Quarks and Hadrons – and the Spectrum in Between

The mass of ordinary matter, due to protons and neutrons, is described with a precision of about five percent [1] by a theory void of any parameters – (massless) Quantum Chromodynamics (QCD). The remaining percent are due to other parts of the Standard Model of Elementary Particle Physics: the Higgs-Mechanism, which explains the existence of quark masses, and a per mil effect due to the presence of Electromagnetism. Only at this stage, free parameters are introduced[1]. Mass is thus generated in QCD without the need of quark masses, an effect termed "mass without mass" [2].

This mass generation is due to the dynamics of the strongly interacting quarks and gluons, the latter mediating the force like the photon in the case of Quantum Electrodynamics. However, in contrast to the photons, which are themselves uncharged and thus do not interact (directly) with one another, the gluons themselves carry the strong (color) charge. This is the essential complication in the dynamics of the strong interaction, since it renders the interaction non-linear. Furthermore, due to the uncertainty relation of quantum physics and relativity, even the number of quarks inside the proton or neutron is not fixed: quark anti-quark pairs are created and annihilated constantly and contribute significantly to the overall mass of the particle. So far, the only known way to analyze QCD at small energies, where its interaction strength is large, is through simulations. These simulations are based on the discretized theory, called

Lattice QCD, which traditionally uses a space-time lattice with quarks on the lattice sites and the gluons located on the lattice links. In the so-called continuum limit, the lattice spacing is sent to zero and QCD and the continuous space-time are recovered. Simulations of Lattice QCD require significant computational resources. As a matter of fact, they have been a driving force of supercomputer development. A large range of special-purpose Lattice QCD machines, e.g. the computers of the APE family, QPACE, and QCDOC among others, have been developed, the QCDOC being the ancestor of the IBM Blue Gene family of supercomputers. Over the last decade, these simulations have matured substantially. In 2008, the first fully controlled calculation of the particle spectrum [1] became available and simpler quantities such as masses and decay constants
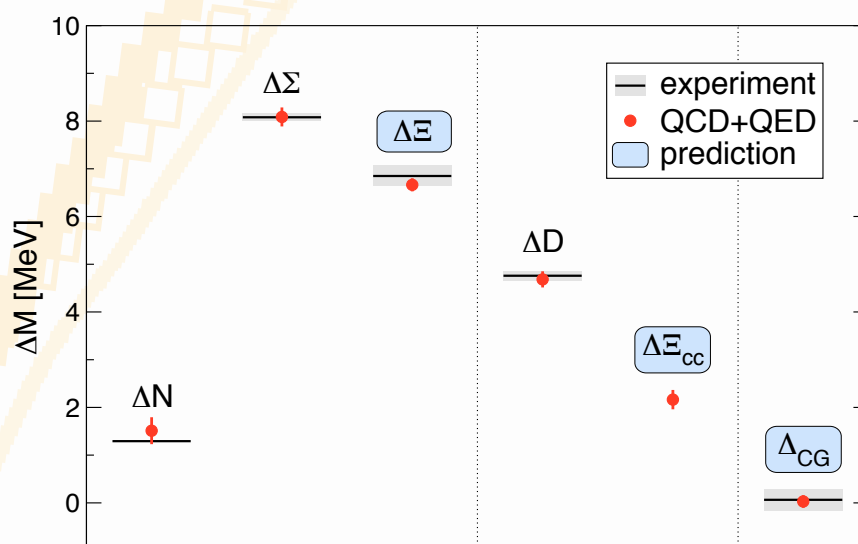

Figure 1: Mass splittings [3]. The horizontal lines are the experimental values and the grey shaded regions represent the experimental errors than those of our predictions. Our results are shown by red dots with their uncertainties. A blue shaded region indicates that no experimental results are available or that these results have larger errors.

[1] These parameters are a coupling (electro-magnetic charge) and the quark masses

are now routinely computed to percent precision.

Neutron, Proton, and the Stability of Matter

In order to increase the precision of the calculations further, one has to address the largest sources of uncertainties, which, in case of the spectrum, are due to Electrodynamics and the difference between the up- and down-quark masses. Once these effects are properly included in the simulations, one can calculate per mil effects of the particle spectrum of the Standard Model, e.g. the difference between the proton and the neutron mass.

For equal light quark masses, Electrodynamics renders the proton slightly heavier, due to energy stored in the electromagnetic field that surrounds it. The light quark mass splitting, conversely, increases the neutron mass, since it contains two of the heavier down-quarks compared to one in case of the proton. The interplay between these effects has significant implications for the stability of matter. If the neutron-proton mass splitting was about a third of the 0.14% found in nature, hydrogen atoms would undergo inverse beta decay, leaving predominantly neutrons. Even with a value somewhat larger than 0.05%, Big Bang Nucleosynthesis (BBN) would have produced much more helium-4 and far less hydrogen than it did in our universe. As a result, stars would not have ignited in the way they did. On the other hand, a value considerably larger than 0.14% would result in a much faster beta decay for neutrons. This would lead to far less neutrons at the end of the BBN epoch and would make the burning of hydrogen in stars and the synthesis of heavy elements more difficult.

Including these effects is, however, non-trivial. The biggest obstacle turns out to be the long ranged nature of electrodynamics. Whereas the strong force is essentially confined inside its "bound-states", the so-called hadrons, the electromagnetic force, falling off according to the well-known $1/r^2$ rule, is still felt at large distances. This introduces significant finite size effects, which are typically larger than the mass splittings one is interested in. In our recent calculation, the correct theoretical framework for a treatment of these effects was established and the finite-size corrections were calculated analytically. A new simulation algorithm for the Electrodynamics part of the calculations was developed, which reduced the autocorrelation by three orders of magnitude. Combined with other advanced methods, such as the latest multi-level solvers, this allowed us to compute the particle splittings using the presently available resources of the Gauss Centre for Supercomputing[2], JUQUEEN at JSC, Hermit at HLRS, and SuperMUC at LRZ (Fig. 1).

From Hadrons to Quark Soup

In the case of the proton and the neutron, quarks and gluons are confined to the hadron. If we, however, increase the temperature of the system sufficiently, both particles will "melt" and quarks and gluons behave as free particles, forming an exotic state of matter called quark-gluon plasma. This (rapid) transition from the quark-gluon to the hadronic phase occurred when the early universe evolved from the "quark epoch", lasting from 10^{-12} to 10^{-6} seconds after the Big Bang, to the following hadron epoch, which ended when the universe was about
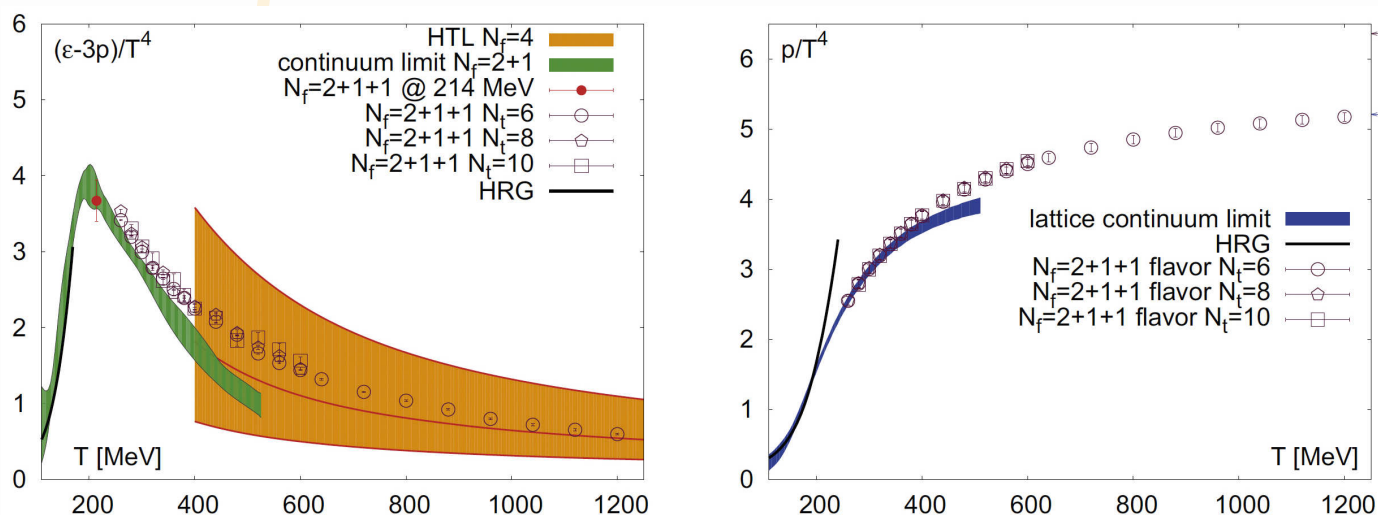
Figure 2: (Left) Preliminary results for the charmed EoS. For comparison, we show the HRG result, the Nf = 2 + 1 band, and, at high Temperatures, the HTL result, where the central line marks the HTL expectation for the EoS with the band resulting from (large) variations of the renormalization scale. (Right) Preliminary results for the pressure, errors indicate the Stefan-Boltzmann value. All errors are statistical only.

one second old. Present heavy-ion experiments (LHC@CERN, RHIC@BNL, and the upcoming FAIR@GSI) create, for a brief moment when two heavy nuclei collide, the extreme conditions of the early universe, allowing us to study this transition and the properties of the quark-gluon plasma some 13 Billion years later.

Considerable theoretical effort is invested attempting to describe these experiments, from collision to detector signals. Here, the Equation of State (EoS) of QCD [4] is a central ingredient for a complete understanding of the experimental findings. At low temperatures, the EoS can be calculated using the so-called "Hadron Resonance Gas" (HRG) model. At high temperatures, perturbative analyses of QCD become possible (e.g. "Hard Thermal Loop" (HTL) perturbation theory). The intermediate region, from ca. 100 MeV to 1 GeV, can be covered systematically through simulations of Lattice QCD.

Presently available Lattice QCD results for the EoS neglect the effects of the

charm quark, which restrict their region of applicability to temperatures below about 400 MeV. In order to reach larger temperatures, we have set up new simulations which take the charm quark into account, using an improved formulation of Lattice QCD. Our preliminary results illustrate the impact of the charm quark for temperatures larger than 400 MeV (Fig. 2), and make contact with both HRG at low and HTL at large temperatures. The EoS is thus becoming available for the whole temperature region.

Computational Aspects

Simulations of Lattice QCD generally happen in three main phases. In the first phase, an ensemble is generated through a Markov process. This phase is thus usually scaled to a large number of cores, minimizing "wall-clock" time. We have, so far, scaled our production code used for the ensemble generation up to 1.8 million parallel threads, running at a sustained performance of over 1.6 PFlop/s (Fig. 3). The second production stage then analyzes the individual "configurations" that

constitute an ensemble one by one. Since an ensemble can contain 1,000 configurations and more, this greatly reduces the need for scaling to a large number of cores. Therefore, we can optimize production at this stage for efficiency (which reaches up to 70% of the hardware peak flop rate) and queue throughput. Physics results are then extracted in the final step of the calculation, which, with our involved blind analysis procedure [1,3], requires a small compute cluster on its own.

Outlook

Simulations of Lattice Quantum Chromodynamics have reached per mil level precision. By now, we are able to reproduce even intricate details of the particle spectrum, such as the neutron-proton and other mass splittings at high precision. The inclusion of Quantum Electrodynamics was essential to archive this level of accuracy, rendering calculations of the combined theory possible in cases where this is needed in the future. Beyond conceptual advances, the correct reproduction of the mass splittings found in nature provides further strong evidence that Quantum Chromodynamics correctly accounts for the properties of strongly interacting matter. Moving beyond the mass spectrum, we can now calculate the properties of the

early universe transition between, and the properties of matter in, the quark and the hadron epoch, starting 10^{-12} seconds after the Big Bang.
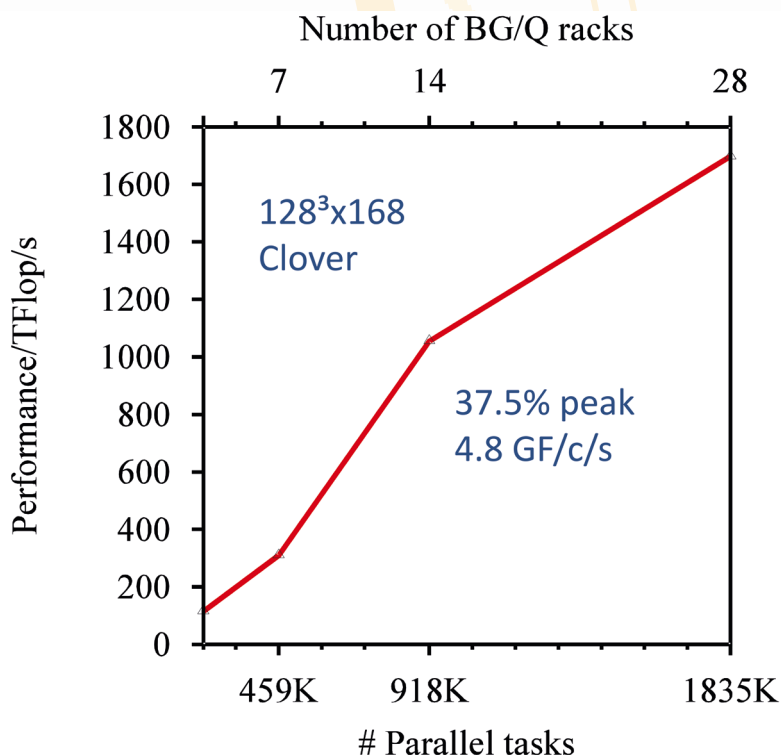
Acknowledgements

Figure 3: Strong scaling analysis of the Lattice QCD simulation code, reaching a sustained performance of over 1.6 Flop/s on the Blue Gene/Q at JSC, Jülich.

References

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