Topics in Theoretical Nuclear Physics: The Quark Structure of Matter on the Lattice

a contribution to the Physics Department Newsletter by Prof. Frank X. Lee
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What is the structure of matter at the deepest level? The current answer to the question is quarks and gluons which make up hadrons (proton, neutron and so on) which make up the nucleus at the heart of an atom. In this sense, quarks and gluons comprise most of the known mass of the universe. The force that holds the quarks together to form hadrons is the strong force, one of the four fundamental interactions in nature, besides the electromagnetic force, the gravitational force and the weak force. The theory behind the interactions of quarks and gluons is called **quantum chromodynamics** (otherwise known as QCD). Incidentally, the 2004 Nobel prize in Physics went to the developers of QCD (see news release http://nobelprize.org/physics/laureates/2004/public.html). Unraveling the quark structure of matter as governed by QCD is key to our understanding of the physical world, and presents one of the most challenging tasks facing contemporary nuclear theory.

What is exactly QCD? The equations of QCD is very simple and can be written down in just one line. Here I venture to write it down for the reader to see, in terms of a quantity called action which is the integral of Lagrangian density over space-time:

$$S_{QCD} = \frac{1}{2}\int d^4x \,\mathrm{Tr}\, F_{mn}F^{mn} + \int d^4x\, \bar{q}(g^m D_m + m_q)q$$

The first term is the gluon action described by the field strength tensor $F_{\mu\nu}$ and the second term is the quark action where m_q is the quark mass. The interaction of the two is through the covariant derivative D_μ. Once the action is known, one basically knows everything about the system by way of ***Feynman path integrals*** which involve one ordinary integral per physical degree of freedom. See Figure 1 for a picture of the proton in QCD.

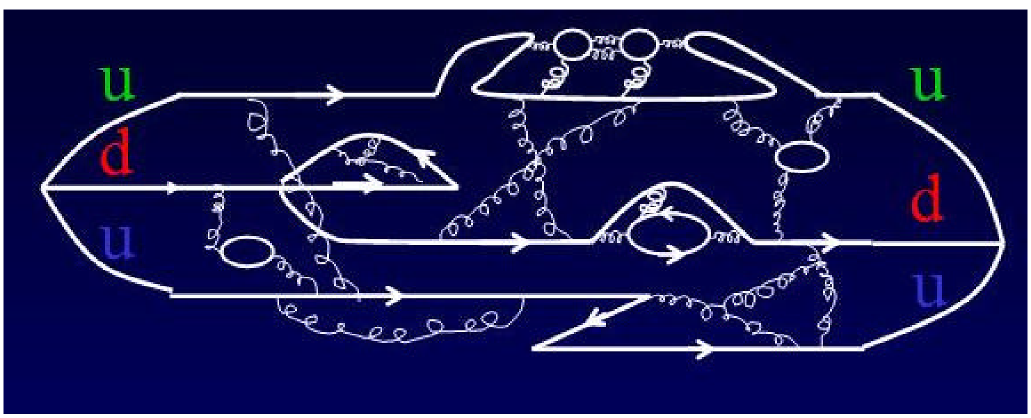

Figure 1: A picture of the proton in QCD. Three quarks are created out of the QCD vacuum. They propagate to another point, while interacting in all manners among quarks and gluons, where they are destroyed into the vacuum. This propagation (called a two-point correlation function) has information about the mass of the proton and its excited states.

So if QCD explains everything about the nucleus of an atom, why don't we have everything answered? The short answer is that it is notoriously difficult to solve. The physics reason is that gluons, the quanta that mediate the interaction between quarks, interact strongly with themselves, unlike the situation in electromagnetism where photons, the quanta that mediate the interactions between electric charges, do not interact with themselves. Since QCD was formulated in the 1970's, directly solving QCD by analytical methods has proven extremely difficult. The only known way to solve QCD is by computer simulations. This is where the concept of QCD on a discrete space-time lattice comes in.

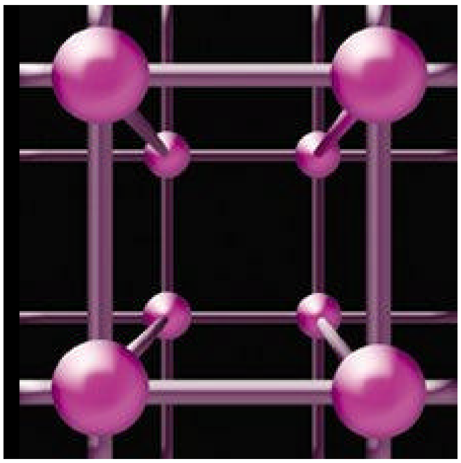

Figure 2: By substituting a grid of discrete links and sites, or a lattice, for continuous space-time, physicists carry out many otherwise insoluble calculations of the QCD theory. Quarks live on the sites, gluons live on the links. The interactions arise from quarks and gluons hopping between sites and links. The time dimension is not depicted here.

What is a discrete space-time lattice? The idea is very simple (see Figure 2). The continuous, unbounded space and time of reality are said to contain infinite degrees of freedom. They can be approximated by a discrete lattice (or grid) of points, somewhat like the vertices of a four-dimensional checkerboard (three dimensions for space and one for time). Quarks live on the sites, while gluons live on the links. The scaffold is restricted to a finite volume but replicated with periodic boundary conditions. In this way, all of space and time are approximated by a finite set of points which can be manipulated by a computer. Of course, the volume should be big enough to accommodate the hadron under study which is typically about 10^{-15} meters(also known as a fermi) in diameter.
For example, a lattice with 10 sites in each dimension(about the smallest size that can provide a rough approximation of reality), and 0.2 fm between neighboring sites, has 2 fm on a side, enough to hold a hadron (with some room to spare).

Results for the real world are approached by performing calculations on a sequence of lattices, shrinking the distance between lattice points to zero and expanding the volume of the network to infinity. However, even on such a small lattice, the number of sums that need to be evaluated is prohibitive: 2^{32000}, which is about one followed by 96,000 zeros. The state-of-the-art simulations use lattice sizes up to 64^4 which is beyond capabilities of today's most powerful supercomputers. In practice, Monte Carlo techniques are used to perform the path integrals which approximate the solution by statistical sampling, much like taking a poll (albeit an elaborate one) to predict an election winner. Another key idea is to use imaginary (Euclidean) time instead of real time. This turns the oscillatory factor e^{-iS} in the path integral into a probability-like distribution e^{-S} which is suitable for numerical simulations.

For these reasons, the field is known as **lattice QCD**.

Why predictions from lattice QCD are hard to come by? Although the basic idea of lattice QCD is fairly simple, it has been difficult to make a reliable calculation with limited computational resources. There are several major obstacles that one must overcome to obtain a credible result. First, the Feynman path integral involves a determinant that is non-local and is very expensive to evaluate numerically. Many simulations simply ignore it by using what is called the *quenched approximation*, which can save computer time by more than a factor of 50. This is significant since realistic calculations take months or years to complete. Second, to approach the continuum limit, small lattice spacings and large number of lattice points are needed, which put increasing demand on computing power. Third, the quark propagation becomes increasingly singular as its mass approaches the physical values of below 10 MeV for up- and down-quarks, causing the phenomenon of critical slowing-down in the matrix-inversion algorithm. For this reason, most calculations are done at relatively large quark masses (50 to 200 MeV) and an extrapolation to the physical quark masses is needed. Recently, however, significant progress has been made with the overlap fermion action which enables us to reach very close to the physical limit. This has led to the observation of the Roper resonance on the lattice for the first time (see Figure 3).

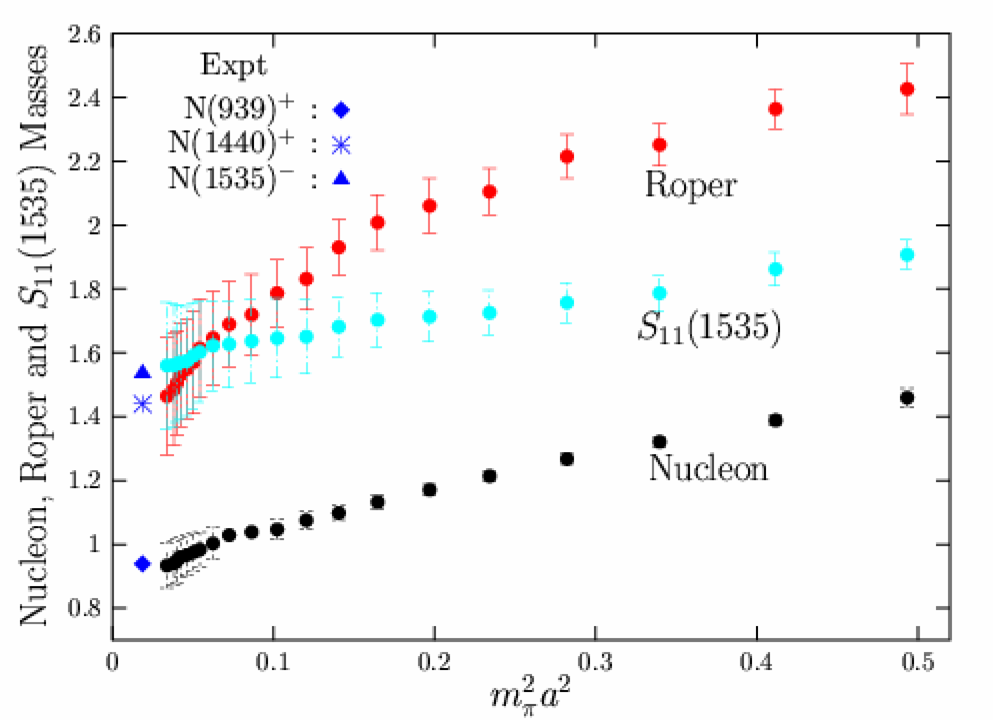

Figure 3: The recently-observed Roper resonance along with the S11 resonance on the lattice with the overlap fermion action. To appear in Phys. Lett. B.

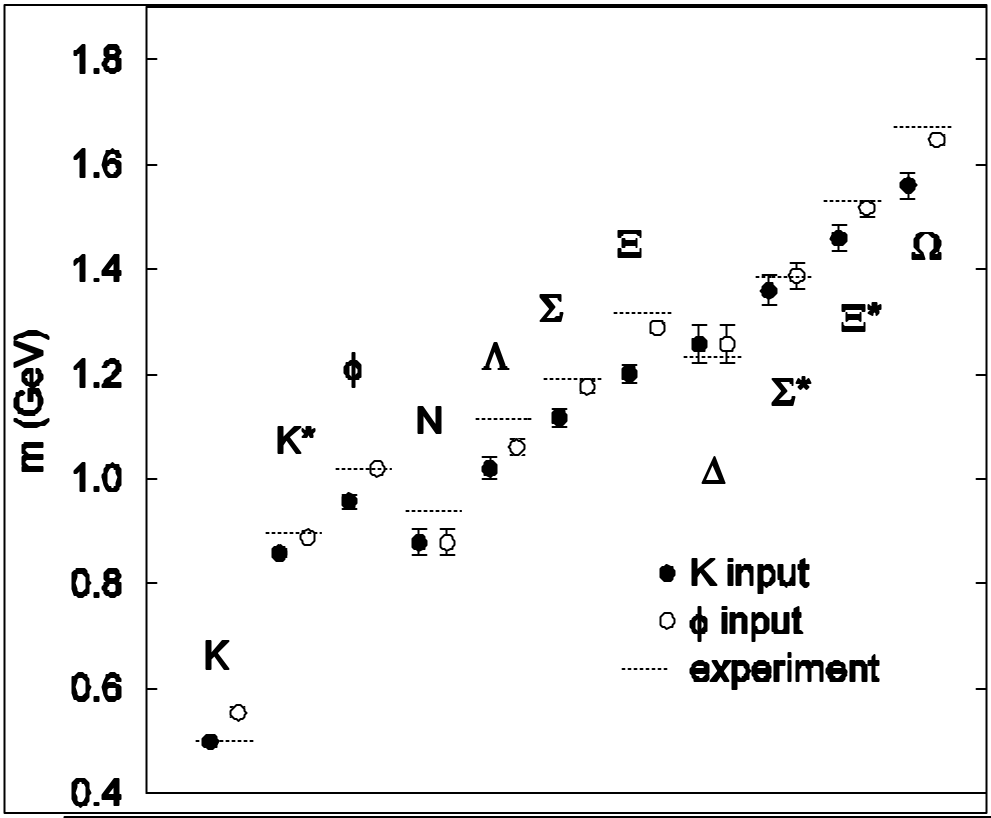

Figure 4: Light hadron spectrum from lattice QCD by the CP-PACS Collaboration, Phys. Rev. Lett. 84, 238 (2000). K input and ϕ input are two different ways of setting the strange quark mass.

What can lattice QCD do? The best calculation performed in the quenched approximation has produced a ground-state hadron spectrum that is within 10% of the observed values (see Figure 4). The remaining discrepancy is attributed to the quenched approximation. The results suggest that the quenched approximation is not as bad as originally suspected. With the savings in computer time, the quenched approximation can be used to explore a variety of physical observables on the lattice without making too serious an error. Plus it is always useful to have the quenched results to compare with the the full calculation to gain additional insight. In addition to hadron masses, one can calculate magnetic moments, form factors, decay constants, matter at finite temperature and density, etc. In fact, almost every aspect involving the strong interaction has been investigated on the lattice to some extent. One thing to bear in mind is that lattice QCD is an exact solution of QCD in the sense that all the systematic errors in lattice QCD can be systematically removed with increasing computing power. Lattice QCD is our best hope to solving QCD.
In some way, lattice QCD is like doing experiments on the computer, albeit with a distinct advantage over real experiments: the ability to change physical parameters and watch how physic observables run with them. One can dial the quark mass to see how the computed quantities depend on it and how they approach the chiral limit, while our experimental colleague must work at the physical quark mass. One can look at the QCD vacuum and quark propagation to identify the degrees of freedom most responsible. One can design and simulate `worlds' with

different space-time dimensions, different number of quark colors and flavors to gain insight into the real world. All on the computer, without leaving your desk. Ultimately, lattice predictions must be compared with real experiments in order to uncover the quark structure of matter from first principles. So we work with experimentalists on how certain observables are measured and learn how to calculate them. Or we make predictions and write proposals to verify them.

Figure 5: Associate Professor Frank X. Lee.

At GW, **Prof. Lee** is pursing a vigorous program in the field of lattice QCD. He has widely published papers and given talks at international conferences on the subject (to find out more, please visit his homepage http://home.gwu.edu/~fxlee). At present, he is doing a number of calculations, working with graduate students **Leming Zhou**, **Scott Moerschbacher**, undergraduates **Ryan Kelly** (Gamow fellow), and **John Bulava**, on JLab-related physics, including the excited baryon mass spectrum, pentaquarks, hadron polarizabilities and magnetic moments. The research is partially funded by the U.S. Department of Energy via a joint grant with **Prof. Bennhold**, and a joint grant with **Prof. Liu** of University of Kentucky. He collaborates with researchers at University of Kentucky; University of Adelaide; and Baylor University. In addition he is the member representing GW in the Lattice Hadron Physics Collaboration whose mission centers on Jlab-related physics. This collaboration is part of a larger, national effort called "National Computational Infrastructure for Lattice Gauge Theory" that was recently awarded a multi-million dollar grant over the next few years by DOE to build several supercomputers dedicated to lattice QCD. Presently, Prof. Lee has access to a variety of computers to carry out his projects. In addition to a fast Unix-based workstation for communications and data analysis; he does calculations from his desk on some of world's most powerful supercomputers; such as those at the DOE-supported National Energy Research Scientific Computing Center (NERSC) (see Figure 6), from which he has an ongoing award for a number of years; and the NSF-supported supercomputers at Pittsburgh and San Diego. He also uses the high-performance cluster at JLab with which he has held a joint appointment.

Figure 6: The 6080-processor IBM-SP supercomputer at NERSC, a DOE sponsored facility located at Lawrence Berkeley National Laboratory. This computer is ranked 14th on the world TOP500 list as of Sept 2004. It is the fastest computer for non-classified research.