The strong running coupling from the gauge sector of Domain Wall lattice QCD with physical quark masses

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We report on the first computation of the strong running coupling at the physical point (physical pion mass) from the ghost-gluon vertex, computed from lattice simulations with three flavors of Domain Wall fermions. We find α_{\text{phys}}(m_\pi^2) = 0.1172(11), in remarkably good agreement with the world-wide average. Our computational bridge to this value is the Taylor-scheme strong coupling, which has been revealed of great interest by itself because it can be directly related to the quark-gluon interaction kernel in continuum approaches to the QCD bound-state problem.

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Introduction. — Quantum Chromodynamics (QCD), the non-Abelian gauge quantum field theory describing the strong interaction between quarks and gluons, can be compactly expressed in one line with a few inputs; namely, the current quark masses and the strong coupling constant, αs. The latter is a running quantity which sets the strength of the strong interaction for all momenta. This running can be, a priori, inferred from the theory and encoded in the Renormalization Group equation (RGE) of αs, the value of which can be thus propagated from one given momentum to any other. The strong coupling is expressed by either the boundary condition for its RGE, generally dubbed Λ_QCD, or its value at a reference scale, typically the Z^n-pole mass. This value is considered one of the QCD fundamental parameters, to be fitted from experiments, and amounts to αs(m_Z^2) = 0.1181(11) [2], in the MS renormalization scheme. Its current uncertainty of about 1 % renders it the least precisely known of all fundamental coupling constants in nature. But at the same time, it is interesting to mention that a plethora of computations of LHC processes depend on an improved knowledge of αs to reduce their theoretical uncertainties [3]. Especially in the Higgs sector, the uncertainty of αs dominates that for the H → c\bar{c}, gg branching fractions and, after the error in the bottom mass, the one for the dominant H → b\bar{b} partial decay. And contrarily to other sources of uncertainty, as parton distribution functions, which reduced substantially [4], that for αs has not significantly changed in the last decade. Moreover, the αs running and its uncertainty also has a non-negligible impact in the study of the stability of the electroweak vacuum, in the determination of the unification scale for the interaction couplings and, generally, in discriminating different New Physics scenarios.

There are many methods to determine the QCD coupling constant based on precision measurements of different processes and at different energy scales. A description of which can be found in the last QCD review of Particle Data Group (PDG) [2] or in specific reviews as, for instance, Ref. [5]. Alternatively, lattice QCD can be applied as a tool to convert a very precise physical observation, used for the lattice spacing setting, into Λ_QCD. Thus, lattice QCD calculations can potentially be of a great help to increase the accuracy of our knowledge of αs. A review of most of the procedures recently implemented to determine the strong coupling from the lattice can be found in Ref. [6]. Among these procedures, there are those based on the computation of QCD Green’s functions (see for instance [7–9]), the most advantageous of which exploits the ghost-gluon vertex renormalized in the so called Taylor scheme [10–17] such that the involved coupling can be computed from two-point Green’s functions. As a bonus, this coupling has many phenomenological implications [18–22] and is connected to the quark-gluon interaction kernel in continuum approaches to the QCD bound-state problem [23–27]. In this letter, we shall focus on this method and evaluate the Taylor-coupling from lattice simulations with three Domain Wall fermions (DWF) at the physical point. DWF (cf. [28–29] for two interesting reviews), owing to their very good chiral properties, are expected to suffer less the impact of discretization artifacts.

The running coupling from QCD two-point Green’s functions. — First, we will sketch how the strong running coupling can be obtained from the gauge sector of QCD, invoking only 2-point Green’s functions. Let F and D be the form factors (dressing functions) of the ghost and gluon propagators in the Landau gauge, the coupling will then read [10, 13]

$$
\alpha_T(k^2) = \frac{g_T^2(k^2)}{4\pi} = \lim_{\Delta \to 0} \frac{g_0^2(a)}{4\pi} F^2(k^2, a) D(k^2, a),
$$

(1)
renormalized in the Taylor scheme, where \( a \) stands for a
regularization cut-off (the lattice spacing that is taken
to vanish in the end of the calculation). The gauge-field
2-point Green’s functions can be obtained from lattice
QCD simulations with an extremely high level of
accuracy, and combined next as Eq. (1) indicates to produce
a precise estimate for the running of the coupling over a
large window of momenta. Roughly above 3.5 – 4 GeV,
this running can be very well described by [14]:

\[
\alpha_T(k^2) = \alpha_T^{\text{pert}}(k^2) \left(1 + \frac{9}{k^2} R(\alpha_T^{\text{pert}}(k^2), \alpha_T^{\text{pert}}(k_0^2))\right)
\]

\[
\times \left(\frac{\alpha_T^{\text{pert}}(k^2)}{\alpha_T^{\text{pert}}(k_0^2)}\right)^{1 - \gamma_0^2/\beta_0} \frac{g_T^2(q_0^2)(A^2)_{R,2g}}{4(N_C^2 - 1)},
\]

where the perturbative result is supplemented by
a leading Operator Product Expansion (OPE) non-
perturbative correction, driven by the dimension-two
gluon condensate \( g_T^2(q_0^2) \langle A^2 \rangle_{R,2g} \), including its anomal-
dous dimension: \( 1 - \gamma_0^2/\beta_0 = 1/4 \) for \( N_f=3 \) [30] 31 and

\[
R(a, a_0) = \left(1 + 1.0588a + 1.61814a^2 + 1.9534a^3\right)
\times \left(1 - 0.62446a_0 - 0.26400a_0^2 - 0.04275a_0^3\right),
\]

obtained here for \( N_f=3 \) as described in the Appendix
of Ref. [14]. The momentum \( q_0=10 \) GeV is chosen as a
subtraction point for the local operator. The per-
turbative \( \alpha_T^{\text{pert}}(k) \) can be approximated at the four-loop
level by the integration of the \( \beta \)-function [2], their coeffi-
cients being defined in the Taylor scheme [13, 32]. Thus,
the purely perturbative running reads as a function of
ln \( k^2/\Lambda_T^2 \), where \( \Lambda_T \) stands for the \( \Lambda_{QCD} \)-parameter
in the Taylor scheme. The confrontation of lattice re-
sults, accurately obtained with Eq. (1), to the running
behavior predicted by Eq. (2) allows for a precise deter-
mination of the parameters \( \Lambda_T \) and the gluon condensate
\( g_T^2(q_0^2) \langle A^2 \rangle_{R,2g} \), both controlling the result displayed by
Eq. (2). Finally, as the running coupling in Taylor and
MS schemes relate as \( \alpha_T = \bar{\alpha}(1 + c_1 \bar{\alpha} + O(\bar{\alpha}^2)) \), where
\( c_1 \) is known [32], the \( \Lambda_{QCD} \)-parameters can be in turn
related, owing to their scale independence, by a subtrac-
tion of the couplings at asymptotically large momenta,
thus obtaining [14]

\[
\frac{\Lambda_{MS}}{\Lambda_T} = e^{-\frac{c_1}{2\beta_0}} = \exp\left(-\frac{507 - 40N_f}{792 - 48N_f}\right).
\]

All the procedure has been described in very detail in
a series of articles, resulting from a long-term research
program aimed at the determination of \( \Lambda_{MS} \) from lattice
QCD, where estimates for \( N_f=0 \) [13], \( N_f=2 \) [14] and
\( N_f=2+1+1 \) (two degenerate light quarks and two non-
degenerate ones with strange and charm flavors) [15] [17]
have been delivered.

The knowledge of \( \Lambda_{MS} \) at a given \( N_f \) defines the per-
turbative running of \( \alpha_{MS} \), known to give a reliable effective
description of the physical world between the energy
thresholds of the \( N_f \)-th and \( (N_f+1) \)-th quark flavors for
\( N_f \geq 3 \) [2]. Then, the matching formula

\[
\alpha^{N_f+1}_{MS}(m_q) = \alpha^{N_f}_{MS}(m_q) \left(1 + \sum_n c_{n0} \left(\alpha^{N_f}_{MS}(m_q)\right)^n\right)
\]
can be applied to extend the running up to the threshold
of the \( (N_f+2) \)-th quark flavor, where \( m_q \) is the MS run-
mass of the \( (N_f+1) \)-th quark and the coefficients
\( c_{n0} \) can be found in Ref. [33] for \( n \leq 4 \). One can proceed
this way up to the \( Z^0 \) mass scale. Thus, the scale \( \Lambda_T \),
obtained for the running coupling in Taylor scheme at
a given \( N_f \), can be related to the benchmark value of
\( \alpha_{MS}(m_Z^2) \).

The running coupling at the physical point. — Our pre-
vious determinations of \( \Lambda_{MS} \) at \( N_f < 3 \) [13, 14] re-
presented nothing but a heuristic effort, paving the way
towards more realistic computations. This is so, first,
because the lattice scale setting made by the confronta-
tion with empiric observations is affected by the presence
of the physical light flavors, up and down but also strange,
thus inducing strong systematic effects. But moreover,
even if one estimates and corrects the strange quark
deviation in the \( N_f=2 \) case as prescribed in Ref. [24],
the matching formula (5) can be hardly trusted at the
uncharged-quark threshold. On the other hand, the one for
\( N_f=2+1+1 \) [15, 17] cannot be considered as a fully realistic
estimate either, as far as it relies on lattice simulations
where the lightest pseudoscalar mass ranges from 270 to
510 MeV and where chiral fits were required to take ex-
perimental \( f_\pi \) and \( m_\pi \) at the physical point [34, 35].

We repeat here the analysis with two ensembles of
gauge-field configurations with \( 2+1 \) DWF simulated at
the physical point and a third one with a pion mass of
around 300 MeV (see Tab. 1). Furthermore, we follow
Ref. [36] and perform a very careful scrutiny of discretiza-
tion lattice artifacts, which corresponds to taking \( a \to 0 \)
in Eq. (1), and approach thus the continuum limit. It can
be outlined as follows: bare coupling and dressing func-
tions are combined as Eq. (1) reads and \( O(4) \)-breaking
artifacts cured by applying the \( H(4) \)-extrapolation [37, 39]; resi-
dual \( O(4) \)-invariant artifacts are then removed by iden-
tifying \( O(a^2) \)-corrections after a thorough com-
parison of results from the two different simulations at
the physical point (as described in Sec.III.B of Ref. [36]);
and, finally, the outcome is checked by applying the same
\( O(a^2) \)-corrections to the third simulation’s results.

Figure 1 shows the coupling data for the three ensem-
bles, exhibiting an excellent overlap and displaying a nice
running behavior. Besides the good chiral properties of
the DWF, a second ace of the exploited ensembles at
the physical point is their large physical volume, which
is made apparent by the absence of finite-volume effects.
when their results compare with those for the half-volume third ensemble. The upper bound of the running window, defined by $k a(2.25) = \pi/2$, corresponds to the largest lattice momenta which, being conservative, can be safely cured for discretization artifacts.

The rightness of Eq. (2) and the need of the gluon condensate $\chi_R(q_0^2)/(A^2)_{R,q_0^2}$ for the appropriate description of the momentum running of MOM-renormalized gauge-field Green’s functions have been very well established \cite{9, 13, 17, 49, 52}. Its nature and implications have been also thoroughly investigated in an exhaustive bunch of different analyses \cite{33, 60}, and its little dependence with the number of dynamical flavors found as well. Indeed, the effect of the heavier flavors can be thought to be negligible. Therefore, we have made the weighted-by-the-errors average of 2.7(1.0) and 4.5(5) GeV$^2$ for the gluon condensate at, respectively, $N_f=2$ \cite{14} and $N_f=4$ \cite{16}; and thus finding for $N_f=3$: $\chi_R^2(q_0^2)/(A^2)_{R,q_0^2} = 4.1(1.1)$ GeV$^2$, where the uncertainty has been conservatively estimated by adding the errors in quadrature. We have then applied this value to Eq. (2) and inverted it numerically for all the lattice calculations at the physical point of $\alpha_T(k^2)$, with $k > 3$ GeV, and obtained thus the estimates of $\Lambda_T$, converted to $\Lambda_{\overline{\text{MS}}}$ through Eq. (4) and displayed in Fig. 2. The plot shows a slow systematic decreasing below 3.62 GeV which, as proven in refs. \cite{16, 17} for $N_f=4$, reflects that in this range higher-order nonperturbative corrections need to be included in Eq. (2). Above 3.62 GeV, a small plateau appears: 11 points for which their central values differ as much as one per mil, their statistical errors being of the order of one per cent. However, the plateau is too small to apply the same fitting strategy developed in refs. \cite{16, 17}, with two free parameters and the lowest bound of the fitting window to be determined by the minimization of $\chi^2$. We make here no fit but take from literature the value of the condensate and evaluate $\Lambda_{\overline{\text{MS}}}$ instead from the largest available momentum: $\Lambda_{\overline{\text{MS}}}=320(4)(13)$ MeV; the first quoted error results from propagating the one of $\alpha_T$ for this momentum into $\Lambda_{\overline{\text{MS}}}$ determined by Eq. (2), while the second one propagates the larger uncertainty from the condensate value. The central values for $\Lambda_{\overline{\text{MS}}}$ and the condensate applied to Eq. (2) produce the black solid curve in Fig. 1.

Beyond this, one can also incorporate the same sort of higher-order nonperturbative correction effectively identified in Ref. \cite{16} and try thus the same fit made therein. In so doing, one would obtain a nice plateau for momenta ranging from 2 to 3.7 GeV and a very consistent best-fit for $\Lambda_{\overline{\text{MS}}}=313$ MeV, which will be used here only to estimate an uncertainty of 7 MeV resulting from the possible impact of higher-order nonperturbative corrections. Thus, following the matching procedure described in the previous section, we will be left with

$$
\alpha_{\overline{\text{MS}}}(m_Z^2) = 0.1172(3)(9) \, ,
$$

\footnote{We have also considered the 6% of correction resulting from the strange quark in the lattice scale setting prescribed by \cite{24}.}
where the first error propagates the uncertainty in the lattice determination of the Taylor coupling, the second does so for the value of the condensate and the last one stands for higher-order nonperturbative corrections.

\( N_f = 2 + 1 + 1 \) versus \( N_f = 2 + 1 \) results. — Let us complete this analysis by relating the current results with our previous ones for \( N_f = 2 + 1 + 1 \) [16]. The lattice actions employed for the fermionic sector differ, twisted-mass for the latter and DWF for the former, although consistent results from both are expected in the continuum limit, if all discretization artifacts are indeed under control. The benchmark value of \( \alpha_{\overline{\text{MS}}}^\text{MS}(m_Z^2) \) here is 0.1172(11), all the errors combined in quadrature, and 0.1200(14) in Ref. [16]; both compatible with the current PDG world average [2], 0.1181(11), but not with each other within their 1-\( \sigma \) errors. This little difference might be due to a simple statistical deviation but can also reflect a small systematic effect in [16], caused by the larger pion mass\(^2\). This new updated result from the Taylor coupling, now at the physical point, lies closer to the FLAG lattice average\(^3\): 0.1182(12) [6]; but even closer to the non-lattice average of PDG: 0.1174(16) [2]. The PDG lattice unweighted average is in turn 0.1188(13), including the ghost-gluon determination [16, 17] among a few others [67–71]. However, updating for the ghost-gluon with the current result, one is left with 0.1184(13), closer to the FLAG central value. A very accurate \( \alpha_{\overline{\text{MS}}}^\text{MS}(m_Z^2) \) = 0.11852(84), obtained from the Schrödinger functional and renormalized couplings defined via the Gradient flow, has been also recently reported [72], with which our estimate agrees as well. It is noteworthy that this agreement demonstrates and strongly confirms, the approaches being radically different, that lattice systematics are well under control. In [72] DWF have also been employed for the extraction of \( \alpha_\text{a} \) from the hadronic vacuum polarization function albeit not at the physical point. Their result is less precise, 0.1181(27), but anyhow in good agreement with ours.

Beyond this, Fig. 3 displays a direct and striking comparison of the Taylor couplings for \( N_f = 2 + 1 \) and \( 2 + 1 + 1 \). It is very apparent that, for momenta above the charm quark mass threshold, the 3-flavors coupling decreases faster than the 4-flavors one, extending down to nonperturbative momenta a well-known perturbative result: the beta function, the logarithmic derivative of the coupling with opposite sign, lessens when the number of flavors gets bigger. Around the charm threshold and below, within the deep IR domain, 4- and 3-flavors couplings appear to be the same, both reaching strikingly the same peak. Lightened by a few recent works [29–27], bridging the gauge sector and phenomenological applications in QCD in connection with the bound-state problem, this feature can be well understood: the Taylor coupling can be related to the quark-gluon interaction kernel [24], both differing only by a small correction rooting in the ghost sector and not depending very much on the number of flavors. Fig. 3 thereby implies that the IR quark-gluon interaction strength does not depend on whether the charm quark becomes active or not. Although expected, to our knowledge, this outcome has never been so remarkably exposed.

Conclusions. — In this article we presented our results on the first computation of the strong running coupling at the physical point from the ghost-gluon vertex, computed from lattice simulations with \( N_f = 2 + 1 \) DWF. We therewith update the last results [16] [17] obtained from applying the same procedure with four flavors but relatively large pion mass. The continuum limit treatment has been also herein improved. Thus, we have been left with an estimate for the benchmark value of \( \alpha_{\overline{\text{MS}}}^\text{MS}(m_Z^2) \) more accurate, closer to the central value of the current lattice (FLAG) average [6] and in remarkably good agreement with the non-lattice average of PDG [2]. Moreover, lattice and non-lattice averages of PDG would come closer after updating the ghost-gluon determination. The convergence of lattice and non-lattice averages is very welcome, implying first that theory meets experiments but, not less important, that systematics effects from the discretization are under control and one can thereby take at face value the lattice errors, approaching thus the goal of getting the \( \alpha_{\overline{\text{MS}}}^\text{MS}(m_Z^2) \) uncertainty below the one per cent level.

On the other hand, the strong coupling in Taylor

\(^2\) The pion mass effect on the UV momentum running is seen to be very small in Fig. 7 but effects on the physical scale setting and on the impact of the discretization artifacts cannot be excluded. Specially the latter would require a very accurate control of the continuum limit that might not have been achieved in Ref. [16].

\(^3\) The FLAG average includes determinations from current two-point correlators [67–69], Schrödinger functional [70] and Wilson loops [71].
scheme, by itself, is an interesting quantity, as it can be directly related to the quark-gluon interaction kernel in continuum approaches to the QCD bound-state problem. It has been herein obtained for three dynamical quarks at the physical point, and has been shown to compare very well with previous results for four dynamical quarks but non-physical pion mass, qualitatively but also quantitatively, beyond the small deviations due, presumably, to the larger pion mass and that impacts on the very delicate extraction of $\alpha_m(m_Z^2)$. Such a comparison shows that the activation of the charm quark does not significantly affect the infrared quark-gluon interaction strength, and it only makes the running coupling decrease slower, above the charm threshold, as suggested by the $\beta$-function.

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