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QCD Spectroscopy with Three Light Quarks

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Numerical simulations in Quantum Chromodynamics – the theory of the strong interactions of elementary particles – are performed with light dynamical quark degrees of freedom. At present the main emphasis is put on the lightest quarks – the u- and d-quark – in order to confront the results with expectations arising from spontaneously broken chiral symmetry. The extension to include the third light quark (the s-quark) is straightforward and is postponed to a later stage of our project.

1 Introduction

Most massive matter in the Universe consists of nucleons (protons and neutrons) which are bound states of quarks held together by strong interactions. The theory of strong interactions is Quantum Chromodynamics (QCD). The quarks bound within the nucleons have very small masses compared to the mass of the nucleon itself: the sum of the masses of the three constituent quarks is only about a percent of the mass of the nucleon bound state. This means that about 99% of the nucleon mass is a consequence of the strong interaction. One of the most beautiful features of QCD is that the nucleon mass, together with a large number of other hadron masses and many other strong interaction parameters, can be calculated – at least in principle – by numerical simulations on space-time lattices (for an introduction and references to QCD on the lattice see Ref. 1).

Numerical simulations in Lattice Quantum Chromodynamics (LQCD) are being performed already since more than twenty years but, in spite of impressive developments both in theoretical insights and in numerical simulation techniques, up to now no satisfactory precision of the results has been achieved. The basic reason is the smallness of the masses of the three "light" quarks (u-, d- and s-quark) because the known simulation algorithms show a considerable slowing down when going towards small quark masses. However, at present there is a growing optimism in our scientific community that the combination of the achieved understanding and the possibility to use Tflops computers for LQCD will lead to first reliable results with controlled (and small) errors on some basic parameters of QCD within the next few years.

Besides being the main obstacle to achieve good precision in numerical simulations, the smallness of the u-, d- and s-quark masses ($m_u \simeq m_d$ and m_s, respectively) is also the most important characteristic feature of the low energy strong interaction dynamics.

It implies that there exists an approximate $\mathrm{SU}(3) \otimes \mathrm{SU}(3)$ chiral flavor symmetry. From the spontaneous breaking of this symmetry by the non-zero vacuum expectation value of the *quark condensate* it follows that there exist eight light pseudo-Goldstone bosons (the pions, kaons and η-meson) which dominate strong interactions at low energies.

The low energy dynamics in the pseudo-Goldstone boson sector of QCD is constrained by the non-linear realization of spontaneously broken chiral symmetry[2]. In an expansion in powers of momenta and light quark masses a few low energy constants – the Gasser-Leutwyler constants – appear which parameterize the strength of interactions in the low energy chiral Lagrangian[3]. The Gasser-Leutwyler constants are free parameters which can be constrained by analyzing experimental data. In the framework of lattice regularization they can be determined from first principles by numerical simulations. In experiments one can investigate processes with different momenta but the quark masses are, of course, fixed by Nature. In numerical simulations there is, in principle, much more freedom because, besides the possibility of changing momenta, one can also freely change the masses of the quarks. This allows for a precise determination of the Gasser-Leutwyler constants – once the simulations reach high precision.

In order to exploit the regime of light quark masses in LQCD our collaboration applies the two-step multi-boson (TSMB) algorithm[4] which has been developed and extensively used in our previous NIC-project on supersymmetric Yang-Mills theory (for summary and references see Ref. 5, 6). The TSMB algorithm allows to perform simulations with small quark masses within the range of applicability of next-to-leading order (NLO) ChPT[7,8].

An important aspect of investigating the quark mass dependence for light quarks in numerical simulations is the possibility to use ChPT for the extrapolation of the results to the physical values of u- and d-quark masses which is difficult to reach otherwise. In fact, ChPT can be extended by changing the *valence quark masses* in quark propagators independently from the *sea quark masses* in virtual quark loops which are represented in the path integral by the *quark determinant*. In this way one arrives at Partially Quenched Chiral Perturbation Theory (PQChPT)[9]. The freedom of changing valence and sea quark masses substantially contributes to the power of lattice QCD both in performing quark mass extrapolations and in determining the values of the Gasser-Leutwyler constants[10].

For a fast convergence of numerical results to the continuum limit it is important to explicitly deal with the leading $\mathcal{O}(a)$ lattice artifacts (a denotes the lattice spacing). This can be achieved by applying *chiral perturbation theory for the Wilson lattice action*[11,12]. In this method the original Wilson lattice action is used in the Monte Carlo generation of gauge configurations and the $\mathcal{O}(a)$ effects are compensated in PQChPT itself. Our calculations showed that in practice this method gives results with good precision[13].

In the next section the TSMB algorithm and the results of our collaboration concerning its perfomance in LQCD simulations are shortly summarized. In section 3 recent results on the quark mass dependence of masses and decay constants of the pseudo-Goldstone bosons in QCD are discussed. The final section contains a short summary of the present status and an outlook to our future plans.

2 The TSMB Algorithm for Light Quarks

The difficulty of numerical simulations with dynamical fermions comes, in general, from the non-locality of the effective lattice action for the bosonic (in case of QCD, the glu-

onic gauge-) fields. In the effective gauge action the logarithm of the determinant of the *fermion matrix* (Q) appears which becomes more and more non-local for fermions with small masses. It would be too much expensive to calculate exactly this determinant in every Monte Carlo updating step. A stochastic evaluation is the only possibility.

In case of the TSMB algorithm[4] the fermion determinant for N_f equal mass flavors of quarks is represented as

$$|\det(Q)|^{N_f} \simeq \frac{1}{\det P_{n_1}^{(1)}(\tilde{Q}^2)\ \det P_{n_2}^{(2)}(\tilde{Q}^2)} . \tag{1}$$

Here the hermitean fermion matrix $\tilde{Q} = \tilde{Q}^\dagger = \gamma_5 Q$ is used and the product of the two polynomials $P_{n_1}^{(1)}(x)\, P_{n_2}^{(2)}(x)$ of orders n_1 and n_2, respectively, satisfies

$$\lim_{n_2\to\infty} P_{n_1}^{(1)}(x)\, P_{n_2}^{(2)}(x) = x^{-N_f/2} , \qquad x \in [\epsilon, \lambda] . \tag{2}$$

The interval $[\epsilon, \lambda]$ is chosen in such a way that it covers the spectrum of $\tilde{Q}^2$. The first polynomial $P_{n_1}^{(1)}(x)$ gives a first crude approximation of $x^{-N_f/2}$ and it is taken into account in the local updating sweeps of the gauge field variables ("first step"). The second polynomial $P_{n_2}^{(2)}(x)$ with $n_2 \gg n_1$ gives a good approximation and is realized in a global accept-reject Monte Carlo step after several sweeps over the gauge fields ("second step").

The TSMB algorithm was originally developed for numerical simulations in the supersymmetric Yang-Mills theory[5,6] but, after appropriate tuning, it can also be applied to QCD with light quarks. In the present version of TSMB several modern ideas on fermionic updating are incorporated: the local update step is based on Lüscher's *multi-boson representation* of the fermion determinant[14], the idea of a *global correction step* in the update is taken over from Boriçi and de Forcrand[15], the final *reweighting correction* has been proposed by Frezzotti and Jansen in Ref. 16 and the clever trick of *determinant breakup* boosting the performance has been inspired by the work of Anna Hasenfratz and Alexandru[17].

The polynomial approximations for TSMB are optimized for delivering a good update performance with the smallest possible polynomial orders. It turned out that for this purpose *least-square optimization* is the best. (This is better than, for instance, Chebyshev-typesapproximations minimizing the maximal relative deviation.) An important technical advantage of least-square optimization is its flexibility for different types of functions to be approximated, for instance, in case of $P_{n_2}^{(2)}(x)$ which is an approximation to $[x^{N_f/2} P_{n_1}^{(1)}(x)]^{-1}$. For the practical determination of least-square optimized polynomials a numerical package based on arbitrarily high precision arithmetics has been developed[18].

The features of least-square optimization are particularly important for the first polynomial $P_{n_1}^{(1)}$. The reason is that in a typical situation $P_{n_1}^{(1)}$ gives a much better approximation in the upper part of the interval $[\epsilon, \lambda]$ than in the lower part closest to zero. Typically, most of the deviation is concentrated on the lowest 2-5% of the interval $[\epsilon, \lambda]$. In this way the two-step updating procedure realizes a simple and effective separation of the small fermion action modes from the larger fermion action modes in such a way that the latter are effectively dealt with in the first step and the former ones in the second step. This *large action filtering* is a basic feature which essentially contributes to the good overall performance of TSMB in case of light fermions.

The first task for our collaboration has been to tune the algorithmic parameters of TSMB for simulation runs with light quarks. At the same time the "cost" of simulations had to be estimated in order to facilitate future planning of the runs. It turned out[7,8,19,20] that the computational cost of producing statistically independent gauge field configurations can be well approximated by the empirical formula

$$C \simeq F(am_q)^{-2}\,\Omega\,, \tag{3}$$

where am_q is the quark mass in lattice units and Ω is the number of lattice points. The factor F depends on the type of measured quantity. The "worst case" situation occurs for quantities which are characteristic to the gauge field alone, for instance, the average plaquette or the Sommer scale parameter r_0. For them we have $F \simeq 10^7$ floating point operations (per independent configuration). For other quatities, as for instance the pion mass m_π, the factor F can be 5-10 smaller, furthermore, in this case even the inverse power of the quark mass seems to be somewhat smaller (about $-3/2$). The pion decay constant f_π has an even shorter autocorrelation in such a way that in our runs its values practically never show any autocorrelation.

The estimate in (3) implies that on a $16^3 \cdot 32$ lattice with $\Omega \simeq 1.3\,10^5$ lattice sites we have $C \simeq 1.3\,10^{12}(am_q)^{-2}$. This means that, for instance, for a quark mass $am_q = 0.01$ we need about $1.3\,10^4 s$ per independent configuration on an 1 Tflops computer. Another consequence of (3) is that the computer time grows as a^{-6} if for $a \to 0$ the physical parameters like quark mass and lattice volume are kept constant.

Concerning the question of double versus single precision arithmetics in the update process our experience shows[21,22] that for larger lattices (about $\Omega > 10^5$) double precision becomes necessary in the global correction step.

3 Pion Masses and Decay Constants

As discussed in the introduction, our first goal is to confront the results of numerical simulations with the (PQ)ChPT formulas. For this it is necessary to reach the range of light quark masses where the NLO (PQ)ChPT formulas give a good approximation. Previous estimates and our first results at relatively large lattice spacings ($a \simeq 0.27\,\mathrm{fm}$) showed[7,8,23,13] that one has to reach roughly $m_{u,d} \simeq \frac{1}{5} m_s \simeq 20\,\mathrm{MeV}$.

Our first series of runs[24] with systematically chosen parameters have been performed on 16^4 lattices with $N_f = 2$ light degenerate quark flavours at the gauge coupling parameter $\beta = 5.1$ and three values of the hopping parameter: $\kappa_0 = 0.176$, $\kappa_1 = 0.1765$ and $\kappa_2 = 0.177$. The sample sizes of statistically independent gauge configurations were relatively large, between 750 and 1800 per point. The lattice spacing determined from the Sommer scale parameter r_0 turned out to be $a = 0.189(5)\,\mathrm{fm} \simeq (1.04\,\mathrm{GeV})^{-1}$ giving lattice extensions of about $L \simeq 3\,\mathrm{fm}$. The pion masses built out of "sea" quarks corresponding to the above κ values are in lattice units: $am_\pi = 0.6747(14),\ 0.6211(22),\ 0.4354(68)$, respectively. In physical units these correspond to $m_\pi \simeq 702,\ 646,\ 452\,\mathrm{MeV}$, respectively. The estimates for the sea quark masses are between $\frac{2}{3} m_s$ for the first κ value and $\frac{1}{3} m_s$ for the third one (approximately $60\,\mathrm{MeV}$ to $30\,\mathrm{MeV}$). The "valence" quark masses for partial quenching were chosen in the range $\frac{1}{2} m_{sea} \le m_{valence} \le 2 m_{sea}$.

In order to cancel the Z-factors of multiplicative renormalization, which in the case of a mass-independent renormalization only depend on the gauge coupling but not on the

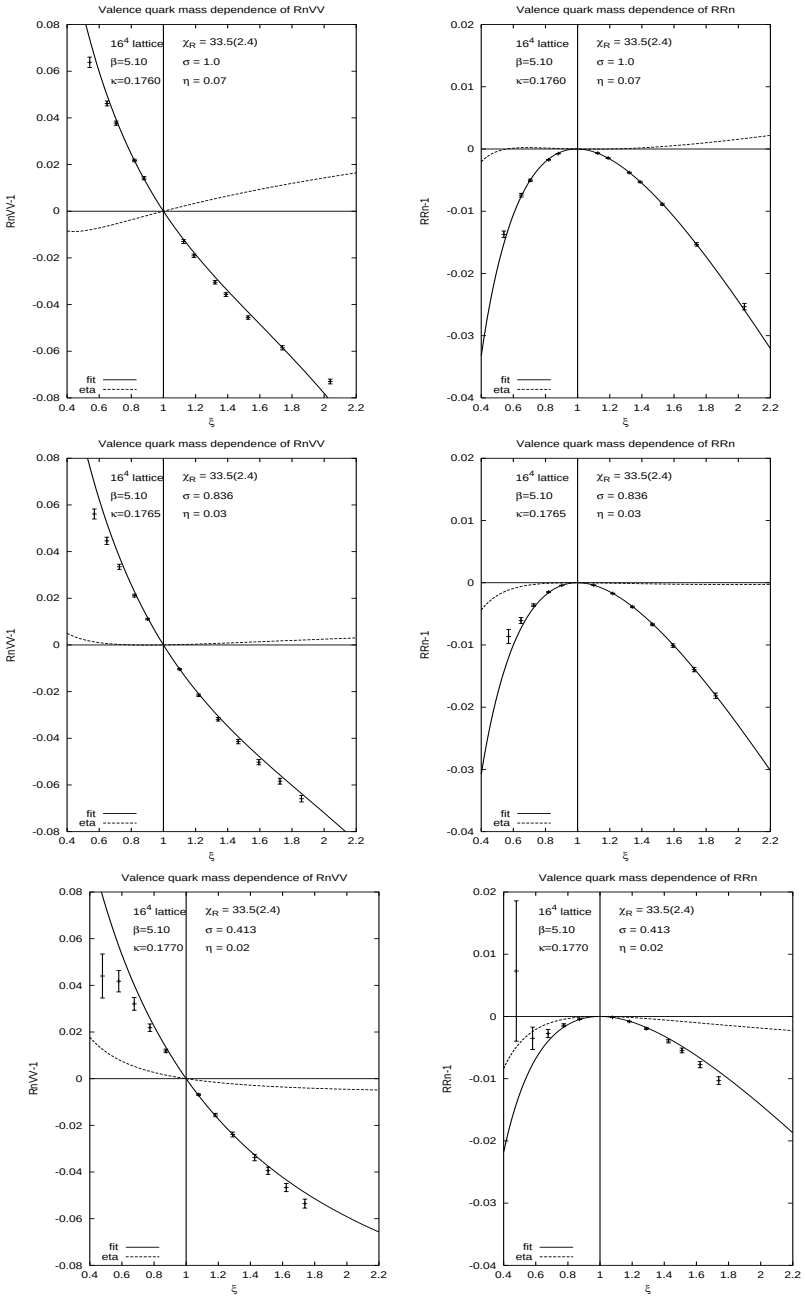

Figure 1. PQChPT fits of $(Rn_{VV} - 1)$ and $(RRn - 1)$ for three different sea quark mass values.

quark mass, we considered ratios of quark masses (m_q) and of pion decay constants (f_π). Specifically, the ratio of the valence to sea quark masses (ξ) and the ratios of different sea quark masses ($\sigma_{1,2}$) are defined as

$$\xi \equiv \frac{m_{qV}}{m_{qS}} , \qquad \sigma_i \equiv \frac{m_{qSi}}{m_{qS0}} , \quad (i = 1, 2) . \tag{4}$$

We investigated the ξ-dependence of the following ratios of decay constants:

$$Rf_{VV} \equiv \frac{f_{VV}}{f_{SS}} , \quad Rf_{VS} \equiv \frac{f_{VS}}{f_{SS}} , \quad RRf \equiv \frac{f_{VS}^2}{f_{VV} f_{SS}} \tag{5}$$

and pion mass squares:

$$Rn_{VV} \equiv \frac{m_{VV}^2}{\xi m_{SS}^2} , \quad Rn_{VS} \equiv \frac{2m_{VS}^2}{(\xi + 1)m_{SS}^2} , \quad RRn \equiv \frac{4\xi m_{VS}^4}{(\xi + 1)^2 m_{VV}^2 m_{SS}^2} . \tag{6}$$

Examples of fits of these quantities by the PQChPT formulas are shown by figure 1. In the formulas the NLO terms including $\mathcal{O}(a)$ lattice artifacts are taken into account together with the leading (i. e. tree-graph or "counter-term insertion") contributions given in Ref. 25.

The results of the simultaneous fits of the valence quark mass dependences at the three sea quark masses (i. e. $\kappa = \kappa_{0,1,2}$) show a satisfactory description of the Monte Carlo data, except for some points near both ends of the ξ-intervals. It is remarkable that the $\mathcal{O}(a)$ terms taking into account leading lattice artifacts are surprisingly small: their fitted ratios to the sea quark masses satisfy $0 < \eta_{0,1,2} < 0.1$. Contrary to expectation, there is a tendency that the values of the η's decrease for decreasing sea quark mass, which could be the consequence of the effective inclusion of some higher order contributions by the fits. Another observation is that in our present quark mass range the NNLO contributions (quadratic in the quark mass) are rather important. Their influence can, however, be diminished by goint to smaller quark masses.

The results from the fits of the valence quark mass dependence can also be used in the investigation of the sea quark mass dependence. In particular, the values of

$$\chi_S \equiv \frac{2B_0 m_{qS}}{f_0^2} , \qquad \eta_S \equiv \frac{\rho_S}{\chi_S} , \qquad \left(\rho \equiv \frac{2W_0 a}{f_0^2} \right) \tag{7}$$

are relevant there. (Here B_0 and f_0 are the parameters of lowest order ChPT and W_0 is a parameter characterizing the magnitude of $\mathcal{O}(a)$ terms.) Since we have for the moment only three different sea quark mass values (and hence only two independent ratios) the only possibility is to extract the NLO parameters in the formulas of Ref. 12. The estimates obtained for these parameters approximately correspond to the phenomenological expectations[26].

4 Discussion and Outlook

The results obtained in our paper[24] for the Gasser-Leutwyler constants can only be taken as estimates of the values in continuum. In order to deduce continuum values with controlled error estimates the left out lattice artifacts have to be removed by performing simulations at increasing β values and extrapolating the results to $a = 0$. The possibility of a precise

continuum extrapolation seems to be rather promising because the fitted $\mathcal{O}(a)$ terms are small and the scaling tests between our previous results at a lattice spacing $a \simeq 0.27\,\mathrm{fm}$ ($\beta = 4.68$)[13] and the results at $a \simeq 0.19\,\mathrm{fm}$ ($\beta = 5.1$)[24] turn out to be unexpectedly good (for examples see figure 2 and in Ref. 27).

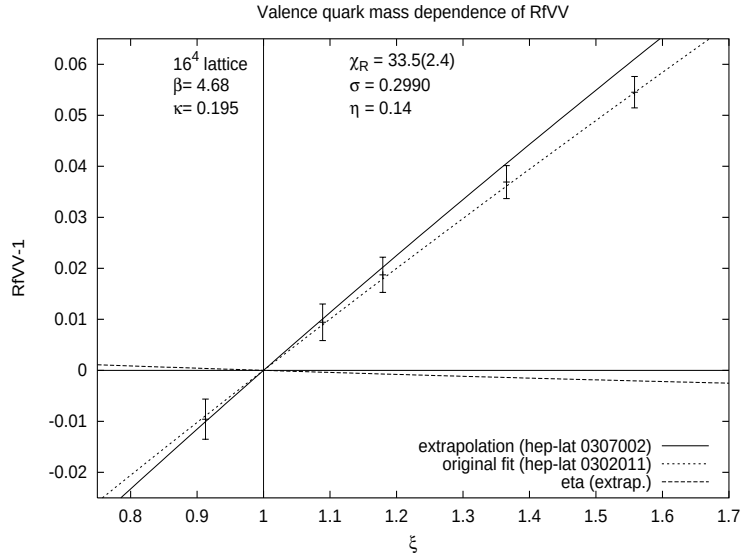

Figure 2. Comparison of the extrapolation of the fit of Rf_{VV} at $\beta = 5.1$ from Ref. 24 with the previous fit at $\beta = 4.68$ as given in Ref. 13.

Comparing our results to those obtained by the CP-PACS Collaboration[28] it turns out their data show substantially larger scale breaking lattice artifacts, which they actually fit by large $\mathcal{O}(a^2)$ terms, although they are at smaller lattice spacings: $0.09\,\mathrm{fm} \leq a \leq 0.22\,\mathrm{fm}$ (and at larger quark masses: $40\,\mathrm{MeV} \leq m_q \leq 200\,\mathrm{MeV}$). They use a clover improved Wilson fermion action[29] and the Hybrid Monte Carlo algorithm[30]. This shows that our choice of the lattice action and of the simulation algorithm is more economic.

Since in our present quark mass range the NNLO terms are rather important, it is desirable to perform simulations at still lighter quark masses. In fact, besides going from 16^4 to the better suited $16^3 \cdot 32$ lattice, our next aim is to decrease the quark mass. A promising approach for this is to choose the lattice action according to *twisted mass LQCD*[31]. In addition to having some favourable theoretical features, this approach also has advantages in the simulation costs because the overall cost factor F of TSMB on the right hand side of the estimate (3) can be decreased from $F \simeq 10^7$ to $F \simeq 10^6$ floating point operations.

Most of the computations reported here were carried out on the APEmille systems installed at NIC Zeuthen, the Cray T3E systems at NIC Jülich and the PC cluster at DESY Hamburg. Some parts of the simulations were performed on the Sun Fire SMP-Cluster at the Rechenzentrum - RWTH Aachen and at the Eötvös University parallel PC cluster supported by Hungarian Science Foundation grants OTKA-T349809/T37615.

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