Probing renormalized perturbation theory with data from lattice QCD at high energies

Stefan Sint (Trinity College Dublin)

work in collaboration with:

Mattia Dalla Brida, Patrick Fritzsch, Tomasz Korzec, Alberto Ramos, Rainer Sommer



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- Status of $\alpha_s(m_Z)$
- The ALPHA collaboration project & results
- Non-perturbative finite volume couplings & SF couplings
- $\bullet~$ The Λ parameter or how to test perturbation theory
- Step-scaling functions and continum extrapolations & some results

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- $\bullet\,$ Alternative route: passing via the $\overline{\rm MS}$ scheme
- Conclusions & outlook

References:

- Mattia Dalla Brida, Patrick Fritzsch, Tomasz Korzec, Alberto Ramos, Stefan Sint, Rainer Sommer [ALPHA Collaboration],
 "Determination of the QCD Λ-parameter and the accuracy of perturbation theory at high energies,"
 Phys. Rev. Lett. 117, no. 18, 182001 (2016) arXiv:1604.06193 [hep-ph].
- Mattia Dalla Brida, Patrick Fritzsch, Tomasz Korzec, Alberto Ramos, Stefan Sint, Rainer Sommer [ALPHA Collaboration], "Slow running of the Gradient Flow coupling from 200 MeV to 4 GeV in $N_{\rm f}=3$ QCD," Phys. Rev. D **95**, no. 1, 014507 (2017), arXiv:1607.06423 [hep-lat].
- Mattia Bruno, Mattia Dalla Brida, Patrick Fritzsch, Tomasz Korzec, Alberto Ramos, Stefan Schaefer, Stefan Sint, Hubert Simma Rainer Sommer [ALPHA Collaboration], "QCD Coupling from a Nonperturbative Determination of the Three-Flavor Λ

Parameter," Phys. Rev. Lett. **119**, no. 10, 102001 (2017), arXiv:1706.03821 [hep-lat].

• A very nice summary has been given by Tomasz Korzec at Lattice '17:

Tomasz Korzec, "Determination of the Strong Coupling Constant by the ALPHA Collaboration," $\!\!$

arXiv:1711.01084 [hep-lat], to appear in the proceedings

- $\alpha_s(m_Z)$ is a fundamental parameter of the Standard Model;
- Important input for LHC physics: accuracy < 1% is required!

Current status & world averages:



Reducing the error to $\Delta \alpha_s(m_Z) \approx 0.0006$ (ie. 0.5%)is a challenge!



ALPHA collaboration project

Build on CLS effort [Bruno et al, JHEP 1502 (2015) 043]:

- $N_f = 2 + 1$ state of the art lattice QCD simulations
- nonperturbatively O(a) improved Wilson quarks & Lüscher-Weisz gauge action;
- open boundary conditions (avoids topology freezing)

Use 3 input parameters from experiment, e.g.

 $F_K, m_\pi, m_K \Rightarrow m_u = m_d, m_s, q_0$

 \Rightarrow everything else becomes a prediction, for instance

 $\alpha_{\circ}^{(N_f=3)}(1000 \times F_K)$ (in any renormalization scheme)

Final goal: $\alpha_s^{(N_f=5)}(m_Z)$ in the \overline{MS} -scheme

- Controlled systematics: avoid the use of perturbation theory except at high energies of $O(m_Z)!$
- Solve the problem of large scale differences using recursive finite volume techniques ("step-scaling").
- Has been accomplished in N_f = 3 QCD (s. next page)
- $\Rightarrow \alpha_s(m_Z)$ currently still requires perturbative matching from N_f = 3 to N_f = 5 across the charm and bottom thresholds! ◆□▶ ◆□▶ ◆ ≧▶ ◆ ≧▶ ○ ≧ · ⑦ Q (?) 6/21

Result for $\alpha_s(m_Z)$ by the ALPHA collaboration



• SF ("Schrödinger functional") from μ_0 to high energies $\mu_{\rm PT}$

This talk will focus on the high energy running in the SF scheme!

Wanted: QCD observables, O, which ...

 are gauge invariant & non-perturbatively defined through the (Euclidean) QCD path integral:

$$\langle O \rangle = \mathcal{Z}^{-1} \int D[A, \psi, \overline{\psi}] O[A, \psi, \overline{\psi}] \exp\{-S\}$$

- depend on a single scale μ = 1/L, with L⁴ the space-time volume. Other dimensionful parameters (momenta, distances,..) are scaled with L or set to zero (quark masses);
- can be expanded perturbatively in $\alpha_s(\mu) = \bar{g}^2(L)/(4\pi)$:

$$\langle O \rangle = c_0 + c_1 \alpha_s(\mu) + c_2 \alpha_s^2(\mu) + \dots$$

 \Rightarrow give rise to non-perturbatively defined couplings:

$$\alpha_O(\mu) \stackrel{\text{def}}{=} \frac{\langle O \rangle - c_0}{c_1} = \alpha_s(\mu) + c_1' \alpha_s^2(\mu) + c_2' \alpha_s^3(\mu) + \dots$$

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Example: a family of SF couplings

• Dirichlet b.c.'s in Euclidean time, abelian boundary values C_k , C'_k :

$$A_k(x)|_{x_0=0} = C_k(\eta, \nu), \qquad A_k(x)|_{x_0=L} = C'_k(\eta, \nu)$$

⇒ induce family of abelian, spatially constant background fields B_{μ} with parameters η , ν (→ 2 abelian generators of SU(3)):

$$B_k(x) = C_k(\eta, \nu) + \frac{x_0}{L} \left(C'_k(\eta, \nu) - C_k(\eta, \nu) \right), \qquad B_0 = 0.$$

- Induced background field is unique up to gauge equivalence
- Effective action

$$e^{-\Gamma[B]} = \int D[A, \psi, \overline{\psi}] e^{-S[A, \psi, \overline{\psi}]}, \qquad \Gamma[B] = \frac{1}{g_0^2} \Gamma_0[B] + \Gamma_1[B] + O(g_0^2)$$

Define family of SF couplings, parameter ν:

$$\frac{1}{\bar{g}_{\nu}^{2}(L)} \stackrel{\text{def}}{=} \left. \frac{\partial_{\eta} \Gamma[B]}{\partial_{\eta} \Gamma_{0}[B]} \right|_{\eta=0} = \left. \frac{\langle \partial_{\eta} S \rangle}{\partial_{\eta} \Gamma_{0}[B]} \right|_{\eta=0} = \frac{1}{\bar{g}^{2}(L)} - \nu \bar{v}(L)$$

⇒ response of the system to a change of a colour electric background field. [Narayanan et al. '92]
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Testing perturbation theory: use the Λ -parameter I

• Non-perturbatively defined coupling $\bar{g}^2(L)$ implies non-perturbative definition of β -function:

$$\beta(\bar{g}) \stackrel{\text{def}}{=} -L \frac{\partial \bar{g}(L)}{\partial L}, \qquad \beta(g) = -b_0 g^3 - b_1 g^5 + \dots$$

with universal coefficients b_0 , b_1 (i.e. b_i , $i \ge 2$ scheme dependent)

$$b_0 = (11 - \frac{2}{3}N_f)/(4\pi)^2, \qquad b_1 = (102 - \frac{38}{3}N_f)/(4\pi)^4.$$

• Exact solution of Callan-Symanzik equation $[L\partial/\partial L + \beta(\bar{g})\partial/\partial\bar{g}]L\Lambda = 0$

$$L\Lambda = \varphi(\bar{g}(L))$$

$$\varphi(\bar{g}) = \left[b_0\bar{g}^2\right]^{-\frac{b_1}{2b_0^2}} e^{-\frac{1}{2b_0\bar{g}^2}} \exp\left\{-\int_0^{\bar{g}} dg\left[\frac{1}{\beta(g)} + \frac{1}{b_0g^3} - \frac{b_1}{b_0^2g}\right]\right\}$$

Scheme dependence of Λ <u>almost</u> trivial:

$$g_{\rm X}^2(\mu) = g_{\rm Y}^2(\mu) + c_{\rm XY} g_{\rm Y}^4(\mu) + \dots \quad \Rightarrow \quad \frac{\Lambda_{\rm X}}{\Lambda_{\rm Y}} = {\rm e}^{c_{\rm XY}/2b_0}$$

 $\Rightarrow \text{ use } \Lambda = \Lambda_{\text{SF},\nu = 0} \text{ as reference.}$ $\underbrace{ \underbrace{\text{Note:}}_{N_f = 3} \Lambda_{\overline{\text{MS}}} \text{ is now } \underline{\text{non-perturbatively}} \text{ defined by } \Lambda = 0.3829 \times \Lambda_{\overline{\text{MS}}} \text{ (for } N_f = 3)$

Testing perturbation theory: use the Λ -parameter II

• Introduce a reference scale $1/L_0$ through:

$$ar{g}^2(L_0) = 2.012 \quad \Rightarrow \quad rac{1}{ar{g}_
u^2(L_0)} = rac{1}{2.012} -
u imes 0.1199(10)$$
 (s. later)

Consider

$$L_0 \Lambda = \underbrace{L_0/L}_{\text{known}} \times \underbrace{\Lambda/\Lambda_{\nu}}_{\exp(-\nu \times 1.25516)} \times \varphi_{\nu}\left(\bar{g}_{\nu}(L)\right)$$

- Non-perturbative results for $1/L_0 \le \mu \le 1/L$ (s. below)
- Perturbation theory for $\mu > 1/L$ by replacing $\beta_{\nu}(g) \rightarrow \beta_{\nu,3\text{-loop}}(g)$ in:

$$\begin{split} \varphi_{\nu} \left(\bar{g}_{\nu}(L) \right) & \propto & \exp\left\{ -\int_{0}^{\bar{g}_{\nu}(L)} dg \left[\frac{1}{\beta_{\nu}(g)} + \frac{1}{b_{0}g^{3}} - \frac{b_{1}}{b_{0}^{2}g} \right] \right\} \\ \beta_{\nu,3\text{-loop}}(g) &= -b_{0}g^{3} - b_{1}g^{5} - b_{2,\nu} g^{7}, \\ b_{2,\nu} &= (-0.06(3) - \nu \times 1.26)/(4\pi)^{3} \quad \text{[Bode, Weisz, Wolff '99]} \end{split}$$

• <u>N.B.</u>: $L_0\Lambda$ must be independent of L and $\nu \Rightarrow$ excellent test of PT!

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Non-perturbative running in steps and determination of L_0/L

Vary scale by factor 2, define step-scaling function [Lüscher, Weisz, Wolff '91]:

$$\sigma(u) = \left. \bar{g}^2(2L) \right|_{u = \bar{g}^2(L)}$$

• Connection to β -function:

$$\int_{\sqrt{u}}^{\sqrt{\sigma(u)}} \frac{dg}{\beta(g)} = -\ln 2$$

- σ(u) can be constructed as the continuum limit of lattice approximants (s. below)
- Once $\sigma(u)$ is available for a range of values $u \in [u_{\min}, u_0]$
- \Rightarrow iteratively step up the energy scale:

$$u_0 = \bar{g}^2(L_0), \quad u_n = \sigma(u_{n+1}) = \bar{g}^2(L_n) = \bar{g}^2(2^{-n}L_0), \quad n = 0, 1, \dots$$

 \Rightarrow scale ratios are $L_0/L_n = 2^n$, where n is the number of steps.

Lattice approximants $\Sigma(u, a/L)$ for $\sigma(u)$

- choose g_0 and L/a = 4, measure $\bar{g}^2(L) = u$ (defines value of u)
- double the lattice and measure

$$\Sigma(u, 1/4) = \bar{g}^2(2L)$$

- now choose L/a = 6 and tune g'_0 such that $\bar{g}^2(L) = u$ is satisfied
- double the lattice and measure
 - $\Sigma(u, 1/6) = \bar{g}^2(2L)$

• . . .

.

$$\sigma(u) = \lim_{a/L \to 0} \Sigma(u, a/L)$$

• change *u* and repeat...

$\Sigma(2,u,1/4)$



g₀²

(gʻ)²

$\Sigma(2,u,1/6)$



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Step scaling function for $\nu = 0$

$$\Sigma(u, a/L) = \bar{g}^2(2L)|_{\bar{g}^2(L)=u}, \qquad \sigma(u) = \lim_{a/L \to 0} \Sigma(u, a/L)$$

- Simulate for a range of u-values ∈ [1, 2.012] on lattices with L/a = 4, 6, 8, 12.
- Double lattice size and measure $\Sigma(u, a/L) = \bar{g}^2(2L)$
- analyze $\Sigma(u, a/L)$ directly
- Alternatively, reduce cutoff effects perturbatively up to 2-loop order:

$$\delta(u, a/L) = \frac{\Sigma(u, a/L) - \sigma(u)}{\sigma(u)} = \delta_1(L/a)u + \delta_2(L/a)u^2 + O(u^3)$$

 $\delta_{1,2}(L/a)$ are known [Bode, Weisz & Wolff '99]

 \Rightarrow cutoff effects in

$$\Sigma'(u, a/L) = \frac{\Sigma(u, a/L)}{1 + \delta_1(L/a)u + \delta_2(L/a)u^2}$$

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start at order u^4 !

Continuum extrapolation of $\Sigma(u, a/L)$

Example for global fit ansatz:

$$\Sigma(u, a/L) = u + s_0 u^2 + s_1 u^3 + c_1 u^4 + c_2 u^5 + \rho_1 u^4 \frac{a^2}{L^2} + \rho_2 u^5 \frac{a^2}{L^2}$$

• s_0 , s_1 fixed to perturbative values: $s_0 = 2b_0 \ln 2$, $s_1 = s_0^2 + 2b_1 \ln 2$

• 4 parameters: c_1, c_2, ρ_1, ρ_2 ; 19 data points, $\chi^2/d.o.f. \approx 1$



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Main disadvantage of SF boundary conditions:

- cutoff effects linear in *a* generated by the boundaries.
- Counterterms are $tr(F_{0k}F_{0k})$ and $\overline{\psi}D_0\psi$, localized at the boundaries $x_0 = 0, L$
- can be cancelled by tuning the counterterm coefficients c_t and \tilde{c}_t .
- In PT: $c_{\rm t}$ known to 2-loops and $\tilde{c}_{\rm t}$ to one-loop order
- To avoid terms linear in a in the continuum extrapolations, we
 - measure the sensitivity at the larger couplings to a variation of c_t and \tilde{c}_t ;
 - interpolate with the perturbative behaviour \Rightarrow model for sensitivity
 - estimate the effect of imperfect tuning by shifting all data in either direction with Δc_{t} and $\Delta \tilde{c}_{\mathrm{t}}$ taken to be the last known order in PT.
 - carry out the continuum limit with $O(a^2)$ terms only and add the differences in the central values in quadrature to the error.
 - the error is subdominant in all cases.



• All results agree at $\alpha = 0.1$, we quote

$$L_0 \Lambda = 0.0303(8)$$
 error $< 3\%$!

- For $\nu=0.3$ this result could be inferred from larger values of $\alpha,$ but not for $\nu=-0.5!$
- As expected, all results have corrections $\propto \alpha^2;$ effective coefficients can vary dramatically
- ⇒ Some luck is required to pick a "good scheme", i.e. with small higher order corrections.

Continuum results $\bar{v} = \omega(u) = v_1 + u \times v_2 + \dots$



- Continuum extrapolation analogous to $\sigma(u)$, but much more data between L/a = 6 to L/a = 24 covering a factor 4 in resolution!
- consider 2 continuum parameterizations (v1, v2 are known from PT):

$$\begin{split} \omega(u) &= v_1 + v_2 u + d_1 u^2 + d_2 u^3 + d_3 u^4 \\ \omega(u) &= v_1 + d_1 u + d_2 u^2 + d_3 u^3 + d_4 u^4 \end{split}$$

- $L_0\Lambda$ calculation for $\nu \neq 0$ requires $\bar{v}(L_0) = \omega(2.012) = 0.1199(10)$ $(u = 2.012 \Leftrightarrow \alpha = 0.16)$
- Observe large deviation from perturbation theory at $\alpha = 0.19$:

$$\left(\omega(\bar{g}^2) - v_1 - v_2\bar{g}^2\right)/v_1 = -3.7(2)\alpha^2$$

• The coefficient is too large for PT to be trustworthy at these couplings!

Idea: First match the SF coupling to the $\overline{\rm MS}\xspace$ -scheme then evaluate the $\Lambda\xspace$ -parameter using up to 5-loop order PT available for this scheme.

• Relation between couplings, allowing for a scale factor s:

$$4\pi\alpha_{\overline{\mathrm{MS}}}(s/L) = \bar{g}_{\overline{\mathrm{MS}}}^2(L/s) = \bar{g}_{\nu}^2(L) + p_1^{\nu}(s)\bar{g}_{\nu}^4(L) + p_2^{\nu}(s)\bar{g}_{\nu}^6(L) + \mathcal{O}(\bar{g}^8)$$

 $\bullet\,$ Same as earlier, except now in the $\overline{\rm MS}$ scheme:

$$\Lambda_{\overline{\rm MS}} L_0 = \frac{sL_0}{L} \varphi_{\overline{\rm MS}} \left[\bar{g}_{\overline{\rm MS}}(L/s) \right] = s \, 2^n \varphi_{\overline{\rm MS}} \left[\sqrt{\bar{g}_{\nu}^2(L) + p_1^{\nu}(s) \bar{g}_{\nu}^4(L) + p_2^{\nu}(s) \bar{g}_{\nu}^6(L)} \right]$$

- expect to see independence of the number of steps n, scale factor s and parameter ν.
- Look at $\nu = 0$, dependence on n and s.
- <u>Note</u>: The neglected order for Λ :

$$\Delta g^2 \frac{d\varphi}{dg^2} \propto \Delta g^2 \left\{ g\beta(g) \right\}^{-1} = \Delta g^2 \times \mathcal{O}(g^{-4})$$

 $\Rightarrow \mbox{ truncation error: } {\rm O}(g^8) \times {\rm O}(g^{-4}) = {\rm O}(g^4) = {\rm O}(\alpha^2).$

Alternative test via the $\overline{\mathrm{MS}}\text{-scheme II}$

$$\alpha(sq) = \alpha_{\nu}(q) + c_{1}^{\nu}(s)\alpha_{\nu}^{2} + c_{2}^{\nu}(s)\alpha_{\nu}^{3}(q) + \dots, \qquad p_{i}^{\nu} = c_{i}^{\nu}/(4\pi)^{i}$$



- Choice of scale factor is important, coefficients can get large.
- "fastest apparent convergence" principle: $c_1(s^*)=0$ which means $s^*=\Lambda_{\overline{\rm MS}}/\Lambda\approx 2.612$ seems like a good idea.

Conclusions and outlook

- Perturbative calculations are subject to errors which are difficult to estimate
- Lattice QCD provides a testing ground for perturbation theory at high energies/small volumes
 - finite volume becomes essential part of observables
 - ⇒ infinite volume calculations are of limited use;
 - PT remains feasible with careful choice of b.c.'s.
 - finite volume protects against infrared/renormalon problems; for SF coupling find a secondary minimum with an action gap of $5\pi/(6\alpha) \approx 2.62/\alpha$
 - \Rightarrow negligible here, e.g. $\exp(-2.62/0.2 \approx 2 \times 10^{-6})$.
- Similar studies are possible with quark masses (cf. David Preti's talk)
- Gradient flow couplings:
 - requires perturbative calculations
 - ⇒ could be done using NSPT [Dalla Brida & Hesse '13, Dalla Brida & Luscher '17]
- BUT: Perturbation theory at low scales often can and should be avoided by using recursive finite size scaling techniques!

Thank you!