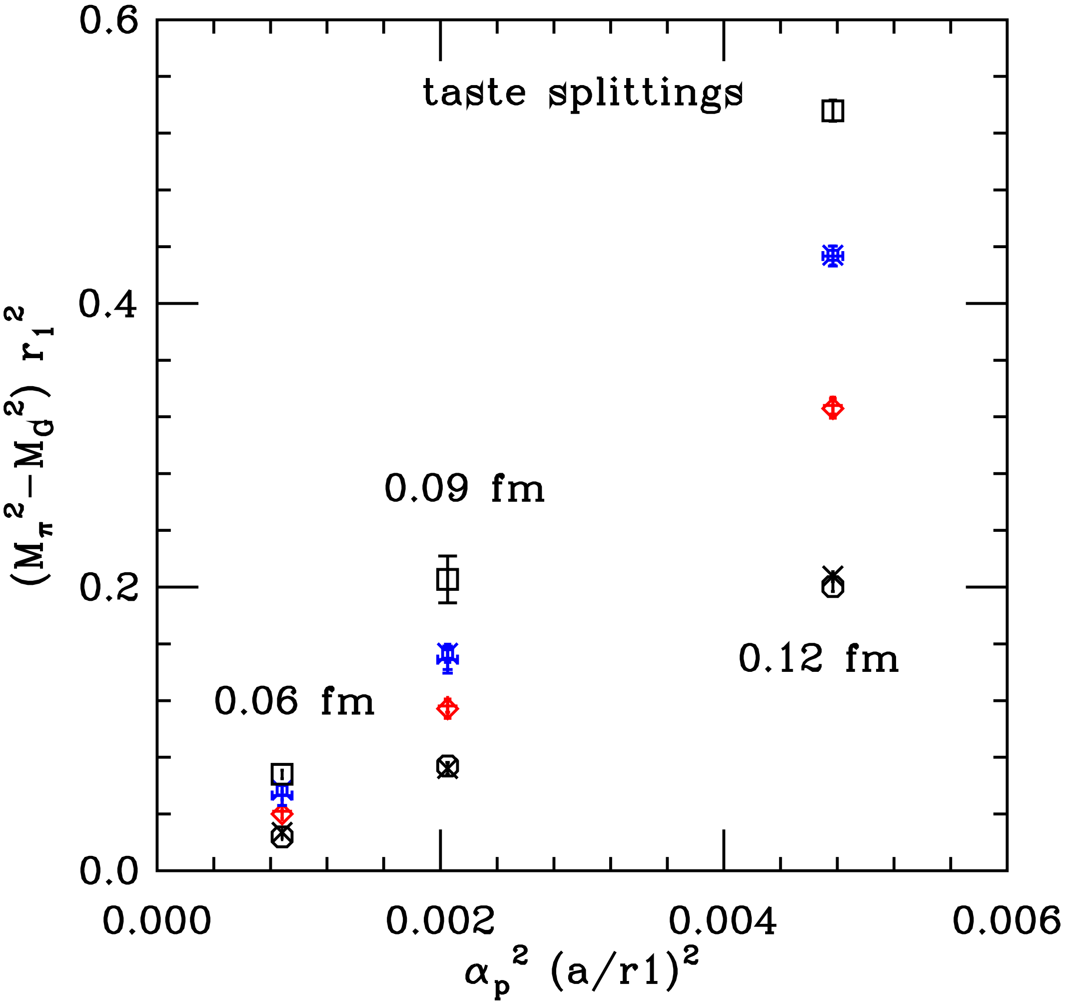


Figure 10: Taste splitting among the pions for lattice spacings 0.12, 0.09 and 0.06 fm with $m_l = 0.4 m_s$. The splittings are plotted as a function of $a^2\alpha_s^2$, the variable in which they are expected to be linear at small lattice spacings. These splittings are important input for including the "taste symmetry breaking" effects in chiral perturbation theory. They also provide a good test of whether the taste symmetry is restored in the expected way as the continuum limit is approached.

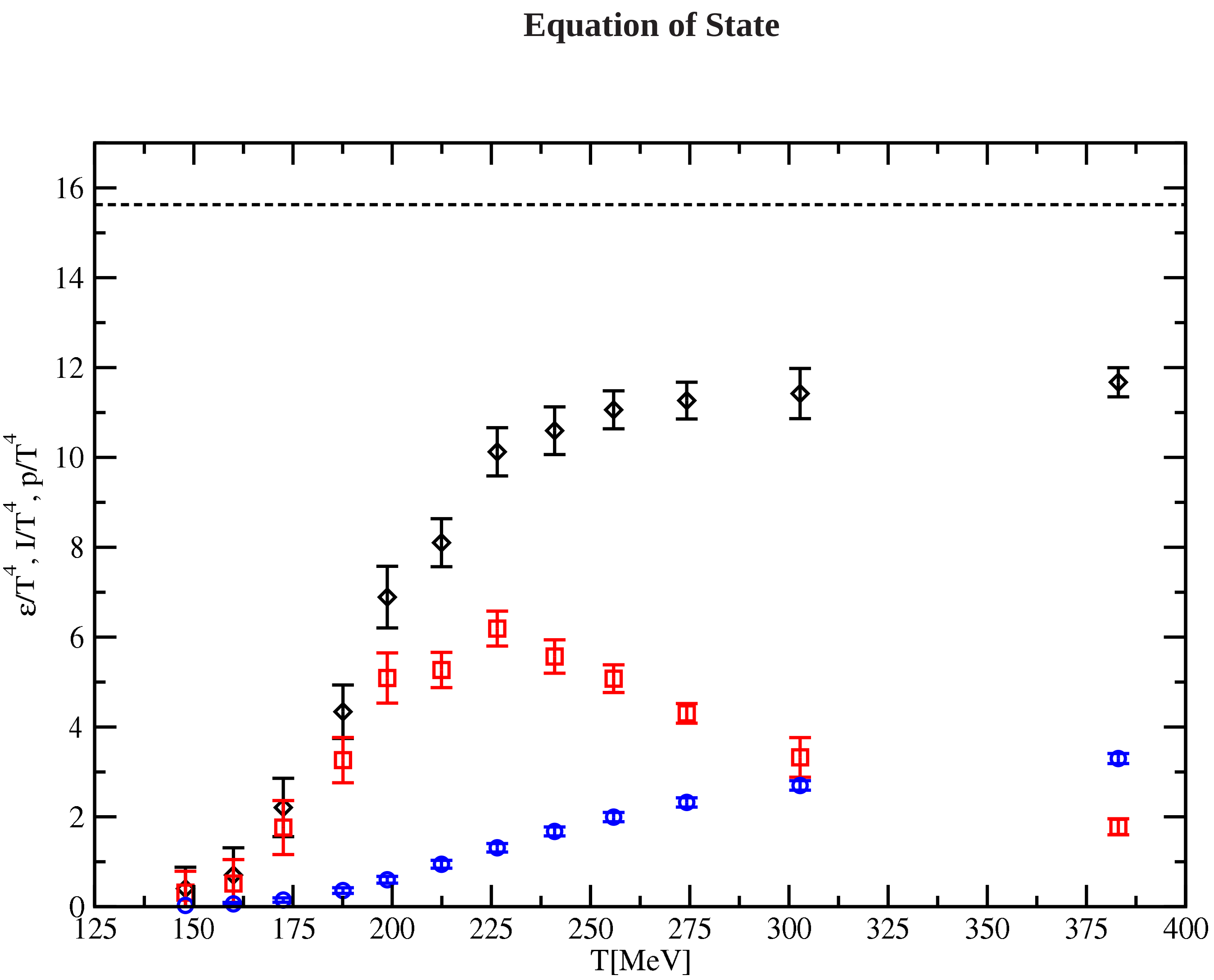


Figure 11: The energy density ε (black diamonds), interaction measure I (red squares) and pressure p (blue circles) in units of T^4 as a function of the temperature T on lattices with six time slices for $m_l = 0.1\,m_s$. The horizontal dashed line is the continuum result for three flavors of massless, non-interacting quarks.