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Lattice computations for high energy and nuclear physics

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Abstract. An overview is given on present lattice field theory computations. We demonstrate the progress obtained in the field due to algorithmic, conceptual and supercomputer advances. We discuss as particular examples Higgs boson mass bounds in lattice Higgs-Yukawa models and the baryon spectrum, the anomalous magnetic moment of the muon and nuclear physics for lattice QCD. We emphasize a number of major challenges lattice field theory is still facing and estimate the computational cost for simulations at physical values of the pion mass.

1. Introduction

When quantum chromodynamics as our theory of the strong interaction was developed, it became clear that one would have to deal with very non-perturbative phenomena. The interaction between the postulated quarks and gluons can not be addressed by perturbation theory anymore when distances of about 1fm or, correspondingly energy scales below 1GeV are considered. However, this is exactly the energy regime where the observed particles such as the proton and the neutron appear. This let K. Wilson to state in his 1977 Cargese lectures [1]

Unfortunately, it is not known yet whether the quarks in quantum chromodynamics actually form the required bound states. To establish whether these bound states exist one must solve a strong coupling problem and present methods for solving field theories don't work for strong coupling.

This observation then led to the development of lattice field theory as a non-perturbative tool to address the fundamental question raised by K. Wilson who then himself [2] suggested to reformulate the theories of elementary particle interactions on a 4-dimensional lattice in order to establish a well-defined and regulated formulation of field theories which are furthermore amenable to non-perturbative computations.

Whereas Wilson was thinking of strong coupling expansions to evaluate the theories [3], it was shown in [4, 5], by drawing analogy to statistical physics, that such lattice gauge theories can also be calculated numerically. This opened a much broader road to carry through ab-initio calculations of theories in high energy physics with techniques that can cover an energy range from large scales, where perturbation theory can be applied, up to very low scales where truly non-perturbative phenomena play the dominant role.

In this article I want to provide an overview how far lattice field theory has progressed in the understanding of the question “whether the quarks in quantum chromodynamics actually form the required bound states”. We will see that there is in fact a tremendous development. There is substantial improvement of the used algorithms and a much better conceptual understanding of



lattice field theories. In addition, there are new supercomputer architectures reaching now the multi-petaflop regime. All this furthered the field to a point where lattice computations make contact to and has an impact on experiments and phenomenology. In addition, we will provide an example that lattice field is not only a tool to address QCD to answer Wilson's original question, but also other field theories such as the Higgs-Yukawa model discussed here.

2. Lattice field theory

The principles of lattice field theory can already be explained at the example of the Schwinger model [6] which describes quantum electrodynamics in two dimensions. In the continuum, the model is defined through the path integral [7]

$$\mathcal{Z} = \int \mathcal{D}A_\mu \mathcal{D}\Psi \mathcal{D}\bar{\Psi} e^{-S_{\text{gauge}} - S_{\text{ferm}}} \quad (1)$$

which is taken here in Euclidean time. In this form, the path integral resembles a partition function in statistical mechanics and, in fact, this resemblance goes much deeper and the study of phase transitions, critical phenomena and also algorithmic developments are common to both fields. The path integral is determined through the actions S_{gauge} for the gauge field and S_{ferm} for the fermion fields, where S_{ferm} is given by

$$S_{\text{ferm}} = \int d^2x \bar{\Psi}(x) [D_\mu + m] \Psi(x) \quad (2)$$

with m being the fermion mass and the gauge covariant derivative

$$D_\mu \Psi(x) \equiv \gamma_\mu (\partial_\mu - ig_0 A_\mu(x)) \Psi(x) , \quad (3)$$

where $\Psi, \bar{\Psi}$ denote anti-commuting fermion fields, A_μ is the gauge potential and g_0 the gauge coupling. The $2 \otimes 2$ matrices γ_μ are the standard Pauli-matrices. The gauge field action is given as

$$S_{\text{gauge}} = \int d^2x F_{\mu\nu} F_{\mu\nu} , \quad F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) . \quad (4)$$

Taking the gauge field action S_{gauge} and deriving the equations of motion will give the Maxwell equations in Euclidean time. It is worth noting that this simple field theory has already a number of interesting properties such as a dynamical generation of a mass gap of bound states or the non-perturbative generation of a fermion condensate [8, 9].

Going to a lattice description of this model, one introduces a lattice spacing a and places the fermion fields on the integer valued lattice sites $x = (t, \mathbf{x})$. The lattice fermion action then assumes the form

$$S \rightarrow a^2 \sum_x \bar{\Psi} [\gamma_\mu \partial_\mu - \partial_\mu^2 + m] \Psi(x) \quad (5)$$

with the most obvious choice of the lattice derivative assuming nearest neighbour differences,

$$\partial_\mu = \frac{1}{2} [\nabla_\mu^* + \nabla_\mu] \quad (6)$$

with, neglecting for a moment the gauge fields,

$$\nabla_\mu \Psi(x) = \frac{1}{a} [\Psi(x + a\hat{\mu}) - \Psi(x)] , \quad \nabla_\mu^* \Psi(x) = \frac{1}{a} [\Psi(x) - \Psi(x - a\hat{\mu})] \quad (7)$$

which in the limit of vanishing lattice spacing will lead to the desired continuum derivative. The second order derivative term ∂_μ^2 in (5) appears in order to remove unwanted modes on the

lattice, the so-called doubler modes. The conceptual drawback of this term is that it breaks a most important symmetry of the continuum action, namely continuum chiral symmetry¹, i.e. the invariance of the action under exchange of mass-less left- and right-handed fermions. Thus it seems that there is a price to pay when putting fermions on the lattice and, in fact, already at an early stage of lattice field theory a no-go theorem was established. It states that on the lattice either the fermion spectrum, the locality of the theory, chiral symmetry or the correct dispersion relation has to be altered compared to the continuum theory [12, 13, 14]. Only in the limit when the lattice spacing a vanishes, the continuum theory with all the desired properties listed above is expected to be recovered. However, this expectation needs, of course, to be explicitly verified. Therefore, it is very important to have different lattice fermion formulations since taking the continuum limit from these alternative theories, which break different continuum properties, physical results have to agree.

Let us now look at the gauge part of the Schwinger model. It was Wilson's essential observation that not the gauge potentials themselves, but the parallel transporters,

$$U(x, \mu) = e^{iaA_\mu(x)} \in U(1) \quad (8)$$

are the fundamental objects for a lattice formulation of gauge theories. Employing the parallel transporter, a lattice covariant derivative can be defined,

$$\nabla_\mu \Psi(x) = \frac{1}{a} [U(x, \mu) \Psi(x + \mu) - \Psi(x)] \quad (9)$$

which guarantees the gauge invariance of the lattice theory. The gauge interaction is then realized through a so-called plaquette variable,

$$U_{(x,p)} = U(x, \mu)U(x + \mu, \nu)U^\dagger(x + \nu, \mu)U^\dagger(x, \nu) \rightarrow F_{\mu\nu}F^{\mu\nu}(x) \text{ for } a \rightarrow 0. \quad (10)$$

As indicated in (10) the so defined plaquette variable assumes the continuum expression for the gauge field interaction. Using the plaquette variable, a lattice action for the Schwinger model can be formulated,

$$S = a^2 \sum_x \left\{ \beta [1 - \text{Re}(U_{(x,p)})] + \bar{\psi} \left[m_0 + \frac{1}{2} \{ \gamma_\mu (\nabla_\mu + \nabla_\mu^*) - a \nabla_\mu^* \nabla_\mu \} \right] \psi \right\}. \quad (11)$$

This action, with $\beta = 1/g_0^2$ and m_0 the fermion mass on the lattice, can be used to compute now expectation values of physical quantities, $\langle \mathcal{O} \rangle$ in close analogy to statistical mechanics by

$$\langle \mathcal{O} \rangle = \frac{1}{\mathcal{Z}} \int_{\text{fields}} \mathcal{O} e^{-S} \quad (12)$$

where $\mathcal{Z} = \int_{\text{fields}} e^{-S}$ is the path integral or partition function. Having now formulated the Schwinger model in Euclidean space-time on a discrete lattice, using a finite number of lattice points, the integral in (12) can be solved numerically. Since in the integrand the Boltzmann factor e^{-S} strongly favors only certain field configurations, Monte Carlo methods relying on importance sampling are used for this task; see [15, 16] for introductions of simulation algorithms used in lattice field theory. Having established the lattice theory of the Schwinger model, a corresponding action for quantum chromodynamics (QCD), our target theory for describing the strong interaction, can be given. Here, one has to go to four dimensions and the $U(1)$ gauge fields of (8) are replaced by non-abelian $SU(3)$ valued gauge fields which represent the gluon fields. The fermions, i.e. the quark fields carry now a colour charge through which they interact with

¹ It is possible to establish a modified but exact chiral symmetry on the lattice [10], based on the Ginsparg-Wilson relation [11]; see also section 4

the gluons and also a Lorentz index thus leading to the fact that they are represented as twelve component Grassman valued fields. We will not detail the lattice QCD action but refer the interested reader to [17, 18, 19, 20].

3. Evaluation of the fermion action

Having established an Euclidean space-time lattice action and correspondingly the pathintegral for lattice field theory, in principle numerical evaluations for calculating physical quantities become possible. However, there is a major and severe obstacle in computing the fermionic part of the pathintegral which leads to very computer time consuming calculations when fermions are employed such as in lattice QCD or also in lattice Higgs-Yukawa models as discussed below. To understand why this is so, let us have a look at the generic form of the fermion part of the partition function,

$$\mathcal{Z}_{\text{ferm}} = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-\bar{\psi} \{D_{\text{ferm}}\} \psi}, \quad (13)$$

where D_{ferm} is a given, generic lattice Dirac operator. The key observation is that fermions, as Grassman variables, cannot be handled on a computer directly. However, since the action is quadratic in the fermion fields, the fermion degrees of freedom can be integrated out leading to the expression

$$\mathcal{Z}_{\text{ferm}} \propto \det[D_{\text{ferm}}] \quad (14)$$

and hence to the evaluation of a determinant. The difficulty arises from the fact that present days lattice computations are performed for lattices with a number of sites $48^3 \cdot 96$. Since, as discussed above, in QCD the fermion field per lattice site has 12 components we would have to compute a determinant of a huge matrix of size $[48^3 \cdot 96 \cdot 12] \otimes [48^3 \cdot 96 \cdot 12]$ which is, of course, prohibitive.

The way out is to represent the fermion determinant as an integral over bosonic degrees of freedom which can be handled on a computer,

$$\det[D_{\text{ferm}}] \propto \int \mathcal{D}\Phi^\dagger \mathcal{D}\Phi e^{-\Phi^\dagger \{D_{\text{ferm}}^{-1}\} \Phi}. \quad (15)$$

To evaluate this representation of the fermionic path integral, we therefore need to compute a vector $X = D_{\text{ferm}}^{-1} \Phi$, or equivalently, we have to solve a set of linear equations

$$D_{\text{ferm}} X = \Phi. \quad (16)$$

Still, given the huge size of the matrix D_{ferm} this looks like an unsurmountable task. What helps here is that the matrix D_{ferm} is a sparse matrix and hence well suited algorithms such as conjugate gradient can be used.

Nevertheless, in the algorithms used to simulate the fermion degrees of freedom, the set of linear equations of (16) needs to be solved $O(100)$ times to generate just one of the gauge field configurations on which eventually physical measurements are to be performed. And, the goal is to reach finally a set of $O(1000 - 10000)$ of such gauge field configurations. If in addition, one keeps in mind that, say, in a conjugate gradient computation for the solution of (16) $O(100 - 1000)$ iterations are needed, one can easily estimate the extremely large number of matrix vector operations, scalar products and norms that is needed for just one simulation point.

All this led in the 20th century to the fact that lattice simulations were performed in the so-called quenched approximation where the above sketched determinant evaluation was completely neglected. It was then the CP-PACS collaboration situated in the home country of

the Conference on Computational Physics 2012, i.e. Japan, which showed in a remarkable paper [21] that this quenched approximation must be dismissed to perform QCD calculations.

In this paper [21], for the first time, the complete low-lying hadron spectrum was computed. By fixing two input masses, all the rest of the baryon masses were “predicted” by lattice QCD. The precision reached in this calculation was so high that in fact significant deviations between the quenched lattice QCD computation and the experimentally determined baryon masses were detected. As a conclusion, it became clear that the quenched approximation is a much too strong truncation of the theory and that the quarks have to be taken as truly dynamical degrees of freedom into account.

The problem of taking the step to keep the determinant in the simulation became very clear at the Berlin lattice symposium in 2001 [22]. At this conference a number of collaborations, using their particular formulation of lattice QCD, showed results for the simulation costs when the pion mass was shifted from an unphysically large value of around 700MeV towards its physical value of 140MeV.

It was found that the simulation costs grow with an inverse power of the pion mass m_π as m_π^{-s} with $s = 1 - 2$. In addition, when decreasing the lattice spacing while keeping the physical extent of the box fixed, the number of lattice points to be simulated needs to be increased leading to a scaling of a^{-4} . When studying the actual lattice spacing dependence of the simulation cost, it was found that there is an additional dependence, leading to a total scaling of a^{-t} with $t = 6 - 7$. All this led to the conclusion that simulations close to the physical point, i.e. at physical values of the pion mass, seemed unreachable [23].

The hope at that time was then that chiral perturbation theory could be used to extrapolate results obtained at too large pion masses to the physical point. However, in the course of the years, it turned out that there are significant challenges in performing chiral extrapolations of baryon quantities; see e.g. [24] for a recent discussion of the subject.

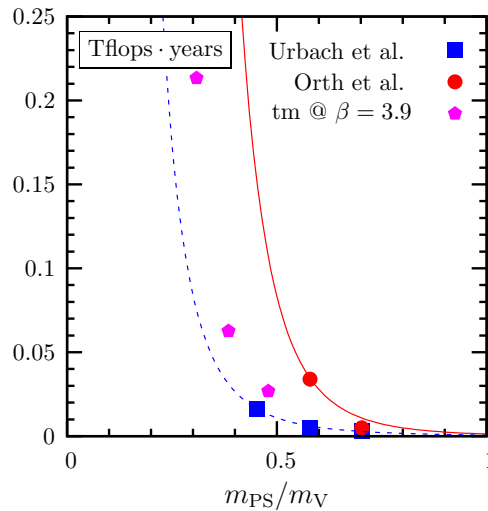


Figure 1. The simulation cost of lattice QCD calculations is shown. The ratio m_{PS}/m_V in the graph assumes a physical value of about 0.18 and the graph shows how the computation costs, expressed in teraflop years increases when m_{PS}/m_V is moved to the physical value. In the past, these costs were several hundred or even thousands of teraflop years. The figure demonstrates the improvement in developing algorithms since it demonstrates that nowadays an amount of teraflop years is necessary that can be reasonably realized on present supercomputer architectures.

In this somewhat desperate situation, around 2005, a number of publications appeared [25, 26, 27] which demonstrated that the standard Hybrid Monte algorithm [28] used for

simulations of fermion system can be supplied with very substantial improvements. This led to a scaling with the pion mass as shown in figure 1, as one example. The graph shows the typical simulation cost in teraflop years to solve a problem of lattice QCD as a function of the ratio of the pion to the vector meson mass m_V with a physical value of this ratio to be $m_\pi/m_V = 0.18$. The finding of the Berlin 2001 lattice conference was that the simulation cost at the physical value of the this ratio becomes several hundred or even more teraflop years. In figure 1, with the mentioned algorithmic improvements implemented, the simulation costs stay at a reasonable level and given present days supercomputers it seems to become perfectly reasonable to simulate directly at the physical point, an enterprise that is in fact started by many collaborations world-wide. The status of such simulations of lattice QCD over the last years is summarized in the reviews of [29, 30, 31, 32].

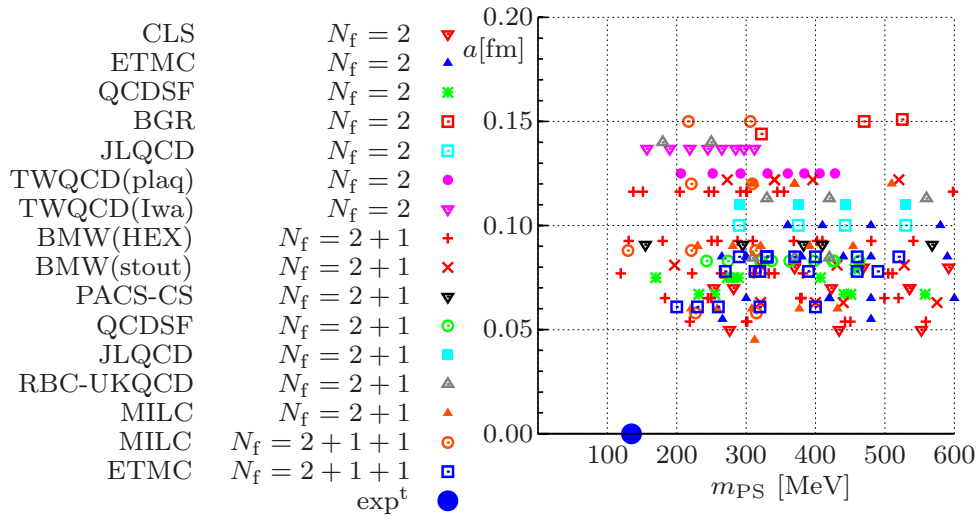


Figure 2. The simulation landscape of present lattice QCD calculations. In the graph, we show the values of the lattice spacing a and pion masses m_{PS} where present simulations are performed world-wide today. Note that already a number of simulations are carried out at the physical point where the pion mass assumes its experimentally measured value.

The progress in supercomputer architectures and, in particular, in the algorithmic improvements are documented in the “landscape” graph of figure 2. This figure shows the lattice spacing and the pion mass where simulations are performed. It can be clearly seen that nowadays simulations with small lattice spacings, $a \lesssim 0.1\text{fm}$ and pion masses well below 500MeV are performed. Even more, there are already simulations at the physical value of the pion mass. As a result of these calculations a first ever computation of the baryon spectrum could be achieved treating the quarks as truly dynamical degrees of freedom [33], see figure 3. Such a calculation has by now been repeated by many lattice collaborations world-wide; see the review [34].

The calculation of the light hadron spectrum can certainly be considered as a breakthrough for lattice QCD computations since this was taken as a most important benchmark result. However, the lattice community has gone already significant steps forward. Following the theoretical basis developed in [35], it is now possible, to address also resonances on the lattice. In figure 4. we show an example for a calculation of the phase shift for the ρ -meson resonance [36]. For a comprehensive review of the status of resonance calculations from lattice field theory, see [37]. An alternative way to compute phase shifts on the lattice is by using a partial wave analysis of a hadron wave function computed on the lattice; see section 6. Even more, as the lattice

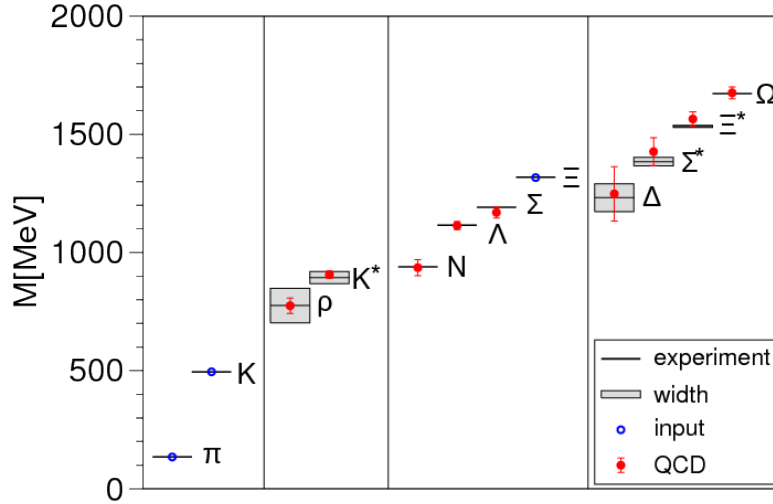


Figure 3. The hadron spectrum calculation of [33]. Using only two input masses, all the rest of the hadron masses are directly computed from lattice QCD. The nice agreement between the lattice calculation and experimental measurement is very reassuring that lattice QCD can provide non-perturbative results that can be directly compared to experiment.

calculations become more and more precise, groups have taken the effects of electromagnetism and an explicit breaking of isospin into account, [38, 39, 40]. In fact, it is now possible to even disentangle the effects of electromagnetism and isospin breaking on the mass splitting of hadrons (see [41]). This is a truly remarkable result since these effects are on the MeV level, while the hadron masses are on a scale of GeV.

In the discussion above, we have seen that there has been a tremendous progress in lattice field theory calculations. In the following, we will discuss two particular examples for such present computations. The first example describes results for bounds on the Higgs boson mass. These bounds can be directly related to the energy scale up to which the standard model of particle interaction can be valid. The second example discusses a computation of the leading order hadronic contribution to the muon anomalous magnetic moment.

After this discussion, we will emphasize some open demanding problems and challenges to lattice field theory. These problems and challenges will for sure necessitate the usage of today's supercomputers of the K-machine class.

4. Higgs-Yukawa

The Higgs-Yukawa sector of the Standard Model (SM) describes the generation of fermion masses via the non-vanishing vacuum expectation value (v_{ev}) acquired by the Higgs field which couples through a Yukawa coupling to the fermions. The essential element in this picture is that the coupling of the fermions to the Higgs field is chirally invariant which leads to the gauge invariant electroweak sector of the SM in the presence of gauge fields.

In principle, the involved couplings of the theory, the quartic self-interaction of the Higgs field and the Yukawa-coupling between the Higgs field and the fermions, can grow strong. This happens, when the involved masses are large and then perturbation theory might fail to analyze the theory. There are indeed examples where the applicability of perturbation theory is questionable. The first is the upper Higgs boson mass bound which is based on triviality arguments [42]. Here the Higgs boson mass can become large, resulting in a strong value of the quartic coupling such that perturbation theory may not work anymore. The second is the lower Higgs boson mass bound which is based on vacuum instability arguments [43, 44, 45, 46]. Here

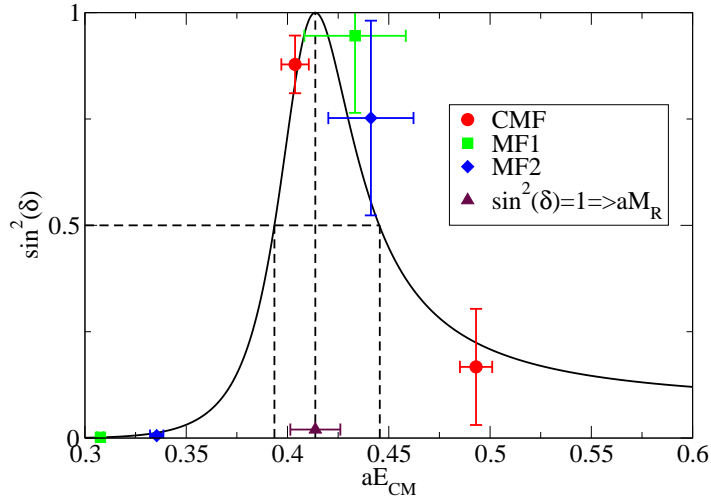


Figure 4. We show the scattering phases calculated in the center of mass frame (CMF), as well as in two moving frames (MF1 and MF2) together with the fits to an effective range formula; see [36]. At the position where the scattering phase passes $\pi/2$, the resonance mass m_ρ (denoted as aM_R in the graph) is determined. Through the fit, the coupling constant $g_{\rho\pi\pi}$ and the decay width Γ_ρ are also extracted.

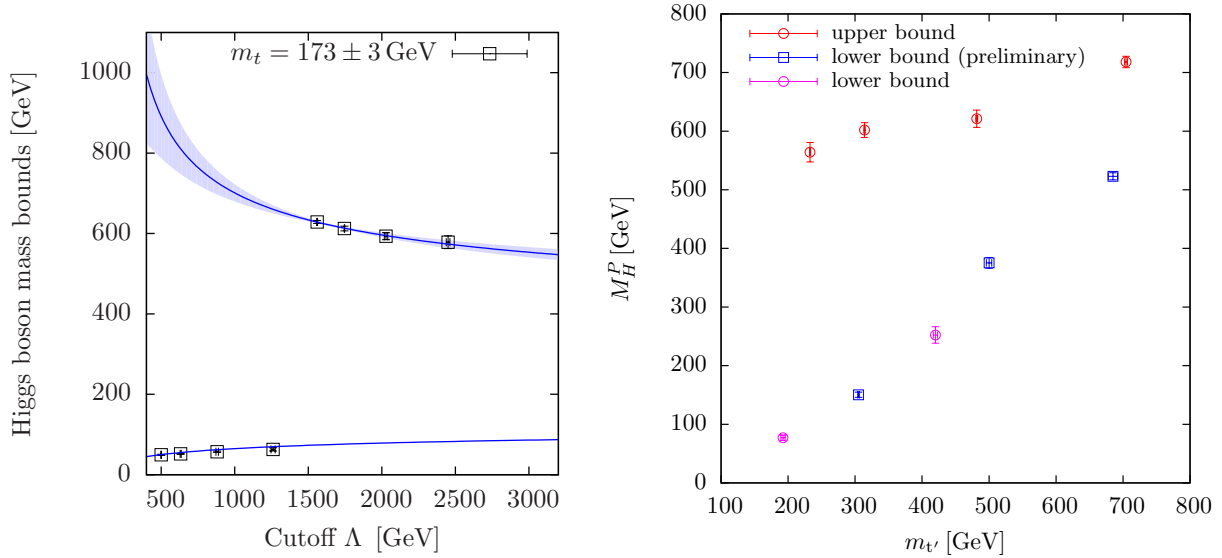
it is unclear whether this instability is not an artifact of perturbation theory applied at large values of the Higgs field such that an expansion around the minimum of the effective potential is not justified anymore.

It is important to stress that both the lower and the upper Higgs boson mass bounds are intrinsically related to the cut-off of the theory. Thus, a calculation of the Higgs boson mass bounds can in turn be used to determine the cut-off up to which the SM is valid, once the SM Higgs boson mass has been determined. If, for example, the recent result for a scalar particle at the Large Hadron Collider (LHC) [47, 48] is confirmed as a SM Higgs boson with a mass of about 125 GeV, the SM could be valid up to very high energies before violating the Higgs boson mass bounds; see [49] for a recent analysis at next-to-next leading order of perturbation theory.

Another example where non-perturbative calculations are necessary is the possibility of a heavy fourth fermion generation [50, 51] which would lead to a large value of the corresponding Yukawa coupling.

Conceptually clean investigations of Higgs-Yukawa models on the lattice became possible when it was realised that –based on the Ginsparg-Wilson relation [11]– there exists a consistent formulation of an exact lattice chiral symmetry [52], which emulates the chiral character of the Higgs-fermion coupling structure of the SM. This triggered a number of lattice investigations of Higgs-Yukawa like models [53, 54, 55, 56, 57, 58, 59, 60, 61].

As an example, we show here the results of the Higgs boson mass bound calculations discussed in [61, 62]. In the left graph of figure 5 the upper and lower bounds were computed at several choices of the cut-off scale, with the fermion masses m_f at the physical top-quark mass. The right graph of this figure shows the fermion mass dependence of the lower and upper Higgs boson mass bounds at a fixed value of the cut-off of about 1.5 TeV. It can be clearly seen that while the upper bound is relatively unaffected when using a heavy fermion mass, the lower bound increases substantially.



(a) The cut-off dependence of the upper and lower Higgs boson mass bounds for fermion a mass of about $\sim 173\text{GeV}$. (b) The mass dependence of the lower and upper Higgs boson mass bounds at a cut-off of about 1.5TeV .

Figure 5. Results for the Higgs boson mass bounds.

The graphs in figure 5 have a very interesting interpretation in the light of the SM and also the fourth fermion generation. Concerning the SM, a Higgs boson mass of about 125GeV just seems to escape the Higgs boson mass bounds leading the SM to be valid up to very high energies. On the other hand a fourth fermion generation seems to be ruled out for fermion masses larger than about 300GeV . Combining this with phenomenological analyses of allowed fermion masses to be larger than about 500GeV , this indicates that a simple extension of the SM with a fourth fermion generation is not compatible with the experimental finding of a possible 125GeV Higgs boson mass.

The discussion of the Higgs boson mass bounds here, as they are interesting by themselves, served as an example that lattice field theory can also provide important information for non-QCD like theories. We note in passing that for the Higgs-Yukawa model considered here, the Higgs boson has also been treated as a true resonance [63]. In addition, the model is studied at non-zero temperature and also at very strong values of the Yukawa-coupling to explore whether a generic non-perturbative interaction can take place that is different from standard model physics [62].

5. The muon anomalous magnetic moment

Let us now turn back to lattice QCD, the original target theory. Here we want to discuss one particular example, namely the anomalous magnetic moment of the muon.

In Dirac's theory the electron is described as a spin $1/2$ particle with the positron as its anti-particle. Like in the classical theory the angular momentum, the spin \vec{S} leads to a magnetic moment of the electron

$$\vec{\mu}_m = -g_e \mu_0 \vec{S} \quad (17)$$

with $\mu_0 = e/4m_e$, e being the electric charge and m_e the mass of the electron. The quantity g_e is the gyro-magnetic ratio of the electron and assumes in Dirac's theory a value of $g_e = 2$.

When a quantum field theory is considered, deviations from $g_e = 2$ appear, originating from

a virtual photon exchange which leads to an *anomalous magnetic moment*

$$a_e = \frac{g_e - 2}{2} . \quad (18)$$

The most simple correction to g_e is just the one *virtual* photon exchange between the charged electrons. This correction, first considered by Schwinger [64], can be directly computed from quantum electrodynamics (QED), the relativistic theory of electromagnetic interaction. The seminal work by Schwinger revealed that the quantum correction $\delta(a_e)$ is

$$\delta(a_e) = \frac{\alpha}{2\pi} . \quad (19)$$

Experimental measurements [65] found a value for $g_e = 2.00238(10)$ and Schwinger's calculation yielded $g_e = 2.00232$. The agreement of these results established the theoretical and experimental fact that quantum corrections lead indeed to deviations from the classical value of $g_e = 2$. Subsequent more precise theoretical calculations and experimental measurement confirmed the agreement between QED predictions and observation (see [66]).

Today, the theoretical efforts have been driven to enormously complicated calculations involving the computation of thousands of diagrams. The calculations of [67] involve nowadays diagrams including four loops, we speak of a 4-loop order calculation and even a 5-loop order calculation is in sight. The theoretical computations are based on a systematic expansion of the theory in the fine structure constant α . Employing such high loop order quantum field theoretical calculations and extremely accurate and subtle experimental measurements, one finds an incredible agreement between experiment and standard model predictions for the anomalous magnetic moment of the electron, i.e. (see e.g. [68])

$$\begin{aligned} a_e(\text{th}) &= 1159652201.1(2.1)(27.1) \cdot 10^{-12} \\ a_e(\text{exp}) &= 1159652188.4(4.3) \cdot 10^{-12} . \end{aligned} \quad (20)$$

This establishes the electron magnetic moment as one of the most precisely determined quantity in nature and the agreement between the two numbers in (20) achieved with such an amazing accuracy is one of the cornerstone results to make us confident that indeed quantum field theories are the correct method to describe particle interactions.

However, the story does not end here. Nature has decided, for an unknown reason, that it comprises three particle generations. Besides the electron, which belongs to the first generation, there are further so-called leptons, the muon with a mass of about 105.7MeV and the τ having a mass of 1777MeV. Comparing these values to the mass of the electron of 0.511MeV, we see that the masses of the leptons of the second (the muon) and the third (the τ) generations are much larger than the electron mass. This fact will play an important role in the discussion below. Being leptons, also the muon and τ carry spin, leading to magnetic moments which become, due to the discussed quantum corrections, anomalous. For example, a comparison for the case of the muon anomalous magnetic moment, a_μ , between experiment and theory yields [66]

$$\begin{aligned} a_\mu^{\text{exp}} &= 1.16592080(63) \times 10^{-3} \\ a_\mu^{\text{theory}} &= 1.16591790(65) \times 10^{-3} . \end{aligned} \quad (21)$$

Here the agreement between theory and experiment is not as nice as in the case of the electron and in fact, one finds $a_\mu^{\text{exp}} - a_\mu^{\text{th}} = 2.90(91) \times 10^{-9}$ which leads to a larger than 3σ level discrepancy.

However, this is a very interesting result. It means that either in the theoretical calculation something has been neglected or has not properly been included. Or, somewhat much more exciting, the discrepancy points to a breakdown of the standard model of particle interactions and the inconsistency stems from effects of some yet unknown new physics beyond the standard model.

Indeed, calculations show that these new physics effects would lead to a correction to the anomalous magnetic moment of size

$$\delta(a_l^{\text{newphysics}}) = m_{\text{lepton}}^2 / M_{\text{newphysics}}^2 \cdot \quad (22)$$

Here m_{lepton} is the mass of one of the leptons and $M_{\text{newphysics}}$ represents the mass (or scale) of a particle originating from the (unknown) new physics beyond the standard model. The formula in (22) shows that in the case of the muon anomalous magnetic moment the effect of new physics would show up about $(m_\mu/m_e)^2 \approx 4 \cdot 10^4$ times stronger than in the case of the electron. In principle, the τ -lepton would be even more suitable to detect these new physics effects, but unfortunately due to the very short lifetime of the τ lepton the experimental measurements of the anomalous magnetic moment of the τ are presently much too imprecise to unveil a possible new physics contribution. This leaves us then with the muon anomalous magnetic moment as the ideal place to look for new physics and indeed a large number of works has been devoted to explore this possibility (see [66]).

As we discussed for the case of the electron, theoretically the anomalous magnetic moment is computed in an expansion of the theory in the fine structure constant to a given loop order. In the loops, in principle all particles of the standard model can appear, if allowed by symmetries and quantum numbers. Therefore, besides leptons and photons, also the vector bosons, W and Z , of the weak interaction and the quarks and gluons of the strong interaction, described by quantum chromodynamics (QCD) can and will contribute. It can be shown that the contribution of the W and Z bosons are first of all rather small and can be, secondly, well controlled by perturbation theory [66].

However, the strong interaction of quarks and gluons in QCD lead to so-called hadronic contributions a_μ^{had} which are intrinsically of non-perturbative nature. Taking these contributions into account by perturbation theory is therefore rather doubtful. Employing additional model assumptions to estimate a_μ^{had} will not provide a fully controlled and reliable calculation of the hadronic contributions and hence an unambiguous and stringent test whether the standard model is correct or must be extended by some new physics cannot be performed.

It is exactly at this point where lattice field theory methods applied to quantum chromodynamics can help – at least in principle. Of course, the discretization itself induces a systematic error which must be removed by making the lattices finer and finer until the continuum of space time points is recovered by some suitable extrapolation process, a procedure which is called the *continuum limit*. In addition, the simulations necessarily demand a finite number of lattice points which can lead to *finite size effects* when the lattice is not large enough in physical units. Finally, often the simulations need to be performed at values of hadron masses that are larger than observed in nature. The reason is that, as discussed above, for smaller and smaller hadron masses the computational costs increase rapidly such that one is restricted to values of, say, pion masses that are a factor of about two larger than the ones observed in nature.

All these systematic effects that appear in lattice simulations need to be controlled in a quantitative way. For example, to reach physical values of the pion masses, an extrapolation to the physical point where the pion mass assumes its physical value needs to be performed. This appeared to be very problematic in the past. This is illustrated in figure 6(a) by the lowest lying points which were obtained in the past by the standard way of computing a_μ^{had} . The figure shows that these older lattice results for a_μ^{had} are significantly below the experimental number. An extrapolation to the physical point, reconciling the lattice data with experiment becomes

in this situation very difficult and even needs some additional model assumptions. This all has led to an error of a_μ^{had} as obtained from lattice simulations that is about a factor of 10 larger than the phenomenological one [69]. The lattice community has been therefore rather sceptical in the past that lattice QCD can provide a significant contribution to our understanding of the discrepancy in $g_\mu - 2$.

One additional suspicion has been that so-called dis-connected (singlet) contributions could be substantial. In all existing lattice calculations these contributions were neglected, however. The reason is simply that these contributions are very noisy and therefore hard to compute reliably. In [70] a dedicated effort to calculate these contributions was undertaken for the first time. As a result, it could be established that the dis-connected contributions are in fact small and can be safely neglected. In addition, also the effects of non-zero values of the lattice spacing and the finite volume turned out to be small. Thus the difficulty to reconcile lattice data with the experimental result, shown in figure 6(a), is rather puzzling.

A resolution of this puzzle was only given in [70] where it was observed that by a suitable redefinition of the lattice observable needed to compute a_μ^{had} a much smoother and much better controlled approach to the physical point can be achieved.

To illustrate the idea, let us give the definition of a_μ^{had} ,

$$a_\mu^{\text{had}} = \alpha^2 \int_0^\infty dQ^2 \frac{1}{Q^2} \omega(r) \Pi_R(Q^2) . \quad (23)$$

Here α is the electromagnetic coupling and $\Pi_R(Q^2)$ the renormalized vacuum polarization function, $\Pi_R(Q^2) = \Pi(Q^2) - \Pi(0)$. The functional form of $\omega(r)$ is analytically known and the argument r is given by $r = Q^2/m_\mu^2$ where m_μ denotes the mass of the muon and Q a generic momentum. The key observation is now that on the lattice there is a large freedom to choose a definition of r . The only requirement is that in the limit of reaching a physical pion mass the continuum definition of $r = Q^2/m_\mu^2$ is recovered. Hence, one may define

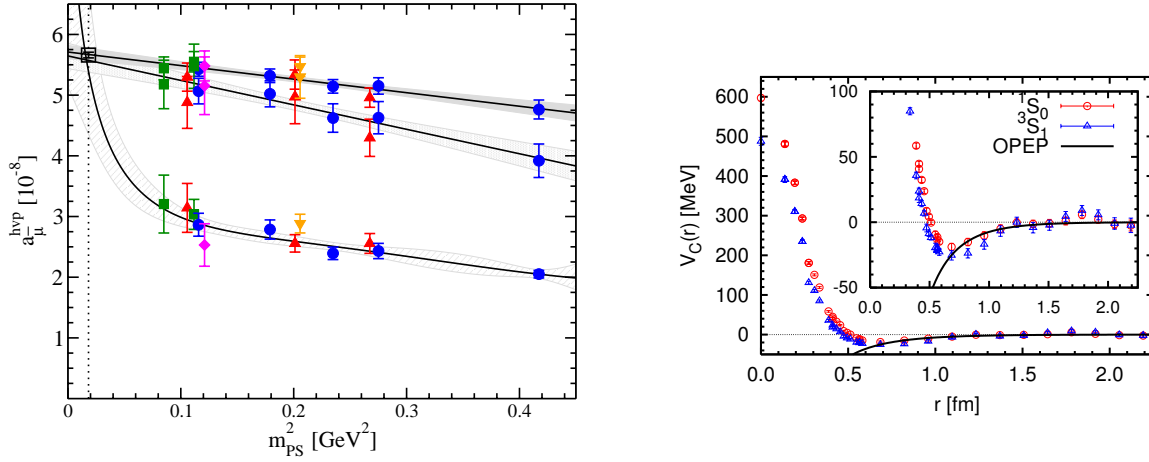
$$r_{\text{latt}} = Q^2 \cdot \frac{H^{\text{phys}}}{H} \quad (24)$$

with possible choices for H

$$\begin{aligned} r_1 : \quad & H = 1 \quad H^{\text{phys}} = 1/m_\mu^2 \\ r_2 : \quad & H = m_V^2(m_{\text{PS}}) \quad H^{\text{phys}} = m_\rho^2/m_\mu^2 \\ r_3 : \quad & H = f_V^2(m_{\text{PS}}) \quad H^{\text{phys}} = f_\rho^2/m_\mu^2 . \end{aligned} \quad (25)$$

Here, $m_V(m_{\text{PS}})$ is the mass of the ρ -meson and $f_V(m_{\text{PS}})$ the ρ -meson decay constant as determined on the lattice at unphysical pion masses m_{PS} . Furthermore, m_ρ and f_ρ denote the corresponding ρ -meson mass and decay constant at the physical point. All the definitions in (25) guarantee that indeed the desired definition of r is recovered in the limit of a physical pion mass since then by definition $m_V(m_{\text{PS}})$ and $f_V(m_{\text{PS}})$ assume their physical values. In figure 6(a) we show the results for a_μ^{had} for all three definitions of r . Clearly, for the definitions r_2 and r_3 the behaviour of the lattice data towards physical pion masses is simply linear and allows for a controlled extrapolation to the physical point. As a result, one finds using definition r_2 in (25) values from the lattice computations and experiment

$$\begin{aligned} a_{\mu, N_f=2}^{\text{had, latt}} &= 5.72(16) \cdot 10^{-8} \\ a_{\mu, N_f=2}^{\text{had, exp}} &= 5.660(47) \cdot 10^{-8} . \end{aligned} \quad (26)$$



(a) We show a result for the hadronic contribution to the muon anomalous magnetic moment using different choices for r in (25). The curves correspond to the definitions r_1 , r_2 and r_3 in (25) from bottom to top. Clearly, the improved definitions, r_2 and r_3 , show a much milder pion mass dependence than the standard definition, r_1 .

(b) The lattice QCD result of the effective central part of the NN potential $V_C(r)$ ($V_C^{\text{eff}}(r)$) in the 1S_0 (3S_1) channel for $m_\pi/m_\rho = 0.595$. The inset shows its enlargement. The solid lines correspond to the one-pion exchange potential (OPEP).

Figure 6. The leading order hadronic contribution to the muon anomalous magnetic moment and an example of a nuclear potential computed in lattice QCD.

One can notice that the lattice result is not only consistent with the experimental determination, but also that the error of the lattice calculation assumes a comparable magnitude as the experimental one. This opens the very interesting possibility that lattice computations can significantly contribute to resolve the discrepancy between the standard model and experimental determinations of the anomalous magnetic moment of the muon.

The hear discussed results for a_μ^{had} have been achieved for the case of two mass-degenerate quark flavours. What is needed in the future is the inclusion of the strange and the charm quarks to allow for a direct comparison to the experimental results. In addition, newly planned experiments at Fermilab [71] and J-PARC [72] are aiming at an accuracy of below 0.5% for the hadronic contribution to the muon anomalous magnetic moment. To match this accuracy, lattice simulations have possibly to include explicit effects of isospin breaking and electromagnetism. All this is in principle reachable within lattice QCD, see section 3, but, it constitutes a real challenge for the lattice community. An even larger challenge are contributions to $g_\mu - 2$ that appear at higher order of the electromagnetic coupling, most notably the so-called light-by-light contributions (see also section 7.1). However, the lattice community is ready to attack these challenges and a large activity has been started to compute a_μ^{had} at leading order and beyond [73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 70].

6. Nuclear physics

The examples discussed above were concerned with questions in high energy physics. However, there is also a significant activity in the lattice community to address problems in nuclear physics; see [83, 84] for reviews of different approaches.

Let me discuss here the method described in [85]. The starting point here is the Schrödinger equation,

$$[H_0 + V(x)] \phi_k(x) = \epsilon_k \phi(x)_k \quad (27)$$

with the energy $\epsilon_k = \frac{k^2}{2\mu}$, the reduced mass $\mu = m_N/2$ and the free Hamiltonian $H_0 = \frac{-\nabla^2}{2\mu}$. $V(x)$ denotes the nuclear potential. The basic idea, pioneered in [85] is to revert this equation. If we would know the exact QCD wave function at wavenumber k , $\phi_k(x)$, for a certain physical situation, we can compute the corresponding potential by solving

$$[\epsilon_k - H_0] \phi_k(x) = \int d^3y V(x, y) \phi_k(y) . \quad (28)$$

Examples for such wave functions could be the nucleon wave function, three body wave functions etc. The basic idea is then to use the potential calculated in finite volume within lattice QCD to solve the Schrödinger equation in infinite volume obtaining in this way the wave function in infinite volume at a given wave number k .

The wave function can be computed on a lattice in a straightforward way. E.g., if we want the nucleon wave function, it can be obtained via

$$\phi_k(r) = \langle 0 | N(x+r) N(x) | NNW_k \rangle \quad (29)$$

using solely lattice QCD. Here $W_k = \sqrt{k^2 + m_N^2}$, $N(x)$ a nucleon interpolating operator and $|NNW_k\rangle$ a 2-nucleon state with energy W_k . Knowing the wave function ϕ_k a partial wave analysis can be performed,

$$\phi_k^l \rightarrow A_l \frac{\sin(kt - l\pi/2 + \delta_l(k))}{kr} \text{ for } r \rightarrow \infty \quad (30)$$

which eventually allows access to the scattering phase shifts $\delta_l(k)$. The strategy can be summarized with the following steps:

- compute the wave function within lattice QCD in *finite volume*
- determine the potential $U(x)$ in *finite volume*
- use this potential to solve the Schrödinger equation in *infinite volume*
- determine scattering phases or binding energies from the so obtained wave function and the partial wave analysis

Following these steps it then becomes, at least in principle, possible to address questions in nuclear physics, neutron stars, supernovae or other related areas. Note that the here described way of calculating phase shifts can be considered as an alternative way to the methods proposed in [35] which has by now extensively been used in lattice QCD computations; see [37] for a recent review.

In the work of [85] following the above sketched strategy it was demonstrated that it is possible to compute directly from lattice QCD the nucleon-nucleon potential (see figure 6(b)). This work, which has been selected as one of 21 papers in Nature Research Highlights 2007, opened the road for further investigations of nuclear physics from lattice QCD, following this approach. Demanding problems that are targeted now are in-elastic scattering, resonances and the extension to weak interactions; see [83] for a recent overview.

7. Challenges

In the previous sections we have discussed a number of topics where lattice field theory has been very successful and important results could be obtained that directly influence the interpretation of experiments or enter phenomenological analyses. However, there are still “big rocks on the road” that constitute major challenges for lattice field theory calculations. In this section, I only want to discuss a few of them.

7.1. Anomalous magnetic moment of the muon

As described above, the lattice can now provide very promising results for the leading order hadronic contribution to the anomalous magnetic moment of the muon. However, getting this contribution more and more precise, it becomes very important to also consider the next to leading order contributions. The dominant piece here is the so-called light-by-light contribution which is given by a 4-point function

$$\Pi_{\mu\nu\alpha\beta}(q_1, q_2, q_3) = \int_{xyz} e^{iq_1 \cdot x + iq_2 \cdot y + iq_3 \cdot z} \langle j_\mu(0) j_\nu(x) j_\alpha(y) j_\beta(z) \rangle \quad (31)$$

with the electromagnetic quark current

$$j_\mu = \frac{2}{3} \bar{u} \gamma_\mu u - \frac{1}{3} \bar{d} \gamma_\mu d - \frac{1}{3} \bar{s} \gamma_\mu s + \frac{2}{3} \bar{c} \gamma_\mu c. \quad (32)$$

To compute $\Pi_{\mu\nu\alpha\beta}(q_1, q_2, q_3)$ at all momenta needed, one would have to solve the linear set of equation in (16) $O(V^3)$ times, with V the lattice volume. Having again lattices of size $V = 48^3 \cdot 96$ in mind, a straightforward calculation of this light-by-light contribution is clearly prohibitive. The lattice community is therefore very active to find better methods to obtain information on $\Pi_{\mu\nu\alpha\beta}(q_1, q_2, q_3)$ but, it is rather clear that this will be a very demanding task in any case, needing presumably supercomputer capabilities well beyond the K-computer class.

7.2. Hadron structure

One main activity of the lattice community is the exploration of the quark and gluon structure of a hadron [86, 87, 88, 89]. There is clearly a need from the lattice to provide inside into the hadron structure since this is, by nature of the problem, a non-perturbative task. There are two basic benchmark observables which are relatively easily accessible to lattice QCD calculations. The first is the axial charge of the nucleon and the second is the average momentum of the quark in a nucleon. Both quantities can be determined on the lattice rather precisely and they can be measured accurately experimentally or can be extracted from a global phenomenological analysis of deep inelastic scattering data.

Thus, similar to the hadron spectrum computation, it would be very important and reassuring if g_A and $\langle x \rangle$ as computed within lattice QCD would agree with experiment or phenomenology. However, presently this is not so, as can be seen in figures 7 and 8; see [87] for a more detailed discussion on this topic. The lattice results for g_A and $\langle x \rangle$ which are obtained at still unphysically large pion masses clearly deviate from the experimental or phenomenological values.

It needs to be stressed that the lattice community has undertaken a large effort to understand the discrepancies shown in figure 7 and figure 8. Many possible systematic effects were studied such as lattice spacing or finite volume artifacts, contaminations of excited states or the extrapolations to the physical point where the pion mass assumes its experimentally determined value (see the above listed reviews). None of these attempts could resolve the tension and it is presently a real puzzle what the origin of the discrepancy can be. To answer this question, most probably only a calculation directly at the physical point, on large enough lattices, several lattice spacings and with a sufficiently high accuracy would be needed.

7.3. Nuclear physics

The benchmark calculation for nuclear physics that has been discussed above has been done in the quenched approximation, see section 2, i.e. with infinitely heavy sea quark masses. Since the exploratory work in [85] was intended to provide a proof of concept, truncating the theory in such a way is justified as a first step. However, to make really contact to nuclear physics in the real world, also these computations need to be performed at the physical point with active quark degrees of freedom and preferably in large volume. Thus, there is also in this field of lattice research a very big challenge awaiting.

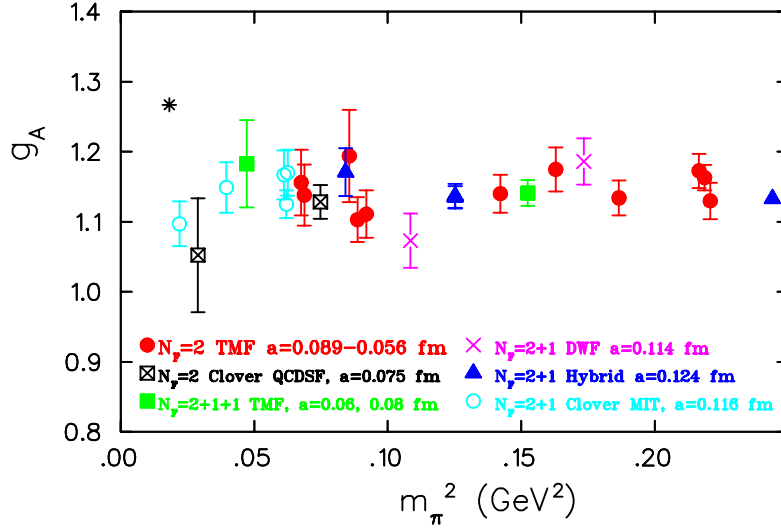


Figure 7. The nucleon axial charge g_A as determined by several lattice computations. Lattice results, taken at unphysical values of the pion mass undershoot the experimental value significantly. The graph is taken from [87].

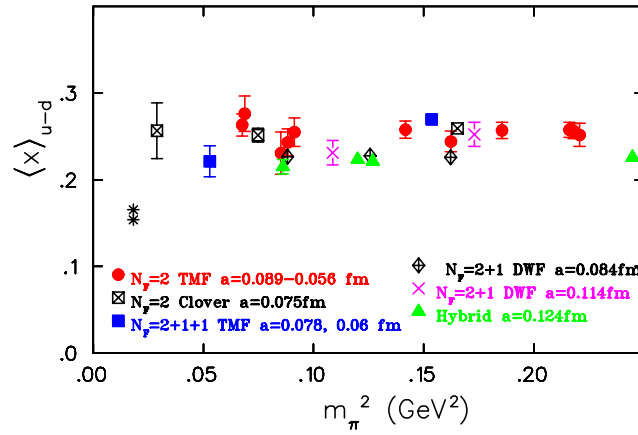


Figure 8. The average momentum of a quark in a nucleon. The lattice results in this case are systematically higher than the phenomenological value. The graph is taken from [87].

7.4. The physical point

As emphasized above, it would be highly desirable to have lattice calculations at the physical point for many physical quantities available to eliminate the systematic effect of working at unphysical values of the pion mass. From our knowledge today, it seems that the coarsest value of the lattice spacing should not exceed $a = 0.1\text{fm}$. At the same time, we want $L \cdot m_\pi > 5$ to suppress unwanted large finite volume effects. Combining this with the physical value of the pion mass of $m_\pi \approx 140\text{MeV}$, this leads to a linear extent of the box of $L \approx 5\text{fm}$. Thus to even

start simulations at the physical point, a lattice with $48^3 \cdot 96$ lattice points is needed. However, this is typically already the largest lattice size that is used today.

In addition and even more demanding, one would like to perform a continuum limit and employ at least $a = 0.05\text{fm}$ thus needing a box with $96^3 \cdot 192$ number of lattice points. Such a box size establishes challenges from the algorithmic point of view, the computational demand and also the storage requirement and builds a real challenge for the future.

Moreover, the lattice community has discovered that going to small values of the lattice spacing, the computational strategies used for coarser values cannot be simply taken over. The reason is that the system starts to freeze in certain topological charge sectors [90] and thus the configuration space is not fully explored and the simulations are not ergodic. Therefore the lattice community is presently exploring new strategies [91] for the computations which raises just another challenge for the future.

8. Concluding remarks

In a presentation like this one, necessarily a selection of topics addressed by the lattice community has to be made. I have left out such interesting directions as B-physics, the excited state spectrum of mesons and nucleons, computations of the quark masses and the strong coupling constant as fundamental parameters of QCD, decay constants or calculations at non-zero temperature and even efforts to look at QCD at non-vanishing chemical potential. The reader who is interested in these directions and others are referred to the annual lattice symposia which are published in [92, 93, 94, 95, 96] for the last five years. Especially the plenary presentations covering the different topics addressed by lattice field theory can provide good overviews about the status of lattice field theory computations in the different areas of modern research.

What I wanted to provide with these proceedings is to give an overview about the substantial progress that has been made in lattice field theory in the last years. At the examples of the baryon spectrum, Higgs boson mass bounds, the anomalous magnetic moment of the muon and efforts to cover nuclear physics I wanted to show the variety and quality of results as well as the accuracy modern lattice calculations can achieve today.

It is important for me to stress that the lattice does not only cover problems within QCD but also goes beyond. In these proceedings I have discussed the example of Higgs-Yukawa models, but there also large activities in the area of conformal field theories (see [97] for a review) and supersymmetry (see [98] for a review).

I hope, that I could convey that lattice field theory has developed into a mature field that has more and more an impact for experiments and phenomenological analyses. At the same time, it is becoming clear that there are major challenges for lattice computations on the way which can only be solved with new computational strategies, further improved algorithms and, last but not least, new supercomputer architectures towards the exaflops regime.

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