Computing $\alpha_{\rm s}$ and light quark masses on the lattice

Francesco Knechtli
Bergische Universität Wuppertal

Quark Masses and the Strong Coupling Constant, Aachen, February 21, 2007

Outline

- Introduction
- Non-perturbative renormalization
- The running strong coupling $\alpha_{\rm s}$
- The running quark masses: light quarks
- Conclusions and Outlook

Introduction

$$\overbrace{\begin{bmatrix} F_\pi \\ m_\pi \\ m_\mathrm{K} \\ m_\mathrm{D} \\ m_\mathrm{B} \end{bmatrix}}^{\text{Experiment}} \quad \begin{matrix} \mathcal{L}_\mathrm{QCD}(g_0, m_q) \\ \Longleftrightarrow \end{matrix} \quad \overbrace{\begin{bmatrix} \Lambda_\mathrm{QCD} \\ \hat{M} = (M_\mathrm{u} + M_\mathrm{d})/2 \\ M_\mathrm{s} \\ M_\mathrm{c} \\ M_\mathrm{b} \end{bmatrix}}^{\text{QCD parameters (RGI)}} + \overbrace{\begin{bmatrix} m_\mathrm{Nucleon} \\ B_\mathrm{K} \\ F_{\mathrm{D_s}} \\ \xi \\ \ldots \end{bmatrix}}^{\text{Predictions}}$$

- QCD coupling and quark masses can be determined only indirectly, through comparison between theory and experiment
- Theory computations are based on
  - *perturbation theory* at high energy $\gtrsim 2 - 10\,\mathrm{GeV}$, where the renormalization group invariant (RGI) parameters Λ_QCD, M_q are defined
  - *lattice theory and simulations* to obtain hadronic properties and their connection to high energy, e.g. $F_\pi/\Lambda_\mathrm{QCD}$, $M_\mathrm{s}/F_\mathrm{K}$, . . .
  - *QCD sum rules*

Introduction

Any theoretical prediction in terms of the QCD coupling and quark masses must make reference to the renormalization scheme and renormalization scale μ used

Running of renormalized parameters is described by renormalization group equations (RGE)

$$\mu \frac{\mathrm{d}\bar{g}}{\mathrm{d}\mu} = \beta(\bar{g}) \,, \qquad \mu \frac{\mathrm{d}\overline{m}_q}{\mathrm{d}\mu} = \tau(\bar{g})\overline{m}_q \,, \quad q = 1, \ldots, N_{\mathrm{f}}$$

Perturbative expansions, but in general non–perturbatively defined!

$$\beta(\bar{g}) \underset{\bar{g}\to 0}{\sim} -\bar{g}^3\{b_0 + b_1\bar{g}^2 + b_2\bar{g}^4 + \ldots\} \,, \qquad \tau(\bar{g}) \underset{\bar{g}\to 0}{\sim} -\bar{g}^2\{d_0 + d_1\bar{g}^2 + \ldots\}$$

Renormalization conditions at zero quark mass $\Rightarrow$ β and τ do not depend on the mass
$\Rightarrow \overline{m}_q(\mu)/\overline{m}_{q'}(\mu) = m_q^{\mathrm{bare}}/m_{q'}^{\mathrm{bare}}$

The $\overline{\mathrm{MS}}$ scheme is the most commonly used for perturbative QCD computations
$b_0, \ldots, b_3$ (van Ritbergen, Vermaseren and Larin, 1997; Czakon, 2005) and
$d_0, \ldots, d_3$ (Chetyrkin, 1997; Vermaseren, Larin and van Ritbergen, 1997) are known

Introduction

Fundamental, RGI parameters of QCD

$$\Lambda = \mu(b_0\bar{g}^2)^{-b_1/2b_0^2}\mathrm{e}^{-1/(2b_0\bar{g}^2)} \exp\left\{-\int_0^{\bar{g}} \mathrm{d}x \left[\frac{1}{\beta(x)} + \frac{1}{b_0 x^3} - \frac{b_1}{b_0^2 x}\right]\right\}$$

$$M_q = \overline{m}_q(2b_0\bar{g}^2)^{-d_0/2b_0} \exp\left\{-\int_0^{\bar{g}} \mathrm{d}x \left[\frac{\tau(x)}{\beta(x)} - \frac{d_0}{b_0 x}\right]\right\}$$

Any physical quantity P can be considered to be a function of Λ and M_q

$$\mu\frac{\mathrm{d}}{\mathrm{d}\mu}P(\mu,\bar{g},\{\overline{m}_q\}) = 0 \quad \Rightarrow \quad P = P(\Lambda,\{M_q\})$$

Simple scheme dependence of RGI quantities between different mass independent renormalization schemes (Sint and Weisz, 1998)

$$\Lambda' = \Lambda \exp\{\mathcal{X}_{\mathrm{g}}^{(1)}/(2b_0)\}\,, \qquad M_q' = M_q$$

$$\bar{g}'^{\,2} = \bar{g}^2(1 + \mathcal{X}_{\mathrm{g}}^{(1)}\bar{g}^2 + \ldots)$$

Non–perturbative renormalization

The scale problem: we want to compute $M_{\rm s}/F_{\rm K}$ on the lattice

$$\underset{\substack{\uparrow \\ \text{box size}}}{L} \gg \frac{1}{F_{\rm K}} \sim \underset{\substack{\uparrow \\ \text{confinement scale}}}{\frac{1}{0.2\,\text{GeV}}} \gg \frac{1}{\mu} \sim \frac{1}{10\,\text{GeV}} \gg \underset{\substack{\uparrow \\ \text{spacing}}}{a}$$

$$\Downarrow$$

$$L/a \gg 50$$

- Spatial lattice size L has to be large to avoid finite–volume effects in $F_{\rm K}$
- In order to extract $M_{\rm s}$, μ has to be in the perturbative regime of QCD
- $\mu \ll 1/a$ to avoid cutoff effects

Solution: take a finite–size effect as the physical observable $\boxed{L = 1/\mu}$

Recursive finite–size scaling technique (Lüscher, Weisz and Wolff, 1991) $\longrightarrow$ left with $L/a \gg 1$

Non–perturbative renormalization

Running mass $\overline{m}_{\rm s}(\mu)$ using recursive (*step scaling*) finite–size technique, $\mu = 1/L$

$L_{\rm max} = {\rm const.}/F_{\rm K} = {\rm O}(0.5\,{\rm fm})$: $\longrightarrow$ $L_{\rm max}\,\overline{m}_{\rm s}(\mu = 1/L_{\rm max})$

$\downarrow$

$L_{\rm max}\,\overline{m}_{\rm s}(\mu = 2/L_{\rm max})$

$\downarrow$

•

always $a/L \ll 1$ •

•

$\downarrow$

$L_{\rm max}\,\overline{m}_{\rm s}(\mu = 2^n/L_{\rm max})$

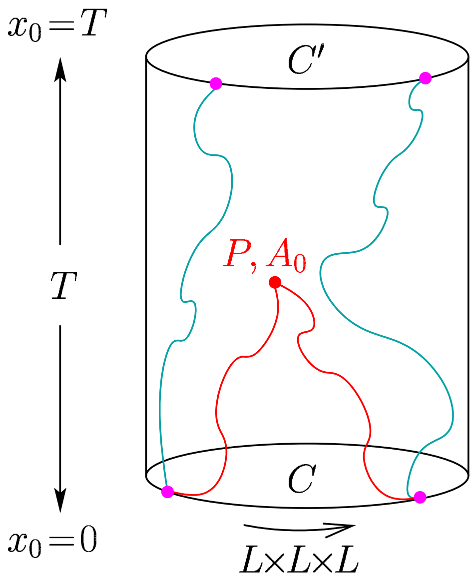
perturbation theory $\downarrow$

$L_{\rm max}\,M_{\rm s} = \#$

Result is a value for $\boxed{M_{\rm s}/F_{\rm K} = \#}$

Non–perturbative renormalization

Schrödinger Functional (SF) renormalization scheme ALPHA Collaboration
(Lüscher, Narayanan, Weisz and Wolff, 1992; Sint, 1994)



Dirichlet boundary conditions at $x_0 = 0$ and $x_0 = T$

- Infrared cutoff $\propto 1/T$ to the frequency spectrum of quarks and gluons $\Rightarrow$ renormalization at zero quark mass
- $\bar{g}(L)$ defined through the variation of the effective action with respect to a change of the boundary gluon fields C, C'

Non–perturbative renormalization

Other solution: $\boxed{\mu^2 = p^2}$ RI–MOM scheme

(Martinelli, Pittori, Sachrajda, Testa and Vladikas, 1995)

- Intermediate momentum subtraction (MOM) scheme:
  - fix the gauge, for example the Landau gauge
  - renormalization of amputated Green functions of operators between quark states of momentum p with $p^2 = \mu^2$, e.g. for a bilinear fermion operator O

$$\frac{Z_O^{\rm MOM}(g_0, ap)}{Z_\psi^{\rm MOM}(g_0, ap)} \times \underbrace{S(p)^{-1} \langle p|O(a)|p\rangle \, S(p)^{-1}}_{\text{computed on the lattice}} \quad = \quad \text{tree level value}$$

  $S(p)$ is the quark propagator, Z_ψ is the quark wave function renormalization (obtained with $O =$ conserved vector current)

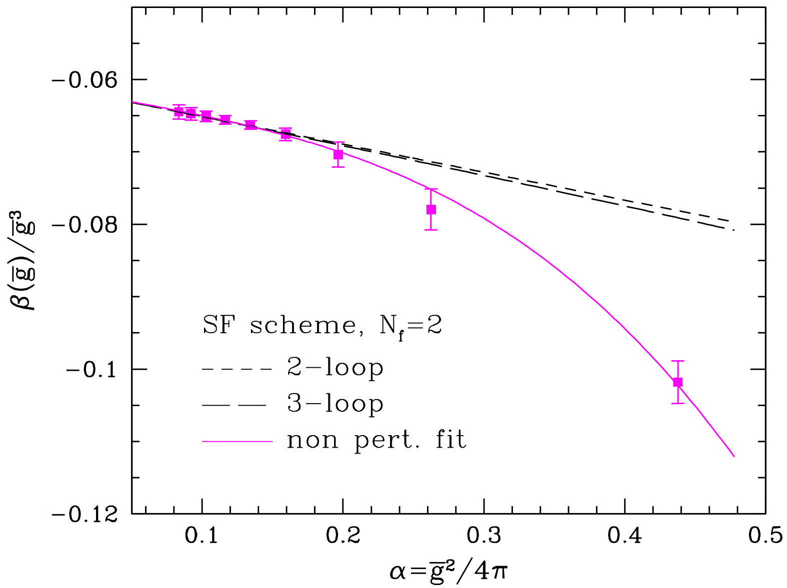
- $Z_O^{\rm MOM}(g_0, ap)$ can be related to $\overline{\rm MS}$ using renormalized perturbation theory
- Problems: gauge fixing, window is required for the momentum

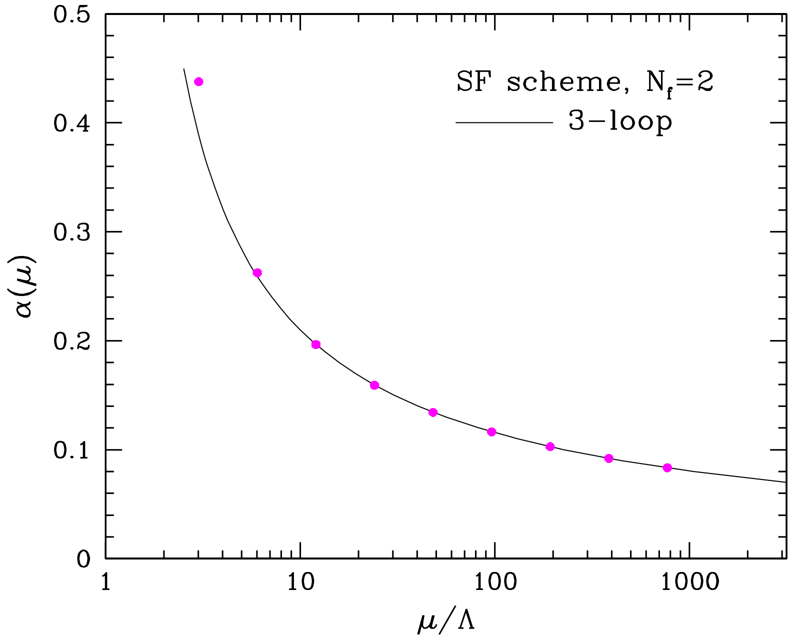
$$\Lambda_{\rm QCD}^2 \ll \quad p^2 \quad \ll a^{-2}$$

The running strong coupling α_s

- The running strong coupling $\alpha_s(\mu) = \bar{g}^2(\mu)/4\pi$ in the Schrödinger Functional scheme (ALPHA, Della Morte, Frezzotti, Heitger, Rolf, Sommer and Wolff, 2005)
- $\alpha_s(\mu)$ from improved bare couplings (HPQCD and UKQCD, Mason, Trottier, Davies, Foley, Gray, Lepage, Nobes and Shigemitsu, 2005)
- Comparison of the Λ parameters

The running strong coupling α_s





Non–perturbative $\beta(\bar{g})$

- Computed from step scaling function of $\bar{g}^2(L)$ $(L \to 2L)$ in the SF
- Deviations from 3–loop for $\alpha_{\rm SF} > 0.25$

- $N_{\rm f} = 2$ flavors of massless quarks
- running starts at $1/L_{\max} \sim 0.4\,\mathrm{GeV}$
- error bars smaller than symbol size

The running strong coupling α_s

- In order to put an MeV scale on L_{max} and Λ computation of e.g. $L_{max}F_K$ is required
- ... at present instead L_{max}/r_0 is used, scale r_0 from static force F (Sommer, 1994)

$$F(r_0)\, r_0^2 \quad = \quad 1.65\,, \quad r_0 = 0.5\,\mathrm{fm} \quad \text{from potential models}$$

- r_0/a has been computed by QCDSF and UKQCD Collaborations (Göckeler, Horsley, Irving, Pleiter, Rakow, Schierholz, Stüben, 2004) at three lattice spacings $a = 0.092\ldots 0.071\,\mathrm{fm}$
- Using $\Lambda^{(2)}_{\overline{\mathrm{MS}}} = 2.382035(3)\Lambda^{(2)}$ (Sint and Sommer, 1996)

$$\boxed{\Lambda^{(2)}_{\overline{\mathrm{MS}}} r_0 \;=\; 0.62(4)(4) \quad \text{or} \quad \Lambda^{(2)}_{\overline{\mathrm{MS}}} \;=\; 245(16)(16)\,\mathrm{MeV}}$$

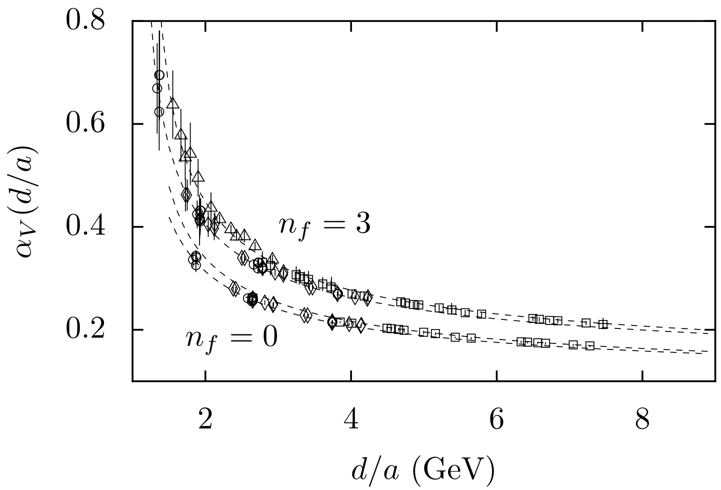
Errors: ΛL_{max}, chiral extrapolation of r_0

The running strong coupling α_s

- Lattice spacing a from Υ mass splitting, $a^{-1} = 1.1 - 2.3\,\mathrm{GeV}$
- α_s from Wilson loops W_{RT}, "tadpole" improvement (Parisi; Lepage and Mackenzie)

$$\ln(W_{RT}) = \sum_{n=1}^{3+\ldots} c_n \alpha_V^n(d/a)$$

  c_n, $n \leq 3$ computed using Feynman diagrams (Mason, Lattice2005)
- 2–loop (third order) relation between α_V and $\alpha_{\overline{\mathrm{MS}}}$ known (Schröder, 1998)
- No continuum limit, must assume *perturbative running and matching* is accurate at scale $a^{-1} \approx 2\,\mathrm{GeV}$



Perturbative inclusion of c and b quarks (Chetyrkin, Kniehl and Steinhauser, 1997)

$$\alpha_{\overline{\mathrm{MS}}}^{(5)} = 0.1170(12)$$

Are $N_f = 3$ flavors of staggered fermion theoretically sound? (fourth root trick)

The running strong coupling α_s

Non–perturbative determinations of the Λ parameter for $N_f = 0, 2$ compared to extractions from high–energy scattering experiments, using higher–order perturbation theory with $r_0 = 0.5\,\mathrm{fm}$

Reference	N_f	$\Lambda_{\overline{\mathrm{MS}}}^{(N_f)} r_0$
ALPHA	0	0.60(5)
QCDSF/UKQCD[a]	0	0.614(2)(5)
ALPHA	2	0.62(4)(4)
QCDSF/UKQCD[a]	2	0.62(4)(2)
DIS @ NNLO[b]	4	0.57(8)
Bethke[c], 2004	4	0.74(10)
Bethke, 2004	5	0.54(8)

[a]: from improved bare couplings

[b]: Blümlein, Böttcher and Guffanti, 2004; Moch, Vermaseren and Vogt, 2004; van Neerven and Zijlstra, 1991

[c]: perturbative matching of effective theories with $N_f = 4$ and $N_f = 5$ massless quarks (Bernreuther and Wetzel, 1982)

The running quark masses: light quarks

Definition of a renormalized quark mass on the lattice

$$\overline{m}^{\overline{\mathrm{MS}}}(\mu) \quad = \quad Z_m(g_0, a\mu)(m^{\mathrm{bare}} - m_{\mathrm{crit}})$$

Wilson fermions Additive mass renormalization $m_{\mathrm{crit}} \propto 1/a$, not there using the Partial Conservation of the Axial Current (PCAC) relation

$$\partial_\mu \underbrace{\bar{u}\gamma_\mu\gamma_5 s}_{A_\mu} \quad = \quad (m_u^{\mathrm{bare}} + m_s^{\mathrm{bare}}) \underbrace{(\bar{u}\gamma_5 s)}_{P} + \mathrm{O}(a^2)$$

by adding O(a) counterterms to the action and to A_μ with coefficients $c_{\mathrm{sw}}(g_0)$ and $c_{\mathrm{A}}(g_0)$ (ALPHA)

Renormalization: $(A_{\mathrm{R}})_\mu = Z_{\mathrm{A}}\, A_\mu$ and $(P_{\mathrm{R}}) = Z_{\mathrm{P}}\, P$, comparing bare and renormalized PCAC relations

$$(\overline{m}_{\mathrm{u}} + \overline{m}_{\mathrm{s}})^{\overline{\mathrm{MS}}}(\mu) \quad = \quad (m_u^{\mathrm{bare}} + m_s^{\mathrm{bare}}) \frac{Z_{\mathrm{A}}(g_0)}{Z_{\mathrm{P}}^{\overline{\mathrm{MS}}}(g_0, a\mu)}$$

The running quark masses: light quarks

Renormalization:

- $Z_{\rm A}(g_0)$ can be computed non-perturbatively using chiral Ward identities (ALPHA)
- At 1–loop in perturbation theory

$$Z_{\rm P}^{\overline{\rm MS}}(g_0, a\mu) \quad = \quad 1 + \frac{g_0^2}{4\pi}[(2/\pi)\ln(a\mu) + k] + {\rm O}(g_0^4)$$

k is a calculable constant. On accessible lattices $g_0 \simeq 1$, applicability of perturbation theory is doubtful, systematic error? $\Rightarrow$ use non-perturbative renormalization

The running quark masses: light quarks

- Computation of the running of the renormalized quark mass and of $M_{\rm s}$ (ALPHA, Della Morte, Hoffmann, Knechtli, Rolf, Sommer, Wetzorke and Wolff, 2005)
- Summary plot for the strange quark's mass
- Recent compilation of unquenched lattice results

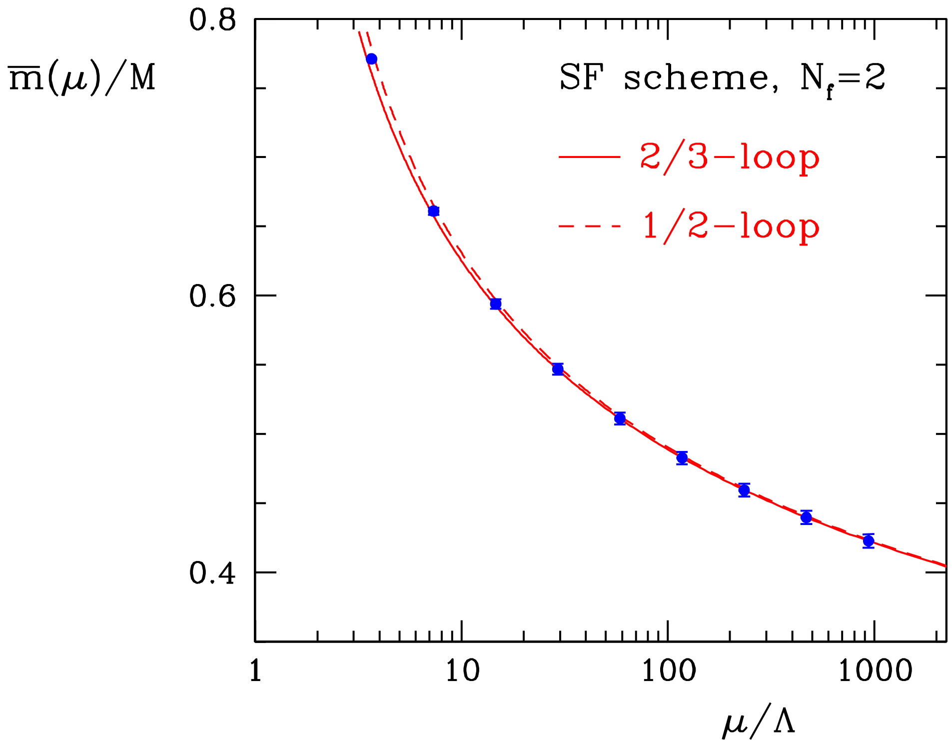
The running quark masses: light quarks

- Running of the mass in the SF for $N_\mathrm{f} = 2$ flavors of mass–less quarks

$$\frac{\overline{m}(\mu)}{\overline{m}(\mu/2)} = \lim_{a\to 0} \frac{Z_\mathrm{P}(g_0, 2L/a)}{Z_\mathrm{P}(g_0, L/a)}\Big|_{\mu=1/L}$$

  independent of the quark flavor q

- *In this case* perturbation theory works surprisingly well down to small energies



$$\overline{m}_\mathrm{s} \;:\; \mu = 1/L_\mathrm{max} \overset{\text{non–pert.}}{\longrightarrow} 2^6/L_\mathrm{max} \overset{\text{pert.}}{\longrightarrow} \text{"}\infty\text{"} \quad \text{(RGI)} \;:\; M_\mathrm{s}$$

$$\alpha_\mathrm{SF}(L_\mathrm{max}) = 0.367$$

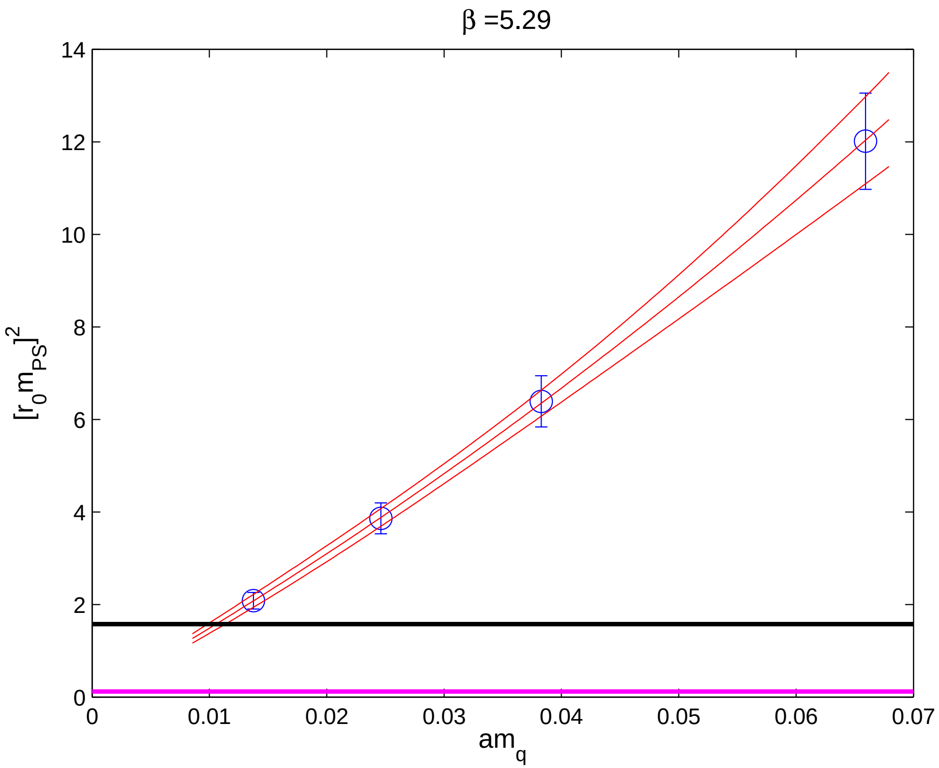
The running quark masses: light quarks

- In order to determine $\overline{m}_s$ need to simulate u and s quark (K^+)
- ... not possible at present, instead simulate two *degenerate* quarks with mass $m_{\rm ref}$ such that

$$m_{\rm PS}(m_{\rm ref}, m_{\rm ref}) = m_{\rm K}$$

- Fit $m_q = m_{\rm ref}$ to QCDSF/UKQCD data

$$r_0 m_{\rm PS}^2 = a m_q (e_1 + e_2 (a m_q)^2)$$



Physical pion point is very far ⇒ only *partially quenched* simulations and chiral extrapolation so far

The running quark masses: light quarks

β	$\kappa_{\rm ref}$	L/a	$am_{\rm ref}$	$M_{\rm ref}$ [MeV]
5.20	0.135680	16	0.01410(30)	58.7(3.2)
5.29	0.136018	16	0.01352(28)	63.5(3.2)
5.40	0.136293	24	0.01300(18)	72.0(2.7)

From $\beta = 5.4$: $M_{\rm ref} = 72(3)(13)\,\mathrm{MeV}$, systematics from difference to $\beta = 5.2$

The result is consistent with the $N_{\rm f} = 0$ number from ALPHA. We *assume* it for $N_{\rm f} = 3$ theory where we relate $M_{\rm ref}$ to $M_{\rm s}$ through Gell-Mann–Oakes–Renner formula

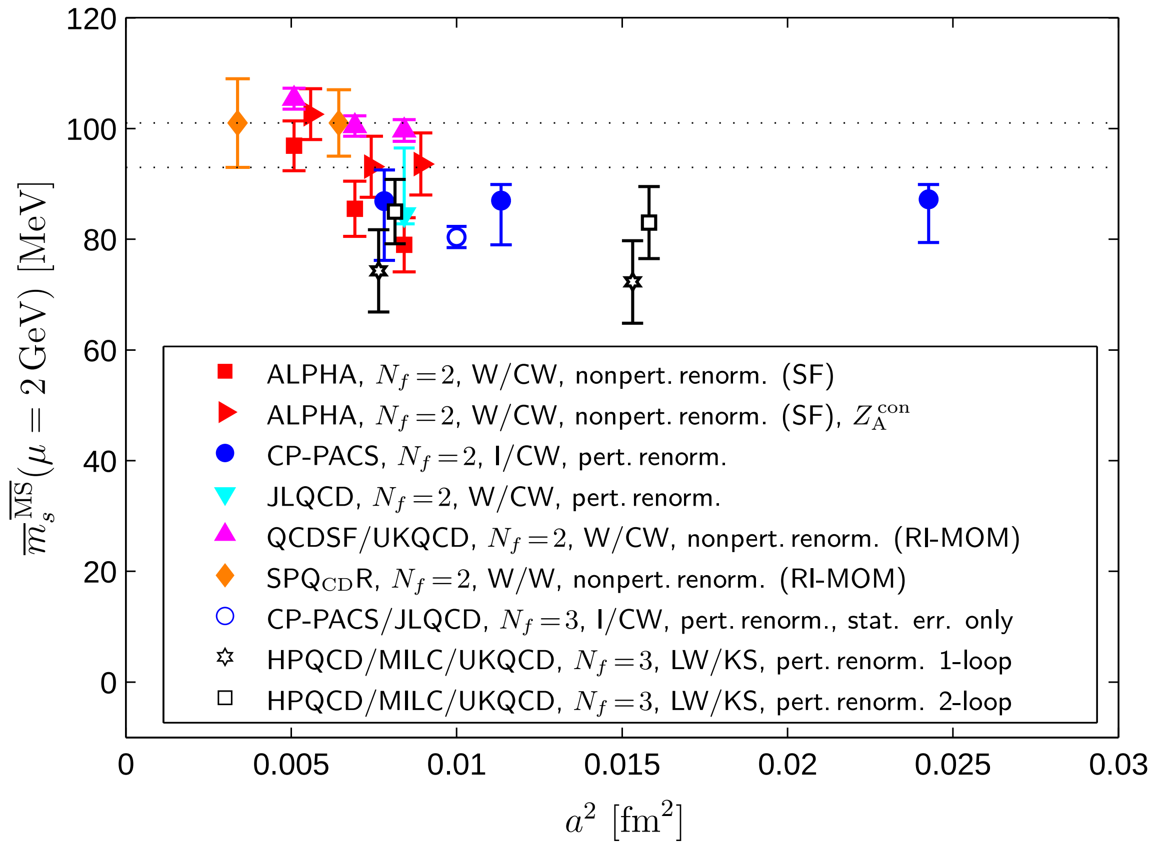
$$m_{\rm K}^2 = \frac{1}{2}\left(m_{\rm K+}^2 + m_{\rm K0}^2\right)_{\rm QCD} = \left(\hat{M} + M_{\rm s}\right) B_{\rm RGI} = 2M_{\rm ref}\, B_{\rm RGI}$$

$$\Rightarrow \quad B_{\rm RGI} = 1.70(38)\,\mathrm{GeV}$$

with $\hat{M} = \frac{1}{2}(M_{\rm u} + M_{\rm d})$. Together with $M_{\rm s}/\hat{M} = 24.4(1.5)$ (Leutwyler, 1996)

$$M_{\rm s} = 138(5)(26)\,\mathrm{MeV} \quad \text{or} \quad \overline{m}_{\rm s}^{\overline{\rm MS}}(\mu = 2\,\mathrm{GeV}) = 97(22)\,\mathrm{MeV} \quad [4\ \text{loop}, N_{\rm f} = 2]$$

The running quark masses: light quarks



- Physical input is the kaon mass
- Comparing bluish to reddish points $\Rightarrow$ non–perturbative renormalization is an effect (points from perturbative renormalization for $Z_{\rm P}$ are systematically smaller), this plot shows that there is a problem (Lattice 2005)

The running quark masses: light quarks

Recent compilation of (unquenched) lattice results in MeV

Reference	N_f	$\overline{m}_s^{\overline{\text{MS}}}(\mu = 2\,\text{GeV})$	$\overline{\hat{m}}^{\overline{\text{MS}}}(\mu = 2\,\text{GeV})$
HPQCD/MILC/UKQCD	3	$76 \pm 3 \pm 7$	$2.8 \pm .1 \pm .3$
HPQCD/MILC/UKQCD update, 2–loop Z_P	3	$86 \pm 3 \pm 4$	$3.2 \pm .1 \pm .2$
CP-PACS/JLQCD	3	$91.8 \pm 3.9 \begin{pmatrix} +6.8 \\ -4.1 \end{pmatrix}$	$3.50 \pm .14 \begin{pmatrix} +.26 \\ -.15 \end{pmatrix}$
SPQ$_{\text{CD}}$R	2	$101 \pm 8 \begin{pmatrix} +25 \\ -9 \end{pmatrix}$	$4.3 \pm 4 \begin{pmatrix} +1.1 \\ -0.4 \end{pmatrix}$
QCDSF/UKQCD ($r_0 = 0.5\,\text{fm}$)	2	$111 \pm 5 \pm 7$	$4.4 \pm .2 \pm .3$
ALPHA	2	97 ± 22	–

Current summary of lattice results (PDG, A.V. Manohar and C.T. Sachrajda, 2006)

$$\overline{\hat{m}}^{\overline{\text{MS}}}(\mu = 2\,\text{GeV}) \;=\; 3.8(8)\,\text{MeV}\,, \quad \overline{m}_s^{\overline{\text{MS}}}(\mu = 2\,\text{GeV}) \;=\; 95(20)\,\text{MeV}$$

Excluding lattice: $\overline{m}_s^{\overline{\text{MS}}}(\mu = 2\,\text{GeV}) = 103(20)\,\text{MeV}$, until 1996 $125(40)\,\text{MeV}$

The running quark masses: light quarks

As pointed out by R. Sommer: present status of quark masses from lattices with $N_\mathrm{f} > 0$ is in a similar stage as 10 years ago with $N_\mathrm{f} = 0$

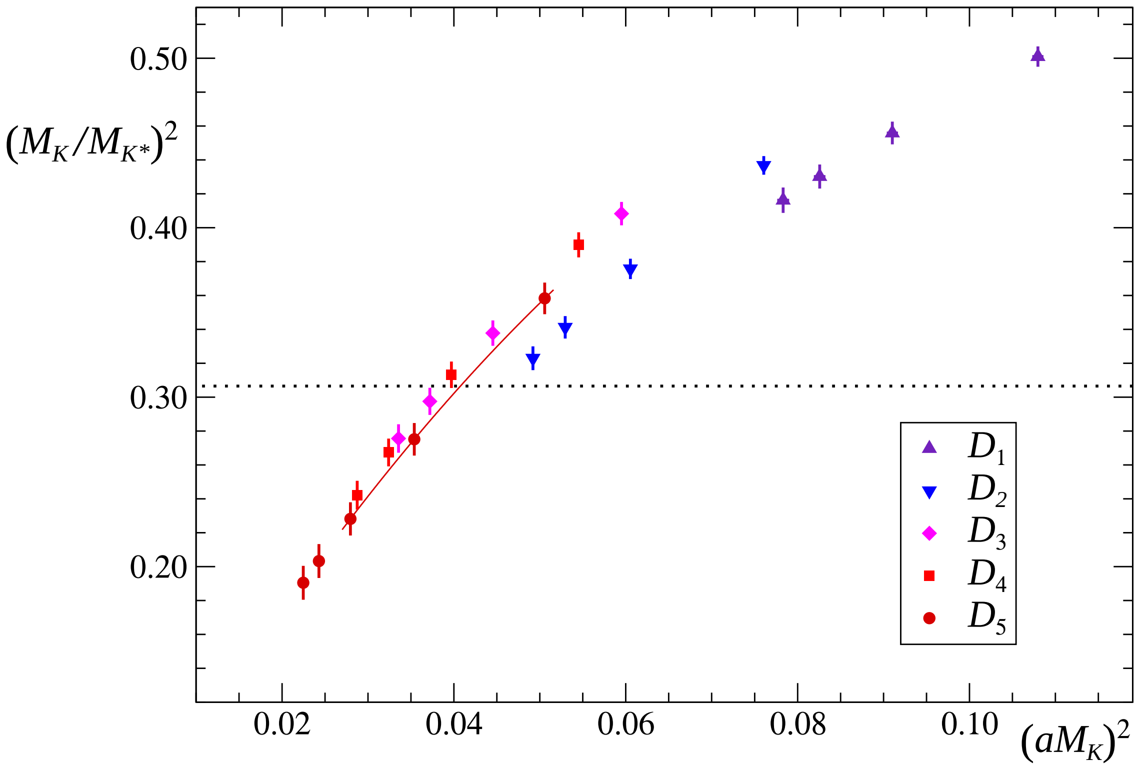
As in the quenched case the errors can be reduced by an order of magnitude, for this we need to control the systematic errors:

- non-perturbative renormalization
- scale setting
- chiral extrapolation
- finite volume effects
- continuum limit

Examples from [Del Debbio, Giusti, Lüscher, Petronzio, Tantalo, 2006]

- Setting the scale with $N_\mathrm{f} = 2$ sea and a valence strange quarks
- Extrapolations to smaller quark masses

The running quark masses: light quarks



W/CW, $\beta = 5.3$

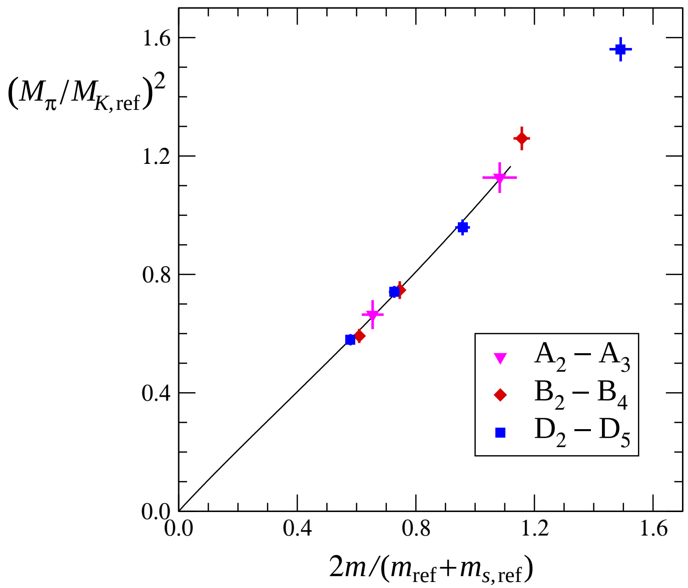
48×24^3

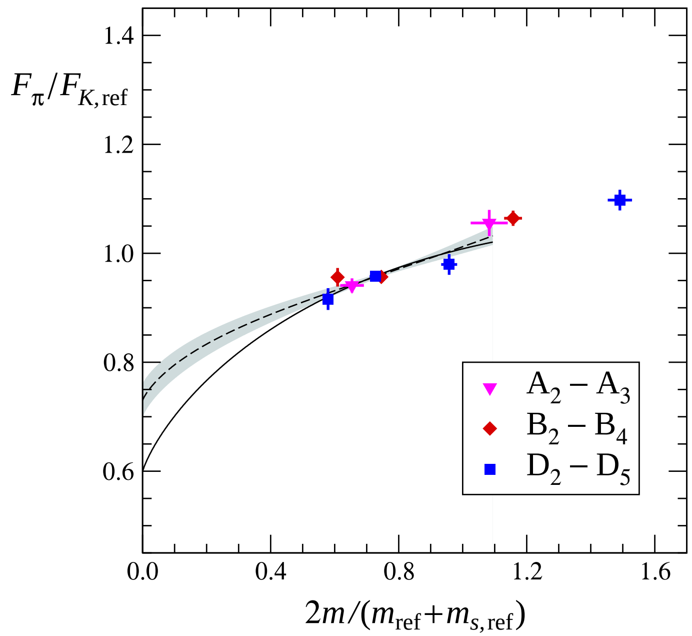
$m \approx m_{\rm s} \ldots m_{\rm s}/4$

$a(g_0) \;=\; 0.0784(10)\,\text{fm}$
(mass independent scheme)

- fix the strange quark mass $m_{\rm s,ref}$ by $m_{\rm K}/m_{\rm K^*} = 0.554$ (physical value)
- fix the sea quark mass $m_{\rm ref}$ by $m_\pi/m_{\rm K} = 0.85 \Rightarrow a = (am_{\rm K})/(495\,\text{MeV})$
- using $r_0 = 0.5\,\text{fm}$ at $r_0 m_\pi = 1.26$: $a = 0.09\,\text{fm}$

The running quark masses: light quarks





1-loop chiral expansion, $N_\mathrm{f} = 2$, $M^2 = 2B$

$$m_\pi^2 = M^2 + \frac{M^4}{32\pi^2 F^2}\ln(M^2/\Lambda_3^2) + \ldots \qquad F_\pi = F - \frac{M^2}{16\pi^2 F}\ln(M^2/\Lambda_4^2) + \ldots$$

Data are compatible but insufficient for a reliable determination of the parameters in the chiral lagrangian

Conclusions and Outlook

- Lattice QCD simulations can determine the fundamental parameters of QCD (Λ, M_q), defined at high energies, using hadronic quantities like m_π, m_K and F_K as input
- The fundamental parameters play a key role in experiments, which aim to test the Standard Model of particle physics and find hints of physics beyond the Standard Model

Shopping list

- simulations with quark masses smaller than $m_\mathrm{s}/4$
- non-perturbative renormalization
- systematic errors in scale setting and continuum limit have to be reduced
- hard but doable work!