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THE STRONG FORCE

Simulation of Quarks and Gluons

ELEMENTARY PARTICLE PHYSICS

The standard model of elementary particles accurately describes our present view of the laws of nature on the smallest resolvable scale. It is briefly summarized in this article. In particular we focus on the theory of strong interactions and describe the technique of computer simulation necessary to reveal some of the predictions of this theory that physicists need to compare with experimental results.

The world of quarks in the standard model of elementary particles

Our present understanding of the structure of matter reaches down to resolutions of about 10^{-16} cm accessible to the presently largest particle accelerators. Experiments at CERN, DESY, Fermilab and other laboratories tell us that the main constituents are fermions with spin one-half: quarks and leptons (see Tab. 1). They interact with each other and with their anti-particles through the exchange of gauge bosons: photons, W- and Z-bosons mediating the electro-weak force (electromagnetism, radioactive decay etc.) on the one hand and gluons responsible for the strong force on the other (see Tab. 2). The latter binds quarks into a large variety of mesons and baryons the most prominent representatives of which are the proton and the neutron as the main constituents of atomic nuclei (see Tab. 3). The existence of three symmetric families of quarks and leptons is experimentally well established. The only missing particles – within the framework of the standard model – are the quanta of the Higgs field whose interaction is responsible for non-vanishing masses of particles. There are good reasons to believe that the standard model is not the end of the story. For example the idea of supersymmetry which relates fermions with bosons and predicts a characteristic pattern of additional (still undiscovered) particles is very exciting. Moreover, the unification of all forces including a consistent quantum theory of gravity has been puzzling physicists since many decades (see the contribution of J. Erdmenger).

quarks			leptons		
u (0.004)	c (1.5)	t (174)	ν_e (??)	ν_μ (??)	ν_τ (??)
d (0.007)	s (0.15)	b (4.7)	e (0.0005)	μ (0.1)	τ (1.8)

Tab. 1
The families of fermionic particles which constitute the fundamental building blocks of matter within the standard model of elementary particle physics. Their masses in units of GeV are quoted in parentheses.

gauge particles	forces	acting on	responsible for
gluons	strong	quarks	stability of nuclear matter
photons, W and Z bosons	electroweak	quarks and leptons	electromagnetism, nuclear reactions
gravitons	gravitational	all particles	stability of stellar systems

Tab. 2
The gauge particles mediating the fundamental interactions under the gauge group SU*(3) x* SU*(2) x* U*(1).*

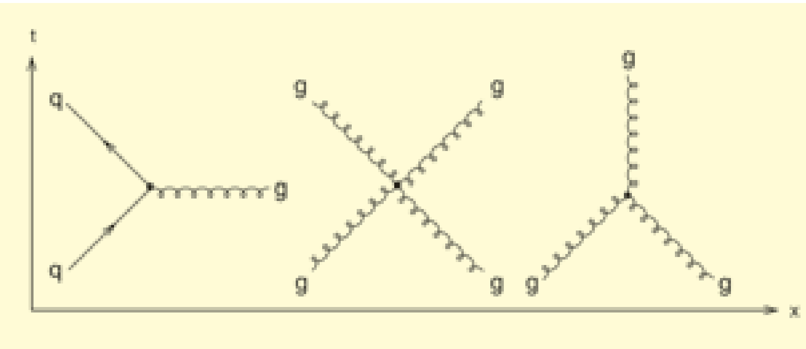

Fig. 1
The interaction vertex diagrams of QCD. Straight lines correspond to the time development of (anti) quark states (q), whereas wiggled lines represent the propagation of gluons (g).

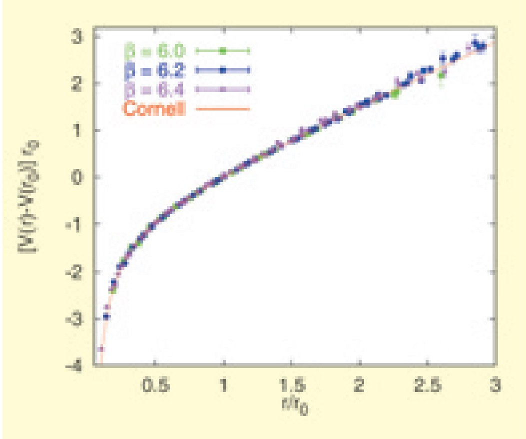

Fig. 2
Potential between an idealized static quark-antiquark pair obtained from Monte Carlo simulations of (quenched) lattice QCD in comparison with the successful phenomenological Cornell heavy quark potential ($r_0 \simeq 0.5$ fermi) [2].

In this contribution we want to restrict ourselves to the strong force, the main research field of the teams *Theory of Elementary Particles/Phenomenology* and *Computational Physics* of the Department of Physics (see the related contribution of our experimental colleague N. Pavel).

The strong force is successfully described by one of the main building blocks of the standard model – *quantum chromodynamics* (QCD). At a first view it looks very similar to quantum electrodynamics (QED). As the exchange of photons generates the electromagnetic force between electrically charged particles the gluon exchange *glues* the quarks together. In Fig. 1 we show interaction vertices of so-called Feynman diagrams which visualize the elementary interactions between quarks and gluons. Such graphical elements are assembled according to well-defined rules and then correspond to mathematical expressions yielding approximate predictions of the theory called perturbation theory. The name derives from the fact that one computes corrections to an idealized (»unperturbed«) theory where particles do not scatter or interact at all. At first sight this seems a very paradoxical starting point for strong interaction physics. Quite remarkably, due to a property named asymptotic freedom, it is nevertheless possible to approximate QCD for scattering processes in the limit of large momentum transfer*. In this limit the effective interaction strength – the coupling constant – gets sufficiently small and the answer emerges in a few diagrams. The vertex diagram on the left in Fig. 1 occurs in both QED and QCD. In the one case it signifies the coupling of photons to electric charge, in the other gluons interact with a mathematically more complicated charge called colour. It corresponds to the generalization of complex phase factors typical for QED to the non-commuting matrices of the non-Abelian group $SU(3)$. The more elaborate colour symmetry necessitates self-interactions of the gluons as shown in the other diagrams which are the reason for the different behaviour of the mediated force compared with the electromagnetic Coulomb force. Although the quark force behaves very similarly at small distances it becomes constant at large distances until there is enough energy to produce new quarks and anti-quarks which shield the colour charge of the original ones. This behaviour of the force or of the corresponding potential explains why quarks behave as weakly bound when they are close together (below 10^{-14} cm), whereas they interact very strongly and remain confined at long distances (above 1 fermi $=10^{-13}$ cm}. The potential computed for an idealized infinitely heavy quark-antiquark pair is drawn in Fig. 2. It explains why quarks are not observed as isolated particles. Unfortunately, the linearly rising part of the potential cannot be obtained from the mentioned perturbation theory which in the case of QED has provided numbers for many (quantum) electromagnetic properties of matter with an unprecedented precision and in agreement with experiment. Perturbation theory as an approximation scheme breaks down when the coupling constant becomes large i.e. of the order of one. In QCD this happens at long distances or, what is equivalent, at small momentum transfer. Perturbation theory also fails if we want to compute the masses and other features of the hadrons as bound states of the (anti)quarks.

»Starke Wechselwirkung« und Computersimulation
Das Standardmodell der Elementarteilchenphysik beschreibt unser gegenwärtiges Verständnis der Naturgesetze bei den kleinstmöglichen, heute experimentell auflösbaren Ausdehnungen. In diesem Artikel beschreiben wir zunächst kurz die Grundzüge des Standardmodells, konzentrieren uns sodann auf die Theorie der starken Wechselwirkungen, ehe wir auf die Technik der Computersimulation eingehen. Sie erlaubt es, wichtige, mit dem Experiment vergleichbare Vorhersagen der Theorie zu extrahieren.

hadron states			(anti)quark constituents
baryons	(anti)proton	$p,\ \bar{p}$	$u\,u\,d,\ \bar{u}\,\bar{u}\,\bar{d}$
	(anti)neutron	$n,\ \bar{n}$	$u\,d\,d,\ \bar{u}\,\bar{d}\,\bar{d}$
	strangeness-1 baryon	Λ	$u\,d\,s$
	…		…
mesons	pion	$\pi^+,\ \pi^-,\ \pi^0$	$u\,\bar{d},\ \bar{u}\,d,\ (u\,\bar{u}-d\,\bar{d})/\sqrt{2}$
	K meson	$K^+,\ K^-,\ \cdots$	$u\,\bar{s},\ \bar{u}\,s,\ \cdots$
	…		…
	D meson	$D^+,\ D^-,\ \cdots$	$c\,\bar{d},\ \bar{c}\,d,\ \cdots$
	…		…

Tab. 3
A few examples for hadronic states and their (anti)quark constituents.

But QCD can also be viewed as a summation over all possible oscillation modes of the gluon and (anti)quark fields weighed with appropriate quantum probability-amplitudes. This so-called path integral representation was invented first by N. Wiener to describe the stochastic Brownian motion of classical particles. It has been generalized by R. P. Feynman and others as a very general way to formulate a quantum(field) theory. The path integral is an in principle infinite dimensional integral over all field values at all possible space-time points. Within this framework particle properties can be predicted by evaluating such integrals. There are many attempts to derive quark confinement and other particle properties from approximation procedures for the path integral that go beyond perturbation theory. The most promising approach, which is »first principles« in using no further model assumptions and can be systematically improved in precision, is QCD on a lattice described in the next section. This has become a research field of its own with a large annual international symposium. *Lattice 2001* actually took place at our university [1] with about 400 participants.

Field theory of quarks and gluons on the computer
In principle the arena where we want to solve the QCD path integral is the infinitely extended four-dimensional space-time continuum, as no experimental sign of any »granularity« has been found. On the other hand on a computer only strictly finite problems can be handled. One therefore needs a truncation of the problem which distorts physical results in a negligible way only. One truncation consists of a finite volume of size L, where the simulated section of »the world« ends. Here our intuition is confirmed by the finding that results quickly become insensitive to the precise value L as soon as it is significantly larger than all scales in our problem. In QCD simulations L is usually a few fermi large. The other truncation affects the resolution. In a continuum of volume L^4 there are still infinitely many points. We therefore introduce a spacing a between neighbouring points that we decide

** That quarks behave asymptotically free has been derived first by the american theoreticians D. J. Gross, F. Wilczek and independently by H. D. Politzer in 1973. For this discovery they have been awarded with the Nobel price in physics this year.*

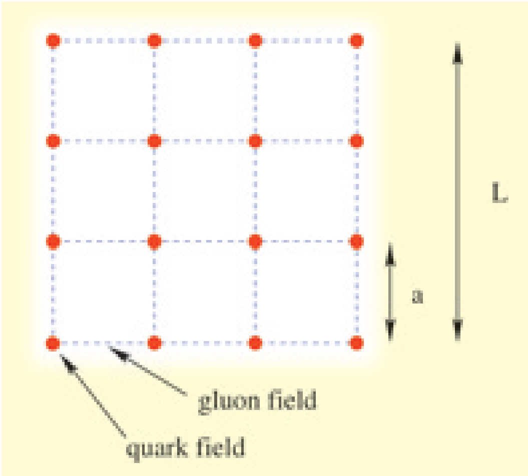

Fig. 3
Two dimensional lattice with quark fields on sites and gluon fields on connecting links.

to keep track of in a simulation. Now fields only exist on the $N = (L/a)^4$ points or sites that we restrict our attention to. A two dimensional (analog) image of the resulting structure is shown in Fig. 3. Such a discretization by a computational grid is in fact used in many places in physics like for instance simulations in fluid dynamics, meteorology or engineering. A continuum limit, where details of the grid become irrelevant, is reached when the relevant field configurations sampled on the grid vary only little over one discretization length a (see Fig. 4 for an illustration). Both truncations introduce errors in physical results that have to be controlled and bounded by varying a and L. Typical discretizations reached in present QCD simulation are a~0.1 fermi. Then there are N~10^6 lattice points with a certain number of field variables per point and the path integral is approximated by a ~10^7-fold integral.

Standard numerical integration methods like for instance the Simpson rule are not suitable for such high dimensional integrals. One has to exploit the fact

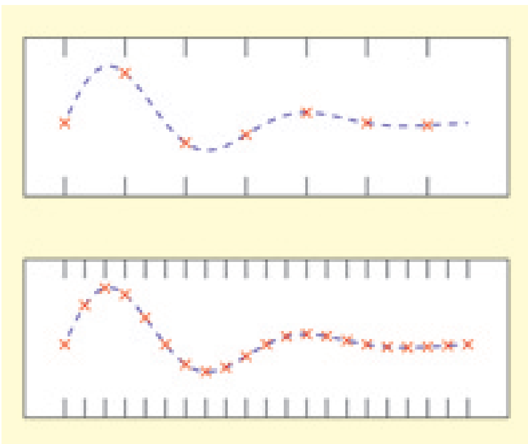

Fig. 4
Discretized sampling of a continuous field with improving resolution.

that very many degrees of freedom also lead to simplifications. This may be compared to the thermodynamics of a gas. Although the phase space of a large number of gas molecules is enormous, in practice most configurations are so unlikely that they can be neglected. Thermodynamics identifies such »equilibrium« configurations and allows for predictions inspite of the complexity of the underlying problem. Similarly the Monte Carlo method stochastically (hence the name) generates a relatively small number of K~100 … 10^6 »typical« lattice field configurations from which the desired physics can be extracted. Here an additional statistical error of the usual form ~$1/\sqrt{K}$ occurs. The look and feel of such computations resembles very much experiments where »data are taken«, »statistics is improved« and systematic errors have to be estimated. Hence one hears lattice theorists talk about »measuring quantities on the lattice« referring to the computer instead of an accelerator. For a given CPU power and computer architecture available one has to pick a lattice size and simulation parameters to minimize the combined error resulting from $a > 0$, $L < \infty$, $K < \infty$. This leads to very high computational demands which explains why lattice projects are often found on the largest parallel computers available. It also motivates that a significant effort of the community goes into research on the improvement of simulation techniques and algorithms with the goal of producing more physical information for a given number of CPU operations.

Coupling constants and quark masses

We now want to take a closer look at the perturbative evaluation of QCD in the limit of high energy. Typical physical theories contain a few »free« parameters that have to be determined experimentally and only thereafter the remaining phenomena in the domain of validity of the theory can be predicted (in principle). As an example one may think of first determining Newton's gravitational constant and then predicting planetary motion. In high energy perturbative QCD one has to take one process, for instance electron-positron scattering, to determine an effective coupling $\bar{g}^2(\mu)$ at some high energy scale μ. In addition, for each of the six quark species, one needs to fix one additonal similar parameter related to their masses. Then a host of other high energy processes has been successfully computed by Feynman diagrams and this constitutes the predictive power of perturbative QCD. As mentioned, for lower energies in the realm of typical hadronic masses (1 GeV) we have to resort to lattice simulations. Here the same number of parameters in the theory has to be adjusted, before predictions can start. Typically, masses in the hadronic spectrum or decay rates are used. So far this looks like two independent theories probed against experiments. Since QCD however is *one* theory for *all* energies, it should be possible to relate one parameter set with the other.

This is precisely the task that the ALPHA collaboration, of which the Humboldt-Universität zu Berlin Computational Physics group forms an important part, has decided to address: we want to compute couplings and quark mass-parameters at high energy *in terms of hadronic quantities*. In this way the whole perturbative sector gets connected to low energy QCD, and the parameters computed are compared to those previously taken from experiment.

Since this calculation involves high and low energies at the same time, a numerical approach is called for. For the same reason this is a particularly challenging numerical problem, since two different physical scales are involved: $E_{\text{hadronic}} \ll E_{\text{perturbative}}$ in addition to the lattice spacing a small and the size L large enough compared to either of them. ALPHA has developed a special so-called step-scaling technique to cope with this [3]. It allows to break up the large scale ratio between $E_{\text{perturbative}}$ and E_{hadronic} into many steps, where only ratios of two in scale have to be managed at one time and the continuum limit is taken for each step. The limited space here does not allow for a more detailed description of the method which has found applications also in several similar problems in the meantime. A key result is shown in Fig. 5 where we see the evolution of a coupling constant over a large range of energies, such that this quantity allows to connect the perturbative with the hadronic sector.

Although very encouraging results have emerged, the project is not yet complete to a degree that allows for a serious comparison with experiment. A complete calculation exists in the quenched approximation [4]. This is a simplified programme that still neglects the creation of virtual quark pairs. The reason for such a pilot study is, that, while it exhibits most of the potential problems, it requires a large factor of 100 or so less compute-power than dynamical simulations that include the mentioned effects of vacuum polarization. Such simulations require a detailed study of algorithmic optimization, which has been conducted. The energy dependence of the coupling has been traced including virtual pairs of the most important lightest quark species [5]. What is still missing is the connection of its low energy behaviour with physical hadronic quantities which requires further extended simulations planned for the near future.

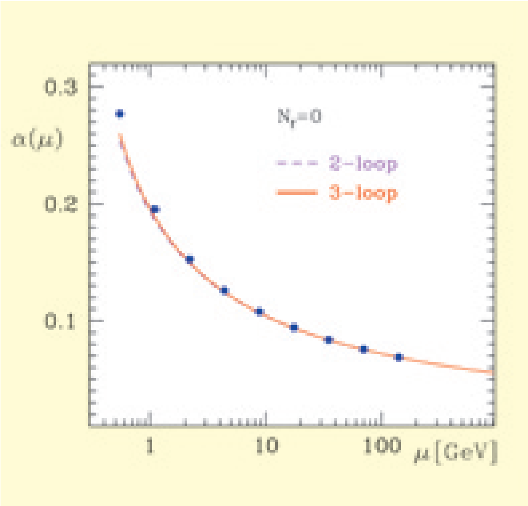

Fig. 5
Energy dependent coupling strength. Points are numerical results, lines derive from perturbative calculations.

The complicated QCD vacuum: quark condensation and confinement

The lattice approach to QCD in combination with numerical simulations allows also structural investigations of the quantized field theory itself.

Non-Abelian gauge theories, in particular QCD, are characterized by a complicated ground state which can be represented by an infinite superposition of gauge-nonequivalent vacuum states mathematically classified by a topological winding number related to a non-trivial homotopy group. Quantum vacuum expectation values of gauge field or quark operators have to take into account the tunnelings between these topologically distinct vacua. Many theorists are convinced that the complicated vacuum structure is the main reason for quark confinement and for the spontaneous breaking of a symmetry of the classical QCD Lagrangian at zero quark masses: the so-called chiral symmetry. This symmetry breaking becomes manifest through a non-vanishing vacuum expectation value $\langle 0|\bar{q}q|0\rangle$ for the spin-half quark fields $q(\chi)$, the »quark condensate« and causes the pseudoscalar mesons like the pion to appear as Goldstone bosons with comparatively small masses. In the Euclidean path integral approach the above mentioned tunneling amplitudes can be semiclassically approximated with the help of classical solutions interpolating between the different vacuum gauge fields: the so-called pseudo-particle solutions or instantons or calorons, the latter are relevant for the case of quark-gluon matter at non-zero temperatures. On the lattice such solutions can be found by successively minimizing the gauge field action functional starting from Monte Carlo generated quantum equilibrium gauge fields. However, whereas these classical solutions do provide a model for chiral

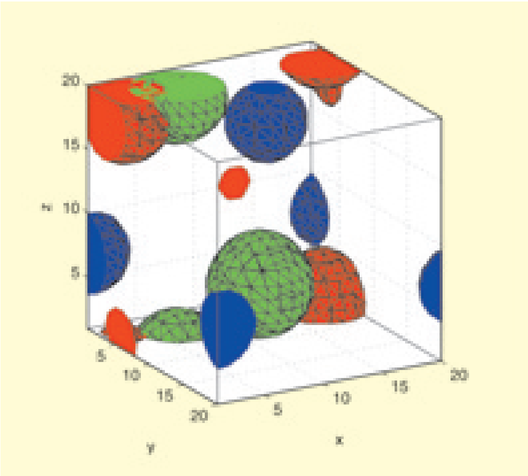

Fig. 6
Isosurface plot for the zero-mode densities of the lattice (improved) Dirac operator (different colours correspond to varying boundary conditions of the fermion fields in Euclidean time direction) shown for a caloron configuration with non-trivial holonomy of topological charge Q_t=2 consisting of 6 monopoles [8].

symmetry breaking, they are not seen to be the source of quark confinement. Our own very recent lattice reinvestigations have shown that the relevant (approximate) solutions differ from the ones used so far in the semiclassical approach by a mathematical property called *holonomy*. The latter characterizes the behaviour of the localized pseudo-particle solutions at spatial infinity. Special solutions of this kind have been constructed a few years ago by T. C. Kraan and P. van Baal (KvB). Within a project supported by the DFG-Forschergruppe *Lattice Hadron Phenomenology* we were able to show that non-trivial holonomy indeed plays an important role and that the semiclassical approach should hence be reconsidered [6]. It is most interesting that the KvB caloron solutions in QCD can dissociate into triplets of extended monopoles (see Fig. 6). This hopefully provides a link to a successful confinement model due to which the condensation of (Abelian) monopoles squeezes the colour-electric flux lines between a quark-antiquark pair into a narrow flux tube similar to the formation of magnetic flux in a normal superconductor due to the condensation of the Cooper pairs.

Unfortunately standard lattice discretizations of the QCD Lagrangian have important drawbacks. The above mentioned chiral symmetry can be violated having bad consequences for those observables, for which the smallness of the masses of the *u*- and *d*-quarks becomes important, e.g. for the masses of the proton or the neutron. Therefore, much effort has been spent since a couple of years in order to introduce and to simulate chiral fermions on the lattice. There are formulations which are chirally exact, but in simulations they turn out to be much more computer-time consuming. Their general properties have to be investigated thoroughly and to be compared with other approaches like the (effective) chiral perturbation theory or random matrix theory until they can be effectively used in phenomenological applications. This research has been successfully started within the Collaborative Research Center SFB/TR 9 *Computational Particle Physics* in collaboration with the John-von-Neumann Institute for Computing/DESY Zeuthen. For the first time the eigenvalue spectrum of the chirally exact lattice Dirac operator was shown to behave exactly as random matrix theory predicts [7]. The final aim is to match lattice QCD with chiral perturbation theory in order to reliably extrapolate lattice simulation results for phenomenological quantities, e.g. for moments of hadron structure functions measured in deep inelastic scattering accelerator experiments, to realistically small *u*- and *d*-quark masses.

Conclusions

The interaction of experimental information and theoretical imagination have led to the standard model of elementary particle physics as the presently accepted theory of matter. In this article we have described how important predictions of this theory are extracted by direct computer simulation of portions of space-time carrying the relevant degrees of freedom. Fuelled by the on-going exponential growth of computer power combined with continuous improvement of algorithms and computational techniques, the lattice method is becoming an indispensable aid to better understand the theory, to compare with experience, and ultimately to promote further our understanding of matter.

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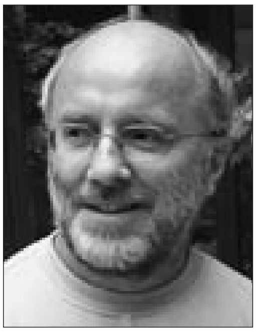

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