

Lattice artifacts and the running of the coupling constant

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We study the running of the Lüscher-Weisz-Wolff (LWW) coupling constant in the two-dimensional $O(3)$ nonlinear σ model. To investigate the continuum limit we refine the lattice spacing from the $\frac{1}{16}$ value used by LWW up to $\frac{1}{160}$. We find larger lattice artifacts than those estimated by LWW and that most likely the coupling constant runs slower than predicted by perturbation theory. A precise determination of the running in the continuum limit would require a controlled ansatz of extrapolation, which, we argue, is not presently available.

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The hallmark of QCD is its alleged asymptotic freedom (AF), that property which expresses the fact that at shorter distances the interactions between quarks and gluons are becoming weaker. This fact, however, has been established only in perturbation theory (PT), an approximation scheme without a mathematical basis and which, moreover, has been shown to be plagued by ambiguities (expectation values of variables of compact support depend upon the boundary conditions (BC) used to reach the thermodynamic limit) [1].

It is therefore most important to establish whether AF is really a property of QCD in a nonperturbative framework. The first step in this direction was taken in 1991 by Lüscher, Weisz, and Wolff (LWW) [2], who proposed a method to investigate the presence of AF in the two-dimensional (2D) $O(N)$ nonlinear σ models, which, perturbatively, are also AF for $N \geq 3$. As a coupling constant they proposed the following renormalization group invariant:

$$\bar{g}^2(\beta, L) = \frac{2L}{(N-1)\xi(L)}. \quad (1)$$

Here $\xi(L)$ is the correlation length of the $O(N)$ model in an infinite strip of width L with periodic BC. It is defined by the following double limit: consider a finite strip of size $L \times T$ with periodic BC in the direction of size L and arbitrary BC in the direction of size T . Then

$$\xi(L) = -\lim_{x \rightarrow \infty} \lim_{T \rightarrow \infty} \frac{x}{\ln[\langle s(0) \cdot s(x) \rangle]}. \quad (2)$$

For the standard $O(N)$ action

$$H_{i,j} = -s(i) \cdot s(j) \quad (3)$$

at inverse coupling constant β , if in Eq. (1) one expressed L in units of the thermodynamic correlation length $\xi_\infty(\beta)$, then in the limit $L \rightarrow \infty$ and $\beta \rightarrow \beta_{\text{crit}}$, holding $z = L/\xi_\infty$ fixed, one would obtain a unique function $\bar{g}^2(z)$ describing the running of \bar{g}^2 with the physical distance z .

As we pointed out in Ref. [3], the interpretation of \bar{g}^2 as a coupling constant is somewhat misleading since it does not measure the strength of the interaction. Indeed in the massive

continuum limit of a free field theory $\bar{g}^2(z)$ is a nontrivial function, running linearly with z . LWW argued in favor of their choice by pointing out that in PT, to lowest order in the bare (lattice) coupling constant $\bar{g}^2(L) \sim 1/\beta$. This argument is also problematic since even if $\beta_{\text{crit}} = \infty$, to construct the continuum limit one would have to let $L \rightarrow \infty$ and thus reach a regime where PT in the bare coupling would clearly not be applicable.

Nevertheless $\bar{g}^2(L, \beta)$ is a renormalization group invariant and if one would discover that for some $\beta < \infty$, $\bar{g}^2(L)$ became independent of L for large L , that would mean that at that β the model is critical, which, as we will explain below, would rule out the existence of AF in the massive continuum limit.

LWW claimed to be able to establish the continuum running of $\bar{g}^2[L/\xi_\infty(\beta)]$ up to physical distances as small as 0.03304(4) and to verify that it approached the perturbative (AF) prediction for the $O(3)$ model. To achieve this they employed a finite size scaling (FSS) technique: one measures $\xi(L)$ at some β and L , then leaving β unchanged, one doubles L and measures $\xi(2L)$. One thus obtains a scaling curve giving $\bar{g}^2(2L)/\bar{g}^2(L)$ versus $\bar{g}^2(L)$. This *step scaling curve*, as LWW called it, allows one to connect small physical distances to large ones [$L/\xi_\infty(\beta) > 7$], where the continuum limit of $\bar{g}^2[L/\xi_\infty(\beta)]$ could be reached.

Similar FSS approaches were used by Kim [4] and Caracciolo *et al.* [5] to predict the value of $\xi(\beta)$ up to $\xi \sim 10^5$, even though the largest lattices involved did not exceed $L = 512$. However, whereas these authors produced their scaling curves simply by observing that the Monte Carlo (MC) data coming from different values of β seemed to fall on the same curve, which they took as their step scaling curve, the LWW paper claimed to have really controlled lattice artifacts (the approach to the continuum). More precisely the problem is this: of course if one knew the continuum value of the step scaling curve one could connect small physical distances to large ones. But in a MC investigation, by necessity, one can only gather data at finite cutoff [$1/\xi_\infty(\beta)$ or alternatively $1/L$]. However, the continuum limit requires letting $\xi_\infty(\beta) \rightarrow \infty$ and $L \rightarrow \infty$. Therefore one must in principle worry about extrapolating the results obtained for the step scaling function at finite cutoff to the continuum limit.

This feat, which the other above quoted authors did not even attempt, was achieved by LWW by assuming a Symanzik-type approach to the continuum limit. Namely, at fixed \bar{g}^2 they assumed that the step scaling function approaches its continuum limit value as $1/L^2$ [strictly speaking, inspired by PT, the Symanzik fit involves $\log(L)/L^2$, however, for $6 \leq L \leq 16$ the log can be approximated by a constant]. They backed this assumption with their MC data. However, the values of L they used ranged only from $6 \leq L \leq 16$. The main point of our paper is to show numerical evidence that if one goes to much larger L values, the Symanzik fit has an unacceptably large χ^2 and an entirely new picture for the running of \bar{g}^2 with the physical distance is suggested.

Before showing our data, we would like to elaborate on a subtlety having to do with the numerical determination of the correlation length $\xi(L)$. Namely, while the definition in Eq. (1) is mathematically well defined, one must adopt a computational procedure for implementing it. LWW used an $L \times T$ lattice with free BC in the T direction, took $T=5L$ and assumed a pure exponential decay for $L < x < T-L$ (see Appendix B of Ref. [2]). We used instead the following numerical estimate of the correlation length ξ : let $P=(p,0)$, $p=2n\pi/T$, $n=0,1,2,\dots,T-1$, $T=10L$. Then

$$\xi = \frac{1}{2 \sin(\pi/T)} \sqrt{G(0)/G(1) - 1}, \quad (4)$$

where

$$G(p) = \frac{1}{LT} \langle |\hat{s}(P)|^2 \rangle; \quad \hat{s}(P) = \sum_x e^{iPx} s(x). \quad (5)$$

It is not clear whether the LWW prescription or the one adopted by us provides an estimate closer to the true exponential correlation length. For finite T the LWW procedure, employing free BC, is likely to produce a value smaller than the true $\xi(L)$. In the procedure adopted by us, there are two effects of opposite sign, which could bring the result closer to the true exponential correlation length.

(1) The periodic BC in the T direction increases the order in the system compared to an infinite strip.

(2) Since our definition is sensitive to the multiparticle states, for $T \rightarrow \infty$ it would produce a value smaller than the true $\xi(L)$. This effect was studied by Campostrini *et al.* [6] using the high-temperature expansion and found to be less than 0.2%.

Since we want to compare our data with those of LWW, we show in Fig. 1 the resulting step scaling functions computed with the two procedures at the same β and L . As can be seen, within numerical accuracy, at these values of \bar{g}^2 the two procedures produce similar results.

Our results for the step scaling function are shown in Figs. 2, 3, and 4 for $L=20, 40$, and 80 , respectively. The values were obtained by measuring the correlation length at given β first on a lattice of size $L \times 10L$, then on $2L \times 20L$. The values of β used (1.815, 1.94, 2.05, 2.16, 2.27, 2.38, and 2.49) were chosen so that \bar{g}^2 took values in the range covered by LWW. The figures contain also two benchmarks taken from LWW [2]: the 3-loop PT curve; the LWW

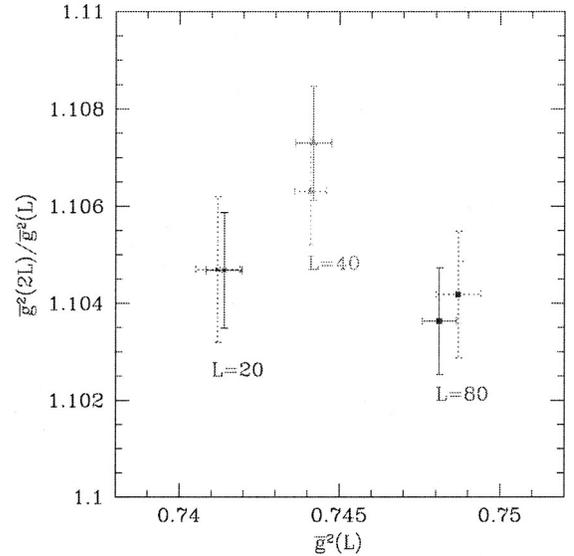


FIG. 1. Step scaling function $\bar{g}^2(2L)/\bar{g}^2(L)$ versus $\bar{g}^2(L)$ for $L=20, 40, 80$ computed with our method of estimating $\xi(L)$ (solid lines) and with the LWW method (dotted line).

estimated continuum values. Figure 4 also contains our value for the step scaling function obtained by doubling L from 160 to 320 at $\bar{g}^2=1.05397(81)$. The error bars were estimated as follows. For each value of β and L we started from a randomly chosen configuration and ran the improved cluster algorithm [7] using 100 000 clusters for thermalization and 1 000 000 clusters for measurements. We then repeated this procedure a minimum of 157 times, except for the value at $L=320$ which contains only 74 runs. We computed the average value over these samples of $G(0)$ and $G(1)$ and from them $\xi(L)$. Since $\xi(L)$ is a nonlinear function of $G(0)$ and $G(1)$, we estimated the error for $\xi(L)$ and $\bar{g}^2(L)$ from

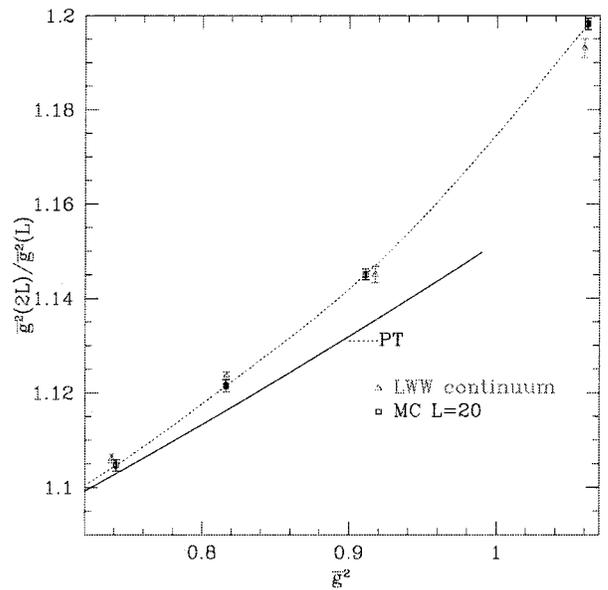


FIG. 2. Step scaling function $\bar{g}^2(2L)/\bar{g}^2(L)$ versus $\bar{g}^2(L)$ for $L=20$. Our MC data are connected by a spline.

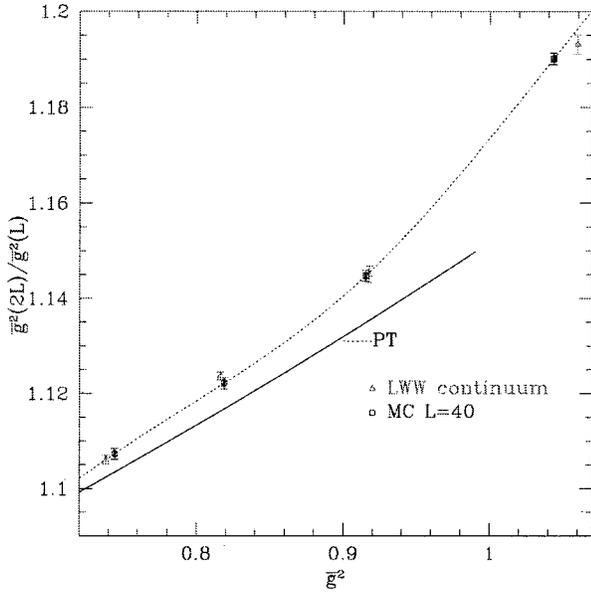


FIG. 3. Step scaling function $\bar{g}^2(2L)/\bar{g}^2(L)$ versus $\bar{g}^2(L)$ for $L=40$. Our MC data are connected by a spline.

our sample of independent values by the jackknife method. The data for $\bar{g}^2(L)$ that were used in the figures are given in Table I.

Our data cast doubt on the LWW prediction [2] for the continuum limit of the step scaling function. The latter was obtained by extrapolating the MC values for L from 6 to 16 via a second order polynomial in $1/L^2$. For illustration in Fig. 5 we show the original LWW data for the step scaling function at $g^2=1.0595$ and the fit just described (the solid line) together with our data at larger L (we used a spline to interpolate our data to extract our values at $g^2=1.0595$). We have arbitrarily changed the abscissa to $1/(\ln L+2.5)$ to better separate the data points at large L horizontally. In the fit, following the procedure described by LWW, we left out the point at $L=5$. Our fit (of the LWW data) reproduces their continuum value pretty well [we obtain 1.2642(13), whereas they give 1.2641(20)]. Note that while our data join the LWW data smoothly, our data at larger L lie below their fit curve.

As already indicated above, LWW expected the data to follow the PT inspired Symanzik ansatz $a/L^2 + b \ln L/L^2$, consequently we tried also a fit of this type to *all* the data. This is shown in Fig. 6. The quality of the fit is not excellent ($\chi^2/N_{DF}=2.8$), and it is only slightly better than the fit obtained following the LWW prescription (quadratic polyno-

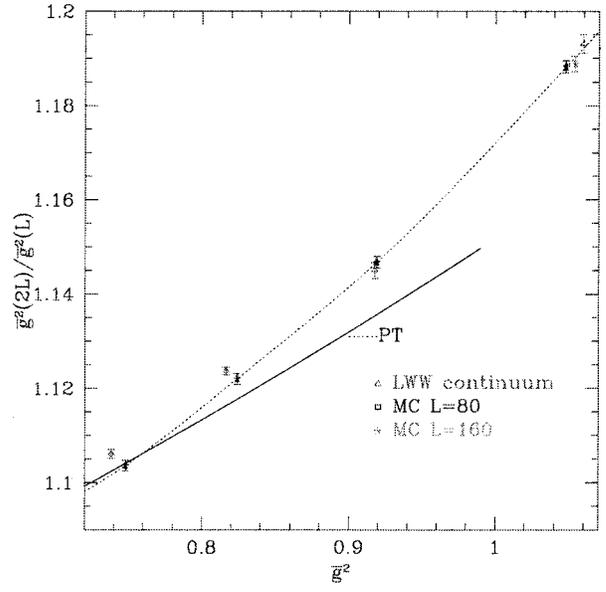


FIG. 4. Step scaling function $\bar{g}^2(2L)/\bar{g}^2(L)$ versus $\bar{g}^2(L)$ for $L=80$ and 160. Our MC data for $L=80$ are connected by a spline.

mial in $1/L^2$, with the point at $L=5$ discarded), whose χ^2/N_{DF} is 3.2. In fact, even with the Symanzik-type fit, our data at $L=80$ and 160 lie below the fit curve, although by less than in Fig. 5.

We did not display the LWW values for $6 \leq L \leq 16$ in Figs. 2, 3, and 4 because that would clutter the plots too much. However, when combined with our values, they reveal a rather complicated approach to the continuum, especially at lower g^2 values. This is not an unexpected fact. Indeed if L is sufficiently small at given β , the (asymmetric) lattice is strongly ordered in the transverse (shorter) direction. On the other hand, as we emphasized several years ago [8], since in the continuum limit one must let $L \rightarrow \infty$ and the Mermin-Wagner theorem guarantees the restoration of the $O(N)$ symmetry in that limit for any finite β , clearly for L sufficiently large this “perturbative” regime, of spins highly ordered in the transverse direction, cannot persist.

In fact we showed in Ref. [8] that even if $\beta_{crit} = \infty$, as predicted by PT, the spins would cease to be highly ordered in the transverse direction for L sufficiently large. Indeed bare PT itself provides a clue as to the distance over which the spins remain well ordered since to lowest order one has

$$\langle s(0) \cdot s(x) \rangle = 1 - \frac{N-1}{\beta} D(x) \quad (6)$$

TABLE I. Monte Carlo data for $\bar{g}^2(\beta, L)$.

β	1.815	1.94	2.05	2.16	2.27	2.38
$L=20$	1.06185(78)	0.91115(67)	0.81616(70)	0.74170(56)		
$L=40$	1.27230(85)	1.04334(76)	0.91530(68)	0.81901(63)	0.74419(57)	
$L=80$		1.24174(85)	1.04778(72)	0.91907(70)	0.82404(60)	0.74811(53)
$L=160$			1.24497(100)	1.05398(81)	0.92457(69)	0.82564(58)
$L=320$				1.2530(15)		

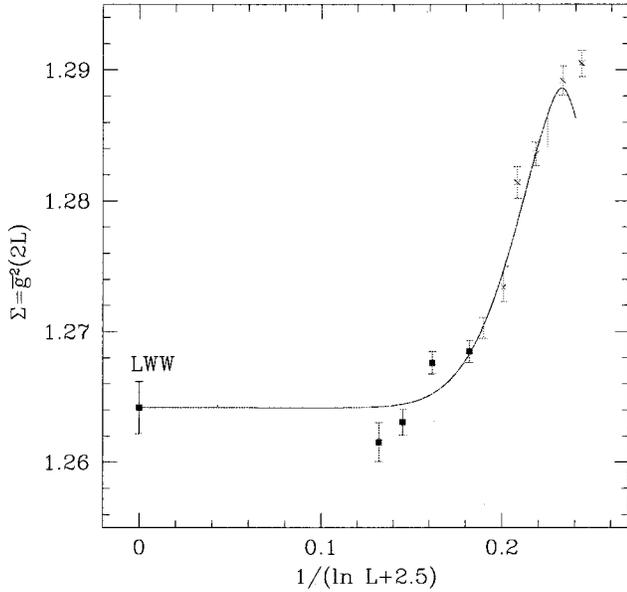


FIG. 5. Step scaling function $\Sigma = \bar{g}^2(2L)$ for $\bar{g}^2 = 1.0595$ versus $1/(\ln L + 2.5)$. Crosses are the LWW data, solid squares our new data. The solid line is the LWW-type fit and the point labeled LWW is the LWW continuum value.

and to a good approximation $D(x) = \frac{1}{4} + (1/2\pi)\ln(x)$. Thus bare PT suggests that spins are well ordered over distances $O\{\exp[2\pi\beta/(N-1)]\}$. On the other hand, the AF formula predicts $\xi = O\{\exp[2\pi\beta/(N-2)]\}$. Thus at fixed physical distance $[L/\xi(L)]$, in taking the continuum limit one would surely leave the regime in which PT in the bare coupling is applicable.

Returning now to the pattern of lattice artifacts, initially, if β is large enough, at small enough L , they should follow the Symanzik pattern used by LWW because the system is essentially in a PT regime. This regime has nothing to do with

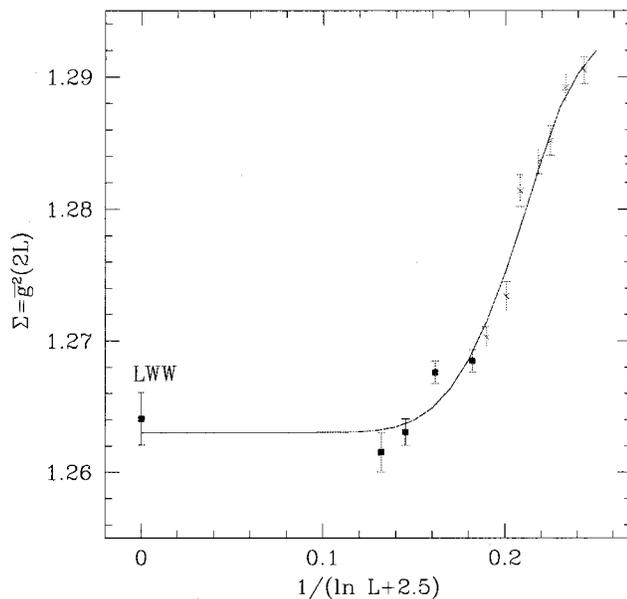


FIG. 6. Step scaling function $\Sigma = \bar{g}^2(2L)$ for $\bar{g}^2 = 1.0595$ versus $1/(\ln L + 2.5)$ as before. The solid line is now the Symanzik type fit.

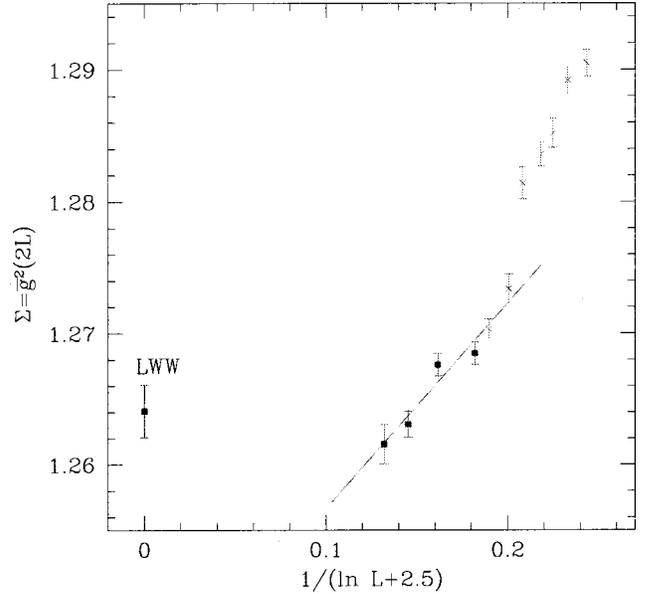


FIG. 7. Step scaling function $\Sigma = \bar{g}^2(2L)$ for $\bar{g}^2 = 1.0595$ versus $1/(\ln L + 2.5)$ as before. The solid line is the fit Eq. (7).

the true approach to the continuum, which occurs only when L is sufficiently large (for given β) so that the $O(N)$ symmetry becomes approximately true. How the true continuum limit is approached can be model dependent. For instance, in the Ising model there are good reasons to expect a $1/L^2$ leading behavior [9]. On the other hand, in the $O(2)$ model there are both theoretical [10] and numerical reasons [11,12] to expect a $1/\ln(L)$ approach.

It is reasonable to expect that the $O(3)$ model, enjoying a continuous symmetry, behaves similar to the $O(2)$ one and not the Ising model. We have attempted a $1/\ln(L)$ fit to our data at $g^2 = 1.0595$. This is shown in Fig. 7. We show the results of fitting only the data with $L \geq 12$ to the ansatz

$$a + \frac{b}{\ln L + c} \quad (7)$$

with $a = 1.2410(3)$, $b = 0.1567(187)$, $c = 2.5$, and $\chi^2/N_{DF} = 5.3/3$. We have no theoretical basis for this ansatz, which was inspired by the behavior of $g^2(L)$ in the critical $O(2)$ model, and present it only as an illustration. Since it is supposed to represent asymptotic behavior for $L \rightarrow \infty$ and it involves $1/\ln L$ rather than $1/L^2$, obviously it should apply only for larger L . Our decision to being with $L = 12$ is arbitrary. It leads to a fit with a reasonable χ^2/N_{DF} and a much lower prediction (1.24 instead of 1.26) for the continuum value of the step scaling function.

Even though we do not have a firm prediction for the continuum step scaling function, our results do not corroborate the original prediction of LWW and suggest that most likely the nonperturbative running of \bar{g}^2 is slower than predicted by PT. This situation is consistent with, though in no way proving, the existence of a transition to a massless phase at finite β_{ct} , as argued by us recently [13]. In that paper we also proved rigorously that for the standard action, the mas-

sive continuum limit cannot be AF if $\beta_{\text{crit}} < \infty$. The result follows from a Ward identity and the reflection positivity of the standard action.

Finally, regarding the running of $\alpha_s(Q)$ in QCD₄, all we can say is that the Symanzik-type fit for the approach to the continuum has no justification there either. Indeed, that fit is inspired by PT. If in fact lattice QCD₄ does undergo a deconfining zero temperature transition at nonzero (bare) coupling, so that the running of $\alpha_s(Q)$ does not follow PT, there is no reason to expect the lattice artifacts to follow the Symanzik ansatz. Therefore it would be very useful if the lattice community employed its resources to establish first the true cutoff effects and the true running of α_s in the pure

Yang-Mills theory by going to larger L , before attempting to handle dynamical fermions; the latter unavoidably can only be done on minuscule lattices, and using the Symanzik fit to extrapolate to the continuum can be misleading, as we have found. As we said many years ago [14], we expect that in the four dimensional Yang-Mills theory as well as in QCD₄ there exists a nontrivial fixed point and that $\alpha_s(Q)$ runs slower than predicted by PT, with the effect becoming pronounced by 1 TeV or less.

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