Computing Properties of Hadrons, Nuclei and Nuclear Matter from Quantum Chromodynamics

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1 Abstract

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The proposal describes the software development effort which the nuclear physics lattice QCD community intends to pursue during the next 5 years. This will ensure that lattice calculations can make optimal use of forthcoming leadership-class and dedicated hardware, including those of the national laboratories, and prepares for the exploitation of future computational resources in the exascale era. This work will greatly advance our ability to perform competitive, high precision calculations of properties of hadrons, nuclei and nuclear matter. It has impact on current heavy ion experiments at RHIC and LHC, the nuclear structure programs at RHICspin and JLab, and the study of excited states by CLAS at JLab, and future experimental research programs including GlueX at JLAb@12GeV and FRIB. If funded, this project will allow us to greatly improve our understanding of interactions in strongly coupled matter under a broad range of conditions.

We intend to further develop and optimize our simulation software for lattice QCD calculations on leadership class computers and on GPU-accelerated heterogeneous architectures. We will improve and extend our software libraries by providing interfaces for heterogeneous computing environments and through the optimization of gauge field evolution algorithms and sparse matrix inverters. The former includes the development of new multi-time scale integrators and the latter will focus on the development of new multi-grid and domain decomposition inverters for several QCD fermion discretization schemes. We furthermore will develop a domain specific language for lattice QCD computations which will enable the generation of highly optimized code within the ROSE compiler framework. This work will be carried out in cooperation with SUPER.

The proposed work is a project of the USQCD Collaboration, which consists of nearly all of the high energy and nuclear physicists in the United States working on the numerical study of lattice gauge theories. It will be carried out by nuclear physicists in USQCD in collaboration with members of the SciDAC SUPER institute and colleagues in the NVIDIA Emerging Applications group.

All our software developments are coordinated with efforts of the US lattice QCD community which is organized through the USQCD collaboration and will be made publicly available through the collaboration WEB page (http://www.usqcd.org).

2 Narrative: Scientific Goals and Software Tasks

2.1 Introduction

A fundamental quest of modern science is the exploration of matter in all its possible forms. The overarching mission of the field of Nuclear Physics is to establish a framework with which to perform high-precision calculations, with quantifiable uncertainties, of the properties and interactions of nuclear matter under a broad range of conditions, including those beyond the reach of laboratory experiment. For the last century, impressive experimental facilities have provided numerous discoveries which have led to the theoretical developments that currently underpin the field. Since the 1970's, quantum chromodynamics (QCD), a non-Abelian quantum gauge field theory constructed in terms of quarks and gluons, has been established as the theory of the strong interactions–which, along with the electroweak interactions, is responsible for all nuclear phenomena. However, many aspects of nuclear physics are dictated by the regime of QCD in which its defining feature–asymptotic freedom–is concealed by confinement and by the structure of its vacuum. The numerical technique of *Lattice QCD* is the only known way to perform *ab initio* QCD calculations of strong interaction quantities in this regime.

The ability to calculate strong interaction observables with quantifiable uncertainties is required in order to better define more complex nuclear systems, and developing such a capability will have profound and transformative impact upon the field. Remarkable progress has been made in the last decade in understanding the structure of hadrons and in establishing bridges between QCD, nuclear interactions and matter under extreme conditions. The 12 GeV upgrade at the Thomas Jefferson National Accelerator Facility (JLab) is designed in part to enable the discovery and exploration of exotic hadrons for which the gluons of QCD may play a visible role in their structure. QCD-consistent forces have emerged from the effective field theory (EFT) framework and are currently being used to calculate the properties and interactions of light nuclei, and are foreseen to be a central component of future calculations of processes involving nucleons. Through collaborative efforts within the nuclear structure community, the field of nuclear physics is presently entering an era in which precise QCD-based calculations of the properties and interactions of nuclei will become possible. Results that emerged from the experimental program at the Relativistic Heavy Ion Collider (RHIC) at Brookhaven National Laboratory and other heavy ion facilities indicate that a new state of matter with a low ratio of viscosity-to-entropy has been produced during the earliest moments of the collision. A complete understanding of these heavy ion collisions, and the development of predictive capabilities for such processes under different conditions requires, at its heart, a detailed map of the QCD phase-diagram and the ability to calculate the properties of matter in each of the phases. QCD-based calculations of nuclear matter at finite temperatures and densities, and of nuclear structure and reactions, will improve the reliability of the input into astrophysical simulations, such as of core-collapse supernovae, enabling the quantification of uncertainties in such simulations.

Lattice QCD is a technique in which strong interaction quantities are calculated by large-scale numerical Monte-Carlo evaluation of the Euclidean space path-integral in a finite-volume discretized space-time, where the effects of the finite volume and the discretization can be systematically removed. With the leadership-class computational platforms that continue to be deployed within the United States, we stand at a new frontier: understanding precisely how the quarks and gluons are assembled to form nucleons and exotic hadrons, and understanding how they interact collectively to generate nuclei and new phases of matter [1].

In order to achieve a precise understanding of the properties of hadrons and of hadronic matter that can confront current and future high precision experiments, and can be used to reliably predict the behavior of matter in environments where experiment is difficult or impossible. Lattice QCD software and algorithms must be upgraded in order to optimally use near-future computational resources on the path to the exascale.

2.2 The Science Case

2.2.1 Matter under extreme conditions (Heavy Ion Collision Physics)

Overview: At low temperatures and densities ordinary hadrons are the prevailing degrees of freedom that determine the properties of nuclear matter. However, under extreme conditions of high temperature or of high density (or both) this is expected to change. The theory of strong interactions (Quantum Chromodynamics (QCD)) predicts that a phase transition occurs that separates the low temperature/density regime from a high temperature/density region where quarks and gluons, the basic constituents of QCD, become the most relevant degrees of freedom. As the temperature and baryon chemical potential are varied, the quark and gluon interactions are modified according to QCD, thereby dictating the properties of matter under extreme conditions.

Deriving detailed predictions for the properties of matter at high temperature and density directly from QCD is paramount in shaping our understanding of nuclear matter in general, as well as for understanding the evolution of the early universe. Large experimental and theoretical programs in the United States and internationally thus exist which explore the properties of matter at high temperature and/or density, with the aim of mapping the boundaries between different phases of strongly interacting matter, and determining quantitatively the properties of matter in this domain.

The progress and future goals of these programs are described in detail in the 2007 Nuclear Science Long Range Plan: The Frontiers of Nuclear Science, a report issued by the DOE/NSF Nuclear Science Advisory Committee (NSAC 2007) [1]. As one of the recommendations it states: "*...Achieving a quantitative understanding of the quark-gluon plasma also requires new investments in modeling of heavy- ion collisions, in analytic approaches, and in large-scale computing...*"

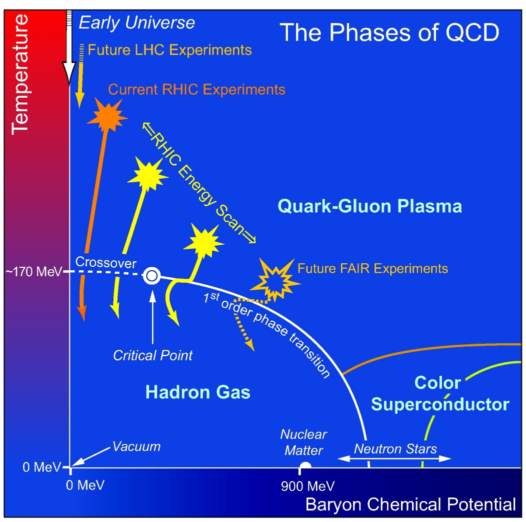

FIGURE 1: Phase diagram of QCD in the temperature and baryon chemical potential plane.

Large scale computation plays a pivotal role in providing answers for the overarching questions in the study of matter under extreme conditions as they have been laid out in the Nuclear Physics Long Range Plan [1],

- What are the phases of strongly interacting matter, and what role do they play in the cosmos?
- What does QCD predict for the properties of strongly interacting matter?
- What governs the transition of quarks and gluons into pions and nucleons?

Past Achievements: During recent years a fairly good quantitative understanding of basic parameters of the transition from ordinary hadronic matter to the quark gluon plasma has been reached in the limiting case of vanishing net baryon number density [2]. The lattice QCD groups in the US contributed significantly to almost all of these new developments. State-of-the art calculations for the thermal transition in QCD [3, 4] led to a first parametrization of the equation of state with almost physical light and strange quark masses. It has been used in the modeling of heavy ion collisions (HIC) [5, 6]. These calculations confirm that the hadron resonance gas, frequently used in phenomenological interpretations of HIC data, provides a fairly good description of the low temperature phase of QCD. A systematic analysis of cut-off effects in calculations with staggered fermions led to a good understanding of the continuum extrapolation of the transition temperature to the quark gluon plasma phase, $T_c = 154(9)$ MeV [7, 8]. Furthermore, it was established that thermodynamics in the transition region is controlled by universal scaling laws that are consistent with those of the three dimensional O(4) universality class [9]. This observation provided a unique way to predict the curvature of the transition line at non-zero chemical potential [10] and characteristic features of cumulants of conserved charge fluctuations [11, 12]. Although these results results still need to be improved so that a controlled continuum extrapolation can be performed, they provide important information about the relative location of the QCD transition line and the freeze-out temperature determined in heavy ion experiments – a prerequisite for the interpretation of the beam energy scan (BES) now underway at RHIC.

A fundamental set of experimental observables that are being analyzed in the BES are fluctuations of conserved charges and their higher order cumulants [13]. They are considered to provide unique signatures for a possible critical point in the QCD phase diagram [11, 14]. Calculations of these observables are computationally demanding. State-of-the-art results for them have been obtained on the USQCD and DOE operated (recently decommissioned) QCDOC computers at BNL [11]. These calculations will be vastly improved through calculations on GPU-accelerated clusters which USQCD operates at JLab [15]. They are crucial for the interpretation of experimental results coming from the BES at RHIC [16].

Any quantitative understanding of electromagnetic signals in heavy ion experiments that emerge from the hot phase has to rely on a hydrodynamic modeling of the expansion of this phase. Such modeling has, for instance, led to an experimental determination of the average emission temperature of dileptons from the quark gluon plasma [17]. Aside from the equation of state, hydrodynamical modeling requires knowledge of transport properties in the quark-gluon plasma. Lattice QCD calculations of bulk and shear viscosities [18] and electrical conductivity [19, 20] have advanced considerably recently. Like the calculation of dilepton rates [19] and thermal masses of hadrons [21], these calculations rely on statistical tools, such as the maximum entropy method, that require input from precise data obtained in lattice calculations on large lattices. The techniques as well as the available data for such an analysis clearly need to be improved in the future.

The state-of-the-art calculations described above would not have been possible without highly optimized software for special purpose (QCDOC) and leadership class (BlueGene L and P) computers that has been developed under the SciDAC-2 program by members of USQCD and the joint effort in the development of software for the rapidly advancing set of applications suitable for calculations on GPU accelerated clusters.

Future Opportunities: Despite the many successes of recent years many questions in the thermodynamics of strongly interacting matter remain open and new ones arise from extensions of the relativistic heavy ion programs in the US and Europe through experiments at the Large Hadron Collider (LHC) at CERN, and the BES at RHIC. These experiments bring new questions into the focus of theoretical studies that are related to (i) the chiral properties of the QCD transition, (ii) transport properties of the Quark-Gluon plasma, (iii) the fate of heavy quark bound states, as well as (iv) the connection between thermal fluctuations of conserved charges, universal critical behavior close to the QCD chiral phase transition and its manifestation in experimentally accessible chemical freeze-out conditions at non-zero net baryon number density.

Properties of the low and high temperature phases and chiral properties of the QCD transition: Many questions in finite temperature QCD are currently being addressed on moderate-sized lattices using improved staggered fermion discretization schemes. All these calculations have been performed in a temperature range up to a few times the QCD transition temperature where it was sufficient to include contributions from the light and strange quark sectors. At the higher temperatures now probed at the LHC, as well as for a proper description of the expansion of the early universe, one needs to also control the contribution of charm quarks to the equation of state. The vastly different energy scale introduced by the charm quarks provides a challenge for such calculations as one needs to control discretization errors on quite different length scales. The highly improved staggered quark (HISQ) action is designed to cope with this problem. Nonetheless systematic thermodynamics studies are missing so far and certainly calculations on larger lattices will be needed.

One of the outstanding problems for future calculations is to confirm the results obtained with staggered fermions by using other fermion formulations. Moreover, subtle features of the QCD transition related to the anomalous axial current, the non-trivial topological structure of the QCD vacuum and its relation to the spectrum of low lying eigenvalues of the Dirac operator at finite temperature may require a chiral discretization scheme to be addressed appropriately. First steps in this direction have been undertaken using the chiral five-dimensional domain wall fermion (DWF) formulation in studies of QCD thermodynamics [22, 23].

Computational Challenge: To make progress with computationally demanding thermodynamic calculations that use the HISQ action and the DWF formulation requires optimized implementations of simulation software on the next generation of leadership class computers, e.g. BlueGene Q, and on GPU accelerated clusters. We have implemented the HISQ action for conventional clusters within the SciDAC-2 software suite. Specific optimizations for BlueGene Q are needed. GPU support for HISQ needs to be developed.

Transport properties, dilepton rates and heavy quark bound states: Unlike thermodynamics calculations for the QCD equation of state, the calculation of transport coefficients, thermal rates and masses requires lattices that are almost two orders of magnitude larger. Recent calculations of the electrical conductivity, performed within the quenched approximation of QCD with vanishing momenta, exploited lattices as large as $128^3 \times 48$. To make contact with experiment these calculations need to be extended to non-zero momenta and a larger temperature range and should include also dynamical light quark effects. A new set of calculations of thermal masses and related screening lengths also becomes important in the context of thermodynamic studies with chiral fermions. The analysis of mass splittings in scalar and pseudo-scalar channels as well as vector and axial-vector channels is needed to disentangle thermal effects related to $SU(2)_L \times SU(2)_R$ chiral symmetry on the one hand and the $U(1)_A$ axial symmetry on the other hand.

The central observables in all these calculations are correlation functions with hadronic quantum numbers. The techniques and the numerical problems one faces in these calculations on large lattices are thus identical to those used in vacuum QCD. Many of these calculations will be ported to GPUs in the future.

Computational Challenge: To make progress we need highly efficient solvers that compute the inverse of the Dirac matrix and codes that support calculations with large lattices and with high statistics. Particularly needed are multicore optimizations specific to the BlueGene Q and to large GPU-enhanced clusters.

The phase diagram at non-zero baryon chemical potential and the QCD critical point: Getting control over the QCD phase diagram at non-vanishing chemical potential is essential for research programs at RHIC and LHC as well as at the future accelerator facilities FAIR in Darmstadt, Germany, and NICA in Dubna, Russia. At present all information on the QCD phase diagram coming from lattice QCD calculations is based on calculations that do not correspond to current state of the art. Likewise, the unsettled question of whether or not a phase transition occurs at non-vanishing net baryon number density is based on calculations that have been performed on rather coarse lattices and thus suffer from large discretization errors.

Direct numerical calculations at non-zero chemical potential or non-zero baryon number are at present not possible; straightforward adoptions of techniques used at vanishing chemical potential are impossible as the high dimensional integrals one needs to analyze do not have positive definite integrands. At present, the Taylor expansion method is most likely to benefit from advances in computing software and hardware, so it looks most promising. The calculation of Taylor expansion coefficients can be performed with HISQ actions at physical quark mass values and vanishing chemical potential. Higher order expansion coefficients need to be calculated at different values of the cut-off. This will allow a direct comparison of higher order cumulants for conserved charge fluctuations with experiment and will provide more reliable estimates for the location of a possible critical point in the QCD phase diagram.

Computational Challenge: The Taylor expansion approach requires the frequent inversion of large sparse matrices with varying random source vectors. These calculations have recently been implemented quite successfully on GPU-clusters. In order to further exploit the potential of GPU-clusters it will be necessary to improve the parallelization and inter-node communication of the QCD code among large GPU arrays as well as to improve algorithms for sparse matrix inversions that take into account the specific structure of the QCD Dirac matrix. Recent successful USQCD work on multi-GPU operation is described in [24, 25]. The outstandingly successful implementation of a multigrid inverter for Wilson fermions is an example of algorithmic improvement [26]. Such a multigrid scheme has yet to be developed for the HISQ action.

2.2.2 Hadron Spectrum (Medium Energy Nuclear Physics)

Overview The calculation of the bound state spectrum of QCD encapsulates our ability to describe the strong interactions, and the confrontation of high-precision calculations with experimental measurements is a vital test of the theoretical framework. The experimental investigation of the excited states of QCD has undergone a resurgence: the observation of new states in the Charmonium system at Belle and at BaBar, the search for the so-called missing baryon resonances of the quark model at CLAS at JLab@6GeV, and the flagship search for so-called exotic mesons at GlueX at the upgraded JLab@12GeV. How do the apparent collective degrees of freedom arise that describe the spectrum arise, and can we identify them?. What role do gluons play in the spectrum, and how are they manifest? The work proposed here will facilitate those calculations both to describe the extant experimental data, and to *predict* the outcomes of future experiments.

Past Achievements In contrast to electromagnetism, the "field-lines" between a quark and antiquark in QCD do not diffuse over large distances, but rather are confined to compact "flux tubes" connecting them. A quark-antiquark pair connected by a flux tube is the simplest picture of a meson. A quark-antiquark pair with relative orbital angular momentum can only possess certain allowed values of J^{PC}, and mesons having quantum numbers outside those allowed values are known as "exotics" and must have a richer structure. The hybrid hypothesis is that these exotic quantum numbers arise from the addition of an excited gluon field, and thus exotic states have attained the status of a "smoking gun" for gluonic degrees of freedom. A recent calculation of the isovector meson spectrum including those of high spin and exotic quantum numbers, suggests the presence of exotics in a regime accessible to GlueX [27, 28], illustrated in Figure 2, and furthermore the existence of both exotic and non-exotic "hybrids". Calculations in the isoscalar sector revealed the hidden flavor-mixing angles describing the admixtures of their light- and strange-quark components [29, 30], and the presence of isoscalar exotics at a mass comparable to their isovector cousins [30].

Baryons, containing three quarks, are emblematic of the non-Abelian nature of QCD, and of SU(3). The search for so-called "missing resonances" focuses on whether the baryon spectrum can be well described by a quark model, or whether an effective theory with fewer degrees of freedom, such as a quark-diquark picture, provides a more faithful description. A recent calculation of the low-lying nucleon and Δ excited spectrum [32] exhibited a counting of levels consistent with the non-relativistic qqq constituent quark model and inconsistent with a quark-diquark picture of baryon structure.

The excited-state spectrum of QCD is characterized by states that are resonances unstable under the strong interaction, and the spectrum is encapsulated within momentum-dependent phase shifts which may then be parametrised in terms of a mass and decay width. In Euclidean space QCD, shifts in the energy spectrum at finite volume can be related to infinite-volume phase shifts at the corresponding scattering momenta [33, 34]. The method has been successfully applied to extract the momentum-dependent phase shifts in non-resonant

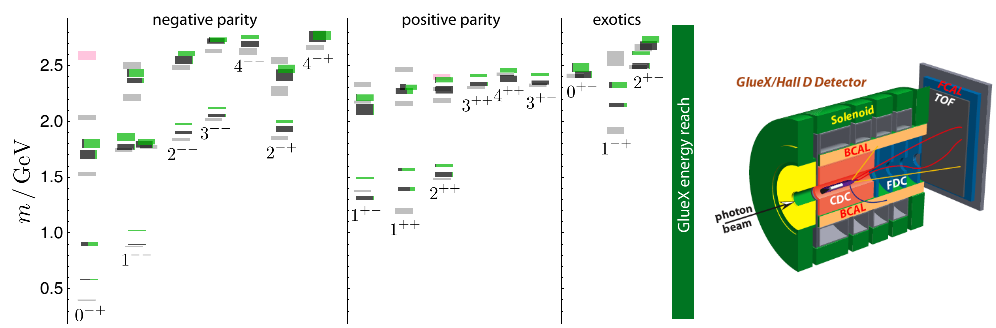

Figure 2: The figure shows the spectrum of states for exotic quantum numbers for both isovectors (grey) and isoscalars (black/green) for light quark masses corresponding to those of a pion of mass 396 MeV [30]. The light/strange quark content is indicated by the fraction of black/green in the rectangle. The pink is the calculation of the pure Yang-Mills glueball [31]. *These results suggest the presence of many exotics in a region accessible to the future GlueX experiment.*

$I = 2\pi\pi$ scattering [35, 36], including those of higher partial waves [35]. The phase shift for the resonant ρ meson has been determined [37, 38], and fitted to obtain a mass and width.

Finally, there have been significant advances in understanding properties of the excited states in QCD, in an approximation in which they are treated as quasi-stable particles. The electromagnetic and axial-vector form factors [39] of the Δ, challenging to determine experimentally, and of the $N \to \Delta$ transition form factors [40, 41], have been computed adding to our understanding of deformations in the baryon spectrum.

Future Opportunities: The work proposed herein will facilitate significant advances towards the precise studies of the spectrum that can reliably confront experiment. Calculations of the excited meson spectrum, with the effect of decay channels included and the momentum-dependent phase shifts determined, at quark masses approaching the physical light-quark masses, will provide *predictions* for the meson spectrum in advance of experiments such as GlueX. Calculations of the radiative transitions between conventional and exotic mesons, advancing methods developed for charmonium [42, 43], will inform expected production rates at GlueX. The calculation of the flavor-singlet spectrum, including in particular the contribution of the predominantly gluonic "glueballs", will be performed in advance of searches such as those at PANDA at GSI.

The calculation of the spectrum of the narrow, double-strangeness Cascade baryons, Ξ, where few states have been discovered and with little knowledge of their quantum numbers, provide an early opportunity for predictions of QCD in the baryon sector in advance of proposed programs at Jefferson Laboratory at 12 GeV, at PANDA, and underpin experimental studies of hypernuclear physics such as those at JPARC.

The spectrum of nucleon and Δ resonances, with the light-quark masses approaching and eventually attaining their physical values, will capitalize on the achievement of the *NSAC performance measures HP3 and HP7* [44]. These calculations will facilitate the interpretation of $N*$ resonance data extracted from experiment, and help address the key questions in our understanding of the hadron spectrum, such as the status and structure of the low-lying *Roper* resonance, and the anomalously light $\Lambda(1405)^-$.'

Measuring the electromagnetic transitions to nucleon resonances is a key effort of CLAS at JLab@12 GeV [47], and their calculation correctly accounting for their decays [48], will provide an important glimpse into their structure. The calculation of the form factors at increasing momentum transfers will elucidate the transition to a perturbative description of QCD in terms of the quark and gluon degrees of freedom [49].

Computational Challenges: The exploitation of leadership-class computers to pursue this program requires that we overcome numerous computational challenges. *Unstable Resonances:* the formalism developed for elastic channels must be extended to inelastic decay channels. *Calculation of hadron correlation functions:* the effective application of the variational method requires a broad variational basis that encompasses the physics, and the resultant efficient computation of many correlation functions including those for multi-hadron states, and for predominantly gluonic states. *High statistical precision:* Calculations of the spectrum are characterized by decreasing signal-to-noise ratios at decreasing quark masses, and with increasing excitation energy. Efficient methods are needed both to generate large lattice ensembles and to make many measurements on those ensembles. *Ensembles at physical quark masses:* Precise comparison with experiment requires large lattice ensembles with the $u-$, $d-$, $s-$ quarks close to their physical values, and of sufficient volume for the reliable determination of the momentum-dependent phase shifts.

2.2.3 Hadron Structure (Medium Energy Nuclear Physics)

Overview: One of the great challenges posed by QCD is understanding how protons and neutrons are made from quarks and glue. Just as calculating the structure of atoms was a cornerstone of quantum mechanics, a cornerstone of our effort is to achieve a quantitative, predictive understanding of the structure of nucleons and other hadrons using lattice QCD. Our lattice calculations are directly relevant to experiments at JLab, RHIC-spin, SLAC, and FNAL, and will have significant impact on future experiments at the JLab 12 GeV upgrade and a planned electron-ion collider. They are explicitly required to meet the *2014 NSAC Performance Measure HP9* [44], and address experimental measurements mandated by 6 of the other 9 Performance Measures.

Past Achievements: Electromagnetic form factors reveal the distribution of charge and current, and recent calculations[50, 51, 52, 53] have shown the emergence of the pion cloud at the periphery of the nucleon. The axial charge, g_A, governing neutron Beta-decay, is the value of the axial form factor at zero momentum transfer. Chiral extrapolations of calculations of g_A at heavy quark masses agree with experiment[50, 54, 55] with errors as low as 7%. Precision calculation will impact the proton-proton fusion rate central to solar models and constrain the weak matrix element $|V_{ud}|$. The scalar and tensor charges, g_S and g_T,[56] will be valuable in searching for physics beyond the standard model in ultra-cold neutron Beta-decay experiments.

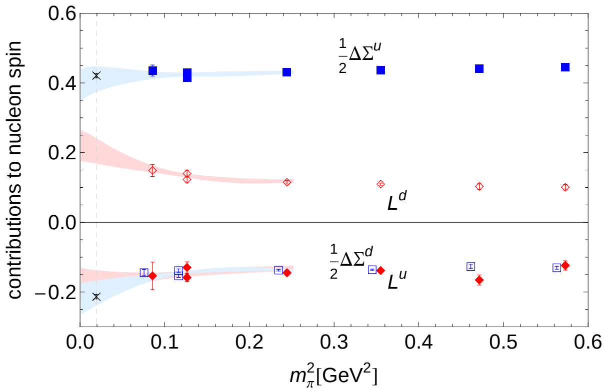

Figure 3: Contributions of quark spin $\Delta\Sigma^{u,d}/2$ (blue error bars) and orbital angular momentum $L^{u,d}$ (red error bars) to the spin 1/2 of the proton for up and down quarks. Chiral extrapolations (shaded error bands) agree with HERMES data (crosses).

Quark parton distributions, measured in deep-inelastic scattering, specify quark density, spin, and transversity distributions as functions of the momentum fraction, x, of the struck quark. Their lowest three moments have been calculated[50, 57, 58, 59] showing, for example, that chiral extrapolations of the fractions of the nucleon spin and momentum arising from quark spin and momentum agree with experiment.

Generalized Parton Distributions (GPD's) specify quark density, spin, and transversely as functions of both the longitudinal momentum fraction x and the transverse position, and if known completely would enable us to calculate a 3-dimensional picture of the nucleon. Their moments in x have been calculated on the lattice[50, 61], and the combination of these moments with convolutions of GPDs measured at JLab and elsewhere will provide a more complete understanding than either effort could obtain separately. Moments of GPD's specify the total angular momentum of quarks in the nucleon, so combined with the quark spin contribution above, the lattice provides a complete determination of quark spin and orbital contributions to the total spin $1/2$ of the nucleon. The results [50, 61, 57, 60] shown in Fig 3, are striking. Only about 30% comes from quark spin and the substantial orbital contributions of up and down quarks cancel so that the remaining 70% must come from gluons. This is of great interest experimentally and a major focus of RHIC-spin and a future electron-ion collider is measuring the contribution of gluons to the nucleon spin. Direct calculation of the gluon contribution to the nucleon spin is clearly desirable, and an important initial step has been taken by calculating the contribution of gluons to the momentum fraction $\langle x \rangle$ of the pion[62].

Transverse momentum distributions show the quark momentum distribution, and initial calculations in a nucleon [63] have opened the way for future results relevant to semi-inclusive deep inelastic and single-spin asymmetry experiments at COMPASS, Hermes, JLab, and a future electron-ion collider. Also, the spin-isospin excitation of the nucleon, the $\Delta(1232)$, has been shown to be deformed by calculating its quark transverse charge densities[64] and the transition form factors to it from the nucleon[41].

Future Challenges: These recent accomplishments and emerging computer resources, combined with the requisite algorithms and software provide the opportunity to meet a range of exciting challenges.

Precision calculations at the physical pion mass Although calculations at the physical pion mass are finally becoming possible, an unexpected challenge has arisen. Instead of following chiral extrapolations of existing calculations that lead to the correct experimental values, calculations[65, 66] in the nucleon for g_A, the momentum fraction, and RMS radius by several groups using standard methodology have shown deviations arising from contamination by excited states. Hence, it will be necessary to dramatically increase statistics to explicitly remove excited states or use distillation[67] to expand in a basis including the relevant multi-particle states.

Disconnected diagrams Disconnected diagrams involve quark propagators that can start at any point on the lattice and are computationally far more expensive than isovector matrix elements that have been the primary focus of past calculations. They are required to calculate flavor singlet quantities such as the properties of a neutron or proton separately, and testing algorithms on large lattices at the physical pion mass and developing efficient software for them will be crucial.

Form factors at high momentum transfer At sufficiently high momentum transfer q, asymptotic scaling sets in and the electric form factor falls off as q^{-4}. To determine this scale for asymptotic scaling, form factor calculations must be extended to high momentum transfer where new techniques[68] need to be explored and applied in large volumes at the physical pion mass.

Higher moments of quark structure functions Due to operator mixing on a discrete lattice, only the lowest three moments of quark distributions can be calculated with present techniques. To reconstruct the full quark distributions, it is necessary to explore new algorithms for calculating higher moments, such as introducing a heavy quark field [69], and to exploit them at the physical pion mass.

Gluon contributions Calculation of gluon contributions to the nucleon mass, momentum, and angular momentum, and gluon mixing with quark disconnected diagrams is complicated by the fact that fluctuations grow strongly as the lattice spacing is decreased. Hence, extracting the continuum limit will require a combination of techniques for obtaining extremely high statistics and new algorithms.

Transverse momentum distributions To relate lattice calculations of transverse momentum distributions to semi-inclusive deep inelastic scattering and Drell-Yan experiments, these calculations must be extended to much higher nucleon momenta and lattice volumes. Because of the rapid decrease of the signal-to-noise ratio with momentum, extremely high statistics will be required.

Computational Challenges: One theme pervading these physics challenges is the need for unprecedentedly large numbers measurements on very large lattices at the physical pion mass. Although deflation is useful for present lattice sizes, evolution to larger lattices will require multigrid algorithms. Optimized inverters implementing these and other algorithmic advances are needed for all the relevant fermion actions on BG/Q, GPU's, and subsequent emerging architectures.

A second theme is the need for nimble exploration of algorithms at scale. Exploration of multigrid methods, distillation, step scaling, schemes for higher moments, noise reduction methods, improved gluon operators as well as performance optimization on each architecture will only be feasible if tools are developed to do this quickly.

2.2.4 Hadron Interactions (Medium and Low Energy Nuclear Physics)

Overview: The strong interactions among baryons are key to every aspect of our existence. The two- and higher-body interactions among protons and neutrons, along with the electroweak interactions, conspire to produce the spectrum of nuclei and the complicated chains of nuclear reactions that allow for the production of the elements forming the periodic table at the earliest times of our universe, in the stellar environments that follow, and in reactors and our laboratories. Decades of experimental effort have provided a precise set of measurements of the nucleon-nucleon scattering cross sections over a wide range of energies, which have given rise to the modern nuclear forces. These experimentally determined two-body forces, encoded by modern potentials such as AV_{18} [70] and the chiral potentials [71], when supplemented with three-body interactions, and implemented using the renormalization group [72], provide the cornerstone of our theoretical description of nuclei and their interactions. Coordinated efforts by the US nuclear physics community during the last several years to develop the computational technology to perform convergent nuclear structure calculations (under the SciDAC2 UNEDF collaboration [73]) show that three-nucleon forces are required to determine the structure of light nuclei [74, 75]. Given the size of the three-nucleon and higher-body interactions, there is considerable uncertainty in their form, and hence in the predictions for systems for which there is little or no experimental guidance, such as arise in extreme nuclear environments [76] that can be found, for instance, in the interior of core-collapse supernova. One of the motivations for building FRIB (Facility for

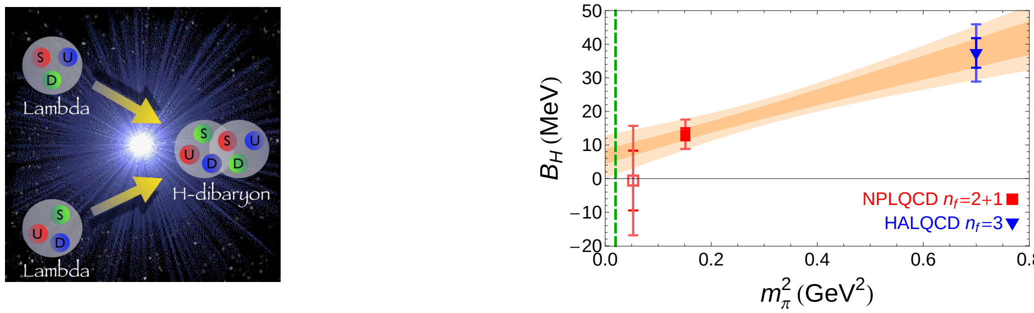

Figure 4: The H-dibaryon has the quantum numbers of $\Lambda\Lambda$ (left panel). The right panel shows the results of Lattice QCD calculations [46, 45, 88, 87]. The green dashed line corresponds to the physical pion mass.

Rare Isotope Beams) is to better constrain the multi-neutron interactions from very neutron-rich nuclei.

The connection between nuclear physics and the underlying theory of fundamental forces, the standard model of the strong and electroweak interactions, will be solidified during the next decade using Lattice QCD. Technology will be developed to reliably calculate the properties and interactions of light nuclei and to quantify, and systematically remove, the uncertainties in such calculations. It is this rationale that underpins the *2014 NSAC Performance Measure HP10* [44]. Fundamental questions regarding the dependence of nuclei and their interactions on the fundamental parameters of nature, and the fine-tunings in nuclear physics, will be answered along the way. Simultaneously, the behavior of exotic matter, such as kaon-condensed matter or hyperonic matter, that is extremely difficult, or impossible, to access in the laboratory but may play an important role in extreme environments, will be quantified. It is exciting to note that the upcoming experimental programs at J-PARC [77], FAIR [78], JLab, and the relativistic heavy ion experiments at BNL and CERN, may be able to observe or constrain the simplest exotic systems.

Past Achievements: A pioneering study of baryon-baryon scattering with Lattice QCD was performed more than a decade ago by Fukugita *et al* [79, 80], but it involved large light-quark masses and did not have dynamical sea quarks (quenched). More recently, Lattice QCD calculations of nucleon-nucleon [81, 82, 83, 84, 85] and hyperon-nucleon [86] interactions were performed but with unphysical pion masses, and the nucleon-nucleon scattering lengths were found to be of natural size. The fine-tunings in nature indicate that LQCD calculations with quark masses much closer to the physical values are needed to extrapolate to the experimental values. During 2010, lattice QCD calculations [46, 45, 87], have provided evidence that the H-dibaryon (with the quantum numbers of $\Lambda\Lambda$) is bound at heavier light-quark masses. While the form of the light-quark dependence of such a system has not been rigorously constructed, possible extrapolations suggest a weakly bound H-dibaryon or a near threshold resonance exists [88, 89, 90] (right panel of Figure 4). It has also been found that the $\Xi^-\Xi^-$ forms a bound state at heavier light-quark masses [45], which is consistent with previous estimates constrained by experimental data and the approximate SU(3) flavor symmetry of QCD. Following work on three-baryon systems [91], in late 2009 the PACS-CS collaboration performed the first, but quenched, calculation of ^{4}He [92]. The pion mass was $m_\pi \sim 800$ MeV and surprisingly the calculated binding energy of ^{4}He was found to be close to its actual value.

Calculations of finite-density, Bose-Einstein condensed multi-meson systems containing up to 12 π^+'s or K^+'s have been performed [93, 94, 95] (and extended up to 72 mesons [96]). Precise determinations of the $\pi^+\pi^+$ scattering length [97] and extractions of the effective range and shape parameter, along with the scattering phase-shift [35, 36], have been performed by combining Lattice QCD calculations with chiral perturbation theory (χPT). Further, analysis of multi-pion systems has led to a determination of the three-pion interaction [93]. A surprising result is that tree-level χPT describes these systems even at the heavy light-quark masses, and hence tree-level χPT should provide reasonable estimates of the properties of a possible kaon-condensed phase in dense matter. However, condensed systems containing baryons have not yet been explored, leaving a significant systematic uncertainty in such calculations. Recursion algorithms have been developed to allow for the Wick contractions contributing to a system with N mesons to be related to those for a system with $N-1$ mesons, requiring only a small number of operations [98].

Future Challenges: A suite of baryon-baryon, multi-baryon and multi-meson calculations must be performed at the physical light-quark masses, and with a range of volumes and lattice spacings in order to quantify the systematic uncertainties associated with using a finite space-time grid. This will provide the first calculations of nuclear forces from QCD that can be compared directly with those of nature, which can then used to make reliable predictions for nuclear systems (without electromagnetism or isospin breaking). The substantial hierarchy of energy-scales contributing to the correlation functions that are used to extract energy-levels and S-matrix elements continues to present a challenge to the Lattice QCD calculations and requires further algorithmic developments. The ongoing efforts to extend the range of calculations to multi-nucleon systems, for instance to p-shell nuclei, requires developments in the algorithms used to calculate Wick-contractions. Once the energy-levels of these multi-hadron systems can be determined with precision, the matrix elements of electroweak operators between such states can be calculated. Further, Lattice QCD will be used to make predictions for the interactions between strange baryons and nucleons, and the structure of the lightest hypernuclei, that may be tested in the upcoming experimental programs.

2.2.5 Fundamental Symmetries (Low Energy Nuclear Physics)

Overview: Research efforts to uncover particles and symmetries beyond those of the standard model of the strong and electroweak interactions are multi-pronged. One of the approaches in this effort is to perform precision measurements of the properties of known particles, such as the magnetic moment of the muon. The E821 experiment at Brookhaven National Laboratory has measured the muon $g-2$ with an uncertainty of 0.7 ppm, which deviates from the theoretical calculation by $\gtrsim 3\sigma$. The approved E-989 experiment at FermiLab is designed to reduce the uncertainty in g-2 below 0.14 ppm, either verifying the discrepancy with theory or resolving it. A major uncertainty in the theoretical calculation arises from strong interactions through quantum loops.

Nature is very nearly invariant under certain symmetry transformations, and the consequences of the slight non-invariance can have widespread implications. A well known example is CP-violation, where the combined operation of charge-conjugation, C, and spatial-inversion, P, is known to be slightly violated, and without CP-violation, the present-day matter and antimatter asymmetry of the universe would not exist. The nEDM collaboration is preparing to measure the electric dipole moment (edm) of the neutron [99], a quantity that vanishes in the absence of time-reversal, T, violation (equivalent to CP-violation when CPT-invariance is exact), with a precision of $\delta d_n \sim 3 \times 10^{-28}$ e cm at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory.

Past Achievements: There have been a number of efforts, part of the broader effort to support the *2020 NSAC Performance Measure FI15* [44], to calculate the neutron edm arising from the QCD θ-term using Lattice QCD [100, 101], but such calculations are found to be sensitive to the topological structure of the gluon fields.

During 2010, the first Lattice QCD calculation of nuclear parity violation was performed [102], in which the "connected diagrams" contributing to the weak one-pion-nucleon vertex, $h^1_{\pi NN}$, were determined. Its value at unphysically large light-quark masses was found to be consistent with the unnaturally small value extracted from theoretical analyses of a number of experimental measurements. An ongoing experimental effort by the NPDGamma Collaboration [103] at the SNS promises to greatly reduce the experimental uncertainties in the value of $h^1_{\pi NN}$, likely in a similar time-frame to the Lattice QCD calculations.

Exploratory Lattice QCD calculations of the muon $g-2$ are underway to understand how to calculate the strong interaction contributions, and this years *Kenneth Wilson Prize* [104] was awarded to Dru Renner and collaborators of the *European Twisted Mass Collaboration* [105] (now at JLab) for calculations of the leading contributions to the magnetic moments of the leptons.

Future Challenges: The currently exploratory calculations of nuclear parity violation must be greatly refined with the inclusion of the currently omitted quark-loop contributions. The neutron edm calculations have to

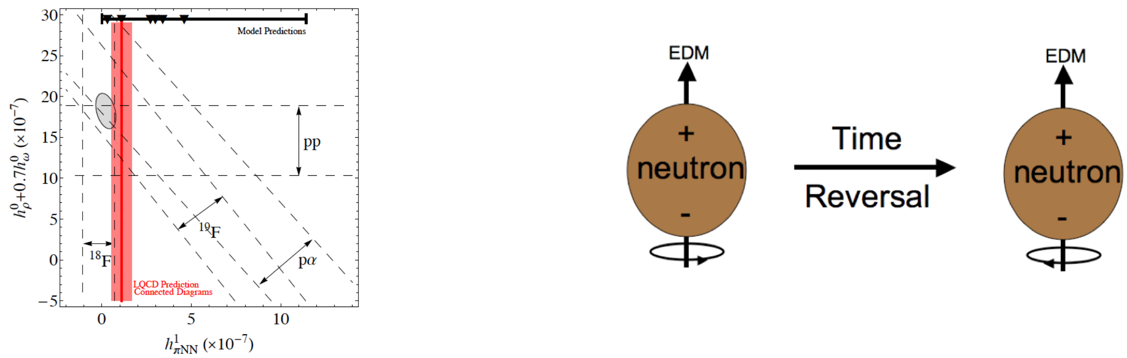

Figure 5: The left panel shows constraints on nuclear parity-violating interactions including the recent Lattice QCD result [102] (shaded (red) region), and the experimental 1σ uncertainty ellipse (gray). The upper panel is a cartoon showing the behavior of the neutron electric dipole moment under time-reversal.

be performed at the physical quark masses, and the impact of higher dimension operators evaluated. Efforts must be made to determine the strong interaction contributions to the light-by-light contributions to the muon $g-2$.

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