Dynamical simulations of lattice QCD.

Working towards vanishing lattice spacing, infinite volume and physical quark masses

Simulations of quantum chromodynamics (QCD) on a discrete lattice have progressed substantially in the past decade, thanks not only to faster computers, but also to the development of algorithms that make better use of properties of the underlying physics of QCD. The John von Neumann Institute for Computing (NIC) group at DESY is engaged in two international lattice QCD simulation efforts, with the goal of ultimately being able to predict results at vanishing lattice spacing, in the infinite volume and at physical quark masses.

Decisive progress

Lattice QCD computations have come a long way from the parameters at which they were performed at the beginning of the 2000s to the control that can be achieved today. In these computations, QCD is formulated on a four-dimensional lattice with a lattice constant *a*, and to be able to treat it on the computer, only a finite volume is considered. As they are computationally much "cheaper", quark masses larger than the physical ones are frequently employed.

In a famous analysis presented at the Lattice 2001 conference in Berlin, Akira Ukawa of the University of Tsukuba in Japan predicted that with the algorithms of the time, even using the computers that we have today, it would be impossible to do computations at quark masses close to the physical ones, or on lattices fine and large enough to have the effects of finite lattice spacing and size under control. Realistic simulations seemed to be confined to the distant future.

Nowadays, a number of groups are performing computations on lattices that are fine and have a large volume, using quark masses close to their physical values. All these parameters are varied between simulations to study their impact. Not only have computers become faster – at least equally important are the many improvements to the algorithms: While in 2001 general-purpose algorithms were used, today's algorithms incorporate significant insight into the physics of the underlying system. They can, for example, separate long-distance physics from effects at short distances, and the computational cost of numerically solving the Dirac equation was reduced drastically by taking into account physical properties in the preconditioning of the system.

A lattice simulation is split in two parts: the generation of the gluon fields and a "measurement", i.e. the computation of observables for the generated fields. The NIC group at DESY contributes in leading positions to two such simulation efforts, which include members from all over Europe: the European Twisted Mass Collaboration (ETMC) and the Coordinated Lattice Simulations (CLS) initiative. Both are generating gluon field configurations at many values of the lattice spacing and volume and for different quark masses in order to study the effects of these parameters on the observables and to ultimately predict results at vanishing lattice spacing, in the infinite volume and at physical quark masses.

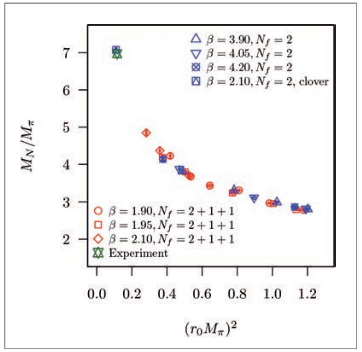

Figure 1
Ratio of the nucleon mass over the pion mass, indicating that in contrast to earlier simulations, the physical values are now met.

ETMC

Along with the $N_f = 2 + 1 + 1$ simulations pursued by ETMC in recent years, there has been a renewed interest in $N_f = 2$ flavour simulations [1]. The leading discretisation effects of twisted-mass fermions at maximal twist always come at $O(a^2)$, but by adding the clover term with a suitably tuned coefficient, their magnitude has been reduced. These simulations are performed at the physical value of the masses of the up and down quark.

So far, the simulations are restricted to one lattice spacing and a relatively small volume ($m_\pi L \approx 3$ at the physical point). However, varying the lattice size *L* allows the volume effects to be studied and estimates for their relevance to be given. An example of how much closer the current simulations are to the physical masses compared to previous simulations is given in Fig. 1.

CLS

CLS has a programme to simulate $N_f = 2 + 1$ flavours of non-perturbatively improved Wilson fermions. The project, which started in 2013, has by now generated lattices at four different lattice spacings between 0.085 fm and 0.05 fm and for a range of quark masses [2]. Both parameters can bring significant corrections with respect to the physical situation. An example is given in Fig. 2, where the product of the pion decay constant with the gluonic scale parameter $t_0 \approx (0.15 \text{ fm})^2$ is displayed. As can be seen, the accuracy that can be reached in such a quantity is at the level of 1%.

The extrapolation towards the continuum limit $a = 0$ fm agrees with leading scaling violations of $O(a^2)$, as expected for this non-perturbatively $O(a)$-improved theory. From Fig. 2, it is also obvious that only the fine lattices used here can lead to such a 1% accuracy – the points at 0.085 fm and 0.065 fm being approximately 5% away from the continuum result.

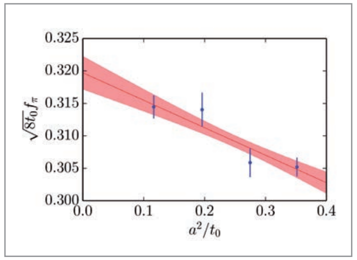

Figure 2
Continuum extrapolation of the dimensionless product $f_\pi (8t_0)^{1/2}$ of the pseudoscalar decay constant f_π and the gluonic scale t_0 along the line $m_\pi = m_K \approx 420$ MeV. Fine lattices are needed to reach a percent-level result.

Conclusion

These lattice simulations have laid the foundation for a large variety of projects currently pursued by a number of European groups. First results have been published, and many more are expected for the next years. The progress of the past decade highlights that it is worth investing in the improvement of computational methods, which now allow us to determine many quantities at percent-level accuracy.

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References:
[1] A. Abdel-Rehim et al., Simulating QCD at the Physical Point with N_f=2 Wilson Twisted Mass Fermions at Maximal Twist [arXiv:1507.05068]
[2] Mattia Bruno et al., Simulation of QCD with N_f =2+1 flavors of non-perturbatively improved Wilson fermions, JHEP (02) 043, 2015.