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Karl Jansen

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The Quest for Solving QCD by Numerical Simulations: The NIC Research Group Elementary Particle Physics

Karl Jansen

NIC, DESY Zeuthen
Platanenallee 6, 15738 Zeuthen, Germany
E-mail: Karl.Jansen@desy.de

We discuss the activities of the NIC research group Elementary Particle Physics and show that the group could achieve important results over the last two years in the field of lattice gauge theory.

1 Introduction

Results from lattice QCD simulations enter more and more the particle data booklet (pdg)[1] which can be considered to be the "bible" for high energy physicists. In fig. 1 we show the relative difference between lattice QCD predictions and the experimental findings of only those physical observables for which lattice results have been taken by the particle data group itself[1]. The figure demonstrates that some of the observables are known from lattice QCD simulations already rather precisely. Moreover, no deviation from the predictions of QCD are detected presently, confirming thus QCD as our theory of the strong interaction at least to the accuracy obtained so far in experiment and from lattice simulations.

Although it is certainly very much encouraging that lattice results are taken seriously as a theoretical input to interprete and to compare experimental data, it has to be admitted

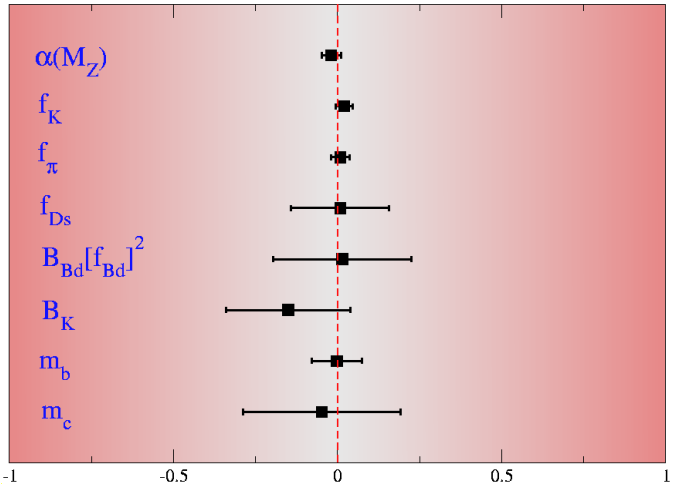


Figure 1. Comparison of lattice and experimental results for a number of physical quantities taken from the particle data booklet. Shown is the relative difference between the lattice prediction from QCD and the experimental finding.

that lattice calculations still have a number of systematic errors and that full dynamical simulations still present a challenge. The NIC research group Elementary Particle Physics focuses in its work in understanding and controlling these systematic errors and facing and overcoming the problem of dynamical quarks. This report about the work of the group will summarize the results of these attempts and presents some very important achievements that could be obtained over the last two years.

Before entering the main research area of lattice QCD, I would like to mention that the research group is also concerned with aspects of non-perturbative aspects of quantum field theories different from QCD:

- In the 2-dimensional Schwinger model, a prototype model to study aspects of much harder to tackle 4-dimensional QCD, a detailed scaling test of various fermion actions could be achieved with a precision that showed in part deviations from analytical, approximative predictions[2]. In addition, new ways of simulating chiral invariant overlap fermions dynamically were addressed[3].

- In another 2-dimensional model, the Gross-Neveu model, the phase structure in the large-N approximation could be computed analytically, revealing interesting insights that can also be relevant for QCD[4].

- A special class of gauge actions were investigated that are constructed such that the topology of the gauge fields is fixed in the numerical simulations. It could be demonstrated that the topology is indeed stabilized using these actions, although a complete fixation could not be achieved[5].

2 Results for Lattice QCD

2.1 Phase Diagram of Lattice QCD

The NIC research group achieved for the first time a comprehensive picture of the phase diagram of lattice QCD[6–11]. The knowledge about the existence and the structure of the Wilson lattice QCD phase diagram can certainly be considered as a breakthrough in lattice field theory and the work by the group received a lot of attention and has been represented at numerous conferences and workshops.

The reason is that, somewhat surprisingly, the phase structure turns out to be rather complicated. Instead of a single phase transition line at which the pseudo scalar mass vanishes as suggested by the continuum picture, various phase transitions were found. The most relevant for a continuum limit is a first order phase transition with the peculiar property that unlike in the continuum the pseudo scalar mass does not vanish, but assumes a non-zero, minimal value. Our present understanding of the lattice QCD phase diagram is sketched in fig. 2.

The phase structure and many properties of the corresponding phase transitions can be computed both, numerically and analytically using tools from chiral perturbation theory[12–17]. Both of these approaches provide a consistent picture that leads to the phase diagram of fig. 2. For a more detailed discussion of the properties and consequences of the existence of the first order phase transition, we refer to our project discussion in this proceedings volume.

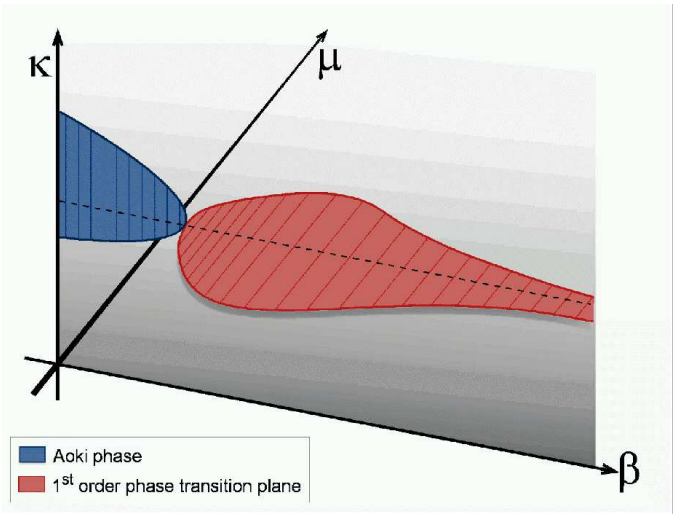


Figure 2. Current knowledge of the lattice QCD zero-temperature phase diagram with Wilson fermions as a function of the inverse gauge coupling $\beta \propto 1/g^2$, the hopping parameter κ (which is inversely proportional to the quark mass) and the twisted mass parameter μ.

Another major part of the work of the NIC research groups was a detailed scaling test of a new formulation of lattice fermions, so-called twisted mass fermions[18,19]. This test came out very positive[20–23]. Again we refer to the report about this project in these proceedings.

2.2 The Strange Quark Mass

One important and essential strength of lattice QCD simulations is that even the fundamental parameters of QCD, the strong coupling α_s and the values of the quark masses can be directly and ab-initio computed from the QCD Lagrangian alone. Lattice QCD is presently the only method that allows for such an ambitious goal. The recent years have seen even progress in calculating these fundamental parameters in the very demanding situation of dynamical quarks, see the discussion below. The NIC research group has very actively pursued such simulations and were one of the first to give a number for a value of the strange quark mass[24–26]. We show a compilation of world-wide results for the strange quark mass m_s in fig.3. Here the lattice results are converted to the more commonly used $\overline{\rm MS}$ renormalization scheme and a scale of 2GeV was taken.

2.3 Algorithmic Improvements – Shifting of the Berlin Wall

The biggest obstacle today in "solving" QCD at least numerically is the shear cost of the numerical simulations for which even nowadays state of the art supercomputers are not sufficient. The dilemma has been most drastically discussed a the 2001 Berlin lattice symposium. A number of research groups world-wide has been asked to present their status of dynamical simulations and estimate the cost. The example of the CP-PACS collaboration, represented by A. Ukawa at the conference provided the rightmost curve in fig. 4.

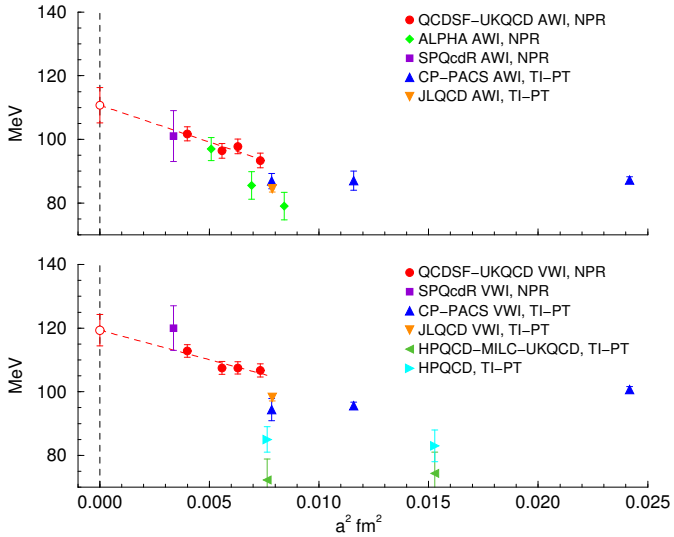


Figure 3. Results for $m_s^{\overline{\rm MS}}(2GeV)$ versus $a^2\mathrm{fm}^2$ using the axial Ward identity (AWI, upper plot) and vector Ward identity (VWI, lower plot). The results are presented with the collaborations preferred units and scales. NPR denotes non-perturbative renormalisation, while TI-PT denotes tadpole improved perturbation theory. The results from the HPQCD collaboration are for $N_f = 2+1$ flavours, the other results are all for $N_f = 2$ flavours.

This result showed that the simulation cost increases dramatically when the ratio of the pseudo scalar to the vector meson mass are driven to its value as observed in experiment and which is represented by the arrow in the plot. The vertical axis shows the teraflop years needed to generate 1000 configurations. The sharp, wall-like increase of the simulation cost triggered the name "Berlin wall" and plots showing this behavior are titled nowadays as Berlin wall plots.

By combining several algorithmic techniques to simulate dynamical quarks, the NIC research group[27,28] has been able to substantially shift this Berlin wall, see fig. 4. Indeed the shift is so dramatic that simulations with realistic values of of the pseudo scalar and vector meson masses seems perfectly feasible, at least for a value of the lattice spacing of $a \approx 0.09$fm and a box length of about 2.4fm. Although lowering the value of the lattice spacing and increasing the box length to 3fm (or even larger) would increase the computation cost again, such simulations seem not to be completely out of range as the old location of the Berlin wall had suggested.

2.4 apeNEXT

We close this section with a remark about the status of the massively parallel apeNEXT system, the latest development in the APE-line[29–31]. These machines are constructed for a peak performance of 10 teraflops. The hardware of the apeNEXT systems is now ready, tested and working in prototype installations. The APE group is starting to install large systems Europe-wide in Italy (12Teraflops), France (2Teraflops) and Germany (3Teraflops DESY, 5Teraflops Bielefeld). It is to be expected that these installations will provide a major and most important computer resource for lattice physicists in Germany.

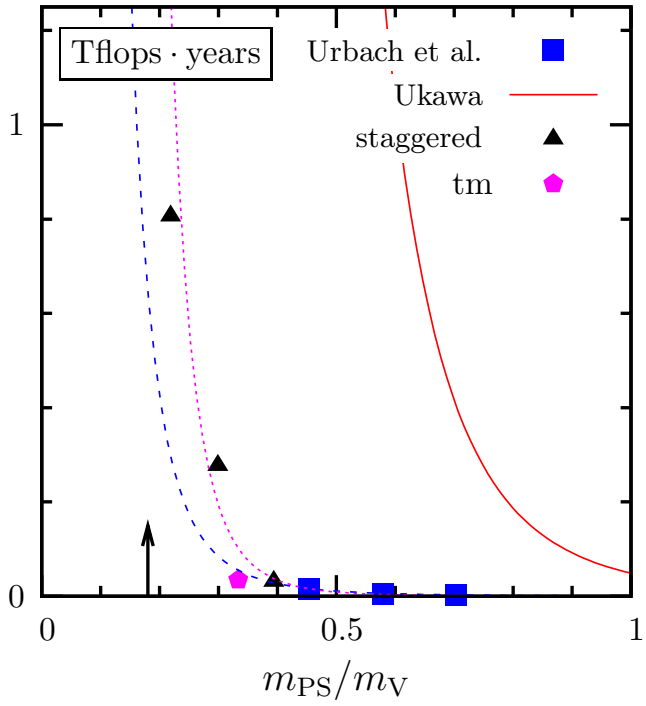


Figure 4. Shift of the Berlin wall through recent algorithmic improvements.

3 Conclusion

The NIC research group has worked very successfully in the last years. It has tested the Wilson twisted mass formulation of lattice QCD and found it to be a most promising tool for future QCD simulations. The group has explored the phase diagram of lattice QCD and obtained for the first time a comprehensive picture of the phase structure which is, moreover, in accordance with analytical results from chiral perturbation theory. As an example of a physics result we presented the computation of the mass of the strange quark in the case of dynamical quarks which is one of the most important quantities to come from lattice simulations.

The group found a new version of an algorithm to simulate dynamical quarks which shifted the Berlin wall considerably such that even simulations at the physical point where the pion mass assumes its experimentally measured value become possible. In parallel, machines of the apeNEXT type are now ready to be installed, providing computer power in the 10 teraflops regime.

All these results of the NIC research group are substantial improvements, if not breakthroughs in lattice gauge theory and the next years will certainly see the fruits of this work resulting in the computation of many physically relevant quantities.

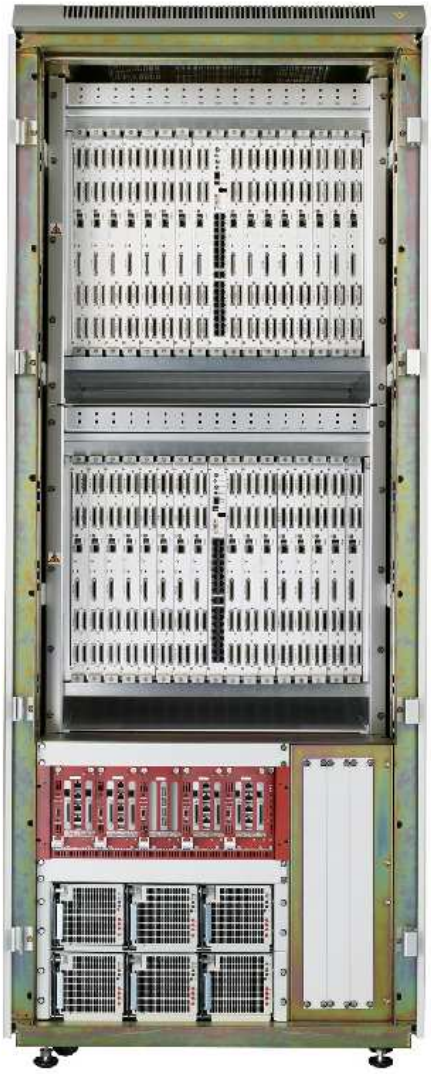


Figure 5. One rack of the apeNEXT installation in Zeuthen. A rack as shown here, has 512 nodes and can deliver 640 gigaflops

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