Two-Loop Computation of the Schrödinger Functional in Pure SU(3) Lattice Gauge Theory

Achim Bode and Ulli Wolff
Institut für Physik, Humboldt Universität
Invalidenstr. 110, D-10099 Berlin, Germany

Peter Weisz
Max-Planck-Institut für Physik
Föhringerring 6, D-80805 München, Germany

Abstract
We compute the Schrödinger functional (SF) for the case of pure SU(3) gauge theory at two-loop order in lattice perturbation theory. This allows us to extract the three-loop $\beta$-function in the SF-scheme. These results are required to compute the running coupling, the $\Lambda$-parameter and quark masses by finite size techniques with negligible systematic errors. In addition, we can now implement two-loop $O(a)$ improvement in simulations and extend and study series in alternative ("tadpole-improved") bare couplings.
1 Introduction

Traditionally, in computer simulations of lattice QCD physicists have been concerned with the computation of low energy quantities which are inacces-
sible to perturbation theory. Typical examples are ratios of hadron masses,
the static quark potential at large separations and glueball masses. At high
energy, where QCD was first established as a promising theory of strong in-
teractions, perturbation theory in the dimensionally regularized continuum
theory is the standard computational tool. Here it provides predictive power
by reproducing a host of high energy data in terms of a renormalized run-
ning coupling and running quark masses at that energy scale. As a result the
coupling in the \( \overline{\text{MS}} \)-scheme at the scale of the mass of the \( Z \)-boson is fixed to
be \( \alpha_{\overline{\text{MS}}} (M_Z) \approx 0.11 \). For a long time the two energy sectors — though they
are believed to belong to one and the same theory — have coexisted rather
independently. Only in recent years was the task of connecting them by
computing \( \alpha_{\overline{\text{MS}}} \) in the theory that is completely parameterized at low energy,
taken up (see [1, 2, 3] for reviews).

Referring also to low energy this result has to be obtained by simulation
on the lattice. The extraordinary difficulty of this computation is caused
by the fact that we seem to have to simultaneously control the continuum
limits of two widely separated physical energies. Naively this requires un-
feasibly large lattices. The problem is circumvented by the somewhat indi-
rect strategy developed by the ALPHA-collaboration in recent years [2, 3].
Here we numerically trace the evolution of the coupling \( \alpha_{\text{SF}} \) defined by the
Schrödinger functional from low to high energy. While not being a directly
physical quantity, it is nevertheless expected to possess a well defined con-
tinuum limit and the motivation for this particular choice is explained in
[4]. Due to its definition on a finite system, it runs with the size \( L \). Once
its evolution is known, it remains to connect both its low and high energy
values to more experimentally accessible quantities. At low energy (i.e. at
large physical volume) this is done by numerical simulation, which however
no longer involves unmanageable scale ratios. At high energy, \( \alpha_{\text{SF}} \) on small
systems can be perturbatively related to \( \alpha_{\overline{\text{MS}}} \). It has turned out that with
the precision that is both experimentally required and achievable in the var-
ious simulation steps, this connection is needed at two-loop order. Due to
the difficult structure of lattice perturbation theory one usually has to con-
tent oneself with one-loop results. In fact, the results presented here and its
analogue for gauge group SU(2) [5] are the only lattice two-loop results of
renormalized quantities known to us.

The perturbative relation between \( \alpha_{\text{SF}} \) and \( \alpha_{\text{MS}} \) is established in two steps through the bare lattice coupling \( g_0 \) as an intermediate quantity. The two-loop relation between \( \alpha_{\text{MS}} \) and \( g_0 \) has been worked out in [6] for Yang-Mills theory with gauge group SU(\( N \)) for general \( N \). The present paper completes the two loop relation for quenched QCD by deriving the connection between \( g_0 \) and \( \alpha_{\text{SF}} \) for the realistic case of SU(3). The analogous SU(2) calculation was reported in [5]. We note that here Feynman diagrams have to be evaluated and extrapolated numerically. This cannot be done for general \( N \), and the more complex group structure of SU(3) represents a very significant complication.

After this introduction, we define the problem for SU(3) and give a few hints to details of the computation in section 2. In section 3 we compile results for finite lattices and analyze and extrapolate them. Finally in section 4 some applications of our results are reviewed. Some preliminary results of this work were already given in [8].

2 Perturbation theory for gauge group SU(3)

In the Schrödinger functional approach [9] we compute the free energy \( \Gamma \) given by the lattice path integral

\[
e^{-\Gamma} = \int D[U] e^{-S(U)}. \tag{2.1}
\]

The geometry is a finite box of size \( L \) with periodic boundary conditions in the spatial directions and Dirichlet boundary conditions in time. In the lattice realization the latter means that the spatial links \( U(x, k), k = 1, 2, 3, \) are frozen to fixed SU(3)-elements for the layers at time coordinate \( x^0 = 0, L, \)

\[
U(x, k)|_{x^0=0} = \exp(aC) = \exp \left[ \frac{ia}{L} \text{diag}(\phi_1, \phi_2, \phi_3) \right], \tag{2.2}
\]

\[
U(x, k)|_{x^0=L} = \exp(aC') = \exp \left[ \frac{ia}{L} \text{diag}(\phi_1', \phi_2', \phi_3') \right]. \tag{2.3}
\]

Here \( a \) is the lattice spacing, and \( \phi_i, \phi_i' \) are certain dimensionless numbers that depend on one free parameter \( \eta \) that we shall vary later on to probe the system. Both our perturbative calculation here and simulations reported in

\[\footnote{Results reported here are based on ref. [7] where more details can be found.}\]
and more recently in [10, 11] are restricted to the choice “A” of [4] for these numbers. All other links interior to the box are integrated over with the invariant SU(3) measure in (2.1). The action is defined by the usual sum over oriented plaquettes,

\[ S(U) = \frac{1}{g_0^2} \sum_p w(p) \text{tr}(1 - U_p). \]  

(2.4)

The weight \( w(p) \) is unity for all plaquettes except those at the boundary that contain the time-direction and one of the frozen spatial links where we put

\[ w(p) = c_t(g_0) = 1 + c_t^{(1)} g_0^2 + c_t^{(2)} g_0^4 + \ldots \]  

(2.5)

The freedom of adjusting this weight is required for improvement of O(\( a \)) lattice artefacts that are otherwise introduced by the surfaces. We set \( \alpha_{SF} = \bar{g}^2/4\pi \) and the SF-coupling \( \bar{g} \) is defined from the response in the energy \( \Gamma \) to infinitesimal changes in the surface fields by varying \( \eta \),

\[ \bar{g}^2 = k/\Gamma', \]  

(2.6)

where \( \Gamma' \) is the derivative with respect to \( \eta \) at \( \eta = 0 \) and \( k \) is a constant. It is fixed by normalizing the leading term in the perturbative expansion

\[ \bar{g}^2(L) = g_0^2 + m_1(L/a) g_0^4 + m_2(L/a) g_0^6 + \ldots \]  

(2.7)

The one loop coefficient \( m_1 \) was computed in ref. [4]. Our objective here is the computation of \( m_2 \) for gauge group SU(3). In order to determine the improvement coefficients in (2.5) we need to explicitly exhibit the dependence of the coefficients \( m_i \) on them. Inspection of the structure of the contributions leads us to write

\[ m_1 = m_1^0 + c_t^{(1)} m_1^b, \]  

(2.8)

\[ m_2 - m_1^2 = m_2^0 + c_t^{(1)} m_2^b + \left[ c_t^{(1)} \right]^2 m_2^c + c_t^{(2)} m_2^d. \]  

(2.9)

To work out the perturbative expansion of \( \Gamma \) we fix the gauge as discussed in [7]. It is an important advantage of the SF-framework that there is a unique background field of minimal action that interpolates between the surface values (2.2), (2.3),

\[ V(x, k) = \exp\left[a(C + (C' - C)x^0/L)\right], \quad V(x, 0) = 1, \]  

(2.10)
and all fluctuation modes receive gaussian damping. To deal with the SU(3) Lie-algebraic structure of the fluctuations it is advantageous to introduce a suitable basis. We used generators proportional to

\[
T^0 = \text{diag}(0, 1, -1) \propto (C' - C),
\]
\[
T^1 = \text{diag}(2, -1, -1),
\]
\[
(T^{\alpha\beta})_{kl} = \delta_k^\alpha \delta_l^\beta, \quad (\alpha\beta) = (12), (13), (23),
\]

such that \(T^0, T^1\) span the Cartan subalgebra. The \(T^{\alpha\beta}\) and their adjoints are natural generalizations of the ladder-operators in SU(2). Now covariant derivatives in the background field acting in the adjoint representation, — an ubiquitous structure in our perturbation theory — are diagonalized in group space,

\[
[T^0, T^{\alpha\beta}] = h_{\alpha\beta} T^{\alpha\beta}
\]

with numbers \(h_{\alpha\beta}\). In this basis the numerical construction of the propagators in the background field is reduced to the SU(2) case. We just have to apply the procedure described in section 5 of ref. [5] several times for various effective background field parameters.

While the vertices for SU(2) were still ‘hand-coded’ in Fortran, the SU(3) structure was so much more complicated that we let Maple do the work. The three-gluon vertex, for instance, consists of 532 terms. As for SU(2), we performed the summations in position space, so that the most demanding big-mac diagram shown in fig. [4] has only \(O((L/a)^5)\) instead of \(O((L/a)^8)\) terms in momentum space. Its total number of contributions for \(L/a = 32\) after all possible reductions is however still about \(5 \cdot 10^{12}\). Along with each vertex amplitude and propagator we computed their exact \(\eta\)-derivatives to form \(\Gamma'\). To enhance the confidence in our numbers we took the same precautions as in [4]: test of all symmetries before using them to reduce the number of terms by a factor of 36 altogether, check of gauge independence and comparison with a slow but independent code for the smallest lattices.
3 Extraction of results

Some of the coefficients in (2.9) can be given in closed form. Since the background field (2.10) leads to constant plaquettes it is easy to see that

$$m^b_1 = m^d_2 = -\frac{2a}{L}. \quad (3.1)$$

The tree-level contribution $m^c_2$ can be evaluated in closed form. The ensuing expression is however a complicated function of the background field parameters and for our purposes the leading behavior is sufficient

$$m^c_2 = \frac{2a}{L} - \frac{4a^2}{L^2} + O(a^5). \quad (3.2)$$

The remaining contributions $m^a_1$, $m^a_2$ and $m^b_2$ are tabulated in table 1. The generically expected behavior for 2-loop lattice Feynman diagrams suggests an asymptotic expansion

$$m^a_2 = \sum_{n=0}^{\infty} [r_n + s_n \ln(L/a) + t_n \ln^2(L/a)](a/L)^n. \quad (3.3)$$

For $m^a_1$ we expect the same structure without ln$^2$-terms and the same is true for the two-loop diagrams contributing to $m^b_2$ which in addition starts at $n = 1$ only. The coefficients of these expansions are extracted from the series of finite lattices and errors are estimated by the blocking procedure described in [12]. The Callan-Symanzik equation

$$L \frac{\partial}{\partial L} \bar{g}(L) = -\beta(\bar{g}) = b_0 \bar{g}^3 + b_1 \bar{g}^5 + b_2 \bar{g}^7 + \ldots \quad (3.4)$$

implies $t_0 = 0$ and fixes all logarithmic divergences in terms of the universal coefficients

$$b_0 = \frac{11}{(4\pi)^2}, \quad b_1 = \frac{102}{(4\pi)^4}. \quad (3.5)$$

These values were first verified to high accuracy from the data and then assumed to be exact to extract subleading terms. Cancellation of all terms of $O(a)$ in $m_1$ and $m_2$ is achieved to our numerical accuracy by choosing

$$c_t = 1 - 0.08896(23)g_0^2 - 0.0301(25)g_0^4 + O(g_0^6). \quad (3.6)$$

5
Table 1: List of $L/a$-dependent coefficients $m_1^a$, $m_2^a$ and $m_2^b$. Numerical errors are beyond the quoted digits.

With these values, referred to as 2-loop perturbative $O(a)$ improvement, we finally quote

$$m_1 = 2 b_0 \ln(L/a) + 0.36828215(13) + O(a^2), \quad (3.7)$$
\[ m_2 - m_1^2 = 2b_1 \ln(L/a) + 0.048085(63) + O(a^2), \]  
for the relation (2.7) between \( g_0^2 \) and \( \bar{g}^2 \).

The two-loop connection between two different couplings determines the difference between the non-universal three-loop coefficients of their respective \( \beta \)-functions. Hence we can employ the results in [8], where use is made of the three-loop \( \beta \)-function in the MS-scheme to determine

\[ b_2 = \frac{0.4828(88)}{(4\pi)^3} \]  
for the third coefficient in (3.4). This is of the order of magnitude of the effective two-loop coefficient \( b_2^{\text{eff}} = 1.5(8)/(4\pi)^3 \) which was used in ref. [4] to represent the data.

A central quantity in the ALPHA-collaboration’s approach is the step scaling function which generalizes the \( \beta \)-function to finite rescalings,

\[ \sigma(s, u) = \bar{g}^2(sL) \big|_{u=\bar{g}^2(L)}. \]  
On the lattice, it emerges as the continuum limit of a finite lattice spacing approximant \( \Sigma \),

\[ \sigma(s, u) = \lim_{a \to 0} \Sigma(s, u, a/L). \]  
All perturbative information about the convergence speed for \( s = 2 \) is conveniently summarized in coefficients \( \delta_1 \) and \( \delta_2 \) defined by

\[ \delta^{(k)}(u, a/L) = \frac{\Sigma(2, u, a/L) - \sigma(2, u)}{\sigma(2, u)} = \delta_1^{(k)}(a/L) u + \delta_2^{(k)}(a/L) u^2 + \ldots, \]  
where the upper index \( k = 0, 1, 2 \) refers to varying the degree of improvement by using an action with one, two or three terms in the expansion of \( c_t \) in (3.6). Our results are collected in table 2.

4 Applications

The perturbative coefficients, whose computation we described in the previous sections, have already found some applications which we now briefly discuss. Once the SF-coupling \( \bar{g} \) is known for small box-size, it is to be converted to the MS-coupling at high energy. One could conventionally choose
The conversion to $\Lambda_{\overline{\text{MS}}}$ then amounts to an additional known factor. If we insert a small $\bar{g}(L)$ belonging to a very small $L$ into formula (4.1), then the exponentiated integral is close to unity. In [10] the $\Lambda$-parameter in the MS scheme at zero flavor number has been estimated to be

$$\Lambda_{\overline{\text{MS}}}^{(0)} = 251(21)\text{MeV}.$$  

The quoted error is the statistical error from the simulations of the couplings. The three-loop term of the $\beta$-function has been used and this renders the systematic error due to further orders negligible. Without the three loop term, a hard to quantify systematic error of the order of the statistical one would have remained.
In [13] the continuum limit of $L_{\text{max}}/r_0 = 0.718(16)$ is computed. The box-size $L_{\text{max}}$ is defined [4] via the Schrödinger functional by $\bar{g}^2(L_{\text{max}}) = 3.48$. The distance $r_0$ is fixed though the relation $r_0^2 F(r_0) = 1.65$, where $F$ is the force between static quarks [14]. It is expected to be close 0.5 fm in physical units. Some of the lattice artefacts derive from the definition of $L_{\text{max}}$ and are expected to be $O(a)$. Series of simulations have been conducted both with the one-loop and two-loop forms of $c_t$, eq. (3.6). In fig. 5 of [13] the effect of $c_t^{(2)}$ is very clearly visible. It practically eliminates the $O(a)$ term in the continuum extrapolation which thus becomes more reliable and accurate.

We conclude with some remarks on the numerical quality of perturbative expansions in the bare coupling, $\alpha_0 = g_0/4\pi$, or improved bare couplings [15] like $\alpha_P = \alpha_0/P$, where $P$ is the average plaquette (in infinite volume) for the corresponding bare coupling. There are few occasions to investigate such series beyond one-loop order as we can do now in the case of $\alpha_{\text{SF}}$. The well-known problem with bare perturbation theory shows up in the size of the coefficients at scale $q = 1/a$,

$$\alpha_{\text{SF}}(1/a) = \alpha_0 + 4.628 \alpha_0^2 + 29.0 \alpha_0^3 + O(\alpha_0^4). \quad (4.3)$$

If we choose a scale $s/a$ where the 1-loop term is cancelled, then $s$ is unnaturally large and the next term is still not small

$$\alpha_{\text{SF}}(14.06/a) = \alpha_0 + 4.18 \alpha_0^3 + O(\alpha_0^4). \quad (4.4)$$

If we change to the boosted coupling the analogous formulas look somewhat better,

$$\begin{align*}
\alpha_{\text{SF}}(1/a) &= \alpha_P + 0.439 \alpha_P^2 + 2.43 \alpha_P^3 + O(\alpha_P^4), \\
\alpha_{\text{SF}}(1.285/a) &= \alpha_P + 1.91 \alpha_P^3 + O(\alpha_P^4). \quad (4.5, 4.6)
\end{align*}$$

The same tendency is obtained if we minimise the two-loop coefficient instead of cancelling the one-loop term because the scale ratio $r$ between the former and latter method comes out to be

$$r = \exp(b_1/(4b_0^2)) \quad (4.7)$$

which is close to unity. With typical couplings like $\alpha_P \simeq 0.11$ for $\beta = 6.5$ it still is difficult to be confident about systematic errors incurred by truncating the series.

9
As the ALPHA collaboration moves to the inclusion of two massless flavors of quarks into simulations of $\alpha_{SF}$ we plan to extend the present two-loop calculation by the required diagrams with quarks. We hope to report on this in the near future.
References

[1] P. Weisz, Nucl. Phys. B (Proc.Suppl.) 47 (1996) 71

[2] R. Sommer *Non-perturbative renormalization of QCD*, Lectures given at 36. Internationale Universitätswochen für Kern- und Teilchenphysik, Schladming 1997, hep-ph/9711243

[3] M. Lüscher, *Advanced Lattice QCD*, Lectures given at Les Houches Summer School 1997, hep-lat/9802029

[4] M. Lüscher, R. Sommer, P. Weisz and U. Wolff, Nucl. Phys. B413 (1994) 481

[5] R. Narayanan and U. Wolff, Nucl.Phys.B444 (1995) 425

[6] M. Lüscher and P. Weisz, Phys. Lett. B349 (1995)

[7] A. Bode, PhD thesis (in German), Humboldt University, August 1998

[8] A. Bode, Nucl. Phys. B (Proc.Suppl.) 63 (1998) 796

[9] M. Lüscher, R. Narayanan, P. Weisz and U. Wolff, Nucl. Phys. B384 (1992) 168

[10] S. Capitani et al. (ALPHA collaboration), Nucl. Phys. B (Proc. Suppl.) 63 (1998) 153

[11] S. Capitani, M. Lüscher, R. Sommer and H. Wittig, in preparation

[12] M. Lüscher and P. Weisz, Nucl. Phys. B266 (1986) 309

[13] M. Guagnelli, R. Sommer and H. Wittig, hep-lat/9806005

[14] R. Sommer, Nucl. Phys. B411 (1994) 839

[15] G. Parisi, *in*: High-Energy Physics — 1980, XX. Int. Conf., Madison (1980), ed. L. Durand and L. G. Pondrom (American Institute of Physics, New York, 1981)
G.P. Lepage and P. B. Mackenzie, Phys. Rev. D 48 (1993) 2250