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Lattice Fields in the LHC Era

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Lattice QCD

Lattice field theory was invented by Wilson (1974) to try to explain how the strong force, described by Quantum Chromodynamics (QCD), binds quarks permanently into the observed hadrons. He replaced space-time by a regular four-dimensional lattice with quark fields at the sites and gluon fields on the links between neighbouring sites, retaining the local gauge invariance of the theory at the sites. This controls the infinities of the quantum field theory by defining it as the zero-lattice-spacing, or "continuum", limit of the lattice theory. The number of degrees of freedom is proportional to the number of sites and hence is finite on a finite-volume lattice, permitting physical quantities to be computed within a fully controlled approximation, if the volume is large enough. QCD is "asymptotically free" – its beta function is negative and has a fixed point at zero gauge coupling the existence of which can be established using perturbation theory, and, because of this, tuning the gauge coupling to zero reduces the lattice spacing to zero relative to any physical scale, such as the size of a hadron. Thus, dimensionless ratios of physical quantities become insensitive to the lattice spacing and equal to their continuum values in this limit. Of course, the volume of the lattice must be kept larger than any of the important physical scales as this limit is taken, which means that the number of lattice sites and the computational cost grow, actually very rapidly. There are many ways of formulating lattice QCD so that the correct continuum theory is recovered. It is sufficient to ensure that the lattice theory either retains QCD's essential symmetries (e.g. gauge invariance), or breaks them in ways that vanish in the continuum limit (e.g. Lorentz invariance). Lattice QCD is now so well underpinned theoretically that it is widely accepted as the best way to define QCD.

Lattice QCD explains the confinement of quarks inside hadrons when the gauge coupling (and hence the lattice spacing) is large, because the potential energy of a static quark-antiquark pair grows linearly with their separation. It has not yet been established that this property remains true in the continuum limit. However, lattice QCD did not become a viable tool for computing the properties of hadrons until Creutz, Jacobs and Rebbi (1979) realised that the path integral in Euclidean space-time could be estimated by computer simulation using Monte Carlo methods. It has taken over 30 years of effort developing the theory, algorithms and computer technology to reach the point today where we can compute the values of many hadron masses and matrix elements for continuum QCD to a precision of a few percent and start to confront experimental measurements. For most practical purposes, QCD can now be solved from first principles, although the computations are enormously demanding and many are still too expensive. This will change as computer performance continues to increase exponentially for problems of this type. The lattice approach can be applied to other quantum field theories and there has been a surge of interest in applying it to possible models of electroweak symmetry breaking in anticipation of discoveries at the LHC. All that is needed is an understanding of how to realise the symmetries of the continuum theory correctly and a fixed point at which to define the continuum limit. However, neither is guaranteed to be easy for any particular theory.

The Origin of Mass

Asymptotic freedom of QCD enables us to use perturbation theory to determine how physical quantities, such as hadron masses, depend on the lattice spacing when this is small (because then the coupling is also small). All quantities with dimensions can be expressed as a computable number times the appropriate power of a fixed energy scale, Λ_{QCD}, which is related to the inverse of the lattice spacing (the "cut-off") by a factor that becomes exponentially small at small coupling. If we imagine QCD to be embedded in a more complete theory, so that new physics enters when the lattice spacing reaches a small enough value, the energy scale of this new physics can be much larger than Λ_{QCD} and, consequently, the masses of hadrons. Thus, asymptotic freedom explains why hadrons can be "light" compared, say, to the Planck mass.

Computer simulation of lattice QCD may be used to compute the numbers that relate physical quantities to Λ_{QCD}, or, equivalently, dimensionless ratios of physical quantities. The first such calculation of the nucleon mass by Hamber and Parisi (1981) obtained 950±100 MeV. This illustrates the challenge for the field – to decide whether QCD is correct requires reducing the uncertainties in such calculations to something comparable to the experimental uncertainty. Hamber and Parisi did not correctly include the effects of virtual quark loops (or "sea quarks"), but it was not until 1998 that CP-PACS announced at the annual Lattice Conference that this gives the wrong result for the nucleon mass and other light hadron masses (Aoki et al., 2000). Ten years later, the light hadron spectrum computed in 2+1 flavour QCD (i.e., including all the effects of *u*, *d* and *s* quarks, with *u* and *d* assumed to be degenerate in mass so that isospin is an exact symmetry) was shown to agree with experiment to within a few percent (Dürr et al., 2008). The inputs to this computation are the observed masses of the (isospin averaged) pion, kaon and Ξ baryon, used to fix the average *u* and *d* mass, the *s* mass and the scale – the quark masses in the simulation are varied until the computed ratios of the pion to Ξ baryon masses and the kaon to Ξ baryon masses match experiment. In this way, the quark masses are determined.

Since the masses of the *u* and *d* quarks turn out to be only a few MeV, roughly 99% of all the visible mass in the Universe is, therefore, explained as the binding energy of QCD. It remains for us to understand the origin of the masses of the quarks, leptons, electroweak gauge bosons and, presumably, the Higgs. Lattice QCD enables precision determination of the quark masses, which is an important first step towards understanding their origin. Today's QCD simulations typically include *u*, *d*, *s* and *c* quarks in the isospin-symmetric limit for the sea quarks. Isospin breaking and QED effects are included for the valence quarks to account, at least approximately, for the mass difference of the neutron and proton. The current world averages for the light quark masses obtained this way are (Laiho et al., 2010)

$$m_u = 2.09\pm0.09 \text{ MeV}, \quad m_d = 4.73\pm0.11 \text{ MeV}, \quad m_s = 93.6\pm1.1 \text{ MeV}.$$

The result for the *u* quark rules out the possibility that it is massless and, consequently, that this could be an explanation for the "strong CP problem". Evidently, lattice QCD has not only established that QCD is a good description of hadrons at low energies, but also that it can be used to determine precisely otherwise inaccessible parameters of the Standard Model.

The Search for Physics Beyond the Standard Model

In the absence of the discovery of new particles, the search for new physics is proceeding through tests of the Standard Model. Lattice QCD is starting to provide a tool of sufficient precision to confront predictions of the Standard Model with experiment and to seek discrepancies. The focus of this search is flavour physics, because the existence of only three generations of quarks and leptons, inherent in the Standard Model, imposes a constraint on the parameters which specify the strengths of the mixings between different quark flavours. Like the quark masses, these parameters, or "CKM matrix elements", are inputs to the Standard Model, presumably originating in some more fundamental underlying theory, and they must be inferred from experimental measurements. If there are only three generations, the 3×3 CKM mixing matrix must be unitary – a statement that the probabilities of all possible mixings of a given flavour must add up to one and a set of "unitarity triangle" constraints. It is possible that new physics violates these constraints and this can be observed if we can determine the mixing parameters precisely enough. Also, like the quark masses, since the quark mixings can only be observed in hadronic processes, QCD effects must be computed to extract the mixing parameters from experimental measurements. The strength of these tests of the Standard Model then depends on our ability to reduce the uncertainties of both the computations and the experiments. Until recently, the computational uncertainties dominated. As the precision of lattice QCD calculations of hadronic matrix elements steadily improves, this situation is changing.

Our most stringent test of CKM unitarity is for the mixing of the *u* quark with *d*, *s* and *b* quarks. The mixing with the *b* quark is so tiny that it can be ignored. The other two mixing parameters can be determined from kaon semileptonic decays (using the computed form factor at zero momentum transfer), and kaon and pion leptonic decays (using the computed ratio of the decay constants), where there are reliable lattice QCD computations of the hadronic decay matrix elements from both 2 flavour (degenerate *u* and *d* quarks only in the sea) and 2+1 flavour (*u*, *d* and *s* quarks) simulations. The former have larger systematic uncertainties, but both give values for the mixing parameters that satisfy the unitarity constraint (at the level of 4% and 2% respectively). Taking the *ud* mixing from the more precisely measured nuclear beta decay confirms CKM unitarity at the per mille level (Colangelo et al., 2011).

The progress achieved over the past 20 years in lattice QCD computations of hadronic weak matrix elements is nicely illustrated by B_K, the matrix element needed to extract the size of *CP* violation in the Standard Model from measurements of neutral kaon mixing (Lunghi & Soni 2011). A crucial feature of CKM mixing in the Standard Model is that *CP* violation is determined by a single parameter. Thus, the same value should be obtained from kaon and from *B* meson decays. The construction of the two *B*-Factories in the 1990s was motivated in large part by this test of the Standard Model. So the beautiful experimental measurements of *B* mixing to an accuracy of a few percent that were achieved could only impact the underlying theory if B_K could be computed to a similar precision. Early lattice QCD results in the 1990s using the quenched approximation (no sea quarks) were comparable to those using non-lattice methods, obtaining values for the (renormalisation group invariant) matrix element around 0.70±0.10, but with no control over the systematic error. In the last five years, simulations with 2+1 flavours have achieved remarkable consistency in the central value and a steady reduction in the uncertainty, so that the current world average is 0.74±0.02.

Using the most reliable lattice QCD results available today (specifically, excluding results for the *cb* and *ub* mixing parameters obtained from inclusive and exclusive semileptonic *b* decays, because they differ by around 2σ), the unitarity triangle, whose area is proportional to the size of *CP* violation, exposes a 3σ tension in the CKM matrix. If this is due to new physics, then it seems predominantly to affect *B* mixing (Laiho et al., 2010, Lunghi & Soni 2011).

The central role that lattice QCD is now playing in the search for new physics is due to the 30 years of effort understanding the theoretical formulation, improving the algorithms and speeding up computer performance finally paying off. So we now have full control over all sources of uncertainty for some phenomenologically important matrix elements and consistent results for them from different lattice formulations providing an independent check. We can expect the range of computable matrix elements to grow and the uncertainties in the results to reduce as the methodology and computer performance continue to improve.

Thermodynamics and the Quark-Gluon Plasma

Lattice field theory provides a theoretical laboratory in which we can explore the properties of QCD with different choices for its quark content. This has been exploited in the historical development by starting with a model in which only valence quarks are present (the "quenched approximation"), which substantially reduces the computational cost. Subsequently, at growing cost and edging ever closer to the Standard Model, two degenerate quark flavours were included in the sea, then 2+1 flavours (the 2 referring to degenerate *u* and *d* quarks), until today most simulations include 2+1+1 flavours of sea quark with isospin breaking effects incorporated in the valence quarks. These simulations may be performed at zero or non-zero temperature, enabling us to map out the phase diagrams. Unfortunately, the Monte Carlo algorithm fails at non-zero baryon chemical potential, so this region of the phase diagram is not accessible (yet) to direct simulation.

The phase structure is sensitive to the sea-quark content, although we have had to learn this the hard way. The temperature of the transition from the confining to the quark-gluon plasma phase turns out to be close to m_s, so it is essential to include the *s* quark in the sea, requiring at least 2+1 flavour simulations. (In fact, there is not a sharp transition, but rather a smooth cross-over between the two phases.) This is one reason why QCD thermodynamics has proved to be a harder problem than the computation of the zero-temperature spectrum and matrix elements (another is that zero-temperature results are needed as input to set the scale and quark masses). Furthermore, most non-zero temperature studies have used the staggered-quark formulation, which has additional copies of the quark flavours in the sea, called "tastes", that decouple only in the continuum limit. The effects of tastes at non-zero lattice spacing can be reduced by modifying the staggered-quark action. After some initial discrepancies, results for the transition temperature and other properties derivable from the equation of state, such as the speed of sound and the pressure, obtained with different formulations are now converging. A typical result for the transition temperature is T_c = 154±9 MeV (Bazavov et al., 2012).

The goal of lattice QCD thermodynamics is to obtain a precise determination of the equation of state of QCD over the temperature range of 150 – 700 MeV that is being explored by experiments at RHIC and the LHC. Along with the determination of the transition temperature and transport coefficients, this will enable us to parametrise hydrodynamical models describing the quark-gluon plasma. The inclusion of the *c* quark in simulations is likely to be necessary at high temperatures, and these can be expected to follow close behind the zero-temperature 2+1+1 flavour simulations currently underway.

Dynamical Electroweak Symmetry Breaking

While the idea that electroweak symmetry is broken by the condensation of techniquarks, which feel a new technicolor gauge interaction, simply replicates what already happens to a limited extent in QCD, extending this to give masses to the quarks runs into trouble – the scale of the technicolor theory, Λ_{TC}, is either too big to generate the heavy-quark masses, or too small that it generates flavour-changing neutral current (FCNC) interactions in contradiction with experiment. A popular solution is to seek a technicolor gauge theory whose dynamics is different from QCD, being governed by a beta function that has an infrared stable (i.e. "conformal") fixed point at non-zero gauge coupling. A suitable choice of techniquark content and masses should destabilise this fixed point so that, between two scales, the gauge coupling is trapped close to the fixed-point value and stops running, a property called "walking", before eventually running down to zero as in QCD. This dynamics introduces two scales: a high scale which generates acceptably small FCNCs and a low scale that generates big enough quark masses.

Lattice field theory is the only first-principles method available to search for fixed points at non-zero coupling. The challenge is that the set of possible technicolor theories is huge and, for each gauge group, there are many choices for the techniquark content (a classification of theories based on an approximate beta function provides a guide, see Sanino 2009). Simulating each specific choice is computationally demanding even with the most powerful algorithms developed for QCD. So work has so far concentrated on the simplest gauge groups, SU(2) and SU(3), for which efficient simulation codes already exist, and has varied the fermion content looking for a zero of the beta function. Since staggered fermions provide efficient implementations of theories with multiples of four flavours in the fundamental representation, the most systematic studies have been carried out for 8, 12 and 16 fundamental flavours with an SU(3) gauge group. This has established that the 16-flavour theory has a conformal fixed point, the 8-flavour theory does not, while the 12-flavour theory remains controversial, with the balance in favour of a conformal fixed point (Hasenfratz, 2010 and 2012).

Thus, these simulations are providing some encouragement for "walking" technicolor to be a viable theory of dynamical electroweak symmetry breaking. Of course, there is not a shred of experimental evidence yet that Nature exploits this possibility. If we are to explain electroweak symmetry breaking through some underlying strong dynamics, computer simulation of lattice field theory is likely to be the only technique available to us, both to construct the theory and to extract predictions that can be used to confront experiment. The computational cost of doing this will far exceed that which has been required for QCD, because we will not have asymptotic freedom and perturbation theory to guide our approach to the continuum limit.

Computers for Lattice Field Theory

The progress achieved in lattice QCD is generally ascribed equally to advances in algorithms and in computer technology. While the former is hard to plan for in the future, technological advances are expected to continue for the next ten years at the exponential "Moore's Law" rate that we have benefited from for the past 50 years. Throughout its history, lattice QCD, more than any other application area, has driven the development of the most powerful supercomputers. This is because the translational symmetry and local interactions of the lattice theory make the simulations very efficient to implement on parallel computers. Also the balance between computations and memory accesses in lattice QCD turns out to be a good design target for machines to support a wide range of scientific applications. Thus, we have seen computers designed and built specifically for lattice QCD, design elements from them incorporated into commercial machines, and lattice QCD codes used to optimise performance of and to stress-test commercial systems.

This concept of "co-design", in which the computer architecture, its system software, the algorithm and application software are all developed together, has been adopted as the plan for the next big step in supercomputer performance from the current petascale to exascale (10^{18} operations per second). This is expected to be accomplished around 2018, by scaling up today's machines with hundreds of thousands of computational units operating in parallel, to systems with hundreds of millions, even billions. Memory access rates will be unable to keep pace and energy requirements will have to be driven down dramatically to keep operating costs at an acceptable level. This will be a huge engineering challenge and, even for lattice QCD, it will not be straightforward to exploit exascale systems efficiently. The key point, though, is that computer performance should not present a limitation on lattice field theory, at least for the first decade of the LHC.

Prospects for the LHC Era

After 30 years of sustained effort to develop the theoretical formulation, speed up algorithms and build faster computers, lattice QCD has reached the point where it is delivering high-precision, model-independent results for a growing range of phenomenologically important quantities, in which all sources of uncertainty are under control and can be systematically reduced further. In flavour physics tests of the Standard Model, a combination of efforts to drive down both theoretical and experimental uncertainties is putting the Standard Model under increased stress and has already exposed a 3σ tension in the *B* meson sector. Independent of the discovery of new particles at the LHC, this work will tighten the constraints on Standard Model processes and will very likely expose areas where new physics is necessary.

Lattice simulations of QCD thermodynamics are reaching a similar point of sophistication, where the lattice approximations are fully under control. This should permit reliable determinations of a wide range of thermodynamic and transport properties of the quark-gluon plasma phase that will guide our interpretation of heavy-ion experiments. A major theoretical challenge remains to find a way to simulate QCD at non-zero baryon density to explore the properties of cold dense nuclear matter.

Beyond QCD, lattice field theory offers the only known way to understand strong dynamics which is not controlled by a perturbatively accessible fixed point and yet may explain electroweak symmetry breaking. Computationally, this will require a major step up in our capabilities, because we will not have perturbation theory to provide a guide. Fortunately, there is no end in sight to the exponential growth of computer power. With the full discovery potential of the LHC also yet to be realised, the only limit to our understanding further how Nature works at the most fundamental level will be our own ingenuity.

References

Aoki, S., Boyd, G., Burkhalter, R., Ejiri, S., Fukugita, M., Hashimoto, S., Iwasaki, Y., Kanaya, K., Kaneko, T., Kuramashi, Y., Nagai, K., Okawa, M., Shanahan, H.P., Ukawa, A., & Yoshié, T. (2000). Quenched Light Hadron Spectrum. *Physical Review Letters 84,* 238-241.

Bazavov, A., Bhattacharya, T., Cheng, M., DeTar, C., Ding, H.-T., Gottlieb, S., Gupta, R., Hegde, P., Heller, U. M., Karsch, F., Laermann, E., Levkova, L., Mukherjee, S., Petreczky, P., Schmidt, C., Soltz, R. A., Soeldner, W., Sugar, R., Toussaint, D., Unger, W., & Vranas, P. (2012). The chiral and deconfinement aspects of the QCD transition. *Physical Review D85,* 054503.

Colangelo, G., Dürr, S., Jüttner, A., Lellouch, L., Leutwyler, H., Lubicz, V., Necco, S., Sachrajda, C.T., Simula, S., Vladikas, A., Wenger, U., & Wittig, H. (2011). Review of lattice results concerning low-energy particle physics. *The European Physical Journal C71,* 1695.

Creutz, M., Jacobs, L., & Rebbi, C. (1979). Experiments with a gauge-invariant Ising system. *Physical Review Letters 42,* 1390-1393.

Dürr, S., Fodor, Z., Frison, J., Hoelbling, C., Hoffmann, R., Katz, S. D., Krieg, S., Kurth, T., Lellouch, L., Lippert, T., Szabo, K. K., & Vulvert, G. (2008). Ab Initio Determination of Light Hadron Masses. *Science 322,* 1224-1227.

Hamber, H., & Parisi, G. (1981). Numerical estimates of hadronic masses in a pure SU(3) gauge theory. *Physical Review Letters 47,* 1792-1795.

Hasenfratz, A. (2010). Conformal or walking? Monte Carlo renormalization group studies of SU(3) gauge models with fundamental fermions. *Physical Review D82,* 014506.

Hasenfratz, A., (2012). Infrared fixed point of the 12-fermion SU(3) gauge model based on 2-lattice MCRG matching. *Physical Review Letters 108,* 061601.

Laiho, J., Van de Water, R. S., & Lunghi, E. (2010). Lattice QCD inputs to the CKM unitarity triangle analysis. *Physical Review D81,* 034503 and http://www.latticeaverages.org.

Lunghi, E., & Soni, A. (2011). Demise of CKM & its aftermath. arXiv:1104.2117v3 [hep-ph].

Sannino, F. (2009). Conformal Dynamics for TeV Physics and Cosmology. *Acta Physica Polonica B40,* 3533-3743.

Wilson, K. G., (1974). Confinement of quarks. *Physical Review, D10,* 2445-2459.