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The Fundamental Constants of Nature from Lattice Gauge Theory Simulations

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Abstract. The fundamental laws of nature as we now know them are governed the fundamental parameters of the Standard Model. Some of these, such as the masses of the quarks, have been hidden from direct observation by the confinement of quarks. They are now being revealed through large scale numerical simulation of lattice gauge theory.

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1. The Standard Model and beyond

The Standard Model of particle physics describes the laws of matter at the most fundamental level currently known.. It contains six quarks (dubbed up, down, charm, strange, top, and bottom), and six leptons (the electron, muon, and tau leptons, and their associated neutrinos). They are organized by the weak interactions into three generations:

$$\begin{pmatrix} u \\ d \end{pmatrix} \quad \begin{pmatrix} c \\ s \end{pmatrix} \quad \begin{pmatrix} t \\ b \end{pmatrix}, \tag{1}$$

$$\begin{pmatrix} e \\ \nu_e \end{pmatrix} \quad \begin{pmatrix} \mu \\ \nu_\mu \end{pmatrix} \quad \begin{pmatrix} \tau \\ \nu_\tau \end{pmatrix}. \tag{2}$$

There are three forces in the Standard Model, the strong, the weak, and the electromagnetic interactions. They are superficially quite different from one another. The W and Z bosons that mediate the weak interactions are very heavy, unlike the massless photons of electromagnetism. The gluons of the strong interactions are also massless, but a free gluon has never been observed. Quarks and gluons seem to be permanently confined in hadrons by the strong interactions.

The parameters of the Standard Model govern its interactions. They are

- the coupling constants of the strong, weak, and electromagnetic interactions, α_s, α_w, and α_{em},
- the masses of the six quarks and six leptons,
  - m_u,m_d,m_c,m_s,m_t,m_b,
  - m_e,m_μ,m_τ,m_{e_ν},m_{ν_μ},m_{ν_τ},
- the matrices of fermion mixings

– among the quarks (the Cabibbo-Kobayashi-Maskawa matrix),

$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix} \tag{3}$$

– and among the leptons,

$$\begin{pmatrix} V_{e\nu_1} & V_{e\nu_2} & V_{e\nu_3} \\ V_{\mu\nu_1} & V_{\mu\nu_2} & V_{e\mu\nu_3} \\ V_{\tau\nu_1} & V_{\tau\nu_2} & V_{\tau\nu_3} \end{pmatrix}, \tag{4}$$

- the mass of the W or Z boson.

At present, these quantities could simply be decrees of the deity as far as we know for sure. Where do they come from? Can we predict them with a more fundamental theory.

The strong interactions confine the quarks, such as the up and down quarks of ordinary matter, into nucleons. The weak interactions are responsible for radioactive decay, such as when a d quark turns into a u quark by emitting an electron and a neutrino.

The Standard Model is maddeningly successful. It agrees with every particle physics experiment performed so far, sometimes to great precision. (The anomalous magnetic moment of the electron, for example, is predicted to a precision of better than one part in a billion.)

Why the word *maddeningly*? The Standard Model contains many gaps and puzzles. These have led particle physicists to conclude that there must be a more fundamental theory of particle physics than the ones yet discovered. We have searched, so far in vain, for evidence of new particles and interactions.

As a glaring example, consider the phenomena that go under the rubric of "Higgs particle". There exist no consistent quantum field theories of heavy vector bosons like the Ws and Zs that do not contain addition scalar particles coupled to the vector bosons. The simplest possibility is a single additional elementary scalar, called the "Higgs", but reality is likely to be more complicated. Consider the force of gravity, which I did not mention earlier. This is because there exists no quantum theory of gravity. The two pillars of twentieth century physics, the theory of Relativity (Einstein's theory of gravity) and quantum mechanics, are inconsistent with each other at very short distances. At least one of them must be modified significantly in a more complete theory. Why is there more than one generation of fermions, when all the matter in the natural world is composed of only particles of the first generation? What is the relation between the three forces? After quantum field theories were developed for each of them, they were seem to all be gauge theories with mathematically very similar structures. It was soon shown how to combine them into a single more fundamental theory, a "Grand Unified Theory". So far, though, experiment has not revealed which, if any, of the possible such theories might be correct.

The list of puzzles and potential clues goes on and on. There is abundant reason to believe in a more fundamental theory "Beyond the Standard Model". So far, experiment has cast little light on which of the many possibilities might be right. Physicists are eagerly searching for any slight deviation from the predictions of the Standard Model to point them in the right direction.

One element of this search is the quest to pin down the parameters of the Standard. Factories for mesons containing heavy quark flavors are pouring out data for determining the CKM matrix elements at accelerators at Stanford, Cornell, and KEK. Another element is the search for new particles and forces. Proton colliders at Fermilab and, soon, at CERN are extending the search for the Higgs to higher and higher masses.

Lattice calculations are essential to this program in two ways. First, they are required to extract properties of quark from properties of hadrons (particles that contain quarks). Experiments examine hadron processes to discover the properties of quarks, and they examine

neutrino processes to discover the properties of neutrinos. The neutrinos are observed directly, and can be analyzed using perturbation theory. The quarks are not observed directly, but are confined permanently within hadrons. Their properties must be inferred using lattice gauge theory calculations.

Secondly, lattice gauge theory calculations are essential to prepare for possible new nonperturbative phenomena in coming experiments. Lattice gauge theory is the first and only general tool for nonperturbative quantum field theory. Of the interactions known to particle physics, only one (quantum electrodynamics) is known to be described by a perturbative theory, whose properties can be expressed as a power series in the electromagnetic coupling constant, $\alpha_{\rm em}$. Strong interactions are known to be described by a nonperturbative theory, quantum chromodynamics or QCD. Consider the "Higgs" of the weak interactions. Is it

- an elementary, perturbative Higgs?
- a bound state of a new strong interactions (technicolor, topcolor)?
- accompanied by very high energy gluino condensates (some supersymmetric models)?

QCD provides an excellent test bed to sharpen our nonperturbative tools to prepare for such questions.

2. Quarks, gluons, and lattice QCD

Quark masses and mixings can't be directly observed. Quarks are permanently confined inside hadrons. As evidence for quarks became stronger in the sixties and early seventies, this nonobservation of quarks became harder and harder to understand in light of another property of quarks that became clear during that period. In electron-proton scattering experiments at Stanford, it became clear that at high energies, the protons behaved as if they were bags full of weakly interacting, almost-free constituents. Why should such almost-free constituents be permanently confined? This paradox was resolved in 1973 with the discovery of the "asymptotic freedom" of QCD. The self-coupling of the gluons mediating the strong force caused the effective value of the strong coupling "constant" to become larger and larger at long distances (long compared with the proton radius), contrary to the well-known behavior of the electromagnetic coupling constant. This meant that even though the quarks were indeed weakly interacting at short distances, the force between them did not die off at long distances, leading to their permanent confinement. Gross, Politzer, and Wilczek shared the Nobel Prize for this discovery in 2004.

The consequence for particle physics is that even though perturbation theory may be used to analyze quark-quark scattering at high energies, to infer the properties of quarks from the relatively low energy dynamics of hadron constituents, the nonperturbative methods of lattice QCD are required.

Quantum field theories are defined by their path integrals. For gauge theory, this may be written schematically as

$$Z = \int d\left[A_{x\mu}\psi_x, \overline{\psi}_x\right] \exp\left(-S(A,\psi,\overline{\psi})\right). \tag{5}$$

The quantum amplitude for a state of quarks and gluons at a given time to evolve into another state at a later time is obtained by integrating over all possible intervening classical field configurations. In principle, one integrates over independent fields defined at each space-time point. A quantum field theory is in principle defined by an infinite dimensional integral (not a very well-defined object). Quantum field theories must therefore be "regulated".

A lattice quantum field theory regulates the continuum theory by defining the fields on a four dimensional space-time lattice. Quarks are defined on the sites of the lattice, and gluons on the

Table 1. Properties of typical sets of gauge configurations for lattice QCD phenomenology calculations.

Lattice spacing (fm)	Quark mass	Volume	Number of configurations	CPU time (teraflop years)
.15	.03	$16^3 \times 48$	500	0.003
	.02		500	0.005
	.01		500	0.011
	...		...	
.10	.012	$28^3 \times 48$	500	0.024
	.006		500	0.08
	.003		500	0.5
	...		...	
.06	.008	$48^3 \times 144$	500	0.4
	.004		500	1.6
...	...		...	

links. Continuum quantum field theory is obtained in the zero lattice spacing limit. This limit is computationally very expensive, which is why large-scale computer simulations are required.

Operationally, lattice QCD calculations consist of the following steps. First, sets of gauge configurations are computed that approximate the integral over classical gauge fields in the vacuum. They are constructed in long Markov chains with Monte Carlo methods, such as the venerable Metropolis method, of the more modern Hybrid Monte Carlo algorithm. Configurations are accumulated at several lattice spacings, and at several values of the masses of the light quarks in the fermi sea, heavier than the physical light quark masses. The results must be extrapolated to the continuum and light quark mass limits. An idealized representative set of gauge configuration parameters is shown in Table 1. To give an idea of the scale of computing involved, to generate the sets of 500 configurations of 0.06 fm, volume $48^3 \times 144$ lattices that is planned this year will take 0.5–1.5 TF-year each, depending on the light quark mass. This step consumes most of the CPU power.

Second, the propagation of quarks through the gauge configurations is calculated. This means solving the Dirac equation on each gauge configuration. On the lattice, this is a sparse-matrix problem, solved with relaxation methods, such as the biconjugate gradient algorithm. This step takes perhaps a quarter to a half of the compute power of the first step.

Thirdly, hadron correlators and amplitudes are computed from the quark propagators. This is a computationally cheap step, consisting mostly of I/O.

State-of-the-art price/performance for computing hardware for this type of calculation is about \$1.3/MF. Larger projects are of order a few Teraflop-years. Our group at Fermilab is currently involved in a joint effort with the MILC Collaboration to calculate the properties of heavy flavor mesons with improved staggered light fermions, on a data set something like the one in Table 1. This year's computational step will be performed on the purpose-built QCDOC computer at Brookhaven and on large clusters at Fermilab. A new set of gauge configurations will be generated on the QCDOC, consuming around 2 TF-years of compute power. These configurations, a few TB of data, will be shipped to Fermilab for quark and hadron analysis on clusters, consuming around 0.7 TF-years of compute power. The QCDOC computations are done with a single, highly optimized program, consist of a few, very long single tasks, and have moderate I/O needs. The cluster programs have large, heterogeneous code bases, consist of many small, individual jobs, and have heavy I/O needs. Either piece of hardware, with work, could have done all the computing jobs required for the entire project. Having both approaches available makes it possible to optimize the running in a robust way.

Progress in numerical science comes from both larger computers and from improvement of methods. A methodological improvement that has been particularly important for the work I'll discuss is improved discretizations. Numerical analysis tells us that if a derivative is approximated by a discrete difference, the resulting discretization errors vanish as the square of the lattice spacing:

$$\frac{\partial \psi(x_i)}{\partial x} = \Delta_x \psi(x_i) + \mathcal{O}(a^2), \tag{6}$$

where $\Delta_x \psi(x_i) \equiv (\psi(x_i + a) - \psi(x_i - a))/(2a)$. By incorporating next-to-nearest neighbor interactions, we can write down an approximation to the derivative whose errors vanish as a higher power of the lattice spacing:

$$\frac{\partial \psi(x_i)}{\partial x} = \Delta_x \psi(x_i) - \frac{a^2}{6} \Delta_x^3 \psi + \mathcal{O}(a^4). \tag{7}$$

This allows control of discretization errors with far less computing power than the simpler derivative. A quark action correcting for all quadratic discretization errors is called the improved staggered fermion "asqtad" action. [1] It is the light quark action used in the calculations of the next section.

3. Lattice QCD confronts experiment

Progress in unquenched lattice QCD. In the last few years, there has been dramatic progress in our ability to perform precise calculations of simple quantities. For twenty years after the first lattice Monte Carlo calculations appeared around 1980, almost all lattice phenomenology was done in the quenched approximation, meaning ignoring the effects of light quarks loops. Although computationally much than correct unquenched calculations, this introduced ten per centish errors into the calculation which supplied an irreducible lower bound on the uncertainties of lattice predictions, as shown in the left-hand graph of Fig. 1. Recently, unquenched calculations with improved staggered fermions (called "asqtad" fermions in the jargon) have matured to the point that these errors can be removed for simple enough quantities. The right-hand graph of Fig. 1 shows the same quantities as on the left, but unquenched and now showing good agreement with experiment at the few per cent level. [2] For these calculations, the masses of some quantities like the pion and kaon masses are used as inputs to fix the fundamental parameters of QCD, the quark masses and the strong coupling constant. Three different groups using this method than compared notes on their predictions for the simplest quantities they were calculating, with the results shown. These results are for the simplest quantities we know how to calculate, and it will be interesting to extend the calculations to more complicated quantities. Likewise, the results shown are obtained with staggered fermions, the least computationally costly of the fermion methods, and it will be interesting to verify that one obtains the same answers with more costly methods. Nevertheless, the progress is striking.

The B_c. Most of the particle masses and other simple quantities that are to be "predicted" by lattice QCD have been well known for fifty years, so that real prediction is impossible. An exception has been the mass of The B_c meson, a meson made of a bottom quark and a charm antiquark. Bottom quarks were discovered in only in the 1970's, and since they are rarely produced in association with charm quarks, B_c mesons were not observed until this past year. Fig. 2 shows the predictions of unquenched lattice calculations done before the observation of the B_c. [3] In December of 2004, the CDF experiment at Fermilab announced the discovery of the B_c. Their result for the mass is shown in the gold bar across the graph, in good agreement with the lattice prediction.

The strong coupling constant. Asymptotic freedom means that the effective coupling "constant" of QCD, $\alpha_s(E)$, is small at in collisions at high energy, E. This means that perturbation theory can be used to analyze high energy collisions, and the strong coupling constant can be measured in a large number of high-energy processes, some of which are shown in the plot in Fig. 3. One can also obtain the strong coupling constant with lattice methods. One obtains α_s on the lattice by using it as a parameter in particle spectroscopy calculations, as in Ref. [2]. One then converts it to the form used in perturbation theory analyses; the result is shown in the next-to-bottom point in Fig. 3. It agrees well with continuum results, as it should. Since the plot was made, a more accurate result has been produced by the authors of the point just discussed, incorporating three-loop lattice perturbation theory. The result is $\alpha_s(M_Z) = 0.1170(12)$, still in agreement with the world average, but now more accurate than any other result.

The light quark masses. When results can be obtained both with lattice QCD and with other methods, the results should agree. Many of the parameters of the Standard Model, however, such as the light quark masses, can only be obtained with lattice QCD. Quark models and other models gave guesses of around $m_s \sim 150$ MeV for the strange quark mass, and $m_l \sim 6$ MeV for the average of the up and down quark masses. With lattice QCD, we can determine these masses with first-principles calculations, for example, by tuning the quark masses to obtain the correct masses for pions and kaons. The result is that the early guesses were simply wrong, the correct answers are about a factor of two lower. A recent paper from one particular group using the set of methods discussed here gives [6]

$$m_s = 76(3)(7) \text{ MeV}, \tag{8}$$

$$m_l = 2.8(1)(3) \text{ MeV}. \tag{9}$$

There is a wide consensus throughout the lattice community that the correct answer for m_s is somewhere in the range 75-105 MeV, and that the earlier guesses were simply wrong.

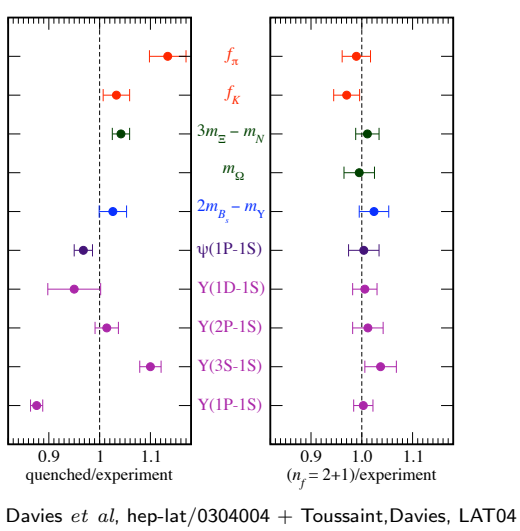

Figure 1. Lattice predictions compared with experiment for simple quantities in quenched and unquenched lattice QCD.

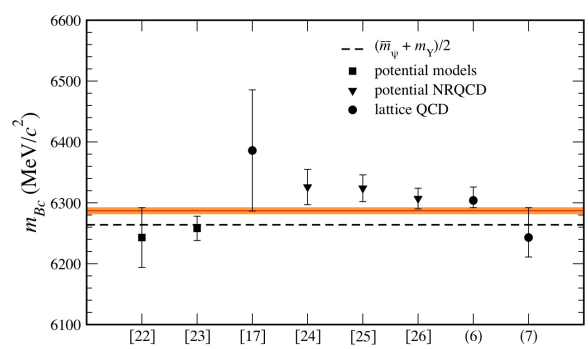

Figure 2. B_c meson observed by the CDF collaboration (gold bar across the figure) compared with predictions of lattice QCD made before the observation (rightmost two data points).

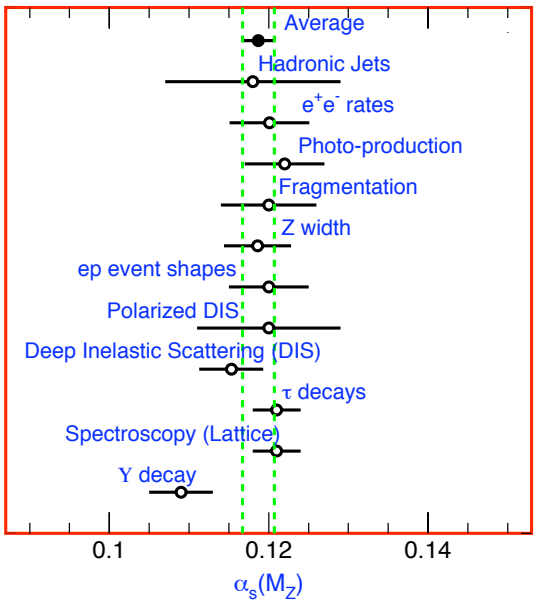

Figure 3. Determinations of the strong coupling constant from a variety of high energy processes, evaluated by convention at the mass of the Z boson, M_Z. [4]

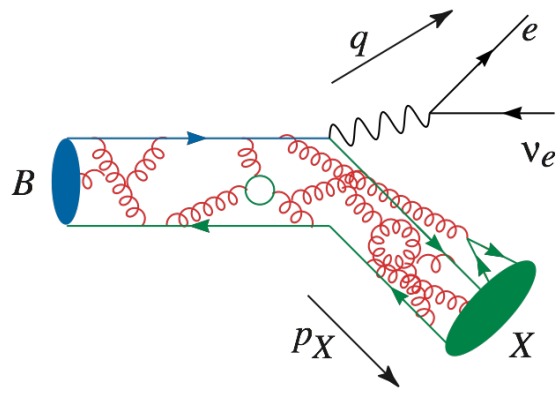

Figure 4. The decay of a B meson into leptons plus hadrons X, where X might be a pion or a D meson. [5]

Table 2. The Cabibbo-Kobayashi-Maskawa matrix elements, with particle processes by which they can be measured.

$$\begin{pmatrix} \begin{array}{c} V_{ud} \\ f_\pi \\ \\ \end{array} & \begin{array}{c} V_{us} \\ f_K \\ K \to \pi l \nu \end{array} & \begin{array}{c} V_{ub} \\ \\ B \to \pi l \nu \end{array} \\ \\ \begin{array}{c} V_{cd} \\ f_D \\ D \to \pi l \nu \end{array} & \begin{array}{c} V_{cs} \\ f_{D_s} \\ D \to K l \nu \end{array} & \begin{array}{c} V_{cb} \\ \\ B \to D l \nu \end{array} \\ \\ \begin{array}{c} V_{td} \\ < B_d | \overline{B_d} > \end{array} & \begin{array}{c} V_{ts} \\ < B_s | \overline{B_s} > \end{array} & \begin{array}{c} V_{tb} \\ - \end{array} \end{pmatrix}$$

Golden quantities and the CKM matrix elements. Most of the results discussed so far are for a particularly simple kind of quantity for lattice QCD: stable meson processes with a single meson present at a time. These are golden quantities for lattice QCD, with uncertainties that are smaller and easier to understand than for most quantities. Although this is a restricted set, many of the most important tasks of lattice gauge theory can be accomplished with quantities of this type. In particular, almost all of the CMK matrix elements and quark masses can be determined with lattice calculations in this category.

CKM matrix elements are measured in decay processes in which a quark of one flavor turns into a quark of another flavor, as given in Table 2. Fig. 4 illustrates B meson "semileptonic" decay, that is, decay into two leptons plus one or more hadrons. In the experimentally observed

Table 3. The values (red) of Cabibbo-Kobayashi-Maskawa matrix elements, measured from semileptonic decay processes (blue). [8]

$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ D \to \pi l \nu & D \to K l \nu & B \to D l \nu \\ 0.24(1)(2)(2) & 0.97(4)(8)(2) & 3.8(1)(1)(6) \times 10^{-2} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}$$

process, a B meson decays into two leptons. the electron and a neutrino, plus hadrons (labeled X), for example a pion. The experimental rate depends on a QCD amplitude, which must be supplied by lattice QCD, and on the CKM matrix element V_{ub}, which is the amplitude connecting a bottom quark and an up quark. Purely leptonic decays, such as a pion decaying into an electron plus a neutrino, are parameterized by decay constants such as f_π. Pion leptonic decay depends on the QCD amplitude f_π and on V_{ud}, the CKM matrix element connecting up and down quarks. The amplitudes for mesons like K, B, and B_s to mix with their antiparticles are proportional to other combinations of CKM matrix elements. In all, eight of the nine CKM matrix elements can be determined from relatively simple lattice QCD calculations combined with experiment.

Semileptonic decays. In semileptonic decay, the shape of the decay amplitude as a function of the momentum of the decay products is predicted by lattice QCD and can be measured in experiment. Fig. 5 shows the decay amplitude for $D \to K l \nu$ semileptonic decay as a function of t, the square of the four-momentum transfered to the leptons, l and ν. The green points are lattice QCD predictions, the blue points are from the experiment of the Focus collaboration which appeared after the lattice predictions. [8] As can be seen, the agreement is excellent.

The shape of a semileptonic decay amplitude is predicted by lattice QCD. The normalization of semileptonic decay amplitudes is give by a lattice calculation times a CKM matrix element. The elements of the second row of the CKM matrix can all be measured from semileptonic decay processes. This makes it possible to determine the entire second row of the CKM matrix from lattice calculations of a similar type, plus experiment. The results of such a set of calculations is shown in Table 3. In the Standard Model, the CKM matrix is an SU(3) special unitary matrix. One component of the search for Beyond the Standard Model physics is checking for evidence of nonunitarity in the CKM matrix. From Table 3, we can check from lattice calculations alone that the second row normalizes to one, as required by unitarity:

$$\left(|V_{cd}|^2 + |V_{cs}|^2 + |V_{cb}|^2\right)^{1/2} = 1.00(4)(8)(2), \tag{10}$$

as required by unitarity. More powerful checks of unitarity are obtained by combining lattice results with those of other methods.

The challenge ahead. To illustrate the challenge ahead, consider the $\rho - \eta$ plane, shown in Fig. 6. In the Standard Model, the CKM matrix may be parameterized by four parameters, two of which are called ρ and η. ρ and η have the form $\rho - i\eta \propto V_{ub}$. They parameterize the CP violation in the Standard Model. CP is a symmetry relating the properties of particles to those of their antiparticles. Understanding the source of CP violation in nature is key to

understanding the abundance of matter over antimatter in the visible universe. The plot is one of the most famous graphs in particle physics at the moment, and reducing its uncertainties is an important goal of particle physics.

Several of the uncertainties in the plot arise from estimates of the uncertainties in lattice QCD calculations. For example, the bounds in the purple curves, labeld ϵ_K, arise from measuring the mixing between K mesons and their antiparticles, analyzed with lattice QCD. Similarly, the bounds in the orange semicircles, labeld ΔM, arise from the mixing between B mesons and their antiparticles. The experimental errors on the mixings that have been measured are of order 1%. The 10 or 20 % uncertainties in the quantities shown in the graph are estimates of the uncertainties of lattice calculations. The current round of calculations aims at reducing these to something of order 5%. Clearly, to profit fully from the experiments that have been done, one needs to aim at lattice uncertainties of around 1%, a very long way beyond where we are today! The progress has been exciting, but the challenge ahead is large.

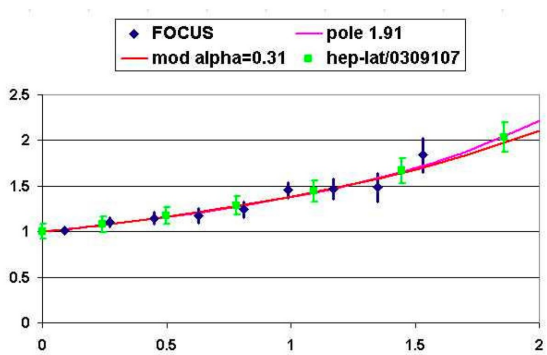

Figure 5. Figure caption for second of two sided figures.

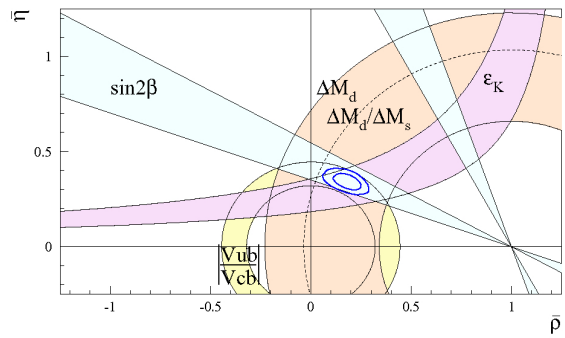

Figure 6. Current bounds on ρ and η, which parameterize CP violation in the CKM matrix. [9]

4. Summary

There has been terrific progress in understanding the dynamics of quarks and gluon with quantitative, first-principles calculations. Some simple things are now done, such as the prediction of the stable meson spectrum and the determination of the strong coupling constant and quark masses. Many other important things look doable with current methods, including determinations of almost all the elements of the CKM matrix. A rich array of further challenges awaits us in QCD and in Beyond the Standard Model physics.

References

[1] S. Naik, Nucl. Phys. B **316**, 238 (1989); D. Toussaint and K. Orginos [MILC Collaboration], Nucl. Phys. Proc. Suppl. **73**, 909 (1999) [arXiv:hep-lat/9809148]; G. P. Lepage, Phys. Rev. D **59**, 074502 (1999) [arXiv:hep-lat/9809157].

[2] C. T. H. Davies *et al.* [Fermilab, HPQCD, MILC, UKQCD Collaborations], Phys. Rev. Lett. **92**, 022001 (2004) [arXiv:hep-lat/0304004].

[3] I. F. Allison, C. T. H. Davies, A. Gray, A. S. Kronfeld, P. B. Mackenzie and J. N. Simone [HPQCD Collaboration], Phys. Rev. Lett. **94**, 172001 (2005) [arXiv:hep-lat/0411027].

[4] S. Eidelman *et al.* [Particle Data Group], Phys. Lett. B **592**, 1 (2004).

[5] Graphic from talk of M. Luke at CKM 2005.

[6] C. Aubin *et al.* [HPQCD, MILC Collaborations], Phys. Rev. D **70**, 031504 (2004) [arXiv:hep-lat/0405022].

[7] C. Aubin *et al.* [Fermilab, MILC Collaborations], arXiv:hep-lat/0506030.

[8] M. Okamoto *et al.*, Nucl. Phys. Proc. Suppl. **140**, 461 (2005) [arXiv:hep-lat/0409116].

[9] M. Ciuchini, E. Franco, F. Parodi, V. Lubicz, L. Silvestrini and A. Stocchi, eConf **C0304052**, WG306 (2003) [arXiv:hep-ph/0307195].