The (Lattice) QCD Potential and Coupling: How to Accurately Interpolate Between Multi-Loop QCD and the String Picture

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Abstract

We present a simple parameterization of the running coupling constant $\alpha_V(q)$, defined via the static potential, that interpolates between 2-loop QCD in the UV and the string prediction $V(r) = \sigma r - \frac{\pi}{12r}$ in the IR. Besides the usual $\Lambda$-parameter and the string tension $\sigma$, $\alpha_V(q)$ depends on one dimensionless parameter, determining how fast the crossover from UV to IR behavior occurs (in principle we know how to take into account any number of loops by adding more parameters). Using a new ansatz for the lattice potential in terms of the continuum $\alpha_V(q)$, we can fit quenched and unquenched Monte Carlo results for the potential down to one lattice spacing, and at the same time extract $\alpha_V(q)$ to high precision. We compare our ansatz with 1-loop results for the lattice potential, and use $\alpha_V(q)$ from our fits to quantitatively check the accuracy of 2-loop evolution, compare with the Lepage-Mackenzie estimate of the coupling extracted from the plaquette, and determine Sommer’s scale $r_0$ much more accurately than previously possible. For pure SU(3) we find that $\alpha_V(q)$ scales on the percent level for $\beta \geq 6$.

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1 Introduction

In a situation where quarks are non-relativistic their dynamics is much slower than that of the massless gluons. In the limit of infinitely heavy quarks, or, equivalently, static sources, their interaction can be described by a local, instantaneous potential $V(r)$. This static potential will for the purposes of this paper always refer to the potential between a quark and an anti-quark in the fundamental representation of SU($N$).

For very short distances, $V(r)$ is Coulomb like, with a running charge that is known to two loops in terms of the (unknown) $\Lambda$-parameter. The strong coupling expansion of lattice gauge theory suggests a string picture, where a flux tube connects two widely separated quarks, in accord with the idea of confinement [2] (we here ignore the string breaking in the presence of dynamical fermions). In addition to a linear term involving the string tension $\sigma$, the potential has a universal large $r$ correction [3] due to the zero point energy of the transverse fluctuations of the flux tube, so that in the IR

$$ V(r) = \sigma r - \frac{e_{IR}}{r} + \ldots, \quad (1) $$

up to a non-universal constant. The “IR charge” $e_{IR} = \pi(D - 2)/24$ in $D$ space-time dimensions, assuming the transverse fluctuations are described by the simplest bosonic string theory.\(^2\)

At present the only way to obtain quantitative information on $V(r)$ is through the Monte Carlo simulation of Wilson loops. These are nowadays very precise; the lattice potential can be measured with a relative accuracy approaching $10^{-4}$ at short distances and $10^{-3}$ at long distances. The lattices used are typically of size $32^4$ for pure gauge theory and $16^4$ in the presence of dynamical quarks. The spacing of the finest lattices available for SU(3) is about 0.04 fm, corresponding to 5 GeV, just where 2-loop perturbation theory is expected to become good. However, at these distances the potential suffers from large lattice artifacts, which obscure the view of perturbative QCD. These lattice artifacts are on the order of 10% at one lattice spacing if one uses the standard (unimproved) Wilson action for the gluons, and fall roughly like $1/r^2$ at larger distances. One therefore has to go to many lattice spacings before rotational invariance is restored within errors.

In early studies, the lattice potential, at least restricted to on-axis points, was fitted to an ansatz of the form $-c/r + \sigma r + V_0$, i.e. it was assumed to behave as in

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\(^1\)The situation is more subtle in the presence of a non-perturbative gluon condensate. But it is now clear that the presence of a gluon condensate is not necessarily incompatible with the existence of a local potential. See [1] for a review and references.

\(^2\)Nowadays [4] this universal correction is easily recognized as the Casimir energy of the (bosonic) conformal field theory in a finite geometry with free boundary conditions that describes the transverse fluctuations of the flux tube; $D - 2$ being the central charge of this theory.
the IR, eq. (1). Not just does this ansatz completely ignore the lattice artifacts, it strictly speaking contradicts QCD at short distances. The number $e$ has to be interpreted as some kind of effective average coupling. It is not even clear that $e$ is an effective short-distance quantity, since it usually comes out rather close to the IR charge $e_{\text{IR}} = \pi/12$ in eq. (1).

To partially accommodate lattice effects, Michael [5] has suggested to add a term to this ansatz, proportional to the difference between the lattice and the continuum Coulomb potential. This takes into account at least the tree-level lattice artifacts. Also, since recent Monte Carlo data [5, 6, 7] on fine lattices are accurate enough to see that $e$ really is a running charge, Michael [5] proposed to take this into account in a phenomenological way by replacing $e$ with $e - f/r$, with some new parameter $f$. If necessary, we will distinguish these kind of ansätze from the naive Coulomb + linear one, by calling them “modified Coulomb + linear ansätze” (or fits).

With this setup one can include smaller $r$-values in the fit, but the first few still have to be left out — and more and more as the data get more precise and the lattice spacings smaller. Furthermore, the short-distance parameters are not very stable with respect to varying the fit range, in particular on fine lattices. This is not surprising, since asymptotic freedom is not properly incorporated in this ansatz; the short-distance parameters are all effective parameters. Therefore, the only physical result one obtains from these fits is, at best, an (improved) estimate of the string tension $\sigma$; no information about short-distance QCD, e.g. the $\Lambda$-parameter, is gained.

To learn about $\Lambda$ another idea of Michael [5] is now widely used. Namely, one defines a running coupling $\alpha_F(r)$ in the “force scheme” by

$$r^2 V'(r) \equiv C_F \alpha_F(r). \quad (2)$$

Here $C_F = (N^2 - 1)/2N$ is the Casimir invariant of the fundamental representation of SU($N$). One then fits numerical derivatives of the potential data to a 2-loop formula for $\alpha_F(r)$. Lattice artifacts, errors from taking numerical derivatives, and the fact that 2-loop evolution is only on the verge of becoming reliable, lead to quite large errors in $\Lambda$. Furthermore, it is hard to estimate the systematic errors of this $\Lambda$-determination; one might simply be determining an effective $\Lambda$, that is still quite far from the true $\Lambda$. This could be true even if some consistency checks involving different lattice spacings, e.g. scaling of quantities involving $\Lambda$, work quite well. In fact, our results indicate that this is exactly what happens.

We here describe a new method that allows for a unified fit of potential data at all distances by incorporating lattice artifacts and the running of the coupling in a more fundamental way. The general idea is to express the lattice potential in terms of a running coupling. More precisely there are three ingredients:
1. As advocated in refs. [8, 9], for example, use the continuum static potential to define a physical running coupling \( \alpha_{V}(q) \) via

\[
V(q) \equiv -C_{F} \frac{4\pi \alpha_{V}(q)}{q^{2}}. \tag{3}
\]

This scheme for the coupling will be referred to as the V scheme. With this definition the effect of multi-gluon exchange is absorbed into \( \alpha_{V}(q) \). Fourier transforming eq. (3), the continuum potential is by definition given by

\[
V(r) = -C_{F} \int_{-\infty}^{\infty} \frac{d^{3}q}{(2\pi)^{3}} e^{-iqr} \frac{4\pi \alpha_{V}(q)}{q^{2}} = -\frac{2C_{F}}{\pi} \int_{0}^{\infty} dq \frac{\sin qr}{qr} \alpha_{V}(q). \tag{4}
\]

2. Globally parameterize \( \alpha_{V}(q) \) to take into account 2-loop QCD in the UV in terms of \( \Lambda \), the string prediction of eq. (1) in the IR in terms of \( \sigma \), and to have another parameter determining how fast the crossover from the UV to the IR behavior occurs. [Actually we will see that by introducing further parameters we can take into account any number of loops in the UV.]

3. Finally, make the ansatz that in terms of the continuum \( \alpha_{V}(q) \) the potential on an infinite lattice of spacing \( a \) can be accurately represented as,

\[
V_{a}(r) = V_{0} - C_{F} \int_{-\pi/a}^{\pi/a} \frac{d^{3}q}{(2\pi)^{3}} e^{-iqr} \frac{4\pi \alpha_{V}(\hat{q})}{q^{2}}, \quad \hat{q}_{i} \equiv \frac{2}{a} \sin \frac{aq_{i}}{2}, \tag{5}
\]

except presumably for \( r = 0 \), where the whole underlying picture of gluon exchange breaks down (which is why we have to add the constant \( V_{0} \) after making the integral convergent by subtracting its value at \( r = 0 \)).

The three parameters in \( \alpha_{V}(q) \) and the constant \( V_{0} \) are then fitted by matching eq. (5) to the Monte Carlo data for the potential.

To be sure, the above equation for the lattice potential in terms of the continuum coupling must be regarded as an ansatz. The motivation for this ansatz is that it appears to be the most natural expression that (a) gives the exact tree level lattice potential, that is, the lattice Coulomb potential (corresponding to the case \( \alpha_{V}(q) \equiv \text{const} \)), and (b) has the right continuum limit. The fact that eq. (5) will allow us to obtain excellent fits of the lattice potential of a wide variety of theories down to one lattice spacing, provides indirect empirical evidence for its accuracy. Additional evidence will be discussed later.

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^3The “lattice momentum” \( \hat{q} \) in eq. (5) is appropriate for the usual Wilson action. If an improved action is used, \( \hat{q} \) should be replaced by the corresponding “improved momentum”, yielding an improved potential \( V_{a}(r) \), etc.
The outline of this paper is as follows. In sect. 2 we provide the details of the parameterization of $\alpha_V(q)$ satisfying the required UV and IR behavior. In particular, we prove an elementary theorem showing how the running coupling can be written in terms of “iterated logarithms” to all orders of the loop expansion of the $\beta$-function. This theorem then suggests a natural way of avoiding the perturbative Landau pole, motivating our ansatz for the running coupling.

In sect. 3 we discuss the efficient evaluation of the three-dimensional integral in eq. (5), and details of our fitting and error analysis procedure. In sect. 4 we apply our results to Monte Carlo data for the lattice potential of various gauge theories; with gauge group SU(3) or SU(2), with or without dynamical fermions (Wilson and staggered). Using eq. (5) leads to excellent fits of the data down to one lattice spacing. To check for systematic errors in the running coupling $\alpha_V(q)$ extracted from these fits, we perform fits with an $\alpha_V(q)$ that partially incorporates 3-loop effects. We compare our results with the Lepage-Mackenzie estimate [10] of $\alpha_V(q)$ in the UV, in particular also on very fine lattices. We then compare the 1-loop expansion of eq. (5) with the 1-loop results of [11] for the on-axis lattice potential. Curiously enough, our 1-loop expansion agrees much better with the Monte Carlo data than the results of [11]. These comparisons provide good evidence for the accuracy of representing the lattice potential as in eq. (5). Finally, we check how accurate 2-loop evolution is compared to our non-perturbative $\alpha_V(q)$.

Sect. 5 is devoted to scaling. We use the intermediate scale $r_0$ introduced by Sommer [12] to determine the ratios of lattice spacings of various theories much more accurately than previously possible. For pure SU(3) we find that $\alpha_V(q)$ scales on the percent level for $\beta \geq 6.0$. In sect. 6 we compare our approach with other schemes to define and extract a running coupling from Monte Carlo simulations. In particular, we provide some details about the force scheme and its close relation to the V scheme. We conclude in sect. 7 by summarizing our findings and outlining various applications and extensions.

In [13] we presented a brief summary of our results. Due to the fact that our error analysis is somewhat involved, some of the results given in [13] were slightly preliminary (also, in one case we only had preliminary potential data).

2 Parameterizing the Running Coupling

2.1 The Ultraviolet Regime

We will first describe some general results concerning the integration of the $\beta$-function

$$\beta(\alpha) \equiv q^2 \partial_q \alpha(q) = -\beta_0 \alpha^2 - \beta_1 \alpha^3 - \beta_2 \alpha^4 - \ldots ,$$

(6)
of the coupling $\alpha = g^2/4\pi$ in a generic scheme. Recall that the 1- and 2-loop coefficients are scheme independent and equal to [14]

$$4\pi \beta_0 = \frac{11}{3} N - \frac{2}{3} n_f, \quad (4\pi)^2 \beta_1 = \frac{34}{3} N^2 - \left(\frac{10}{3} N + \frac{N^2 - 1}{N}\right) n_f$$

in QCD with gauge group $SU(N)$ and $n_f$ flavors of massless fermions. The higher coefficients depend on the scheme (none are presently known in the V scheme). In terms of $\hat{\alpha}(q) \equiv \beta_0 \alpha(q)$ the integration of the $\beta$-function immediately leads to

$$\frac{1}{\hat{\alpha}} = t + b \ln \left(\frac{1 + b\hat{\alpha}}{\hat{\alpha}}\right) - \int_0^{\hat{\alpha}} dx \left(\frac{1}{\hat{\beta}(x)} + \frac{1}{x^2(1 + bx)}\right) = t + b \ln \frac{1}{\hat{\alpha}} + b_2 \hat{\alpha} + b_3 \hat{\alpha}^2 + \ldots,$$

where $\hat{\beta}(\hat{\alpha}) \equiv -\hat{\alpha}^2(1 + \hat{\beta}_1 \hat{\alpha} + \hat{\beta}_2 \hat{\alpha}^2 + \ldots)$, $\hat{\beta}_i \equiv \beta_i / \beta_0^{i+1}$, and

$$t \equiv \ln\left(\frac{q^2}{\Lambda^2}\right), \quad b \equiv \hat{\beta}_1, \quad b_2 \equiv \hat{\beta}_1^2 - \hat{\beta}_2, \quad b_3 \equiv \hat{\beta}_1^2 - 1/2 \hat{\beta}_3 - 1/2 \hat{\beta}_3.$$

(8)

We have followed the usual convention of defining the integration constant, the $\Lambda$-parameter, so that there is no constant term on the rhs of (8). Note that as long as the $\beta$-function has a power series expansion in $\alpha$, there is only one logarithmic term on the rhs of (8), coming from the first two loops. Solving (8) iteratively gives

$$\frac{1}{\hat{\alpha}} = t + b \ln t + \frac{1}{t} \left[b^2 \ln t + b_2\right] + \frac{1}{t^2} \left[-\frac{1}{2} b^3 \ln^2 t + (b^3 - b b_2) \ln t + b b_2 + b_3\right] + \ldots.$$  

(10)

As an aside we would like to point out that the full 2-loop expression for $1/\hat{\alpha}$ involves not just the leading terms $t + b \ln t$ usually quoted, but also the subleading 2-loop term $b^2 \ln t/t$.

Recall that the above expansion has a Landau pole, i.e. the perturbative $\hat{\alpha}(q)$ diverges for some $q > \Lambda$ as $q$ approaches $\Lambda$ from above. One of the goals of the ansatz we will later use for $\alpha_V(q)$ is of course to avoid this unphysical Landau pole. To motivate our ansatz we now describe a different way of solving (8) for $\alpha(q)$. Namely, consider the following recursively defined function

$$R(t) \equiv R^{(0)}(t), \quad R^{(k)}(t) \equiv b \ln \left[a_k(t + R^{(k+1)}(t))\right], \quad k = 0, 1, 2, \ldots.$$  

(11)

We now prove that by suitably choosing the coefficients $a_k > 0$ the running coupling can be written as

$$\frac{1}{\hat{\alpha}} = t + R(t).$$  

(12)

This is equivalent to showing that $R(t) = t - \frac{1}{\hat{\alpha}}$ can be rewritten in terms of $\hat{\alpha}$ in the form $R = b \ln \frac{1}{\hat{\alpha}} + b_2 \hat{\alpha} + b_3 \hat{\alpha}^2 + \ldots$. The proof is simple: By substituting
\( t = \frac{1}{\alpha} - R^{(0)} \) in the definition of \( R^{(k)} \) we have

\[
R^{(k)} = b \ln \left( \frac{a_k}{\alpha} \right) + b \ln \left[ 1 + \hat{\alpha}(R^{(k+1)} - R^{(0)}) \right].
\]  

(13)

All we have to do is to iterate these equations, starting with \( R^{(0)}(k) = b \ln(a_k/\alpha) \). By induction one therefore proves

\[
R^{(k)} = b \ln \left( \frac{a_k}{\alpha} \right) + b \sum_{n=1}^{\infty} R^{(k)}_n (b\hat{\alpha})^n,
\]  

(14)

where \( R^{(k)}_n = \ln a_{k+n} + \text{terms involving only } \ln a_j \text{ with } j < n + k \). This completes the proof.

Specifically, \( R^{(1)}_1 = \ln(a_{k+1}/a_0) \), \( R^{(2)}_2 = \ln(a_{k+2}/a_1) - \frac{1}{2} \ln^2(a_{k+1}/a_0) \), etc. So the first few \( a_k \) are determined by

\[
a_0 = 1, \quad b^2 \ln a_1 = b_2, \quad b^3(\ln a_2 - \ln a_1 - \frac{1}{2} \ln^2 a_1) = b_3.
\]  

(15)

Note that to obtain the \( 1/\hat{\alpha} \) expansion to \( n \) loops one can truncate the iterative definition of \( R(t) \) by setting \( R^{(n-1)} = b \ln t \). For example, to get two loops we can simply set \( R(t) = b \ln(t + b \ln t) \), cf. (10).

Our iterated form of \( R(t) \) still has a Landau pole, but now a simple way to avoid it suggests itself by the replacements:

\[
\frac{1}{\hat{\alpha}(q)} = t + R^{(0)}(t) \to \frac{1}{\hat{\alpha}(q)} = \ln \left[ 1 + e^t e^{R^{(0)}(t)} \right],
\]  

(16)

and

\[
e^{R^{(k)}(t)} \to \ln b \left[ c_k + e^{a_k t} e^{a_k R^{(k+1)}(t)} \right],
\]  

(17)

with some constants \( c_k \geq 1 \). [The constant 1 in eq. (16) is chosen to get the right IR behavior for \( \alpha_V(q) \), see below. In a scheme where the coupling “freezes out” in the IR some constant \( > 1 \) should be chosen.] Note that the \( c_k \) are non-perturbative parameters. Obviously the new \( \hat{\alpha}(q) \) has no Landau pole.

To two loops we can now write as ansatz for \( \alpha_V(q) \)

\[
\frac{1}{\beta_0 \alpha_V(q)} = \ln \left[ 1 + e^t \ln \left[ c_0 + e^t \lambda(t) \right] \right], \quad b = \beta_1/\beta_0, \quad t = \ln(q^2/\Lambda^2_V),
\]  

(18)

where we know that \( \ln \lambda(t) = R^{(1)}(t) = b \ln t \) in the UV limit. A natural Landau pole free form of \( \lambda(t) \) is

\[
\lambda(t) = \ln b \left[ c_1 + c e^t \right],
\]  

(19)
with a new parameter \( c > 0 \). We will see below that \( c_0 \) and \( c_1 \) are fixed by the required IR behavior in terms of \( \Lambda_V, \sigma \) and \( e_{\text{IR}} \). \( c \) is the crossover parameter mentioned in the introduction.

The relation of the \( \Lambda \)-parameter in the \( V \) scheme, \( \Lambda_V \), to that in another scheme is fixed by a 1-loop calculation [15]. For instance, the relation to the \( \overline{\text{MS}} \) scheme is given by [16, 17, 18],

\[
\Lambda_V / \Lambda_{\overline{\text{MS}}} = \exp[(31N - 10n_f)/(66N - 12n_f)].
\]

If one wants to incorporate three loops, one would write

\[
\lambda(t) = \ln^b \left[ c_1 + e^{a_1 t} e^{a_1 R(2)(t)} \right],
\]

and for \( e^{R(2)(t)} \) use the form \( \ln^b (c_2 + c e^t) \), say. Note that the leading 3-loop effects are given by the \( e^{a_1 t} \) term. They are included if we simply replace \( e^{a_1 R(2)(t)} \) by a constant \( c \).

Eq. (18) is a generalization of Richardson’s ansatz [19], who writes \( \beta_0 \alpha_R(q) = 1/\ln[1 + q^2 / \Lambda_R^2] \). His potential, defined as in (4), has the advantage of simplicity, containing only the single parameter \( \Lambda_R \). However, by the same token, the corresponding potential can be fitted to describe only the UV or the IR or the crossover region, but not all three or even two of them. For potential models mainly the crossover region is relevant, explaining why the Richardson potential works so well in that context.

### 2.2 The Infrared Regime

To build the IR behavior given by eq. (1) into our ansatz we have to transform eq. (1) to momentum space. \textit{A priori} the Fourier transform of \( \sigma r \) is ill-defined. However, the potential corresponding to \( \alpha_V(q) = q^{-n} \) can be defined by analytic continuation in \( n \) to be

\[
V(r) = -C_F \frac{r^{n-1}}{\Gamma(n+1) \cos \frac{\pi n}{2}},
\]

as long as \( n \) is not an odd integer. So (1) corresponds to the small \( q \) expansion

\[
\alpha_V(q) = \frac{2}{C_F} \frac{\sigma}{q^2} + \frac{e_{\text{IR}}}{C_F} + \ldots,
\]

and matching this to eq. (18) leads after a small amount of algebra to

\[
\ln^b c_0 = \frac{C_F \Lambda_V^2}{2 \beta_0 \sigma}, \quad \ln^b c_1 = \left(1 - \frac{2}{C_F} \beta_0 e_{\text{IR}}\right) \frac{c_0}{2b} \ln^{b+1} c_0.
\]

For given \( N, n_f \) and \( \Lambda_V \), the string tension determines \( c_0 \). \( c_1 \) is then fixed by the IR charge. In other words, \( c_0 \) and \( c_1 \) parameterize the leading and subleading IR behavior, respectively. This was of course already obvious from their definition in eqs. (18) and (19).
2.3 Summary

The ansatz defined by eqs. (18), (19) and (23) will be referred to as our “standard ansatz”. It is consistent with 2-loop QCD in the UV and in the IR reproduces the leading and subleading prediction of the string picture. For given $N$, $n_f$ and $e_{IR}$ we have to fit three parameters in $\alpha_V(q)$: $\Lambda_V$, $\sigma$ and the crossover parameter $c$. The leading 3-loop effects can be taken into account by adding one more parameter, $a_1$ in eq. (20). At this point we fix the IR charge at $e_{IR} = \frac{\pi}{12}$, leaving a check of this value to future high precision studies.

3 Fitting and Error Analysis

3.1 Numerical Evaluation of $V_{a^2}(r)$

It is crucial to have an efficient way of numerically evaluating $V_{a^2}(r)$ if one wants to perform fits. Recall first of all, that our approach is not expected to work for $r = 0$. So we can not simply subtract off the $r = 0$ value of our ansatz when comparing with the Wilson loop potential, which is normalized to vanish for $r = 0$, by such an (implicit) subtraction. For simplicity we have therefore added a constant in eq. (5), after performing the subtraction. [The subtraction is still useful, since then the integral has an integrable singularity at $q = 0$, and does not have to be defined by analytic continuation.]

Since the integrand of $V_{a^2}(r)$ is a periodic function in each $q_i$ one can quite efficiently evaluate the integral as follows (cf. [20, 21]): First introduce a small gluon mass, i.e. replace $1/\hat{q}^2$ by $1/(\hat{q}^2 + m^2)$. Next approximate the integral by a sum; schematically

$$\int_{-\pi/a}^{\pi/a} d^d q F(q) \approx \left(\frac{2\pi}{aL}\right)^d \sum_n F\left(\frac{2\pi n}{aL}\right),$$

(24)

(where each component of $n$ runs from $-L/2$ to $L/2 - 1$ in integer steps) but only after applying the following change of variable to the integral: $q_i \rightarrow q_i - \epsilon \sin q_i$, where for given $m$, $\epsilon$ is determined by the equations $\epsilon = 1/\cosh u$, $u - \tanh u = m$. Using the Poisson resummation formula and a contour deformation argument one sees that this choice of $\epsilon$ greatly accelerates the convergence of the sum towards the integral as $L$ is increased. Finally, extrapolate to zero gluon mass. For the

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4This normalization is related to the overall constant in the potential (defined, for instance, by the behavior of the potential in the IR). Although this constant is physical — it determines the absolute energy of heavy quark bound states, for example — it has not yet been possible to calculate it in the Wilson loop approach, basically because it is difficult to separate from self-energy contributions. Therefore one defines the Wilson loop potential to automatically vanish at $r=0$. See [1] for a discussion of issues related to the constant in the potential.
accuracy desired here, about $10^{-5}$ for small $r$ and $10^{-4}$ for large $r$ to be safely below the Monte Carlo errors, we can dispense with the last step and simply use a fixed small mass such as $am = 10^{-4}$.

For small $r$ we find that $L = 20$ is sufficient. As the components of $r$ increase the integral becomes more and more oscillatory, so $L$ must increase correspondingly. If one needs to evaluate $V_{\alpha^2}(r)$ for many $r$-values, as we do, one should make sure to evaluate the $r$-independent part of the integrand only once for a given $2\pi n/aL$, instead of doing so again and again for different $r$.

For sufficiently large $r$ (depending on the accuracy of the potential data; typically when at least one component of $r$ is greater than $16a$) one can simply use the continuum $V(r)$ given by eq. (4). This integral is divergent in the IR and converges slowly in the UV. One can (define and) evaluate it efficiently as follows: To improve the convergence in the UV, add and subtract the Richardson potential with suitably chosen $\Lambda_R$. This potential has a quickly convergent integral representation [19]. Then cancel the $q^{-2}$ singularity of the new integrand by subtracting a term with $\alpha(q) \propto q^{-2}$ and add it on again in the analytically continued form of eq. (21). In the end add a suitable constant to match $V(r)$ to $V_{\alpha^2}(r)$.

3.2 Fitting Procedure

As it stands, we would perform fits of the MC data to the ansatz (5) by varying the overall constant $V_0$ and the parameters $\Lambda_V$, $\sigma$ and $c$ in $\alpha_V(q)$. However, it turns out that $\Lambda_V$ is strongly correlated with $c$ (and $V_0$), leading to a large error in $\Lambda_V$ without a corresponding large error in $\alpha_V(q)$. Clearly, the $\Lambda$-parameter is a bad parameterization of the physics. It is a much better idea to use $\alpha_V(q^*)$, where $q^*$ is some UV scale, as independent fit parameter. For easy comparison with the Lepage-Mackenzie method of estimating $\alpha_V(q^*)$ (see sect. 4.2) we choose $aq^* = 3.4018$.

We will therefore fit $V_0$, $\alpha_V(q^*)$, $\sigma$ and $c$. At present all our fits are uncorrelated, i.e. we do not take into account correlations between the potential data at different $r$ (we will comment on this in sect. 4.1.2). Instead, we form the usual, naive $\chi^2$ from our ansatz and the Monte Carlo data, which are available to us in the form $V_{MC}(r) \pm \delta V_{MC}(r)$. To find the minimum of $\chi^2$ we use Powell’s method [22], which does not require knowledge of any derivatives.

3.3 Error Analysis

We will find that the optimal value of $c$ is always quite small, with an error that can be of the same order as the average value of $c$. This is unfortunate, since, we recall, for $\alpha_V(q)$ to be consistent with full 2-loop evolution, any $c > 0$, but not
$c = 0$ is allowed. The optimal value is somewhat irrelevant, though, because the distribution of $c$ is often very non-gaussian, with a long tail towards larger values of $c$.

We will also find that $c$ can be quite strongly correlated with $V_0$ and $\alpha_V(q^*)$, whose distribution is then also skewed. The reason for this correlation is that, in particular for coarse lattices, only the first few points really “see” perturbative QCD, and we then have an over-parameterization of the UV and intermediate regime in terms of $V_0$, $\alpha_V(q^*)$ and $c$. As one would expect, these problems tend to go away as the data become more precise and the lattice spacings smaller.

The correlation between the parameters $\alpha_V(q^*)$, $c$ and $\sigma$ is usually such that they tend to move up and down together. The distribution of $\alpha_V(q^*)$ and $c$ can usefully, if somewhat simplified, be visualized as a narrow and relatively flat ridge, whose maximum is close to the end of the ridge where both parameters are small. In such a situation, error estimates based on the covariance matrix at the optimal parameter values are very misleading.\footnote{It does not help, by the way, to consider $\ln c$ instead of $c$ as fit parameter. Note, first of all, that this would correspond to a different assumption about the prior distribution of $c$ (in the sense of Bayes’ theorem) — now all values of $\ln c$, not $c$, are considered equally likely \textit{a priori}. In this case the distribution of $\ln c$ is strongly skewed in the opposite direction, with a long tail towards negative values of $\ln c$ and a sharp fall-off in the positive direction. In some cases the distribution even seems to become unnormalizable, since the tail to the left does not vanish sufficiently fast. We therefore stick to fitting $c$, using the $\ln c$ fits as one measure of systematic errors.}

To obtain reliable error estimates in all cases we have decided to use the following procedure. Once the optimal values of the fit parameters are known, we sample the total distribution around these values by varying the fit parameters, accumulating \textit{all} quantities of interest by weighing each sample volume $dV$ with a relative probability $dV \exp(-\chi^2/2)$. [Confer the maximum likelihood justification of the $\chi^2$ method.] For the fit parameters themselves the number of distinct values sampled was only $10 - 20$, so to estimate the 1-sigma band and similar statistical measures from the corresponding histograms we suitably interpolated the distribution between these values. For other quantities, like $\Lambda_V$ or $r_0$ (cf. sect. 5.2), the number of different values accumulated is very large and no interpolation is necessary. We have checked with various toy examples that this procedure gives reliable error estimates. In the long run one should of course perform the error analysis by bootstrapping the potential data — an option we do not have at this point.

For the error analysis it would of course be nice if we could replace $c$ by a more well-behaved fit parameter for the intermediate regime, namely one that is less correlated with $\alpha_V(q^*)$ and $V_0$ and whose distribution is more gaussian. We have tried various options — \textit{e.g.} replacing $c$ by $q_0$ or $q_0/\sqrt{\sigma}$ of sect. 5, or by $\alpha_V(q^*/3)$
— but with the present data all have problems of one sort or another in at least one case. It is possible though, we think, that some of these problems will not exist for more accurate potential data.\(^6\)

The above concerns the statistical errors. Since systematic errors affect different quantities to different extents, they will be discussed in the next two sections where we present explicit results for various quantities.

## 4 Results and Comparison with Other Methods

### 4.1 Overview

We applied our scheme to potential data obtained by Monte Carlo simulations of Wilson loops in the following lattice gauge theories:

- **Pure SU(3) at** \(\beta = 6.0, 6.4\) [7] on a \(32^4\) lattice and at \(\beta = 6.8\) [23, 24] on a \(48^3 \times 64\) lattice. Potential data exist, basically, at all lattice points that are multiples of \((1, 0, 0), (1, 1, 0), (1, 1, 1), (2, 1, 0), (2, 1, 1)\) or \((2, 2, 1)\), and have no component larger than 16 for \(\beta = 6.0\) and 6.4, and no component larger than 24 for \(\beta = 6.8\). For orientation we jump ahead and remark that the lattice spacings of these theories are between roughly 0.10 fm and 0.038 fm. We should mention that the \(\beta = 6.8\) data from [7], which we had first analyzed, turned out to suffer from large finite-size effects — even though they are nicely linear at large \(r\) — as the comparison with the new data shows. We will see later that the new \(\beta = 6.8\) data also show signs (much smaller though) of finite-size and/or other systematic errors. Finally, we should point out that the \(\beta = 6.8\) data used in [13] are from the same Wilson loop data, but used a preliminary extraction [23] of the potential from these Wilson loops. New SU(3) data will be analyzed with our method in [25].

- **SU(3) with two flavors of of dynamical staggered fermions of mass** \(am = 0.01\) at \(\beta = 5.6\) [26], and two Wilson fermions \((\kappa = 0.1675)\) at \(\beta = 5.3\) [26]. The lattice size is \(16^3 \times 32\) in both cases, with a spacing of about 0.10 fm and 0.14 fm, respectively. The potential was calculated at all points in a plane with no component larger than 8. There was no sign of string breaking for the \(r\)-values considered. It seems that the main effect of the non-zero fermion

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\(^6\)For example, if one uses \(q_0\), the problem is that the mapping from \(\alpha_V(q^*)\) and \(q_0\) to \(\Lambda_V\) and \(c\) becomes nearly degenerate when \(c\) is very small. The fact that in some cases the optimal value of \(c\) is very small, might be an artifact of present data that will disappear with better data (more precisely, once the effective potentials have been extrapolated to large euclidean times, cf. sect. 4).
masses is to renormalize the fit parameters. [We will see however that the effect of quenching can not be absorbed in a "\(\beta\)-shift" with respect to quenched QCD.]

- Pure SU(2) at \(\beta = 2.85\) [6] on a \(48^3 \times 56\) lattice. Potential data\(^7\) were available at all points with no component larger than 3 and at all even on-axis points \(r/a = 4, 6, 8, \ldots, 24\). The lattice spacing is about 0.028 fm.

Recall that \(\beta\) is related to the bare lattice couplings \(g_0\), respectively \(\alpha_0\), by \(\beta \equiv 2N/g_0^2 = N/2\pi\alpha_0\).

### 4.1.1 Results from the Standard Ansatz

Using our standard ansatz of sect. 2 we could fit all data down to one lattice spacing, with the uncorrelated \(\chi^2 \approx N_{DF}\). In sect. 4.1.2 we will discuss in detail what possible effect the neglect of correlations has on our results. To convince the reader that our fits really are much better than previous ones, let us here just note (more details will be given as we proceed) that in contrast to our ansatz, it is completely impossible, at least on fine lattices, to describe the data within errors down to one, or even several lattice spacings with the modified Coulomb + linear ansätze discussed in sect. 1. This is particularly obvious from plots of the difference between fit and data; we will present such plots below. We also note that our fit parameters are essentially stable with respect to variations of the fit range, which can not be said about Coulomb + linear fits on fine lattices.

Our results for the optimal parameters and \(\chi^2\) of the fits are given in table 1. As already mentioned in sect. 3.3, the distribution of \(c\) is quite non-gaussian, and to obtain reliable errors we use the procedure described there. The results are shown in table 2. As it turns out that the 1-sigma band (determined by cutting off 16% of the distribution on each side) is typically rather symmetric around the average of a random variable, even if the distribution itself is quite skewed, we saw no need to quote asymmetric errors. [In some cases we slightly shifted the mean, to put it in the middle of the 1-sigma band.] Note however that the optimal parameters of table 1 usually lie very asymmetrically within the 1-sigma band quoted in table 2, for \(\alpha_V(q^*)\), \(\Lambda_V\) and \(c\) sometimes even outside it!

Note that in the above tables we also included data sets denoted by \(\beta = 6.8'\) and 2.85'. This was done to illustrate the effect that uncertainties of the Monte

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\(^7\)As in the references above, for the SU(2) case and those with dynamical fermions we actually used data for the "effective potential" \(V_T(r)\) obtained from Wilson loops at euclidean times \(T\) and \(T+1\), with \(T = 3\) for the Wilson fermion case, and \(T = 4\) for the SU(2) and staggered fermion cases. The actual potentials, obtained by a large \(T\) extrapolation, will differ somewhat from these effective potentials.
| Group | \( n_f \) | \( \beta \) | \( \alpha_V(q^*) \) | \( a\Lambda_V \) | \( a^2\sigma \) | \( c \) | \( \chi^2/N_{DF} \) |
|---|---|---|---|---|---|---|---|
| SU(3) | 0 | 6.0 | 0.1460(18) | 0.140(18) | 0.0486(5) | 0.0011(9) | 65.2/62 |
| SU(3) | 0 | 6.4 | 0.1299(7) | 0.0997(28) | 0.01513(25) | 0.012(6) | 89.6/66 |
| SU(3) | 0 | 6.8 | 0.11514(12) | 0.0603(4) | 0.00690(5) | 0.0070(8) | 188.8/104 |
| SU(3) | 0 | 6.8' | 0.11468(17) | 0.0587(5) | 0.00658(7) | 0.0036(7) | 135.0/68 |
| SU(2) | 0 | 2.85 | 0.1675(5) | 0.0484(19) | 0.00398(25) | 0.003(7) | 36.2/26 |
| SU(2) | 0 | 2.85' | 0.1685(8) | 0.0510(25) | 0.00387(9) | 0.00045(37) | 21.8/26 |
| SU(3) | 2W | 5.3 | 0.1895(16) | 0.1749(10) | 0.1001(5) | 0.00689(5) | 6.84 \cdot 10^{-3} |
| SU(3) | 2S | 5.6 | 0.1674(11) | 0.1262(10) | 0.0485(3) | 0.0011(9) | 40.0/37 |

Table 1: Optimal fit parameters and uncorrelated \( \chi^2 \) for our standard ansatz. \( W, S \) indicates Wilson, respectively, staggered fermions. The \( \beta = 6.8' \) and 2.85' data sets are explained in the main text. Note that \( \Lambda_V \) is not a fit parameter in our procedure; it is quoted for reference purposes.

| Group | \( n_f \) | \( \beta \) | \( \alpha_V(q^*) \) | \( a\Lambda_V \) | \( a^2\sigma \) | \( c \) |
|---|---|---|---|---|---|---|
| SU(3) | 0 | 6.0 | 0.1470(18) | 0.140(18) | 0.0486(5) | 0.0011(9) |
| SU(3) | 0 | 6.4 | 0.1299(7) | 0.0997(28) | 0.01513(25) | 0.012(6) |
| SU(3) | 0 | 6.8 | 0.11514(12) | 0.0603(4) | 0.00690(5) | 0.0070(8) |
| SU(3) | 0 | 6.8' | 0.11468(17) | 0.0587(5) | 0.00658(7) | 0.0036(7) |
| SU(2) | 0 | 2.85 | 0.1675(5) | 0.0484(19) | 0.00398(25) | 0.003(7) |
| SU(2) | 0 | 2.85' | 0.1685(8) | 0.0510(25) | 0.00387(9) | 0.00045(37) |
| SU(3) | 2W | 5.3 | 0.1895(16) | 0.1749(10) | 0.1001(5) | 0.00689(5) |
| SU(3) | 2S | 5.6 | 0.1674(11) | 0.1262(10) | 0.0485(3) | 0.0011(9) |

Table 2: Average fit parameters and 1-sigma band for our standard ansatz, obtained with the error analysis procedure of sect. 3.3.

Carlo potential data have an impact on our fit parameters. For the \( \beta = 6.8' \) SU(3) data set we omitted data points at large distances, namely all points with at least one component larger than 16\( a \). This gives us an idea if there are finite-size (or other large \( r \)) artifacts. These seem to exist, since the string tension from these two fits are not consistent. These effects are probably not quite as large as table 2 indicates, since by incorporating 3-loop effects we will later find better fits, where the difference is less significant. But the difference is still larger than in all other cases, where the string tension is completely stable when varying the fit range over comparable scales (in physical units).

For the \( \beta = 2.85' \) SU(2) set, we increased the errors of the potential at the first two lattice points from \( 1 \cdot 10^{-4} \) to \( 2 \cdot 10^{-4} \). From the tables in ref. [6] the extrapolation of the effective potential to large times might easily change the values by this.
amount, and, in contrast to changes at large \( r \), that presumably can be absorbed into a change of the string tension without otherwise affecting the fit, it is not obvious that an analogous statement will be true for short distances, where errors are much smaller. In this case, increasing the errors at small \( r \) significantly reduces \( \chi^2 \), but does not lead to much different values for the fit parameters. We regard the two “primed” data sets as somewhat more reliable than the corresponding “unprimed” ones.

One might wonder why the fractional error of \( \alpha_V(q^*) \), although quite small, is much larger than that of the lattice potential at \( r = a \), which in the worst case is a few times \( 10^{-4} \). The main reason for this is that \( \alpha_V(q^*) \) is strongly correlated with the overall constant \( V_0 \) of the potential; an increase, say, of \( V_0 \) can be partially compensated by a decrease of \( \alpha_V(q^*) \) (and smaller changes of \( c \) and \( \sigma \)). If the potential data at small \( r \) are correlated, fits that take this into account should give a more precise \( \alpha_V(q^*) \) (see below).

Note the relatively large statistical error of \( \Lambda_V \) in table 2, to which, as we will see below, we have to add a systematic error that in some cases is even larger. This large error is not just due to the fact that only the logarithm of \( \Lambda_V \) enters in \( \alpha_V(q) \). Instead, the main contribution to its error comes from the correlation with \( c \). Since both parameters are, roughly speaking, intermediate range parameters, one should not be surprised that their correlation is such that it leads to a much smaller error in the running coupling than expected from naive error propagation. This was the reason we chose \( \alpha_V(q^*) \), not \( \Lambda_V \), as the fit parameter for the UV region.

From table 2 we see that the quenched \( \beta = 6.0 \) and the unquenched \( \beta = 5.6 \) SU(3) theory have almost the same string tension. In previous studies it has often been found empirically that the effect of unquenching can be absorbed into such a change of \( \beta \). Of course, strictly this can not be true, since it would contradict QCD at short distances. And indeed, we find in table 2 that these two theories have very different UV couplings \( \alpha_V(q^*) \).

### 4.1.2 Correlated versus Uncorrelated Fits, Systematic Errors

We should comment on our use of naive, uncorrelated fits (cf. sect. 3), that ignore any correlations the potential data might have between different \( r \)-values. Of course, one should eventually take these into account, preferably by bootstrapping. We do not have this option at present, but would like to dispel any worries one might have, that we are, say, underestimating the errors because of this.

To investigate this question we have performed fits of all potential data to modified Coulomb + linear ansätze (cf. sect. 1) using the uncorrelated \( \chi^2 \), and compared them to previous results from correlated fits with the same ansatz and
fit range [6, 7, 26, 23, 27]. We estimate the errors from the covariance matrix, which for these fits should be reasonably accurate, since in contrast to the crossover parameter $c$ in our ansatz, for example, none of the parameters here is expected to be strongly non-gaussian \textit{(a posteriori} this is also justified by the excellent agreement with errors from bootstrapping for weakly correlated data). We find:

(i) The uncorrelated $\chi^2$ is smaller than the correlated one; slightly if the data are weakly correlated, \textit{much} smaller if the data have large correlations.

(ii) The central values of the fit parameters are largely unaffected, even if the correlations are strong.

(iii) The errors from uncorrelated fits tend to be too \textit{large}, significantly so if the data are strongly correlated.

Basically, these features are well known [23, 27, 28]. In fact, thinking about how $\chi^2$ is affected by (positive) correlations, and how this in turn affects the “$\Delta \chi^2 = 1$” method of estimating errors, the above features are more or less obvious. The first point, that our fits will underestimate $\chi^2$ if the data are correlated, is of no big concern. Our aim in this paper is (a) to show that our ansatz for the potential is much better than Coulomb + linear ansätze, and (b) give an estimate of the errors of the running coupling extracted from our fits. If point (a) is not clear already on purely theoretical grounds — assuming QCD is correct — then one only needs to look at some pictures of the fractional difference between our fit and the data (see below) and compare them with corresponding pictures from Coulomb + linear fits (see \textit{e.g.} [7]).

For the cases at hand, the only potential data that have strong correlations are those for pure SU(2). In this case, our errors for the parameters of $\alpha_V(q)$ are likely to be over- not underestimates, according to (iii). [In cases where the first few $r$-values had to be omitted from the Coulomb + linear fits, we can not exclude that the potential data have non-negligible correlations among these points. If so, correlated fits with our ansatz would allow us to determine $\alpha_V(q^*)$ more precisely.]

We add some remarks from our experience of comparing (uncorrelated) fits to our ansatz and to modified Coulomb + linear ansätze. We found that it is somewhat of an art to extract parameters from Coulomb + linear fits, in particular on finer lattices. Even with the lattice artifacts taken into account as described in sect. 1, and the Coulomb charge $e$ replaced by the mock running charge $e - f/r$, one has to omit many small $r$ points from the fit, and it is often not so clear if one ever reaches a plateau at which the parameters stabilize. For the $\beta = 6.8$ SU(3) data, for instance, neither $e$, $f$, or the coefficient of the lattice correction seems to stabilize; $f$ even becomes negative at some point. One clearly sees that this type of ansatz does not incorporate the correct physics.
Table 3: Optimal fit parameters and $\chi^2$ for $a_1 \neq 1$ ansätze.

| Group | $n_f$ | $\beta$ | $\alpha_V(q^*)$ | $a\Lambda_V$ | $a^2\sigma$ | $c$ | $a_1$ | $\chi^2/N_{DF}$ |
|-------|-------|---------|-----------------|--------------|-------------|----|-------|------------------|
| SU(3) | 0     | 6.0     | 0.1450          | 0.1081       | 0.0488      | 2.32 $\cdot 10^{-4}$ | 0.5  | 64.1/62 |
| SU(3) | 0     | 6.4     | 0.1286          | 0.0876       | 0.01530     | 8.77 $\cdot 10^{-3}$ | 0.5  | 88.8/66 |
| SU(3) | 0     | 6.8     | 0.11440         | 0.0549       | 0.00718     | 1.23 $\cdot 10^{-2}$ | 0.5  | 153.5/104 |
| SU(3) | 0     | 6.8'    | 0.11405         | 0.0532       | 0.00686     | 7.03 $\cdot 10^{-3}$ | 0.5  | 119.0/68 |
| SU(2) | 0     | 2.85    | 0.1663          | 0.0482       | 0.00387     | 3.37 $\cdot 10^{-6}$ | 1.5  | 26.2/26 |
| SU(2) | 0     | 2.85'   | 0.1667          | 0.0487       | 0.00379     | 3.84 $\cdot 10^{-6}$ | 1.5  | 17.8/26 |
| SU(3) | 2W    | 5.3     | 0.1883          | 0.2021       | 0.0994      | 6.12 $\cdot 10^{-5}$ | 1.5  | 35.6/37 |
| SU(3) | 2S    | 5.6     | 0.1664          | 0.1391       | 0.0480      | 3.01 $\cdot 10^{-5}$ | 1.5  | 37.0/40 |

Out fits, in contrast, are stable with respect to varying the fit range. Furthermore, we can at least argue — and we will in sect. 4.2 — that our UV parameter $\alpha_V(q^*)$ is most accurately determined at the shortest distances, but no such argument is possible for the unphysical “running charge” $e - f/r$.

We now turn to the systematic errors of $\alpha_V(q^*)$, $\sigma$ and $c$ in our ansatz. There are two potential sources of such errors: (i) our ansatz for the continuum running coupling, and (ii) remaining lattice artifacts not taken into account in our ansatz for the lattice potential in terms of the continuum coupling, eq. (5). Of course, in general we can not rigorously disentangle and separately investigate these two effects, since our fit necessarily involves both. [We can disentangle them at the 1-loop level, as we will discuss in sect. 4.3.] It is pretty clear, however, that lattice effects will have a very small direct influence on $\sigma$ and probably also on $c$. They might have an effect on $\alpha_V(q^*)$, and through the correlations of the fit parameters this would then indirectly influence $c$ and to a smaller extent also $\sigma$.

The question whether $\alpha_V(q^*)$ has errors due to lattice artifacts is sufficiently important to be discussed separately in the next subsection. Here we will discuss the errors of the fit parameters due to our ansatz for the coupling. Our fits in themselves give no indication of significant systematic errors in this ansatz.

The only real check of our ansatz for $\alpha_V(q)$, then, is to try to find other ansätze that give similarly good or better fits. This is not so easy. From sect. 2 we know how to incorporate higher loops into $\alpha_V(q)$. However, each loop adds at least two new parameters (one corresponding to the coefficient in the $\beta$-function, the other is a non-perturbative parameter arising from our method of avoiding the Landau pole), and this often leads to stability problems with the fits, since the limited

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8There is a slight but noticeable dependence on the fit range for the $\beta=6.8$ SU(3) data, where (cf. the previous remarks on the $\beta=6.8'$ data set, and below) it is just as likely to be due to the data, rather than our ansatz.
Table 4: Average fit parameters and 1-sigma band for $a_1 \neq 1$ ansätze.

| Group | $n_f$ | $\beta$ | $\alpha_V(q^*)$ | $a\Lambda_V$ | $a^2\sigma$ | $c$ | $a_1$ |
|-------|-------|----------|-----------------|-------------|-------------|-----|-------|
| SU(3) | 0     | 6.0      | 0.1462(15)      | 0.118(12)   | 0.0492(7)   | 0.0010(8) | 0.5  |
| SU(3) | 0     | 6.4      | 0.1289(7)       | 0.0892(37)  | 0.01545(33) | 0.014(8)  | 0.5  |
| SU(3) | 0     | 6.8      | 0.11443(13)     | 0.0550(5)   | 0.00719(6)  | 0.0129(17)| 0.5  |
| SU(3) | 0     | 6.8'     | 0.11408(17)     | 0.0533(8)   | 0.00689(10) | 0.0076(18)| 0.5  |
| SU(2) | 0     | 2.85     | 0.1669(7)       | 0.0496(17)  | 0.00385(9)  | 0.000012(9)| 1.5  |
| SU(2) | 0     | 2.85'    | 0.1682(11)      | 0.0521(27)  | 0.00376(10) | 0.000042(37)| 1.5  |
| SU(3) | 2W    | 5.3      | 0.1916(27)      | 0.225(18)   | 0.0993(6)   | 0.0007(6) | 1.5  |
| SU(3) | 2S    | 5.6      | 0.1685(16)      | 0.152(9)    | 0.0479(3)   | 0.00022(18)| 1.5  |

part of the intermediate and UV region available in practice has effectively been vastly overparameterized. Another way of saying this, is that with present data non-perturbative and all-order effects apparently become important before we can clearly discern 3-loop effects.

We have tried various ansätze that fully or partially take into account 3- and 4-loop effects. Even if they give stable results, most give significantly better fits only for one of the theories we are considering. This might simply reflect a (not even large) fluke of the data in question. The overall best method we found has one new parameter $a_1$, that takes into account the leading 3-loop effects. It corresponds to the choice $\lambda(t) = \ln^b(c_1 + c e^{a_1 t})$ in eq. (18). Even these fits are not always stable and so in tables 3 and 4 we show results for suitably chosen fixed $a_1$. The values of $\chi^2$ are significantly better for the last four theories shown. None of the other “sporadically” better fits we found seems to lead to a much larger variation in fit parameters (or other quantities obtained from $\alpha_V(q^*)$, cf. sect. 5) than that observed when comparing tables 1 and 2 with tables 3 and 4.

Comparing tables 2 and 4 we see that the systematic errors of $\alpha_V(q^*)$ and $\sigma$ are never much larger, if larger at all, than their statistical errors. It is significantly larger in some cases for $\Lambda_V$. Since $c$ is really a different parameter for different $a_1$, it is not surprising that it can also change significantly. More relevant, however, is the question of how much $\alpha_V(q)$ from different fits differ in the intermediate region. We find, not surprisingly, that in this region $\alpha_V(q)$ is typically even better determined than at its “edges”.

For illustration, one of our fits is shown in figure 1. One sees that every little bump and wiggle of the data is reproduced by our fit. Since the errors are too small to be resolved in graphs of the potential itself, we show in figures 2 and 3 examples of the fractional difference between our fit and the Monte Carlo data.

Though these plots do not in any obvious way indicate that there are lattice
Figure 1: Comparison of Monte Carlo data (circles with error bars) for the lattice potential in pure SU(3) gauge theory at $\beta=6.0$ with $V_{a}(r)$ from our standard fit (lines), calculated on the lattice points and connected with straight lines to guide the eye. Shown is an overview (a) and the small $r$ region (b).
Figure 2: Fractional difference between our $a_1 = 1.5$ fit and the Monte Carlo results for the $\beta = 2.85'$ pure SU(2) potential in the small $r$ region.

Figure 3: Same as figure 2, for our $a_1 = 1.5$ fit of the potential of $\beta = 5.6$ SU(3) with two staggered fermions.
artifacts not reproduced by our ansatz, one could take the fact that the small $r$ region contributes a relatively larger fraction to the total $\chi^2$ as a hint of such a systematic error. However, this is at present just as likely to come from slight underestimates of the error or shifts in the central values of the potential data (compared to the true values) than from systematic errors in our ansatz. We recall that obtaining the true potential involves an extrapolation to large euclidean times. Uncertainties in the data arise, because either this extrapolation is not done and one simply quotes an effective potential from a fixed time, or, if the extrapolation is done, it is hard to independently assess its reliability for small $r$ (where the quoted errors are very small), since there was no theoretical expectation of what exactly the answer should be. This is underscored by the fact that slightly different procedures of extracting the potential from Wilson loops tend to lead to correlated changes of the potential. This can have a large effect on the $\chi^2$ of our fit, and lead to significant changes of the fit parameters.

From tables 1 to 4 it seems the theories under consideration fall into two classes: Pure SU(3), and the rest. For the former better fits are obtained for \( a_1 < 1 \) instead of \( a_1 = 1 \), whereas for the latter \( a_1 > 1 \) is preferable. Presumably related is the fact that in the pure SU(3) cases \( c \) is consistently larger than for the other theories.

The optimistic view would be that this is due to the size of the third \( \beta \)-function coefficient. It is not known in the V scheme, but if the \( \overline{\text{MS}} \) scheme is any guide, this can certainly not be sole explanation, since in this scheme [29] \( a_1 \simeq 0.600 \) is the same for pure SU(2) and SU(3), and \( a_1 \simeq 0.625 \) for SU(3) with \( n_f = 2 \).

In certain respects the pure SU(3) data seem not to behave as “nice” as the others. For example, the $\chi^2$ of the fits are not as good, and various quantities are less stable with respect to changing the form of our ansatz for $\alpha_V(q)$ or when leaving out small $r$ data points (cf. also sect. 5). The latter is true even though for pure SU(3) the decrease of $\chi^2$ when allowing $a_1 \neq 1$ is relatively smaller than for the other theories. One reason that might at least partially explain the relative stability and other “nice” features of the SU(2) data, as compared with the $\beta = 6.8$ data which naively would be expected to behave quite similar, is that at large $r$ the SU(2) data consist only of on-axis points. Another reason could be that the SU(2) data have significant correlations in $r$, at least for large distances [6]. However,

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9In the process of searching for possible systematic errors due to lattice artifacts, we have also checked what happens if we use $\alpha_V(q)$ instead of $\alpha_V(\tilde{q})$ in eq. (5). It turns out that despite the slow running of the coupling this does have a significant effect: It is not possible to get good fits at small $r$; the points $r/a = \sqrt{2}, \sqrt{3}, 2$ are impossible to fit simultaneously. It is of course not too surprising that one should use $\alpha_V(\tilde{q})$ in (5), since the integrand of $V_{\alpha V}(r)$ should be periodic in all $q_i$.

10We know for a fact that this is true for the existing $\beta = 6.8$ pure SU(3) data, where Gunnar Bali generously provided us with potentials extracted by slightly different procedures from the Wilson loop data.
this does not distinguish the $n_f=2$ theories from the other pure SU(3) cases.

One fact that does differentiate the two classes is that only for the pure SU(3)
data was the potential extrapolated to large euclidean times; in the other cases
only effective potentials were available. Another point to note is that for the pure
SU(3) theories potential data exist for much larger distances. We performed a fit
of the $\beta = 6.0$ data where we only included points that also exist for unquenched
SU(3) at $\beta = 5.6$. The value of $c$ decreases significantly, and, more generally, the
SU(3) data behave more similar to those of the second class also in other (though
not all) respects.

Although we do not understand why $c$ should decrease, the facts mentioned in
the last paragraph would seem to provide the best guess, at present, of why the
theories under consideration should appear to fall in two classes.\textsuperscript{11} The “nicer”
behavior of the second class might disappear once extrapolated to large euclidean
times. In fact, it was observed in [6] that the difference between the (on-axis)
effective SU(2) potential and the extrapolated one is not smooth in $r$. If this is
the problem, one should investigate if it is possible to perform the extrapolation
in a smoother way.

Note that in itself the small value of $c$ in the second class of theories is somewhat
questionable, since $c=0$ is not consistent with full 2-loop evolution. On the one
hand, it is only $\ln c$ that enters into the UV expansion, so a small value of $c$ does
not necessarily violate the principle of naturalness. However, note that the value
of $c$ is even smaller for the $a_1 > 1$ fits than for the $a_1 = 1$ ones. This makes a certain
mathematical sense, but one might question it on physical grounds: Recall that
the $\chi^2$ of these fits is significantly better than those with $a_1 = 1$. If we take this
to mean that we are really seeing 3-loop effects, then it is surprising that at the
same time the 2-loop effects are suppressed due to the small value of $c$. However,
since a small $c$ always suppresses both 2-loop and (the leading) 3-loop effects, this
argument is not conclusive. Only new data, with careful consideration of finite-size
and extrapolation effects, will help to clarify these questions.

4.1.3 Estimate of the String Tension

For future reference we would like combine our results and quote estimates of the
string tension for the various theories we studied. To obtain the best values we
should not just take into account the results in tables 2 and 4, but also the following:
We are performing a global fit and do not want any potential uncertainties at
small $r$ to distort the fit at large $r$. Therefore we fix $\alpha_V(q^*)$ at its average value
obtained from a fit with all data points, and leave out successive short-distance

\textsuperscript{11}To be sure, note that the “smoother” behavior of the second class is not due to smaller errors.
Despite the extrapolation, it is the pure SU(3) data that have much smaller errors.
Table 5: Comparison of our estimate of the string tension in lattice units with previous ones from (modified) Coulomb + linear fits.

| Group | \( n_f \) | \( \beta \) | \( a^{2}\sigma \) (our fit) | \( a^{2}\sigma \) (C+L fit) |
|-------|--------|--------|----------------|----------------|
| SU(3) | 0      | 6.0    | 0.0491(8)      | 0.0513(25)     |
| SU(3) | 0      | 6.4    | 0.0153(4)      | 0.0139(4)      |
| SU(3) | 0      | 6.8    | 0.0070(3)      | 0.00705(14)    |
| SU(2) | 0      | 2.85   | 0.00375(14)    | 0.00354(26)    |
| SU(3) | 2W     | 5.3    | 0.0992(9)      | 0.0976(9)      |
| SU(3) | 2S     | 5.6    | 0.0480(5)      | 0.0481(5)      |

As expected, our results are generally in good agreement with previous estimates, though often more precise. An exception is \( \beta = 6.4 \) pure SU(3), where our result is significantly higher than the latest Coulomb + linear estimate (though it agrees much better with a previously published estimate [7] and our own estimate from uncorrelated Coulomb + linear fits).

Since our method takes into account the corrections to the asymptotic linear behavior more accurately, one would expect that it gives better estimates of the string tension than previously possible. That our errors are not always smaller than previously quoted ones, is due to the fact that we were rather careful about systematic errors. In particular, for \( \beta = 6.8 \) the quoted error is almost completely of systematic origin. If one were similarly careful about systematic errors for Coulomb + linear fits, their errors would be as least as large, often much larger.

### 4.2 Lattice Artifacts, \( \alpha_V(q^*) \), and the Lepage-Mackenzie Method

Our precise estimate of \( \alpha_V(q^*) \) depends on including all points down to \( r = a \) in our fits. Leaving out \( r = a \) does in some cases lead to significant shifts in the central value. This is illustrated in table 6, where we show results from fits where data points at small \( r \) have been ignored.

If one had very precise data on a relatively fine lattice, leaving out \( r = a \) should not prevent an accurate determination of \( \alpha_V(q^*) \). This seems to be the case for
The SU(2) data, as table 6 indicates. However, if the data are not that precise, leaving out \( r = a \) is expected to lead to much larger errors, for the following reason: We will see in sect. 5 that the momentum scale \( q^* \) corresponds to a distance scale of roughly \( r^* \sim 1.53/q^* \sim 0.45a \). So, ignoring \( r = a \) will make it much harder to obtain precise information at scale \( r^* \).

One therefore should not be surprised that the determination of \( \alpha_V(q^*) \) rapidly deteriorates as one leaves out data points on the coarser lattices. A bit surprising is the fact that for the \( \beta = 6.8 \) SU(3) case the value of \( \alpha_V(q^*) \) from a full fit seems incompatible (on the 3−4 sigma level) with that from fits without \( r = a \), which still have very small errors and a much better \( \chi^2 \) (for the \( \beta = 6.8 \) results shown in table 6 the error of \( \alpha_V(q^*) \) is always less than \( 4 \cdot 10^{-4} \)).

Since it is not obvious that our ansatz (5) really incorporates lattice artifacts with sufficient accuracy at one lattice spacing, the question arises whether our method indeed breaks down at \( r = a \) in this case (then the value of \( \alpha_V(q^*) \) from fits ignoring \( r = a \) would be more accurate), or if instead the value of \( \alpha_V(q^*) \) from the full fit is more reliable, and the change when leaving out the first point is just the kind of “edge effect” that one might expect if one has data with very small (perhaps slightly underestimated) errors, and considers a quantity that depends mainly on the “boundary” of the data set.

Although this question can not really be answered with certainty at present, we would like to argue that the second possibility is more likely, i.e. the value of

| Group | \( n_f \) | \( \beta \) | \( \alpha_V(q^*) \) | \( a\Lambda_V \) | \( a^2\sigma \) | \( c \) | \( a_1 \) | \( r_{\text{min}} \) | \( \chi^2/\hat{N}_{\text{DF}} \) |
|-------|---------|----------|-----------------|---------------|---------------|-----|---------|---------------|-----------------|
| SU(3) | 0       | 6.0      | 0.1450          | 0.1081        | 0.0488        | 2.3 \( \cdot 10^{-4} \) | 0.5 | 1       | 64.1/62        |
|       |         |          | 0.154           | 0.165         | 0.0502        | 1.8 \( \cdot 10^{-2} \) | 0.5 | \( \sqrt{2} \) | 59.8/61         |
|       |         |          | 0.149           | 0.139         | 0.0497        | 3.2 \( \cdot 10^{-3} \) | 0.5 | \( \sqrt{3} \) | 59.0/60         |
| SU(3) | 0       | 6.8      | 0.1144          | 0.0549        | 0.00718       | 1.2 \( \cdot 10^{-2} \) | 0.5 | 1       | 153.5/104      |
|       |         |          | 0.1163          | 0.0611        | 0.00758       | 4.9 \( \cdot 10^{-2} \) | 0.5 | \( \sqrt{2} \) | 102.3/103      |
|       |         |          | 0.1163          | 0.0610        | 0.00758       | 4.9 \( \cdot 10^{-2} \) | 0.5 | \( \sqrt{3} \) | 102.3/102      |
|       |         |          | 0.1160          | 0.0602        | 0.00754       | 4.1 \( \cdot 10^{-2} \) | 0.5 | 2       | 91.4/101       |
| SU(2) | 0       | 2.85     | 0.1663          | 0.0482        | 0.00387       | 3.4 \( \cdot 10^{-6} \) | 1.5 | 1       | 26.2/26        |
|       |         |          | 0.1677          | 0.0485        | 0.00374       | 1.2 \( \cdot 10^{-6} \) | 1.5 | \( \sqrt{2} \) | 15.6/25        |
|       |         |          | 0.1667          | 0.0488        | 0.00377       | 3.8 \( \cdot 10^{-6} \) | 1.5 | \( \sqrt{3} \) | 13.8/24        |
| SU(3) | 2S      | 5.6      | 0.1664          | 0.1391        | 0.0480        | 3.0 \( \cdot 10^{-5} \) | 1.5 | 1       | 37.0/40        |
|       |         |          | 0.168           | 0.148         | 0.0477        | 6.7 \( \cdot 10^{-5} \) | 1.5 | \( \sqrt{2} \) | 35.9/39        |
\(\alpha_V(q^\star)\) from the full fit is quite reliable also for SU(3) at \(\beta = 6.8\). We already mentioned that there are some uncertainties in the \(\beta = 6.8\) data at large \(r\), so the same might be true at small \(r\) (where previously no independent check of the data was possible), in particular in view of the fact that the pure SU(2) data do not seem to have this problem. The lattice spacing in this case is comparable to that of the SU(3) theory, even smaller, and the errors at short distances are about as good. [At \(r = a, \sqrt{2}a\) the potential in the SU(2) case has relative errors of \(4 \cdot 10^{-4}, 3 \cdot 10^{-4}\), respectively, whereas for SU(3) the corresponding numbers are \(2 \cdot 10^{-4}, 4 \cdot 10^{-4}\).]

These arguments would be more convincing if we had a completely independent estimate of \(\alpha_V(q^\star)\) that we could compare with. Fortunately, such an estimate exists. Namely, Lepage and Mackenzie [10] have argued that the running coupling \(\alpha_V(q)\) at some UV scale can be determined by comparing the non-perturbative expectation value of the plaquette operator, \(W_{11} \equiv \frac{1}{N} \langle \text{Tr } U_{\text{plaq}} \rangle\), as measured in the Monte Carlo simulation, with its expansion in terms of \(\alpha_V(q)\). From the results of [16, 17, 18, 11, 27] this expansion can be written as

\[
- \ln W_{11} = \pi C_F \alpha_V(q) \left[ 1 - \alpha_V(q) \left( \frac{11N}{12\pi} \ln \left( \frac{6.7117}{aq} \right)^2 + (\delta_f + \frac{1}{6\pi} \ln(aq)^2) n_f \right) \right] + O(\alpha_V(q)^3), \tag{25}
\]

where \(\delta_f = -0.060\) for staggered and \(\delta_f = -0.105\) for Wilson \((r = 1)\) fermions.

The next question is what \(q\) to choose in eq. (25). Were the expansion known to large orders, one could extract \(\alpha_V(q)\) at basically any \(q\). For a given truncation of the series, however, there is an “optimal scale” \(aq^\star\) at which to extract \(\alpha_V(q)\). Intuitively \(q^\star\) is the “natural scale” of the “physical process” in question. Let us write the leading non-trivial contribution to a lattice quantity as \(\alpha_V(q^\star) \int_{-\pi/a}^{\pi/a} d^4q F(q)\). [Depending on the quantity in question this might be the 1-loop or the tree level contribution.] To this order the natural definition of \(q^\star\) is\(^\text{12}\)

\[
\alpha_V(q^\star) \int_{-\pi/a}^{\pi/a} d^4q F(q) \equiv \int_{-\pi/a}^{\pi/a} d^4q \alpha_V(q) F(q). \tag{26}
\]

Using the 1-loop expansion of \(\alpha_V(q)\) around \(q = q^\star\) leads to an explicit formula for \(q^\star\),

\[
\ln q^{\star 2} = \frac{\int_{-\pi/a}^{\pi/a} d^4q F(q) \ln q^2}{\int_{-\pi/a}^{\pi/a} d^4q F(q)}. \tag{27}
\]

\(^{12}\)According to our philosophy it would seem more natural to use \(\alpha_V(\hat{q})\) in eq. (26) to define a quantity \(\hat{q}\). If this is done, one would also have to use \(\hat{q}\) in eq. (25), for example. However, in that equation one wants to think of \(\alpha_V(q)\) as a continuum object, so the use of \(\hat{q}\) might not appear natural. We will not pursue this question here, since in the context of the scale determination the use of \(q\) or \(\hat{q}\) will not make much difference in the final results.
Table 7: The expectation value of the plaquette, the coupling at the UV scale $aq^* = 3.4018$ determined by the Lepage-Mackenzie prescription, and the value of the $\Lambda$-parameter obtained by assuming $\alpha_V(q)$ to be given by the leading part of 2-loop evolution.

| Group | $n_f$ | $\beta$ | $W_{11}$ | $\alpha_V(q^*,W_{11})$ | $\alpha\Lambda_V^{(2)}(W_{11})$ |
|-------|------|--------|---------|---------------------|--------------------------|
| SU(3) | 0    | 6.0    | 0.59368 | 0.1519 (35)         | 0.169 (13)               |
| SU(3) | 0    | 6.4    | 0.63064 | 0.1302 (22)         | 0.0968 (64)              |
| SU(3) | 0    | 6.8    | 0.65922 | 0.1153 (15)         | 0.0581 (34)              |
| SU(2) | 0    | 2.85   | 0.70571 | 0.1712 (50)         | 0.0554 (74)              |
| SU(3) | 2W   | 5.3    | 0.53354 | 0.1991 (79)         | 0.255 (26)               |
| SU(3) | 2S   | 5.6    | 0.56500 | 0.1788 (57)         | 0.185 (19)               |

The integrands $F(q)$ appropriate for planar Wilson loops can be found, for example, in [11]. For the plaquette $W_{11}$ or $\ln W_{11}$ one gets the right $q^*$ if one simply uses $F(q) \equiv \text{const}$. Using the methods of sect. 3.1 we obtain $aq^* = 3.4018$.

Expressed in terms of the physical coupling $\alpha_V(q^*)$ the expansion of $\ln W_{11}$ is expected to be well-behaved, i.e., at least the first few higher order coefficients in the square bracket of eq. (25) are expected to roughly follow the pattern established by the first two, which in this case both are $\mathcal{O}(1)$. Using the measured $W_{11}$ to determine $\alpha_V(q^*)$ from (25) with the higher order coefficients set to 0, we will therefore quote it with nominal error $\alpha_V(q^*)^3$, which would be the actual error (for small $\alpha_V(q^*)$) if the next coefficient had magnitude 1.\textsuperscript{13} The value of $\alpha_V(q^*)$ obtained in this way will be denoted by $\alpha_V(q^*,W_{11})$. These numbers are collected in table 7 for the theories under consideration.

Note that other quantities besides $W_{11}$ can be used in the Lepage-Mackenzie prescription (see figure 4 below). Each quantity comes with its own $q^*$. What distinguishes $W_{11}$ is that among all simple quantities whose $\alpha_V(q)$ expansion is known to second order it has the largest $q^*$. It should therefore give the most reliable results for the coupling in the UV.

By assuming 2-loop evolution to be accurate at $q^*$, one can obtain an estimate of the $\Lambda$-parameter from $\alpha_V(q^*)$. For future reference we quote in table 7 the value of $\Lambda_V$ obtained from $\alpha_V(q^*,W_{11})$ by assuming that $\alpha_V(q)$ is given by the leading part of 2-loop evolution, $\beta_0 \alpha_V(q) = 1/(t + b \ln t)$. This value is denoted by $\Lambda_V^{(2)}(W_{11})$.

Comparing with tables 1 to 4 we see that our and the Lepage-Mackenzie es-

\textsuperscript{13}Actually, for gauge group SU(2) the second coefficient is smaller by a factor $2/3$ (for $n_f = 0$) when compared to SU(3), and we indeed find that various errors in the SU(2) case are smaller by roughly a factor $(2/3)^2$.  

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estimate of $\alpha_V(q^*)$ are consistent within their errors, our values being somewhat smaller (in particular for theories on coarser lattices). It would be nice to compare our and the Lepage-Mackenzie estimate in a situation where the errors are much smaller. This is indeed possible. In [32] Wilson loops up to size $8 \times 8$ were generated for pure SU(3) on very fine $16^4$ lattices. We used their $\beta=9.0$ and $18.0$ data to extract the potential (using times $T=7$ and $8$) at the first seven on-axis points, and then fitted them to our standard ansatz. Obviously $\sigma$ can not be fitted from such data, so we simply set it to some reasonably value estimated by scaling, the precise value being irrelevant. For simplicity we also fixed $c=0.001$ (again, the precise value of $c$ has hardly any effect). We performed fits using all $r\geq a$ data, and also fits with the first point left out. In table 8 we show our results for $\alpha_V(q^*)$ and the corresponding results obtained by the Lepage-Mackenzie method, which is very accurate for these fine lattices. Note the perfect agreement for the $r\geq a$ fits. When leaving out the first point, the central value of the fitted $\alpha_V(q^*)$ becomes significantly worse — despite the much better $\chi^2$ — though with its larger errors it is still (barely) consistent with the Lepage-Mackenzie estimate.

A significant change of $\alpha_V(q^*)$ combined with a much better value for $\chi^2$ when leaving out the first data point — this was exactly the kind of behavior that raised some doubts about our estimate of $\alpha_V(q^*)$ for the SU(3) theory at $\beta=6.8$. But table 8 suggests that our estimate of $\alpha_V(q^*)$ from fits with all data points is reliable. Before we can draw this conclusion with certainty, it will, however, be necessary to apply our method to more, in particular more accurate data. In the next subsection we perform one more important check of our method; it allows us to separately test our ansatz for the lattice potential, independent of any assumption about the form of the running coupling beyond perturbation theory.

To conclude this subsection, we mention that we investigated another aspect

| $\beta$ | $W_{11}$ | $\alpha(q^*,W_{11})$ | $\alpha_V(q^*)$ $r\geq a$ | $\chi^2/N_{\text{DF}}$ | $\alpha_V(q^*)$ $r\geq 2a$ | $\chi^2/N_{\text{DF}}$ |
|-------|---------|----------------|----------------|----------------|----------------|----------------|
| 9.0   | 0.75614 | 0.0731 (4)     | 0.0733 (4)     | 2.4/5          | 0.0747 (12)    | 0.4/4          |
| 18.0  | 0.88450 | 0.03040 (3)    | 0.03049 (11)   | 3.1/5          | 0.0311 (4)     | 0.8/4          |

Table 8: Comparison of $\alpha_V(q^*)$ for pure SU(3) from our fits (fourth and sixth columns) with results from the Lepage-Mackenzie prescription. The latter is quoted with error $\alpha_V(q^*)^3$.

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14Note that at fixed $r/a$ fractional lattice artifacts do not vanish as the lattice gets finer. So there is no obvious reason why our method should work well on fine lattices — meaning not just that we get a good fit of the potential data, but also, that this involves no significant compensating error between our handling of the lattice artifacts and the $\alpha_V(q)$ extracted from the fit — but not very well on coarser ones (it should work somewhat better on fine lattices, since the coupling is smaller).
of the Lepage-Mackenzie prescription, namely to what extent \( \alpha_V(q^*) \) agrees with 
\[
(2\pi)^{-1} \int_{-\pi/a}^{\pi/a} d^4q \ \alpha_V(q).
\]
Using \( \alpha_V(q^*) \) and \( \alpha_V(q) \) from our fit, we find that the integral is always slightly larger, but the difference is well within the expected \( \alpha_V(q^*)^3 \) error (the difference is never more than half this error).

4.3 The 1-Loop Expansion of the Potential

We would now like to compare the 1-loop expansion of our ansatz for the lattice potential with the 1-loop results for the on-axis lattice potential that can be obtained from the more general results for planar Wilson loops in finite volume presented in [11].

Expanding the coupling of a generic scheme around \( q = \mu \) to one loop gives 
\[
\alpha(q) = \alpha(\mu) - \alpha(\mu)^2 \beta_0 \ln q^2/\mu^2.
\]
Inserting this into eq. (5)\(^{15}\) we obtain
\[
V_a^2(r) = \alpha(\mu) V_a^2[1](r) + \alpha(\mu^2) \beta_0 V_a^2[\ln \mu^2/q^2](r) + \mathcal{O}(\alpha^3), \tag{28}
\]
where we use the notation \( V_a^2[\alpha] \) to denote the “potential” in eq. (5) as a functional of the “running coupling” \( \alpha(q) \). For any given \( \alpha(q) \) these functions can easily be evaluated numerically as described in sect. 3.1. Remember that \( V_a^2[1](r) \) is the lattice Coulomb potential. The expansion in (28) can easily be extended to higher orders.

On the other hand, the 1-loop expansion of the on-axis potential given in [11] in terms of the bare coupling \( \alpha_0 \) can be reexpressed in terms of a continuum coupling. For the latter we choose the V scheme. Restricting ourselves to pure \( SU(N) \) from now on, we have (cf. the references given above eq. (25))
\[
\alpha_0 = \alpha_V(\mu) \left[ 1 - \alpha_V(\mu) \left( \beta_0 \ln \left( \frac{1}{a\mu} \right)^2 + 2.409830 N - \frac{\pi}{2N} \right) \right] + \mathcal{O}(\alpha^3), \tag{29}
\]
which allows us to rewrite the on-axis potential of [11] (in the infinite volume limit) as
\[
V_a^{(1)}(r) = \alpha_V(\mu) V_a^2[1](r) + \alpha_V(\mu) \left[ \beta_0 \ln \left( \frac{a\mu}{10.3295} \right)^2 V_a^2[1](r) + (N^2 - 1) \tilde{X}(r) \right] + \mathcal{O}(\alpha^3). \tag{30}
\]
Here, in terms of the notation of Heller and Karsch [11],
\[
\tilde{X}(R) \equiv (4\pi)^2 \lim_{T \to \infty} \frac{1}{2} \left[ W_2(R,T)^2 - W_2(R,T-1)^2 \right], \tag{31}
\]
\(^{15}\)Where one should ignore the constant \( V_0 \) in the following. In the end we will consider potential differences anyhow.
Let us now consider the difference $\Delta V_{a^2} \equiv aV_{a^2}((2a,0,0)) - aV_{a^2}((a,0,0))$ of the lattice potential at the first two on-axis points. For this quantity the optimal choice of $\mu$ according to the Lepage-Mackenzie prescription is $\mu = 1.028/a$, which we will denote by $q^*_\Delta$. Using this value, our ansatz gives

$$\Delta V_{a^2} = C_F \alpha_V(q^*_\Delta) \left[ 0.54255 - 0.08186 \beta_0 \alpha_V(q^*_\Delta) \right] + O(\alpha^3). \tag{32}$$

From ref. [11] and unpublished results of Heller [27] on $32^4$ lattices we estimate $\tilde{X}(2a) - \tilde{X}(a) = 0.331(1)$, so that

$$\Delta V_{a^2}^{(1)} = C_F \alpha_V(q^*_\Delta) \left[ 0.54255 - 0.234(7) \beta_0 \alpha_V(q^*_\Delta) \right] + O(\alpha^3). \tag{33}$$

In table 9 we compare Monte Carlo results for $\Delta V_{a^2}$ with the tree level and 1-loop estimate from our ansatz and from ref. [11]. The errors of the Monte Carlo results were obtained by quadratically adding those of the individual potential values, which is almost certainly an overestimate because of correlations. To keep all estimates strictly perturbative, we did not calculate $\alpha_V(q^*_\Delta)$ from our fitted $\alpha_V(q)$, but instead used the Lepage-Mackenzie value of $\alpha_V(q^*)$ from the plaquette and 2-loop evolution.\(^{16}\)

Note that the 1-loop estimate from our ansatz is consistently and significantly better than the result of [11]. This is somewhat odd; why should the 1-loop result from our ansatz be better than what is presumably the exact answer? Probably we are just lucky with our ansatz. The difference between the Monte Carlo results and

\(^{16}\)If we use our fitted $\alpha_V(q)$ to calculate the value of $\alpha_V(q^*_\Delta)$ to be inserted in eq. (32), the agreement between our 1-loop result and the Monte Carlo data becomes even better. For example, in the SU(2) case we then obtain $\Delta V_{a^2} = 0.0941$.\)
those of ref. [11] is consistent with a 2-loop contribution of $1.5(2) \, C_F \, \beta_0^2 \, \alpha(q_\Lambda^2)^3$ to $\Delta V_{\alpha^2}$. The coefficient $1.5(2)$ seems a bit large, perhaps, but it is a nontrivial fact that this value is consistent with all data in table 9. We have checked that the contribution to $\Delta V_{\alpha^2}$ from zero-modes [33], which was not included in [11], is negligible in the cases considered.

The situation illustrated in table 9 requires further investigation. But we can certainly conclude that our ansatz incorporates the lattice artifacts very well. We emphasize that our results in table 9 do not involve any assumption about the form of $\alpha_V(q)$ beyond one loop. It is therefore a check of our ansatz for the lattice potential that is completely independent of our ansatz for the continuum running coupling $\alpha_V(q)$.

### 4.4 Comparing $\alpha_V(q)$ with 2-Loop Approximations

We would now like to address the question to what extent the running coupling obeys 2-loop evolution. The first question, though, is, which form of 2-loop evolution we should use. There is $\beta_0 \alpha(q) = 1/(t + b \ln(t + b \ln t))$, which incorporates the leading and subleading 2-loop contribution. More commonly used are however the expressions $\beta_0 \alpha(q) = 1/(t + b \ln t)$, or $\beta_0 \alpha(q) = (1 - b \ln t)/t$, which incorporate only the leading part of the 2-loop contribution to the running coupling. We will refer to these expressions as the “full”, the “leading”, and the “other leading” form of 2-loop evolution of the coupling, respectively, and generically denote them as $\alpha^{(2)}_\Lambda(q)$.

We would like to compare these expressions with our fitted $\alpha_V(q)$, which, though not exact, ought to be much closer to the exact answer than any of the above expressions. In table 10 we compare pure SU(3) fits for $\alpha_V(q)$ with the various forms of 2-loop evolution. The $\Lambda$-parameter used in the 2-loop expressions is $\Lambda_V$ from our fit. We used the relative scales of these theories, as determined in sect. 5 below, to give a comparison at the same physical momenta for the different theories. The momenta are quoted in units of the lattice spacing of the $\beta = 6.0$ theory. Using either $r_0 \simeq 0.5$ fm (cf. sect 5) or $\sqrt{\sigma} \simeq 440$ MeV, one sees that the momenta chosen are roughly 1 GeV, 2 GeV, 10 GeV and 80 GeV.

Somewhat surprisingly, the leading form of 2-loop evolution is closer to our fitted $\alpha_V(q)$ than the full one, except for the highest momenta, even though our $\alpha_V(q)$ was designed to contain all 2-loop contributions. The reason for this is that up to moderate UV momenta (around 10 GeV) there is a partial cancellation between the subleading 2-loop and non-perturbative contributions. Note that the other form of leading 2-loop evolution always fares worse in our comparison than either the leading or the full expression. This is not surprising, since compared to the full 2-loop formula it has a subleading 2-loop term of the wrong sign. This
The main point is that we have a non-perturbative, numerically accurate running coupling, and can quantify how good 2-loop evolution is.
Figure 4: Log-log plot of $\alpha_V(q)$ for $\beta = 6.0$ pure SU(3) from our standard fit (the solid lines delineating the error), its leading 2-loop approximation (dotted line), and results obtained by applying the Lepage-Mackenzie method to various Wilson loops and Creutz ratios (circles), shown with error $\alpha_V(q)^3$.

5 Scaling

5.1 Introduction

By the term scaling we circumscribe three related but distinct issues that one faces in simulating a quantum field theory on a lattice. First, choosing and then calculating a dimensionful quantity from (results of) the simulation. This quantity will then be known in lattice units, and one can use it to determine the relative scales of different lattice theories. Secondly, one must determine the absolute scale of a lattice theory by equating a dimensionful quantity from the simulation with its experimentally measured value. Thirdly, one must extrapolate to the continuum limit by simulating the theory on several (sufficiently small) lattice spacings; or at least check that one is in the scaling region where dimensionless ratios of physical quantities are independent of the lattice spacing within some acceptable error.

The absolute scale determination is of course not really meaningful unless one is sufficiently close to the continuum limit — and to the real world, which might involve further extrapolations, e.g. in various masses or the number of flavors.

Note that there is no reason for the relative and the absolute scales to be determined from the same quantity. In fact, this is probably not a good idea, since it would be rather surprising if the quantity that can be determined most precisely from the simulation happens to also be the observable most suitable
for precise experimental determination. One should therefore clearly separate the absolute from the relative scale determination. Once the latter has been calculated for various theories, one just has to determine the absolute scale for one of these theories — using perhaps a quite different observable — to know it for all theories.

In the past it was customary to use the string tension $\sigma$ to set the scale. However, since it is an asymptotic (large $r$) quantity, it has relatively large statistical and systematic errors. Furthermore, $\sigma$ is not really well-defined in the presence of sea quarks, due to string breaking.\footnote{Though in practice the string tension is at present “quite well-defined”, since clear signs of string breaking have not been seen yet; instead one observes a large linear regime in the static potential (cf. the fermionic theories of sect. 4). That such a regime should exist before the potential flattens and keels over is also clear from the success of Coulomb + linear potentials in describing heavy quarkonium systems.} Is is therefore also experimentally not particularly well determined. The situation is even worse for the $\Lambda$-parameter, whose error is much larger, due to, as we discovered, its correlation with higher order and non-perturbative contributions to the running coupling at small and intermediate distances. We now describe a better way of setting the scale.

## 5.2 The Scales $q_0$ and $r_0$

Instead of using a parameter describing the asymptotic long or short distance behavior of the running coupling to set the scale, it is clearly a much better idea to do so using the value of the coupling itself at some intermediate distance. Sommer\cite{Sommer} proposed to determine a scale $r_0 = r_0(c_r)$ using the interquark force,

$$C_F \alpha_F(r_0) = c_r,$$

for some fixed constant $c_r$ of $O(1)$. [For details about the coupling in the force scheme we refer to sect. 6.1.] This is basically equivalent, as we will see below, to defining a momentum scale $q_0 = q_0(c_q)$ via

$$C_F \alpha_V(q_0) = c_q,$$

for suitably chosen $c_q$.

In\cite{Sommer} it was suggested to take $c_r = 1.65$, since in various phenomenological potential models of heavy quarkonium systems this gives $r_0 \simeq 0.5$ fm, roughly the distance at which these effective potentials are best determined empirically. Since the relation between the static potential and these effective potentials is not well understood at present, $r_0$ does not seem to provide the best way to determine the absolute scale. The various extrapolations required to connect Monte Carlo data to the real world are much better understood — in particular have been explored by simulations — for spin-averaged level splittings in heavy quarkonium systems.
systems [34, 35], which are of course also accurately known experimentally. When available, this approach seems to provide the best method for an absolute scale determination (for a review of the controversy over the difference in the absolute scale determinations from this method versus those from light quark spectroscopy, see [35]). Be that as it may, we will here concentrate on determining relative scales, for which a quantity like \( r_0 \) is ideally suited.

The scale \( r_0 = r_0(1.65) \) has already been used in the literature, so for comparison we will calculate it too, using the exact relation between \( \alpha_V(q) \) and \( \alpha_F(r) \). From our point of view, it is however to some extent more natural to define a scale \( q_0 \) directly in terms of \( \alpha_V(q) \) using eq. (35). The question is if one can find a simple relation between \( q_0 \) and \( r_0 \). In practice this is indeed the case. We will see in sect. 6.1 that to two loops \( \alpha_F(r) = \alpha_V(q) \) with \( r = e^{1-\gamma}/q = 1.526205/q \).\(^{18}\) The scales we are interested in are however not in the perturbative region, so this equality does not hold very well. Nevertheless, one might suspect that by either

(i) setting \( c_q = c_r \) there is an almost universal relation \( r_0 = c_{rq}/q_0 \) with some \( c_{rq} \neq e^{1-\gamma} \), or

(ii) still requiring \( r_0 = e^{1-\gamma}/q_0 \) there is an almost universal constant \( c_q(c_r) \neq c_r \) that achieves this.

Studying the different theories of sect. 4 we find that both of the constants \( c_{rq} \) in (i) and \( c_q \) in (ii) are universal on the permille level for \( c_r = 1.65 \). We decided to basically follow approach (ii) and define \( q_0 \equiv q_0(1.45) \). With \( r_0 \equiv r_0(1.65) \) from now on, we find that \( q_0 r_0 = 1.524(4) \) holds for all theories and all parameterizations of \( \alpha_V(q) \) discussed in sect. 4. [Considering only the standard parameterization of \( \alpha_V(q) \) we find \( q_0 r_0 = 1.5266(12) \).] This simple relation between \( q_0 \) and \( r_0 \) is useful for quick translations between scale determinations in the two schemes. Below we will however always calculate \( r_0 \) and \( q_0 \) from their original definitions, given by eqs. (34) and (35).

### 5.3 Results

Using our standard fit and the exact relation between \( \alpha_V(q) \) and \( \alpha_F(r) \) we obtain the results in table 11 for \( q_0, r_0 \) and the dimensionless quantities \( q_0/\sqrt{\sigma} \) and \( r_0\sqrt{\sigma} \). These estimates were obtained in the same analysis that lead to the results in table 2, including the error estimates from the method described in sect. 3.3. In particular, the error of a “composite” quantity like \( r_0\sqrt{\sigma} \) was not calculated by

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\(^{18}\)It is in this sense that a momentum scale \( q \) corresponds to a distance scale \( r \approx 1.53/q \), as mentioned in sect. 4. Note, however, that one could use other prescriptions to define numerically different momentum versus distance scale relations. In the present context the above seems the most natural one.
$$\text{SU}(3) \quad \bar{\beta} = 6.0 \quad aq_0 = 0.2884(8) \quad aq_0 / \sqrt{\sigma} = 1.308(6) \quad r_0 / a = 5.292(14) \quad r_0 \sqrt{\sigma} = 1.167(5)$$

$$\text{SU}(3) \quad \bar{\beta} = 6.4 \quad aq_0 = 0.1600(6) \quad aq_0 / \sqrt{\sigma} = 1.301(10) \quad r_0 / a = 9.535(36) \quad r_0 \sqrt{\sigma} = 1.173(8)$$

$$\text{SU}(3) \quad \bar{\beta} = 6.8 \quad aq_0 = 0.10640(13) \quad aq_0 / \sqrt{\sigma} = 1.281(4) \quad r_0 / a = 14.34(2) \quad r_0 \sqrt{\sigma} = 1.190(3)$$

$$\text{SU}(3) \quad \bar{\beta} = 6.8' \quad aq_0 = 0.0824(8) \quad aq_0 / \sqrt{\sigma} = 1.306(5) \quad r_0 / a = 18.54(17) \quad r_0 \sqrt{\sigma} = 1.168(5)$$

$$\text{SU}(3) \quad \bar{\beta} = 2.85 \quad aq_0 = 0.0813(11) \quad aq_0 / \sqrt{\sigma} = 1.306(8) \quad r_0 / a = 18.76(27) \quad r_0 \sqrt{\sigma} = 1.167(7)$$

$$\text{SU}(3) \quad \bar{\beta} = 2.85' \quad aq_0 = 0.1054(3) \quad aq_0 / \sqrt{\sigma} = 1.300(4) \quad r_0 / a = 14.48(5) \quad r_0 \sqrt{\sigma} = 1.175(3)$$

$$\text{SU}(2) \quad \bar{\beta} = 2.85 \quad aq_0 = 0.0812(9) \quad aq_0 / \sqrt{\sigma} = 1.307(6) \quad r_0 / a = 18.80(19) \quad r_0 \sqrt{\sigma} = 1.1667(7)$$

$$\text{SU}(2) \quad \bar{\beta} = 2.85' \quad aq_0 = 0.0802(11) \quad aq_0 / \sqrt{\sigma} = 1.308(7) \quad r_0 / a = 19.02(26) \quad r_0 \sqrt{\sigma} = 1.1657(9)$$

$$\text{SU}(3) \quad \bar{\beta} = 5.3 \quad aq_0 = 0.4225(9) \quad aq_0 / \sqrt{\sigma} = 1.334(18) \quad r_0 / a = 3.616(8) \quad r_0 \sqrt{\sigma} = 1.1448(15)$$

$$\text{SU}(3) \quad \bar{\beta} = 5.6 \quad aq_0 = 0.2944(7) \quad aq_0 / \sqrt{\sigma} = 1.356(11) \quad r_0 / a = 5.190(12) \quad r_0 \sqrt{\sigma} = 1.1437(10)$$

Table 11: Average values and errors of the scales $q_0$ and $r_0$ in units of the lattice spacing and the string tension, obtained from our standard ansatz and error analysis. The $\beta = 6.8'$ and $2.85'$ data sets are explained in sect. 4.1.

Table 12: Same as table 11, for $a_1 \neq 1$ fits.
The dimensionless quantities $q_0/\sqrt{\sigma}$ and $r_0\sqrt{\sigma}$, on the other hand, can have significant systematic errors, inherited from $\sigma$. For the SU(2) case these systematic errors are still almost negligible, whereas for SU(3) at $\beta=6.8$ and the unquenched theories the systematic errors are much larger than the statistical ones.\footnote{Note, by the way, that the statistical error of $r_0\sqrt{\sigma}$ for the last three entries of tables 11 and 12 is much smaller than for the pure SU(3) cases, even though the opposite is true for the errors of the potential data themselves. We had observed and discussed similar features already in sect. 4.1}

We combine our results, including those from fits where small $r$ data points have been left out, and in table 13 give estimates of $r_0$ and $r_0\sqrt{\sigma}$ that include systematic errors. We compare our results with estimates from various other methods: The $\beta=6.0$ and 6.4 values of $r_0$ [31] were obtained by the method of ref. [12] using force data from [7, 23]; the value of $\sigma$ used in $r_0\sqrt{\sigma}$ is from the same reference. The $\beta=6.8$ results were obtained with a modified Coulomb + linear fit [23], as were the $n_f=2$ results [26]. The $\beta=2.85$ SU(2) value of $r_0$ was obtained in a simulation using the Schrödinger functional coupling $\alpha_{SF}(q)$ [36] (cf. sect. 6.2).

We recall (sect. 4.1.2) that our errors for a given fit of the $\beta=2.85$ SU(2) data might not be accurate due to correlations. However, we saw that our uncorrelated fits tend to overestimate errors in such a situation, so all errors in table 13 should be on the safe side.

As another check we have determined $r_0$ and $r_0\sqrt{\sigma}$ using uncorrelated fits to modified Coulomb + linear ansätze. Despite the uncertainties of the short-distance parameters of these fits, in the intermediate range these fits are rather well-determined and we obtain results in good agreement with the estimates from our ansatz.

We hope that an analysis of new data at other $\beta$-values for pure SU(3) will lead to smaller errors for $r_0\sqrt{\sigma}$ [25]. Even as it stands, though, our errors for $r_0$ and $r_0\sqrt{\sigma}$ are much smaller than those obtained previously (except for $r_0\sqrt{\sigma}$ in the $\beta=6.8$ case, where the Coulomb + linear estimate in table 13 does not include all systematic errors). Note in particular that for the first time we can see a significant difference in $r_0\sqrt{\sigma}$ for theories with and without dynamical fermions.

As table 13 indicates, for pure SU(3) $r_0\sqrt{\sigma}$ scales within errors of about 2\% for $\beta \geq 6.0$ (perhaps even for smaller $\beta$ which we have not studied so far). Note that if we just consider our standard fit results in table 11, $r_0\sqrt{\sigma}$ even scales at the 0.5\% level. Scaling of the string tension is shown in another way in table 14, where we used our estimates of $\sigma$ from table 5 and rescaled them to the $\beta=6.0$ lattice spacing with the help of the relative scales obtained from $r_0$ in table 13.

In this table we also show, as check of UV scaling, results for $\alpha_V(q)$ at the scale $q_{6.8}^*=3.4018/a_{6.8}$ for different $\beta$. [A rough check of UV scaling, without error bars, was already provided by the $\alpha_V(q)$ entries in table 10.] We used our $a_1=0.5$ fits
and evolved the $\beta = 6.0$ and 6.4 results using the appropriate ratios of $r_0$. The error from the scale uncertainty is negligible. Instead, the error is dominated by the error of our fit (where one must be careful to take into account the correlation of the fit parameters) and by the systematic error of $\alpha_V(q^*)$, which we took to be the difference between the central values in tables 2 and 4 (for $\beta = 6.8$ we averaged over the 6.8 and 6.8' results). We see that scaling violations, if existent, are just slightly larger than the error of $1 - 2\%$.

Without presenting explicit results here, we note that scaling holds at the same or even slightly better level of accuracy also in the intermediate regime\(^{20}\) (to some extent this can be seen, again, in table 10). We hope to provide more accurate results for pure SU(3) in [25], including a more stringent check of the scaling of $\alpha_V(q)$ at all momenta.

Finally, we have repeatedly stressed the large systematic errors of the $\Lambda$-parameter, that are usually ignored. To underscore this point, we compare in table 15 three different determinations of this parameter: First the value from our

\(^{20}\)One should not be worried about the fact that the crossover parameter $c$ does not scale too well (for given $a_1$; it obviously should not scale when comparing results with different $a_1$). It is an effective parameter, representing small subleading effects, and therefore prone to amplify even small flukes in the data.
6.2 The Force Scheme

We already mentioned this scheme at various points in this paper. We now discuss it in more detail. Let us first describe the close relation of the coupling in this scheme, \( \alpha_F(r) \), to \( \alpha_V(q) \). Recall that \( \alpha_F(r) \) is defined in terms of the continuum potential as

\[
r^2 V'(r) \equiv C_F \alpha_F(r).
\]

(36)

So just from their definitions we have an explicit exact relation between these two couplings. This relation can be rewritten as

\[
\alpha_F(r) = \frac{\sigma}{C_F} r^2 + \frac{2}{\pi} \int_0^\infty \frac{dq}{q} \sin qr \left[ q \partial_q \tilde{\alpha}_V(q) + \tilde{\alpha}_V(q) \right],
\]

(37)
where the “IR subtracted” $\alpha_V(q)$ is defined by

$$\tilde{\alpha}_V(q) = \alpha_V(q) - \frac{2\sigma}{C_F} \frac{1}{q^2}. \quad (38)$$

Besides this exact though perhaps not directly illuminating relation, there is a “deeper” relationship between these two couplings. Namely, $\alpha_F(r)$ is in a rather literal sense a position space analog of $\alpha_V(q)$. To see this, note first of all that, like any continuum coupling, $\alpha_F(r)$ obeys the $\beta$-function equation with the first two universal coefficients. In particular, it has an expansion of the form (10), where now $t \equiv \ln(\Lambda_F r)^{-2}$. The relation between $\Lambda_F$ and $\Lambda_V$ can be obtained by a direct calculation of the 1- and 2-loop terms in $V(r)$, written as a Fourier transform of $\alpha_V(q)$. We obtain $\Lambda_F = e^{\gamma-1} \Lambda_V$, where $\gamma = 0.57721566 \ldots$ is Euler’s constant.

Next, note that for long distances

$$\alpha_F(r) = \frac{\sigma}{C_F} r^2 + \frac{e_{\text{IR}}}{C_F} + \ldots, \quad (39)$$

which is to be compared to the IR expansion (22) of $\alpha_V(q)$. So we see that one can use the same ansatz (18) for $\alpha_F(r(t))$ as for $\alpha_V(q(t))$.

We mentioned in the introduction that the force scheme has been widely used [5, 6, 7, 37, 40] to obtain an estimate of the $\Lambda$-parameter by matching force data to the (leading) 2-loop expression for $\alpha_F(r)$. In sect. 5 we also discussed how $\alpha_F(r)$ is used to define the useful intermediate scale $r_0$ by $C_F \alpha_F(r_0) = 1.65$. Sommer [12] determined $r_0$ from force data. Let us note some potential and real problems in using the force scheme to determine $\Lambda_F$ or $r_0$, and to what extent some of these problems can be circumvented.

- To get the force from potential data involves taking numerical derivatives, which generically increases the errors dramatically. Only if the potential data at neighboring points are strongly correlated will this not be the case.

- Lattice artifacts in the force can easily be taken into account at tree level, cf. [12]. However, we know that at short distances this is not sufficient to describe the lattice artifacts accurately. For the $r_0$ determination this will presumably lead to significant errors only, if at all, on rather coarse lattices, where $r_0/a$ is not much larger than 1, cf. table 13. But for the $\Lambda_F$ estimate this will induce sizable systematic errors even on fine lattices.

- Global versus local fits: To determine $r_0$ from force data one only needs a locally accurate interpolation between two neighboring points [12]. $r_0$ can therefore be obtained without any assumption about the global from of the force. By the same token, however, one misses the opportunity of obtaining
a more precise value for \( r_0 \) offered by a globally accurate ansatz (or accurate at least in the intermediate region) that takes into account information from many more data points. For the \( \Lambda_F \) estimates one often has the worst of both worlds, namely, \( \Lambda_F \) is typically extracted locally from the force using the (leading) 2-loop formula for \( \alpha_F(r) \), which can not be expected to hold very accurately. This problem in itself could be mitigated by fitting to a global ansatz like (18). However, lattice artifacts would still be a problem.

Note that none of the above problems occurs in our approach: We have a globally accurate\(^{21}\) ansatz for the potential that takes lattice artifacts into account much better than at tree level. What we have not done yet, is to take into account correlations of the potential data. If these were strong, so that the force could be extracted with great accuracy, the best method to fit the force data would presumably be to match them to the corresponding differences of the lattice potential as given by our ansatz. This would solve the one problem that our approach has, namely that we have to fit the overall constant of the potential, whose correlation with \( \alpha_V(q^*) \) provides the main contribution to the latter’s error.

However, in most cases the correlations of the potential data do not seem to be strong enough to outweigh the other disadvantages of using the force. And, in any case, since the potential data are primary even in the presence of correlations, the cleanest method of extracting a running coupling would be to append our fitting routine to that for the lattice potential and perform fits on bootstrap copies of the potential data. This would automatically take care of all correlations, presumably in the best way possible.

6.2 The Schrödinger Functional Coupling

Lüscher et al [41, 30, 31] have introduced and studied in some detail a completely different running coupling. It is defined by the response of the partition function ("Schrödinger functional") of a lattice gauge theory on a finite lattice to a constant background field, with the extent of the lattice providing the running scale. This coupling is denoted by \( \alpha_{SF}(q) \). The great advantages of this method are (i) that the coupling is defined so that it can be extracted from the Monte Carlo simulation with basically no systematic error and (ii) that it is relatively easy to cover a large energy range by varying the size of the lattice. Its disadvantages are (i) that it involves "special purpose" simulations due to the gauge field configurations required and (ii) that there are apparently large higher order coefficients relating this scheme to more common ones, see below (the 2-loop relation to the \( \overline{MS} \) scheme will be known soon [42]).

\(^{21}\)Recall that we checked that leaving out points at small or large distances from the fit does not significantly change our estimate of \( r_0 \).
6.3 A Comparison

We would like to end this section with a quantitative comparison of $\alpha_F$, $\alpha_V$ and $\alpha_{SF}$ at a suitable physical scale. For pure SU(3) at $\beta=6.5$ the most accurate value of $\alpha_F$ obtained by the UKQCD collaboration from force data [40] turns out to be at $r/a=2.5322$, where they find $\alpha_F=0.248(2)$. On the other hand, translating results for $\alpha_{SF}(q)$ via perturbative matching formulas gives $\alpha_F=0.205(7)(9)$ at the same physical scale [31] (we quote $\alpha^3_F \simeq 0.009$ as the second, systematic error from the perturbative matching). We do not have results at $\beta=6.5$. But using $r_0/a=11.23(21)$ for $\beta=6.5$ (from [31], obtained using data of [40]) and our values of $r_0$ we obtain $\alpha_F=0.231(5)$, 0.237(5), 0.231(4) at the same physical scale for $\beta=6.0$, 6.4, 6.8, respectively. In our error estimate we linearly added the contributions from our $\alpha_V(q)$ and those from expressing the above scale $r$ in the appropriate lattice units. The systematic error from the $a_1=1$ versus $a_1=0.5$ fits is negligible. The non-monotonicity of the $\alpha_F$-values as a function of $\beta$, which we previously saw for $\alpha_V(q)$ (cf. tables 10 and 14), is perhaps due to systematic errors of the potential data we used in our fits. We therefore simply quote $\alpha_F=0.236(6)$ at the above scale. This is in reasonable agreement with the value from force data, but they both differ by about $3\alpha^3$ with respect to the value from the Schrödinger functional. This indicates that perturbative corrections in the translation between $\alpha_{SF}$ and $\alpha_V$ or $\alpha_F$ have quite large coefficients.

7 Conclusions and Outlook

Our ability to fit lattice potential data to very high precision rests on two ingredients. First, our expression for the lattice potential in terms of the continuum running coupling $\alpha_V(q)$, eq. (5), and, secondly, our parameterization of $\alpha_V(q)$ that incorporates both the short distance QCD and the long distance flux tube predictions for the static potential (sect. 2).

Our ansatz for the lattice potential is obviously correct at tree level. At the 1-loop level we found (sect. 4.3), rather confusingly, that our ansatz seems to work much better than what is presumably to be the exact answer [11]. This remains to be understood. Be that as it may, this and other checks, like the comparison with the Lepage-Mackenzie estimate of the short-distance coupling (sect. 4.2), indicate that we are handling the lattice artifacts extremely well. More precisely, the fact that we can reproduce basically all lattice artifacts within the very small errors of the potential data does not seem to involve any significant compensating error between our ansatz for the lattice potential and our estimate of the running coupling $\alpha_V(q)$ at short distances. To be absolutely sure about this conclusion, however, we do need new potential data, since at the level of precision.
we are working many presently available data seem to suffer from slight systematic uncertainties of one sort or another (finite-size effects, extrapolation of Wilson loop ratios to large euclidean times).

Previous methods of fitting the data did not incorporate QCD very well — to the extent that (slight) systematic errors of the data did not make much of a difference; they could not be detected anyhow. Our method is precise enough to make it necessary to carefully check the data for finite-size effects and extrapolate the effective potentials to large euclidean times. Put in another way, there is a large payoff again for precise potential data. Particularly exciting is the prospect of potential data from improved actions [43], for which our method is ideally suited (cf. the introduction), since what eventually will prevent us from using our method to extract $\alpha_V(q)$ ever more accurately, are lattice artifacts, and not, for example, a 2-loop approximation used in other methods.

We believe that performing fits of potential data with our method allows for the first time a realistic error assessment, in contrast with the hard to estimate systematic errors afflicting (modified) Coulomb + linear fits and the method of estimating the $\Lambda$-parameter by matching force data to 2-loop formulas.

We showed that the $\Lambda$-parameter has a relatively large error (cf. sect. 4.1.1) — without leading to a large error in $\alpha_V(q)$ itself — because $\Lambda$ is strongly correlated with higher order and non-perturbative contributions at an intermediate range, appearing here in the form of the crossover parameter $c$. This is not surprising, if one remembers that the true UV regime is $q \gg \Lambda$, i.e. $\Lambda$ is really more an intermediate range parameter; it must be correlated with higher order effects. We therefore regard previous estimates of $\Lambda$ as overly optimistic.

Within our approach the error of $\Lambda$ is largely a red herring. We only use $\Lambda$, which is clearly a bad way to parameterize the physics, because it is otherwise difficult to write down a closed form expression for the running coupling. But the physics is contained in $\alpha_V(q)$, which has much smaller statistical and systematic errors.

The scale $r_0$ is now widely used to compare the lattice spacings of different theories. For such relative scales, this is certainly much more accurate than using the $\Lambda$-parameter or the string tension. Sommer [12] described a careful procedure, taking lattice artifacts into account at tree level, to determine $r_0$ locally from force data. We determine $r_0$ from our fit of potential data, using the exact relation between the force and potential schemes. Our values for $r_0$ (sect. 5) are significantly more accurate than those from the procedure of ref. [12] — or those obtained using a modified Coulomb + linear ansatz for the potential — because (a) we use potential data, that in the cases considered have much smaller errors than force data, (b) we can take lattice artifacts into account more accurately, and (c) we have a globally accurate ansatz for the potential, so that information from many
points, not just two neighboring ones, can be taken into account.\footnote{We carefully checked that the one potential problem with global fits, systematic errors from the form of the ansatz, does not lead to significant errors in the intermediate region where $r_0$ is situated.}

Using $r_0$ to set the (relative) scale of different lattice theories, enabled us to check the scaling of $\alpha_V(q)$ for pure SU(3), cf. sect. 5.3. If existent, the scaling violations are not much larger than the error, which is about 2\%. Unfortunately, the pure SU(3) data on the finest lattice, corresponding to $\beta=6.8$, show some signs of systematic errors, making a more accurate check of scaling impossible, since we investigated only two other $\beta$ values, 6.0 and 6.4. A more complete study of SU(3) data is in preparation [25], and will provide a more stringent test of scaling.

When comparing quenched and unquenched QCD we clearly see that the effect of adding fermions can not be absorbed into a “$\beta$-shift”. If one matches the string tensions in this manner, one finds that the running coupling in the UV is quite different (sect. 4.1.1). Also, our results are accurate enough to show, for the first time, that the dimensionless quantity $r_0\sqrt{\sigma}$ is different in quenched and unquenched QCD (sect. 5.3).

Till now we performed only uncorrelated fits, ignoring the correlations between the potential at different $r$-values. Except for the case of the SU(2) potential [6], the data we used are not strongly correlated. In such cases previous experience with (modified) Coulomb + linear fits [23, 27, 28] indicates, that neither the fit parameters nor their errors change significantly when employing correlated fits. We have explicitly checked this (sect. 4.1.2) by performing fits of the potential data to modified Coulomb + linear ansätze and comparing them with previous results from correlated fits. For strongly correlated data we find that our naive uncorrelated fit over- not underestimates the errors (what uncorrelated fits do underestimate, is $\chi^2$). It is easy to understand why this is true. So in all cases our errors seem to be on the safe side.

However, what clearly should be done, is to merge our fitting routine with that for the potential and perform fits on bootstrap copies of the potential; this would automatically take into account all correlations in an optimal manner and simplify the error analysis. Note that once this has been done, another nice feature of our approach can be fully exploited. Namely, that our method just needs one fit of potential data to obtain the running coupling $\alpha_V(q)$ at all (accessible) scales; in particular, we obtain estimates of the UV coupling $\alpha_V(q^\ast)$ (or $\Lambda_V$, if desired), the string tension $\sigma$, and $r_0$ in one fell swoop. At present one usually performs a separate fit (or even simulation) for each of these quantities.

We know how to incorporate QCD to any number of loops in our ansatz for the running coupling (sect. 2.1). Once the third $\beta$-function coefficient, $\beta_2$, becomes available in the V scheme it should of course be incorporated into our ansatz.
With present data we can not determine this parameter reliably by fitting. It is suggestive, though, that pure SU(3) on finer lattices seems to favor a value of $a_1$ (which is related to $\beta_2$) that is in the neighborhood of the value this quantity has in the $\overline{\text{MS}}$ scheme (cf. sect. 4.1). With future high precision data it therefore might be possible to determine $\beta_2$ by fitting. On the other hand, non-perturbative effects might become important before 3-loop effects are clearly visible.

Besides fitting lattice potential data and extracting the running coupling along the way, our results should have various other applications in the upcoming era of high precision Monte Carlo calculations. For example, Monte Carlo simulations are now competing (see [35] for a recent review) with — or have already surpassed — experiment in determining the running coupling of real world QCD at high energy (this is due to the fact that in the simulation one can use a more suitable observable, like level splittings in bottomonium [34, 35], to set the scale than is possible in accelerator experiments). To minimize the systematic error in these calculations it is crucial to be able to extrapolate the running coupling to different energy scales and to a number of fermions different from those used in a specific simulation.

Another obvious application is to potential models (on the lattice or in the continuum). As far as we know, previously no simple analytic expression incorporating both 2-loop QCD and the leading and subleading string picture prediction for the potential was known. Although the relation between the static potential and heavy quark potentials is not well understood, in high precision studies of the heavy quark spectrum our form of the potential might also present an improvement. More generally, our parameterization of the running coupling should be useful for just about any phenomena where one would like to extend perturbation theory without running into the Landau pole.

Finally, we note that our scheme can accommodate string breaking in the presence of light quarks. If the onset of string breaking (before the Yukawa-like potential between the pair-created mesons becomes relevant) is modeled by a potential $V(r) = \frac{\sigma}{\mu} (1 - e^{-\mu r})$ for large $r$, the small $q$ behavior of the running coupling is

$$\alpha_V(q) = \frac{2}{C_F} \frac{\sigma q^2}{(q^2 + \mu^2)^2} + \ldots.$$ \hspace{1cm} (40)

To take this into account we add a suitable term to eq. (18),

$$\frac{1}{\beta_0 \alpha_V(q)} = \frac{C_F}{2\sigma \beta_0} \frac{1}{q^2} + \frac{C_F}{\sigma \beta_0} \frac{1}{1 + q^4/\Lambda_V^4} + \ln \left[ 1 + \frac{q^2}{\Lambda_V^2} \ln \left( c_0 + \frac{q^2}{\Lambda_V^2} \lambda(q) \right) \right],$$ \hspace{1cm} (41)

where there is some freedom in the exact choice of the second term on the rhs.

Another, less trivial extension would be to generalize our ansatz for the infinite lattice potential to one for a finite lattice. It is well known, at least empirically,
that the right potential on a finite lattice is not obtained from some infinite lattice expression by simply replacing the integral over the Brillouin zone by a corresponding sum over the lattice. In understanding this problem it will be necessary to take into account the exact definition of the finite-volume potential, e.g. via Wilson loops, a consideration that played no role in the present work.

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