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Quarks in a Box

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The determination of the masses of the light quarks requires solving the hadronic binding problem of quantum chromodynamics (QCD), the fundamental theory describing the strong interactions between the quarks. Due to asymptotic freedom, the high-momentum sector of QCD can be treated by perturbative methods, however, on the low energy hadronic scale the running coupling of QCD becomes large. As a consequence, perturbative methods are not adequate for the hadronic binding problem, the scenario of which is dominated by the QCD vacuum state. The only known way to *solve* rather than *model* the problem is through *ab-initio* numerical simulations by high-end computers on a finite discrete space-time lattice. In this paper, which is intended for a non-expert audience, we give an illustrated introduction to the hadronic binding problem and its treatment by computer simulation on Tera-scale computers. We focus on the finite-size approach as pursued by the GRAL project to Go to more Realistic And Lighter quark masses, the main obstacle to current simulations.

1 The Hadronic Binding Problem

Half a century of experimental research in elementary particle physics has revealed a plethora of information on the properties of sub-nuclear matter. Symmetry, the primary building principle of twentieth century physics, allowed Gell-Mann and Ne'eman to arrange the complicated empirical patterns of the particle states in terms of higher representations of a special unitary group—the so-called *flavor* SU(3), SU(3)$_f$. At this time, the three unknown entities associated with the fundamental representation of SU(3)$_f$, according to Gell-Mann named *up* (u), *down* (d) and *strange* (s) quarks, were considered as purely mathematical objects. According to the first naive quark model, nucleons like the proton and the neutron are composed of three constituent quarks as depicted in Fig. 1a, while mesons are built up from a quark joined by its anti-quark, see Fig. 1b. At the time the simple quark model was quite an un-orthodox proposal as quarks carry only a fraction of the electron's charge[1].

It then took physicists nearly ten years to formulate a dynamical description of the interaction which binds quarks into hadrons. The key step was to generalize the principle of local gauge invariance, based on the abelian group U(1), that has been so successful for the description of electrodynamics, to a non-abelian form, the so-called *color* SU(3), SU(3)$_c$: In addition to the electric charge as carried by the electron, quarks come with three new charges conventionally labeled by colors. And the electromagnetic force between electrons, mediated by the uncharged photon, is generalized to the strong force between the quarks, resulting from the exchange of gluons basically coming in eight different color charge combinations. The number eight is reflected in the dimension of the adjoint representation of SU(3)$_c$. Fig. 2 shows a cartoon of a gluon exchanging the colors between two of the three constituent quarks within the proton.

Actually, the picture in Fig. 2 is not at all the entire story as it does not capture the

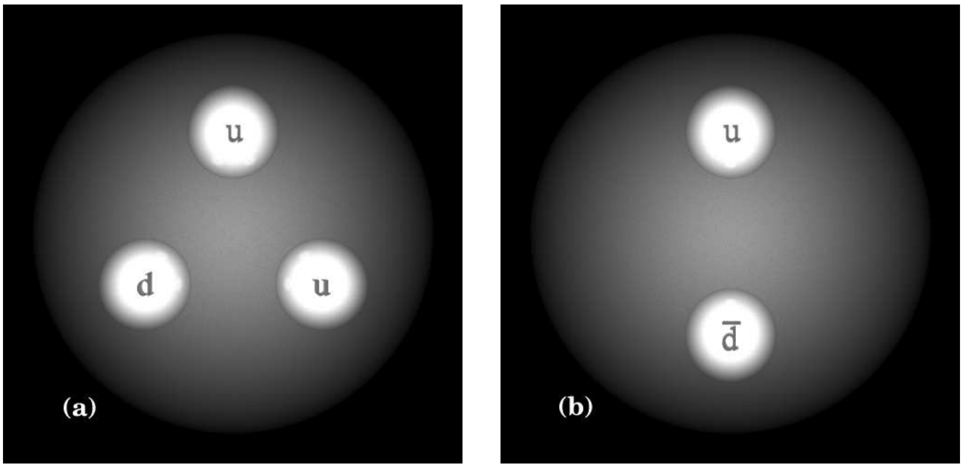

Figure 1. Simple constituent quark model of (a) a nucleon (proton) with two *u* quarks and one *d* quark, (b) a π^+ meson with *u* quark and $\bar{d}$ anti-quark.

phenomenon of quantum fluctuations. In fact, it was one of the great triumphs of relativistic quantum field theory to provide a very accurate explanation for the tiny Lamb-shift, which is—according to quantum electrodynamics (QED)—due to quantum fluctuations that lift the degeneracy of the $2s_{\frac{1}{2}} - 2p_{\frac{1}{2}}$ levels of hydrogen[1] contrary to the previous predictions of Dirac's equation. In QED, a photon, for instance, can virtually fluctuate into an electron-positron pair that exists for a short time in accordance with Heisenberg's uncertainty principle $\Delta E\, \Delta T \approx \hbar$, as schematically depicted as Feynman diagram in Fig. 3a.

In QCD one would expect quantum fluctuations to be all the more important since due to the strong coupling, α_s, which is by about two orders of magnitude larger than the electromagnetic coupling $\alpha = \frac{e^2}{\hbar c}$, the probability for pair creation is much larger. Therefore, the proton is not just made up of constituent quarks and gluons but is a "soup" of quarks, anti-quarks and gluons. From the outside the proton looks like a particle carrying an effective quark number of 3, an electric charge 1 and color charge 0. Theoretically, it often is a good approximation to distinguish between "valence" quarks and a *sea* of virtual quark-anti-quark pairs and gluons, in order to explicitly express the appearance of a net quark number. An artist's impression of the sea of quarks, anti-quarks and gluons is given in Fig. 4.

All our experimental evidence shows that quarks cannot be isolated but always form bound hadronic states with color charge zero, a phenomenon denoted as confinement of quarks. Confinement prevents us from direct experiments with quarks. In particular, we are not able to determine the masses of quarks as for instance the masses of isolated electrons.

Why then bother about the masses of quarks, if such objects cannot be isolated anyway? Well, the clue to further progress in elementary particle physics is an understanding of the violation of quark flavor symmetry in *weak interactions*, as for instance evident in the decay $K \to \pi\pi$. Within the Glashow-Salam-Weinberg (GSW) theory, weak interactions between quarks are readily formulated as the exchange of the massive gauge bosons W^+, W^- and Z. A quantitative understanding of flavor dynamics therefore requires knowl-

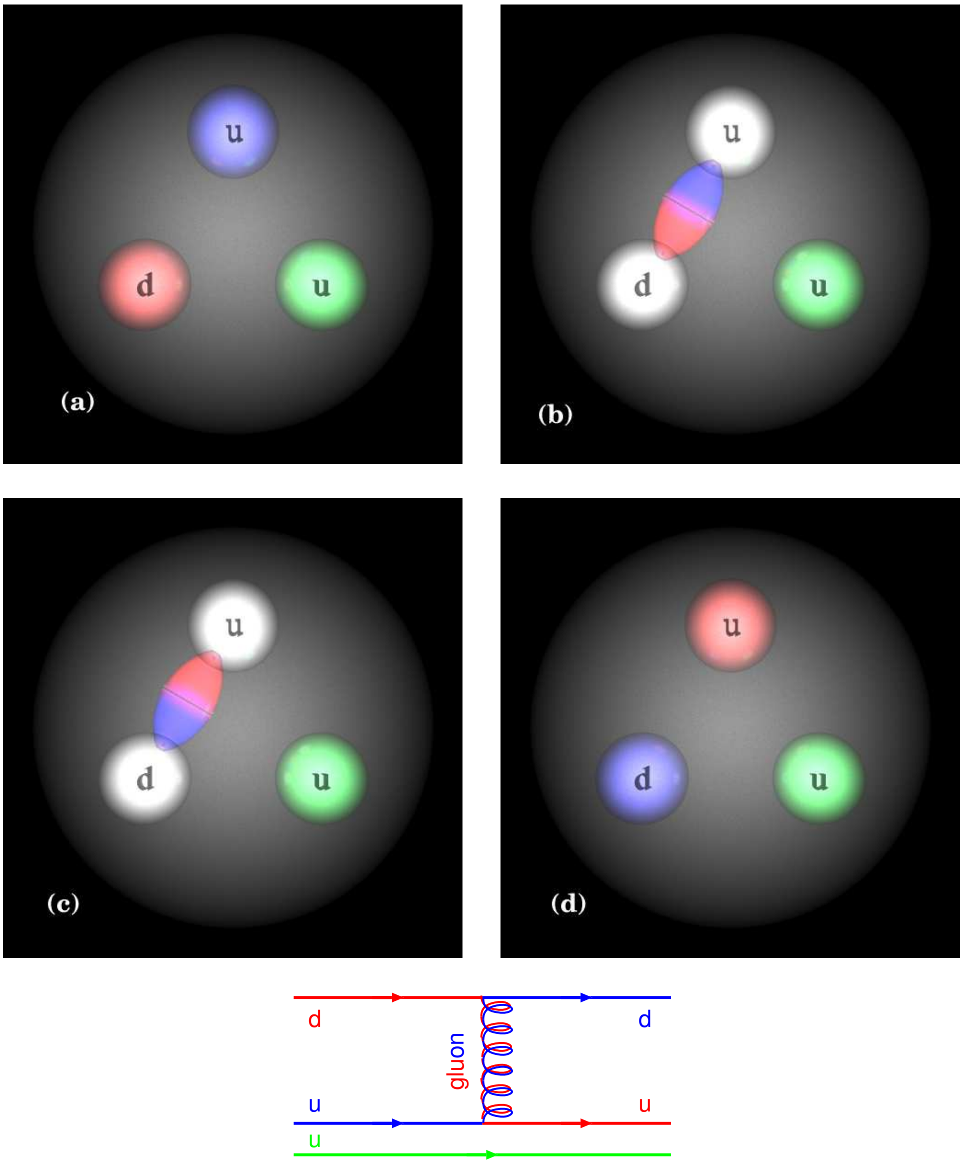

Figure 2. Visualization of the interaction between two quarks within the nucleon by color exchange via a gluon. The sequence corresponds to the Feynman diagram as drawn in the lower part of the picture.

edge of the properties of the quarks. In fact their masses are important input parameters of the current standard model (SM) of elementary particles, a combination of QCD and GSW. Accessing the quark masses thus implies solving the problem of how quarks, the fundamental objects, bind into hadrons, the "elementary" particles of the pre-quark-era.

Let us discuss the binding problem as a Gedanken-experiment by considering the sim-

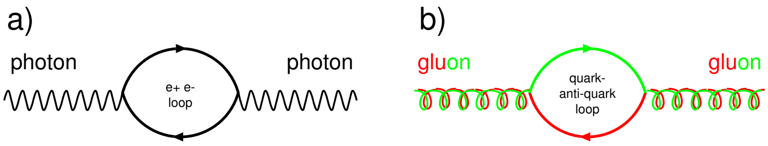

Figure 3. Virtual pair creation process in QED (a) and QCD (b).

ple case of the hydrogen atom. Suppose that electrons occur only confined within atoms. How could we still determine the mass m_e of such elusive electrons? The answer is to solve Schrödingers equation, which predicts the energy levels

$$E_n(m_e) = -\frac{1}{2} m_e c^2 \frac{\alpha^2}{n^2} \tag{1}$$

and charge radii

$$r_n(m_e) = \frac{n^2}{\alpha} \frac{\hbar}{m_e c}. \tag{2}$$

From the measurements of the transition energy $E_2 - E_1$ and Bohr's radius one can determine the mass of the "confined" electron using the ratio $\frac{(E_2-E_1)(m_e)}{r_n(m_e)}$.

Quite analogously, if in QCD the theoretician could determine hadron masses $M_{h_i}(m_{q_j})$ as functions of the quark masses m_{q_j} (the indices i, j numbering hadrons and quarks, respectively), it would be possible to infer the quark masses from ratios of the experimental values of M_{h_i}. This finally brings us to the *hadronic binding problem*, which is considerably more complex than the atomic one. While the electron carries a mass of 511 keV and the hydrogen binding energy is of the order of 10 eV only, we are faced here with very heavy bound states (with a nucleon of 931 MeV) composed of very light quarks (u and d carry masses of 1 to 10 MeV). Thus, contrary to atomic scale physics, the femtoworld of hadrons is a relativistic world *par excellence*, where in accordance with Einstein's equation $E = mc^2$ the nucleon mass mostly consists of binding energy.

Given this situation, the obvious way to tackle the binding problem of the strong interaction is to start out from the ubiquitous sea of strongly interacting virtual gluons and quark-antiquark pairs as the basic entity. The state of lowest energy of this medium is denoted as the QCD "vacuum" state. Knowledge about the vacuum state would enable us to determine the propagation of quarks through the quark-gluon sea and subsequently to determine the properties of hadrons composed of quarks interacting through the medium. Note that this scenario is quite different from the above-mentioned situation of the Lamb-shift: there, the quantum fluctuations are computed as a perturbation of eigenstates of the hydrogen atom, which are a simple solution of Dirac's equation. On the other hand, in QCD, hadrons themselves can be considered as small distortions of the vacuum. The determination of the QCD vacuum, however, as might already be clear from Fig. 4a, is an extremely complicated computational task.

It is well known that the propagation of electrons and photons through the vacuum of QED can be treated to high accuracy by low-order power expansion in α, as $\alpha \ll 1$. At the hadronic energy scale, however, the running coupling of QCD becomes large ($\mathcal{O}(1)$), and consequently the QCD vacuum state turns out to be a non-perturbative problem.

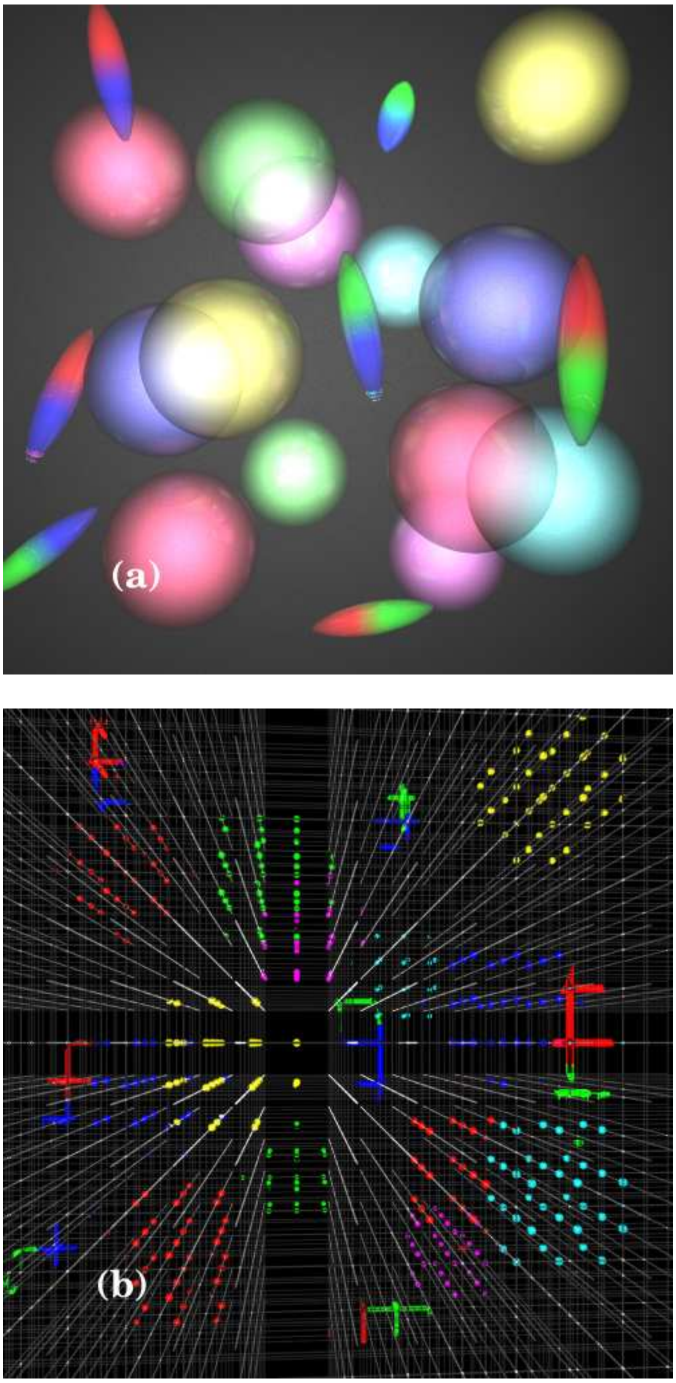

Figure 4. (a) Artist's snapshot of the fluctuating quark-antiquark-gluon sea. (b) Same situation on the lattice. The quark fields are restricted to the lattice sites, the gluonic fields are exchanged only along the links of the lattice.

2 QCD Vacuum States from Lattice Simulations

Currently, the only known way to *solve* the hadronic binding problem beyond *modeling* is through *ab-initio* numerical simulations on high-end computers using a finite discrete space-time lattice[2]. The lattice essentially serves two purposes, namely (a) to provide a suitable regularization scheme for the quantum field theory and (b) to make the problem computationally tractable by shifting it from real-space into a finite box.

(a) The need for regularization is well known in the context of the perturbative analysis of quantum field theories. In that case infinities arise in the computation of higher-order Feynman diagrams which have to be compensated for by adding infinite counter terms. The integration process itself must of course avoid infinities. The regularization prescription renders the integrals finite by means of a regularization parameter (corresponding to a high-momentum cut-off), which is subsequently taken to infinity. Analogously we cannot implement a non-countable, infinite number of space-time points on a computer. A lattice with regularization parameter a, the lattice spacing, renders the space-time points countable, and by Fourier transform we recognize that the inverse lattice spacing a^{-1} is just a cut-off at large momentum. Of course one has to send the cut-off to zero, $a \to 0$, performing a sequence of simulations, in order to be able to extrapolate eventually to continuum results—the so-called continuum limit.

(b) It is evident that we cannot handle an infinite number of lattice sites on a computer, even if it is countable. This fact is a fundamental problem for interactions with infinite range like, for instance, gravity. Fortunately, strong interactions are short ranged, *i. e.*, they fall off rapidly enough outside the proton, a feature already described by the early effective Yukawa theory of pion exchange between nucleons. Thus, we are allowed to restrict our lattice laboratory to a finite box containing the hadron to be investigated. A finite box size L essentially serves as a low-momentum cut-off. Below, we shall demonstrate how to take advantage from the finite size L of the lattice by provoking finite-size-effects.

The analogous picture to Fig. 4a for the lattice world is presented in Fig. 4b. The quark fields are restricted to the sites of the lattice, gluons are restricted to the links.

We describe quantum fluctuations of this lattice system by considering the superposition of all its conceivable wave mechanical time evolutions ("paths"). In analogy to the famous Huygens principle of light propagation, the underlying wave mechanics is characterized by a phase factor, $\exp(-iS/\hbar)$, where the functional $S[\bar{\psi}, \psi, A]$ is nothing but the QCD action. This leads to the "path integral" which is a functional integral in the configuration space $[\bar{\psi}, \psi, A]$:

$$Z = \int \mathcal{D}A_\mu(\mathsf{x})\mathcal{D}\bar{\psi}_\mathsf{x}\mathcal{D}\psi_\mathsf{x}\, e^{-\frac{i}{\hbar}[\bar{\psi},\psi,A]}. \tag{3}$$

Actual lattice calculations use the Euclidean form of quantum field theory, which renders the path integral a real-valued partition function, as known from statistical mechanics. The Euclidean form of Eq. (3) is achieved by the analytic continuation of the time variable $t \to -i\tau$. The ensuing effect is a transformation of the Minkowski metric into a Euclidean metric, while a positive definite Boltzmann weight $\exp(-\beta S)$ emerges. This form of the path-integral is well suited for statistical evaluation,

$$Z = \int \left(\prod_{\mathsf{n},\mu} [dU_\mu(\mathsf{n})][d\bar{\psi}_\mathsf{n}][d\psi_\mathsf{n}] \right) e^{-\beta S_g[U] - S_f[\bar{\psi},\psi,U]}. \tag{4}$$

S_g is the action due to the gluon fields, S_f is the part of the action due to the quarks. The gluonic field is described by SU(3) matrices $U_\mu(\mathsf{n})$ extending from lattice point $\mathsf{n} = (n_1, n_2, n_3, n_4)$ to $\mathsf{n} = (n_1, n_2, n_3, n_4) + e_\mu$, ψ_n denotes the quark fields located at the sites n. As the latter are Grassmann variables, and S_f is a bilinear form, the fermionic variables can be integrated out, leaving us with

$$Z = \int \prod_{\mathsf{n},\mu} [dU_\mu(\mathsf{n})] \det(M[U]) e^{-\beta S_g}. \tag{5}$$

The Euclidean path-integral Eq. (5) is evaluated by means of stochastic Monte Carlo algorithms. It suffices to generate a representative ensemble of fluctuating vacuum gauge fields $\{U_i\}$, $i = 1, \ldots, N$ which incorporate the effects of virtual fermion-anti-fermion pairs via the determinant of M, the lattice Dirac matrix. The ensemble of such vacuum states contains the complete physical information as pictured in Fig. 4. Given the ensemble of say N vacuum configurations, any observable, like operators which describe valence quarks propagating in the vacuum or even objects built from sea quarks loops, can be "measured" as ensemble average together with their statistical error,

$$\langle O \rangle = \frac{1}{N} \sum_{i=1}^{N} O_i[U_i] \quad \text{and} \quad \sigma_O^2 = \frac{2\tau_{\text{int}}}{N} \left(\frac{1}{N} \sum_{i=1}^{N} |O_i[U_i]|^2 - \langle O \rangle^2 \right). \tag{6}$$

Let us for the moment set $\det(M)$ equal to 1 in Eq. (5). In this case, the vacuum state is of purely gluonic nature. Lattice QCD based on such a kind of vacuum states is called "quenched approximation" because sea quarks are decoupled. Often this approximation describes the physics situation accurately enough. The advantage is that such a quenched simulation is substantially cheaper than the full one, because one can make use of a simple Markov transition by applying stochastic modifications link-wise to the variables $U_\mu(\mathsf{n}) \rightarrow {U'}_\mu(\mathsf{n})$ with a local Metropolis decision.

However, using Metropolis for full QCD, the Metropolis decision

$$P(U \rightarrow U') = \min \left[1, \exp(-\Delta S_g) \frac{\det(M[U'])}{\det(M[U])} \right] \tag{7}$$

requires the computation of the fermionic determinant for each link $U_\mu(\mathsf{n})$ separately, which is prohibitively expensive. A better way to proceed is to compute a global update of the links as achieved by the ingenious hybrid Monte Carlo algorithm[3], the standard method for simulations of full QCD. Nevertheless realistic full QCD simulations require computers of the class of hundreds of teraflops, as we shall see next.

Let us illustrate these statements by presenting a picture of a typical lattice QCD experiment in Fig. 5, the determination of the flux tube between two heavy quarks that are being drawn apart. The underlying gauge configurations have been generated in the quenched approximation. Subsequently, the potential was computed on these configurations by means of a simple operator, the Wilson loop. The color encodes the result for the action density. Note the fluctuations due to the stochastic method. As the problem has a cylindric symmetry, it can be plotted in two dimensions. The sequence of sheets corresponds to increasing quark-antiquark separations.

The energy between the quarks grows linearly with their distance—confinement at work! As we did not include sea-quark loops, one expects the flux tube not to break up into two mesons.

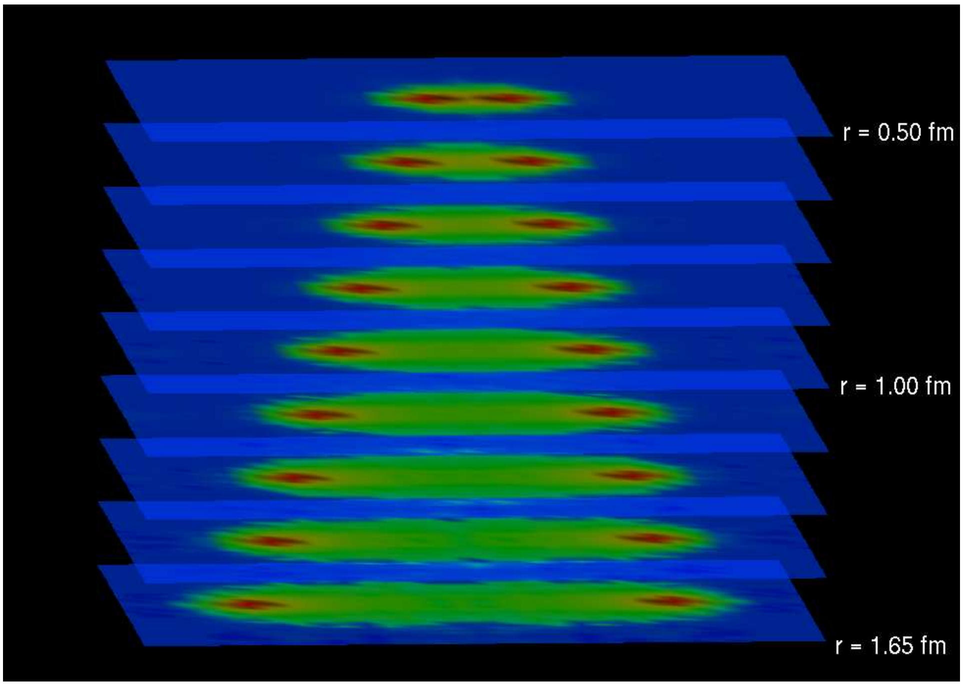

Figure 5. Flux between a pair of very heavy quark and antiquark. The sheets correspond to increasing distances (Bali, Schlichter, Schilling 1997).

3 The Multi-Scale Problem of QCD

Our previous considerations already have shown how lattice gauge theory merges quantum field theory with the techniques of statistical physics. The approach to the continuum limit ($a \rightarrow 0$) is carried out on a sequence of lattices with decreasing spacings a. In order to vary a, we have to tune the parameter $\beta \propto \frac{1}{g^2}$ suitably—with g being the bare strong coupling constant. For $a \rightarrow 0$ lattice physics would become insensitive to the spacing of the lattice. Such behavior typically occurs near a second-order phase transition, where the correlation length diverges. In practice, one never can achieve $a = 0$. Hence, results from different finite lattice spacings are extrapolated to $a = 0$.

In lattice QCD, a correlation length is associated to an inverse physical mass, $\xi = 1/m$. Our box size L must fulfill $\xi \ll L$, so that ξ can be accommodated in the finite box. The lightest particle of the strong spectrum with the largest correlation length is the π meson. Therefore, L must be larger than ξ_π, because otherwise finite size effects will spoil the results.

On the other hand, the lattice spacing a has to be chosen small enough to resolve the objects to be investigated. However, decreasing the lattice spacing decreases the finite box size unless we compensate for this effect by increasing the number of lattice sites. The crucial point is that we are limited in L/a by the available computer power. Presently, we can only choose between too coarse a lattice spacing a or too large a pion mass. We see that lattice QCD is a typical multi-scale problem.

Future realistic QCD simulations with dynamical fermions would require to operate beyond the $\rho \to \pi\pi$ decay threshold and closer to the continuum limit than achieved so far. In order to estimate the simulation efforts we have determined the costs of full QCD simulations from the results of our large scale simulation projects SESAM and TχL. In these lattice experiments we have used the hybrid Monte Carlo algorithm with two degenerate flavors of Wilson fermions.

SESAM/TχL has generated 10 ensembles of full QCD vacuum configurations with $O(5000)$ HMC trajectories each, at $\beta = 5.6$ and 5.5 in the region $0.57 < \frac{m_\pi}{m_\rho} < 0.85$. The lattice sizes are $16^3 \times 32$ (SESAM) and $24^3 \times 40$ (TχL), corresponding to physical sizes of $1.372(36)$ fm (SESAM) and of $1.902(34)$ fm (TχL) after chiral extrapolation. Running primarily on APE100 systems of the NIC at DESY/Zeuthen, DFG/Bielefeld and INFN/Rome, the total costs of the simulations sum up to about 0.06 Tflops-yrs. The configurations which have been generated on APE100 systems are stored at the ZAM/FZ-Jülich storage facilities for detailed physics evaluation on the Cray T3E systems.

In table 3 we try to convey to the reader an idea about the characteristics of full QCD lattice simulations by presenting some key quantities from SESAM/TχL. $\frac{m_\pi}{m_\rho}$ is the value of the π mass divided by the ρ mass as obtained in the simulation (the experimental value being 0.1724). The third row shows the so-called integrated autocorrelation time $\tau_{\rm int}$ that determines the actual statistical significance of a Markov chain based simulation, see Eq. (6). These numbers tell us that we have about 200 stochastically independent configurations per ensemble.

β		$16^3 \times 32$				$24^3 \times 40$	
5.6	$\frac{m_\pi}{m_\rho}$	0.83	0.81	0.76	0.68	0.70	0.57
	$T_{\rm equi}$	5200	5400	5250	4950	4700	4000
	$\tau_{\rm int}$		19(4)	25(6)	33(4)	36(4)	50(5)
5.5	$\frac{m_\pi}{m_\rho}$	0.85	0.80	0.75	0.68		
	$T_{\rm equi}$	3500	4000	5000	5000		
	$\tau_{\rm int}$	19(2)	24(3)	38(2)	47(3)		

Table 1. Some characteristic quantities from SESAM/TχL simulations.

From our determination of autocorrelation times and the CPU time measurements we are in the position to estimate the costs of full QCD simulations. Suppose we aim for an accuracy comparable to state-of-the-art quenched simulations. The standard has been set by the CP-PACS group at Tsukuba/Japan. They have carried out quenched simulations[4] in 1997 on the 600 Gflops CP-PACS/Hitachi SR2001 parallel system built at Tsukuba university. They achieved finite a results for light hadrons with errors $< 1\%$ and subsequently could extrapolate to continuum results with errors between 1 and 3%. Using their setting, we find the upper bounds to the CPU time (see table 3) needed to carry out an analogous simulation with $n_f = 2$ Wilson fermions. We conclude that such a full QCD simulation will be a task for a 100 Teraflops system.

$a[fm]\backslash\frac{m_\pi}{m_\rho}$	0.75	0.70	0.60	0.50	0.40	$\sum$ [Tflops-yrs]	z_2	L/a	# of confs
0.102	0.46	0.79	0.21	0.58	18	25(8)	4.3	32	800
0.076	1.2	1.8	3.5	7.0	15	28(9)	2.8	40	600
0.064	3.7	6.7	12	23	50	95(35)	2.8 (!)	48	400
0.050	17	28	60	120	260	485(150)	2.8 (!)	64	200

Table 2. Extrapolation of costs for the determination of light hadron masses with 2 flavors of Wilson fermions in analogy to the quenched setting of the CP-PACS group.

4 Going Realistic And Light–The GRAL Project

What ways are there at present to extend the range of full QCD simulations towards smaller quark masses? A crucial parameter for the costs of QCD simulations is the number of lattice sites, $(L/a)^4$. In previous simulations L/a has in general been chosen such that finite-size-effects were largely suppressed at given quark mass.

The idea of our new project called GRAL (Going Realistic And Light) is to reverse the strategy and to perform a comprehensive study of finite-size-effects. Deliberately accepting finite-size-effects allows one in principle to extend full QCD simulations into the regime of lighter quark masses. For given bare coupling and quark mass, QCD vacua will be generated on a sequence of box sizes that will allow for an extrapolation in L/a. For such a finite-size-scaling analysis we expect a formula like that of Fukugita, Parisi et al.[5] to be applicable: $m(L) = m_\infty + cL^{-\nu}$.

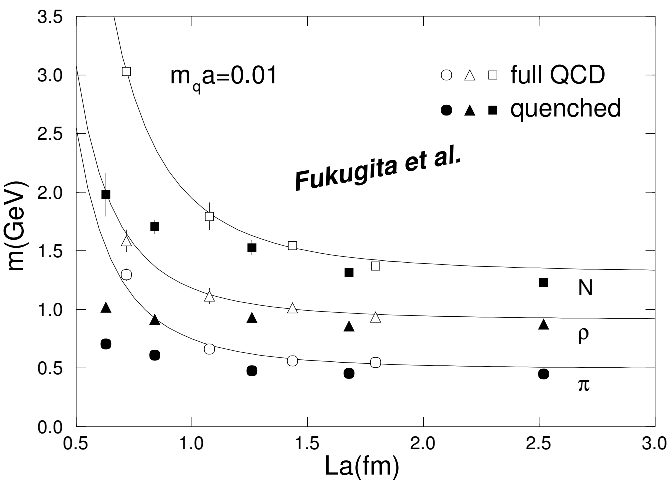

Figure 6. Infinite volume extrapolation.

Before embarking on a large-scale production, however, this program requires an extensive scanning of parameter space (spanned by the bare coupling β, the bare quark mass and the number of lattice sites) in order to locate the physically interesting and computationally feasible operating region.

To this end we specify, for a start, $L/a = 16$ as the maximal spatial extent of a series of lattices employed. Furthermore we require the simulation on this lattice to yield meson masses with $\frac{m_\pi}{m_\rho} = 0.4$ (*i. e.* below the decay threshold at 0.5) and a finite-size-parameter of $\xi_\pi/L = 0.2$. This particular value for ξ_π/L has been chosen in view of a recent SESAM/TχL quark mass analysis[6], where 0.2 was found to mark the onset of significant finite-size-effects in the hadronic spectrum.

In summary, the envisaged properties of our target point on a $16^3 \times 32$-lattice are as follows:

$\frac{m_\pi}{m_\rho}$	$\frac{\xi_\pi}{L}$	ξ_π	am_π	am_ρ	a[fm]	L [fm]
0.4	0.2	3.2	0.31	0.78	0.116	1.86

The lattice spacing a has been estimated on the basis of the SESAM and TχL data at $\beta = 5.6$ and 5.5. As can be seen from the table, the price for sticking to $L/a = 16$ is a fairly coarse lattice. According to our scaling cost extrapolations, we expect a total cost of approximately $0.2\ \mathrm{TFlop/s} \cdot \mathrm{h}$ to produce 100 statistically independent gauge field configurations at the target point. For more details see Ref. 7.

With shrinking box size local fluctuations in the vacuum field configurations will eventually destabilize the global updating process of the Hybrid Monte Carlo Algorithm. The crucial issue regarding the feasibility of our strategy is the question of when this breakdown occurs. Thus, our first task will be to establish a suitable "window" of lattice volumes were our sampling algorithm remains stable.

5 Summary

With this contribution we aimed at illustrating the lattice approach to the determination of hadronic properties for a non-expert audience. We argued that the hadronic binding is a highly relativistic problem, where quarks with small masses form nucleons which are about a factor of 100 heavier. We have emphasized the important role of the QCD vacuum fields. Such fields can be generated by lattice gauge simulations. Given an ensemble of vacuum gauge fields we can compute the propagation of quarks that combine to hadrons through the fluctuating quark-gluon sea. We have estimated the huge costs of future simulations of the full theory, assuming accuracies similar to those of state-of-the-art quenched simulations. These considerations demonstrate that new ideas are required to approach the regime of small realistic quark masses. One promising idea is pursued by our GRAL project, which means to Go Realistic And Light using finite-size techniques. In this manner we will attempt to go beyond the previous milestones of SESAM/TχL.

Acknowledgments

We acknowledge the essential support of the SESAM/TχL projects and the current GRAL project by the John von Neumann Institute for Computing (former HLRZ) with about 150 Tflops-hrs compute time on APE100 computers at DESY/Zeuthen and about 50 Tflops-hrs on the Cray T90 and T3E systems at Jülich for post-processing of our field configurations. The availability of multi-Tbyte storage space at ZAM/FZ-Jülich played an essential rôle in our Europe-wide simulation project. We heartily thank the members of these computer centers for their friendly support.

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