

Current correlators at four loops and heavy quark mass determinations

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Outline

- 1 Quark Mass Determination
 - Why precise quark masses?
 - From hadron production to quark masses: sum rules
 - Status
- 2 Reduction techniques
 - Basics: Integration-by-Parts
 - Laporta algorithm
 - Gröbner bases
 - Combined techniques
- 3 Results
 - Third moment of the vacuum polarization at four loops
 - Reconstruction of the full energy dependence
 - Charm and bottom quark masses from $R(s)$
 - m_c and α_s from lattice QCD
 - Conclusion

Why precise quark masses?

Precise predictions require precise knowledge of the theory's parameters.

In QCD: strong coupling α_s and masses of the 6 quarks u, d, s, c, b, t

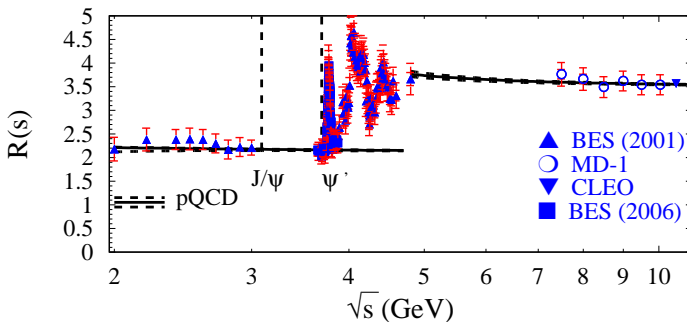
here: focus on m_c and m_b

Applications:

- Weak decay rates of heavy mesons, e. g. $\Gamma(B_{c/d} \rightarrow \ell \nu K) \propto m_b^5$
- Quarkonium spectroscopy
- Decay rates and branching ratios of light Higgs: $\Gamma(H \rightarrow b\bar{b}) \propto m_b^2$
- GUT predictions for m_t/m_b (Yukawa unification at M_{GUT})
- ...

From hadron production to quark masses I

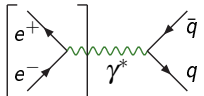
Information about quark masses is found in the threshold region of the cross section for hadron production from e^+e^- .



Resonance behaviour is not accessible by perturbative QCD

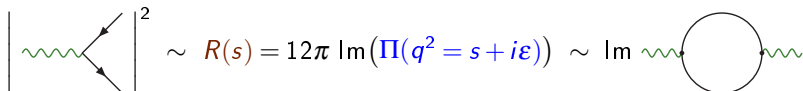
→ sum rules [Shifman, Vainshtein, Zakharov]

From hadron production to quark masses II

Process:  + higher order corrections

The diagram shows an incoming electron (e^-) and positron (e^+) pair on the left, meeting at a vertex. A wavy line representing a virtual photon (γ^*) connects this vertex to another vertex on the right. From the second vertex, a quark (q) and an antiquark (\bar{q}) emerge.

Optical theorem: total production cross section $R(s)$
 \propto imaginary part of forward scattering amplitude
 (Vacuum Polarization $\Pi(q^2)$)



The diagram shows a wavy line on the left that splits into two lines, representing the production of a quark-antiquark pair. This is equated to the imaginary part of a vacuum polarization loop diagram, which consists of a circle with two wavy lines entering and exiting.

$$\left| \text{wavy line} \rightarrow \text{quark-antiquark pair} \right|^2 \sim R(s) = 12\pi \text{Im}(\Pi(q^2 = s + i\epsilon)) \sim \text{Im} \text{wavy line} \rightarrow \text{vacuum polarization loop}$$

Vacuum Polarization: Correlator of electromagnetic currents $j_\mu = \bar{\psi}\gamma_\mu\psi$

$$(q_\mu q_\nu - g_{\mu\nu} q^2) \Pi(q^2) = i \int dx e^{iqx} \langle 0 | T j_\mu(x) j_\nu(0) | 0 \rangle$$

R-Ratio:
$$R(s) = \frac{\sigma(e^+e^- \rightarrow \text{hadrons})}{\sigma(e^+e^- \rightarrow \mu^+\mu^-)_{LO}}$$

From hadron production to quark masses III

The connection between $R(s)$ and $\Pi(q^2)$ leads to a

Dispersion Relation:
$$\Pi(q^2) - \Pi(0) = \frac{q^2}{12\pi^2} \int ds \frac{R(s)}{s(s - q^2)}$$

Expansion for small q^2 on both sides:

$$\mathcal{M}_n^{\text{th}} = \frac{12\pi^2}{n!} \left(\frac{\partial}{\partial q^2} \right)^n \Pi(q^2) \Big|_{q^2=0} = \frac{9}{4} Q_q^2 (4m^2)^{-n} C_n$$

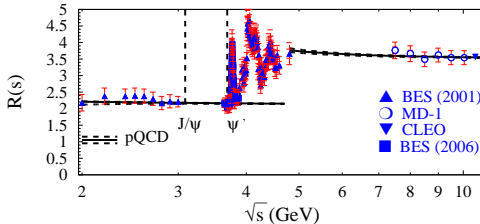
$$\mathcal{M}_n^{\text{exp}} = \int_0^\infty ds \frac{R(s)}{s^{n+1}}$$

$$\mathcal{M}_n^{\text{th}} = \mathcal{M}_n^{\text{exp}}$$

$$\Rightarrow m = \frac{1}{2} \left(\frac{9Q_q^2 C_n}{4\mathcal{M}_n^{\text{exp}}} \right)^{\frac{1}{2n}}$$

Features of the sum rule approach

Advantages and disadvantages of C_n for different n ?

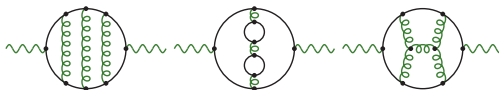


Long distance effects average out for small n

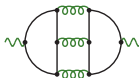
- larger n
- suppresses continuum region (no data; no m dependence)
 - reduces influence of experimental error
 - growing long distance effects
 - increasingly difficult to calculate

What do we have to calculate?

At four loops 700 Feynman integrals contribute



Singlet contributions come into play:



Perform Taylor expansion in the external momentum q^2

reduces the number of scales:

propagator-type integrals (q^2, m^2) \rightarrow tadpoles (m^2)

(light quarks are treated as massless)

Express integrals in terms of master integrals

Status of current correlators in the low energy limit

At three loops, i. e. $\mathcal{O}(\alpha_s^2)$

- first 8 moments [Chetyrkin, Kühn, Steinhauser (1996)]
- moments up to $n = 30$ for
 - vector current [Boghezal, Czakon, Schutzmeier (2006)]
 - all diagonal currents (including singlet) [Maier, PM, Marquard, (2007)]

At four loops, i. e. $\mathcal{O}(\alpha_s^3)$

- first physical moment of the vector current (non-singlet) [Chetyrkin, Kühn, Sturm; Boghezal, Czakon, Schutzmeier (2006)]
- all orders result for n_l^{z-1} at $\mathcal{O}(\alpha_s^z)$ [Grozin, Sturm (2005)]
- moments up to $n = 30$ for n_f^2 [Czakon, Schutzmeier (2007)]
- second (including singlet) and third moments for all diagonal currents [Maier, PM, Marquard (2008/2009)]

Integration-by-Parts

Tadpole integrals are mapped to six topologies



All appearing integrals can be expressed as linear combination of 13 master integrals with rational coefficients in the space-time dimension d .



[Schröder, Vuorinen (2005)]

Basic tool: Integration-by-Parts identities (IBP) [Chetyrkin, Tkachov (1981)]

$$0 = \int d^d k_1 \dots d^d k_\ell \frac{\partial}{\partial k_i^\mu} \frac{\{k_j^\mu, p_j^\mu\}}{D_1^{a_1} D_2^{a_2} \dots D_n^{a_n}}$$

give relations between integrals with different propagator powers.

- Usage:**
- generate and solve a system of equations → Laporta algorithm
 - construct recursion relations → Gröbner bases

A Simple two-loop example

Consider the two-loop tadpole with two massive and one massless line:

$$J(x, y, z) = \text{Diagram} = \int dk_1 dk_2 \frac{1}{(k_1^2 + m^2)^x (k_2^2)^y ((k_1 + k_2)^2 + m^2)^z}$$

The diagram is a circle with a vertical dashed line through its center. The left side of the circle is labeled 'x', the right side 'y', and the bottom side 'z'. There are dots at the top and bottom of the dashed line.

$$\begin{aligned} \Rightarrow 0 &= \int dk_1 dk_2 \frac{\partial}{\partial k_2^\mu} k_2^\mu I(x, y, z) \\ &= (d - 2y - z)J(x, y, z) + zJ(x - 1, y, z + 1) + zJ(x, y - 1, z + 1) \end{aligned}$$

For $x = y = z = 1$: $J(1, 1, 1) = \frac{1}{d - 3} J(1, 0, 2)$

Diagrammatically: $\text{Diagram} = \frac{1}{d - 3} \text{Diagram}$

The diagram on the left is the same as in the first equation. The diagram on the right is a figure-eight shape.

Laporta algorithm

“Standard” method to solve IBPs: [Laporta algorithm](#) [Laporta (2000)]

- define ordering of integrals
- generate IBPs for all permutations of propagator powers and scalar products up to the required sums of powers
- solve systematically for the most difficult integrals by a Gauss elimination-like algorithm

Generally very powerful, but:

- system of equations is overdetermined by $\mathcal{O}(3-5)$
- complicated intermediate expressions
- expensive simplifications needed at each step
- bad combinatorics for large propagator powers
- most of the solved integrals are not needed in the calculation

Limitations of the Laporta algorithm

In our case: each q^2 derivative adds two propagator powers and one irreducible scalar product to the integrands.

For C_3 :

- $4.5 \cdot 10^6$ integrals needed
- up to 12 additional propagator powers (“dots”)
- up to 8 irreducible scalar products
- distributed on 10 indices ($\sim 10^{13}$ permutations)

⇒ naïve approach fails because of combinatorics

In principle the problems can be avoided by using recursion relations.

- calculate exactly what is needed
- size of expressions is limited by the number of master integrals (“backwards substitution”)

Systematic approach: Gröbner bases

Gröbner bases

Consider multivariate polynomials and conditions of the form

$$b_1 = 0, \dots, b_n = 0$$

How to find out, if a polynomial p is zero, i. e. a representation

$$p = f_1 b_1 + \dots + f_n b_n$$

with polynomial coefficients f_i exists?

→ Divide out the elements of the basis

If we have a Gröbner basis, the remainder is unique.

Gröbner bases can be constructed by the Buchberger algorithm.

- Guaranteed to terminate after a finite number of steps, but not on real computers.

Gröbner bases for Feynman integrals

For Feynman integrals:

- consider algebra of shift and multiplication operators
 - IBP identities are polynomials in these operators
 - construct a Gröbner basis from the IBP identities
 - take an integral and divide out the elements of the basis
- remainder is the desired reduction to master integrals.

Example: $J(a, b) = (S_1^+)^{a-1} (S_2^+)^{b-1} J(1, 1)$

$$(S_1^+)^{a-1} (S_2^+)^{b-1} = f_1 b_1 + f_2 b_2 + R$$

$$\Rightarrow J(a, b) = (f_1 b_1 + f_2 b_2 + R) J(1, 1) = R J(1, 1)$$

S-Bases

Problem: Buchberger algorithm is too slow even for simple problems

Better: S-bases (modified Buchberger algorithm)

[Smirnov & Smirnov]

- much faster, but not guaranteed to stop
- strongly dependent on ordering of the integrals
- sometimes doesn't find a basis even after many tries
- public implementation in Mathematica available:

FIRE [A. V. Smirnov]

Unfortunately, there is no solution to this problem in sight.

→ Has to be combined with other methods.

FIRE has a Laporta part for that reason;
a C++ implementation is in development.

Self energy reduction

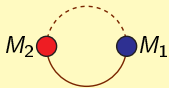
S-Bases tend to fail for integrals with self energy insertions.
 These integrals have the highest propagator powers (*here*: +2).

→ most difficult for Laporta algorithm.

Idea: Apply tensor reduction to self energy subgraphs to remove scalar products and reduce the self energies to master integrals.



= 2-loop SE × 1-loop SE × connecting propagator
 × scalar products between self energies



Treat self energy master integrals als objects,
 which depend only on their external momentum.
 → effective one-loop integral!

Very efficient, but limited to special topologies.

Combination of reduction techniques

The reduction techniques have complementary strengths.

Strategy:

- use self energy formalism where it is applicable
→ two dots less for Laporta
- keep the system for Laporta algorithm as small as possible:
don't generate all equations, but adapt to the needed integrals
- use Gröbner bases in combination with self energy formalism
if something is missing (and for checks)

**A sophisticated combination of reduction techniques
can handle problems which are difficult for Laporta alone.**

Results

First three moments of the vacuum polarization up to $\mathcal{O}(\alpha_s^3)$
(with n_l light quark flavours)

$$C_1^V = 1.06666 + 2.55473 \left(\frac{\alpha_s}{\pi} \right) + (0.50988 + 0.66227 n_l) \left(\frac{\alpha_s}{\pi} \right)^2 \\ + (1.87882 - 2.79472 n_l + 0.09610 n_l^2) \left(\frac{\alpha_s}{\pi} \right)^3,$$

$$C_2^V = 0.45714 + 1.10955 \left(\frac{\alpha_s}{\pi} \right) + (1.41227 + 0.45491 n_l) \left(\frac{\alpha_s}{\pi} \right)^2 \\ + (-6.23488 + 0.96156 n_l - 0.01594 n_l^2) \left(\frac{\alpha_s}{\pi} \right)^3,$$

$$C_3^V = 0.27089 + 0.51939 \left(\frac{\alpha_s}{\pi} \right) + (0.35222 + 0.42886 n_l) \left(\frac{\alpha_s}{\pi} \right)^2 \\ + (-8.30971 + 1.94219 n_l - 0.03959 n_l^2) \left(\frac{\alpha_s}{\pi} \right)^3$$

+ correlators of the scalar $j^S = \bar{\psi}\psi$, pseudoscalar $j^P = \bar{\psi}\gamma_5\psi$
and axial vector $j_\mu^A = \bar{\psi}\gamma_\mu\gamma_5\psi$ currents

Third moment of the vacuum polarization

$$C_n = C_n^{(0)} + \left(\frac{\alpha_s}{\pi}\right) C_n^{(1)} + \left(\frac{\alpha_s}{\pi}\right)^2 C_n^{(2)} + \left(\frac{\alpha_s}{\pi}\right)^3 C_n^{(3)} + \dots$$

$$C_n^{(3)} = C_F T_F^2 n_\ell^2 C_{\ell\ell,n}^{(3)} + C_F T_F^2 n_h^2 C_{hh,n}^{(3)} + C_F T_F^2 n_\ell n_h C_{\ell h,n}^{(3)}$$

$$+ C_F T_F n_\ell \left(C_A C_{\ell NA,n}^{(3)} + C_F C_{\ell A,n}^{(3)} \right) + C_{n_f^0,n}^{(3)} + C_F T_F n_h \left(C_A C_{h NA,n}^{(3)} + C_F C_{h A,n}^{(3)} \right)$$

$$C_{ll,3}^{(3),v} = + \frac{31556642272}{49228003125} - \frac{256}{405} \zeta_3,$$

$$C_{hh,3}^{(3),v} = + \frac{56877138427}{12609717120} - \frac{6184964549}{1556755200} \zeta_3,$$

$$C_{lh,3}^{(3),v} = + \frac{60361465477}{29393280000} - \frac{1765}{31104} c_4 + \frac{86485}{41472} \zeta_4 - \frac{57669161}{17418240} \zeta_3,$$

$$C_{lNA,3}^{(3),v} = - \frac{1475149211788337}{6452412825600000} - \frac{8529817}{77414400} c_4 + \frac{1510937903}{14745600} \zeta_4 - \frac{561258009401}{6193152000} \zeta_3,$$

$$C_{lA,3}^{(3),v} = + \frac{983812946922223}{4389396480000} + \frac{8529817}{38707200} c_4 + \frac{21972351293}{17203200} \zeta_4 - \frac{28995540810097}{21676032000} \zeta_3,$$

$$C_{hNA,3}^{(3),v} = - \frac{454880458419083629}{5854170457175040000} - \frac{7110196837}{1117670400} c_4 + \frac{1068488091383}{7451136000} \zeta_4$$

$$+ \frac{4448}{315} \zeta_5 - \frac{43875740175477222611}{433642256087040000} \zeta_3,$$

$$C_{hA,3}^{(3),v} = - \frac{2327115263308753}{2489610816000} - \frac{16870125343}{39916800} c_4 + \frac{286864384271}{26611200} \zeta_4 - \frac{377837317054807}{61471872000} \zeta_3,$$

$$c_4 = 24 a_4 + \log^4 2 - 6 \zeta_2 \log^2 2;$$

$$a_n = \text{Li}_n(1/2)$$

Padé approximations I

What if we want more moments?

Direct calculation not reasonable at the moment.

Full q^2 dependence of correlators?

Needed e. g. for contour improved perturbation theory.

Padé approximations: [Broadhurst, Fleischer, Tarasov '93; Baikov, Broadhurst '95; Chetyrkin, Kühn, Steinhauser '96; Hoang, Mateu, Zerbarjad '08; Masjuan, Peris '08]

use
$$\rho_{m,n}(x) = \frac{a_0 + a_1x + a_2x^2 + \dots + a_mx^m}{1 + b_1x + b_2x^2 + \dots + b_nx^n}$$

to approximate $\Pi(x = \frac{q^2}{4m^2})$. Fix a_i, b_j by $\rho_{m,n}^{(k)}(x_0) = \Pi^{(k)}(x_0)$.

Input:

- low energy expansion
- threshold expansion
- high energy expansion

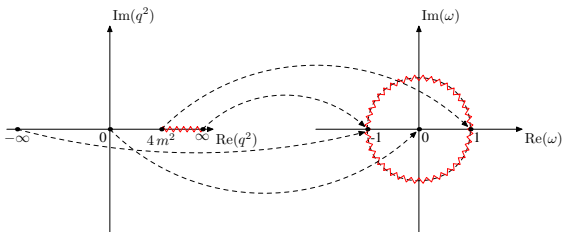
Padé approximations II

Problem 1: Padé approximations cannot predict logarithms $\log\left(\frac{q^2}{4m^2}\right)$
→ subtract an appropriate function

$$\Pi(q^2) = \Pi_{reg}(q^2) + \Pi_{log}(q^2)$$

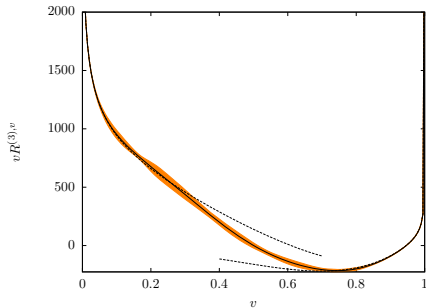
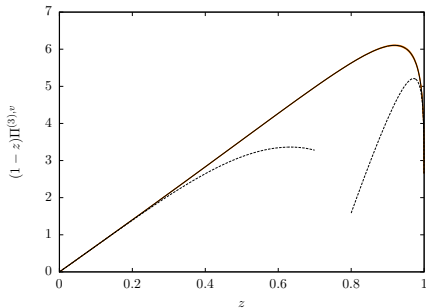
Problem 2: Branch cut above threshold
→ conformal mapping to the unit circle

$$\frac{q^2}{4m^2} = \frac{4\omega}{(1+\omega)^2}$$



Padé approximations: Results

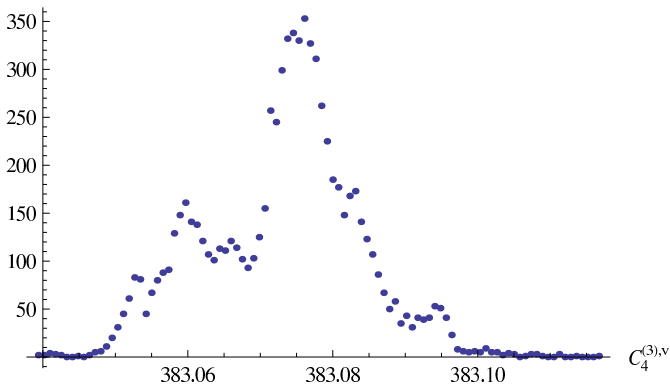
Padé approximations below and above threshold



The plots show the low energy and threshold resp. the threshold and high energy expansion and the Padé approximations including a 3σ error band.

Padé approximations: Error estimation

Exploit the freedom of choosing numerator / denominator degree of the approximation and the freedom in the choice of the subtraction function to estimate errors.



Padé approximations: Prediction of higher moments

	$n_l = 3$	$n_l = 4$	$n_l = 5$
$C_1^{(3),v}$	366.1748	308.0188	252.8399
$C_2^{(3),v}$	381.5091	330.5835	282.0129
$C_3^{(3),v}$	385.2331	338.7065	294.2224
$C_4^{(3),v}$	383.073(11)	339.913(10)	298.576(9)
$C_5^{(3),v}$	378.688(32)	338.233(32)	299.433(27)
$C_6^{(3),v}$	373.536(61)	335.320(63)	298.622(54)
$C_7^{(3),v}$	368.23(9)	331.90(10)	296.99(9)
$C_8^{(3),v}$	363.03(13)	328.33(14)	294.94(12)
$C_9^{(3),v}$	358.06(17)	324.78(18)	292.72(16)
$C_{10}^{(3),v}$	353.35(20)	321.31(22)	290.44(19)
$K_0^{(3),v}$	17(11)	17(29)	16(10)
$D_2^{(3),v}$	2.0(42)	1.2(83)	1.4(21)

Results for m_c

n	exp	α_s	μ	np	total	$m_c(3 \text{ GeV})$
1	0.009	0.009	0.002	0.001	0.013	0.986
2	0.006	0.014	0.005	0.000	0.016	0.976
3	0.005	0.015	0.007	0.002	0.017	0.978
4	0.003	0.009	0.031	0.007	0.033	1.004

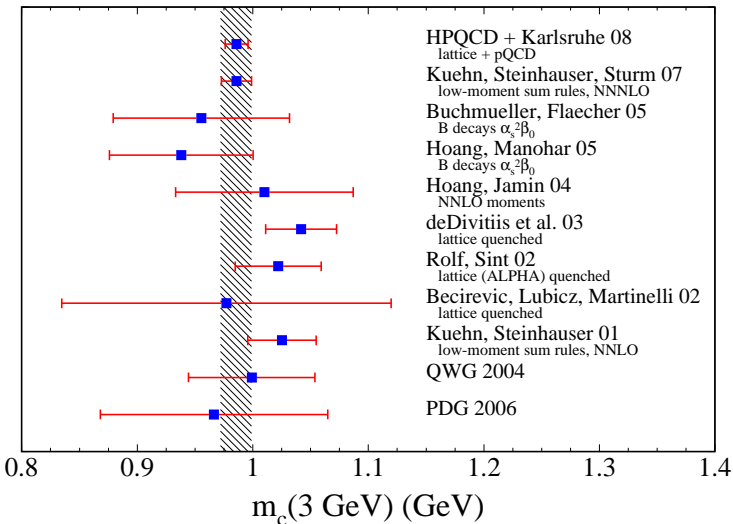
Error sources:

- experimental (exp)
- uncertainty of α_s
- renormalisation scale dependence (μ)
- non-perturbative effects (np);

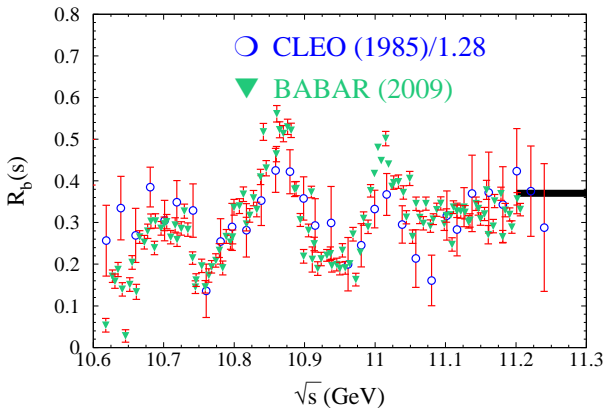
Operator product expansion:

$$\Pi(q^2) = \Pi_{\text{perturbative}}(q^2) + C_{\psi\bar{\psi}} \langle \psi\bar{\psi} \rangle + C_{G^2} \langle G^2 \rangle + \dots$$

Results for m_c : Comparison



Bottom threshold



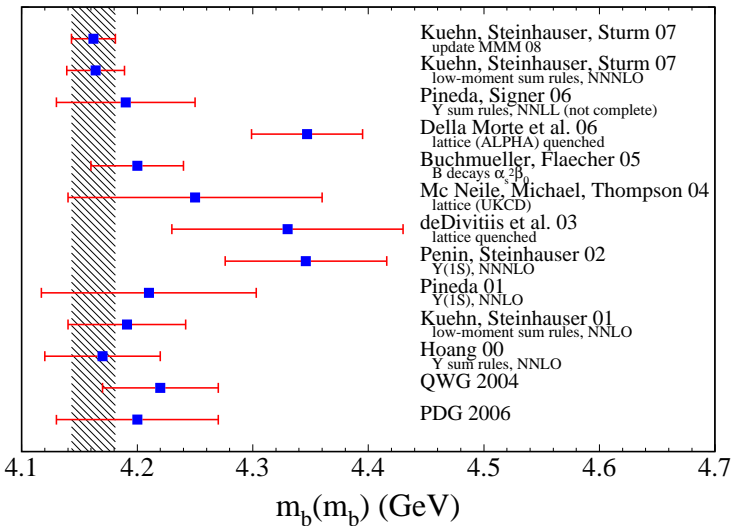
Barbar data from 2009 significantly reduced the error compared to m_b determinations from CLEO data.

Results for m_b

n	exp	α_s	μ	total	$m_b(10 \text{ GeV})$	$m_b(m_b)$
1	0.014	0.007	0.002	0.016	3.597	4.151
2	0.010	0.012	0.003	0.016	3.610	4.163
3	0.008	0.014	0.006	0.018	3.619	4.172
4	0.006	0.015	0.020	0.026	3.631	4.183

Note the discussion about m_b from sum rules vs. m_b from semi-leptonic B decays.

Results for m_b : Comparison



α_s and m_c from lattice QCD

Instead of experimental data for $R(s)$ one can use lattice QCD simulations to determine α_s and m_c .

Pseudoscalar current correlator is best suited. [HPQCD & Karlsruhe] (really?)

Experimental input: m_π^2 , $2m_K^2 - m_\pi^2$, m_{η_c} , m_Υ

$$\alpha_s(M_Z) = 0.1174(12)$$

nice agreement with other determinations

$$m_c(3 \text{ GeV}) = 0.986(10) \text{ GeV}$$

perfect agreement with determinations from $R(s)$

Correlators of non-diagonal currents are of interest for future applications.

Conclusion

- Current correlators in combination with $R(s)$ or lattice data allow for precise determinations of quark masses
- A combination of reduction techniques for Feynman integrals led to the calculation of the second and third moment of current correlators at four loops
- Full energy dependence can be reconstructed by Padé approximations
- Results led to the most precise values for the charm and bottom quark masses up to date
- Don't rely only on C_1 , higher moments are crucial for consistency checks