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Lattice calculations

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Abstract. In this contribution we describe how an exact chiral symmetry can be realized on the lattice. A practical realization of a lattice Dirac operator that leads to a chiral invariant lattice action is discussed and a simulation with this operator is presented that aims at testing the phenomenon of spontaneous chiral symmetry breaking in QCD.

PACS. 11.15.Ha Lattice gauge theory – 12.38.Gc Lattice QCD calculations

1 Introduction

Since its formulation in 1974 [1], lattice QCD has matured to a well-established part of theoretical high-energy physics and it nowadays provides many non-perturbatively obtained, *ab initio* computations and results in a variety of fields. These include, besides QCD, the electroweak standard model, spin systems, tests of semi-classical pictures (instantons etc.) and even quantum gravity (see, *e.g.*, [2]). One of the reasons why the impact of lattice calculations is becoming stronger and stronger is the fact that (parallel) computers, the workhorses for lattice physicists, have become more and more powerful. However, a certainly equal important reason is that over the years a number of conceptual developments have been established that help in making simulations faster and much better controlled:

- *Accelerating the continuum limit*
Lattice QCD actions that are used in the past give rise to lattice discretization errors that are linear in the lattice spacing a. Considering pure gauge theories, these effects are only quadratically in the lattice spacing [3, 4] and hence simulations including fermions slow down the approach to the continuum limit substantially. Following the concept of *Symanzik improvement* [5,6], this drawback can be overcome: it can be shown that at $O(a)$ only one additional term can be added to the standard Wilson fermion action. This term, called the *Sheikoleslami-Wohlert* term [7], is multiplied by a free, tunable parameter c_{sw}. It is possible to compute this coefficient non-perturbatively in such a way that it exactly cancels the linear lattice discretization effects coming from the standard Wilson fermion action and hence the discretization errors are reduced from $O(a)$ to $O(a^2)$ [8,9]. Of course, the continuum limit itself still has to be performed, but it is reached with a much faster rate by using these so-called *non-perturbative O(a)-improved Wilson fermions*.
- *Finite-size effects*
Lattice simulations have necessarily to be done in a finite, 4-dimensional box of physical size L^4. In order to fit physical quantities like a proton into this box, it is necessary that the physical size is large enough. The linear physical extent L is given by $L = Na$, where N is the number of lattice points. If the lattice spacing a is kept small enough to avoid large discretization effects, the number of points to be simulated becomes easily very large. Therefore, trying to avoid finite-size effects results in very costly and demanding simulations.
However, in many circumstances it is possible to turn this drawback around and promote it to an advantage. It is possible to use the finite volume as a probe of the system and extract from the finite-volume effects of physical quantities infinite-volume properties of the system under consideration. One prominent application is to use the finite size of the box as the scale used in non-perturbative renormalization (see the reviews [10,11]). Another strategy is to develop finite-size formulae that actually describe the finite-size effects analytically and allow for a well-controlled determination of infinite-volume quantities. An example of this strategy is given below.
- *Dynamical fermions*
QCD, as a quantum field theory allows for the creation and annihilation of virtual quark-antiquark pairs that lead to renormalization effects like the running of the strong-coupling constant, *i.e.* the value of the strong-coupling constant depends on the energy where it is measured. In order to take these effects into account, the full theory including the fermionic degrees of

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freedom has to be simulated. The algorithms that are known today for these simulations lead to very costly simulations [12]. Although, by a continuous development of the algorithms it was possible to gain a factor about 20 in the, say, last 10 years, physical results with well-controlled errors would need computers that can deliver 10–100 teraflops performance, something that cannot be reached today.
Therefore, many simulations performed so far neglect the dynamical quark effects and work in the so-called *quenched approximation*. It is surprising —and not really understood— that this approximation (or better truncation) of the theory still gives results that often differ from experimental data by only 20% to 30%. Of course, eventually the quenched approximation has to be given up and the lattice community worldwide is in a transition period to switch to real dynamical-fermion simulations.

– *Chiral symmetry*
The lattice and chiral symmetry, *i.e.* the invariance of the action under exchange of left-handed and right-handed massless quarks, were two concepts that did not seem to fit together for a very long time. Only recently a solution to this longstanding problem could be found and in the remaining part of this contribution we explain this new development.

2 Spontaneous chiral symmetry breaking

In our theory of strong interactions, quantum chromodynamics, chiral symmetry is assumed to be spontaneously broken. This symmetry allows for an interchange of left-handed and right-handed quarks while leaving physics invariant —at least when these quarks are massless. In this case a scalar quark-antiquark $q\bar{q}$ condensate is assumed to be developed and the Goldstone particles are identified with the light pions that are observed in nature.

As stated above, the occurrence of spontaneous symmetry breaking *is an assumption*. The phenomenon is inherently non-perturbative and cannot be addressed with approximative methods like perturbation theory. However, even with numerical simulations it is difficult to test spontaneous chiral symmetry breaking (SχSB). The reason for this becomes clear when the way to detect SχSB is considered. Let us choose a system that has a finite physical volume V, as would be required for numerical simulations. Further, we introduce a quark mass m. SχSB is tested in a double limit, where first the volume of the system is sent to infinity and then the quark mass is sent to zero. If a non-vanishing scalar quark condensate remains, SχSB is identified. Obviously, such a procedure is infeasible within the approach of numerical simulations.

The way out is the use of chiral perturbation theory [13]. In this approach chiral symmetry breaking is also taken as an assumption with the consequences of the appearance of non-vanishing field expectation values and Goldstone particles. A special situation arises when the size of the box becomes comparable to or even smaller than the Compton wavelength of the Goldstone particle. Then, the corresponding field can be considered as being uniform and it is possible to set up a systematic expansion that starts in the lowest order with an effective Lagrangian of this constant mode and then taking systematically higher-order fluctuations into account [14].

3 Chiral symmetry on the lattice

Chiral perturbation theory as well as the lattice method was developed for quantum chromodynamics in order to deepen our understanding of the strong interactions. Still, until relatively recently, both approaches could not really come together, at least in the region of very small quark masses where chiral symmetry starts to get restored. The reason was that the lattice seemed to be lacking the concept of chiral symmetry and for many years the infamous Nielson-Ninomiya theorem [15] has been telling us that it would even be impossible to implement chiral symmetry in a consistent way on a lattice.

The situation only changed a few years ago, when an old work by Ginsparg and Wilson [16] was rediscovered [17]. The Ginsparg-Wilson paper contained actually a clue for answering the problem of chiral fermions on the lattice. The interaction of the fermions is described by some particular operator, the Dirac operator, the details of which should not be discussed here. In the continuum theory this Dirac operator anti-commutes, of course, with γ_5. On a lattice with non-vanishing lattice spacing a, such an anti-commutation property cannot be demanded. If the anti-commutation property is insisted on, the fermion spectrum of the lattice theory does not correspond to the one of the target continuum theory.

The suggestion of Ginsparg and Wilson was to replace the anti-commutation condition by a relation (now known as the Ginsparg-Wilson (GW) relation) for a lattice Dirac operator D:

$$\gamma_5 D + D\gamma_5 = aD\gamma_5 D \; . \tag{1}$$

Clearly, in the limit that the lattice spacing vanishes, the usual anti-commutation relation of the continuum theory is recovered.

The fact that renders the relation eq. (1) conceptually extremely fruitful is that it implies an exact chiral symmetry on the lattice even if the value of the lattice spacing does not vanish [18]. The notion of a chiral symmetry on the lattice is a conceptual breakthrough and renders the lattice theory in many respects to behave like its continuum counterpart with far-reaching consequences.

However, as nice as the theoretical progress that followed the rediscovery of the Ginsparg-Wilson relation was, as much of a challenge are realizations of operators D that satisfy the Ginsparg-Wilson relation (see [19–21] for reviews). Let us give a particular example for such a solution as found by H. Neuberger [22] from the overlap formalism [23], based on the pioneering work of D. Kaplan [24]. To this end, we first consider the standard Wilson Dirac operator on the lattice:

$$D_{\rm w} = \frac{1}{2}\left\{\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - a\nabla_\mu^*\nabla_\mu\right\} \tag{2}$$

with ∇_μ, ∇^*_μ the lattice forward, backward derivatives, *i.e.* nearest-neighbour differences, acting on a field $\Phi(x)$:

$$\nabla_\mu \Phi(x) = \Phi(x+\mu) - \Phi(x)\,,$$
$$\nabla^*_\mu \Phi(x) = \Phi(x) - \Phi(x+\mu)\,.$$

We then define

$$A = 1 + s - D_{\mathrm{w}} \tag{3}$$

with $0 < s < 1$ a tunable parameter. Then Neuberger's operator D_{N} with mass m is given by

$$D_{\mathrm{N}} = \left\{ 1 - \frac{m}{2(1+s)} D_{\mathrm{N}}^{(0)} + m \right\}\,, \tag{4}$$

where

$$D_{\mathrm{N}}^{(0)} = (1+s)\left[1 - A(A^\dagger A)^{-1/2}\right]\,. \tag{5}$$

What is important here in the definition of Neuberger's operator is the appearance of the square root of the operator $A^\dagger A$. This means that D_{N} connects all points of the lattice with each other. Note, however, that despite this the operator is a local operator in the field-theoretical sense [25]. In practice, the operator $A^\dagger A$ is represented by a matrix that is, unfortunately, very large. Having a physical volume of size L^4, the number of sites is $N^4 = (L/a)^4$. As the internal number of degrees of freedom per lattice point is 12, we end up with A being a $(12N^4) \otimes (12N^4)$ complex matrix with N typically in the range $10 < N < 30$ for present days simulations. Hence we have to construct the square root of a very large matrix. What is worse, to compute relevant physical observables, we don't need the operator D_{N} itself but its inverse. Such an inverse is constructed by iterative methods like the conjugate gradient algorithm and its relatives [26].

The square root can be constructed by a polynomial expansion, normally based on a Chebyshev approximation, or by rational approximations. Both methods give comparable performances in practice. The convergence of the approximation to the square root is determined by the condition number of the (positive definite) matrix $A^\dagger A$. When the matrix $A^\dagger A$ is normalized such that the largest eigenvalue is 1, the condition number is given by the inverse of the lowest eigenvalue.

It was shown that very low-lying eigenvalues of the operator $A^\dagger A$ can appear in numerical simulations resulting in large condition numbers [27]. In such situations the convergence of the approximations chosen can be rather slow and special tricks have to be implemented to accelerate the convergence. The most fruitful improvement is to treat a part of the low-lying end of the spectrum exactly by projecting this part out of the matrix $A^\dagger A$ [28, 27]. Further improvements can be implemented, examples of which are discussed in ref. [27].

Despite all these technical improvements it is found that a typical value for the degree of a polynomial is $O(100)$ and a typical value for the number of iterations to compute the inverse of D_{N} is again $O(100)$. Since in each iteration to compute D_{N}^{-1} the Chebyshev polynomial has to be evaluated, this means that for a value of a physical observable on a single configuration ten thousand applications of a huge matrix on a vector has to be performed. To compute the expectation value of some observable, this observable has to be averaged over many gluonic configurations. Clearly, this results in a very demanding computational effort.

4 The scalar condensate

The existence of an exact lattice chiral symmetry allows the use of finite-size effects to test for SχSB in QCD. Using a chiral invariant formulation of lattice QCD, it is possible to reach the region of very small quark masses where it is to be expected that chiral symmetry starts to get restored.

The order parameter of chiral symmetry breaking in quantum chromodynamics is the condensate of a quark-antiquark state $\Sigma = \langle \psi\bar{\psi} \rangle$. A (standard) caveat here is the fact that all computations are done in the quenched approximation. In QCD there is a peculiarity: the field configurations can have topological properties, characterized by the so-called topological charge which can be measured —unambiguously— through the number of zero modes of the operator D_{N}. In fact, the formulae from quenched chiral perturbation theory are parameterized by the topological charge and it is hence very important to be able to identify the topological charge of the gauge field configurations. Without the special properties of lattice Dirac operators that satisfy the Ginsparg-Wilson relation such an identification would be very difficult.

The complete theoretical formula from quenched chiral perturbation theory in lowest order is

$$\begin{aligned}\Sigma_\nu(m,V) = \Sigma\, z\, [I_\nu(z)K_\nu(z) \\ + I_{\nu+1}(z)K_{\nu-1}(z)] + C\cdot m/a^2\,.\end{aligned} \tag{6}$$

The only important thing to notice here is that this relatively involved combination of Bessel functions only depend on one scaling variable,

$$z = \Sigma m V\,, \tag{7}$$

that contains the quantity of interest, namely the infinite volume, chiral limit scalar condensate Σ. The additional term $C \cdot m/a^2$ is a power divergence that comes from the renormalization properties of the theory. We will not discuss this field-theoretical aspect here but just notice that this term has to be included in the fit.

In fig. 1, we show the result of our numerical computation of the scalar condensate [29] in a fixed topological charge sector $|\nu| = 1$ as a function of the quark mass at several volumes. The solid line is a fit to the prediction of chiral perturbation theory, eq. (6). We find that the simulation data are described by this prediction very well. This means that we find evidence for the basic assumption on which the theoretical prediction relies: the appearance of spontaneous chiral symmetry breaking in (quenched) QCD.

We want to remark that this work was the first of this kind. After this work, a number of other groups repeated

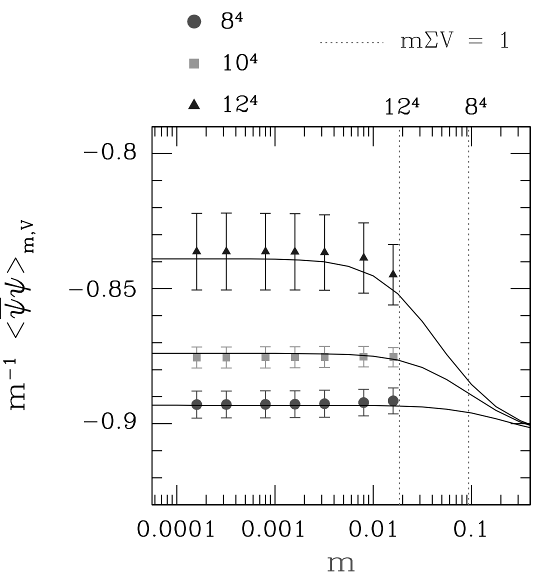

Fig. 1. The scalar condensate computed on lattices of various size as a function of the quark mass. The solid lines are 2-parameter (Σ and the constant C of eq. (6)) fits, according to the prediction of chiral perturbation theory.

such an analysis [30–32] and it was reassuring to observe that very consistent results were found. In a sub-sequel work [33,34] we developed also a quite general method for renormalizing the value of the bare scalar condensate as extracted from the finite-size scaling analysis performed here.

5 Conclusion

In this contribution we have demonstrated that by a combination of theoretical ideas, improved numerical methods and the use of powerful supercomputer platforms it is possible to test basic properties of field theories. Of particular interest was the question of whether the phenomenon of spontaneous symmetry breaking (SSB) does occur in certain field theories important in elementary-particle physics. The phenomenon of SSB leads to far-reaching consequences in theories like QCD or the scalar sector of the electroweak interactions. In the work performed here, we found strong evidence for the appearance of spontaneous chiral symmetry breaking in quenched lattice QCD.

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