

Quantum chromodynamics with advanced computing

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Abstract. We survey results in lattice quantum chromodynamics from groups in the USQCD Collaboration. The main focus is on physics, but many aspects of the discussion are aimed at an audience of computational physicists.

1. Introduction and background

Quantum chromodynamics (QCD) is the modern theory of the strong nuclear force. The physical degrees of freedom are quarks and gluons. The latter are the quanta of gauge fields, in some ways analogous to photons. The crucial difference is that gluons couple directly to each other, whereas photons do not. A consequence of the self-coupling is that the force between quarks does not vanish at large distances (as the Coulomb force $e^2/(4\pi r^2)$ does) but becomes a constant $F_{\text{QCD}} \approx 800 \text{ MeV fm}^{-1} \approx 15,000 \text{ N}$. It would, thus, require a vast amount energy to separate quarks out to a macroscopic distance. Indeed, long before the separation becomes large enough to measure, the energy stored in the gluon field “sparks” into quark-antiquark pairs. This phenomenon of QCD explains why freely propagating quarks are not observed in nature, and it is called confinement.

QCD is a quantum field theory, which means that from the outset one must deal with mathematical objects that are unfamiliar even to many physicists. The most widely used theoretical tool for quantum field theories is relativistic perturbation theory, as developed for quantum electrodynamics (QED) by Feynman, Schwinger, Tomonaga and others sixty years ago (1). Perturbation theory provides the key connection between the mathematical theory with experiments in QED (2) and the Glashow-Weinberg-Salam theory merging QED with the weak nuclear force (3).

A textbook example of perturbative quantum field theory is to calculate how virtual pairs induce a distance dependence on the coupling in quantum gauge theories. In QED, one considers the fine structure constant,

$$\alpha = \frac{e^2}{4\pi\hbar c}, \quad (1)$$

where $-e$ is the charge of the electron. In QCD, one has the strong coupling α_s , related to the gauge coupling g by analogy with equation (1). When virtual pairs are taken into account, α and α_s are not constant but depend on distance; they are said to “run.” The running, depicted in figure 1, is completely different in the two theories. In QED α becomes constant at distances $r > \hbar/m_e c$ (the electron’s Compton wavelength), but at short distances it grows. In QCD α_s grows at long distance; perturbative running no longer makes sense once r is in the confining

regime. At short distances—or, equivalently, high energies—the QCD coupling is small enough that perturbation theory can again be used. For example, the cross section for an electron-positron pair to annihilate and produce a quark-antiquark pair can be reliably computed as a power series in α_s . The quark and antiquark each fragment into a jet of hadrons—mostly pions, but some protons and neutrons, too—and general properties such as the energy flow and angular distributions of these jets can be traced back to the quark and antiquark. In this way, the experiments can measure quark properties, and these are found to agree with theoretical calculations (4).

QCD and the electroweak theory form the foundation of the Standard Model of elementary particles. They are so well established that many particle physicists consider the chromodynamic and electroweak gauge symmetries, and the associated quantum-number assignments of the quarks and leptons, to be laws of nature. We cannot conceive of a more comprehensive theory that does not encompass them. But there is more to the Standard Model. We know that something must spontaneously break the electroweak symmetry and that something (perhaps the same thing) must generate masses for the quarks and leptons. The Standard Model contains interactions that *model* these phenomena. The model interactions are consistent with observations yet also incomplete. It is hoped that insights obtained with the Large Hadron Collider (LHC), to commence operations at CERN later this year, will enable particle physicists to solve many of the puzzles raised by the Standard Model.

The purpose of this paper is to cover QCD, particularly in the strong-coupling regime where perturbation theory is insufficient. It is worth bearing in mind, however, that there is a close connection between many of the results discussed below and some of the big questions in particle physics. A simple example is the masses of the quarks. To determine the quark masses (which because of confinement cannot be measured), we have to calculate the relation between quark masses and measurable quantities, such as hadron masses. Quark masses are interesting for many reasons, the most unsettling of which is as follows. The mass of the top quark is larger than that of the bottom quark; see figure 2. Similarly, the mass of the charmed quark is larger than that of the strange quark. If this simple pattern held with the up and down quarks—the ones that make up proton and neutrons—then the up quark would be more massive than the down. But then protons would decay to neutrons, positrons, and neutrinos ($p \rightarrow ne^+\nu$). The positrons would find electrons and annihilate to photons.

This universe would consist of neutron stars surrounded by a swarm photons and neutrinos, and nothing else. Our universe is not at all like this, because neutrons are more massive than

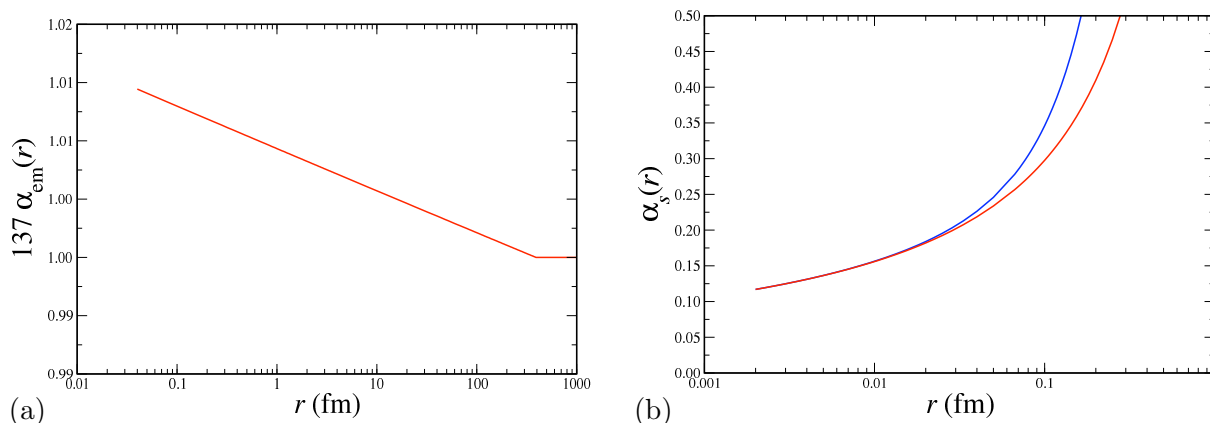


Figure 1. Running of (a) the QED and (b) the QCD coupling with distance. For QCD the red curve shows the perturbative result, and the (higher) blue show the effect of confining forces.

protons. The allowed decay reaction is $n \rightarrow pe^- \bar{\nu}$, leading to an abundance of protons and electrons, and making possible chemistry and biochemistry. With QCD we trace the neutron-proton mass difference back to the down-up quark masses and then to the deeper origin of quark masses. The pattern of quark masses is necessarily not simple, and the search for simple explanation of a messy pattern occupies many particle theorists. Below we give further examples where QCD is essential for working out the mysteries of particle physics.

QCD is also the cornerstone of modern nuclear physics. The simplest nucleus is nothing but the proton, a bound state of two up quarks and one down quark. The neutron is a bound state of two down quarks and one up quark. The confining force is very, very strong. By comparison, the force traditionally called the strong nuclear force is a residue of the fundamental chromodynamic force. This is similar to van der Waals forces among molecules, which are electromagnetic forces between neutral objects with structure leading to a distribution of electric charge. Some basic problems are, therefore, to understand nucleon structure directly from QCD, to study the excitation spectrum of nucleons (and their cousins with strangeness and other flavors), and to see how few-nucleon (or, more generally, few-hadron) systems interact.

Another active area of research in nuclear QCD is the properties of quark matter at high temperature and density. This regime is important to cosmology, because an epoch of the early universe consisted of hot quark matter, and to astrophysics, because, for example, neutron stars are composed of dense quark matter. In the laboratory, nuclear physicists create hot, dense quark matter by colliding heavy ions, at present with Brookhaven's RHIC, soon with (the heavy-ion mode of) CERN's LHC, and someday with GSI's FAIR.

At strong coupling it is necessary to go beyond perturbation theory. In a relativistic quantum field theory, such as QCD, this is not easy. An important obstacle is that a quantum field associates one (or perhaps a few) degrees of freedom with every point in space-time. Hence, the number of degrees of freedom is uncountably infinite. Furthermore, the fluctuations at short distances, if added up naively, contribute an ultraviolet divergence to anything of interest. These fluctuations are treated by a set of ideas known as *renormalization* (5). In short, one must find a tool that (correctly) handles both strongly coupled fields and the renormalization of short-distance fluctuations.

This tool is lattice field theory or, for gauge theories like QCD, lattice gauge theory. The idea, which goes back at least as far as Heisenberg, is to replace continuous space (or, in practice, space-time) with a discrete grid, or lattice. Then the number of degrees of freedom is countable. If the lattice is of finite extent, it occupies a finite physical volume, and, moreover, the number of degrees of freedom is finite. In 1974, Kenneth Wilson showed how to maintain gauge symmetry with a discrete lattice (6). In this and subsequent work, he and others elaborated how the lattice provides a mathematically rigorous definition of quantum field theory via functional integrals (7).

The functional integral for quantum fields on a finite lattice is a familiar object, a multi-dimensional integral, that can be evaluated on a computer. Before downloading some publicly available code (8) and trying to run it on a laptop, let us pause to contemplate how many variables of integration are reasonable (for physics). One wants to have the spacing between

Quark flavors in the Standard Model:

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

$m_u < m_d \quad m_c > m_s \quad m_t > m_b$

!!!

What explains the pattern of masses?

Figure 2. The six *flavors* of quarks come the three *generations* with a doublet in each generation. The doublet structure plays a role in the electroweak interactions. For example, the upper (lower) entries have electric charge $+2/3$ ($-1/3$).

sites on the lattice small enough to resolve hadron structure, and one wants the volume large enough that the boundary conditions do not modify the structure. If one supposes that the ratio of these two lengths is 32, then the dimensions of the integrals of interest are

$$\text{gluon d.o.f.} = 8 \times 4 \times 32^3 \times 128 > 10^8, \quad (2)$$

because gluons come in 8 colors with 4 polarization states each. The factor 128 presumes a space-time lattice with a time extent long (in relativistic units) compared to the spatial extent; this is common practice.

To cope with integrals of such large dimension, the only practical technique is Monte Carlo integration with importance sampling. The weight guiding the importance sampling is e^{-S} , where S is the classical action for the random sample of gluon variables. In functional integral formalisms for quantum mechanics, the expression for the action is the defining equation of the physical system. The development of algorithms to generate these samples is a vibrant subject, covered in part by Bálint Joó's poster here at the SciDAC conference. This paper will not dwell on algorithms, but it is important to mention one more complication.

Quarks are fermions and, as such, must satisfy the Pauli exclusion principle. In the functional integral formalism, this is handled by introducing anticommuting Grassmann variables for fermions. The integration is no longer Riemann (or Lebesgue) integration but a formal procedure called Berezin integration. To make a long story short, in lattice QCD we always can and do carry out the Berezin integration by hand. The outcome is that the weight for the importance sampling becomes $\det M \exp(-S_{\text{gluons}})$, where M is a sparse matrix with space-time indices. The matrix M is $N \times N$, where

$$N = \text{quark d.o.f.} = n_f \times 3 \times 2 \times 2 \times 32^3 \times 128 > 10^8. \quad (3)$$

The quark field represents n_f flavors with 3 colors and 2 spin states of quark and antiquark for every flavor and color. The matrix M is sparse because it is a lattice version of a differential operator, the Dirac operator (generalized to QCD). Incorporating $\det M$ into the weight is computationally demanding, increasing by two or three orders of magnitude the amount of floating-point operations needed to generate a new configuration of gluons.

The lattice is a helpful device mathematically and computationally, but it is not physical. To obtain a real result of the chromodynamics of continuum spacetime, one must work out the integrals for a sequence of lattices, and take the limit $a \rightarrow 0$ in a way that respects renormalization. Taking a smaller and smaller increases the computing burden as onerously as $a^{-(4+z)}$. The exponent z depends on the algorithm and is typically around 1 or 2. The 4 in the exponent is the key reason why numerical lattice QCD requires the most advanced computing facilities available. No algorithm can reduce it, because it is the dimension of space-time.

Most lattice-QCD calculations are carried out in two steps. The first is to generate an ensemble of gluon fields, with a certain lattice spacing and quark masses. This requires the computationally super-demanding $\det M$. To generate an ensemble of useful size, one needs several hundred, perhaps even a few thousand, samples of the gluon field. Computers of the highest available capability are needed for this step. In recent years, lattice gauge theorists have carried out this step with the special-purpose computer QCDOC, large clusters of PCs, and, more recently, leadership-class machines constructed under the auspices of the DOE's Office of Advanced Scientific Computing Research (ASCR). These ensembles of gluon fields are valuable: within the U.S. they are generated by and for particle and nuclear physicists and shared under various agreements. File-sharing is facilitated by formats and software developed by the International Lattice Data Grid (9).

The second step is to mine these ensembles for physics. A simple example is to compute the quantum mechanical amplitude for a proton to propagate from one point to another, and

study the behavior of the amplitude as the separation varies: this is what one does to compute the proton mass, in fact. The key ingredients are a few rows of the inverse of the matrix M , introduced above. With the same ensemble one can study protons, pions, and more uncommon hadrons such as the charmed strange pseudoscalar meson (or D_s for short). Different rows of M^{-1} (i.e., different flavors, colors, spins, and space-time separations) are combined in various ways to obtain the quantum numbers of the hadrons in the problem at hand. Because each problem is different, and there are so many of them, we must attack this problem with the highest capacity computers. The job mix here is heterogeneous, with many users whose job streams range from many large jobs to extremely many medium-sized jobs. The challenge is to develop systems that scale well (for the large jobs), while maintaining the flexibility needed to handle the heterogeneity. The USQCD Collaboration has designed clusters of PCs that deliver this capacity in a cost-effective way (10).

The remainder of this paper focuses on physics. It is organized according to four principal themes of lattice gauge theory:

- Determination of fundamental parameters of the Standard Model of particle physics
- Study of nucleon structure, the hadron spectrum, and hadron interactions
- Simulation of the thermodynamic properties of QCD at nonzero temperature and density
- Lattice gauge theories beyond QCD, such as those appearing in models of electroweak symmetry breaking

Roughly speaking, the first and last are particle physics, and the second and third are nuclear physics. But the lines are blurry: for example, some of the simplest calculations of proton structure (the second item) may play a role more accurate calculations of pp scattering cross sections at the LHC. The way that scientific goals drive the computing needs of lattice gauge theory are discussed further, along the lines of these themes, in public whitepapers of the USQCD Collaboration (8).

2. Standard Model particle physics

In quantum electrodynamics, the fundamental parameters are the masses of electrically charged particles and the fine structure constant α . Similarly, in quantum *chromodynamics*, the fundamental parameters are the masses of colored particles (the quarks) and the strong coupling α_s . Just as α can be determined in many ways (2), α_s can be determined at high energies from jet cross sections with perturbative QCD, and at low energies from the hadron spectrum with lattice QCD. Two recent results are (evaluated at distance $r = \hbar/m_{Z^0}c$)

$$\alpha_s = \begin{cases} 0.1172 \pm 0.0022 & \text{perturbative QCD} & \text{jet shapes} & \text{Ref. (11)} \\ 0.1170 \pm 0.0012 & \text{lattice QCD} & \text{hadrons} & \text{Ref. (12)} \end{cases}, \quad (4)$$

where both error bars reflect experimental and theoretical uncertainties. The first result is determined at high energies, around 100 GeV, in the regime where quarks can be treated as nearly free. The second is determined at low energies, of a few GeV and lower, where quarks are confined. Both are linked soundly to the defining equations of QCD. The agreement demonstrates the richness and broad validity of QCD and should make any enthusiastic scientist say “Wow!”

A straightforward application of lattice QCD is to work out how hadron masses depend on quark masses. Quark masses are interesting for several reasons. As fundamental constants of nature, they are interesting in their own right. As discussed in the introduction, the pattern of quark masses is puzzling and, hence, a motivation to search for extensions of the Standard Model that would contain a simple explanation.

Three flavors of quarks—top, bottom, and charm—have masses large enough to influence some high-energy scattering and decay processes. Their masses can be determined with perturbative QCD as well as lattice QCD. (The results agree (13).) The other three quarks—up, down, and strange—have masses so small that the full bound-state problem must be considered. Lattice QCD, therefore, provides the best information. Some recent results are the following (14; 15):

$$m_u = 1.9 \pm 0.2 \text{ MeV}/c^2, \quad (5)$$

$$m_d = 4.6 \pm 0.3 \text{ MeV}/c^2, \quad (6)$$

$$m_s = 88 \pm 5 \text{ MeV}/c^2. \quad (7)$$

One remarkable aspect of these results is that the strange quark’s mass is somewhat smaller than had been thought on the basis of less reliable techniques for attacking strongly-coupled QCD. This point is, perhaps, of interest mostly to particle physicists, but a further one is of broader interest. The up and down masses—the constituents of protons and neutrons and, thus, everyday matter—are very small, within an order of magnitude of the electron mass ($0.511 \text{ MeV}/c^2$). Only about 1–2% of the proton mass ($938.3 \text{ MeV}/c^2$) or neutron mass ($939.6 \text{ MeV}/c^2$) is accounted for by the quark masses. Consequently, most of their masses—and the mass of everyday matter—arises from confinement, namely, the binding energy of the gluons and the (relativistic) kinetic energy of bound quarks. This is a stunning insight, to be revisited in Section 5.

The caption of figure 2 states that the pairings of quarks in each doublet stem from the electroweak interactions. That is not the full story. There is no reason for the eigenstates of mass to be the eigenstates of the interaction term with W gauge bosons. The two are related by a unitary transformation, V_{CKM} , namely,

$$\begin{pmatrix} d \\ s \\ b \end{pmatrix}_W = V_{\text{CKM}} \begin{pmatrix} d \\ s \\ b \end{pmatrix}_{\text{mass}}, \quad V_{\text{CKM}} = \begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}. \quad (8)$$

Here the initials CKM stand for Cabibbo-Kobayashi-Maskawa; Cabibbo introduced equations (8) for two generations, and Kobayashi and Maskawa were the first to study the ramifications for three generations.

The left-hand side of the first equation denotes the electroweak basis. The labels on the elements of V_{CKM} are the weak isopartner and the mass eigenstate, because the transition amplitude for $W \rightarrow \bar{b}u$, for example, is proportional to V_{ub} . The study of physical processes related to V_{CKM} is called flavor physics, because the central issues are to understand why there are several flavors of quarks and what lends them their separate identities.

As a unitary matrix, V_{CKM} contains complex entries. Some of the phases can be absorbed into unobservable phases of the quark wave functions. For only two generations, one physical parameter remains, and it is real. For three generations, as in nature, three physical parameters are real and one phase remains. The complex couplings imparted by the phase lead to physical processes that proceed at different rates for particles and the corresponding antiparticles. Such reactions are needed to explain the abundance of matter and the dearth of antimatter in the universe. Among particle physicists, this phenomenon is called CP violation. It is clearly intriguing to know whether the CP violation of the CKM matrix is enough to account for the matter-antimatter asymmetry of the universe. According to present measurements and theoretical understanding, it is insufficient, so one would like to know what other interactions violate CP .

In the Standard Model, there is a scalar boson called the Higgs boson. Section 5 will explain more about it. For now let us note that both the quark masses and the CKM matrix have their

Table 1. Decay constants f_P of pseudoscalar mesons (here $P \in \{\pi, K, D, D_s\}$). Values in MeV. Experimental determinations assume a suitable element of the CKM matrix element consistent with all flavor data.

Meson	MILC (15)	FNAL (23)	HPQCD (24)	Experiment (Ref.)	Deviation
π	128 ± 3	–	132 ± 2	130.7 ± 0.4 (13)	0.4σ
K	154 ± 3	–	157 ± 2	159.8 ± 1.5 (13)	1.7σ
D^+	–	201 ± 19	207 ± 4	206 ± 9 (33)	0.1σ
D_s	–	249 ± 17	241 ± 3	277 ± 9 (34)	3.8σ

origin in matrices of couplings between quark fields and the Higgs field. Therefore, the puzzles of CP violation and the pattern of the quark masses are tied together by the Standard Model.

To make progress in flavor physics, lattice-QCD calculations are needed to interpret the experimental measurements. In a schematic form the rate Γ is given by

$$\Gamma = \left(\begin{array}{c} \text{known} \\ \text{factor} \end{array} \right) \left(\begin{array}{c} \text{CKM} \\ \text{factor} \end{array} \right) \left(\begin{array}{c} \text{QCD} \\ \text{factor} \end{array} \right), \quad (9)$$

where the “known factor” consists of well-measured physical constants and numerical factors like 4π . The paradigm is to measure as many flavor-changing processes as possible, and use the Standard-Model formulae to over-determine the CKM matrix. If all the determinations are consistent, then one can set limits on non-Standard sources of flavor and CP violation. To do so, the QCD factor must be computed, and often the only way to do so is with lattice QCD.

There are dozens of relevant measurements, but because the CKM matrix is unitary, the elements of the CKM matrix must satisfy constraints. A particular vivid one is the unitarity triangle that stems from the orthogonality of columns of a unitary matrix:

$$V_{ud}^* V_{ub} + V_{cd}^* V_{cb} + V_{td}^* V_{tb} = 0, \quad (10)$$

which traces out a triangle in the complex plane. The triangle and the present uncertainties from various constraints is shown in figure 3, dividing each side by $V_{cd}^* V_{cb}$. Except for the wedge labelled $\sin \beta$ the uncertainties can be reduced with lattice calculations of the QCD factor.

Lattice calculations for a wide range of observables relevant to the CKM matrix have appeared over the past few years, and further improvements are under way. These include calculations of properties of strange kaons (15; 17; 18; 19; 20; 21), charmed D and D_s mesons (22; 23; 24), and beautiful B and B_s mesons (25; 26; 27; 28; 29; 30). For recent reviews, including references to work in Asia, Australia, and Europe, see (31; 32).

The past several months witnessed an unexpected development in flavor physics, in the field of leptonic decays of pseudoscalar mesons. (Pseudoscalar bosons have spin 0 and negative parity; the most common examples are the pion and kaon.) One can consider the measured decay rates to determine a QCD matrix element called the decay constant, and denoted f_π (for the pion), f_K (for the kaon), and so on. Table 1 shows the results of some SciDAC-supported calculations of decay constants and the corresponding measurements. The calculations agree very well with the measurements, except in the case of the charmed strange pseudoscalar meson D_s .

This set of circumstances is odd, because the computation is easiest for the D_s . Algorithms for the propagators of light quarks slow down as the quark mass m_q is decreased. As a consequence, properties of hadrons containing up or down quarks are reached via a (controlled) extrapolation in m_q . This introduces a source of uncertainty that is absent for the D_s , which, as the lightest bound state of a charmed quark and a strange antiquark, can be computed by working directly at the physical quark masses.

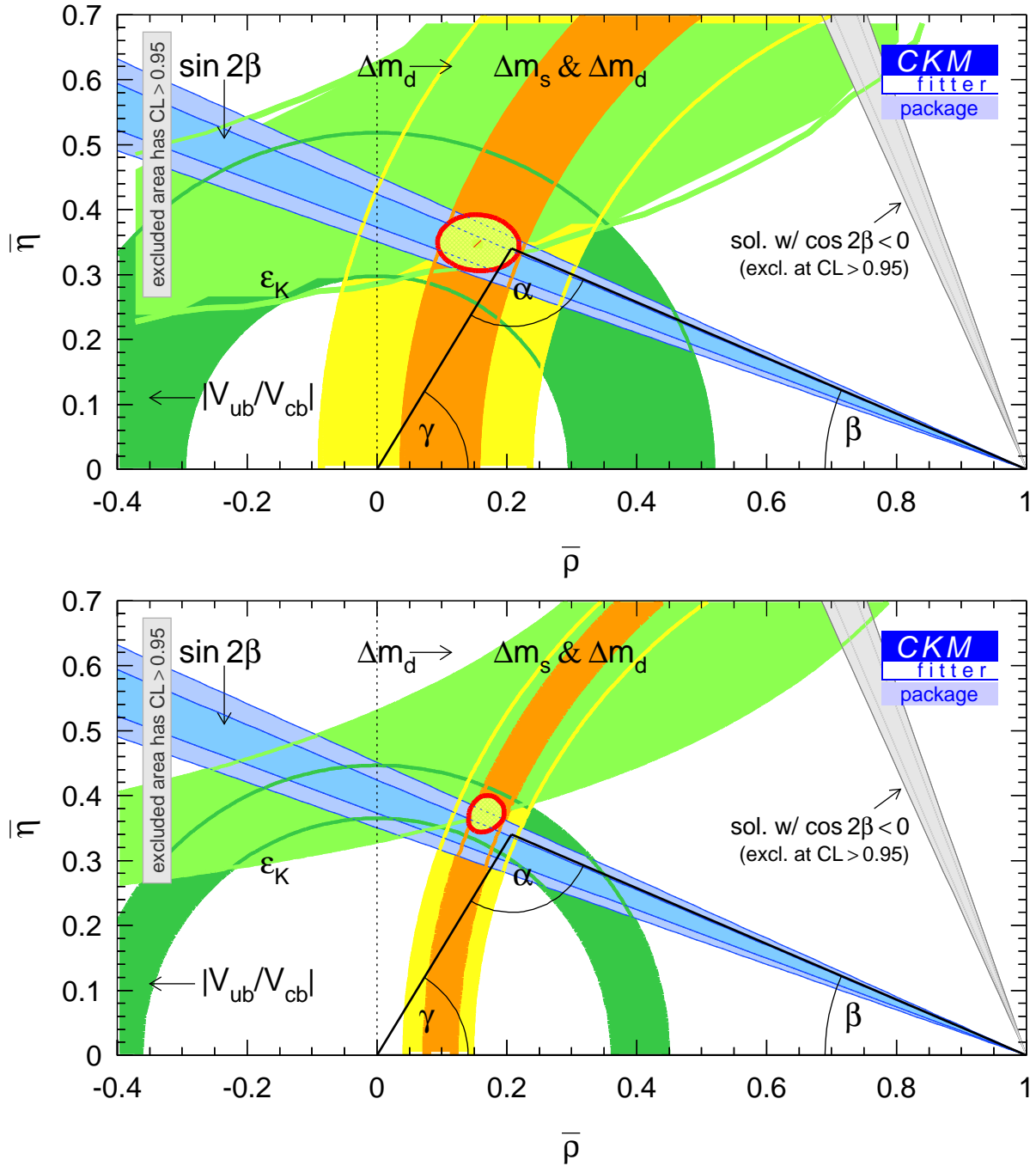


Figure 3. Constraints on the CKM unitarity triangle from experiments and QCD calculations, highlighting those where lattice QCD plays a role. The upper panel shows the current status, and the lower a forecast of how the uncertainties can be reduced with lattice QCD (16). In the lower panel, one can envision tension between the lime-green hyperbola and the blue wedge, depending on how the central values evolve and measurements and lattice-QCD computations improve. The current status of the angles α and γ is omitted, because better measurements are needed; they are expected from LHC**b**.

There is no obvious explanation for this discrepancy within the Standard Model. Unless there is a real blunder somewhere, the discrepancy points to a non-Standard particle mediating the decays $D_s \rightarrow \mu\nu$ and $D_s \rightarrow \tau\nu$, thereby changing the interpretation of the “measured” f_{D_s} . It turns out to be rather easy to devise models of such interactions (34). Given the agreement of CLEO’s new measurement of f_{D^+} (33), new W' bosons and charged Higgs bosons seem unlikely, making leptoquarks—particles with baryon and lepton number—are the most plausible agents of decay.

3. Nucleon structure and nuclear physics

Let us turn now to nuclear physics, where the importance of lattice QCD is difficult to overstate. Many nuclear laboratories, such as Jefferson Laboratory in the U.S., have turned their attention to the structure of the proton (the simplest nucleus!) (35), the excitation spectrum of baryons (36), and processes that may produce glueballs. On the theoretical side, the previous decade witnessed dramatic growth in the application of effective field theories to understand nuclear interactions (37). These techniques connect a wealth of nuclear and hadronic data to the QCD Lagrangian. Lattice QCD is an irreplaceable tool to interpret the new and upcoming experiments at JLab and to compute the so-called low-energy constants of the effective theory (38).

A topic at the interface between nuclear and particle physics concerns the distributions of partons (a generic term for quarks and gluons) inside the proton. In high-energy collisions of $p\bar{p}$ (at the Tevatron) or pp (at the LHC), the transverse motion of partons can be neglected. To compute cross sections (to produce, say, a Higgs boson), the key property needed is the distribution of the longitudinal momentum. From a nuclear perspective, this is also one of the most basic aspects of proton structure. Usually one studies parton distributions q as a function of the fraction x of longitudinal momentum carried by a parton, $0 < x < 1$. Fits to scattering data can determine $q(x)$ only over a range, $x_{\min} < x < x_{\max}$, limited by kinematics and statistics. Lattice QCD can compute moments of q : $\langle x^n \rangle_q = \int_0^1 dx x^n q(x)$. Clearly the two kinds of information are complementary. The experimental range can be extended with *ad hoc* functions possessing the right asymptotic forms at the endpoints, and in this way an Ansatz-guided experimental determination of $\langle x^n \rangle_q$ is possible. One finds good agreement with lattice calculations (39). To explore nucleon structure further, the next step is to probe the transverse structure and compute the so-called generalized parton distributions (39).

The axial charge of the nucleon is another topic of keen interest, because it appears in the description of β decay. It is also related to the relative spin polarization of up and down quarks in the proton. Some recent results with lattice QCD are

$$g_A = \begin{cases} 1.21 \pm 0.08 & \text{Ref. (40)} \\ 1.20 \pm 0.07 & \text{Ref. (41)} \end{cases}, \quad (11)$$

showing good agreement with experiment ($g_A = 1.269 \pm 0.003$). Work is under way to reduce the theoretical uncertainty.

In all fields of physics, spectroscopy is a time-honored approach to learn about the dynamics of the underlying phenomena of interest. In nuclear and hadronic physics, therefore, an important area of investigation is the excitation spectrum of hadrons, particularly baryons. Excited states present additional challenges for lattice QCD, but the tools needed are available and have been demonstrated to work (42; 43). This subject extends to include topics such as the intriguing Roper resonance (44) and electromagnetic transitions of the form $\gamma N \rightarrow N^*$, where N^* is an excited nucleon (45).

Because the gluons couple to each other, it is conceivable that there are hadrons consisting essentially of gluons, with no valence quarks. (Virtual quark-antiquark pairs appear in all

hadrons.) The most persuasive evidence that glueballs do indeed exist come from lattice-QCD calculations. In an approximation omitting virtual quark pairs, the evidence is clear that stable gluon-only bound states arise (46; 47). There are two challenges with glueballs. One, obviously, is to extend the lattice calculations to full QCD with virtual quark-antiquark pairs. The other is to identify them unambiguously in the laboratory (48). Experiments with γp collisions are expected to produce such states and are planned at the 12 GeV upgrade of CEBAF, the accelerator at Jefferson Lab. To plan this program it is essential to know the photocouplings of the mesons (exotic or not). It is possible to compute these photocouplings in lattice QCD, as has been demonstrated for charmonium ($\bar{c}c$ mesons) (49). An extension of this work to light mesons, including exotics and glueballs, is under way.

A long-term goal of nuclear physics is to compute many-body interactions from QCD. In addition to providing a better understanding of the nucleus, these calculations are relevant to mesonic atoms, namely, those containing a positively and negatively charged meson, and to strangeness in neutron stars. Although in some cases lattice QCD results can be compared to measurements, the more interesting situation is where this cannot be done. The aim here is to gain confidence in the reliability of these difficult calculations, so that one can use them (with robust uncertainty estimates) in applications where it is otherwise impossible to acquire the needed information any other way.

An interesting example is the lattice calculation of the πK scattering lengths, of which there are two, $a_{1/2}$ and $a_{3/2}$, depending on whether the πK system has isospin $I = \frac{1}{2}$ or $\frac{3}{2}$. A recent lattice-QCD calculation finds (50)

$$a_{1/2}m_\pi c/\hbar = +0.1725 \pm 0.0017^{+0.0023}_{-0.0156}, \quad (12)$$

$$a_{3/2}m_\pi c/\hbar = -0.0574 \pm 0.0016^{+0.0024}_{-0.0058}, \quad (13)$$

in convenient dimensionless units. These are in rough, but not spectacular, agreement with other determinations using chiral perturbation theory or the Roy-Steiner equations. For example, an analysis based on the Roy-Steiner method (51) finds

$$a_{1/2}m_\pi c/\hbar = +0.224 \pm 0.022, \quad (14)$$

$$a_{3/2}m_\pi c/\hbar = -0.0448 \pm 0.0077, \quad (15)$$

employing an extrapolation from high energies down to the threshold (where the scattering length is defined); see (38) for more discussion. A more direct experimental determination is proposed by the DiRAC Collaboration, which would form $\pi^- K^+$ atoms (52). In this sense, Eqs. (12) and (13) represent something exciting: a theoretical prediction awaiting definitive experimental confirmation.

Multimeson systems are proving to be a fruitful area of research, with further work on $\pi\pi$ (53), KK (54), and even states with as many as twelve pions (55). Once methods have been vetted in mesonic systems, the next step is to consider nucleon-nucleon (56) and nucleon-hyperon (57) systems. This is more difficult, because the signal-to-noise ratio in the Monte Carlo estimate of baryonic correlation functions is worse. Here the methods of effective field theories can be used to extend feasible lattice-QCD calculations to a wider range of nuclear phenomena. The hyperon-nucleon interaction is of interest, because there is speculation that the large Fermi energy may make it energetically favorable for some nucleons to transmute to hyperons (58).

4. QCD thermodynamics

The discussion in the introduction of the computational scope of numerical lattice QCD mentions that, but does not explain why, the spacetime lattice usually has a time extent much longer than

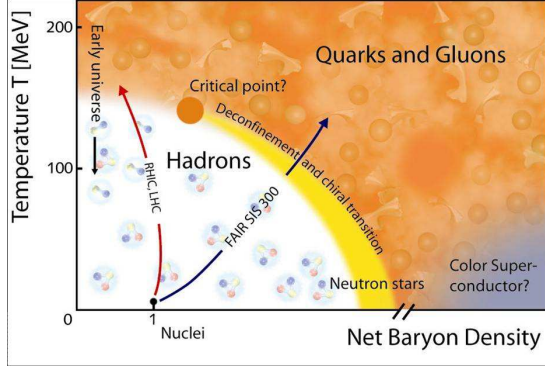


Figure 4. Phase diagram of QCD, showing conjectured phases and phenomena of physical interest. Accelerator experiments at RHIC and LHC probe small chemical potential, around the crossover regime. At the planned Facility for Antiproton and Ion Research (FAIR) experiments can reach larger chemical potential. Image from the CBM Collaboration (60).

the spatial dimension, for example, $32^3 \times 128$. The reason is that the functional integral actually describes a grand canonical ensemble (in the sense of thermodynamics) at temperature T ,

$$k_B T = \hbar c / N_t a, \quad (16)$$

where N_t is the number of sites in the time direction, a is the lattice spacing, and k_B is Boltzmann's constant. In the applications to particle and nuclear physics discussed in Sections 2 and 3, one wants $T = 0$ and, hence, takes N_t large enough for the Boltzmann suppression $e^{-mc^2/k_B T} = e^{-N_t a m c / \hbar}$ to eliminate thermal effects, where m is a hadron mass.

There are, however, many areas of research where a nonzero temperature and a nonzero chemical potential arise. For nonzero temperature, one simply makes N_t smaller, typically $4 \leq N_t \leq 12$ in current work. Such lattices take somewhat less memory, but not less computing because thermodynamics obviously requires calculations at several temperatures. It is conceptually easy to introduce a nonzero chemical potential into lattice gauge theory, but the conceptually clean approach is computationally beyond present resources. For small chemical potential, several approaches are available and efficient (59).

The physical phenomena of interest are summarized by the phase diagram in figure 4. The key feature is a phase transition from hadronic matter to a substance called the quark-gluon plasma. The transition is expected to be first order and end at a critical point at chemical potential $\mu \neq 0$. Between the critical point and the $\mu = 0$ axis the transition is a rapid crossover. Lattice-QCD calculations, as well as measurements of heavy-ion collisions at RHIC and LHC, probe the crossover, which is relevant to the cooling of the early universe. Neutron stars appear at high baryonic density, namely, high μ . At even higher densities, several phases with color superconductivity are thought to exist. Apart from heavy-ion collisions (so far at small μ) much of this phase diagram is unexplored, and lattice gauge theory offers the only *ab initio*, quantitative, theoretical tool to see if it really reflects QCD.

The central concept in QCD thermodynamics is the equation of state (EoS), namely, the relationship between the pressure p and energy density ϵ as the temperature T and chemical potential μ are varied. The EoS reveals the relevant degrees of freedom. In QCD, are they hadrons? Or quarks and gluons? At low temperatures, hadrons are clearly present, and phenomenological models of hadron gases can describe QCD thermodynamics. At very high temperatures, perturbation theory in $\sqrt{\alpha_s}(\hbar c/k_B T)$ can be used. But near the transition, nonperturbative methods are needed.

The first step is to find the transition temperature, which has now been done with 2+1 flavors of realistic sea quarks (61; 62). The different physics below, near, and above the critical temperature T_c also has ramifications for controlling systematic errors. Discretization effects from the lattice, for example, depend on the basic degrees of freedom. (For a crossover it is, strictly speaking, incorrect to speak of a critical temperature. But the critical point in the phase diagram is close enough to the $\mu = 0$ axis that thermodynamic variables change rapidly at T_c .)

The next step is to map out the thermal contribution to the trace of the energy-momentum tensor, $\text{tr } \Theta = \epsilon - 3p$. From the temperature dependence of $\epsilon - 3p$ other thermodynamic variables, such as the entropy density, can be worked out. This also has now been done with 2+1 flavors of realistic sea quarks (63; 64), including at small μ (65). As the system is heated, even to $2T_c$, the behavior of $\epsilon - 3p$ shows that the system does not turn rapidly into weakly interacting quarks and gluons.

To make contact with heavy-ion collisions, the last step would be to take the output of lattice QCD as input to hydrodynamic models. With these models one would then compute experimental observables, such as elliptic flow and quarkonium suppression. With current computing resources, the EoS has been pinned down with 20–25% accuracy. To make a big impact on hydrodynamic modeling, however, it will be necessary to reduce the error to 5%. This is conceptually straightforward to achieve, but it will be computationally challenging. Part of the strategy is to reduce discretization effects, which scale as a^2 (a is the lattice spacing), while the net cost scales as a^{-11} .

5. Non-Standard particle physics

As mentioned above, particle physics awaits a new era when the LHC starts producing physics results. Commencing later this year, the LHC will collide two beams of 7 TeV (TeV = teraelectronvolt) protons. (Amusingly, some particle physicists now call this energy scale the terascale, deliberately alluding to terascale computing. It would be unkind to tell them that in computing we are moving on to the petascale.) In particular, the LHC will address the central problem of particle physics, which is the origin of the W and Z boson masses. The fact that these masses do not vanish demonstrates that some mechanism breaks the electroweak gauge symmetry spontaneously. “Spontaneous symmetry breaking” means simply that, although the equations of motion are symmetric, the solution chosen is not symmetric. For example, in the Standard Model a scalar field breaks electroweak symmetry, via a technique invented by Higgs. Interactions between the Higgs field and the fermions also generate (in the Standard Model) the quark and charged lepton masses and the CKM matrix. Therefore, flavor physics will remain interesting in the LHC era, and the physics program discussed in Section 2 will need to be continued and extended.

In this section, however, I would like to consider applications of lattice gauge theory to understanding the mechanism of electroweak symmetry breaking. Since we suspect that the Standard Higgs sector is far from the full story, it is possible (some would say likely) that strongly coupled fields are involved. For example, instead of being an elementary field, the Higgs boson (and its siblings, the longitudinal polarization states of the W and Z bosons) could be composite. The constituents would then form a whole spectrum of states, just as quarks bind into many different hadrons. Even if the Higgs is elementary at the terascale, other agents of electroweak symmetry breaking could be strongly coupled.

Numerical work on theoretical bounds on the Higgs mass are a long-standing topic in lattice field theory (66; 67). The issue is that the Higgs mass is proportional to its self-coupling, which runs at short distances in a way similar to α in QED; see figure 1. The perturbative running becomes invalid once the coupling is too large, and nonperturbative methods are required. A subtle relation arises between the Higgs mass and a scale where new phenomena imply that the Standard Model breaks down. To make a long story short, one can in this way bound the Higgs mass from above. A similar analysis applied to the Yukawa coupling between the Higgs field and the top quark leads to a lower bound on the Higgs mass, as discussed in a recent comprehensive analysis (68).

A popular class of non-Standard models is to replace the Higgs sector with a strongly interacting sector that is, in some respects at least, analogous to QCD. In fact, absent a stronger source of symmetry breaking, the pions of QCD would break the electroweak symmetry, leading

to W and Z masses around 100 MeV. What one needs, then, is a new quantum number, called technicolor, and a gauge force to bind the corresponding particles, called techniquarks, together. These dynamics are posited to take place at terascale energies and, by analogy with QCD, generate vector boson masses around 100 GeV, as observed. The earliest models of technicolor followed the example of QCD too closely and have been ruled out by experimental measurements. One way around the experimental constraints is to assume that the coupling evolves more slowly than in QCD. This is called “walking” (i.e., slower than running) technicolor. For a wide range of scales below the confining scale, the coupling is too strong for perturbation theory to be relied on, so nonperturbative work with lattice gauge theory is called for. In the past year, the walking hypothesis has indeed been tested, by examining the scaling behavior of the technipion mass, the vector meson mass, and the technipion decay constant (69). Even more recently, the evolution of α_s in (a TeV-scale version of) QCD with several flavors has been computed (70), to see how many flavors are needed to having a walking coupling, and how a walking coupling changes the physics.

The most popular way to relieve the theoretical problems of the Standard Model is to introduce supersymmetry, a symmetry that transforms fermions into bosons, and vice versa. In these models, every known particle (quarks, leptons, gauge bosons) comes with another state known as a superpartner. In the minimal supersymmetric model, the Higgs sector contains three neutral bosons, a charged pair, and their superpartners. No superpartner has been observed, so at the terascale and below supersymmetry must be broken somehow. Usually supersymmetric models are conceived of as weakly coupled, but, since they are gauge theories, strong coupling is not to be dismissed out of hand. It is therefore of great interest to formulate and simulate supersymmetric gauge theories on a spacetime lattice. This has been an extremely fruitful theoretical field during the past several years (71; 72), and now first numerical simulations are being carried out (73; 74). This rapid development yields hope that nonperturbative studies of supersymmetric models will be possible, including studies of supersymmetry breaking.

6. Perspective

Every now and then one hears the question, “How much computing would it really take to solve QCD on a computer?” The questioner is (usually) well meaning, but most experts would agree that the question is not well conceived. The calculations for some of the simplest hadronic quantities are finally becoming mature, with analyses that forthrightly address all sources of uncertainty. This class of observable, sometimes called “gold-plated” (75), consists of masses of particles that are stable (with respect to the strong interactions), not too close to thresholds, and of hadronic transition matrix elements with one or zero of these stable hadrons in the final and initial states. Many, but not all, aspects flavor physics (Section 2), and some aspects of hadronic structure (Section 3), lie in this class, and the first solid round of serious computation is nearing its end.

But this is the end of the beginning. In these nearly mature fields, it turns out that precision is important, at least for the foreseeable future. For example, to gain persuasive evidence of new phenomena in flavor physics, 5–25% accuracy is not enough. A better target (given the stakes and the quality of the corresponding experiments) is 1–3%. If the history of kaon physics is a guide, it will eventually be important to go further. Happily, the need for and clear path to precision has persuaded the particle-physics community that the resources needed for lattice flavor physics are worth the cost.

Even a quick glance at Section 3 reveals that the large majority of interesting problems in nuclear physics require much more computing resources than gold-plated observables. By definition the excited hadrons are not stable under the strong interaction. They will be harder to pin down, and it is possible that we will not know how hard until the work currently under way reaches some of its milestones. The calculations of scattering lengths, while impressive,

must be repeated with several values of the physical volume to ensure that the mathematical formalism used to extract them works as it should. Given the importance of nuclear lattice QCD in guiding nuclear experimentation, one would hope for full support from experimenters for the needed computing resources.

The “how much?” question should be rephrased. It is really a class of questions, “How much computing would it take to compute my favorite observable?” Of course, the answer depends on your observable and its wider context. It should be clear, however, that physics with either precision and complexity leads to questions whose answers will need one or two orders of magnitude more computing than what is available now.

Another reason the “how much?” question is ill-conceived is that it often overlooks the heterogeneous job mix needed to attack many problems in lattice QCD. It is not enough to generate huge ensembles of lattice gauge fields, with ever smaller lattice spacing and ever smaller quark masses, on the world’s highest-capability computer. This step is necessary, creating a gold mine of information. It is not enough, however, merely to open a mine; the gold must be extracted and, here, we need a large capacity of computing that is flexible in every way (while having significant capability of its own).

We do not know how broad the future of lattice gauge theory will be. If the LHC discovers a strongly interacting sector beyond the Standard Model, it is likely that chiral fermions play a role. This is simply because, at the terascale, we already know that left-handed fermions and right-handed fermions are different fields. But chiral fermions possess some conceptual and computational challenges not found in QCD. A strongly coupled terascale will bring many more particle theorists to lattice gauge theory, and this larger community will clamor for computing that is up to the task.

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