How Strong are the Strong Interactions?

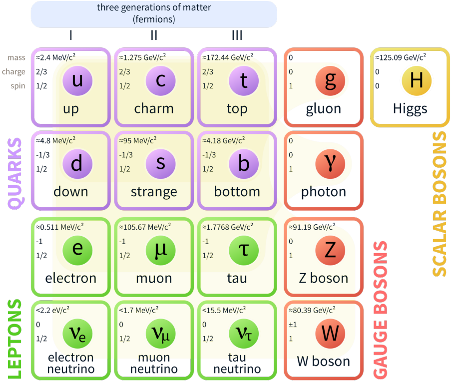
T. Korzec

ALPHA Collaboration

NIC Symposium 2018

The Standard Model

Building blocks of matter +
interactions among them:



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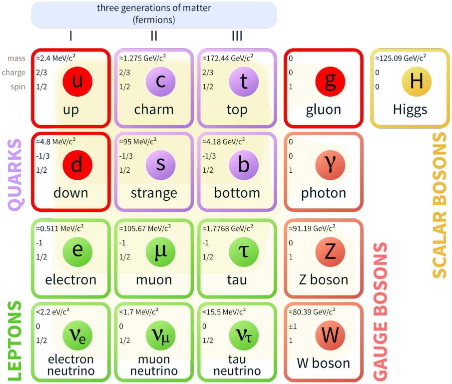

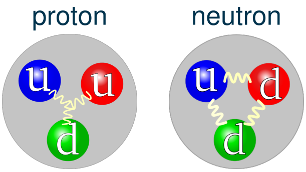

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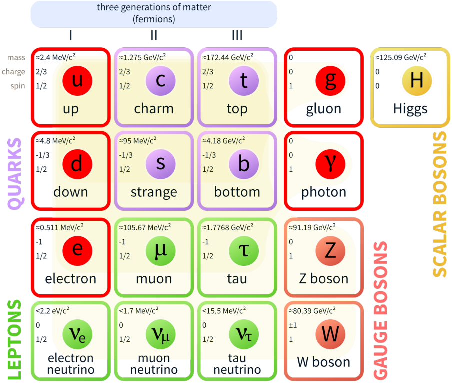
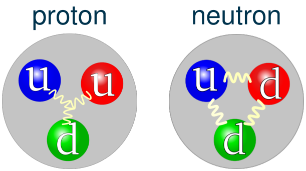
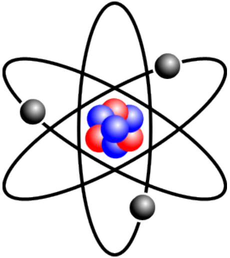




atoms



$$
\begin{aligned}
\mathcal{L}_{SM} = & -\tfrac{1}{2}\partial_\nu g^a_\mu \partial_\nu g^a_\mu - g_s f^{abc}\partial_\mu g^a_\nu g^b_\mu g^c_\nu - \tfrac{1}{4}g_s^2 f^{abc}f^{ade}g^b_\mu g^c_\nu g^d_\mu g^e_\nu - \partial_\nu W^+_\mu \partial_\nu W^-_\mu - \\
& M^2 W^+_\mu W^-_\mu - \tfrac{1}{2}\partial_\nu Z^0_\mu \partial_\nu Z^0_\mu - \tfrac{1}{2c_w^2}M^2 Z^0_\mu Z^0_\mu - \tfrac{1}{2}\partial_\mu A_\nu \partial_\mu A_\nu - igc_w(\partial_\nu Z^0_\mu(W^+_\mu W^-_\nu - \\
& W^+_\nu W^-_\mu) - Z^0_\nu(W^+_\mu \partial_\nu W^-_\mu - W^-_\mu \partial_\nu W^+_\mu) + Z^0_\mu(W^+_\nu \partial_\nu W^-_\mu - W^-_\nu \partial_\nu W^+_\mu)) - \\
& igs_w(\partial_\nu A_\mu(W^+_\mu W^-_\nu - W^+_\nu W^-_\mu) - A_\nu(W^+_\mu \partial_\nu W^-_\mu - W^-_\mu \partial_\nu W^+_\mu) + A_\mu(W^+_\nu \partial_\nu W^-_\mu - \\
& W^-_\nu \partial_\nu W^+_\mu)) - \tfrac{1}{2}g^2 W^+_\mu W^-_\mu W^+_\nu W^-_\nu + \tfrac{1}{2}g^2 W^+_\mu W^-_\nu W^+_\mu W^-_\nu + g^2 c_w^2(Z^0_\mu W^+_\mu Z^0_\nu W^-_\nu - \\
& Z^0_\mu Z^0_\mu W^+_\nu W^-_\nu) + g^2 s_w^2(A_\mu W^+_\mu A_\nu W^-_\nu - A_\mu A_\mu W^+_\nu W^-_\nu) + g^2 s_w c_w(A_\mu Z^0_\nu(W^+_\mu W^-_\nu - \\
& W^+_\nu W^-_\mu) - 2A_\mu Z^0_\mu W^+_\nu W^-_\nu) - \tfrac{1}{2}\partial_\mu H \partial_\mu H - 2M^2\alpha_h H^2 - \partial_\mu \phi^+ \partial_\mu \phi^- - \tfrac{1}{2}\partial_\mu \phi^0 \partial_\mu \phi^0 - \\
& \beta_h\left(\tfrac{2M^2}{g^2} + \tfrac{2M}{g}H + \tfrac{1}{2}(H^2 + \phi^0\phi^0 + 2\phi^+\phi^-)\right) + \tfrac{2M^4}{g^2}\alpha_h - \\
& g\alpha_h M\left(H^3 + H\phi^0\phi^0 + 2H\phi^+\phi^-\right) - \\
& \tfrac{1}{8}g^2\alpha_h\left(H^4 + (\phi^0)^4 + 4(\phi^+\phi^-)^2 + 4(\phi^0)^2\phi^+\phi^- + 4H^2\phi^+\phi^- + 2(\phi^0)^2H^2\right) - \\
& gMW^+_\mu W^-_\mu H - \tfrac{1}{2}g\tfrac{M}{c_w^2}Z^0_\mu Z^0_\mu H - \\
& \tfrac{1}{2}ig\left(W^+_\mu(\phi^0\partial_\mu\phi^- - \phi^-\partial_\mu\phi^0) - W^-_\mu(\phi^0\partial_\mu\phi^+ - \phi^+\partial_\mu\phi^0)\right) + \\
& \tfrac{1}{2}g\left(W^+_\mu(H\partial_\mu\phi^- - \phi^-\partial_\mu H) + W^-_\mu(H\partial_\mu\phi^+ - \phi^+\partial_\mu H)\right) + \tfrac{1}{2}g\tfrac{1}{c_w}(Z^0_\mu(H\partial_\mu\phi^0 - \phi^0\partial_\mu H) + \\
& M\left(\tfrac{1}{c_w}Z^0_\mu\partial_\mu\phi^0 + W^+_\mu\partial_\mu\phi^- + W^-_\mu\partial_\mu\phi^+\right) - ig\tfrac{s_w^2}{c_w}MZ^0_\mu(W^+_\mu\phi^- - W^-_\mu\phi^+) + igs_w MA_\mu(W^+_\mu\phi^- - \\
& W^-_\mu\phi^+) - ig\tfrac{1-2c_w^2}{2c_w}Z^0_\mu(\phi^+\partial_\mu\phi^- - \phi^-\partial_\mu\phi^+) + igs_w A_\mu(\phi^+\partial_\mu\phi^- - \phi^-\partial_\mu\phi^+) - \\
& \tfrac{1}{4}g^2 W^+_\mu W^-_\mu\left(H^2 + (\phi^0)^2 + 2\phi^+\phi^-\right) - \tfrac{1}{8}g^2\tfrac{1}{c_w^2}Z^0_\mu Z^0_\mu\left(H^2 + (\phi^0)^2 + 2(2s_w^2 - 1)^2\phi^+\phi^-\right) - \\
& \tfrac{1}{2}g^2\tfrac{s_w^2}{c_w}Z^0_\mu\phi^0(W^+_\mu\phi^- + W^-_\mu\phi^+) - \tfrac{1}{2}ig^2\tfrac{s_w^2}{c_w}Z^0_\mu H(W^+_\mu\phi^- - W^-_\mu\phi^+) + \tfrac{1}{2}g^2 s_w A_\mu\phi^0(W^+_\mu\phi^- + \\
& W^-_\mu\phi^+) + \tfrac{1}{2}ig^2 s_w A_\mu H(W^+_\mu\phi^- - W^-_\mu\phi^+) - g^2\tfrac{s_w}{c_w}(2c_w^2 - 1)Z^0_\mu A_\mu\phi^+\phi^- - \\
& g^2 s_w^2 A_\mu A_\mu\phi^+\phi^- + \tfrac{1}{2}ig_s\lambda^a_{ij}(\bar{q}^\sigma_i\gamma^\mu q^\sigma_j)g^a_\mu - \bar{e}^\lambda(\gamma\partial + m^\lambda_e)e^\lambda - \bar{\nu}^\lambda(\gamma\partial + m^\lambda_\nu)\nu^\lambda - \bar{u}^\lambda_j(\gamma\partial + \\
& m^\lambda_u)u^\lambda_j - \bar{d}^\lambda_j(\gamma\partial + m^\lambda_d)d^\lambda_j + igs_w A_\mu\left(-(\bar{e}^\lambda\gamma^\mu e^\lambda) + \tfrac{2}{3}(\bar{u}^\lambda_j\gamma^\mu u^\lambda_j) - \tfrac{1}{3}(\bar{d}^\lambda_j\gamma^\mu d^\lambda_j)\right) + \\
& \tfrac{ig}{4c_w}Z^0_\mu\{(\bar{\nu}^\lambda\gamma^\mu(1+\gamma^5)\nu^\lambda) + (\bar{e}^\lambda\gamma^\mu(4s_w^2 - 1 - \gamma^5)e^\lambda) + (\bar{d}^\lambda_j\gamma^\mu(\tfrac{4}{3}s_w^2 - 1 - \gamma^5)d^\lambda_j) + \\
& (\bar{u}^\lambda_j\gamma^\mu(1 - \tfrac{8}{3}s_w^2 + \gamma^5)u^\lambda_j)\} + \tfrac{ig}{2\sqrt{2}}W^+_\mu\left((\bar{\nu}^\lambda\gamma^\mu(1+\gamma^5)U^{lep}{}_{\lambda\kappa}e^\kappa) + (\bar{u}^\lambda_j\gamma^\mu(1+\gamma^5)C_{\lambda\kappa}d^\kappa_j)\right) + \\
& \tfrac{ig}{2\sqrt{2}}W^-_\mu\left((\bar{e}^\kappa U^{lep\dagger}{}_{\kappa\lambda}\gamma^\mu(1+\gamma^5)\nu^\lambda) + (\bar{d}^\kappa_j C^\dagger_{\kappa\lambda}\gamma^\mu(1+\gamma^5)u^\lambda_j)\right) + \\
& \tfrac{ig}{2M\sqrt{2}}\phi^+\left(-m^\kappa_e(\bar{\nu}^\lambda U^{lep}{}_{\lambda\kappa}(1-\gamma^5)e^\kappa) + m^\lambda_\nu(\bar{\nu}^\lambda U^{lep}{}_{\lambda\kappa}(1+\gamma^5)e^\kappa\right) + \\
& \tfrac{ig}{2M\sqrt{2}}\phi^-\left(m^\lambda_e(\bar{e}^\lambda U^{lep\dagger}{}_{\lambda\kappa}(1+\gamma^5)\nu^\kappa) - m^\kappa_\nu(\bar{e}^\lambda U^{lep\dagger}{}_{\lambda\kappa}(1-\gamma^5)\nu^\kappa\right) - \tfrac{g}{2}\tfrac{m^\lambda_\nu}{M}H(\bar{\nu}^\lambda\nu^\lambda) - \\
& \tfrac{g}{2}\tfrac{m^\lambda_e}{M}H(\bar{e}^\lambda e^\lambda) + \tfrac{ig}{2}\tfrac{m^\lambda_\nu}{M}\phi^0(\bar{\nu}^\lambda\gamma^5\nu^\lambda) - \tfrac{ig}{2}\tfrac{m^\lambda_e}{M}\phi^0(\bar{e}^\lambda\gamma^5 e^\lambda) - \tfrac{1}{4}\bar{\nu}_\lambda M^R_{\lambda\kappa}(1-\gamma_5)\hat{\nu}_\kappa - \\
& \tfrac{1}{4}\overline{\bar{\nu}_\lambda M^R_{\lambda\kappa}(1-\gamma_5)\hat{\nu}_\kappa} + \tfrac{ig}{2M\sqrt{2}}\phi^+\left(-m^\kappa_d(\bar{u}^\lambda_j C_{\lambda\kappa}(1-\gamma^5)d^\kappa_j) + m^\lambda_u(\bar{u}^\lambda_j C_{\lambda\kappa}(1+\gamma^5)d^\kappa_j\right) + \\
& \tfrac{ig}{2M\sqrt{2}}\phi^-\left(m^\lambda_d(\bar{d}^\lambda_j C^\dagger_{\lambda\kappa}(1+\gamma^5)u^\kappa_j) - m^\kappa_u(\bar{d}^\lambda_j C^\dagger_{\lambda\kappa}(1-\gamma^5)u^\kappa_j\right) - \tfrac{g}{2}\tfrac{m^\lambda_u}{M}H(\bar{u}^\lambda_j u^\lambda_j) - \\
& \tfrac{g}{2}\tfrac{m^\lambda_d}{M}H(\bar{d}^\lambda_j d^\lambda_j) + \tfrac{ig}{2}\tfrac{m^\lambda_u}{M}\phi^0(\bar{u}^\lambda_j\gamma^5 u^\lambda_j) - \tfrac{ig}{2}\tfrac{m^\lambda_d}{M}\phi^0(\bar{d}^\lambda_j\gamma^5 d^\lambda_j) + \bar{G}^a\partial^2 G^a + g_s f^{abc}\partial_\mu\bar{G}^a G^b g^c_\mu + \\
& \bar{X}^+(\partial^2 - M^2)X^+ + \bar{X}^-(\partial^2 - M^2)X^- + \bar{X}^0(\partial^2 - \tfrac{M^2}{c_w^2})X^0 + \bar{Y}\partial^2 Y + igc_w W^+_\mu(\partial_\mu\bar{X}^0 X^- - \\
& \partial_\mu\bar{X}^+ X^0) + igs_w W^+_\mu(\partial_\mu\bar{Y}X^- - \partial_\mu\bar{X}^+ Y) + igc_w W^-_\mu(\partial_\mu\bar{X}^- X^0 - \\
& \partial_\mu\bar{X}^0 X^+) + igs_w W^-_\mu(\partial_\mu\bar{X}^- Y - \partial_\mu\bar{Y}X^+) + igc_w Z^0_\mu(\partial_\mu\bar{X}^+ X^+ - \\
& \partial_\mu\bar{X}^- X^-) + igs_w A_\mu(\partial_\mu\bar{X}^+ X^+ - \\
& \partial_\mu\bar{X}^- X^-) - \tfrac{1}{2}gM\left(\bar{X}^+ X^+ H + \bar{X}^- X^- H + \tfrac{1}{c_w^2}\bar{X}^0 X^0 H\right) + \tfrac{1-2c_w^2}{2c_w}igM\left(\bar{X}^+ X^0\phi^+ - \bar{X}^- X^0\phi^-\right) + \\
& \tfrac{1}{2c_w}igM\left(\bar{X}^0 X^-\phi^+ - \bar{X}^0 X^+\phi^-\right) + igMs_w\left(\bar{X}^0 X^-\phi^+ - \bar{X}^0 X^+\phi^-\right) + \\
& \tfrac{1}{2}igM\left(\bar{X}^+ X^+\phi^0 - \bar{X}^- X^-\phi^0\right).
\end{aligned}
$$

The Standard Model

Achievements

- No major discrepancy with experiments observed so far, e.g.

$$a_e^{\mathrm{sm}} = 0.00115965218164\,3(76) \qquad \sim \text{electron's magnetic moment}$$
$$a_e^{\mathrm{exp}} = 0.00115965218073(28)$$

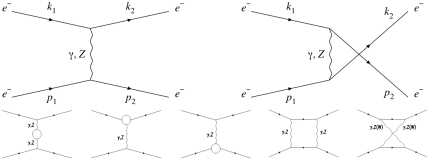
- All predictions have come true. Latest: existence of the Higgs boson
- Calculations are difficult, but possible: hundreds of processes

Open issues

- No gravity
- No explanation for dark matter
- Many parameters (18 or more)
- "Triviality"

Perturbation Theory

- Almost all results from Quantum Field Theories are obtained in an approximation: perturbation theory
- PT = expansion in a coupling g around $g = 0$
  $\to$ power-series $c_0 + c_1 g + c_2 g^2 + c_3 g^3 + \dots$
- The terms correspond to sums of "Feynmans diagrams"



- In QED, QCD, the standard model: the series is not convergent! (asymptotic expansion)

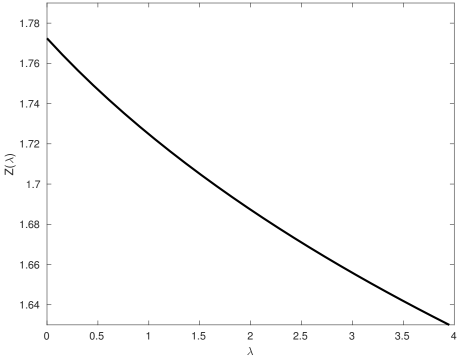
1-D toy example:

$$Z(\lambda) \quad = \quad \int_{-\infty}^{+\infty} dx\, e^{-x^2 - \frac{\lambda}{4!} x^4}$$

$$\overset{\lambda \to 0}{\sim} \quad c_0 + c_1\lambda + c_2\lambda^2 + c_3\lambda^3 + c_4\lambda^4 + \ldots$$

Coefficients c_i are calculable:

$c_0 = \sqrt{\pi}, \quad c_1 = -\sqrt{\pi}/32, \quad c_2 = \sqrt{\pi}\, 35/6144, \quad c_3 = -\sqrt{\pi}\, 385/196608, \ldots$



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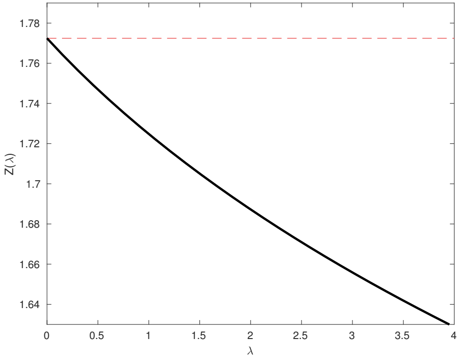

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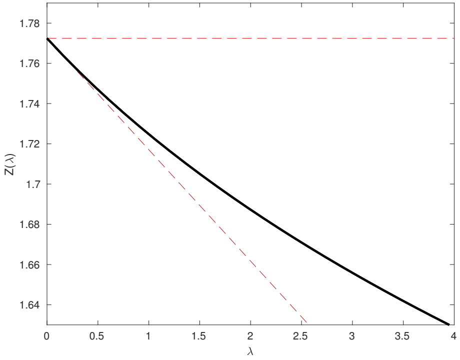

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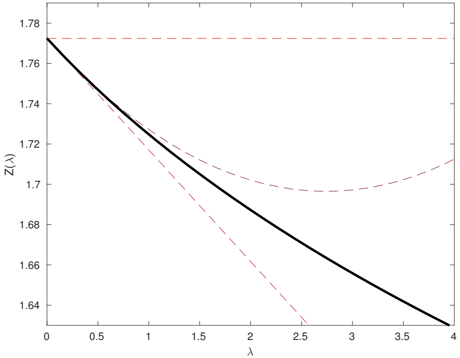

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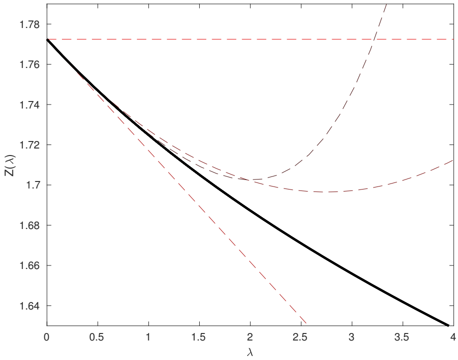

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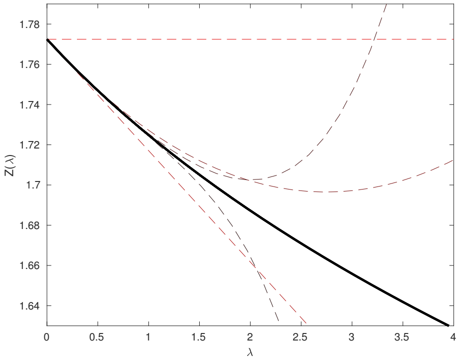


ED vs QED

Classical Electrodynamics (ED)

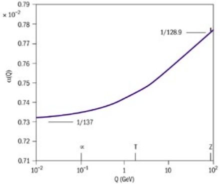
Coulomb's law (natural units, charges in multiples of e)

Force between two charges: $F(r) = \alpha \frac{Q_1 Q_2}{r^2}$

Fine structure constant $\alpha = \frac{e^2}{4\pi} \approx 1/137$

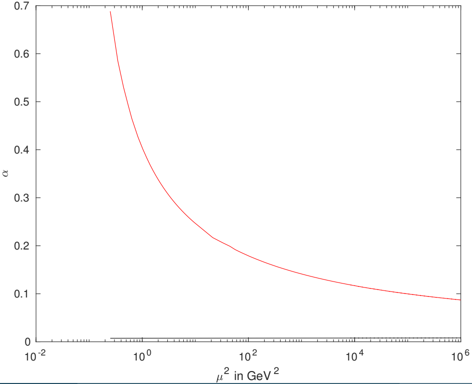
Quantum Electrodynamics (QED)

Coupling α depends on scheme and the energy-scale
E.g. $\alpha(q) \equiv r^2 F(r)/(Q_1 Q_2)$



- Strong interactions: Quantum-Chromodynamics (QCD)
- As in QED: energy dependent "running" coupling $\alpha_s \equiv \frac{\bar{g}_s^2}{4\pi}$
- Running is given by the renormalization-group β-function

$$\mu \frac{d\bar{g}_s}{d\mu} = \beta(\bar{g}_s) \overset{\bar{g}\to 0}{\sim} -\bar{g}_s^3 \left(b_0 + b_1 \bar{g}_s^2 + b_2 \bar{g}_s^4 + \ldots\right)$$



Determination of α_s

- Fix QCD parameters $\alpha_S(\mu), \overline{m}_u(\mu), \overline{m}_d(\mu), \ldots$ from experiments
  $\Rightarrow$ everything else is a prediction

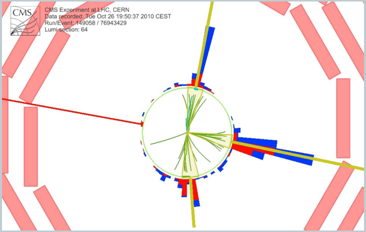
Example

differential inclusive jet production cross section

$$\frac{d\sigma}{dp_T} \overset{\text{NLO}}{=} \alpha_S^2(\mu)\,\hat{X}^{(0)}(\mu_F, p_T) \times [1 + \alpha_S(\mu) K1(\mu, \mu_F, p_T)]$$

- Measure $\frac{d\sigma}{dp_T}$ at LHC for transverse jet momenta $p_T = 74 - 2500$ GeV
- Best fit $\rightarrow \alpha_S(\mu)$
  with $\mu \approx p_T$
- E.g. $p_T = 1410 - 2500$ GeV
  $\rightarrow \alpha_S(1508.04\text{ GeV}) = 0.0822^{+0.0034}_{-0.0031}$

[V. Khachatryan et al. (CMS), JHEP 03, 156 (2017)]



[CMS, CERN]

Determination of α_s

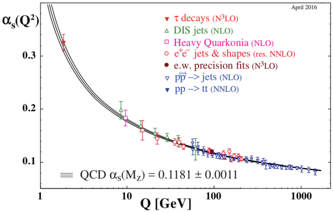
[Particle Data Group, Chin. Phys. C, 40, 100001 (2016)]

- Various experiments
  $\leftrightarrow$ various high Q
- Use $\beta^{\text{5-loop}}$

  [P.Baikov, K.Chetyrkin, J.Kühn, PRL 118 (2017)]

  [F.Herzog, B.Ruijl, T.Ueda, J.Vermaseren, JHEP 02 (2017)]

  $\alpha_{\overline{\text{MS}}}(Q) \to \alpha_{\overline{\text{MS}}}(M_Z)$
- Experiment at $Q \approx 100$ MeV
  Needs $\beta^{\text{non-perturbative}}$
  $\to$ not with $\overline{\text{MS}}$
- We use:
  finite volume schemes
- Use PT to relate our α to $\alpha_{\overline{\text{MS}}}$
  at high energies



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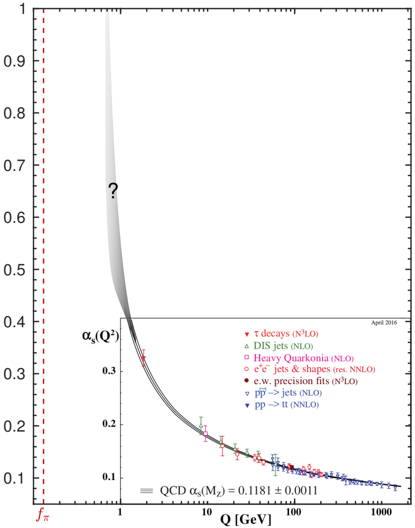

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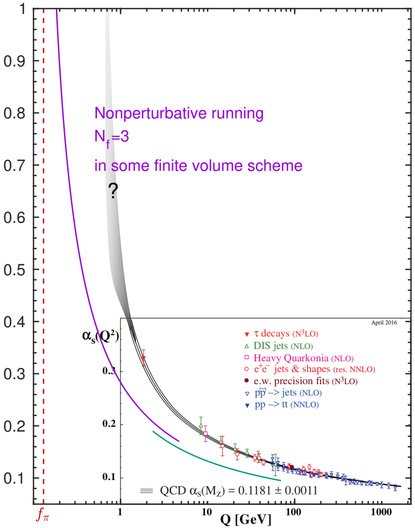

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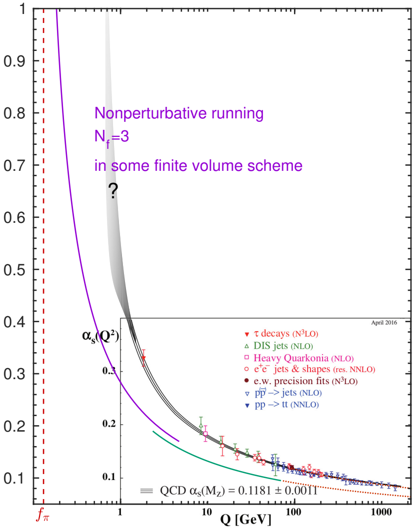
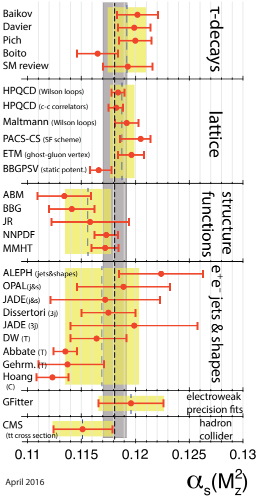
  $\to$ not with $\overline{\text{MS}}$
- We use:
  finite volume schemes
- Use PT to relate our α to $\alpha_{\overline{\text{MS}}}$ at high energies

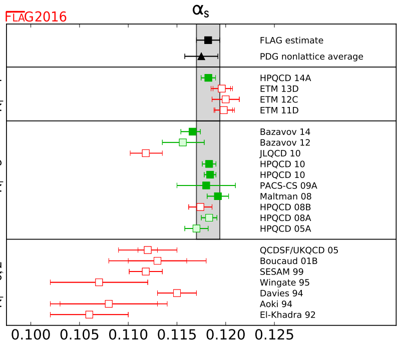
[Particle Data Group, Chin. Phys. C, 40, 100001 (2016)]



The QCD Coupling Constant: $\alpha_{\overline{\mathrm{MS}}}^{N_f=5}(M_Z)$



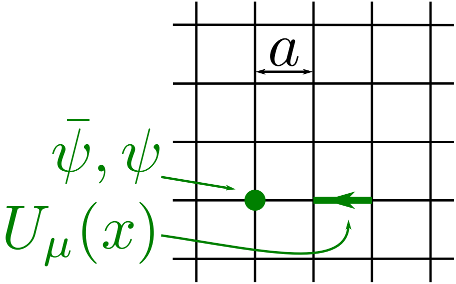
[Particle Data Group, Chin. Phys. C, 40, 100001 (2016)]



[FLAG Working Group, Phys. J. C (2017)]

Lattice QCD

- Discretize hypercubic piece of space-time of size $T \times L^3$. Lattice spacing: a
- Put matter fields $\psi(x), \bar{\psi}(x)$ on the sites
- Put gauge fields, i.e. SU(3) matrices, $U_\mu(x)$ on the links
- Integrate-out the matter fields



remaining task: compute the following integral:

$$\langle \mathcal{O} \rangle = \int DU \underbrace{\frac{1}{Z} e^{-S_g[U]} \det[D_u] \det[D_d] \det[D_s] \det[D_c] \det[D_b] \det[D_t]}_{\equiv p[U]} \mathcal{O}[U]$$

- $\int DU$: high dimensional integral, 8 dimensions for each link of the lattice
  e.g. $192 \times 64 \times 64 \times 64$ lattice $\Rightarrow$ 1.6×10^9 dimensional integral
- $S_g[U]$: gauge action
  e.g. plaquette-action $\square$
- D_x: Dirac operator for flavor x. Very large sparse matrix, depends on U
  e.g. $192 \times 64 \times 64 \times 64$ lattice $\Rightarrow$ $603,979,776 \times 603,979,776$ matrix
- Z: normalization, so $\langle 1 \rangle = 1$
- $\mathcal{O}[U]$: "observable", usually contains D_x^{-1}

Systematic Errors

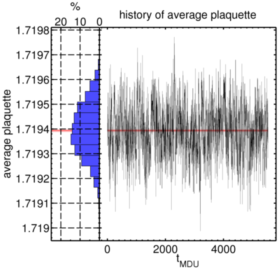
- Finite lattice spacing $\Rightarrow$ continuum extrapolation $a \to 0$
- Finite size effects $\Rightarrow$ infinite volume extrapolations $L \to \infty$
- (partial) quenching, e.g. $\det[D_c]\det[D_b]\det[D_t] \approx$ constant
- Unphysical masses, e.g. $m_u = m_d > m_u^{\mathrm{phys}}$ $\Rightarrow$ chiral extrapolation

Importance Sampling Monte Carlo

$$\langle \mathcal{O} \rangle = \int DU\, p[U]\, \mathcal{O}[U]$$

- Generate a sequence of random gauge configurations distributed according to $p[U]$
  $U_1, U_2, \ldots, U_N$
- Then

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}[U_i] \qquad + \qquad O(1/\sqrt{N})$$



Algorithms: HMC

$D^\dagger D$: positive definite, sparse $M \times M$ matrix,
$M = 12 \cdot$ number-of-sites, e.g. $M = 603,979,776$

$$
\begin{aligned}
\langle \mathcal{O} \rangle &= \int DU \, \frac{1}{Z} e^{-S_g[U]} \det[D]^2 \, \mathcal{O}[U] \\
&= \int DU \, \frac{1}{Z'} e^{-S_g[U]} \int d^M\phi \, e^{-\phi^\dagger [D^\dagger D]^{-1} \phi} \, \mathcal{O}[U] \\
&= \int DU \, \frac{1}{Z''} e^{-S_g[U]} \int d^M\phi \, e^{-\phi^\dagger [D^\dagger D]^{-1} \phi} \int D\Pi \, e^{-(\Pi,\Pi)} \, \mathcal{O}[U] \\
&\equiv \int_{\text{fields}} \frac{1}{Z''} e^{-H[U,\Pi,\phi]} \, \mathcal{O}[U]
\end{aligned}
$$

- Global heatbath: generate random momenta Π, generate random pseudo-fermions ϕ
- Molecular Dynamics: solve Hamilton's equations of motion
  $(U, \Pi) \xrightarrow{t_{\text{MDU}} \to t_{\text{MDU}} + \tau} (U', \Pi')$
  $H = H'$! But numerical solution (e.g. leap-frog): $H' - H = \Delta H$
- Correction: accept reject step, $p_{\text{acc}} = \min[1, e^{-\Delta H}]$

Algorithms: Mass preconditioning

Useful factorization

[M. Hasenbusch Phys.Lett. B519 (2001)]

$$\det[D^2] = \det[D^\dagger D + \mu_0^2] \times \frac{\det[D^\dagger D + \mu_1^2]}{\det[D^\dagger D + \mu_0^2]} \times \ldots \times \frac{\det[D^\dagger D]}{\det[D^\dagger D + \mu_{N_H}^2]} \, .$$

- $\mu_0 > \mu_1 > \ldots > \mu_{N_H}$ algorithmic parameters
- Separate pseudo-fermions (ϕ-fields) for every factor
- Smoother MD-forces $\Rightarrow$ allow coarser discretization of t_{MDU}
- Multi-level integration:
  - Cheap and large forces: fine integration
  - Expensive and small forces: coarse integration

Algorithms: RHMC

Non-degenerate quarks only possible if D is a positive matrix

$$\det[D] = \det[\sqrt{D^\dagger D}] = W \det[R^{-1}]$$

- R: rational approximation to $[D^\dagger D]^{-1/2}$

$$\frac{1}{\sqrt{x}} \approx a_0 \frac{(x+a_1)(x+a_3)\cdots(x+a_{2n-1})}{(x+a_2)(x+a_4)\cdots(x+a_{2n})}$$

- Optimal a_i: minimize maximal deviation between R and $\frac{1}{\sqrt{x}}$ in an interval
- Split R into factors e.g.
  $\det[R^{-1}] \propto \det[P^{-1}_{1,6}]\det[P^{-1}_{7,9}]\det[P^{-1}_{10,10}]$
  with $P_{k,l}(x) = \prod_{j=k}^{l} \frac{x+a_{2j-1}}{x+a_{2j}}$
- Separate pseudo-fermions for separate P-factors.
  (partial fraction decomposition of $P \rightarrow$ actions as for HMC)
- Correction $W = \det[DR]$: reweighting-factor

$$\begin{aligned}\langle \mathcal{O} \rangle &= \int DU\, p[U]\, \mathcal{O}[U] \\ &= \int DU\, p'[U]\, \mathcal{O}[U] \frac{p[U]}{p'[U]} \\ &= \frac{\langle W\mathcal{O} \rangle'}{\langle W \rangle'}\end{aligned}$$

with
$W[U] \propto p[U]/p'[U]$

- Computing W allows to correct, if a slightly “wrong” PDF was used

Algorithms: Solvers

Most expensive part of the simulation (and also in $\mathcal{O}[U]$): “inversions”

$$Dx = b, \qquad b \text{ given, find } x$$

- Krylov space methods
  - Find best solution in subspace spanned by $\{\eta, D\eta, D^2\eta, \ldots\}$
  - Successively enlarge the subspace
  - convergence rate $\leftrightarrow$ condition number of D
- Preconditioning
  - even-odd preconditioning
  - SAP preconditioning
  - low mode deflation
- Efficient implementation
  - mixed precision
  - hand-coded asm

openQCD

[M.Lüscher, S.Schaefer, Comput.Phys.Commun. 184 (2013)]

CLS Data Set: the Ensembles

- Generation of "large volume" ensembles is very expensive
  $\Rightarrow$ Form a "consortium" of groups. Share the load
- Later: each subgroup can focus on different "observables"
- >cls Coordinated Lattice Simulations

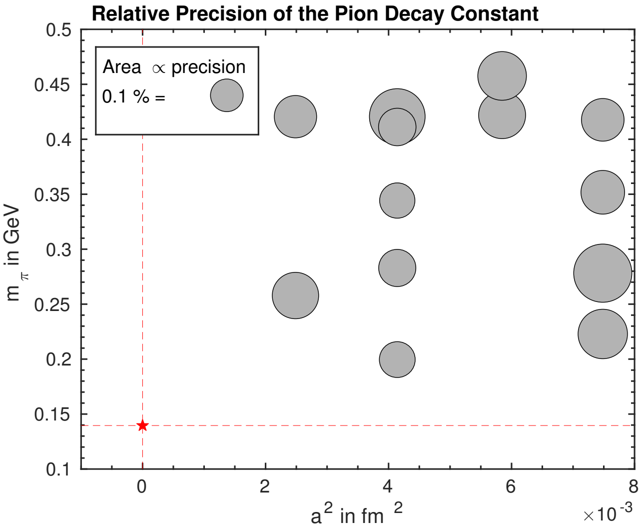
  Berlin, Dublin, Geneva, Madrid, Mainz, Milan, Münster, Odense, Regensburg, Rome, Valencia, Wuppertal, Zeuthen (NIC!)

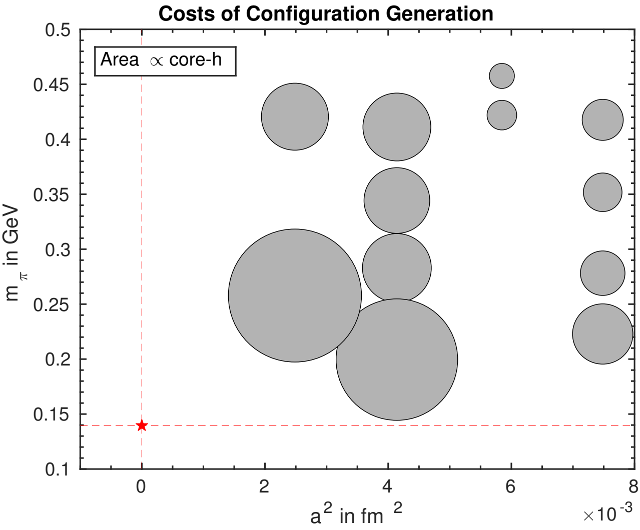
Dataset that entered our coupling determination:

[M.Bruno et al., JHEP 1502 (2015)]+newer runs

- Actions
  - Lüscher-Weisz gauge action  , 
  - 2+1 flavors of improved Wilson fermions
    non-perturbative c_{sw} [J.Bulava, S.Schaefer, Nucl.Phys. B874 (2013)]
  - Open boundary conditions in time
- Chiral trajectory with $m_u + m_d + m_s = \mathrm{const}$
- Many lattice spacings (also quite fine ones)
- Various pion masses, down to $\sim$ 200MeV

Costs and Precision




Costs of Configuration Generation
Area ∝ core-h
0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
m_π in GeV
0
2
4
6
8
a² in fm²
×10⁻³

Scale Setting

Simulation parameters: bare masses $m_{u,d}, m_s$ and bare coupling g_0
Lattice spacing a is not an input parameter!
$\Rightarrow$ needs to be "measured"
The experimental input is

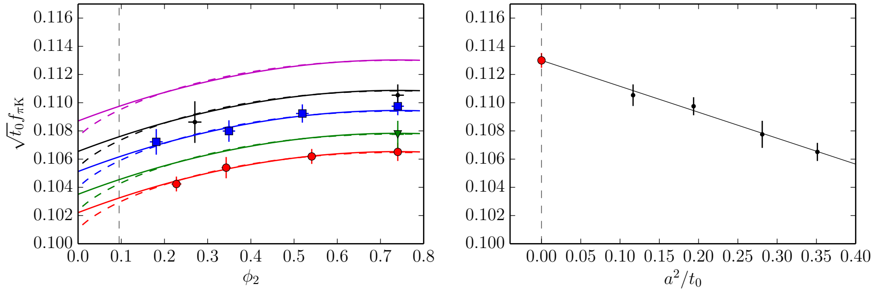
- $m_\pi = 134.8(3)$ MeV, $m_K = 494.2(3)$ MeV
  [FLAG Working Group, Phys. J. C (2017)]
- $f_{\pi K} \equiv \frac{2}{3} f_K + \frac{1}{3} f_\pi = 147.6(5)$ MeV
  [Particle Data Group, Chin.Phys. C38 (2014)]
  has a weaker quark mass dependence than f_π or f_K
  (along our chiral trajectory)
  [W. Bietenholz et al., Phys.Lett. B690 (2010)]

Scale setting

- Adjust bare masses such that $m_\pi / f_{\pi K}$ and $m_K / f_{\pi K}$ are correct
- Compute $af_{\pi K}$, divide by experimental $f_{\pi K}$
  $\rightarrow a$ in fm

In practice: no simulation at the physical mass point $\rightarrow$ extrapolation
Use intermediate scale t_0. $\phi_2 = 8t_0 m_\pi^2$

1. Determine $\sqrt{t_0} f_{\pi K}$ at the physical mass-point in the continuum
   $\Rightarrow \sqrt{8t_0^{\mathrm{phys}}} = 0.415(4)(2)$ fm
2. Measure for all lattice-spacings $t_0/a^2 \Rightarrow$ determine a in fm



“Single-Lattice” Approach

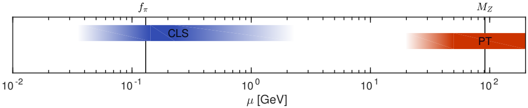
Now that a is known, we could

- Measure the force between two static quarks $a^2 F(r)$ for $r = a, 2a, 3a, \ldots$
- Continuum-extrapolate the dimensionless combination $r^2 F(r)$ (needs interpolations in r)
- Define a strong coupling $\alpha_{qq}(\mu) = \frac{3}{4} r^2 F(r), \qquad \mu = 1/r$
- Study μ dependence. At high μ: relate perturbatively to $\alpha_{\overline{\mathrm{MS}}}$

Problem

- Need $r \gg a$ otherwise: big lattice artifacts
- Need $L \gg m_\pi^{-1}$ otherwise: big finite-size effects
- Need $\mu = r^{-1}$ large (e.g. $\approx$ 100 GeV), otherwise α_{qq} too large for PT

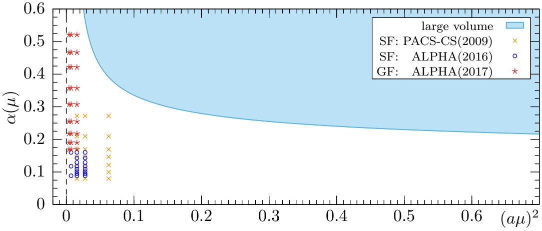
$\Rightarrow$ Needs enormously large L/a



- A “single lattice” approach is impossible without compromises

$$L \gg \frac{1}{m_\pi} \quad \text{and} \quad a \ll \frac{1}{\mu} \qquad \Rightarrow \frac{L}{a} \approx O(1000)$$

- Solution: finite-size scaling, $\mu \equiv 1/L \qquad \Rightarrow \frac{L}{a} \approx O(10)$
  But: requires separate sets of simulations for each value of μ



Choosing a Good Finite Volume Scheme

We need

- Non-perturbative definition
- Accessible with Monte-Carlo methods
  often: massless=impossible
- Good statistical precision from low to high energies
- Mild lattice artifacts
- Available perturbation theory
  - Normalization
  - Relation to $\overline{\text{MS}}$-scheme
  - For precision also: $\beta^{\text{3-loop}}$

Finite Volume Couplings

Schrödinger Functional $=$ Dirichlet boundaries in one direction
$\Rightarrow$ massless simulations possible (even with odd N_f)

SF-coupling

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

- $\bar{g}_{\mathrm{SF}}$: response of system to a change of boundaries
- Excellent theoretical understanding, $\beta^{\text{3-loop}}$ known
- Good statistical precision at high energies

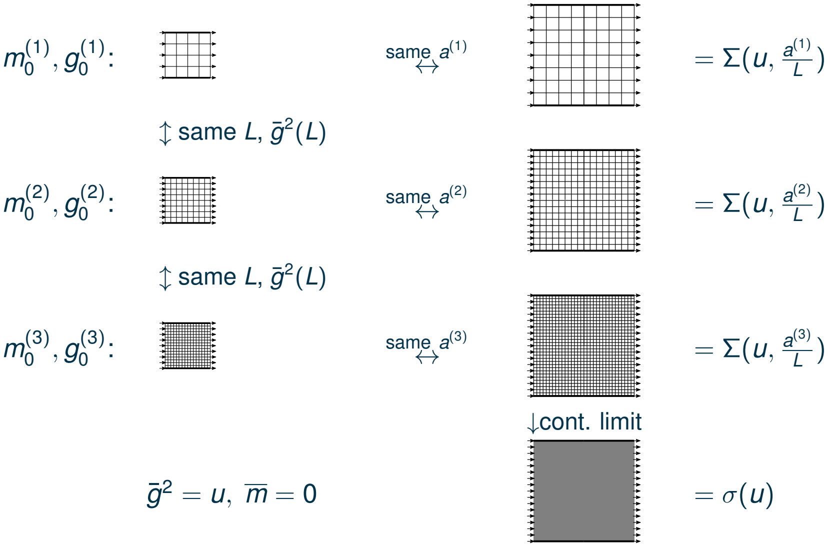
GF-coupling

[P.Fritzsch, A.Ramos, JHEP 1310 (2013)]

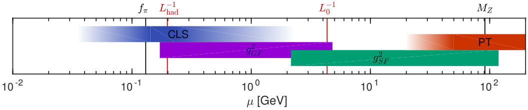
- $\bar{g}_{\mathrm{GF}}$: action density at “finite flow time”
- Very good statistical precision also at low energies

Computing Step Scaling Functions

Instead of $\beta(\bar{g})$, compute: $\sigma(u) = \bar{g}^2(\mu/2)|_{u=\bar{g}^2(\mu)}$



Overall Strategy



- Define two scales: $L_{\rm had}$ and L_0 implicitly via

$$\bar{g}^2_{\rm GF}(L_{\rm had}) \equiv 11.31\,, \qquad \bar{g}^2_{\rm SF}(L_0) \equiv 2.012$$

- Compute step scaling functions
  - GF coupling: $\sigma_{\rm GF}(u)$ in the range $u \in [\bar{g}^2_{\rm GF}(2L_0), \bar{g}^2_{\rm GF}(L_{\rm had})]$
    LW-action, SF boundaries, no background field
  - SF coupling: $\sigma_{\rm SF}(u)$ in the range $u \in [\bar{g}^2_{\rm SF}(L_{\rm PT}), \bar{g}^2_{\rm SF}(L_0)]$
    plaquette action, SF boundaries, background field: $\eta = \nu = 0$
- Nonperturbative scheme matching at L_0: compute $\bar{g}^2_{\rm GF}(2L_0)$
- Large volume simulations (CLS): obtain $1/\sqrt{t_0}$ in GeV

  LW-action, open boundaries in time
- Relate the scales $L_{\rm had}$ and $\sqrt{t_0}$

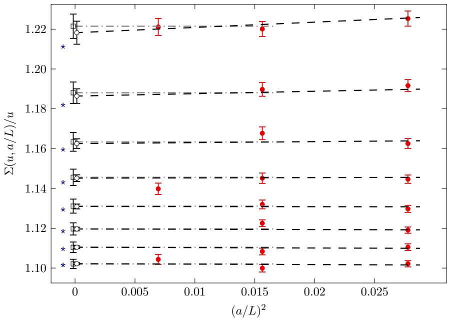
$$\bar{g}_{\rm GF}\Big(\underbrace{\frac{f_{\pi K}\sqrt{t_0}}{f_{\pi K}^{\rm PDG}}}_{\text{scale setting}} \times \underbrace{\frac{L_{\rm had}}{\sqrt{t_0}}}_{\text{con. to CLS}}\Big) \overset{\sigma_{\rm GF}}{\longleftrightarrow} \bar{g}_{\rm GF}(2L_0) \overset{\text{matching}}{\longleftrightarrow} \bar{g}_{\rm SF}(L_0) \overset{\sigma_{\rm SF}}{\longleftrightarrow} \bar{g}_{\rm SF}(L_{\rm PT}) \overset{\rm PT}{\longleftrightarrow} \alpha^{(5)}_{\overline{\rm MS}}$$

Step Scaling Functions

$$\bar{g}_{\rm GF}\Big(\underbrace{\frac{f_{\pi K}\sqrt{t_0}}{f_{\pi K}^{\rm PDG}}}_{\text{scale setting}} \times \underbrace{\frac{L_{\rm had}}{\sqrt{t_0}}}_{\text{con. to CLS}}\Big) \overset{\sigma_{\rm GF}}{\longleftrightarrow} \bar{g}_{\rm GF}(2L_0) \overset{\text{matching}}{\longleftrightarrow} \bar{g}_{\rm SF}(L_0) \overset{\sigma_{\rm SF}}{\longleftrightarrow} \bar{g}_{\rm SF}(L_{\rm PT}) \overset{\rm PT}{\longleftrightarrow} \alpha^{(5)}_{\overline{\rm MS}}$$

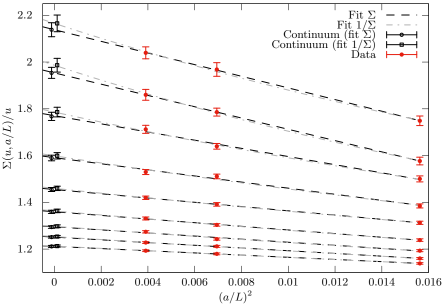
SF-coupling

[M. Dalla Brida, P. Fritzsch, T. K., A. Ramos, S. Sint, R. Sommer, PRL 117 (2016)]



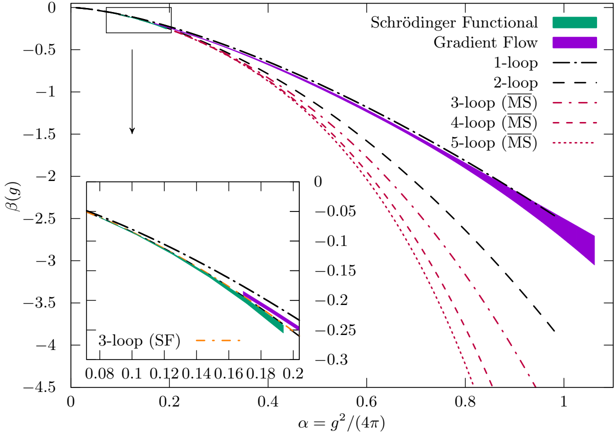
GF-coupling

[M. Dalla Brida, P. Fritzsch, T. K., A. Ramos, S. Sint, R. Sommer, PRD 95 (2017)]



Relation $\sigma \leftrightarrow \beta$:

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

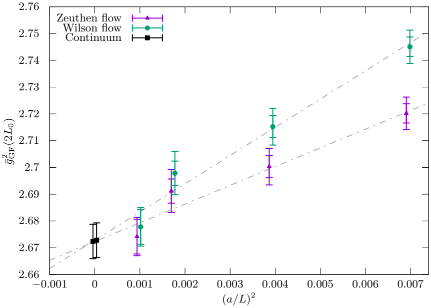


Matching GF and SF Schemes

$$\bar{g}_{\mathrm{GF}}\Big(\underbrace{\frac{f_{\pi K}\sqrt{t_0}}{f_{\pi K}^{\mathrm{PDG}}}}_{\text{scale setting}} \times \underbrace{\frac{L_{\mathrm{had}}}{\sqrt{t_0}}}_{\text{con. to CLS}}\Big) \overset{\sigma_{\mathrm{GF}}}{\longleftrightarrow} \bar{g}_{\mathrm{GF}}(2L_0) \overset{\text{matching}}{\longleftrightarrow} \bar{g}_{\mathrm{SF}}(L_0) \overset{\sigma_{\mathrm{SF}}}{\longleftrightarrow} \bar{g}_{\mathrm{SF}}(L_{\mathrm{PT}}) \overset{\mathrm{PT}}{\longleftrightarrow} \alpha^{(5)}_{\overline{\mathrm{MS}}}$$

[M. Dalla Brida, P. Fritzsch, T. K., A. Ramos, S. Sint, R. Sommer, PRD 95 (2017)]

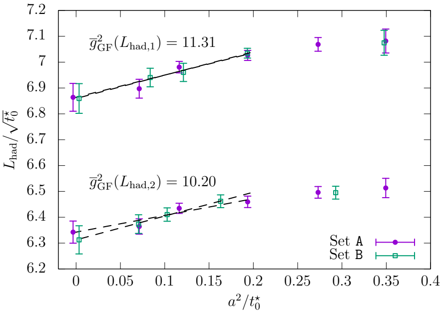
- $\bar{g}^2_{\mathrm{SF}}(L_0) = 2.012$
- compute: $\bar{g}^2_{\mathrm{GF}}(2L_0)$
  - $\Phi(u, a/L) = \bar{g}^2_{\mathrm{GF}}(2L)\Big|_{\bar{g}^2_{\mathrm{SF}}(L)=u}$
  - $\phi(u) = \lim_{a\to 0} \Phi(u, a/L)$



$$\bar{g}^2_{\mathrm{GF}}(2L_0) \overset{\text{matching}}{=} 2.6723(64), \qquad \frac{L_{\mathrm{had}}}{L_0} \overset{\text{GF running}}{=} 21.86(42)$$

Connecting SF to Large Volume

$$\underbrace{\bar{g}_{\rm GF}\Big(\frac{f_{\pi K}\sqrt{t_0}}{f_{\pi K}^{\rm PDG}}}_{\text{scale setting}} \times \underbrace{\frac{L_{\rm had}}{\sqrt{t_0}}}_{\text{con. to CLS}}\Big) \overset{\sigma_{\rm GF}}{\longleftrightarrow} \bar{g}_{\rm GF}(2L_0) \overset{\text{matching}}{\longleftrightarrow} \bar{g}_{\rm SF}(L_0) \overset{\sigma_{\rm SF}}{\longleftrightarrow} \bar{g}_{\rm SF}(L_{\rm PT}) \overset{\rm PT}{\longleftrightarrow} \alpha^{(5)}_{\overline{\rm MS}}$$



$$\frac{L_{\rm had}}{\sqrt{t_0}} = 6.825(47)$$

Perturbative Decoupling

Decoupling:

$$\bar{g}^{N_\mathrm{f}}(\mu) = \bar{g}^{N_\mathrm{f}+1}(\mu) \times \xi\left(g^{N_\mathrm{f}}(\mu), \overline{m}_h/\mu\right) \quad + \quad O(\overline{m}_h^{-2})$$

- $O(\overline{m}_h^{-2})$ are very small already for $\overline{m}_h = \overline{m}_c$

  [M. Bruno, J. Finkenrath, F. Knechtli, B. Leder, R. Sommer, Phys.Rev.Lett. 114 (2015)]

  [F. Knechtli, T.K., B. Leder, G. Moir, arXiv:1706.04982 (2017)]

- ξ known in perturbation theory to 4 loops

  [K. Chetyrkin, J. Kühn, C. Sturm, Nucl. Phys. B744 (2006)]

  [Y. Schröder, M. Steinhauser, JHEP 01, 051 (2006)]

- Perturbation theory looks surprisingly well-behaved already at $\mu = \overline{m}_c$

n (loops)	$\alpha_{\overline{\mathrm{MS}}}^{(N_\mathrm{f}=5)}$	$\alpha_n - \alpha_{n-1}$
1	0.11699	
2	0.11827	0.00128
3	0.11846	0.00019
4	0.11852	0.00006

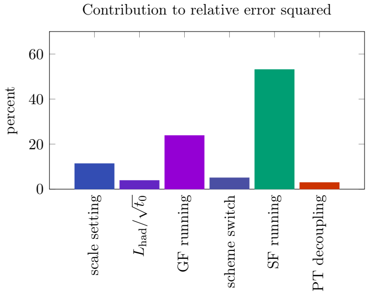
conservative error (within PT):
$\alpha_4 - \alpha_2 \approx 0.0003$

Everything Together

Final Result

$$\alpha_{\overline{\text{MS}}}(M_Z) = 0.1185(8)(3)$$

0.1174(16) PDG non-lattice



Everything Together

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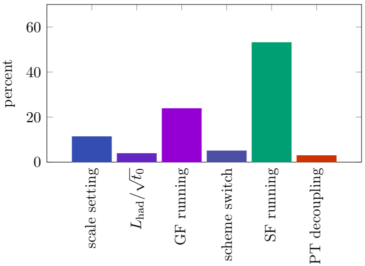
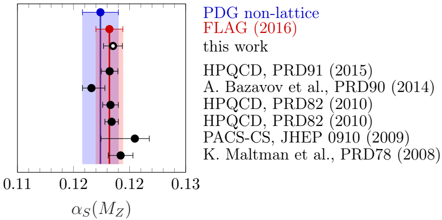
0.1174(16) PDG non-lattice

Contribution to relative error squared





Conclusions and Outlook

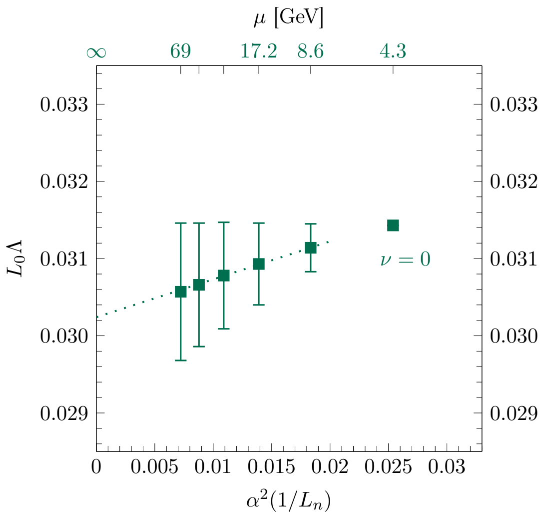
Conclusions

- For the first time: sub-percent error in α_S with fully controlled systematic errors.
- Connection to perturbation theory is a delicate issue
  works at $\alpha \approx 0.1$ but not always safe at $\alpha \approx 0.2$
- With increased precision goals, systematic errors become more and more difficult to control
- Switching to a gradient-flow scheme pays off: the usually expensive low-energy running contributes a small error

Outlook

- Long-term: $\alpha_s^{(3)} \to \alpha_s^{(4)}$ non-perturbatively

- $L_n = 2^{-n} L_0, \qquad \alpha = \bar{g}_\nu^2/(4\pi)$
- Use 3-loop PT at $\alpha(1/L_n) \Rightarrow$ Residual error $O(\alpha^2)$



Warning 1: Accuracy of Perturbation Theory

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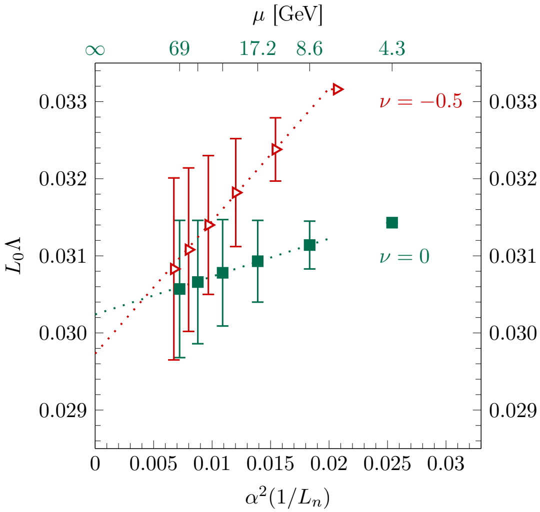

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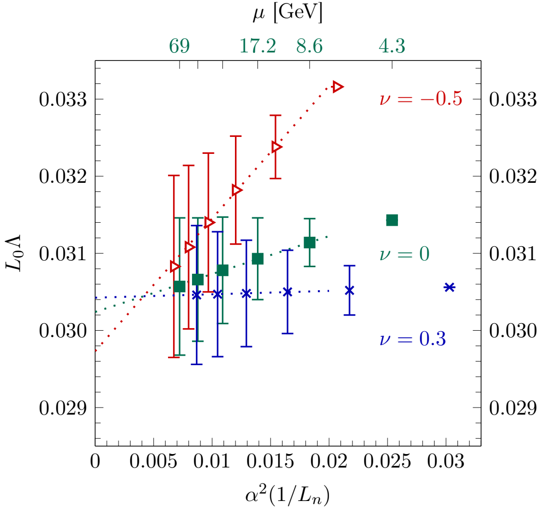
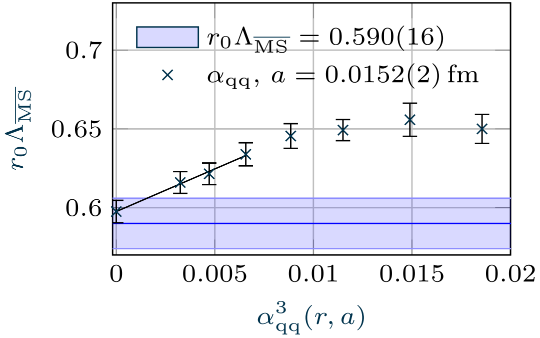


- Similarly: α_{qq} = coupling from the static force
- at $\alpha_{qq} < 0.22$: $\frac{\Lambda^{\text{4-loop}}_{\overline{MS}} - \Lambda_{\overline{MS}}}{\Lambda_{\overline{MS}}} = 7.0(5)\alpha^3_{qq}$



[N.Husung, M.Koren, P.Krah, R.Sommer, arXiv:1711.01860]

Warning 2: Scale Setting

- There is some tension in the value of $\sqrt{t_0}$
- Could become relevant in future, more precise Λ determinations