FINITE SIZE TECHNIQUES AND THE STRONG COUPLING CONSTANT

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1. INTRODUCTION

In these lectures I will mainly describe work done by the Alpha Collaboration to extract quantitative results in QCD from numerical simulations. Information on this collaboration, e.g. its members, physics program etc. can be obtained from the web page: www.ifh.de/computing/parallel/ape/alpha/alpha.html

One of the main goals of our collaboration is to determine the running coupling in the $\overline{\rm MS}$-scheme[1] at energies around m_Z to a quotable accuracy of a few percent. Our emphasis is on the control of the systematic errors. So far this has only been achieved in pure Yang-Mills theory[2] and the method, which uses finite size techniques, will be described in section 3. The particular coupling defined there is based on the Schrödinger functional first investigated by Symanzik[3] which turns out to be a very powerful tool to probe the dynamics of quantum field theories (in particular non-abelian gauge theories).

Before going to the 4-dimensional theories I will first focus attention on the 2-d sigma-model. The reason for this is two-fold. Firstly it was in this model that we first tested the finite size scaling method mentioned above[4]. Secondly the extraction of physical results from numerical experiments in practice involves accepting some "conventional wisdom" as a plausible working hypothesis. This includes in particular 1) an assumption on the way the continuum limit is approached, and 2) the applicability of renormalized perturbation theory at high energies, the rational of which is the assumed property of asymptotic freedom. The validity of these hypotheses can be made more plausible by studies in simpler models. One can ask whether the validity of asymptotic freedom is at all phenomenologically relevant in its strict sense because it addresses the properties of the model at infinitely large energies, whereas QCD is (at best) an effective theory at intermediate high energies (at higher energies QCD can hardly be unraveled experimentally from the effects of other interactions). The question whether a particular non-perturbative field theory (e.g. QCD) is asymptotically free is however at the very least an interesting academic question.

In section 2 I will thus first introduce the recent work by Balog, Niedermaier and Hauer[5, 6, 7, 8, 9] on the form factor bootstrap approach[10, 11] in the 2-d O(3) non-linar sigma model because their results represent, in my opinion, the best evidence we have at present for the existence of a non-perturbatively defined field theory with asymptotic freedom. Then I will review the general strategy of the computation of a non-perturbatively defined running coupling using finite size recursive methods and a particular application thereof to the sigma-model[4].

The application of the finite size scaling method to the computation of a running coupling in full QCD will still take a few years to complete. Much preparation needs to be done, in particular development of efficient algorithms for simulating fermions and studies of improvement of the action to reduce cut-off effects. In section 4 I will review the Symanzik improvement program[12] applied to Wilson fermions[13], and some of the work done by the Alpha Collaboration to study improved operators and their non-perturbative renormalization which is required to extract physical matrix elements. In these applications the Schrödinger functional again plays a useful role.

The style of these lectures will be rather informal. The aim will be to emphasize the underlying ideas and issues; however, in so doing, many important technical details will be glossed over and for these the interested reader should refer to the original papers.

2. THE 2-d O(N) NON-LINEAR SIGMA MODEL

The "conventional wisdom"

The sigma model is a field theory in two dimensions formally described by the action

$$S = \frac{1}{2g_0^2}\int \mathrm{d}^2x(\partial_\mu\sigma^a)^2 \tag{1}$$

where the fields $\sigma^a(x),\ a = 1, ..., N$ are restricted to lie on a sphere $\sigma^2 = 1$. The model is asymptotically free in renormalized perturbation theory i.e. renormalized running couplings go to zero as momenta $q \to \infty$ according to

$$g^2(q) \sim 1/b_0 \ln(q^2/\Lambda^2), \tag{2}$$

where Λ is the associated (scheme-dependent) lambda-parameter. The quantum model is supposed to have a mass gap with the lowest states above the vacuum an isovector multiplet of single particle states of mass m. In these respects the sigma-model resembles QCD and it is these features together with its comparative accessibility for numerical experiments which makes it a useful laboratory to study the "conventional wisdom". A wonderful property that makes it even more attractive is that the classical model possesses an infinite number of local[14] and non-local conservation laws[15]. Moreover these conservation laws carry over to the quantum theory[16, 17] and imply that in the scattering of two particles there is no particle production. Contrary to the situation in four dimensions this property does not imply that the theory has a trivial S-matrix. Indeed a proposal of the exact 2-2 particle S-matrix was given by the Zamolodchikov brothers[18]

$$\begin{aligned} S_{ik;jl}(p_1,p_2;p_1',p_2') &= \delta(p_1-p_1')\delta(p_2-p_2')\sigma_2(\theta)\times \\ [\delta_{ij}\delta_{kl} - \frac{2\pi i}{N-2}\{\frac{1}{i\pi-\theta}\delta_{ik}\delta_{jl} &+ \frac{1}{\theta}\delta_{il}\delta_{jk}\}] + (i\leftrightarrow k, p_1\leftrightarrow p_2), \end{aligned} \tag{3}$$

a structure which also follows from the existence of the non-local conservation laws[16]. The multiparticle S-matrix elements are simply products of the 2-2 particle S-matrix elements. In Eq. (3) θ_i are rapidities $p_j = m\sinh\theta_j$ and $\theta = |\theta_1 - \theta_2|$. Properties of unitarity, analyticity and crossing together with the assumption of no bound states and the minimum number of poles and zeros in the physical strip fix the function σ_2[18]. The conjecture for the S-matrix already has an element of asymptotic freedom in the sense that the phase shifts approach zero logarithmically with the energy at high energy. Non-perturbative checks of the proposed S-matrix include agreement with the computation of the amplitudes in $1/N$ expansion to order N^{-2} and at low energy the phase shifts in the O(3) model have been measured by Lüscher and Wolff[19] using lattice simulations and found to be in good agreement with Eq. (3).

A further important result was obtained by Hasenfratz, Maggiore and Niedermayer[20] who established the exact ratio of the mass gap to the Λ-parameter

$$\frac{m}{\Lambda_{\overline{\mathrm{MS}}}} = \frac{(8/e)^{1/(N-2)}}{\Gamma[1+1/(N-2)]}\,. \tag{4}$$

To obtain this result requires the ability to compute a physical quantity both perturbatively and non-perturbatively. The quantity they selected was the free energy of the model with a chemical potential h coupled to a Noether charge. For large h one can compute $F(h) - F(0)$ using renormalized perturbation theory. For general h one can also use the thermodynamic Bethe ansatz (supplemented with some plausible assumptions) to derive an integral equation for $F(h)$. This equation, in which the scattering phase shift enters in the kernel, can be solved analytically at large h. A highly non-trivial consistency condition is that the analytic forms of the high h expansions obtained from the non-perturbative and perturbative computations match; in particular that the non-perturbative method reproduces the universal perturbative 1- and 2-loop beta-function coefficients.

Form factor bootstrap approach

Although the results above have not yet been rigorously derived they are already rather strong indication that conventional wisdom is internally consistent. Further stronger evidence in the O(3) case is supplied by the recent work of Balog and Niedermaier[8, 9]. They have pursued the old so-called bootstrap program[10, 11] which observed that in principle correlation functions of a local operators could be constructed if one knew all the matrix elements by saturation by a complete set of intermediate states. Of course the complication of such an explicit complete reconstruction is comparable to the computation of a partition function in statistical mechanics. However, as we shall see shortly, in certain energy regimes a good approximation to the correlation functions is obtained by truncating the sum over intermediate states.

Consider matrix elements of a local operator $\mathcal{O}$ of "spin" s and dimension Δ:

$$\langle\Omega|\mathcal{O}|n; i_n, \theta_n, ...\rangle = (m\sum_j e^{\theta_j})^{\Delta+s}(m\sum_k e^{-\theta_k})^{\Delta-s} f^{(n)}_{i_n,...,i_1}(\mathcal{O};\theta_n,...). \tag{5}$$

The matrix elements are obtained by solving a set of equations - the so-called Smirnov axioms[11] which have the following structure;
I.a (Watson's theorem):

$$f^{(n)}_{i_n,...,i_1}(\mathcal{O};\theta_n,\theta_{n-1},...) = S^{j_{n-1}j_n}_{i_n,i_{n-1}}(\theta_{n,n-1}) f^{(n)}_{j_n,...,i_1}(\mathcal{O};\theta_{n-1},\theta_n,...), \tag{6}$$

I.b (cyclicity) (for a recent derivation see ref.[21]):

$$f^{(n)}_{i_n,...,i_1}(\mathcal{O};\theta_n+2\pi i,\theta_{n-1},...) = f^{(n)}_{i_{n-1},...,i_1,i_n}(\mathcal{O};\theta_{n-1},...,\theta_1,\theta_n), \tag{7}$$

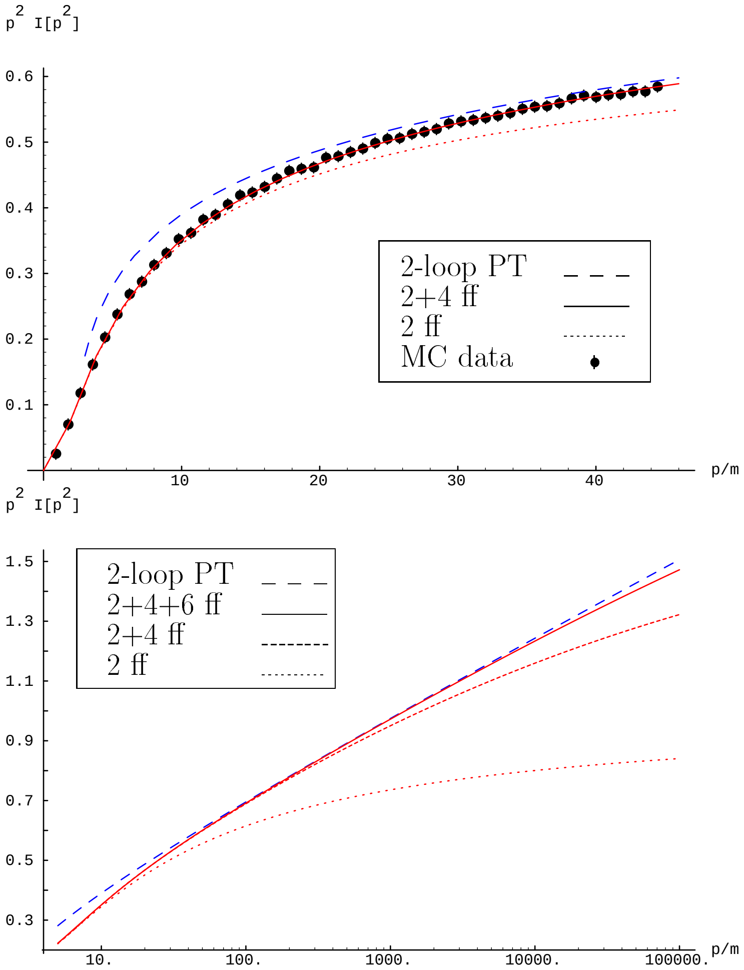

Figure 1. O(3) 2d σ-model current-current correlator (see Eq. (9)).

II. Kinematic residue:

$$\mathrm{Res}_{\theta_n=\theta_{n-1}+i\pi}[f^{(n)}_{i_n,\ldots,i_1}(\mathcal{O};\theta_n,..)] = \mathcal{T}[S]^{j_{n-2},\ldots,j_1}_{i_n,\ldots,i_1}\, f^{(n-2)}_{j_{n-2},\ldots,j_1}(\mathcal{O};\theta_{n-2},..), \tag{8}$$

where $\mathcal{T}$ is determined in terms of the S-matrix[8]. We do not give the explicit form here - the intention of writing down the equations is just to give an impression of the structure; there are two equations inter-relating a fixed particle number and one equation relating an n-particle form factor to a $n-2$ particle form factor. As one can imagine it is highly non-trivial to find a solution of this set of equations, but the problem becomes more tractable in the O(3) case where the S-matrix is a rational function of the rapidity difference θ. Even so the task is formidable but Balog, Niedermaier and Hauer[7] have succeeded to find solutions up to 6-particle matrix elements of the isovector $l=1$ operators: the spin-field σ^a and the Noether current $j^a_\mu = g_0^{-2}\epsilon_{abc}\sigma^b\partial_\mu\sigma^c$ and the isoscalar $l=0$ operators : the energy-momentum tensor $\theta_{\mu\nu} = g_0^{-2}[\partial_\mu\sigma^a\partial_\nu\sigma^a - \frac{1}{2}\eta_{\mu\nu}\partial_\rho\sigma^a\partial_\rho\sigma^a]$ and the topological density $k = \frac{1}{8\pi}\epsilon_{abc}\epsilon_{\mu\nu}\sigma^a\partial_\mu\sigma^b\partial_\nu\sigma^c$. Introducing the current-current 2-point function through

$$\int \mathrm{d}^2x e^{ipx}\langle j^a_\mu(x) j^b_\nu(0)\rangle = \delta^{ab} I(p^2)(p_\mu p_\nu - \delta_{\mu\nu}p^2), \tag{9}$$

a renormalized running coupling can be defined through $\bar{g}(p^2)^{-2} \propto p^2 I(p^2)$. Fig. 1 shows the approximation of including only the intermediate states containing up to 6 particles. There is impressive quantitative agreement with renormalized perturbation theory (using the Hasenfratz-Maggiore-Niedermayer result[20] (4) to convert the 2-loop perturbative result to a function of p/m) up to $p/m \sim 5000$, and up to $p/m \sim 40$ with results obtained from lattice simulations of the standard action[22]. A similar result holds for the spin-spin correlation function.

The Balog-Niedermaier scaling hypothesis

Consider the Källèn-Lehmann spectral decomposition[23]

$$I_{\mathcal{O}}(p^2) = \int_0^\infty d\mu \frac{\rho_{\mathcal{O}}(\mu)}{\mu^2 + p^2} \tag{10}$$

of the invariant amplitude defined by the two-point function of a local operator $\mathcal{O}$ (see e.g. Eq. (9)). From the form factor bootstrap one can show[8] that for $\mu \to \infty$ the n-particle contributions to the spectral function behave as

$$\rho_{\mathcal{O}}^{(n)}(\mu) \sim \frac{A_{\mathcal{O}}^{(n)}}{\mu(\ln\mu)^{4-2l}}, \tag{11}$$

whereas the behavior of the complete spectral function computed in renormalized perturbation theory is given by

$$\rho_1(\mu) \sim \frac{A_{\mathcal{O}}}{\mu}\Big[1 + O\Big(\frac{1}{\ln\mu}\Big) + \ldots\Big], \tag{12}$$

$$\rho_0(\mu) \sim \frac{A_{\mathcal{O}}}{\mu}\Big[\frac{1}{(\ln\mu)^2} + O\Big(\frac{\ln\ln\mu}{(\ln\mu)^3}\Big) + \ldots\Big], \tag{13}$$

for the isospin $l = 1, 0$ operators respectively. Note that each intermediate state with a finite number of particles gives a contribution to the current-current correlation function which is finite as $p \to \infty$. Hence for the asymptotic behavior predicted by perturbation theory to come about the sum of these contributions must diverge.

To get a grasp on the spectral functions involving an arbitrary number of particles Balog and Niedermaier observed that the spectral functions that they had computed so far possessed a remarkable scaling property. Defining new functions $Y_l^{(n)}$ through

$$\rho_l^{(n)}(\mu)/\mu = M_l^{(n)} Y_l^{(n)}\Big(\frac{\ln(\mu/m)}{\xi_l^{(n)}}\Big) \tag{14}$$

where $M_l^{(n)}, \xi_l^{(n)}$ are the values and positions of the maxima of $\rho_l^{(n)}(\mu)/\mu$, they observed that these rescaled functions are strikingly similar even for small n for fixed $l = 0, 1$ as is illustrated in Fig. 2. One can in these cases compare even and odd n (e.g. energy-momentum tensor and topological density spectral functions) since they are related by amazing clustering properties[8].

This similarity encouraged Balog and Niedermaier[9] to make the following scaling hypothesis for $n \to \infty$:

$$Y_l^{(n)} \to Y_l, \quad \xi_l^{(n)} \sim \xi_l n^{1+\alpha_l}, \quad M_l^{(n)} \sim M_l n^{\gamma_l}. \tag{15}$$

Many of the exponents above are connected by consistency conditions and only one must be fitted numerically

$$\alpha_0 = \alpha_1 = \alpha = 0.273, \quad \gamma_0 = 3 + 2\alpha, \quad \gamma_1 = 1. \tag{16}$$

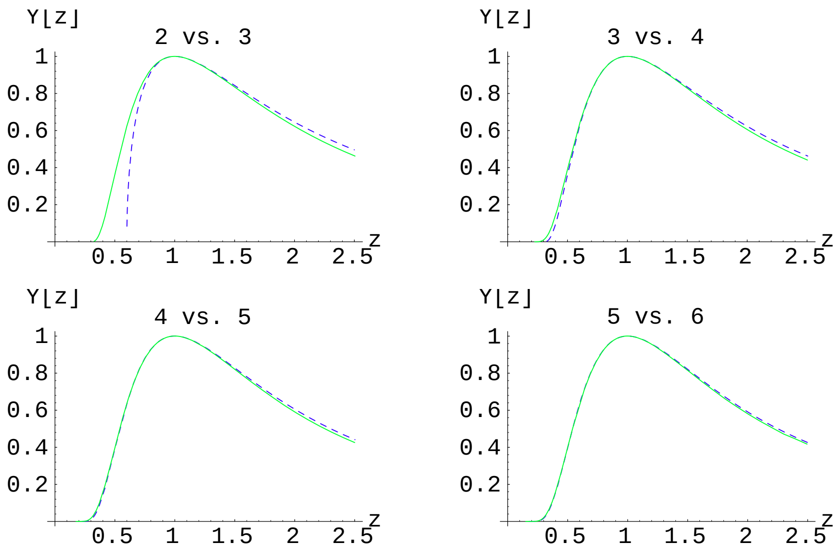

Figure 2. Comparison of consecutive O(3) Isospin 1 n-particle spectral functions.

The consequences of this scaling hypothesis are far-reaching. Firstly if one couples the model to external fermions via the Noether current the n-particle production probability in the fermion scattering is directly related to the spectral function

$$P_{2n} \propto \mu \rho_1^{(2n)}(\mu), \;\; \bar{n} \sim (\ln \mu)^{1/(1+\alpha)}. \tag{17}$$

Thus one finds the form of Koba-Nielsen-Olesen[24] scaling of multi-particle inclusive cross-sections $P_n = \sigma_n(s)/\sigma_{\rm tot}(s)$:

$$\bar{n} P_n \sim \psi(n/\bar{n}) \quad , \quad s \to \infty. \tag{18}$$

Secondly, ultraviolet properties are qualitatively consistent with renormalized perturbation theory and quantities accessible in perturbation theory are typically reproduced to better that 1%. For example e.g. the central charge is given by

$$c = 1.603 + 0.194 + 0.072 + \ldots = 1.997\,, \tag{19}$$

(where the first explicit contributions summing to 1.869 come from the 2,4 and 6 particle states and the rest of the sum obtained using the scaling hypothesis) which is within the systematic errors equal to the expected value[25] 2. Furthermore one finds

$$A^{\rm EM}/A^{\rm EM}_{\rm PT} = 0.99\ . \tag{20}$$

Moreover some normalizations not accessible to PT are fixed[9, 26] e.g.

$$A^{\rm curr} = \frac{\pi}{4} A^{\rm spin}, \;\; A^{\rm EM} = 4 A^{\rm top}\ . \tag{21}$$

Finally the topological density correlation function $\langle k(x) k(0) \rangle$ whose normalization in the form-factor bootstrap approach is fixed by matching with renormalized

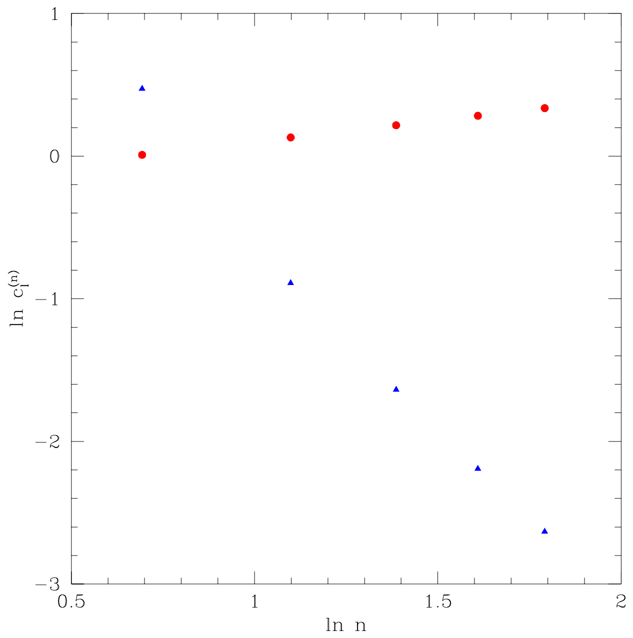

Figure 3. O(3) spectral function integrals $c_l^{(n)}$. The circles correspond to $l = 1$ and the triangles to $l = 0$.

perturbation theory at high energies, agree very well with that obtained by numerical simulations using a geometric definition of the topological charge density. The agreement is obtained only if one assumes that $k(x)$ is not multiplicatively renormalized - a property that would be anticipated for a topological object. Thus some remnant of topology survives although the topological susceptibility $\langle Q^2/V\rangle$ does not seem to have a continuum limit[27] ($\chi/m^2 \to \infty$ as $am \to 0$). The correlation function is everywhere negative for $x \neq 0$ and the susceptibility is rendered positive by the contact term at the origin. Whether a modified physically relevant definition of a topological susceptibility exists is an open question.

In a recent paper Patrascioiu and Seiler[28] have computed the current two-point function in the dodecahedron model (a model of 20 discrete spins arranged on the sphere) and found that up to $p/m = 80$ the amplitude cannot be distinguished from that of O(3) model (after including an overall normalization factor) and seems to have the same continuum limit (incidentally coinciding with the Balog-Niedermaier curve). Since they argue that the dodecahedron model is probably not asymptotically free they conclude the same should be true for the O(3) model. However another plausible interpretation is that their data just shows that for intermediate energies the dodecahedron model is a good "effective asymptotically free model". It is clear that one can not make any definitive statement on which scenario is correct using merely numerical experiments.

A very good indication of the validity of conventional wisdom is however obtained if one looks at Fig. 3 which is a plot of the integrals of the spectral densities

$$c_1^{(n)} = \int d\mu \rho_1^{(n)}(\mu), \quad c_0^{(n)} = 12\pi \int d\mu \rho_0^{(n)}(\mu)\,. \qquad (22)$$

In the scenario of Patrascioiu and Seiler, running couplings approach constants at infinity and hence they would require $c_1^{(n)} \to 0$. There is certainly no sign of this behavior and if it is true then it sets in at high n and hence at astronomic energy scales not accessible to numerical test. Conventional wisdom is thus "effectively true" in this model and any violation would be truly academic.

Measurement of a running coupling using lattice simulations

As in the sigma model a running coupling in QCD can also be defined through a two-point correlation function of currents e.g.

$$\frac{\sigma(e^+e^- \to \text{hadrons})}{\sigma(e^+e^- \to \mu^+\mu^-)} \equiv 3\sum_f Q_f^2\Big(1+\frac{1}{\pi}\alpha_R(q)\Big). \tag{23}$$

However this and other couplings defined in infinite volume are extremely difficult to measure over a wide range of energies while controlling systematic errors at the same time. We will come back to this point in the next section. The proposal to overcome this is to use a recursive finite-size scaling method[4]. Here a running coupling is defined in finite volume $\bar{g}^2(L)$ and its evolution from small to large scales is done recursively. Contact with physical low energy scales is made at large L and at small L we can convert to other schemes e.g. $\overline{\text{MS}}$ using perturbation theory.

Here we outline how the general method proceeds. Consider a theory defined in a volume of finite extent L in some (not necessarily all) directions. Suppose we have defined an "admissible coupling" i.e. a (renormalized) observable $\bar{g}$ depending on L and equal to the bare coupling at tree level perturbation theory. Certainly in the continuum limit there will be a well defined curve $\bar{g}^2(2L)$ versus $\bar{g}^2(L)$ - the so called step scaling function. When we regularize the theory on the lattice the regulated form of the coupling will depend on the number M of points (in the finite directions) and on the bare coupling g_0. A given bare coupling corresponds to a given lattice spacing in units of some inverse physical mass. Thus if we simulate two lattices one with M points and another with $2M$ points at the same bare coupling we are investigating the system with some physical extent and the system with that extent doubled. If we measure $\bar{g}^2(M,g_0)$ and $\bar{g}^2(2M,g_0)$ for a rather random selection of input parameters M,g_0 we will, due to lattice artifacts, obtain a cloud of points (with their associated error bars) from which it would be difficult to precisely extract the continuum step scaling function.

To take the continuum limit one must proceed more systematically. The first step is to consider a sequence of lattices with points $M_1 < M_2 < M_3 ... < M_n$ and for each lattice size M_i determine (through numerical simulation and reweighting) the value of the bare coupling $g_0 = g_{i1}$ so that $\bar{g}$ stays fixed at some given value u_1. Now measure $\bar{g}$ at a sequence of lattices with double the points $2M_i$ but at the same values g_{i1} of the bare couplings. The results of these measurements v_{i1} will not be the same but they should approach a value v_1 corresponding to a point (u_1, v_1) on the continuum curve as $M \to \infty$. If we know the way the continuum limit is approached we can extrapolate v_{i1} without going to very large M_i. Symanzik proposed the limit is approached at a rate proportional to a^p i.e. as the physical length is being held fixed at a rate $\propto 1/M^p$, where p is an integer ≥ 1. It is to be stressed that this is a working hypothesis and it has to be tested. Symanzik's results are within the framework of all orders of perturbation theory but the structural statement is assumed to hold in the non-perturbative framework [the same holds true for renormalizability itself]. Once the continuum limit v_1 is determined we can repeat the procedure with a new fixed value u_2 say $u_2 = v_1$ and so on. In this way we determine a sequence of points on the step scaling function curve.

To carry out such a program and to get confidence that we are controlling the continuum limit it is clear that the coupling must have certain good properties. In

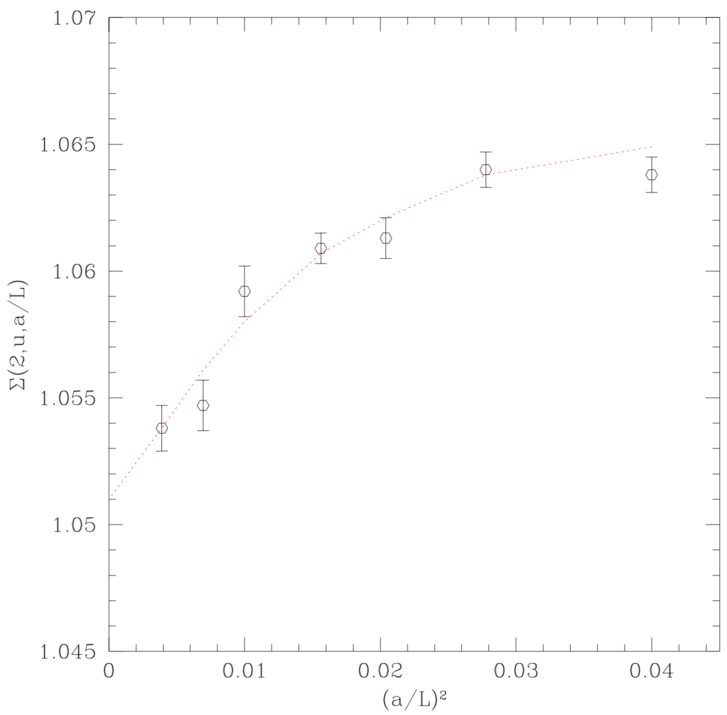

Figure 4. Approach to continuum limit of step scaling function $v = \Sigma(2, u, a/L)$ at $u = 0.9176$. The curve represents a second order fit polynomial in $(a/L)^2$.

particular it must be accurately calculable in numerical simulations. Consider the O(3) sigma-model on an infinite cylinder of circumference L, then a suitable coupling is defined through the (finite volume) mass gap

$$\bar{g}^2(L) = m(L)L. \tag{24}$$

Fig. 4 shows the data of one run of measurements[4], using the standard lattice action, of $\bar{g}^2(2L)$ with $\bar{g}^2(L)$ fixed at the value $u = 0.9176$. The data can certainly be fitted with a form as suggested by Symanzik (here the expected value of p is 2). One observes that in this case the continuum limit is approached from above. This is contrary to what happens at smaller renormalized couplings where perturbation theory predicts the limit to be approached from below. We are thus seeing some non-perturbative behavior at least on the level of cut-off effects. The same qualitative behavior at large coupling is also seen in the leading order of the $1/N$ expansion as illustrated in Fig. 5. Here all computations can be done analytically and one sees that the continuum limit is indeed approached at a rate $O(a^2)$ modulated by possible logarithmic factors.

By performing various steps of factor two we end up with the step scaling function over a wide range of energies. It remains to make contact with the low energy scale. For the particular quantity we are studying here this is rather easy. At a some large attained value of $\bar{g}^2(L)$ we simulate $\bar{g}^2(sL)$ for large s. The physical volume is now so big that we can expect finite volume corrections to be very small[29]

$$m(L) = m\Big(1 + O(e^{-cmL})\Big). \tag{25}$$

We finally obtain the running coupling over a wide range of energies as a function of mL. I will not show this plot here, but instead include Fig. 6 which shows approximations to m/Λ by taking 2,3 and 4 loop approximations to the Λ-parameter as a

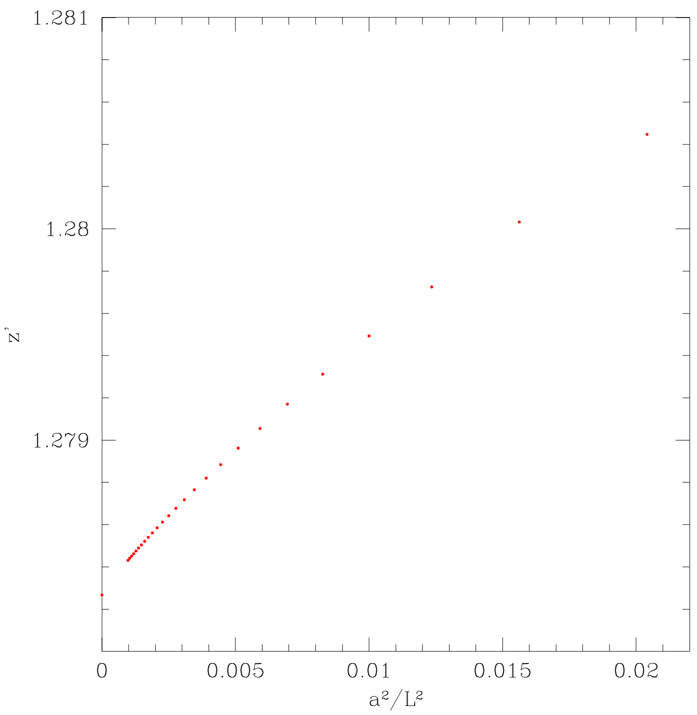

Figure 5. Approach to continuum limit of step scaling function $v = z' = \Sigma(2, u, a/L)$ at $u = 1$ in the limit $N = \infty$.

function of $\bar{g}(L)$. This is an update of the plot in the original paper[4] extended by the 4-loop computation of Shin[30] and new MC data at smaller $\bar{g}^2(L)$ of Hasenbusch[31]. Note that there is an indication of the 3,4-loop curves approaching the limit from below. The result is thus so far well consistent with the theoretical prediction[20, 32].

3. RUNNING COUPLINGS IN THE PURE YANG-MILLS THEORY

As mentioned previously one of the goals of the Alpha Collaboration is to obtain $\alpha_{\overline{\rm MS}}(m_Z)$ with a controlled error of say 1% i.e. without compromising approximations. To reach this goal we need at least four ingredients

- 1. An accurate determination of a reference low energy scale
- 2. A non-perturbatively defined running coupling $\alpha(q)$ accurately computable through numerical simulation over a wide range of q
- 3. A careful extrapolation to the continuum limit
- 4. The perturbative relation of our coupling to that of the $\overline{\rm MS}$-scheme to two loop order

  $$\alpha_{\overline{\rm MS}}(sq) = \alpha(q) + c_1(s)\alpha(q)^2 + c_2(s)\alpha(q)^3 + \ldots \qquad (26)$$

  where s is a so-called boost factor at our disposal.

Points 1-3 were encountered in the study of the sigma-model in the last section. Point 4 enters because once we have indeed checked that the chosen coupling runs at high energy according to the perturbative renormalization group, we can at the highest energies measured relate our coupling via perturbation theory to the $\overline{\rm MS}$-scheme. Since

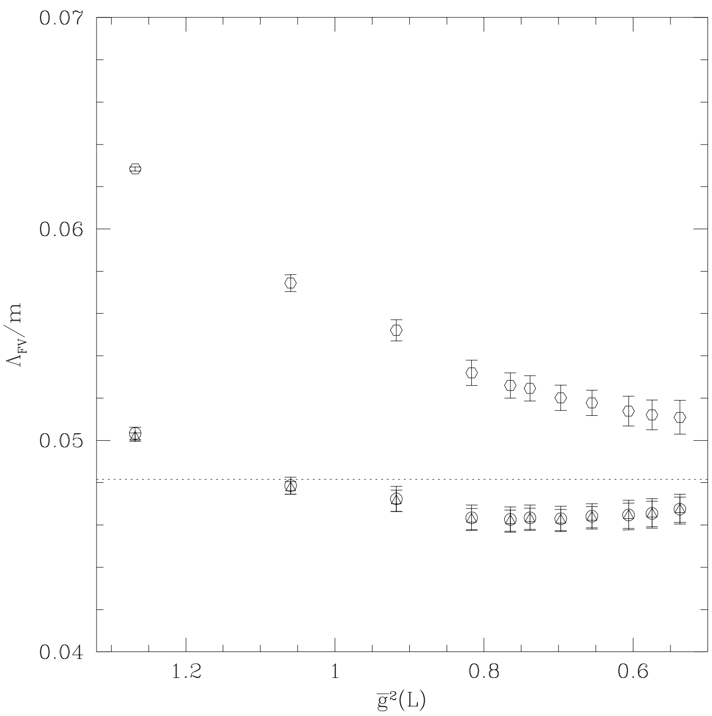

Figure 6. Approximations to m in units of the finite volume Λ-parameter, Λ_{FV}, in the O(3) model. The dotted line is the prediction of Hasenfratz, Maggiore and Niedermayer[20]. The upper points correspond to 2-loop and the lower points to 3,4-loop.

$\alpha_{\overline{\mathrm{MS}}}(m_Z)$ is expected to be ~ 0.1, to achieve 1% accuracy we need the perturbative relation to two loops (at least).

As a first step we consider the pure SU(3) Yang-Mills theory. There are many definitions of running couplings (see e.g. ref.[33]). The basic difficulty is that for a given coupling its low- and high-energy properties must be related to each other. Consider as an example the coupling $\alpha_{\mathrm{q\bar{q}}}$ defined in infinite volume through the force between static quarks at distance r

$$F_{\mathrm{q\bar{q}}}(r) = \frac{4}{3}\frac{\alpha_{\mathrm{q\bar{q}}}}{r^2}. \tag{27}$$

$\alpha_{\mathrm{q\bar{q}}}$ is a "running" coupling at momentum $q = 1/r$ and its relation to the $\overline{\mathrm{MS}}$-coupling is given by

$$\alpha_{\overline{\mathrm{MS}}} = \alpha_{\mathrm{q\bar{q}}} - 0.082 \times (\alpha_{\mathrm{q\bar{q}}})^2 + \ldots \tag{28}$$

Now if we take for example a lattice with 32^4 points and require $L \geq 2$fm to avoid large finite size effects the lattice spacing is $a \geq 0.06$fm. Further to avoid significant cutoff effects we should take $r \geq 3a$ (at the very least) and thus we are restricted to rather low energies $q \leq 2$GeV. The situation is illustrated in Fig. 7 of the force in pure SU(2) gauge theory. Although this plot is rather familiar to workers in lattice theory, I include it again here for the non-experts because it has some beautiful features. Firstly one sees that the force is consistent with tending to a constant K (the string tension) at large r - which is a manifestation of Wilson's criterion of static confinement[13]. Secondly there is evidence of the presence of a $1/r^2$ correction with a coefficient predicted by Lüscher[34] assuming the validity of an effective string picture. Perhaps surprising is that this long distance (i.e. non-perturbative) formula provides also a good quantitative description down to quite short distances.

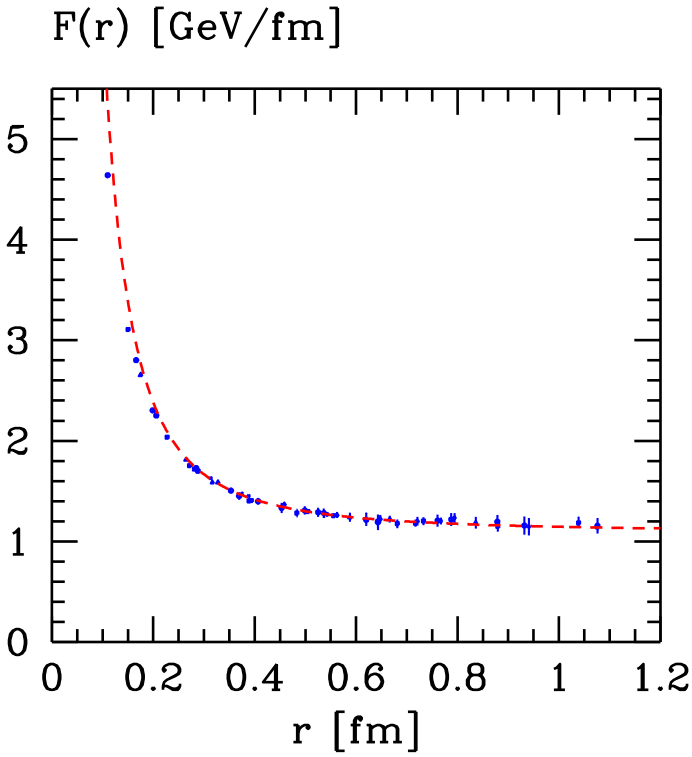

Figure 7. The force in pure SU(2) Yang-Mills theory, the dashed line represents Lüscher's force: $K + \frac{\pi}{12r^2}$.

Also we can see that Sommer's scale[35] r_0 defined as the distance where $r_0^2 F_{q\bar{q}}(r_0) = 1.65$ is rather precisely computable in present simulations and is hence a good low energy reference scale (see point 1 above) in pure gauge theories (and probably also in QCD). In nature (i.e. potential models applied to quarkonium) one finds $r_0 \sim 0.5$fm. (In pure SU(3) gauge theory $r_0\sqrt{K} = 1.18(2)$).

Now one could make (and of course it has been done) the daring assumption that for this coupling perturbative running sets in already at a low scale. But it is obviously better if we can avoid making such ad hoc assumptions.

As we saw illustrated in the sigma model, a way to overcome the difficulty is to define a coupling $\bar{g}(L)$ depending on the volume and use a finite step scaling technique. The finite volume is thus used as probe of the theory instead of being considered a source of systematic error. As stated previously it is important to make a good choice of the non-perturbatively defined $\bar{g}$ so that

- it is accurately computable by numerical simulation
- it has small cutoff effects
- it has an easy perturbative expansion

In our experience these properties are not easy to fulfill. In the next sub-section we will define a coupling through the Schrödinger functional but it is important to realize that there are many other proposals including in particular one which has been systematically studied[36, 37] which is defined by correlations of Polyakov loops in a volume with twisted boundary conditions.

The Schrödinger functional

Consider the SU(N) Yang-Mills theory on a "cylinder" $[0,T]\times S^1\times S^1\times S^1$. We impose periodic boundary conditions in the spatial directions and Dirichlet boundary conditions at the caps $t=0,T$:

$$A_k(x)|_{x_0=0}=C_k(\mathbf{x}),\quad A_k(x)|_{x_0=T}=C'_k(\mathbf{x})\,. \tag{29}$$

The Schrödinger functional[3, 38, 39] is the partition function with these boundary conditions and formally given by the integral

$$\mathcal{Z}[C',C]=\int D[A]\,\mathrm{e}^{-S[A]}. \tag{30}$$

In the continuum one also has to integrate over gauge transformations of the boundary conditions at one end. Going to a Hamiltonian picture one obtains the quantum mechanical interpretation of the Schrödinger functional as a propagation kernel

$$\mathcal{Z}[C',C]=\langle C'|\mathrm{e}^{-\mathrm{H}T}\mathrm{P}|C\rangle \tag{31}$$

where H is the Hamilton operator and P the projector on gauge invariant states.

In the lattice formulation the gauge fields are replaced by a field of matrices $U(x,\mu)\in\mathrm{SU}(N)$, associated with the lattice links. On the boundary the matrices are related to the continuum fields C_k through

$$U(x,k)|_{x_0=0}=\mathcal{P}\exp\left\{a\int_0^1\mathrm{d}t\,C_k(\mathbf{x}+(1-t)a\hat{\mathbf{k}})\right\}. \tag{32}$$

For lattice action we take

$$S[U]=\frac{1}{g_0^2}\sum_{\text{plaquettes }p}w(p)\,\mathrm{tr}\{1-U(p)\} \tag{33}$$

i.e. the standard Wilson one plaquette action. The weights $w(p)$ which differ from 1 only for plaquettes touching the boundary are introduced for the possibility of diminishing some of the O(a) cutoff effects. The lattice regularized Schrödinger functional

$$\mathcal{Z}[C',C]=\int\prod_{x,\mu}\mathrm{d}U(x,\mu)\,\mathrm{e}^{-S[U]} \tag{34}$$

is a well defined gauge invariant functional of C,C'.

For the Schrödinger functional perturbation theory is the expansion about a "background field" i.e the field $B_\mu(x)$ with minimal action satisfying the prescribed boundary conditions. Consider for example constant Abelian boundary fields

$$C_k=\frac{i}{L}\times\mathrm{diag}\{\phi_1,\phi_2,\ldots,\phi_N\},\qquad k=1,2,3, \tag{35}$$

(here L is the circumference of the circles S^1) and similarly C', with angles ϕ_α satisfying

$$\phi_1<\phi_2<\ldots<\phi_N,\quad \phi_N-\phi_1<2\pi,\quad \sum_{\alpha=1}^N\phi_\alpha=0\,. \tag{36}$$

In this case it is easy to see that the induced background field is a constant color-electric field

$$B_0=0,\qquad B_k=\frac{x_0}{T}(C'_k-C_k)+C_k\,. \tag{37}$$

The lattice background field is simply $V_\mu(x) = e^{B_\mu(x)}$. For the specific boundary conditions Eqs. (35,36) one can show[39] that V is the unique global minimum of the action. This is an important result since it guarantees the stability of the perturbative expansion in this case.

The renormalization of the Schrödinger functional was first discussed by Symanzik[3]. He found that, in general, space-time boundaries with Dirichlet boundary conditions induce additional UV divergences, but that these can be cancelled by adding boundary counterterms to the action:

$$\int \mathrm{d}^3\mathbf{x}\, \{\mathcal{L}_\mathrm{b}(x)|_{x_0=0} + \mathcal{L}'_\mathrm{b}(x)|_{x_0=T}\} \ . \tag{38}$$

Here $\mathcal{L}_\mathrm{b}(x)$ is a linear combination of local fields of dimension $d \le 3$, invariant under both spatial and internal symmetries. Indeed in scalar field theories one has boundary counterterms proportional to $\phi^2, \phi\partial_0\phi$. But in pure gauge theory there are no such (gauge invariant) fields which leads us to the conclusion that the effective action $\Gamma[B] - \Gamma[0] = \ln(\mathcal{Z}[B]/\mathcal{Z}[0])$ is finite after renormalization of the coupling (done exactly as in infinite volume). This has been checked explicitly to two loops PT[40, 41].

Now to define a running coupling one notes that

$$\Gamma[B] = \frac{1}{g_0^2}\Gamma_0[B] + \Gamma_1[B] + \ldots \ \propto \ \frac{1}{\bar{g}^2} \, . \tag{39}$$

To render the definition finite one makes the field B dependent on a parameter η and defines the coupling as the response of the system to a change of the boundary conditions

$$\bar{g}^{-2}(L) = \left(\frac{\partial\Gamma}{\partial\eta}/\frac{\partial\Gamma_0}{\partial\eta}\right)\Big|_{\eta=0} \ . \tag{40}$$

For the simulation we set $T = L$ and chose constant Abelian boundary fields as in Eqs. (35,36) with a specific choice of the angles (for the case of SU(3))

$$(\phi_1, \phi_2, \phi_3) = \frac{1}{3}(-\pi, 0, \pi) + \frac{1}{2}(2, -1, -1)\,\eta \, , \tag{41}$$

and a similar expression for $(\phi'_1, \phi'_2, \phi'_3)$. The field (41) was found (after some trial) to represent a good choice in that the resulting coupling has a good signal and relatively small cutoff effects, thus satisfying our selection criteria above. Note that our observable is actually a set of plaquette expectation values at the boundary, which are accurately measurable. For large volumes our coupling is expected to diverge exponentially i.e. the observable becomes very small and hence accurate measurement is more difficult if the fluctuations are relatively large.

Now we have found a suitable definition of the coupling the finite step scaling analysis proceeds as in the sigma model as described in the previous section. An important step is, as we have stressed before, the extrapolation to the continuum limit. Here, if we follow Symanzik's ideas we expect the dominant cutoff effects to be $\mathrm{O}(a)$ and accordingly make a linear extrapolation of the data as illustrated in Fig. 8.

Having carried out this procedure during our investigations[2] in 1993 we ended up with Table 1. Note that by combining the evolution steps we obtained the evolution of $\bar{g}^2(L)$ from 1.243 to 3.474, corresponding to a total scale factor of about 25. In the meantime, in the process of computing the running quark mass in quenched QCD[42], we have refined this analysis and gone to smaller values of $\bar{g}$ and reached a scale factor of around 64.

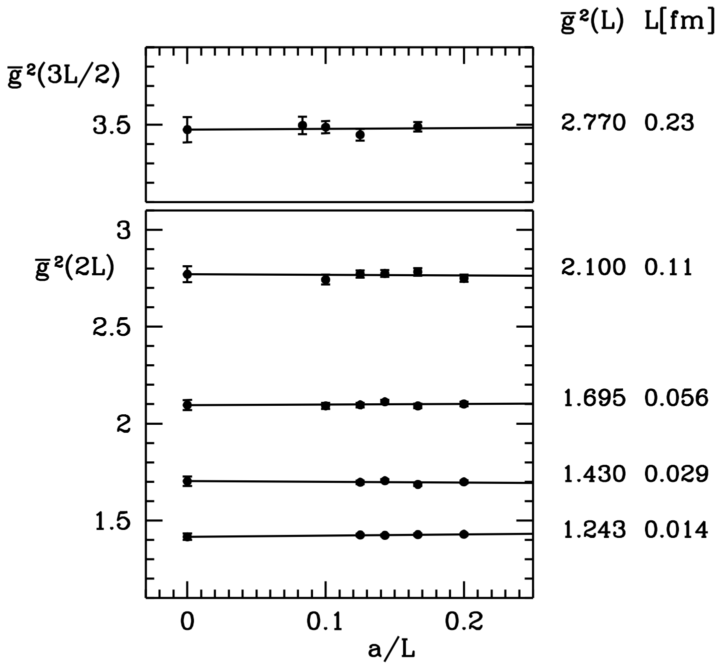

Figure 8. Taking the continuum limit of the step scaling function (SU(3)).

Table 1. Evolution of $\bar{g}^2(L)$ (SU(3)) in the continuum limit

s	$\bar{g}^2(L)$	$\bar{g}^2(sL)$
2	1.243	1.416(16)
2	1.430	1.703(24)
2	1.695	2.095(25)
2	2.100	2.771(41)
3/2	2.770	3.474(65)

Finally we must make contact with the low energy scales. Let us define

$$L_{\max} \equiv \text{value of } L \text{ where } \bar{g}^2(L) = 3.480\,. \tag{42}$$

The question is now: how large is $L_{\max}$ in physical units for example in terms of Sommer's scale r_0? To obtain this we note that both factors on the rhs of

$$L_{\max}/r_0 = (L_{\max}/a)(r_0/a)^{-1} \tag{43}$$

are functions of g_0 that can be determined separately. The procedure is then as follows. We choose a value of g_0 and compute r_0/a on a large lattice, avoiding finite-volume effects. Then at the same g_0 compute $\bar{g}^2(L)$ for a range of L/a and find $L_{\max}/a$ through interpolation. The results are not independent of g_0, but we expect

$$L_{\max}/r_0 = \text{constant} + \mathrm{O}(a/L_{\max}) \tag{44}$$

and this is born out by the data as illustrated in Fig. 9.

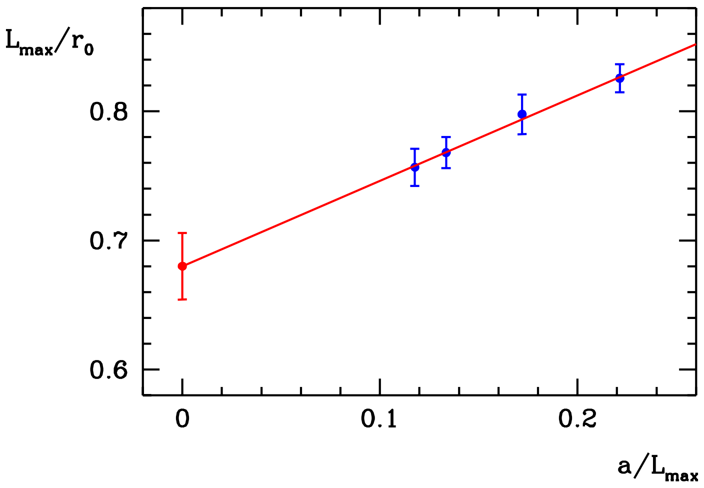

Figure 9. Extrapolation of $L_{\max}/r_0$ to the continuum limit (SU(3)).

Fig. 10 shows the SF running coupling in pure SU(3) Yang-Mills theory[42] as a function of the energy calibrated by r_0. This is a truly impressive plot and clearly demonstrates that the data are well described by perturbative running at large energies. What is perhaps surprising is that the true non-perturbative running is well described by perturbative running right down to low energies. We emphasize that this is not a universal property of couplings; on the other hand it shows that some naturally defined couplings with this striking property exist.

The 3-loop beta-function is now known in this scheme[41] and using this we can extract a quite accurate value of the Λ-parameter in this scheme. Converting to the $\overline{\mathrm{MS}}$-scheme we obtain in pure SU(3) Yang-Mills theory

$$\Lambda^{(0)}_{\overline{\mathrm{MS}}} = 251(20)\mathrm{MeV}\,. \tag{45}$$

Previous estimates using the potential[43, 44, 45] indeed produced similar values but the present analysis certainly has a much better control of the systematic errors.

Some estimates of the running coupling in full QCD using the assumption of perturbative running already at small scales have been made[46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57]. The results are indeed consistent with experiment but it is surely very difficult to make a reliable estimate of the systematic errors. It will still take a few years to do a similarly good job on the running coupling in full QCD as we have now for the quenched theory. One requires accurate measurements which in turn require improved algorithms for fermions and also powerful computers. However the definition of the coupling introduced above can be readily extended to the theory with fermions since, as we shall see in the next section the Schrödinger functional is defined in the full theory with quarks[58]. In fact the Schrödinger functional has a wider range of applications and turns out to be a very useful tool for purposes of studying chiral symmetry and determining renormalization constants of composite operators.

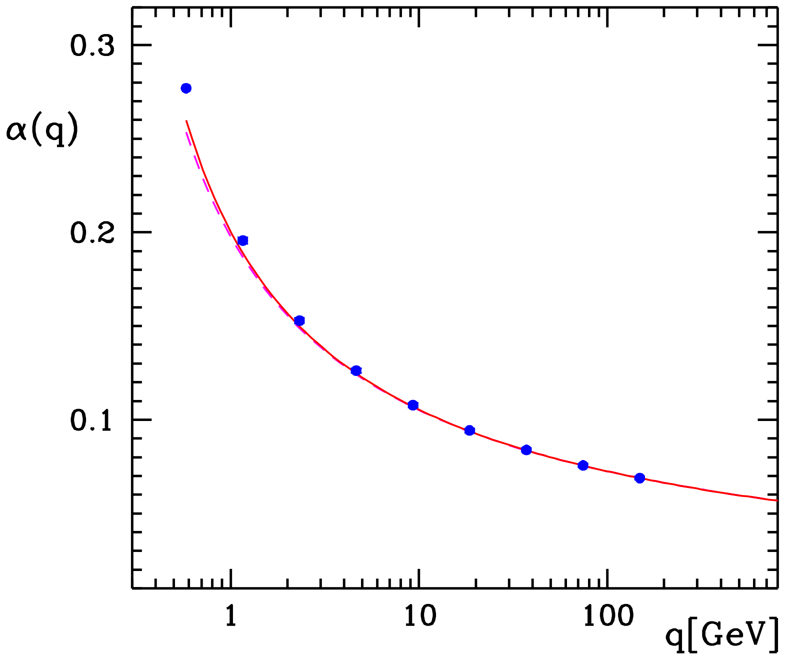

Figure 10. The SF running coupling in pure SU(3) Yang-Mills theory. The curves indicate 2-,3-loop running staring the integration at the highest energy.

4. IMPROVED FERMION ACTION AND NON-PERTURBATIVE RENORMALIZATION

If one constructs a lattice regulated free fermion action naively by just replacing the derivative in the Dirac operator by a simple difference operator one finds that the energy-momentum dispersion has extra minima and the continuum limit of the lattice theory contains 16 particles instead of 1. To lift this degeneracy (at the same time maintaining the usual classical continuum limit) Wilson[13] proposed to use an action which has an additional term of dimension 5

$$S = S_{\rm gluon} + S_{\rm quark}\,, \tag{46}$$

$$S_{\rm quark} = a^4 \sum_x \overline{\psi}(x)(D + m_0)\psi(x)\,. \tag{47}$$

Here m_0 is the bare quark mass and the Wilson-Dirac operator is given by

$$D = \frac{1}{2}\{\gamma_\mu(\nabla_\mu^* + \nabla_\mu) - a\nabla_\mu^*\nabla_\mu\}\,, \tag{48}$$

where ∇_μ, ∇_μ^* are gauge covariant forward and backward difference operators.

The Wilson action has many good properties e.g. a positive definite transfer matrix[59]. But it has one disadvantage - the Wilson term $\nabla_\mu^*\nabla_\mu$ violates chiral symmetry. This has several implications. Firstly chiral Ward identities are violated by terms of $\mathrm{O}(a)$ and thus low-energy theorems are generally affected. Secondly the quark mass requires additive renormalization (in addition to the customary multiplicative renormalization). Another consequence is that the axial current must be renormalized by a finite multiplicative renormalization constant and mixing of composite operators with different chiralities is not excluded. All these difficulties do not represent a fundamental problem but they do imply that, as indicated above, renormalization is more complicated and the continuum limit is reached only very slowly. Indeed, because of the presence of the Wilson term, cutoff effects are expected proportional to the lattice spacing a and this can be rather large for typical values of the Monte Carlo simulation parameters. Decreasing the lattice spacing at constant physical length scales means simulating lattices with a larger number of points and thus a significant increase in the cost (in time) of the simulation.

Diminishing cutoff effects

To make progress in controlling the cutoff effects other than the brute force method of simulating very large lattices, we need some theoretical understanding of cutoff effects in a general lattice theory. There are presently unfortunately very few rigorous non-perturbative statements in this respect. However there is a very plausible framework due to Symanzik[12], which we have already mentioned in previous sections, which he obtained through a systematic study of the continuum limit of lattice Feynman diagrams. Symanzik proposed that the structural properties that he found in perturbation theory should also hold at the non-perturbative level. To be precise he proposed that at energies well below the cutoff, the lattice theory is equivalent to an effective continuum theory with effective action

$$S_{\mathrm{eff}} = S_0 + aS_1 + a^2 S_2 + \dots \tag{49}$$

where S_i are integrals of local operators of dimension $4+i$ having the symmetries of the lattice theory. In Wilson's formulation of QCD we expect the leading correction[60]

$$S_1 = \int \mathrm{d}^4 x \, \mathcal{L}_1(x) \tag{50}$$

where $\mathcal{L}_1$ is a linear combination of local gauge invariant scalar fields of dimension 5. A linearly independent set of such operators is given by

$$\mathcal{O}_1 = \overline{\psi}\, \sigma_{\mu\nu} F_{\mu\nu} \psi, \tag{51}$$

$$\mathcal{O}_2 = \overline{\psi}\, D_\mu D_\mu \psi + \overline{\psi}\, \overleftarrow{D}_\mu \overleftarrow{D}_\mu \psi, \tag{52}$$

$$\mathcal{O}_3 = m \,\mathrm{tr}\left\{F_{\mu\nu} F_{\mu\nu}\right\}, \tag{53}$$

$$\mathcal{O}_4 = m \left\{ \overline{\psi}\, \gamma_\mu D_\mu \psi - \overline{\psi}\, \overleftarrow{D}_\mu \gamma_\mu \psi \right\}, \tag{54}$$

$$\mathcal{O}_5 = m^2\, \overline{\psi} \psi\,. \tag{55}$$

In the effective theory renormalized local lattice fields $\phi_{\mathrm{R}} = Z_\phi \phi$ are represented by

$$\phi_{\mathrm{eff}} = \phi_0 + a\phi_1 + a^2 \phi_2 + \dots \tag{56}$$

(where ϕ_i are local operators in the continuum theory) in the sense that renormalized lattice n-point correlation functions

$$G_n(x_1, \dots, x_n) = (Z_\phi)^n \left\langle \phi(x_1) \dots \phi(x_n) \right\rangle_{\mathrm{con}} \tag{57}$$

at fixed separated points x_k are given by

$$\begin{aligned}
G_n(x_1,\dots,x_n) &= \langle\phi_0(x_1)\dots\phi_0(x_n)\rangle_{\rm con} \\
&-a\int \mathrm{d}^4y\ \langle\phi_0(x_1)\dots\phi_0(x_n)\mathcal{L}_1(y)\rangle_{\rm con} \\
&+a\sum_{k=1}^{n}\langle\phi_0(x_1)\dots\phi_1(x_k)\dots\phi_0(x_n)\rangle_{\rm con}+\mathrm{O}(a^2)\,,
\end{aligned} \tag{58}$$

where the expectation values on the right hand side are taken in the continuum theory.

The effective action above contains a large number of operators even if we are only interested in describing the leading cutoff effects. It is important to remark that the situation is greatly simplified by restricting attention to on-shell quantities[60] since for this purpose some of the operators in the effective action become "redundant". This comes about by considering the field equations which imply for example

$$\mathcal{O}_4 + c\,\mathcal{O}_5 = 0, \qquad c = 2+\mathrm{O}(g^2)\,, \tag{59}$$

which is true when inserted in a correlation function, up to contact terms which can be absorbed by a redefinition of ϕ_1 in Eq. (56). Thus $\mathcal{O}_4$ may be eliminated in favor of $\mathcal{O}_5$ in correlation functions with fields at non-zero physical distances from each other from which all on-shell data can be extracted. Similarly $\mathcal{O}_2$ can also be eliminated and we conclude that $\mathcal{L}_1$ can be expressed as a linear combination of $\mathcal{O}_1,\mathcal{O}_3,\mathcal{O}_5$ as far as on-shell quantities are concerned.

The implications of Symanzik's analysis is that it must be possible to construct an $\mathrm{O}(a)$ on-shell improved lattice action so that the S_1-term in its associated effective action vanishes by adding $\mathrm{O}(a)$ counterterms[12] δS of the form

$$\delta S = a^5\sum_x\left\{c_1\widehat{\mathcal{O}}_1(x)+c_3\widehat{\mathcal{O}}_3(x)+c_5\widehat{\mathcal{O}}_5(x)\right\} \tag{60}$$

where $\widehat{\mathcal{O}}_{\rm i}$ are lattice counterparts of $\mathcal{O}_{\rm i}$. The terms proportional to $\widehat{\mathcal{O}}_3$ and $\widehat{\mathcal{O}}_5$ in (60) may be dropped, because they simply correspond to a renormalization of the bare coupling and mass. An $\mathrm{O}(a)$ improved action in QCD, first proposed by Sheikholeslami and Wohlert[61], is thus given by

$$S_{\rm impr} = S_{\rm Wilson} + a^5\sum_x c_{\rm sw}\,\overline{\psi}(x)\frac{i}{4}\sigma_{\mu\nu}\widehat{F}_{\mu\nu}(x)\psi(x) \tag{61}$$

where $\widehat{F}_{\mu\nu}(x)$ is a lattice version of the field strength tensor (and the conventions for the Dirac matrices are as in ref.[60]). The coefficient $c_{\rm sw}(g_0)$ appearing here must be tuned to achieve cancellation of $\mathrm{O}(a)$ effects in on shell quantities. At small g_0 it can be computed perturbatively and to one-loop order PT

$$c_{\rm sw} = 1+0.2659\times g_0^2+\mathrm{O}(g_0^4) \qquad (N=3,\ \text{any } N_{\rm f}). \tag{62}$$

This was first computed by Wohlert[62] by improving the residue of a pole in the S-matrix (in a volume finite in two directions with twisted boundary conditions), and later checked by improving certain correlation functions constructed using the Schrödinger functional[63] (see later).

The action can in principle be improved further to order a^2, but this involves introduction of many new operators of dimension 6. For the pure Yang-Mills theory the structure of the on-shell $\mathrm{O}(a^2)$ improved action is relatively simple[64], but for the theory with quarks the required set of operators contains also those involving products of 4 quark fields. The fact that the action is then no longer quadratic in the fermion fields causes extra complications for the numerical simulations and becomes impractical. Indeed, in general, improved actions are more difficult to simulate and one must ensure that the gain in reduction of cutoff effects is not swamped by the loss in simulation time. For the SW improved action above this problem is not severe because its structure is comparatively simple; with respect to the Wilson action it has just one extra term which involves the quark fields at the same space-time point.

Another effect of improving the action is that positivity of the transfer matrix is lost in general. Although positivity is a very nice property which one would have preferred to keep if possible it is not a necessity for the regularized theory. Indeed in the cases one can study explicitly one finds that the complex eigenvalues of the transfer matrix occur at energies of the order of the ultra-violet cutoff and hence not dangerous.

Improved operators

If one is only considering spectral quantities it is sufficient to improve the action. But if one is interested in matrix elements of renormalized operators one must also improve the corresponding lattice operators.

Consider for example in the theory with two degenerate flavors the following set of bare isovector operators bilinear in the quark fields:

$$V^a_\mu(x) = \overline{\psi}(x)\gamma_\mu\frac{1}{2}\tau^a\psi(x), \tag{63}$$

$$A^a_\mu(x) = \overline{\psi}(x)\gamma_\mu\gamma_5\frac{1}{2}\tau^a\psi(x), \tag{64}$$

$$T^a_{\mu\nu}(x) = i\overline{\psi}(x)\sigma_{\mu\nu}\frac{1}{2}\tau^a\psi(x), \tag{65}$$

$$S^a(x) = \overline{\psi}(x)\frac{1}{2}\tau^a\psi(x), \tag{66}$$

$$P^a(x) = \overline{\psi}(x)\gamma_5\frac{1}{2}\tau^a\psi(x), \tag{67}$$

where τ^a are the Pauli matrices. By inspection of symmetry properties the corresponding O(a)-improved (unrenormalized) fields are

$$(V_{\rm I})^a_\mu = V^a_\mu + c_{\rm V}a\tilde{\partial}_\nu T^a_{\mu\nu}, \tag{68}$$

$$(A_{\rm I})^a_\mu = A^a_\mu + c_{\rm A}a\tilde{\partial}_\mu P^a, \tag{69}$$

$$(T_{\rm I})^a_{\mu\nu} = T^a_{\mu\nu} + c_{\rm T}a[\tilde{\partial}_\mu V^a_\nu - \tilde{\partial}_\nu V^a_\mu], \tag{70}$$

$$(P_{\rm I})^a = P^a, \tag{71}$$

$$(S_{\rm I})^a = S^a, \tag{72}$$

where $\tilde{\partial}_\mu$ denotes the symmetrized lattice derivative $\frac{1}{2}(\partial_\mu + \partial^*_\mu)$. The coefficients $c_{\rm A}(g_0), c_{\rm V}(g_0)$ and $c_{\rm T}(g_0)$ must be chosen so as to cancel any remaining terms of O(a) in correlation functions involving the corresponding operators. To one-loop order PT[63, 65]

$$c_{\rm A} = -0.005680(2) \times C_{\rm F}g_0^2 + {\rm O}(g_0^4), \tag{73}$$

$$c_{\rm V} = -0.01225(1) \times C_{\rm F}g_0^2 + {\rm O}(g_0^4), \tag{74}$$

$$c_{\rm T} = 0.00896(1) \times C_{\rm F}g_0^2 + {\rm O}(g_0^4), \tag{75}$$

(for any $N_{\rm f}$) where $C_{\rm F} = (N^2-1)/2N$.

Mass-independent renormalization schemes

Before going on to consider methods to determine improvement coefficients let us first discuss the renormalization scheme. For practical purposes it is convenient to use mass-independent renormalization schemes[66]. The only complication is that for compatibility with O(a) improvement mass-independent renormalization schemes require slight modifications from what is usually done and must have the form:

$$g_{\mathrm{R}}^2 = \tilde{g}_0^2 Z_{\mathrm{g}}(\tilde{g}_0^2, a\mu)\,, \tag{76}$$

$$m_{\mathrm{R}} = \widetilde{m}_{\mathrm{q}} Z_{\mathrm{m}}(\tilde{g}_0^2, a\mu)\,, \tag{77}$$

where the modified bare coupling and mass are defined by

$$\tilde{g}_0^2 = g_0^2\,(1 + b_{\mathrm{g}} a m_{\mathrm{q}})\,, \quad m_{\mathrm{q}} = m_0 - m_{\mathrm{c}}\,, \tag{78}$$

$$\widetilde{m}_{\mathrm{q}} = m_{\mathrm{q}}\,(1 + b_{\mathrm{m}} a m_{\mathrm{q}})\,. \tag{79}$$

To see how this more complicated structure comes about consider for example the "pole mass" of a free quark. It is given by

$$m_{\mathrm{p}} = \frac{1}{a}\ln(1 + a m_0) = m_{\mathrm{q}} - \frac{1}{2} a m_{\mathrm{q}}^2 + \ldots \tag{80}$$

and hence to tree level one immediately sees $b_{\mathrm{m}} = -1/2$.

To appreciate the necessity of the factor involving b_{g} in Eq. (78) consider the SF running coupling introduced in the last section. The perturbation expansion in the theory with N_{f} dynamical quarks

$$\bar{g}^2 = g_0^2 + [c^{(1,0)} + c^{(1,1)} N_{\mathrm{f}}] g_0^4 + \ldots \tag{81}$$

has been worked out to 1 loop in ref.[67]. The O(a) counterterms required for the improvement of the Schrödinger functional were taken into account in this calculation. If we insert the definition of the renormalized mass (with the value of b_{m} just obtained) $m_{\mathrm{R}} = m_{\mathrm{q}}(1 - \frac{1}{2} a m_{\mathrm{q}}) + O(g_0^2)$ the result assumes the form

$$c^{(1,0)} = \frac{11N}{24\pi^2}\ln(L/a) + k_1 + O(a^2), \tag{82}$$

$$c^{(1,1)} = -\frac{1}{12\pi^2}\ln(L/a) + k_2 + k_3 a m_{\mathrm{R}} + O(a^2), \tag{83}$$

where k_2 is a function of $m_{\mathrm{R}} L$ and

$$k_3 = 0.012000(2). \tag{84}$$

We can now express $\bar{g}^2$ as a series in the renormalized coupling g_{R}^2 by eliminating the bare coupling. The renormalization factor $Z_{\mathrm{g}}^{(1)}(a\mu)$ should be chosen so as to cancel the logarithmic divergence, but since it may not depend on the quark mass, the additional factor $1 + b_{\mathrm{g}}^{(1)} g_0^2 a m_{\mathrm{q}}$ is necessary to get rid of the term proportional to k_3.

Local operator renormalizations also involve extra factors, e.g. the renormalized improved isovector operators are given by

$$(X_{\mathrm{R}})^a = Z_{\mathrm{X}}(1 + b_{\mathrm{X}} a m_{\mathrm{q}})(X_{\mathrm{I}})^a, \tag{85}$$

for $X = V, A, T, S, P$. A summary of the tree level and one-loop improvement coefficients b_X known to date is given in Table 2[67, 65].

Table 2. Tree level and one-loop improvement coefficients b

X	$b_{\mathrm{X}}^{(0)}$	$b_{\mathrm{X}}^{(1)}$
g	0	$0.012000(2) \times N_{\mathrm{f}}$
m	$-\frac{1}{2}$	$-0.07217(2) \times C_{\mathrm{F}}$
ζ	$-\frac{1}{2}$	$-0.06738(4) \times C_{\mathrm{F}}$
A	1	$0.11414(4) \times C_{\mathrm{F}}$
V	1	$0.11492(4) \times C_{\mathrm{F}}$
P	1	$0.11484(2) \times C_{\mathrm{F}}$
T	1	$0.10434(5) \times C_{\mathrm{F}}$

Non-perturbative determination of improvement coefficients

Although the improvement coefficients are computable in perturbation theory, in practice simulations are carried out at not so very small bare coupling and hence they should be determined non-perturbatively. There are a host of observables one could chose to compute and demand improvement thereof. To fix the $\mathrm{O}(a)$ improved Wilson action it is however natural to investigate the expressions associated with chiral symmetry. For example we can consider the PCAC relation on the lattice and tune c_{sw} and c_{A} so that the error term in

$$\langle \partial_\mu (A_{\mathrm{R}})^a_\mu(x)\,\mathcal{O}\rangle = 2m_{\mathrm{R}}\langle (P_{\mathrm{R}})^a(x)\,\mathcal{O}\rangle + \mathrm{O}(a^p) \tag{86}$$

is reduced from $\mathrm{O}(a)$ to $\mathrm{O}(a^2)$.

To this end we define an "unrenormalized current quark mass" through

$$m = \frac{\langle \partial_\mu \{A^a_\mu(x) + c_{\mathrm{A}} a \partial_\mu P^a(x)\}\mathcal{O}\rangle}{2\langle P^a(x)\,\mathcal{O}\rangle}\,. \tag{87}$$

The PCAC relation then implies

$$m = \frac{Z_{\mathrm{P}}(1+b_{\mathrm{P}} a m_{\mathrm{q}})}{Z_{\mathrm{A}}(1+b_{\mathrm{A}} a m_{\mathrm{q}})}\, m_{\mathrm{R}} + \mathrm{O}(a^p)\,, \tag{88}$$

and the violation of chiral symmetry can be studied by computing m for various choices of $\mathcal{O}$. Note that the sources $\mathcal{O}$ need not be improved (but must be physically separated from x). Again there are many choices of $\mathcal{O}$ that one may consider but a very convenient set is obtained naturally in the framework of the Schrödinger fuctional.

When constructing the Schrödinger fuctional in QCD we impose the same boundary conditions for the gauge fields as we did in the theory without quarks, but we must also supplement boundary conditions for the quark fields. Since the Dirac equation is of first order, only half of the components of the quark and anti-quark fields can be prescribed. Appropriate boundary conditions are found to be[58]

$$\frac{1}{2}(1+\gamma_0)\psi(x) = \rho(\mathbf{x}),\;\; \overline{\psi}(x)(1+\gamma_0)\frac{1}{2} = \bar{\rho}(\mathbf{x}),\;\; \text{at } x_0 = 0, \tag{89}$$

and similar boundary conditions are imposed at $x_0 = T$ with fields ρ'. Note in particular that Dirichlet boundary conditions induce a frequency gap of order $1/L$ on the quark

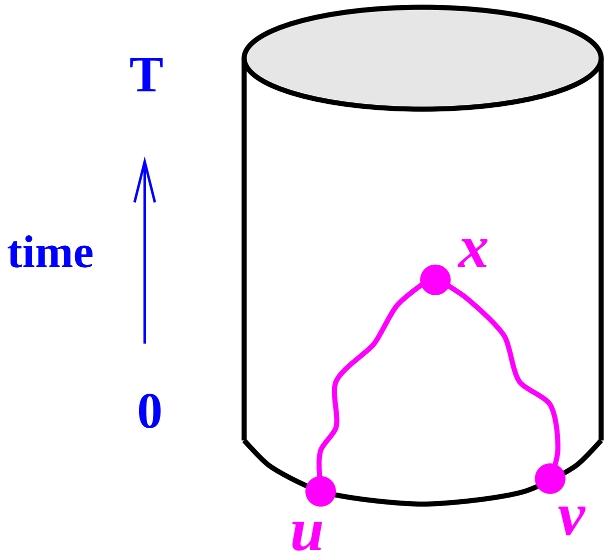

Figure 11. A sketch of a SF correlation function. The sources are at the boundary and the local operator at some point x well away from the boundary.

and gluon fields and hence there is no problem in performing numerical simulations for vanishing quark masses.

Now differentiation w.r.t. $\rho, \bar{\rho}$ produce sources at the boundary. e.g.

$$\mathcal{O}^a = a^6 \sum_{\mathbf{u},\mathbf{v}} \overline{\psi}(u)\gamma_5 \frac{1}{2}\tau^a \psi(v), \qquad u_0 = v_0 = 0\,, \tag{90}$$

and we can study correlation functions such as

$$\langle A_\mu^a(x)\mathcal{O}^a\rangle = \frac{1}{\mathcal{Z}}\int_{\text{fields}} A_\mu^a(x)\mathcal{O}^a\, \mathrm{e}^{-S} \tag{91}$$

illustrated schematically in Fig. 11.

The corresponding SF-mass $m = m_{\rm SF}$ must be independent of the boundary fields C, C', x_0 and the lattice sizes T and L, up to cutoff effects. We first inspect the PCAC relation at tree-level where all computations can be done analytically. Fig. 12 shows results on a 16×8^3 lattice with bare mass $am_0 = 0.01$. The large effects for the Wilson action are due to the fact that non-zero boundary values C and C' induce a background gauge field. Note that on adding the SW improvement term (with $c_{\rm sw} = 1$) the dependence on the boundary values is practically eliminated.

Turning to unimproved quenched QCD e.g. 16×8^3 lattice, $\beta = 6.4$, $a = 0.05$ fm (see Fig. 13) a strong violation of chiral symmetry is again manifest. The situation here can be improved by introducing the improvement terms in the action and axial vector current. This is illustrated in Fig. 14 where we have the same lattice as before, but $c_{\rm sw} = 1.60$, $c_{\rm A} = -0.027$. Similar results are obtained for larger lattices, other boundary values, etc. In each case we find that at lattice spacings $a \leq 0.1$ fm chiral symmetry is effectively restored provided $c_{\rm sw}$ and $c_{\rm A}$ are chosen appropriately.

A typical systematic non-perturbative determination of $c_{\rm sw}$ and $c_{\rm A}$ proceeds as follows[68]. Take three configurations of x_0, C, C', ... and require

$$m_1 = m_2 \quad \text{and} \quad m_2 = m_3\,. \tag{92}$$

For any other configuration Symanzik's analysis then guarantees that $m = m_1 + \mathrm{O}(a^2)$. Different "improvement conditions" yield values of $c_{\rm sw}$ and $c_{\rm A}$ that differ by terms

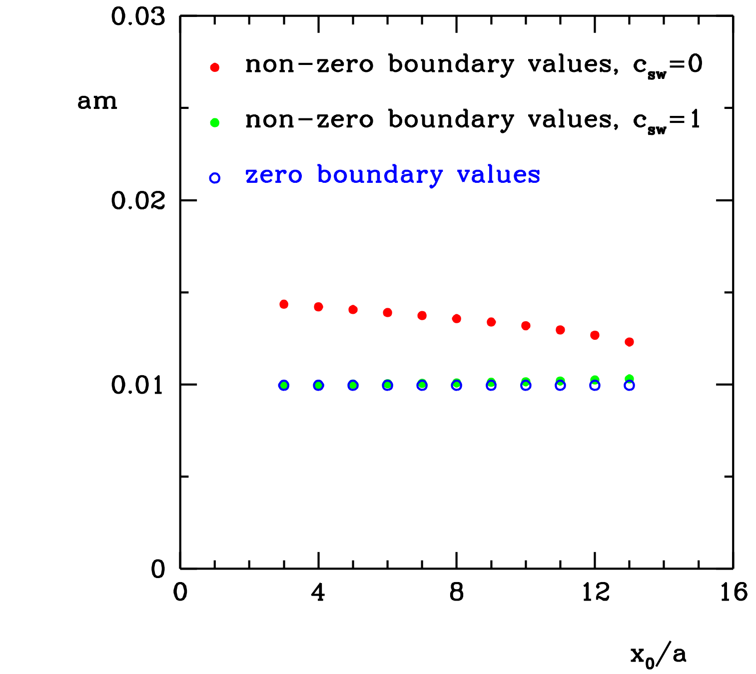

Figure 12. m_{SF} at tree-level. The $c_{\mathrm{sw}} = 1$ results nearly fall on top of those for zero boundary values.

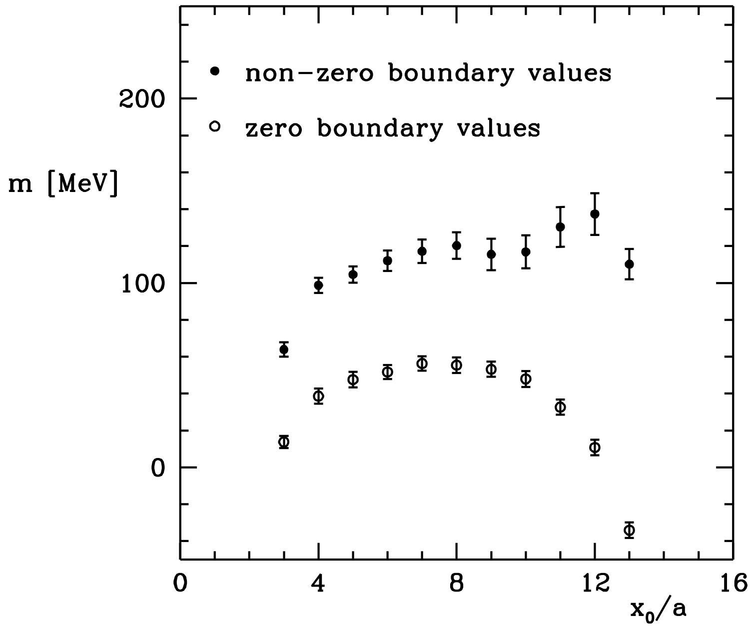

Figure 13. m_{SF} in unimproved quenched QCD.

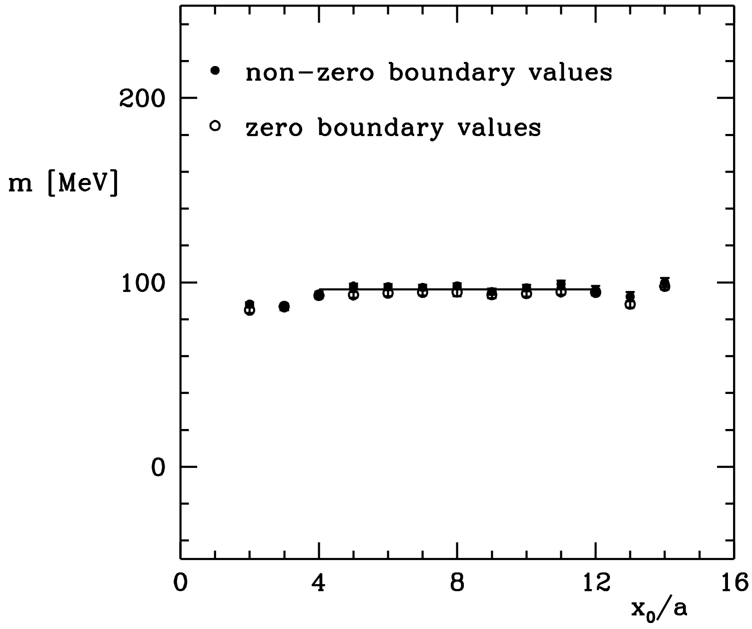

Figure 14. $m_{\rm SF}$ in improved quenched QCD.

of $\mathrm{O}(a)$. Thus improvement conditions should be chosen with care in order to avoid an artificial enhancement of $\mathrm{O}(a^2)$ cutoff effects, albeit this can be rather difficult to control in practice.

In Fig. 15 we show the results for $c_{\rm sw}$ in quenched QCD for a particular choice of improvement conditions[68]. The solid line is a parametrization of the data

$$c_{\rm sw} = \frac{1 - 0.656\,g_0^2 - 0.152\,g_0^4 - 0.054\,g_0^6}{1 - 0.922\,g_0^2}, \qquad 0 \leq g_0 \leq 1\,. \tag{93}$$

This expression is now often taken for the definition of the improved action in various numerical simulations. A similar result is obtained for $c_{\rm A}$ but the analysis[68] is rather delicate and is now being reviewed.

Renormalization constants

For zero quark masses chiral symmetry is expected to become exact in the continuum limit. It is therefore natural to fix the renormalization constants $Z_{\rm A}, Z_{\rm V}$ of the currents by imposing the continuum chiral Ward identities also at finite values of the cutoff[70, 71, 72].

In the case of the axial current the relevant Ward identity can be written in the form

$$\int_{\partial R} {\rm d}\sigma_\mu(x)\epsilon^{abc}\langle A_\mu^a(x) A_\nu^b(y)\mathcal{Q}^c\rangle = 2i\langle V_\nu^c(y)\mathcal{Q}^c\rangle \tag{94}$$

where the integral is taken over the boundary of a region R containing the point y and $\mathcal{Q}^a$ is a source located outside R. In view of on-shell improvement it is important to note that all space-time arguments in Eq. (94) are well separated from one another.

As mentioned above, the Schrödinger functional is also a useful tool for the accurate determination of the renormalization constants of composite operators[73]. For the source

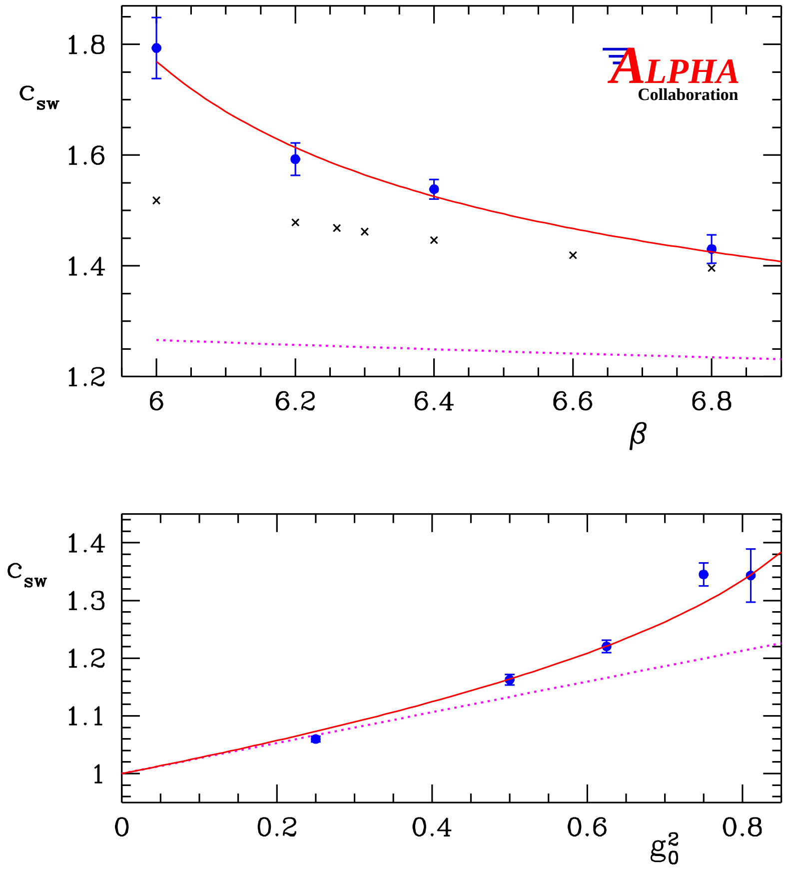

Figure 15. $c_{\rm sw}$ quenched QCD; the dotted line denotes one loop bare PT and the crosses correspond to tadpole improved PT[69].

in Eq. (94) one can take $\mathcal{Q}^a = \epsilon^{abc}\mathcal{O}'^b\mathcal{O}^c$ with $\mathcal{O}^a$ as given in Eq. (90) and $\mathcal{O}'^a$ defined similarly with the primed fields. The region R is taken to be $R = \{x; t_1 \le x_0 \le t_2\}$.

Now introduce correlation functions:

$$f_{\rm V}^{\rm R}(x_0) = \frac{a^3}{6L^6}\sum_{\mathbf{x}} i\epsilon^{abc}\langle \mathcal{O}'^a (V_{\rm R})_0^b(x)\mathcal{O}^c\rangle, \tag{95}$$

$$f_{\rm AA}^{\rm R}(x_0,y_0) = \frac{a^6}{6L^6}\sum_{\mathbf{x},\mathbf{y}} \epsilon^{abe}\epsilon^{cde}\langle \mathcal{O}'^d (A_{\rm R})_0^a(x)(A_{\rm R})_0^b(y)\mathcal{O}^c\rangle, \tag{96}$$

$$f_1 = -\frac{1}{3L^6}\langle \mathcal{O}'^a\mathcal{O}^a\rangle. \tag{97}$$

At zero quark mass, and for the correct values of $c_{\rm sw}$ and $c_{\rm A}$ a lattice version of the chiral Ward identity Eq. (94) is

$$f_{\rm AA}^{\rm R}(x_0,y_0) = f_1 + O(a^2), \;\; x_0 > y_0. \tag{98}$$

Compared to Eq. (94) one has set $\nu = 0$ and included an additional summation over $\mathbf{y}$, thus obtaining the isospin charge the action of which can be evaluated because of the exact isospin symmetry on the lattice. Further the conservation of the axial charge at $m_{\rm q} = 0$ was exploited.

Since the isospin symmetry remains unbroken for non-zero quark mass, one need not restrict the normalization of the vector current to the case $m_{\rm q} = 0$. Using the vector Ward identity analogous to Eq. (94) one obtains

$$f_{\rm V}^{\rm R}(x_0) = f_1 + O(a^2), \tag{99}$$

when $c_{\rm sw}$ is chosen correctly. Note that the improvement coefficient $c_{\rm V}$ is not needed here, because the tensor density does not contribute to the isospin charge.

Now to get precise definitions of the normalization constants starting from Eqs. (98) and (99) further specifications must be made. The following specific normalization conditions were chosen[73]:

$$f_{\rm V}^{\rm R}(T/2) = f_1, \ T = 2L, \tag{100}$$

$$f_{\rm AA}^{\rm R}(2T/3, T/3) = f_1, \ \text{at } m_{\rm q} = 0, \ T = 9L/4, \tag{101}$$

where one also set the boundary fields to zero: $C = C' = \rho = \rho' = 0$. In order to guarantee that cutoff effects of matrix elements of renormalized currents vanish proportional to a^2 when approaching the continuum limit, one completes the normalization conditions by scaling L in units of a physical scale

$$L/a = 8 \text{ at } g_0 = 1, \ \ L/r_0 = \text{constant}. \tag{102}$$

In the simulations the choices Eq. (102) are realized by smooth inter-/extrapolations.

Of course these explicit choices of the normalization conditions are rather arbitrary. One must just take care not to introduce large $\mathrm{O}(a^2)$ effects through an "unfortunate" choice. A study of the cutoff effects in the lattice Ward identities in perturbation theory is often a good guide. Also in the course of the simulations it was checked that $Z_{\rm V}, Z_{\rm A}$ do not change appreciably when parameters such as Eq. (102) are varied within reasonable limits.

Fig. 16 shows that the renormalization constants of the vector and axial vector currents are obtained rather accurately in this way[73]. The solid lines are fits by rational functions which incorporate the leading order perturbative results[74, 75, 76]

$$Z_{\rm V} = 1 - 0.097072(1) \times C_{\rm F} g_0^2 + O(g_0^4), \tag{103}$$

$$Z_{\rm A} = 1 - 0.087344(1) \times C_{\rm F} g_0^2 + O(g_0^4)\,. \tag{104}$$

Since the condition Eq.(99) should hold also for non-vanishing quark mass one can also compute the coefficient b_V non-perturbatively. For quenched QCD the result[73] is shown in Fig. 17. The solid line (incorporating the known 1-loop coefficient) is

$$b_{\rm V} = \frac{1 - 0.7613\, g_0^2 + 0.0012\, g_0^4 - 0.1136\, g_0^6}{1 - 0.9145\, g_0^2}, \qquad 0 \leq g_0 \leq 1 \tag{105}$$

Unfortunately the analogous coefficient $b_{\rm A}$ for the axial current cannot be obtained in the same way since the relevant Ward identity contains a physical mass dependence apart from the $\mathrm{O}(am)$ lattice artifact. A method of determining the combinations $b_{\rm A} - b_{\rm P}$ and $b_{\rm V} - b_{\rm S}$ in the quenched theory have been proposed[78, 79].

In this context it is instructive to note a rigorous result due to Lüscher[80] for the improvement coefficient b_s of the isoscalar scalar density $S(x) = \overline{\psi}(x)\psi(x)$. Let us work on an infinite lattice and consider the pseudoscalar density correlation function; at large x_0 we have

$$\sum_{\mathbf{x}} \langle P^a(x) P^a(0)\rangle \propto \exp(-x_0 m_\pi)\ , \tag{106}$$

and differentiating with respect to the bare mass

$$\frac{\partial}{\partial m_0} \sum_{\mathbf{x}} \langle P^a(x) P^a(0)\rangle \propto \exp(-x_0 m_\pi) \Big\{ x_0 \frac{\partial m_\pi}{\partial m_0} + O(1) \Big\} \ , x_0 \to \infty\,. \tag{107}$$

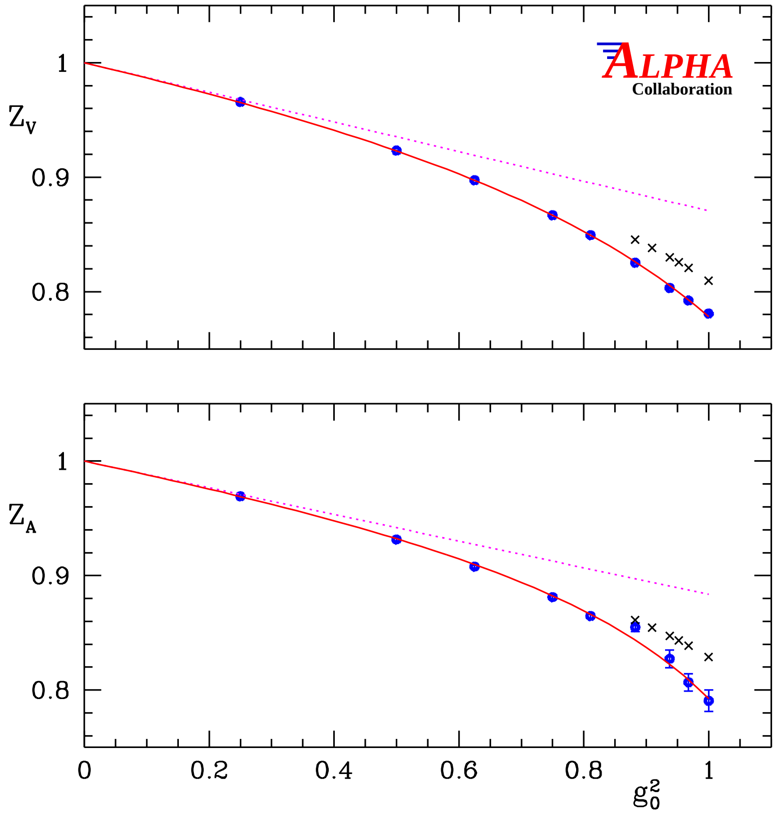

Figure 16. Non-perturbative determination of $Z_{\rm A}, Z_{\rm V}$ for $g_0^2 \leq 1$ in the valence approximation.

On the other hand, from the functional integral one has

$$\frac{\partial}{\partial m_0} \sum_{\mathbf{x}} \langle P^a(x) P^a(0)\rangle = \sum_{\mathbf{x}} \sum_{y} \langle P^a(x) \big[S(y) - \langle S(y) \rangle \big] P^a(0)\rangle \,. \tag{108}$$

One now splits the above summation over y_0 into several ranges

$$y_0 \gg x_0, \;\; y_0 \sim x_0, \;\; x_0 > y_0 > 0, \;\; y_0 \sim 0, \;\; y_0 \ll 0 \,, \tag{109}$$

and observes that the only range which gives a contribution proportional to x_0 is the middle one. It then follows that

$$\frac{\partial}{\partial m_0} \sum_{\mathbf{x}} \langle P^a(x) P^a(0)\rangle \propto \langle \pi | S(0) - \langle S(0) | \pi \rangle \big[x_0 + O(1) \big] \,. \tag{110}$$

In other words, we have

$$\frac{\partial m_\pi}{\partial m_0} = \langle \pi | S - \langle S \rangle | \pi \rangle \,. \tag{111}$$

Finally one notes that

$$\frac{\partial \tilde{m}_0}{\partial m_0} = 1 + 2 b_{\rm m} a m_{\rm q} \tag{112}$$

and concludes that

$$\frac{\partial m_\pi}{\partial \tilde{m}_0} = \langle \pi | S - \langle S \rangle | \pi \rangle \big(1 + 2 b_{\rm m} a m_{\rm q} \big) \,. \tag{113}$$

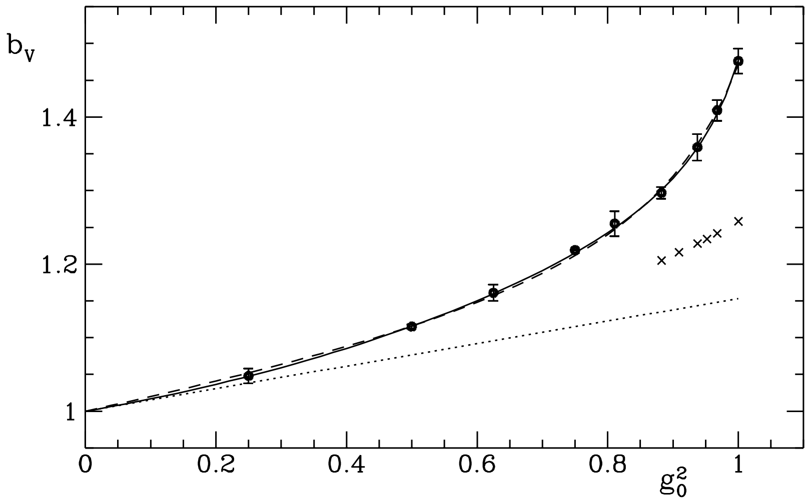

Figure 17. Non-perturbative determination of b_V for $g_0^2 \leq 1$ in the valence approximation (solid line). The dotted line indicates the perturbative estimate and the crosses the perturbative estimate using Parisi's coupling[77].

Since the left hand side is improved one deduces the relationship

$$b_s = -2b_{\mathrm{m}} \, . \tag{114}$$

It should be emphasized that the scalar densities S and S^a may not have the same b's, although this should be the case in quenched QCD as has been explicitly verified to one-loop.

On-going computations

Various computations of improvement coefficients and renormalization constants are under way. Firstly to complete the definition of the renormalized SF-running mass m(L) one must specify a normalization condition for the pseudoscalar density. Defining

$$f_{\mathrm{P}}^{\mathrm{R}}(x_0) = -\frac{a^3}{3L^3} \sum_{\mathbf{x}} \langle (P_{\mathrm{R}})^a(x) \mathcal{O}^a \rangle, \tag{115}$$

one can for example impose the normalization condition

$$f_{\mathrm{P}}^{\mathrm{R}}(T/2)^2 = f_1, \text{ at } m_{\mathrm{q}} = 0. \tag{116}$$

The corresponding non-perturbative running mass is now being measured in the quenched theory[42].

A computation of c_{V} appearing in the definition of the renormalized improved vector current is under way[81].

Finally the extension of non-perturbative improvement program to the theory with dynamical quarks is in principle straightforward. The first step - the non-perturbative determination of c_{sw} in the theory with two dynamical quarks is practically completed[82].

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