Progress in Particle and Nuclear Physics 67 (2012) 140–152

Contents lists available at SciVerse ScienceDirect

Progress in Particle and Nuclear Physics

journal homepage: www.elsevier.com/locate/ppnp

Review

Nuclear physics from lattice QCD☆

M.J. Savage [1]

Department of Physics, University of Washington, Box 351560, Seattle, WA 98195, USA

ARTICLE INFO

Keywords:
Nuclear forces
Lattice QCD
Nuclei

ABSTRACT

I review recent progress in the development of Lattice QCD into a calculational tool for nuclear physics. Lattice QCD is currently the only known way of "solving" QCD in the low-energy regime, and it promises to provide a solid foundation for the structure and interactions of nuclei directly from QCD.

1. Introduction

As discovered by the New Zealand physicist Ernest Rutherford, a nucleus, labeled by its baryon number and electric charge, is at the heart of every atom. Loosely speaking, nuclei are collections of protons and neutrons that interact pairwise, with much smaller, but significant, three-body interactions. We are in the fortunate situation of knowing the underlying laws governing the strong interactions. It is the quantum field theory called quantum chromodynamics (QCD), constructed in terms of quark and gluon fields with interaction determined by a local SU(3) gauge-symmetry, along with quantum electrodynamics (QED), that underpins all of nuclear physics when the five relevant input parameters, the scale of strong interactions Λ_{QCD}, the three light-quark masses m_u, m_d and m_s, and the electromagnetic coupling α_e, are set to their values in nature. It is remarkable that the complexity of nuclei emerges from "simple" gauge theories with just five input parameters. Perhaps even more remarkable is that nuclei resemble collections of nucleons and not collections of quarks and gluons. By solving QCD, we will be able to predict, with arbitrary precision, nuclear processes and the properties of multi-baryon systems (including, for instance, the interior of neutron stars).

The fine-tunings observed in the structure of nuclei and the interactions between nucleons are peculiar and fascinating aspects of nuclear physics. For the values of the input parameters that we have in our universe, the nucleon–nucleon (NN) interactions are fine-tuned to produce unnaturally large scattering lengths in both *s*-wave channels (described by non-trivial fixed-points in the low-energy effective field theory (EFT)), and the energy levels in the ^{8}Be-system, ^{12}C and ^{16}O are in "just-so" locations to produce enough ^{12}C to support life, and the subsequent emergence and evolution of the human species. At a fundamental level it is important for us to determine the sensitivity of the abundance of ^{12}C to the light-quark masses and to ascertain the degree of their fine-tuning.

Being able to solve QCD for the lightest nuclei, using the numerical technique of Lattice QCD (LQCD), would allow for a partial unification of nuclear physics. It would be possible to "match" the traditional nuclear physics techniques—the solution of the quantum many-body problem for neutrons and protons using techniques such as No-Core Shell Model (NCSM), Greens function Monte Carlo (GFMC), and others, to make predictions for the structure and interactions of nuclei for larger systems than can be directly calculated with LQCD. By placing these calculations on a fundamental footing, reliable predictions with quantifiable uncertainties can then be made for larger systems.

☆ Lecture presented at the Erice School on Nuclear Physics 2011: *From Quarks and Gluons to Hadrons and Nuclei*, organized by A. Faessler and J. Wambach.
E-mail address: savage@phys.washington.edu.

[1] [NPLQCD Collaboration].

0146-6410/$ – see front matter
doi:10.1016/j.ppnp.2011.12.008

2. Lattice QCD calculations of nuclear correlation functions

Lattice QCD is a technique in which space–time is discretized into a four-dimensional grid and the QCD path integral over the quark and gluon fields at each point in the grid is performed in Euclidean space–time using Monte Carlo methods. A LQCD calculation of a given quantity will deviate from its value in nature because of the finite volume of the space–time (with $L^3 \times T$ lattice points) over which the fields exist, and the finite separation between space–time points (the lattice spacing, b). However, such deviations can be systematically removed by performing calculations in multiple volumes with multiple lattice spacings, and extrapolating using the theoretically known functional dependences on each. Supercomputers are needed for such calculations due to the number of space–time points (sub grids of which are distributed among the compute cores) and the Monte Carlo evaluation of the path integral over the dynamical fields. In order for a controlled continuum extrapolation, the lattice spacing must be small enough to resolve structures induced by the strong dynamics, encapsulated by $b\Lambda_\chi \ll 1$ where Λ_χ is the scale of chiral symmetry breaking. Further, in order to have the hadron masses, and also the scattering observables, exponentially close to their infinite volume values, the lattice volume must be large enough to contain the lightest strongly interacting particle, encapsulated by $m_\pi L \gtrsim 2\pi$ where m_π is the mass of the pion and L is the extent of the spatial dimension of the cubic lattice volume (this, of course, can be generalized to non-cubic volumes). Effective field theory (EFT) descriptions of these observables exist for $b\Lambda_\chi \lesssim 1$ (the Symanzik action and its translation into χPT and other frameworks) and $m_\pi L \gtrsim 2\pi$ (the p-regime of χPT and other frameworks). The low-energy constants in the appropriate EFT are fit to the results of the LQCD calculations, which are then used to take the limit $b \to 0$ and $L \to \infty$. As the computational resources available today for LQCD calculations are not sufficient to be able to perform calculations at the physical values of the light quark masses in large enough volumes and at small enough lattice spacings, realistic present day calculations are performed at light quark masses that yield pion masses of $m_\pi \sim 200$ MeV. Therefore, present day calculations require the further extrapolation of $m_q \to m_q^{\mathrm{phys}}$, but do not yet include strong isospin breaking or electromagnetism. In principle, the gluon field configurations that are generated in LQCD calculations can be used to calculate an enormous array of observables, spanning the range from particle to nuclear physics. In practice, this is becoming less common, largely due to the different scales relevant to particle physics and to nuclear physics. Calculations of quantities involving the pion with a mass of $m_\pi \sim 140$ MeV are substantially different from those of, say, the triton with a mass of $M(^3\mathrm{H}) \sim 3$ GeV, and with the typical scale of nuclear excitations being $\Delta E \sim 1$ MeV. Present day dynamical LQCD calculations of nuclear physics quantities are performed with $m_\pi \sim 400$ MeV, lattice spacings of $b \sim 0.1$ fm and volumes with spatial extent of $L \sim 4$ fm. Quenched calculations, which unfortunately cannot be connected to nature, are typically performed in larger volumes as the gauge-field configurations are less expensive to generate compared with dynamical configurations.

LQCD calculations are approached in the same way that experimental efforts use detectors to measure one or more quantities—the computer is equivalent to the accelerator and the algorithms, software stack, and parameters of the LQCD calculation(s) are the equivalent of the detector. The parameters, such as lattice spacing, quark masses and volume, are selected based upon available computational resources, and simulations of the precision of the calculation(s) required to impact the physical quantity of interest, i.e. simulations of the LQCD Monte Carlo's are performed. The size of the computational resources required for cutting edge calculations are such that you only get "one shot at it". A typical work-flow of a LQCD calculation consists of three major components. The first component is the production of an ensemble of gauge-field configurations which contain statistically independent samplings of the gluon field configuration resulting from the LQCD action. The production of gauge-fields requires the largest partitions on the leadership class computational facilities, typically requiring $\gtrsim$128 K compute cores. Present day calculations have $n_f = 0, 2, 2+1, 3, 2+1+1$ dynamical light quark flavors and use the Wilson, $\mathcal{O}(b)$-improved-Wilson, staggered (Kogut–Susskind), domain-wall or overlap discretizations, each of which have their own "features". It is the evaluation of the light-quark determinant (the determinant of a sparse matrix with dimensions $\gtrsim 10^8 \times 10^8$) that consumes the largest fraction of the resources. Roughly speaking, $\gtrsim 10^4$ HMC trajectories are required to produce an ensemble of 10^3 decorrelated gauge-fields, but in many instances this is an under-estimate. For observables involving quarks, a second component of production is the determination of the light-quark propagators on each of the configurations. The light-quark propagator from a given source point is determined by an iterative inversion of the quark two-point function, using the conjugate-gradient (CG) algorithm or variants thereof such as BiCGSTAB, an example of which is shown in Fig. 1. During the last couple of years, the propagator production codes have been ported to run on GPU machines in parallel. The GPU's can perform propagator calculations faster than standard CPU's by one or two orders of magnitude, and have led to a major reduction in the statistical uncertainties in many calculations. There have been numerous algorithm developments that have also reduced the resources required for propagator production, such as the implementation of deflation techniques and the use of multi-grid methods. The third component of a LQCD calculation is the production of correlation functions from the light-quark propagators. This involves performing all of the Wick contractions that contribute to a given quantity. The number of contractions required for computing a single hadron correlation function is small. However, to acquire long plateaus in the effective mass plots (EMP's) that persist to short times, Lüscher–Wolff type methods [1,2] involve the computation of a large number of correlation functions resulting from different interpolating operators, and the number of contractions can become large. In contrast, the naive number of contractions required for a nucleus quickly becomes astronomically large ($\sim 10^{1500}$ for uranium), but symmetries in the contractions greatly reduces this number. For instance, there are 2880 naive contractions contributing to the ^{3}He correlation function, but only 93 are independent. As a light-quark propagator can give rise to a pion correlation function ($\sim e^{-m_\pi t}$) and a nucleon correlation