The Mass Difference Between Protons and Neutrons and the Fine Tuning of Physical Constants

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We report on a large scale calculation of the origin of the mass difference between the proton
and the neutron that was carried out to a large extent on the JUQUEEN computer.

1 Introduction

To our current knowledge, the strong nuclear force is described at a fundamental level
by quantum chromodynamics (QCD)[1], a quantum field theory of quarks and gluons that
is strongly coupled at low energies[2,3]. The strong coupling, which gives the theory its
very rich dynamical content is at the same time responsible for the failure of conventional
perturbative approaches that are the usual tool for solving quantum field theories: A small
perturbation on top of the unperturbed "free" theory of quarks and gluons will never be
able to even reproduce the hadrons, i.e. the particles connected to the strong nuclear force
that we observe in experiment like protons and neutrons.

A direct numerical solution of the theory is possible if one discretises it on a space-
time lattice[4]. This lattice approach has matured over the last decade into a reliable tool to
compute otherwise unattainable predictions of QCD[5]. A few years ago, it has eventually
been demonstrated[6], using lattice techniques, that QCD indeed does give the correct masses
to the most common hadrons within a few percent accuracy (see Fig. 1).

With the validity of the approach thus confirmed, one can start to ask more subtle
questions. One of these questions is the origin of the mass difference between proton and
neutron. Although this difference is relatively tiny – the neutron is only 0.14% more mas-
sive than the proton[7] – it does have profound consequences for the evolution and existence
of the universe as we know it. As the more massive particles, neutrons can decay into
protons (plus an electron and a neutrino), but since the mass difference is tiny, the process
is relatively slow: Free neutrons have a half life of about 15 minutes. These properties are
rather crucial, as a more massive proton in a hydrogen atom would decay into a neutron,
obviously leading to an entirely different universe. When the nuclei that predominantly
populate our universe today formed during the first twenty minutes after the big bang, the
value of the neutron half-life and thus the proton neutron mass difference also determined
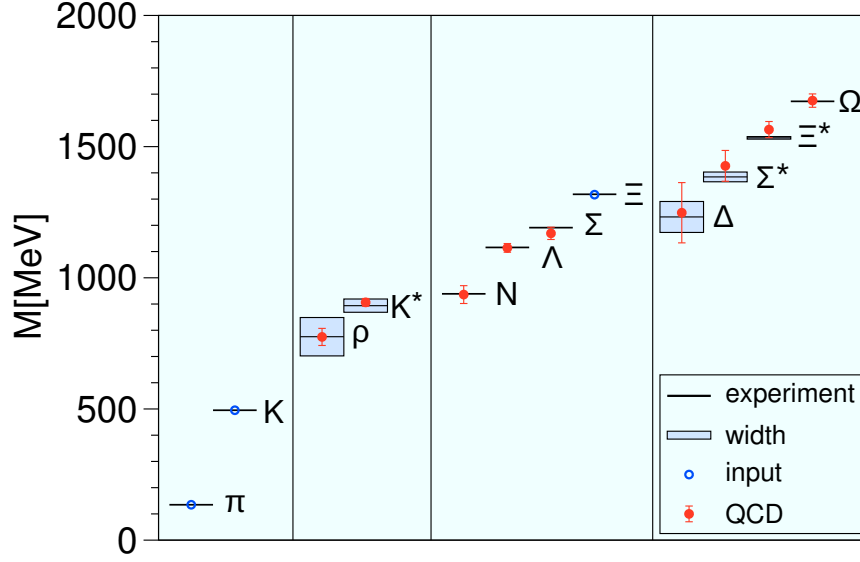
Figure 1. The light hadron spectrum[6].

what fraction of the primordial protons would fuse to helium nuclei. A smaller mass difference and thus longer half-life would have left little hydrogen as fuel for stars[8].

It is therefore very interesting to note, that the mass difference between proton and neutron actually results from a cancellation of two competing effects. On the one hand, the proton as a charged particle has a higher electromagnetic self energy and thus mass than the neutron. This effect is however overcompensated by the neutron consisting of one additional "down" quark as compared to the protons "up" quark. We know that the "down" quark is slightly more massive than the "up" quark and we also know that this is an exceptional situation, as the second and third generation "down" type quarks (the "strange" and the "bottom") are actually lighter than their respective "up" type counterparts (the "charm" and "top")[7].

While these qualitative features are well understood, the complex dynamics of QCD makes any quantitative understanding of the proton-neutron mass difference in terms of the fundamental theory extremely difficult. We report here on a recent calculation that computed the proton-neutron mass splitting and related quantities *ab initio* utilising a lattice formulation of QCD and the quantum field theory of the electromagnetic interaction (QED)[9] which was mostly carried out on the JUQUEEN supercomputer of Forschungszentrum Jülich.

2   Computational Challenges

In order to compute the mass difference between proton and neutron, one has to eliminate two approximations that are usually done in a lattice calculation: The equal mass of up and down quark (usually called the isospin limit) and the neglect of electromagnetic effects.
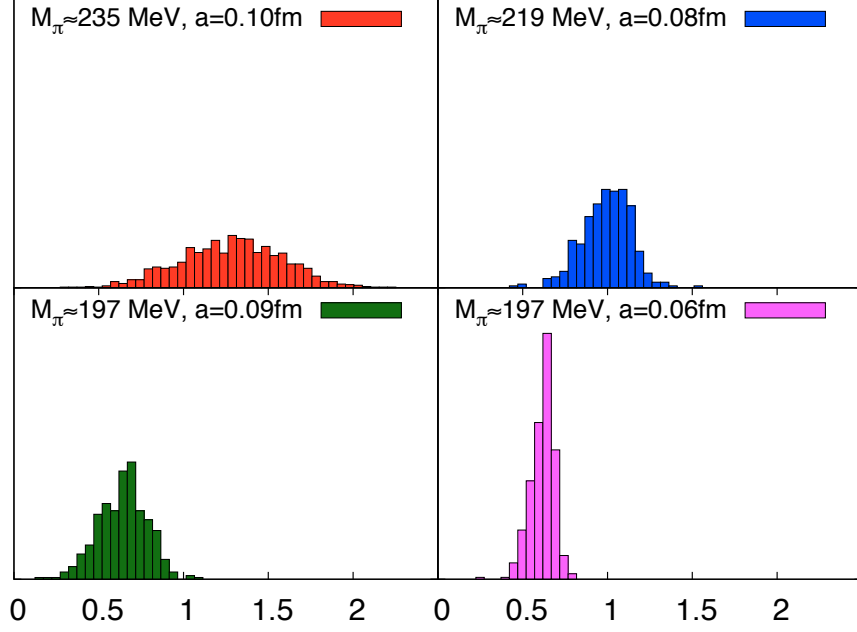
Figure 2. Inverse iteration number for each ensembles with the smallest quark mass at each lattice spacing[9].

2.1 Nondegenerate Up and Down Quarks

In typical lattice computations of QCD, the mass of the up and down quark are usually set to be equal. Although the up quark mass is known to be less than half that of the down quark[10]

$$\frac{m_u}{m_d} = 0.46(2)(2) \qquad (1)$$

the approximation is well justified by the fact that both up and down quark masses are substantially smaller than the dynamical scale of the theory

$$m_u, m_d \ll \Lambda_{\text{QCD}} \sim 300\,\text{MeV} \qquad (2)$$

For the *ab initio* calculation of the mass splittings, however, we had to lift this degeneracy. In principle this is straightforward to achieve by using different masses in the update algorithm. In practice however, the smallness of the up quark mass poses a technical challenge. At the core of the update algorithms are inversions of large, sparse matrices whose condition number is inversely proportional to the quark mass minus a fluctuating offset (see e.g. Ref. 11). In the worst case, the condition number could diverge leading to a so-called exceptional configuration. Because the size of the fluctuations of this offset are related to the quality of the lattice discretisation (more precisely to the chiral symmetry of the fermion operator, see e.g. Ref. 12) an efficient lattice discretisation is essential. We have chosen a highly efficient discretisation that specifically suppresses the couplings of long range physical modes to short range lattice artefacts[13, 14]. As demonstrated in Fig. 2, the
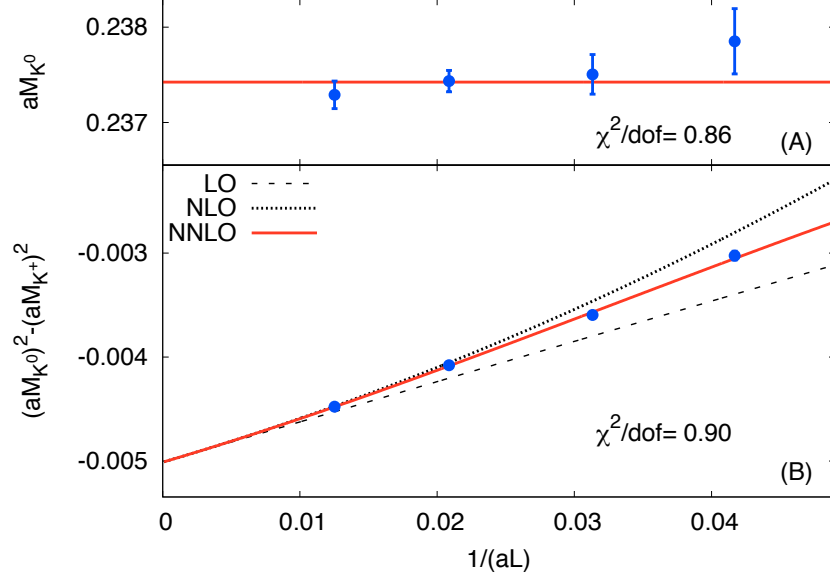
Figure 3. The measured mass of the neutral kaon (top) and the mass square difference between the neutral and charged kaon (bottom) plotted as a function of inverse lattice size[9]. Blue points are lattice data while the lines represent our analytical predictions in leading (LO), next to leading (NLO) and third order (NNLO) in $1/L$.

inverse iteration number remains safely above 0 even for our ensembles with the smallest quark masses and we are thus clear of exceptional configurations.

2.2 QED on the Lattice

The second major challenge one faces when computing the proton neutron mass splitting is the inclusion of electromagnetic effects into the lattice calculation. At first sight this difficulty might seem odd: After all, the quantum field theory of the electromagnetic interaction, quantum electrodynamics (QED) is much better understood and typically simpler than the theory of the strong interaction, QCD. On a fundamental level however, QED poses some conceptual problems that QCD successfully avoids. First of all, the flip side of the strong QCD coupling at low energies is a vanishing coupling at high energies, also known as asymptotic freedom[2,3]. In QCD this property guarantees that at short distances no additional dynamics appears and thus a finer and finer lattice discretisation will ultimately reproduce the continuum theory. In QED the opposite is true: at smaller distance the coupling diverges and no continuum limit exists in principle. We are dealing with an effective theory that is only valid down to a certain distance scale. This scale fortunately is very small so that it can be neglected in our calculations, but it does pose a limit on the electromagnetic coupling we were able to simulate.

A second, potentially more severe problem results from the massless photon present in QED. While the strong interaction is also carried by a massless particle – the gluon – in QCD, these particles can never be observed outside bound states, which are always mas-
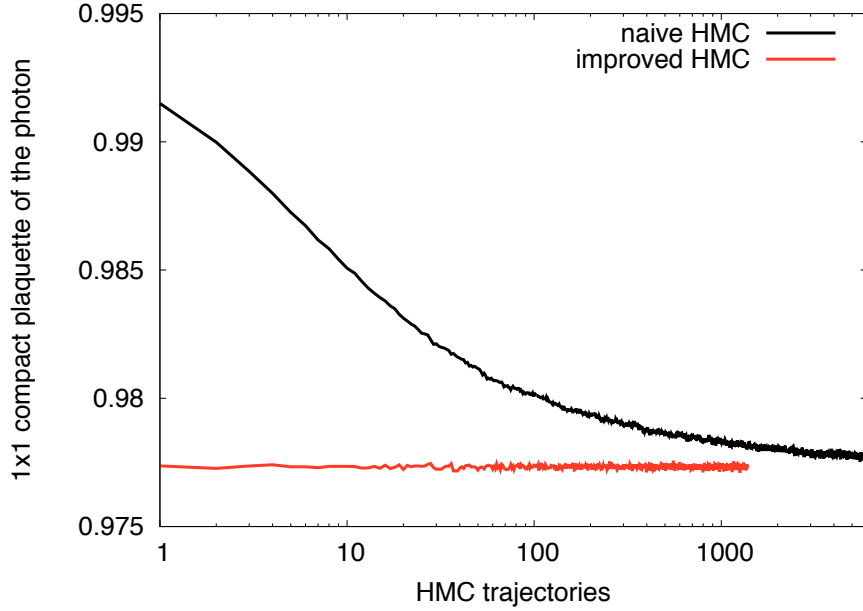
Figure 4. Evolution of the plaquette with simulation time for a standard HMC and the improved momentum space HMC described in the text[9].

sive. Since the propagation of a particle over a long distance is exponentially suppressed by its mass[15], a massive particle usually does not feel the finite extent of its spacetime lattice very strongly. The massless photon on the other hand induces severe self interactions of particles winding around the entire lattice. The most severe of them with vanishing momentum $\vec{p} = 0$ have to be removed in order to render the theory consistent[16]. We demonstrated analytically and numerically that the resulting theory is well defined and computed the remaining finite volume effects to third order in the inverse box length[9] $1/L$ unearthing on the way some subtleties of a nonrelativistic effective description[17] (see Fig. 3).

The long range correlations induced by the massless photons also have a negative effect on the update algorithm. In a standard molecular dynamics based hybrid Monte Carlo (HMC) algorithm[18], long range modes have huge autocorrelations. To counter these effects, we designed a momentum space version of this algorithm that drives modes with different momenta k with a force proportional to $1/k^2$. The resulting speedup is documented in Fig. 4.

There is a further subtlety involved when trying to answer the question of QED contributions to a certain effect like the neutron-proton mass difference. The general strategy to compute QED contributions is to simply switch off the electromagnetic interaction and check for the difference. Although it is easy enough to simply turn off the electromagnetic interaction in our simulations, there is no easy answer to the question of which quantities should be kept constant while doing so to reproduce "nature without QED". Nature can not guide us here since we can not simply turn off electromagnetic interactions between elementary particles. What we can do however is taking a sensible quantity that we do
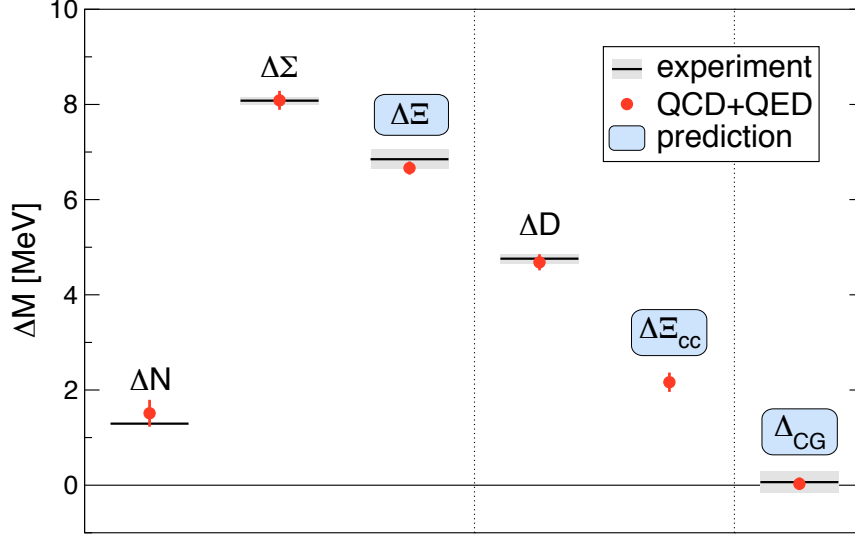
Figure 5. A comparison of the small mass differences between some related hadrons as found in experiment (black lines) and an *ab initio* calculation in QCD+QED (red dots). The grey bands on experimental values show current experimental uncertainties. The leftmost point, ΔN, is the mass difference between neutron and proton. For further details see Ref. 9.

expect to vary very little while changing the electromagnetic coupling and simply define that it stays precisely constant during that process. We could demonstrate[9] that the mass difference between a positively and negatively charged Σ particle is a suitable quantity that, within our statistical accuracy, is not expected to be affected by changing the electromagnetic coupling and consequently used it to define our "nature without QED" point.

3 Data Sets and Analysis

We generated a total of 41 ensembles of lattice discretised QCD+QED gauge fields at different parameter values with four non-degenerate dynamical quarks. Ground state masses were extracted and a statistical analysis of the pertaining fit quality ensured the absence of excited state contaminations. The parameters themselves where chosen such that a safe interpolation and extrapolation to the physical point was possible and the total error of the procedure was minimised. Interpolations to the physical point were carried out in the electromagnetic coupling constant and the strange and charm quark masses. Extrapolations were performed in the lattice spacing, the box size and the light quark mass. All interpolations and extrapolations were performed with a variety of ansätze that covered the possible influence of effects that our data were not accurate enough to discern and thus give a reliable estimate of the possible systematic errors of our analysis procedure. The spread of the results thus obtained, properly weighted by the quality and estimated information content of the respective fit, was used as an estimate of the systematic error.

For further details we refer the interested reader to the supplementary material provided in Ref. 9.
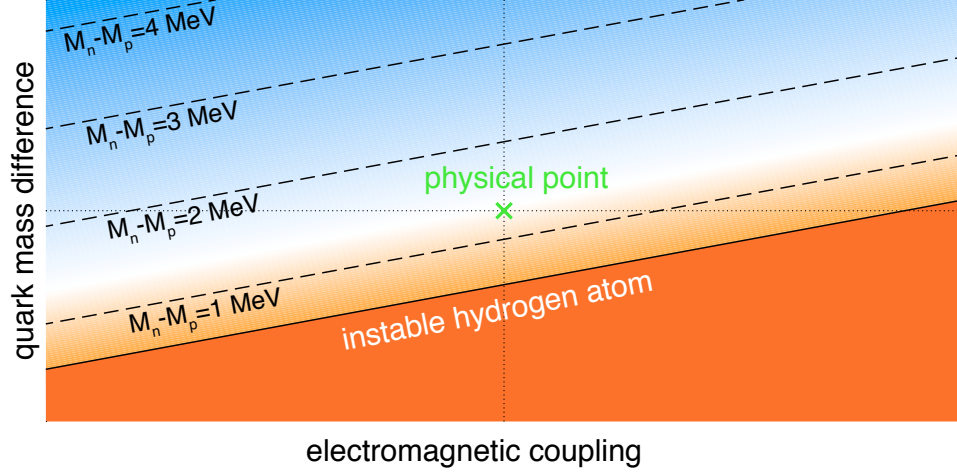
Figure 6. The figure shows a contour plot of the proton neutron mass difference as one varies the electromagnetic coupling (x-axis) and the difference between the "down" and the "up" quark mass from 0 to twice their physical values. The physical point, designating the values actually realised in nature, is marked by a green cross. The red region corresponds to a mass difference between neutron and proton that is less than the mass of the electron. In such a world, the hydrogen atom would not be stable as it would be favourable for the proton in its core to capture the electron and transform into a neutron.

4 Results

Fig. 5 displays the main result of our computation, the small mass differences between some closely related hadrons compared to experimentally known values where available. The leftmost point, ΔN is the mass difference between neutron and proton, which we could confirm to be correctly described by QCD+QED. Our calculations also give a prediction of the mass splittings between the doubly charmed baryons Ξ_{cc}^{++} and Ξ_{cc}^{+}, which have not clearly been observed in experiment yet[7].

Coming back to the original question of quantifying the contribution to the neutron-proton mass difference of electromagnetic effects versus the mass difference of "up" and "down" quarks, Fig. 6 displays a contour plot of the neutron-proton mass difference when hypothetically varying both the electromagnetic coupling and the difference of "down" and "up" quark mass between zero and twice their physical values respectively. This figure illustrates how much wiggle room nature had in choosing the fundamental parameters before our universe would be dramatically different.

Acknowledgements

References

1. H. Fritzsch, M. Gell-Mann, and H. Leutwyler, *Advantages of the Color Octet Gluon Picture*, Phys. Lett., **B47**, 365–368, 1973.
2. H. D. Politzer, *Reliable Perturbative Results for Strong Interactions?*, Phys. Rev. Lett., **30**, 1346–1349, 1973.
3. D. J. Gross and F. Wilczek, *Ultraviolet Behavior of Nonabelian Gauge Theories*, Phys. Rev. Lett., **30**, 1343–1346, 1973.
4. K. G. Wilson, *Confinement of Quarks*, Phys. Rev., **D10**, 2445–2459, 1974.
5. Y. Aoki, G. Endrodi, Z. Fodor, S. D. Katz, and K. K. Szabo, *The Order of the quantum chromodynamics transition predicted by the standard model of particle physics*, Nature, **443**, 675–678, 2006.
6. S. Durr et al., *Ab-Initio Determination of Light Hadron Masses*, Science, **322**, 1224–1227, 2008.
7. K. A. Olive et al., *Review of Particle Physics*, Chin. Phys., **C38**, 090001, 2014.
8. J. Bernstein, L. S. Brown, and G. Feinberg, *COSMOLOGICAL HELIUM PRODUCTION SIMPLIFIED*, Rev. Mod. Phys., **61**, 25, 1989.
9. Sz. Borsanyi et al., *Ab initio calculation of the neutron-proton mass difference*, Science, **347**, 1452–1455, 2015.
10. S. Aoki et al., *Review of lattice results concerning low-energy particle physics*, Eur. Phys. J., **C74**, 2890, 2014.
11. T. DeGrand and C. E. Detar, *Lattice methods for quantum chromodynamics*, 2006.
12. C. Hoelbling, *Lattice QCD: concepts, techniques and some results*, Acta Phys. Polon., **B45**, no. 12, 2143, 2014.
13. S. Capitani, S. Durr, and C. Hoelbling, *Rationale for UV-filtered clover fermions*, JHEP, **11**, 028, 2006.
14. S. Durr et al., *Scaling study of dynamical smeared-link clover fermions*, Phys. Rev., **D79**, 014501, 2009.
15. H. Yukawa, *On the Interaction of Elementary Particles I*, Proc. Phys. Math. Soc. Jap., **17**, 48–57, 1935, [Prog. Theor. Phys. Suppl.1,1(1935)].
16. M. Hayakawa and S. Uno, *QED in finite volume and finite size scaling effect on electromagnetic properties of hadrons*, Prog. Theor. Phys., **120**, 413–441, 2008.
17. Z. Fodor, C. Hoelbling, S. D. Katz, L. Lellouch, A. Portelli, K. K. Szabo, and B. C. Toth, *Quantum electrodynamics in finite volume and nonrelativistic effective field theories*, 2015.
18. S. Duane, A. D. Kennedy, B. J. Pendleton, and D. Roweth, *Hybrid Monte Carlo*, Phys. Lett., **B195**, 216–222, 1987.
19. Jülich Supercomputing Centre, *JUQUEEN: IBM Blue Gene/Q Supercomputer System at the Jülich Supercomputing Centre*, Journal of large-scale research facilities, **1**, A1, 2015, `http://dx.doi.org/10.17815/jlsrf-1-18`.