LATTICE SIMULATIONS FOR THE RUNNING COUPLING CONSTANT OF QCD

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The strong coupling constant \( \alpha_s(\mu_0) \), taken at a fixed reference scale \( \mu_0 \), is the single free parameter of QCD and should be known to the highest available precision. The value of \( \alpha_s \) should also be determined with good accuracy over as large a range of scales as possible, in order to reveal potential anomalous running in the strength of the strong interaction. Lattice QCD is now able to calculate \( \alpha_s \) with accuracy comparable to or better than experiment. We review the status of such lattice calculations in quenched and full QCD.

1 QCD coupling and \( \beta \)-function

The scale dependence of the QCD coupling \( \alpha_s = g_s^2/(4\pi) \) is controlled by the \( \beta \)-function:

\[
\mu \frac{\partial \alpha_s}{\partial \mu} = \beta(\alpha_s) = -\left( \frac{\beta_0}{2\pi} \alpha_s^2 + \frac{\beta_1}{4\pi^2} \alpha_s^3 + \frac{\beta_2}{64\pi^3} \alpha_s^4 + \ldots \right),
\]

(1)

where \( \beta_0 = 11 - 2N_f/3 \), \( \beta_1 = 51 - 19N_f/3 \) and \( N_f \) is the number of flavors of quarks with mass less than the energy scale \( \mu \). The coefficients \( \beta_n \) for \( n \geq 2 \) are renormalization-scheme-dependent.

By solving the differential equation for \( \alpha_s \), a constant of integration is introduced. This constant is the one fundamental constant of QCD. Usually one chooses for this constant the value of \( \alpha_s \) at a fixed reference scale \( \mu_0 \). Equivalently one can consider the dimensional parameter \( \Lambda \), defined for example as

\[
\Lambda(N_f) = \mu \exp \left( \frac{-2\pi}{\beta_0} \frac{\alpha_s(\mu)}{\beta_0} \right) \left( \frac{\beta_0 \alpha_s(\mu)}{2\pi} \right)^{-\beta_1/\beta_0^2} \times \exp \left\{ - \int_0^{\alpha_s(\mu)} du \left( \frac{1}{\beta(u)} + \frac{2\pi}{\beta_0 u^2} - \frac{\beta_1}{\beta_0^2 u} \right) \right\}.
\]

(2)

Note that, by using this relation at the leading order, one gets that \( \Lambda(N_f) \) is known with an accuracy of about 5% if \( \alpha_s(\mu) \) is given with an accuracy of about 1%.
When two different renormalization schemes are considered one can write
\[
\alpha_s^{(1)}(\mu) = \alpha_s^{(2)}(\mu) \left\{ 1 + a \frac{\alpha_s^{(2)}(\mu)}{4\pi} + b \left[ \frac{\alpha_s^{(2)}(\mu)}{4\pi} \right]^2 + \ldots \right\}
\]
and check that
\[
\beta_2^{(1)} = \beta_2^{(2)} - 4a\beta_1 + 2(b - a^2)\beta_0
\]
\[
\Lambda^{(1)}(N_f) = \Lambda^{(2)}(N_f) \exp \left( \frac{a}{2\beta_0} \right).
\]
Using the \( \Lambda \) parameter we can also obtain a parametrization of the \( \mu \) dependence of the QCD coupling\(^a\)
\[
\alpha_s(\mu) = \frac{2\pi}{\beta_0 \log(\mu/\Lambda)} \left[ 1 - \frac{\beta_1}{\beta_0^2} \log(\mu/\Lambda) + \ldots \right].
\]
Clearly the coupling decreases as the scale \( \mu \) increases, corresponding to the property of asymptotic freedom. However, due to the logarithmic dependence one needs to consider a large range of scales \( \mu \) in order to see a variation of \( \alpha_s(\mu) \) by a factor two or three (see Fig. 9.2 in Ref. \(^2\)).

1.1 Experimental results for \( \alpha_s(\mu) \)
The value for a quantity \( A \) from an experiment can be used to extract a value of \( \alpha_s(\mu) \) by considering the following perturbative expansion (in some renormalization scheme)
\[
A = c_0 + c_1 \alpha_s(\mu) + c_2 \alpha_s^2(\mu) + \ldots.
\]
If the scale involved is low one should also try to take into account non-perturbative contributions to \( A \). Clearly the physical result \( A \) does not depend on the chosen renormalization scheme. However, the truncated perturbative series does exhibit renormalization-scheme dependence. In particular, the finite coefficients \( c_i \) (\( i \geq 2 \)) depend on the renormalization scale \( \mu \) and, implicitly, on the chosen renormalization scheme. Therefore, for a given scheme, one should find the best choice\(^b\) for the scale \( \mu \) in order to reduce the scale ambiguity in the expansion (7).

In order to compare the values of \( \alpha_s(\mu) \) from various experiments\(^3,4\), these values must be evolved — using the renormalization group — to a common

\(^a\)Note that this parametrization is not unique but depends on the choice of the constant of integration (see for example problem 13.11 in Ref. \(^1\)).

\(^b\)See Ref. \(^3\) for various methods proposed for choosing the scale \( \mu \).
scale (usually the mass of the $Z^0$ boson) and related to a common scheme (usually the $\overline{MS}$ scheme). The present world-wide average in the $\overline{MS}$ scheme for $\alpha_s(M_Z)^{(N_f=5)}$ is $0.1172 \pm 0.002$.

2 Numerical evaluation of $\alpha_s(\mu = q)$

One can perform the experiment also on a computer, using Lattice QCD. For example, one can evaluate numerically the plaquette $W_{1,1} = < \text{Tr} U_{\mu\nu}/3 >$ — which corresponds to the elementary gluonic action on the lattice — and compare the result with a perturbative expansion. Also in this case one should be careful with the choice of the scheme used for the perturbative expansion and with the choice of the scale $\mu$. For example, it is well known that the expansion of the plaquette $W_{1,1}$ in terms of the lattice bare coupling $\alpha_0 = g_0^2/4\pi$ yields a very poor result. In fact, for $g_0^2 = 1$ one-loop perturbation theory with $N_f = 0$ predicts $-\log W_{1,1} \approx 0.4228$ while the corresponding Monte Carlo result is about 0.5214.

A better expansion is obtained if one considers an effective coupling defined in terms of a physical quantity. For example, if $V(q)$ is the interquark potential one can define

$$V(q) = -\frac{16\pi\alpha_V(q^2)}{3q^2}$$

and work in the $\alpha_V$ scheme. In this scheme one gets, at the one-loop level and with $N_f = 0$,

$$-\log W_{1,1} = c_1 \alpha_V(q^2) \left[ 1 + \tilde{c}_2 \alpha_V(q^2) + \ldots \right],$$

where $\tilde{c}_2 = \frac{11}{4\pi} \log \left( \frac{q^2}{\tilde{\alpha}_V} \right) + \tilde{d}$ and $\tilde{d} \approx 1.329$. In order to fix the value of the scale $q$ the idea introduced in Ref. is to impose the relation

$$\alpha_V(\tilde{q}^2) c_1 = \alpha_V(q^2) \int d^4q \, f(q) = \int d^4q \, \alpha_V(q^2) \, f(q),$$

namely $\tilde{q}$ is the average momentum entering in the one-loop calculation. By expanding both $\alpha_V(\tilde{q}^2)$ and $\alpha_V(q^2)$ in terms of $\alpha_V(\mu^2)$ one gets

$$\log (\tilde{q}^2) \int d^4q \, f(q) = \int d^4q \, \log (q^2) \, f(q).$$

In the case of the plaquette this prescription gives $\tilde{q} \approx 3.4018/a$ where $a$ is the lattice spacing. Clearly, this procedure can be repeated for different Wilson loops $W_{r,t}$, i.e. from the numerical values for $W_{r,t}$ one can obtain $\alpha_V(\tilde{q}_{r,t}^2)$ using a perturbative expansion like eq. (9). As can be seen from Fig.
In Ref. 6, the coupling $\alpha_V(q^2)$ obtained from such calculations runs with $q$ in agreement with a two-loop formula (6).

In order to compare these results with experimental data one needs to fix the lattice spacing $a$, i.e. the scale $\bar{q}$ should be given in physical units. This can be done by comparing lattice data with an experimental input, as has been done7 using the $\Upsilon$ meson spectrum, known experimentally with very good accuracy and for which accurate simulations can be done. Using results for $N_f = 0$ and $N_f = 2$ dynamical fermions, which allows extrapolation to physical case $N_f = 3$, the authors of Ref. 7 obtained a final result — in the $\overline{MS}$ scheme and evolved perturbatively to the $Z^0$ mass scale — of 0.1174 ± 0.0024. Similar results have been obtained by other groups, using different lattice setups, and have been included by the Particle Data Group3 in the evaluation of the world-wide average of $\alpha_s(M_Z)(N_f=5)$.

2.1 Ingredients for a numerical evaluation of the QCD running coupling constant

From the previous analysis it is clear that in order to evaluate the QCD running coupling constant using lattice numerical simulations one needs:

- a good definition for $\alpha_s$ allowing high accuracy, control over finite-size effects and discretization effects,
- an accurate determination of the energy scale (i.e. the lattice spacing $a$),
- a perturbative relation with $\alpha_{\overline{MS}}$,
- the possibility of extending the procedure to dynamical fermions (unquenched simulations).

3 Running coupling in a finite box

The Alpha collaboration9 studies the QCD running coupling using finite boxes (with physical size $L = Na$), a definition for $\alpha_s$ that explicitly depends on the scale $L$, and a non-perturbative finite-size scaling technique.10 To this end one could consider, for example, the force between static quarks separated by a distance $r = L/2$, given by

$$\alpha_{qq}(L) = \left. \frac{3}{4} r^2 F_{qq}(r, L) \right|_{r=L/2},$$

(12)

\textsuperscript{c} See Ref. 8 for a previous review of the numerical determination of $\alpha_s$. 

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or a correlation function\textsuperscript{11} for a separation $r = L/2$. Most of the simulations by the Alpha collaboration have been carried out using as definition for $\alpha_s$ the response of the system to a change of the boundary conditions in the Schrödinger functional approach (for details see Ref.\textsuperscript{12}). In all cases the physical size $L$ of the lattice is the only physical scale on which these couplings depend, i.e. the box size may be regarded as a reference scale, similar to the renormalization scale $\mu$. Thus, one has a coupling running with $\mu = 1/L$.

The key point in considering these couplings is the use of a non-perturbative renormalization group technique. More specifically, one defines the step-scaling function $\sigma(u)$ through the relation $\alpha_s(2L) = \sigma(\alpha_s(L))$. Clearly this function provides the value of the coupling in a box of size $2L$ given a value for the same coupling in a box of size $L$. Thus, $\sigma(u)$ can be regarded as an “integrated” $\beta$-function. The step-scaling function can be evaluated non-perturbatively using numerical simulations by considering several values of $L$, as shown in Fig. 4 in Ref.\textsuperscript{13}. Notice that for each data point in the plot one should carefully check for possible systematic effects, especially discretization errors. In fact, each point is the result of an extrapolation\textsuperscript{d} to zero lattice spacing of data obtained from several simulations, done with the same physical size $L$ but different lattice spacing $a$ and number of sites per direction $N$.

Once the step-scaling function is known, i.e. after fitting the numerical data, one can evaluate the running coupling in a very large box $L_0 = L_{\text{max}}$ and then find the value of the coupling for boxes of sizes $L_i = L_0/2^i$, using a recursive procedure and a numerical inversion of the step-scaling function. [In order to keep errors under control one should avoid using the fit for the step-scaling function outside the range of the numerical data, i.e. one should avoid extrapolating the step-scaling function $\sigma(u)$ to very small values of $u$.] In this way one obtains the values $\alpha_s(\mu_i)$ for the running coupling at the scales $\mu_i = 1/L_i = 2^i/L_{\text{max}}$.

Since all the scales $\mu_i$ are given in term of $L_{\text{max}}$, the last step consists in setting the scale for the largest lattice, i.e. finding the value of $L_{\text{max}}$ in physical units by comparing lattice data with an experimental input. Thus, the use of a non-perturbative finite-size scaling technique avoids the requirement of a non-perturbative evaluation of the scale $L_i$ for very small values of $L_i$: this is in general complicated by finite-size effects and by the fact that small values of $L_i$ correspond to large value of $\beta$ and that simulations at large $\beta$ and small physical volumes are essentially “perturbative”.

The final value\textsuperscript{13} obtained by the Alpha collaboration in pure QCD is

\textsuperscript{d}See Ref.\textsuperscript{14} for possible problems with this extrapolation.
Λ_{MS}^{(N_f=0)} = 251 \pm 21 \text{ MeV}. Preliminary data with dynamical fermions (N_f = 2) have been presented last year\textsuperscript{15}.

4 Numerical determination of \( \Lambda \)

Several groups study the running of the QCD coupling (in some scheme) over a range of energies and then try to fit the data using a two- or three-loop expression for \( \alpha(q) \) as in eq. (6), considering \( \Lambda \) as a fitting parameter. Alternatively, one can evaluate \( \Lambda \) as a function of \( \alpha(q) \) and look for a plateau at high scale [note that in eq. (2) the left-hand side is constant, for a given value of \( N_f \), even though the right-hand side depends explicitly on the scale \( \mu \)].

4.1 Inter-quark potential

One can evaluate the QCD coupling using the static potential \( V(r) \), which can be evaluated for several values of \( r \) with good accuracy using Wilson loop data and the relation\textsuperscript{5}

\[ W(r,t) = C(r)e^{-tV(r)} + \ldots. \]  

This formula should in general be considered in the limit of large \( t \), but using\textsuperscript{6} smearing and noise-reduction techniques one can increase the overlap of the evaluated quantity with the ground state, i.e. increase the value of \( C(r) \), and obtain a good signal already for small values of \( t \). Then, from \( V(r) \) one can obtain the force \( F(r) \) [and the running coupling \( \alpha_{q\bar{q}}(1/r) \), see eq. (12)] using a finite-difference approximation for the derivative \( dV(r)/dr \). In the quenched case\textsuperscript{17} one obtains \( \Lambda_{\text{MS}}^{(N_f=0)} = 246 \pm 7 \pm 3 \text{ MeV}, \) in excellent agreement with the result from the Alpha collaboration. Unquenched simulations (also interesting to study string breaking\textsuperscript{18}) are under way\textsuperscript{19}.

4.2 Three-gluon vertex

In this case one evaluates the three-gluon vertex\textsuperscript{20} in the \( \text{MOM} \) scheme (in Landau gauge). For this quantity perturbative results are known to three loops\textsuperscript{21} (and the corresponding beta function to four loops). In order to obtain good data a careful analysis of breaking of rotational symmetry is required\textsuperscript{22}. From quenched simulations\textsuperscript{23} one obtains the value \( \Lambda_{\text{MS}}^{(N_f=0)} = 295 \pm 5 \pm 15 \text{ MeV}, \) somewhat larger than the previous results. Preliminary unquenched

\textsuperscript{4}For a review of this method see for example Ref. 16.
data\textsuperscript{24} have been presented last year and the authors quote $\Lambda_{\overline{MS}}^{(N_f=2)} = 264 \pm 27$ MeV. A similar study has started recently using the quark-gluon vertex\textsuperscript{25} yielding $\Lambda_{\overline{MS}}^{(N_f=0)} = 300 ^{+150} _{-180} \pm 55 \pm 30$ MeV, in agreement with the result obtained using the three-gluon vertex.

4.3 Gluon propagator

In this case\textsuperscript{26} one evaluates the gluon propagator $D(q)$ (in Landau gauge) and defines $Z_3(q) = q^2 D(q)$. Then, the gluon data can be fitted by considering the two coupled differential equations

$$\frac{d \log Z_3(q)}{d \log q^2} = \Gamma(\alpha) = - \left[ \frac{\gamma_0}{4\pi} \alpha + \frac{\gamma_1}{(4\pi)^2} \alpha^2 + \ldots \right], \quad (14)$$

$$\frac{d \alpha}{d \log q} = \beta(\alpha) = - \left[ \frac{\beta_0}{2\pi} \alpha + \frac{\beta_1}{(2\pi)^2} \alpha^2 + \ldots \right], \quad (15)$$

where $\Gamma(\alpha)$ is the anomalous dimension of the gluon renormalization constant in the $\overline{MOM}$ scheme. At the lowest order these equations imply the well-known result $D(q^2) \sim 1/q^2 \log (q^2/\Lambda^2)$ with $c = \frac{\gamma_0}{2\gamma_0} = 13/22$.

A solution for these two equations depends on the values $Z_3(\mu)$ and $\alpha(\mu)$ given at some scale $\mu$, and a direct fit of the data provides a value for these two constants. The value $\alpha_s(\mu)$ obtained from the fit can then be evolved, using the renormalization group, to the $Z^0$ scale and related to the $\overline{MS}$ scheme, using the perturbative relation between the two schemes. The authors\textsuperscript{26} quote $\Lambda_{\overline{MS}}^{(N_f=0)} = 319 \pm 14 \pm 20$ MeV as final result in the quenched case, in agreement with the results quoted in Sec 4.2.

4.4 Search for power corrections

Recently there have been various attempts of finding power corrections to the perturbative running of $\alpha_s$, following theoretical predictions\textsuperscript{27}. In particular data from the inter-quark potential\textsuperscript{28}, the three-gluon vertex\textsuperscript{29,30} and the gluon propagator\textsuperscript{30} have been reanalyzed. In all cases the authors found that a nonzero contribution proportional to $1/p^2$ improves the fit of the data. In particular, the result obtained in this way for the $\Lambda$ parameter using the three-gluon vertex\textsuperscript{29}, i.e. $\Lambda_{\overline{MS}}^{(N_f=0)} = 237 \pm 3 ^{+10} _{-10}$ MeV, is in much better agreement with the results quoted in Sections 3 and 4.1 than the original value (see Section 4.2).
5 Running couplings at the IFSC-USP

We now describe the simulations being performed since July 2001 at the Institute of Physics of the University of São Paulo, São Carlos (IFSC-USP). In connection with a grant from FAPESP (“Projeto Jovem Pesquisador”, together with Tereza Mendes), we have set up a dedicated PC cluster at the IFSC-USP. The system has 16 nodes with 866 MHz Pentium III CPU and 256 MB RAM memory (working at 133 MHz), a server with 866 MHz Pentium III CPU and 512 MB RAM memory (working at 133 MHz) and is operating with Debian Linux. The machines are connected with a 100 Mbps full-duplex network and in total there are 130 GB in /tmp directories and 24.8 GB for the /home directory.

We are carrying out simulations considering two definitions of the running coupling constant. In the Coulomb gauge we consider

\begin{align}
g_C^2(p) = \frac{11}{12} p^2 V(p) \equiv \frac{11}{12} g_0^2 p^2 D_{44}(p),
\end{align}

where \( V(p) \) is the color-Coulomb potential, \( D_{44}(p) \) is the time-time component (at equal time) of the gluon propagator and the momenta are three-dimensional.\(^9\) Clearly, if \( V(p) \) is governed by a string tension at large distances, i.e. goes like \( 1/p^4 \) at small momenta, then we should find \( g_C^2(p) \sim 1/p^2 \) in the infrared limit. In Landau gauge\(^h\) we consider

\begin{align}
g_L^2(p) = \frac{g_0^2}{4\pi} \left[ p^2 D(p) \right] \left[ p^2 G(p) \right]^2,
\end{align}

where \( D(p) \) is the transverse gluon propagator and \( G(p) \) is the ghost propagator. This expression enters directly in the quark Schwinger-Dyson equation\(^3^3\) and can be interpreted as an effective interaction strength between quarks.\(^i\) In this case one obtains \( g_L^2(p) \sim p^{-2} \) if, for example, \( D(p) \sim \text{const} \) and \( G(p) \sim p^{-4} \) in the infrared limit. On the contrary, if the gluon propagator goes to 0 in the infrared limit and the ghost propagator blows up not faster than \( p^{-4} \) then \( g_L^2(p) \) has an infrared fixed point. The last behavior has also been obtained\(^3^2\) by solving (approximatively) a coupled set of Schwinger-Dyson equations.

\(^f\)Work in collaboration with D. Zwanziger, New York University (NYU). Some of our simulations are done on a PC cluster at NYU.

\(^g\)Remarkably, this definition of the running coupling constant is renormalization-group invariant\(^3^1\).

\(^h\)Work in collaboration with K. Langfeld and J. C. R. Bloch, Tübingen University.

\(^i\)This is also a renormalization-group-invariant quantity since (in Landau gauge) \( \tilde{Z}_1 = 1 \).
In our project we are also interested in a numerical verification of Gribov’s confinement scenarios — written in terms of the infra-red behavior for the propagators considered above — for these two gauges. Theoretical studies\textsuperscript{34,35} predict that in Landau gauge, there should be a strong suppression of the (unrenormalized) transverse gluon propagator $D(p)$ in the infrared limit and an enhancement of the ghost propagator $G(p)$ in the same limit. These results clearly indicate the absence of a massless gluon from the physical spectrum and provide an indication of a long-range effect in the theory that may result in color confinement. The confinement scenario is particularly simple in the minimal Coulomb gauge where the ghost propagator determines directly the Coulomb interaction\textsuperscript{34,31}. In fact, in this case, confinement of color, i.e. the enhancement at long range of the color-Coulomb potential $V(R)$, is due to the enhancement of ghost propagator $G(p)$ at small momenta. At the same time, the disappearance of gluons from the physical spectrum is manifested by the suppression at $p = 0$ of the propagator $D_{ij}(p, p_4)$ of 3-dimensionally transverse would-be physical gluons.

Preliminary results in the pure $SU(2)$ case for the two running coupling constants and Gribov’s confinement scenarios have been presented in Refs.\textsuperscript{36}.

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