Understanding hadron structure from lattice QCD in
the SciDAC era

Lattice Hadron Physics Collaboration:
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Abstract. The structure of neutrons, protons, and other strongly interacting particles in terms
of their quark and gluon constituents can be calculated from first principles by solving QCD on
a discrete space-time lattice. With the advent of SciDAC software and prototype clusters and
of DOE supported dedicated lattice QCD computers, it is now possible to calculate physical
observables using full QCD in the regime of large lattice volumes and light quark masses that can
be compared with experiment. This talk will describe selected examples, including the nucleon
axial charge, structure functions, electromagnetic form factors, the origin of the nucleon spin,
the transverse structure of the nucleon, and the nucleon to Delta transition form factor.

1. Introduction

SciDAC is playing a crucial role in exploiting the full potential of lattice QCD to understand
the structure of hadrons from first principles. The deceptively simple looking QCD Lagrangian

\[ L = \bar{\psi}(i\gamma^\mu D_\mu - m)\psi - \frac{1}{4} F_{\mu\nu}^2 \]

with \( D_\mu = \partial_\mu - igA_\mu \) and \( F_{\mu\nu} = i[D_\mu, D_\nu] \) produces the amazingly rich and complex structure of
the strongly interacting matter in our universe. By asymptotic freedom, the interaction becomes
weak at high energy and thus amenable to perturbation theory, enabling the validity of QCD to
be exhaustively verified experimentally. The flip side of asymptotic freedom, however, is the fact
that the interaction becomes strong and thereby analytically intractable at low energies, and
the only known way to calculate the low energy properties of hadrons from first principles
is numerical evaluation of the QCD path integral on a discrete space time lattice. Since,
as described below, Teraflops years of computation are required for accurate calculations of
Figure 1. First principles calculations using improved staggered quarks of selected decay constants and hadron mass differences showing agreement with experiment at the level of a few percent in full QCD (right) and showing discrepancies up to 10 percent in the quenched approximation, which ignores dynamical quark-antiquark excitations, (left).

hadron observables, SciDAC support of prototype Terascale clusters, support of development of highly optimized code, and encouragement of a coherent national program that shares the use of common QCD configurations for nuclear physics and particle physics applications has enabled us to undertake the first calculations in the physical regime of realistically light quarks in sufficiently large spatial volumes.

In addition to the prospect of precisely calculating the experimentally observable properties of the nucleon from first principles, lattice QCD also offers the deeper opportunity of obtaining insight into how QCD actually works in producing the rich and complex structure of hadrons. Beyond simply calculating numbers, we would like to answer basic questions of hadron structure. For example, what are the dominant components of the nucleon wave function? How does the total spin of the nucleon arise from the spin and orbital angular momentum of its quark and gluon constituents? How does the nucleon quark and gluon structure produce the observed scaling behavior of form factors? What is the transverse, as well as longitudinal structure of the nucleon light-cone wave function? As the quark mass is continuously decreased from a world in which the pion mass is 1 GeV to the physical world of light pions, how does the physics of the quark model and adiabatic flux tube potentials evolve into the physics of chiral symmetry breaking, where instantons, quark zero modes, and the associated pion cloud play a dominant role? What is the role of diquarks in conventional hadrons and exotic states such as pentaquarks? As discussed below, contemporary lattice calculation are beginning to provide insight into these and other fundamental questions in hadron structure.

It has taken the first thirty years since Wilson’s seminal formulation of QCD on a lattice[1] to develop the theoretical techniques and computer technology for quantitative numerical solution of QCD. Reference [2] provides an elementary introduction for non-specialists. The basic practical problem is that one must address the triply demanding limits of a small lattice spacing, a large physical volume, and a small quark mass. Instead of referring to the unobservable bare quark mass, since \( m_q \propto m_{\pi}^2 \), it is convenient to express the quark mass dependence of observables by their dependence on \( m_{\pi}^2 \). To include the essential physics of the pion cloud, the box size must be large compared to the pion Compton wavelength, \( m_{\pi}^{-1} \), and the ultimate computational cost of a full QCD lattice calculation including dynamical sea fermions turns out to have mass dependence \( m_{\pi}^{-9} \). Hence, in the past, full QCD calculations were relegated to what I call the “heavy pion world”, where \( m_{\pi} \gtrsim 500 \text{ MeV} \), and it was conventional to perform theoretically unjustifiable linear extrapolations in \( m_{\pi}^2 \) to obtain first estimates of physics in our world with 140 MeV pions. During the past year, our collaboration has begun a series of full QCD calculations[3] combining computationally economical staggered sea quark configurations generated using the
so-called asqtad improved action by the MILC collaboration[4, 5] with domain wall valence quarks that have the important property of chiral symmetry. As discussed in the talk by Paul Mackenzie at this conference, the MILC configurations have been shown to give very accurate results in heavy quark systems. As an example, Figure 1 shows impressive agreement with experiment at the level of a few percent of decay constants and mass splittings using this theory in full QCD, and also indicates how the quenched approximation, which omits quark excitations from the Dirac Sea, introduces discrepancies at the 10% level[6]. Use of these configurations has enabled us to treat pion masses as light as 359 MeV in volumes with spatial dimension as large as 3.5 fm. Initial results are presented below for five pion masses, 359, 498, 605, 696, and 775 MeV, as well as comparisons from the heavy pion world with SESAM full QCD configurations[7] using Wilson quarks at pion masses 744, 831, and 897 MeV.

2. Nucleon Structure

These proceedings will briefly summarize the experimental observables that are calculable on the lattice and describe selected recent results. More details may be found in a recent review[8], recent publications of our group[9, 10, 11, 12, 3, 13] and of the QCDSF collaboration[14, 15, 16, 17].

Since asymptotic freedom renders QCD corrections to high energy scattering small and calculable, high energy lepton scattering provides precise measurements of matrix elements of the light-cone operator

\[ \mathcal{O}(x) = \int \frac{d\lambda}{4\pi} e^{i\lambda x} \bar{\psi} \left( -\frac{\lambda n}{2} \right) \hat{P} e^{-ig \int_{-\lambda/2}^{\lambda/2} d\alpha \cdot n \cdot A(n)} \psi \left( \frac{\lambda n}{2} \right), \]

where \( n \) is a unit vector along the light-cone and \( \lambda = p^+ x^- \). Expanding \( \mathcal{O}(x) \) in local operators via the operator product expansion generates the tower of twist-two operators

\[ \mathcal{O}^{\{\mu_1 \mu_2 \ldots \mu_n\}} = \bar{\psi} \gamma_5 \{\mu_1 \} D^{\mu_2} \ldots i D^{\mu_n} \psi, \]

whose matrix elements can be calculated in lattice QCD.

The familiar quark distribution \( q(x) \) specifying the probability of finding a quark carrying a fraction \( x \) of the nucleon’s momentum in the light cone frame is measured by the diagonal nucleon matrix element,

\[ \langle P | \mathcal{O}(x) | P \rangle = q(x), \]

and the \((n-1)^{th}\) moment of the quark distribution is specified by the diagonal matrix element

\[ \langle P | \mathcal{O}^{\{\mu_1 \mu_2 \ldots \mu_n\}} | P \rangle \propto \int dx x^{n-1} q(x). \]

Analogous expressions in which the twist-two operators contain an additional \( \gamma_5 \) measure moments of the longitudinal spin density, \( \Delta q(x) \). The generalized parton distributions \( H(x, \xi, t) \) and \( E(x, \xi, t) \) [18, 19, 20, 21] are measured by off-diagonal matrix elements of the light-cone operator

\[ \langle P' | \mathcal{O}(x) | P \rangle = \langle \Gamma | \hat{P} \rangle H(x, \xi, t) + i \frac{\Delta t}{2m} \langle \sigma^{\mu \nu} n_\alpha \rangle E(x, \xi, t), \]

where \( \Delta t = P^{\mu} - P^{\mu}, t = \Delta^2, \xi = -n \cdot \Delta / 2, \) and \( \langle \Gamma \rangle = \hat{U} (P') \Gamma U(P) \) for Dirac spinor \( U \). Off-diagonal matrix elements of the tower of twist-two operators \( \langle P' | \mathcal{O}^{\{\mu_1 \mu_2 \ldots \mu_n\}} | P \rangle \) yield moments of the generalized parton distributions, which in the special case of \( \xi = 0 \), are

\[ \int dx x^{n-1} H(x, 0, t) = A_{n,0}(t), \quad \int dx x^{n-1} E(x, 0, t) = B_{n,0}(t), \]
Figure 2. Nucleon axial charge, $g_A$. The left plot shows our full QCD calculations in spatial box sizes 1.5 fm (right three error bars), 2.6 fm (next five points) and 3.5 fm (second error bar superposed on the left-most point), compared with experiment (data point at far left). The solid line shows a fit to the data using chiral perturbation theory and the dashed lines indicate the error band in this fit. For comparison, the right graph adds the results by RBCK in a 1.9 fm box (three lowest new points that touch the solid line) and by QCDSF/UKQCD (remaining new points).

where $A_{n,i}(t)$ and $B_{n,i}(t)$ are referred to as generalized form factors (GFF’s). The physical observables considered in this work are special cases of these general expressions.

**Nucleon axial charge**

The nucleon axial charge, $g_A = \langle 1 \rangle_{\Delta q} = \int dx \Delta q(x) \propto \int dx \bar{q}(x) \gamma^\mu \gamma^5 q(x)$, is a fundamental property of the nucleon governing $\beta$ decay. It is an ideal test of lattice calculations for several reasons. The isovector combination $\langle 1 \rangle_{\Delta q}$ has no contributions from disconnected diagrams, it is accurately measured by neutron $\beta$ decay, and the functional dependence on $m_\pi^2$ is known from chiral perturbation theory\cite{22}. Furthermore, renormalization to account for the difference between regulating quantum field theory with a lattice cutoff and in the continuum can be performed accurately nonperturbatively using the five dimensional conserved current for domain wall fermions. Thus, conceptually, it is a “gold plated” test of our ability to calculate hadron observables from first principles on the lattice, and in addition, since it is known to be particularly sensitive to finite lattice volume effects that reduce the contributions of the pion cloud, it is also a good test for an adequate lattice volume.

The left panel of Figure 2 shows the results of our calculations in the heavy and light pion regimes, together with a fit to a curve defined by chiral perturbation theory\cite{22} that enables us to extrapolate the calculations to the physical pion mass. Note that the extrapolation goes through the experimental point, and that the dashed lines denote the errors in the extrapolation arising from the statistical errors in the lattice measurement. Also note that at the lowest pion mass, measurements were made in lattice volumes of 2.6 fm and 3.5 fm with statistically indistinguishable results, indicating the absence of finite volume corrections at this lattice size. For comparison, the right hand graph shows the two other calculations of $g_A$ in full QCD. The three points by the RBCK collaboration\cite{23} in a 1.9 fm box are consistent with our results within statistics, whereas the QCDSF/UKQCD results in a smaller volume lie uniformly lower than our results and experiment. The axial charge is the most completely analyzed and theoretically controlled of our calculations in the light quark regime, and clearly demonstrates the quantitative potential of lattice QCD with the emerging level of computational resources.
Figure 3. The left graph shows a curve with chiral perturbation theory behavior at small pion masses adjusted to fit full QCD and quenched results at large pion masses. The right plot shows preliminary full QCD calculations extending down to the chiral regime as described in the text. The left-most data point, denoted by an open circle, corresponds to a 359 MeV pion mass and volume 3.5 fm, and the diamond denoting the same mass in a 2.5 fm volume has been shifted slightly to the right for visual clarity. The star at the left in each graph denotes the experimental value.

Quark momentum fraction

The quark momentum fraction, $\langle x \rangle_q = \int dx x q(x) \propto \int dx \bar{q}\gamma^\mu D^\mu q$, is particularly interesting physically, because it reflects the fact that a large fraction of the momentum is carried by gluons rather than quarks. Figure 3 shows the flavor-nonsinglet difference between the momentum fraction of up and down quarks, which has no contributions from presently uncalculated disconnected diagrams and thus may be compared directly with experiment.

In contrast to the case of the axial charge, chiral perturbation theory yields a significant dependence of the momentum fraction on the pion mass. The left panel indicates this dependence by extrapolating calculations in the heavy pion regime using the functional form

$$a[1 - \frac{(3g_0^2+1)m_\pi^2}{(4\pi f_\pi)^2\alpha}ln\left(\frac{m_\pi^2}{m_\pi^2+\mu^2}\right)] + bm_\pi^2.$$  

This form[12] has the leading behavior described by chiral perturbation theory and contains a phenomenological parameter $\mu$ that joins the chiral behavior to the heavy pion regime.

The right panel shows the results with chiral valence quarks and MILC configurations at the five light masses as well as the heavy quark SESAM results denoted by open diamonds. The light quark calculations are renormalized by calculating in perturbation theory the ratio of the renormalization factor for the operator of interest to the corresponding renormalization factor for the axial current and multiplying by the nonperturbative renormalization constant for the axial current[13]. Since the ratio is close to one, the perturbative treatment should be adequate.

The light quark results are essentially flat, with no indication yet of the chiral turn-over to approach experiment, so calculations underway this year at 300 MeV and 250 MeV will be essential in understanding this regime. The normalizations of the SESAM and MILC results do not agree as well as they did in the case of the axial charge, which we attribute to the fact that the perturbative corrections for the Wilson fermions in the SESAM calculations are much larger, so higher order terms need to be calculated.

Figure 4 shows the ratio of the spin averaged momentum fraction, $\langle x \rangle_q$, to the spin-dependent fraction $\langle x \rangle_{\Delta q}$. In this case, the ratio is nearly mass independent and yields excellent agreement with experiment.
Figure 4. QCD predictions for the ratio of the spin-averaged momentum fraction, $\langle x \rangle_q$, to the spin-dependent momentum fraction, $\langle x \rangle_{\Delta q}$, compared with the experimental result (denoted by the star at the left).

Electromagnetic form factors

Electromagnetic form factors calculated by our collaboration are reported in the proceedings by David Richards\[24\], and will only be mentioned briefly here. The electromagnetic form factors $F_1$ and $F_2$, corresponding to $A_{10}$ and $B_{10}$ defined above, characterize the spatial distribution of charge and current at low momentum transfer and the ability of a single quark to absorb a large momentum transfer and remain in the ground state. Figure 1 of ref.\[24\] shows how the slope of $F_1$ increases and the pion mass decreases, reflecting the increase in the rms radius as the extent of the pion cloud increases. It also shows how the rms radius extracted from the slope lies on a curve parameterized in terms of chiral perturbation theory that is consistent with experiment at the physical pion mass.

One of the early successes of perturbative QCD was the understanding of how the short range quark structure of a hadron governs the behavior of exclusive processes at large momentum transfer. However, whereas simple counting rules suggested that $F_2 \sim F_1/Q^2$, experimental data from JLab\[25\] show that $F_2$ falls off much more slowly. Theoretically, it has recently been shown \[26\] that the next to leading order light cone wave function yields $F_2 \sim F_1 \log^2(Q^2/\Lambda^2)/Q^2$, which agrees with the Jlab data for $\Lambda = 0.3$ GeV. Since the short range quark structure dominates this physics, it is reasonable to expect that suppression of the pion cloud in the heavy pion world should not destroy the qualitative behavior and indeed, this expectation is borne out in Figure 2 of Ref.\[24\].

Origin of the nucleon spin

In the nonrelativistic quark model, the total proton spin of 1/2 arises trivially from adding the spins of the three valence quarks, and the so-called spin crises arose when deep inelastic scattering measurements of the lowest moment of the spin-dependent structure function, $\Delta \Sigma = \langle 1 \rangle_{\Delta u} + \langle 1 \rangle_{\Delta d}$, indicated that only of the order of 30% of the nucleon spin arises from quark spins. Hence, it is interesting to use the lattice to study how the angular momentum decomposition evolves as the pion mass is decreased from the heavy, quark model, limit to its physical value.

The contribution of the quark spin to the total angular momentum is given by the sum of the up and down quark axial matrix elements, $\Delta \Sigma$, and the connected diagram contribution is
Figure 5. Contribution of connected diagrams to the fraction of the total nucleon spin arising from the spin of the quarks, $\Delta \Sigma$, and from the quark orbital angular momentum, $2L_q$, in the heavy pion regime.

shown in Figure 5 for the regime of heavy pions. Note that in contrast to the axial charge, for which the disconnected diagrams cancel, disconnected diagrams should also contribute to this quantity and will be evaluated in the next phase of our SciDAC effort.

The total quark contribution to the nucleon spin [27] is given by the extrapolation to $t = 0$ of $A_{20}^{u+d}(t)$ and $B_{20}^{u+d}(t)$, shown in Figure 6 for the case of an 897 MeV pion. Since $A_{20}^{u+d}(t)$ is calculated directly at $t = 0$ and $B_{20}^{u+d}(t)$ is well fit by a constant that is measured to be nearly zero with small errors [10], the connected contribution to the angular momentum is measured to within a few percent. Combined with the calculation [9] of $\Sigma$, we obtain the connected diagram contributions to the decomposition of nucleon spin in the heavy pion regime shown in Figure 6. Similar results have been obtained in Refs. [14, 28].

As in the case of the axial charge and momentum fraction shown previously, it will be very interesting to see how the quark spin and orbital angular momentum contributions evolve when calculations are completed for lighter pion masses. Just how connected and disconnected diagram contributions combine to produce the experimentally measured contribution from the quark spin, and how the remaining total angular momentum is divided between quark orbital angular momentum and angular momentum carried by gluons will resolve a puzzle that has challenged theorists for decades.

Transverse structure

Whereas structure functions measured in deep inelastic scattering only tell us about the distribution of quarks as a function of the longitudinal momentum fraction, $q(x)$, generalized parton distributions explore the quark distribution in three dimensions, $q(x, r_\perp)$, as a function of the longitudinal momentum fraction $x$ and the transverse spatial coordinate $r_\perp$. Indeed, Burkardt has shown [29] that the quantity corresponding to the mass in a conventional form factor approaches infinity for the transverse form factor in the infinite momentum frame, yielding the familiar non-relativistic relation that the generalized parton distribution $H(x, 0, t)$ is the transverse Fourier transform of the quark distribution,

$$H(x, 0, -\Delta^2) = \int d^2r_\perp q(x, r_\perp) e^{i\vec{r}_\perp \cdot \vec{\Delta}_\perp}.$$  

Hence, the generalized form factor, which can be calculated on the lattice, measures moments...
Figure 6. Generalized form factors $A_{20}$ and $B_{20}$ determining the total quark contribution to the nucleon spin when the pion mass is 897 MeV.

Figure 7. Lattice results for generalized form factors in the heavy pion world have been discussed [8, 10, 11, 15] in some detail, but the key features are shown in this figure. Physically, as $x \to 1$, the struck quark carries all the momentum, the spectator partons contribute negligibly, the transverse distribution approaches a delta-function, and the slope of the form factor therefore approaches zero. As $x$ decreases, successively more spectator partons become relevant, the transverse sizes increase, and the slope of the form factor correspondingly increases. Hence, we expect that as $n$ increases, the moment $x_n - 1$ increasingly weights large $x$ thereby decreasing the slope. The left panel of Figure 7 shows that this change in slope is quite dramatic, with the third moment being far flatter than the first moment.

It is useful to use the slope of the form factors at $t = 0$ to determine the transverse rms radius for each moment:

$$\langle r^2 \perp \rangle (n) = \int d^2 r \perp r^2 \perp \int dx x^{n-1} q(x, r \perp) \frac{1}{\int d^2 r \perp \int dx x^{n-1} q(x, r \perp)}.$$
Figure 7. The left panel shows normalized generalized form factors $A_{n,0}^{u-d}(t)$ for $n=1$ (diamonds), $n=2$ (triangles), and $n=3$ (squares). The right panel shows the transverse rms radius of the proton light cone wave function as a function of the average quark momentum fraction, $x_{av}$, for each measured moment.

Figure 4 of David Richards proceedings[24] shows the results of a new lattice method that for the first time has the precision to measure non-vanishing $R_{EM}$ and $R_{SM}$ ratios[30, 31]. Extrapolation of these quenched results in the heavy pion regime to the chiral limit yields results qualitatively similar to experiment, raising the expectation that calculations presently under way in the chiral regime will provide quantitative agreement with experiment. With this absolute calibration from experiment, comparable lattice calculations of correlation functions in the $\Delta$ can then be used to obtain insight into the magnitude and origin of its deformation[32].

3. New Era of Lattice QCD
From these examples, I hope it is clear that with SciDAC support and dedicated DOE computer resources, we have entered a new era of lattice QCD. We are now solving full QCD well into the chiral regime, and in the coming year have computer resources to include even lower pion masses and to begin calculations at finer lattice spacings.

Lattice QCD is finally becoming a quantitative tool that can be expected to agree with experiment and to complement it where experiments are impractical. When the credibility of ab initio calculations has been well established by agreement with experiment, calculations will also enable a host of illuminating calculations of the internal structure of hadrons. Timely examples include the exploration of diquark components in hadrons and calculation of pentaquarks.

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