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Lattice QCD — from quark confinement to asymptotic freedom *

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Abstract

According to the present understanding, the observed diversity of the strong interaction phenomena is described by Quantum Chromodynamics, a gauge field theory with only very few parameters. One of the fundamental questions in this context is how precisely the world of mesons and nucleons is related to the properties of the theory at high energies, where quarks and gluons are the important degrees of freedom. The lattice formulation of QCD combined with numerical simulations and standard perturbation theory are the tools that allow one to address this issue at a quantitative level.

1. Introduction

Quantum chromodynamics (QCD) is a gauge field theory that looks rather similar to quantum electrodynamics. Apart from the fact that the gauge group is SU(3) instead of U(1), the lagrange density

$$\mathcal{L}_{\text{QCD}} = \frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a + \sum_{q=u,d,s,\dots} \bar{q} \{ \gamma_\mu (\partial_\mu + g A_\mu^a T^a) + m_q \} q \quad (1.1)$$

has the same general form, the first term being the square of the gauge field tensor and the second a sum over the contributions of the up, down, strange and the heavy quarks. No attempt will here be made to explain the detailed structure of eq. (1.1), but an important point to note is that there are no free parameters other than the gauge coupling g and the masses m_u, m_d, \dots of the quarks.

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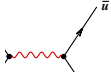


Fig. 1. In QCD the quarks interact by exchanging massless vector bosons (wiggly line) that are referred to as gluons. They carry SU(3) quantum numbers and couple to all flavours of quarks with equal strength proportional to the gauge coupling g .

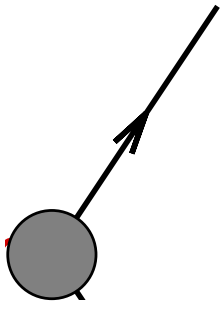
QCD is thus an extremely predictive theory. It is also difficult to work out so that only too often ad hoc approximations need to be made before theory and experiment can be compared. Precision tests of QCD are therefore still rare, and complex strong interaction phenomena (such as those observed in heavy ion collisions) will probably never be explained from first principles.

1.1 Quark confinement & asymptotic freedom

The Feynman rules derived from the QCD lagrangian suggest that the quarks are weakly interacting with each other by exchanging massless vector bosons (see fig. 1). Similar to an exchange of photons, the forces that result from this type interaction fall off like $1/r^2$ at large distances r , and the energy required to break up a quark-antiquark bound state is hence finite. Quarks have, however, never been observed in isolation nor is there any experimental evidence for massless vector bosons other than the photon.

An important hint to the solution of the puzzle comes from perturbation theory itself. Once higher-order corrections are included, it turns out that the strength of the interactions mediated by the vector bosons depends on the magnitude q of the energy-momentum that is transferred between the quarks. Explicitly, if we introduce an effective coupling

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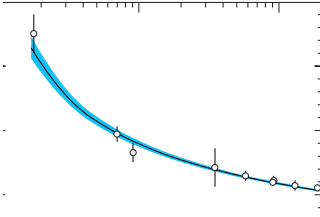


Fig. 2. The experimentally measured values of the effective gauge coupling $\alpha_s(q)$ confirm the theoretically expected behaviour [eq. (1.3)] at high energies (compilation of the Particle Data Group [?]).

$$g(q) = \tag{1.2}$$

where the shaded circle stands for the sum of all vertex diagrams with all possible exchanges of virtual quarks and vector bosons, it can be shown that [?,?]

$$\alpha_s(q) \equiv \frac{g(q)^2}{4\pi} = \frac{c}{\ln(q/\Lambda)} + \dots \tag{1.3}$$

for large momenta q and some calculable constant c . The logarithmic decay of the coupling (which is referred to as *asymptotic freedom*) is actually observed in high-energy scattering experiments (see Fig. 2), and from such measurements the value of the mass scale Λ in eq. (1.3) was determined to be 213^{+38}_{-35} MeV [?] †.

The fact that the gauge coupling is weak at high energies implies that perturbation theory will, in general, be reliable in this regime. On the other hand, as we move towards the other end of the energy scale, the expansion breaks down at some

† The quoted value of Λ refers to a particular definition of the effective coupling that is known as the “ $\overline{\text{MS}}$ scheme of dimensional regularization”.

point and the physical picture associated with the Feynman diagrams consequently becomes invalid. An immediate conflict between theory and the non-observation of isolated quarks is thus avoided.

1.2 Lattice formulation

It remains to be shown, however, that quark confinement is indeed a property of QCD. Moreover, once this is achieved, computational tools need to be developed to determine the basic properties of the quark bound states such as the pions, the kaons and the nucleons.

The lattice formulation of QCD was introduced many years ago as a framework in which these issues can be addressed [?]. Introductory texts on the subject are refs. [?{?}], for example, and to find out about the most recent developments in the field, the proceedings of the yearly lattice conferences usually provide a good starting point [?].

Very briefly lattice QCD is obtained by replacing the four-dimensional space-time continuum through a hypercubic lattice and by restricting the quark and the gauge fields to the lattice points. The expression for the lagrange density (1.1) then needs to be discretized in a sensible way, and the precise relation between the correlation functions calculated on the lattice and the physical quantities of interest must be understood. A few key elements of this construction are

- { The gauge symmetry can be fully preserved, and no additional unphysical degrees of freedom are thus introduced.
- { In general the details of the discretization become irrelevant in the continuum limit, i.e. any reasonable lattice formulation will give the same continuum theory up to finite renormalizations of the gauge coupling and the quark masses.
- { Lattice QCD admits an expansion in Feynman diagrams that coincides with the usual expansion up to terms proportional to the lattice spacing. The consistency of the lattice theory with the standard perturbative approach to QCD is thus guaranteed.

A last point to be mentioned here is that the lattice provides a regularization of the ultra-violet divergences that are usually encountered in quantum field theory. The lattice theory is, therefore, mathematically well defined from the beginning.

1.3 Numerical simulations

The application of numerical simulation methods to solve the theory has been an interesting perspective since the early days of lattice QCD. Today quantitative results

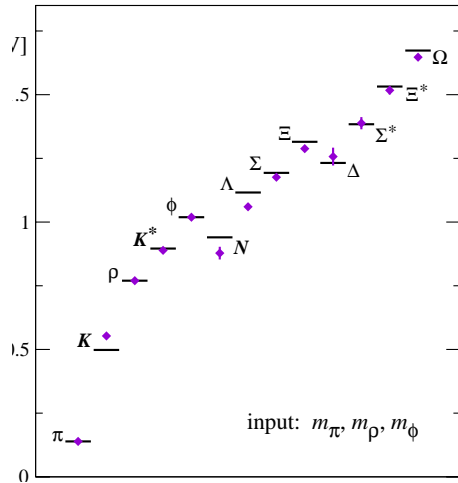


Fig. 3. Recent calculations of the hadron masses m_h (data points) in lattice QCD agree quite well with the observed spectrum (horizontal lines) [?].

are practically all based on such numerical studies.

In the course of these calculations the fields have to be stored in the memory of the computer, and only lattices of limited size can thus be simulated. The progress in computer technology allows the lattice extents to be doubled in all directions roughly every 8 years. At present lattices as large as 128×64^3 can be accommodated on (say) a commodity PC cluster with 128 nodes. The simulation then proceeds by generating a representative ensemble of fields through a stochastic process. Eventually the physical quantities are extracted from ensemble averages of products of gauge-invariant local fields.

In general numerical simulations have the reputation of being an approximate method that mainly serves to obtain qualitative information on the behaviour of complex systems. This is, however, not so in lattice QCD, where the simulations produce results that are exact (on the given lattice) up to statistical errors. The systematic uncertainties related to the non-zero lattice spacing and the finite lattice volume then still need to be investigated, but these effects are theoretically well understood and can usually be brought under control.

Lattice QCD is being used to compute a wide range of physical quantities, including the hadron mass spectrum (e.g. 3), decay constants, form factors and weak transition matrix elements. The technique is not universally applicable, however, and quantities like the inelastic proton-proton scattering cross-section or the nucleon

structure functions at small angles remain inaccessible.

2. Quark confinement

As can be seen from fig. 3, there is currently no perfect match between experiment and the lattice calculations. The experts are not alarmed by this, since the computations are still incomplete in certain respects. However, rather than going into any details here, we now turn to the more fundamental question of quark confinement.

2.1 Static quark potential

Quarks carry SU(3) quantum numbers and are thus sources of the gauge field. As a consequence the latter exerts a force on the quarks, since any change in their positions implies a change in field energy. According to the current understanding, the confinement of quarks is associated with an unbounded increase of the field energy at large quark separations.

The ground state energy of the gauge field hamiltonian in the presence of a static quark-antiquark pair separated by a distance r is referred to as the static quark potential $V(r)$. There are various ways to compute $V(r)$ on the lattice. Perhaps the most elegant approach is to consider Wilson lines that wind around a cylindrical space-time manifold (see fig. 4). The correlation function of any two such loops can be shown to satisfy

$$\langle P(r)P(0)^* \rangle_{T \rightarrow \infty} = e^{-TV(r)} \{1 + O(e^{-T\epsilon})\}, \quad \epsilon > 0, \quad (2.1)$$

where T denotes the circumference of the cylinder, and the potential can thus be determined by calculating the correlation function.

Some recent results for the potential $V(r)$ and the force $V'(r)$ are plotted in fig. 5. They show that $V(r)$ is monotonically rising and eventually grows linearly with a small correction proportional to $1/r$. The force is fairly strong, at least 1 GeV/fm in the whole range of distances, and if this continues to be so at larger values of r it will evidently not be possible to separate the quark-antiquark pair. At short distances, on the other hand, the data points rapidly approach the curves that are obtained in perturbation theory (as it has to be since the effective gauge coupling is small in this regime).

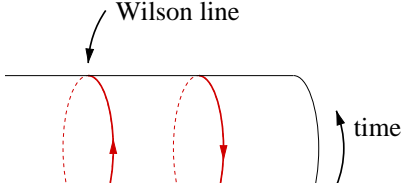


Fig. 4. Polyakov loops are Wilson lines that wind around the space-time manifold in the time direction. In eq. (2.1) we consider the correlation function of two Polyakov loops with opposite orientation that are separated by a distance r in space.

2.2 String model

The data shown in the second plot in Fig. 5 suggest that the force $V'(r)$ approaches a constant $\sigma \simeq 1.06 \text{ GeV/fm}$ at large quark-antiquark separations. σ is referred to as the string tension, because a constant force is what would be obtained if the quarks were held together by an elastic string.

The idea that quark confinement is linked to the formation of string-like flux tubes has in fact been around for very many years. We should then not only see the linear rise in the static potential but also a characteristic $1/r$ correction that derives from the zero-point energy of the transversal string vibrations. Explicitly the prediction is that [?,?]

$$V(r) \underset{r \rightarrow \infty}{=} \sigma r + \mu - \frac{\pi}{12r} + \mathcal{O}(r^{-2}), \quad (2.2)$$

where (from the string theory point of view) σ and the mass μ are free parameters.

The string picture may appear to be somewhat naive, but the simulation data for the second derivative of the static potential shown in Fig. 6 agree very well with eq. (2.2). What is plotted there is the dimensionless combination $-\frac{1}{2}r^3V''(r)$, which, according to string theory, should converge to $\frac{\pi}{12}$ at large r . If we allow for a small higher-order correction proportional to $1/r$, the data are perfectly compatible with this.

An even better matching between string theory and the gauge theory is observed in three space-time dimensions. In this case a string with fixed ends can only vibrate

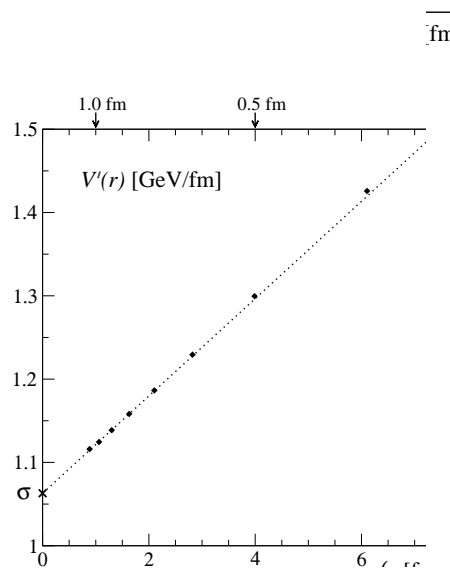
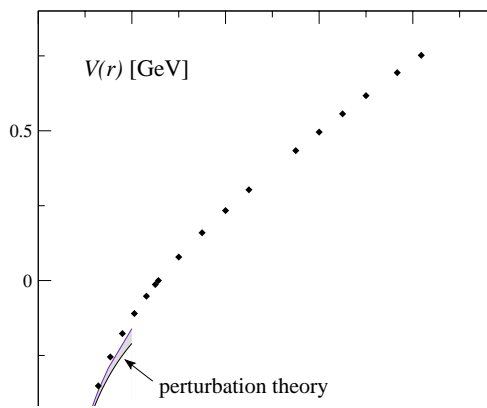


Fig. 5. Simulation results for the static potential $V(r)$ [?] and the force $V'(r)$ [?]. The statistical and systematic errors in these calculations are smaller than or at most equal to the size of the data symbols.

in one transversal direction and the associated zero-point energy is consequently reduced by a factor 2. This is exactly what one finds on the lattice when the three-dimensional gauge theory is simulated (points and curves in the lower half of fig. 6).

2.3 Summary

The lattice studies conducted so far leave little doubt that the quarks are confined

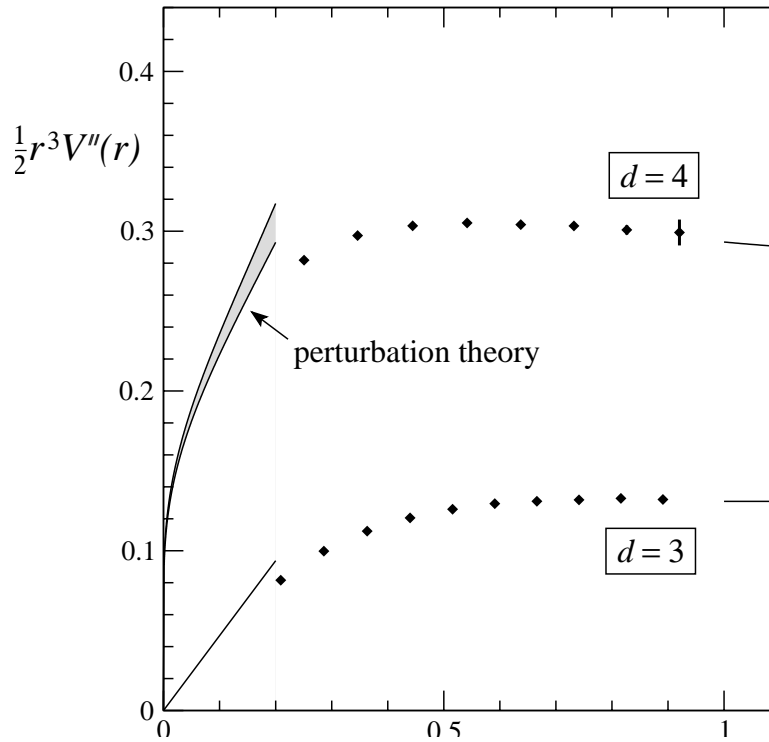


Fig. 6. Simulation results for the second derivative of the static potential in $d = 4$ space-time dimensions (upper curves and data points) and in three dimensions [?].

because the field energy of the surrounding SU(3) gauge field rises linearly at large distances. As far as the static potential is concerned, we have also seen that the behaviour of the gauge theory in this regime is accurately described by an effective string model. This correspondence is, incidentally, expected to extend to the confinement phase of other gauge field theories [??] and to a range of other observables such as the spectrum of excited states in the presence of static quarks [?,?].

3. QCD from low to high energies

As explained above, lattice QCD allows us to study the phenomenon of quark confinement and to compute the basic properties of the light mesons and of the nucleons. Among the most obvious quantities to consider in this low-energy regime are the mass m_π of the charged pions and the pion decay constant f_π . Experimentally the latter is determined by measuring the decay rate $\pi^+ \rightarrow \mu^+ \nu_\mu$, while in QCD it can be expressed as a matrix element

$$\langle 0 | A_\mu | \pi^+ p \rangle = i p_\mu f_\pi \quad (3.1)$$

of the appropriate axial quark current A_μ between the vacuum state and the one-pion state with four-momentum p .

The experiments at the big particle colliders, on the other hand, probe the interactions of the quarks and gluons at high energies (from 10 to 100 and more GeV), where asymptotic freedom has set in and perturbation theory may be applied to calculate the reaction rates. The hadronic decay width of the Z {boson, for example, is given by

$$\Gamma_{Z \rightarrow q\bar{q}} = \text{constant} \times \left\{ 1 + \frac{\alpha_s}{\pi} + \mathcal{O}(\alpha_s^2) \right\}, \quad (3.2)$$

where α_s denotes the gauge coupling (1.3) at momentum transfer q equal to the mass of the Z {boson and the constant includes the (calculable) contributions of the weak and electromagnetic interactions.

3.1 Connecting different energy regimes

From a purely phenomenological point of view, it seems unlikely that there is any connection between (say) the pion mass and the Z {boson decay rate. However, since all strong interaction physics is described by the same underlying field theory, there have to be at least some such relations.

To make this a bit more explicit, first note that in QCD any physical quantity is a function of the parameters that appear in the lagrangian (1.1). The gauge coupling g is one of them, but for the following discussion it is actually more natural to consider the scale Λ in eq. (1.3) to be a basic parameter of the theory. We then infer that there are functions G and F such that

$$m_\pi^2 / f_\pi^2 = G(m_u / \Lambda, m_d / \Lambda, \dots), \quad (3.3)$$

$$f_\pi / \Lambda = F(m_u / \Lambda, m_d / \Lambda, \dots), \quad (3.4)$$

and for the masses of the kaons and the heavier pseudo-scalar mesons similar equations can be written down.

Now if we take the experimental values of the meson masses in units of the pion decay constant as input, the equations for the meson masses can be solved for the quark masses (in units of m_π) and the ratio f_π/m_π then becomes a calculable quantity. Note that this ratio links the physical properties of the pions to the Λ_{QCD} parameter, which is a characteristic scale in the high-energy regime of QCD. Since f_π/m_π is also known experimentally, an interesting test is thus obtained that will only be passed (barring miracles) if QCD is the correct theory at all energies.

3.2 The scale problem

In lattice QCD the calculation of f_π/m_π appears to be a difficult task, because f_π and m_π are physical quantities that refer to the properties of the theory at energies orders of magnitude apart. A straightforward approach then requires the simulation of lattices with a very large number of points.

It is not difficult to obtain an estimate of what would be needed. For the computation of f_π and the meson masses, the spatial lattice size L should be at least 2 fm as otherwise there will be sizeable finite-volume effects. The effective gauge coupling $\alpha_s(q)$, on the other hand, can only be reliably determined at momenta q up to $1/a$ or so (where a denotes the lattice spacing). Moreover, to be able to extract f_π from the asymptotic behaviour (1.3) of the coupling, q must be taken to values deep in the high-energy regime of QCD. The combination of all these requirements then implies that the number L/a of lattice sites in each direction has to be on the order of 100 or maybe even larger than this.

3.3 Finite-size scaling

Such lattices may become accessible at some point, but it is much more efficient to adopt a recursive scheme, where the large scale difference is bridged by a sequence of matching lattices [?] (see ref. [?] for an introduction to the subject). The key idea is to introduce an effective gauge coupling $\alpha(q)$ that measures the interaction strength at a momentum q proportional to $1/L$. In this way the finite lattice size becomes a device to probe the interactions rather than being a source of systematic errors.

There are many ways to define an effective coupling of this kind. We may choose some particular boundary conditions, for example, and take the response of the system to a change in the boundary values of the fields as a measure for the interaction strength [?]. The important point to note is that the final results (such as f_π/m_π) do not depend on any of these details.

$$= L_0, a = a_0$$

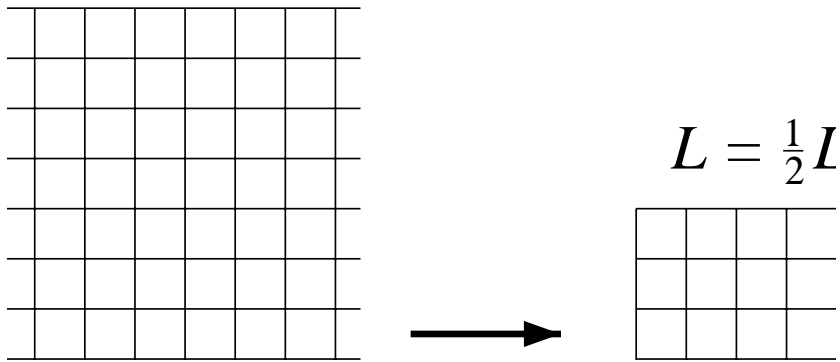


Fig. 7. Finite-size scaling amounts to the construction of a sequence of matching lattices with lattice spacings $a = 2^{-k} a_0$ and decreasing physical sizes L .

The next step is to construct a sequence of lattices with lattice spacings a and sizes L that decrease by factors of 2 as shown in Fig. 7. Starting with some physically large lattice, it is possible to scale the lattices to very small sizes in this way without running into technical difficulties. The coupling $\alpha(q)$ (the one discussed above that is defined at some q proportional to $1/L$) can be calculated on each of these lattices and its evolution can thus be followed over a wide range of momenta.

3.4 Simulation results

So far such computations have been performed in the pure gauge theory and in QCD with two flavours of quarks. As can be seen from Fig. 8, the momentum dependence of the coupling $\alpha(q)$ that has been studied is accurately matched by perturbation theory already at fairly low momenta. Contact with the asymptotic behaviour (1.3)

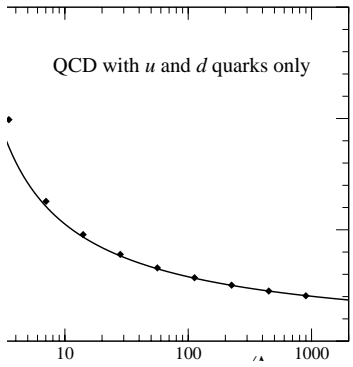
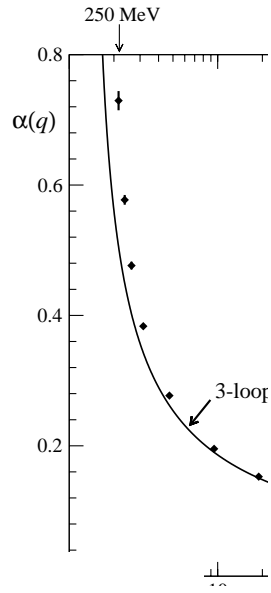


Fig. 8. Momentum-dependence of the effective gauge coupling (in a particular finite-volume scheme) in the pure SU(3) gauge theory [?–?] and in QCD with two flavours of massless quarks [?].

of the coupling can thus easily be made, and since also the low-energy regime is safely reached, these calculations provide the desired link between that regime and the parameter.

For the full theory, with all flavours of quarks properly included, a similar study has not yet been made. The reason partly is that these calculations are exceedingly

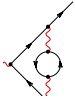


Fig. 9. In the language of Feynman diagrams, quark polarization effects are represented by subdiagrams with closed quark lines. For technical reasons, many results in lattice QCD still do not include these contributions.

expensive in terms of computer time, because the available simulation techniques become very inefficient once the quark polarization effects are taken into account (e.g. Fig. 9). We shall return to this issue in a moment and only note at this point that practically all applications of lattice QCD meet the same difficulty.

Since they are often not very large, it is, however, a sensible and still widely used approximation to neglect the quark polarization effects. The calculations of the pion decay constant and of the pseudo-scalar meson masses that are required to obtain f_π/m_π can then be carried out with the presently available computer resources (see refs. [1,2] for example). As already mentioned, the lattices should be at least 2 fm wide in these computations, but this is not a problem here because the lattice spacing does not need to be extremely small at the same time. Values from 0.05 to 0.1 fm have actually been found to be adequate in this context.

Once all this is done, and a careful analysis of the systematic errors is made, the combination of the results yields the value [1,2]

$$f_\pi/m_\pi = 0.56 \pm 0.05. \quad (3.5)$$

This figure agrees with the experimental number $f_\pi/m_\pi = 0.62 \pm 0.10$ within the quoted errors, which is somewhat unexpected since the quark polarization effects have been neglected. Maybe the ratio is not strongly affected by them, but there is currently no very good theoretical argument for this and the coincidence can, therefore, not be taken as a solid confirmation of QCD at this point. The computation nevertheless provides important insights into how precisely the low- and the high-energy regimes of the theory are connected to each other, and it also shows the potential of the lattice approach to lead, in due time, to some very stringent tests of QCD.

3.5 Real-world lattice QCD simulations

At present the great challenge in lattice QCD is to devise efficient simulation methods for the full theory (including quark polarization effects) that will work well on large lattices and at small quark masses. The fact that the currently available techniques will not lead very far became particularly clear at the lattice conference last year in Berlin [?], where an effort was made to assess the cost of such calculations.

The figure that is usually quoted in this context is the number of arithmetic operations that are required to generate the next statistically independent field configuration. An approximate and mostly empirical formula that was presented at the conference is [?]

$$\frac{\# \text{ operations}}{\text{field configuration}} \simeq 3.3 \left[\frac{140 \text{ MeV}}{m_\pi} \right]^6 \left[\frac{L}{3 \text{ fm}} \right]^5 \left[\frac{0.1 \text{ fm}}{a} \right]^7 \text{ Tflops year}, \quad (3.6)$$

which shows the dependence on the lattice parameters and on the calculated value m_π of the pion mass (which depends on the specified values of the quark masses). The result is given in Tflops years, the number of operations that a computer with a sustained speed of 1 Tflops (10^{12} floating-point operations per second) performs in 1 year of running time.

While such machines will become available to the lattice community in the near future, the poor scaling behaviour of the algorithms (the high powers in the formula) tells us that it will not be possible to vary the lattice parameters over a wide range. If the lattice spacing is decreased by a factor of 2, for example, the simulation time goes up by a factor of 128 or so. Evidently this unfavourable situation calls for new algorithmic ideas, and a significant investment in purely technical R&D work will be required in the coming years to solve the problem.

4. Conclusions

Lattice QCD was introduced nearly 30 years ago and it has since then turned into a powerful quantitative approach to the physics of the strongly interacting particles. Only a few topics have been touched in this talk, but this should not hide the fact that the technique is being used to calculate many quantities of phenomenological interest (hadron masses, decay constants, transition matrix elements, and so on) and also to study some of the more fundamental issues such as the breaking of chiral symmetry and the phase diagram at non-zero baryon density.

All this work has had its share in making QCD the unique candidate of the theory of the strong interactions. In particular, little doubt is left that the non-linearities of the dynamics of the SU(3) gauge field are responsible for the confinement of the quarks. Moreover we have seen that quark confinement and asymptotic freedom are just two complementary aspects of the theory. The fact that the relation between the parameters in the lagrangian and the basic properties of the mesons and nucleons can be worked out on the lattice is the key to showing this, along with the ability to compute the (non-perturbative) evolution of the effective gauge coupling from very low to high energies.

Currently the quark polarization effects are often neglected in the numerical simulations because their inclusion slows down the computations by a large factor. It is mainly for this reason that comparisons of the lattice results with experimental numbers cannot at present be regarded as hard tests of QCD. Once this technical limitation is overcome, it is clear, however, that precision tests will become a reality, and the hope of the experts is that this will happen before the next 30 years have elapsed!

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