Perturbative versus non-perturbative decoupling of heavy quarks

ALPHA **Collaboration**

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We simulate a theory with $N_f = 2$ heavy quarks of mass M. At energies much smaller than M the heavy quarks decouple and the theory can be described by an effective theory which is a pure gauge theory to leading order in $1/M$. We present results for the mass dependence of ratios such as $t_0(M)/t_0(0)$. We compute these ratios from simulations and compare them to the perturbative prediction. The latter relies on a factorisation formula for the ratios which is valid to leading order in $1/M$.

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1. Decoupling of heavy quarks

At low energies $E \ll M$ heavy quarks of mass M decouple. Their effects can then be described by an effective theory [1]. The leading order of this effective theory is a theory where the heavy quarks are removed. Corrections to the leading order in the effective theory involve power corrections $(E/M)^n$ with $n \geq 2$. The heavy quarks leave traces through the renormalization of the gauge coupling and the power corrections. In this contribution we discuss the renormalization effects. Power corrections are discussed in [2, 3].

We consider QCD with N_q quarks and denote its Lambda parameter by Λ_q. We will use the $\overline{\text{MS}}$ scheme. N_l quarks are light and we set their mass to zero in the following. $N_q - N_l$ quarks are heavy and their renormalization group invariant (RGI) mass is M (for its definition see Section 3). The Lagrangian of the effective theory $\mathscr{L}_{\text{dec}}$ is defined only in terms of N_l light quarks and is given by a series in $1/M$

$$\mathscr{L}_{\text{dec}} = \mathscr{L}_{\text{QCD}_{N_l}} + (1/M)^2 \sum_i \omega_i \Phi_i + O((\Lambda_q/M)^4). \tag{1.1}$$

Here Φ_i are fields of dimension 6 and ω_i are dimensionless parameters. At leading order the effective theory is QCD with N_l massless quarks. QCD_{N_l} has only one free parameter, namely the gauge coupling which we denote by $\bar{g}_l(\mu/\Lambda_l)$. One can specify either a value for the coupling at some scale μ or equivalently the Lambda parameter. Matching at leading order the effective theory with N_l quarks to the full theory with N_q quarks (see Section 3) yields a relation $\Lambda_l = \Lambda_{\text{dec}}(M, \Lambda_q)$ which determines the Lambda parameter of QCD_{N_l} as a function of the heavy quark mass M and the Lambda parameter of QCD_{N_q}.

2. Factorisation formula

m^{had} denotes a hadron mass or a hadronic scale like $1/r_0$ [4] or $1/\sqrt{t_0}$ [5]. The non-perturbative matching condition is

$$m_q^{\text{had}} = m_l^{\text{had}} + O((\Lambda_q/M)^2), \tag{2.1}$$

where m_q^{had} (m_l^{had}) is the hadron mass computed in QCD_{N_q} (QCD_{N_l}). Eq. (2.1) leads to the factorisation formula [2]

$$\frac{m_q^{\text{had}}(M)}{m_q^{\text{had}}(0)} = Q_{l,q}^{\text{had}} \times P_{l,q}(M/\Lambda_q) + O((\Lambda_q/M)^2), \tag{2.2}$$

where

$$P_{l,q}(M/\Lambda_q) = \frac{\Lambda_l}{\Lambda_q} \tag{2.3}$$

and

$$Q_{l,q}^{\text{had}} = \frac{m_l^{\text{had}}/\Lambda_l}{m_q^{\text{had}}(0)/\Lambda_q}. \tag{2.4}$$

The factor $P_{l,q}$, Eq. (2.3), can be computed in perturbation theory and depends on M. It is universal in the sense that it does not depend on the hadronic scale. The factor $Q_{l,q}^{\text{had}}$ Eq. (2.4) instead is non-perturbative and independent of M. It depends on the hadronic scale. The independence of M relies on the observation that $m_l^{\text{had}}/\Lambda_l$ is a pure number in QCD_{N_l}. Eq. (2.2) factorises the left hand side into a factor with a perturbative expansion and a non-perturbative, but M-independent factor.

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3. Perturbative matching

At leading order in $1/M$ matching imposes that observables computed in QCD_{N_q} are equal to observables computed in QCD_{N_l}. In perturbation theory this leads to a relation between the $\overline{\mathrm{MS}}$-couplings $\overline{g}_l(\mu/\Lambda_l)$ in QCD_{N_l} and $\overline{g}_q(\mu/\Lambda_q)$ in QCD_{N_q}:

$$\overline{g}_l^2(\mu/\Lambda_l) = \overline{g}_q^2(\mu/\Lambda_q) + \mathrm{O}(\overline{g}_q^4(\mu/\Lambda_q)). \tag{3.1}$$

We choose the renormalization scale $\mu = m_*$ [6, 7] defined through the condition

$$\overline{m}(m_*) = m_*, \tag{3.2}$$

where $\overline{m}(\mu)$ is the running quark mass. The relation Eq. (3.1) is known up to four loops [8, 9]:

$$\begin{aligned}\overline{g}_l^2(m_*/\Lambda_l) &= \overline{g}_q^2(m_*/\Lambda_q)\, C(\overline{g}_q(m_*/\Lambda_q)) \\ C(g) &= 1 + c_2 g^4 + c_3 g^6 + \dots \quad (c_1 = 0).\end{aligned} \tag{3.3}$$

The coefficients c_2 and c_3 can be found in [2]. In the following we use the notation $g_* = \overline{g}_q(m_*/\Lambda_q)$.

From the matching relation Eq. (3.3) we can compute the factor $P_{l,q}$ in Eq. (2.3). The definition of the Λ parameter in QCD with N_f quarks and running coupling $\overline{g}$ is

$$\Lambda = \mu \exp(I_g^{N_f}(\overline{g}(\mu))), \tag{3.4}$$

where $I_g^{N_f}(\overline{g}) = -\int^{\overline{g}} dx \frac{1}{\beta_{N_f}(x)}$. The β_{N_f} function has the perturbative expansion

$$\beta_{N_f}(\overline{g}) \overset{\overline{g}\to 0}{\sim} -\overline{g}^3\left\{b_0 + \overline{g}^2 b_1 + \dots\right\}; \quad b_0(N_f) = \frac{1}{(4\pi)^2}\left(11 - \frac{2}{3}N_f\right),\ b_1(N_f) = \frac{1}{(4\pi)^4}\left(102 - \frac{38}{3}N_f\right). \tag{3.5}$$

The precise definition of $I_g^{N_f}(\overline{g})$ is given by

$$\begin{aligned}\exp(I_g^{N_f}(\overline{g})) &= \left(b_0(N_f)\overline{g}^2\right)^{-b_1(N_f)/(2b_0(N_f)^2)} e^{-1/(2b_0(N_f)\overline{g}^2)} \\ &\times \exp\left\{-\int_0^{\overline{g}} dx \left[\frac{1}{\beta_{N_f}(x)} + \frac{1}{b_0(N_f)x^3} - \frac{b_1(N_f)}{b_0(N_f)^2 x}\right]\right\}.\end{aligned} \tag{3.6}$$

The factor $P_{l,q}$ in Eq. (2.3) is obtained from Eq. (3.4) and Eq. (3.3):

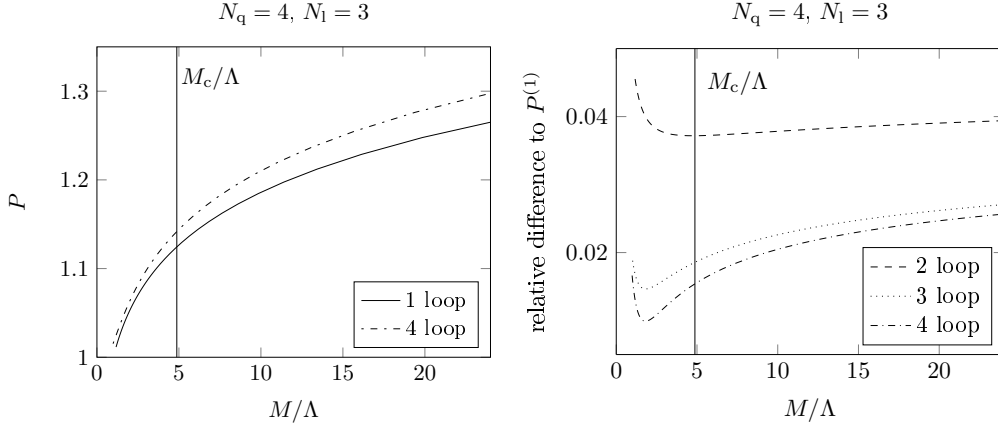$$P_{l,q}(M/\Lambda_q) = \exp\left\{I_g^{N_l}(g_*\sqrt{C(g_*)}) - I_g^{N_q}(g_*)\right\}, \tag{3.7}$$

where M is the RGI mass that corresponds to m_*.

In order to evaluate Eq. (3.7) we need to determine the coupling g_*. The renormalization group invariant quark mass M is defined from the renormalized running mass $\overline{m}(\mu)$ by

$$M = \overline{m}(\mu)\exp(I_m^{N_q}(\overline{g})), \tag{3.8}$$

where $I_m^{N_q}(\overline{g}) = -\int^{\overline{g}} dx \frac{\tau_{N_q}(x)}{\beta_{N_q}(x)}$. The τ_{N_q} function has the perturbative expansion

$$\tau_{N_q}(\overline{g}) \overset{\overline{g}\to 0}{\sim} -\overline{g}^2\left\{d_0 + \overline{g}^2 d_1 + \dots\right\}; \quad d_0 = 8/(4\pi)^2. \tag{3.9}$$

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Figure 1: Perturbative decoupling of the charm quark. The factor $P_{3,4}$ (left plot) and the corrections $(P_{3,4} - P_{3,4}^{(1)})/P_{3,4}^{(1)}$ for different loop orders relative to the one-loop "approximation" $P_{3,4}^{(1)} = (M/\Lambda)^{2/27}$ (right plot).

The precise definition of $I_m^{N_q}(\bar{g})$ is given by

$$\exp(I_m^{N_q}(\bar{g})) = (2b_0(N_q)\bar{g}^2)^{-d_0/(2b_0(N_q))} \exp\left\{ -\int_0^{\bar{g}} dx \left[\frac{\tau_{N_q}(x)}{\beta_{N_q}(x)} - \frac{d_0}{b_0(N_q)x} \right] \right\}. \quad (3.10)$$

Using Eq. (3.4) and Eq. (3.8) we obtain $(\mu = m_*)$

$$\frac{\Lambda_q}{M} = \exp\left\{ I_g^{N_q}(g_*) - I_m^{N_q}(g_*) \right\} = \exp\left\{ -\int^{g_*(M/\Lambda_q)} dx \, \frac{1 - \tau_{N_q}(x)}{\beta_{N_q}(x)} \right\}. \quad (3.11)$$

Inverting this relation determines the coupling g_* as a function of M/Λ_q which in turn allows to compute $P_{l,q}$ through Eq. (3.7). In the following we will use the notation $\Lambda \equiv \Lambda_q$.

For numerical applications we expand the integrands in Eq. (3.6) and Eq. (3.10) using Eq. (3.5) and Eq. (3.9) and we evaluate the integrals numerically. For the n-loop expression we set $b_i = 0$, $d_{i-1} = 0$ for $i \geq n$. A one-loop "approximation" is defined by setting $b_i = 0, i > 0, d_i = 0$:

$$P_{l,q}^{(1)} = (M/\Lambda)^{\eta_0}, \quad (3.12)$$

where $\eta_0 = 1 - \frac{b_0(N_q)}{b_0(N_l)} > 0$. In Fig. 1 we show the convergence of the perturbative expression for $P_{3,4}$, i.e., for the case of decoupling of the charm quark. The one-loop "approximation" is accidentally very close to the four-loop result. In the right plots of Fig. 1 we show the relative correction $(P_{3,4} - P_{3,4}^{(1)})/P_{3,4}^{(1)}$ where $P_{3,4}$ is computed to n-loops $(n = 2,3,4)$. The perturbative expansion appears to behave well even for the case of the charm quark, where one would not have necessarily expected it to be so. More details on the calculation of $P_{l,q}$ will be presented in [10].

4. Non-perturbative results

In order to check the factorisation formula Eq. (2.2) and the applicability of perturbation theory to compute the factor $P_{l,q}$ Eq. (3.7), we study a theory with $N_q = 2$ heavy quarks and compare it to Yang-Mills theory $(N_l = 0)$. We simulate $N_q = 2$ O(a) improved Wilson quarks [11] with plaquette gauge action. The ensembles are listed in Table 1. The simulations with periodic boundary

β	a [fm]	BC	$T \times L^3$	$M/\Lambda_{\overline{\text{MS}}}$	kMDU	τ_{exp}
5.3	0.0658(10)	p	64×32^3	0.638(46)	1.0	0.07
		p	64×32^3	1.308(95)	2.0	0.05
		p	64×32^3	2.60(19)	2.0	0.04
5.5	0.0486(7)	o	120×32^3	0.630(46)	8.5	0.15
		o	120×32^3	1.282(93)	8.1	0.12
		p	96×48^3	2.45(18)	4.0	0.10
5.7	0.0341(5)	o	192×48^3	0.587(43)	4.0	0.28
		o	192×48^3	1.277(94)	4.2	0.24
		o	192×48^3	2.50(18)	8.5	0.20

Table 1: The decoupling ensembles.

conditions (p) are done with the MP-HMC algorithm [12] and those with open boundary conditions (o) with the publicly available openQCD package [13]. We refer to [3] for further explanations.

We consider the scale $m^{\text{had}} = 1/\sqrt{t_0}$ defined from the Wilson flow [5]. The factorisation formula for its mass-dependence reads, cf. Eq. (2.2)

$$\sqrt{t_0(M)/t_0(0)} = 1/(P_{0,2} Q_{0,2}^{\sqrt{t_0}}) + \text{O}((\Lambda/M)^2) \tag{4.1}$$

We compute from the simulations $t_0(M)/a^2$ at three values of the heavy quark mass close to the target values $M_t/\Lambda = 0.59$, 1.28 and 2.50. They correspond to approximately $M_c/8$, $M_c/4$ and $M_c/2$ (M_c is the charm quark mass).

The RGI mass M and the ratio M/Λ are computed as explained in [3]. The data of the simulations in Table 1 are corrected for small mismatches compared to the target values M_t/Λ. This is done by fitting the $\beta = 5.7$ data to the form

$$t_0(M)/a^2 = s_1 (M/\Lambda)^\alpha . \tag{4.2}$$

We get $\alpha = -0.246(5)$ which is close to $-2\eta_0 = -0.242424$. The corrected values $t_0(M_t)$ are computed as

$$\ln(t_0(M_t)/a^2) = \ln(t_0(M)/a^2) + \alpha \ln(M_t/M) . \tag{4.3}$$

In order to keep the O(a) improved coupling $\tilde{g}_0^2 = (1 + b_g(g_0^2) N_q am) g_0^2$ fixed, we correct

$$t_0(M_t)/a^2 \longrightarrow (1 + 2 \times 0.098 N_q am) t_0(M_t)/a^2 , \tag{4.4}$$

where m is the PCAC mass.

In order to compute the ratio in Eq. (4.1) we need the value $t_0(0)/a^2$ in the chiral limit. The latter is known only for $\beta = 5.3$ and $\beta = 5.5$ from [14]. For our smallest lattice spacing $a(\beta = 5.7)$ we use

$$\sqrt{t_0(M)/t_0(0)}\Big|_{a(5.7)} \approx \sqrt{t_0(M)/t_0(M_{\text{ref}})}\Big|_{a(5.7)} \times \lim_{a \to a(5.7)} \sqrt{t_0(M_{\text{ref}})/t_0(0)}, \tag{4.5}$$

where the reference mass is chosen to be our lightest mass $M_{\text{ref}}/\Lambda = 0.59$. The limit in the second factor in Eq. (4.5) is computed by a linear extrapolation of the data $\sqrt{t_0(M_{\text{ref}})/t_0(0)}$ at $\beta = 5.3$ and
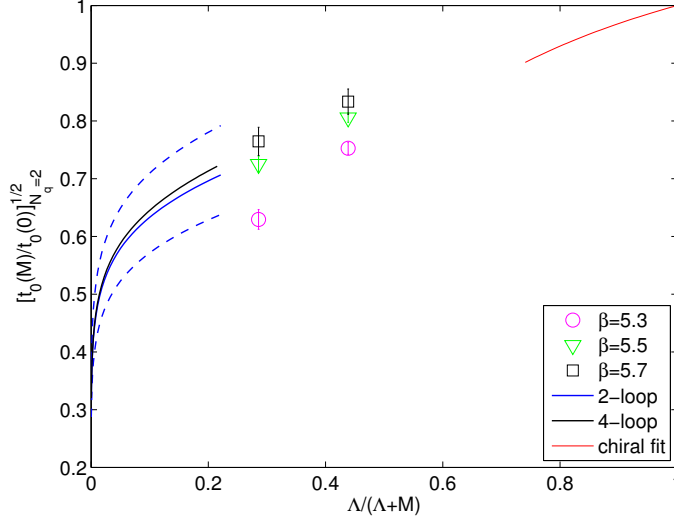
Figure 2: The mass dependence of the ratio $\sqrt{t_0(M)/t_0(0)}$.

5.5 as a function of $a^2/(8t_0(M_{\rm ref}))$. We add to the error of the extrapolation half of the difference between the $\beta = 5.7$ and $\beta = 5.5$ values. This error is added linearly to the total error in Eq. (4.5).

The results for the ratio $\sqrt{t_0(M)/t_0(0)}$ at $M_{\rm t}/\Lambda = 1.28$ and 2.50 are shown by the symbols in Fig. 2. We compare them to the factorisation formula Eq. (4.1), where the factor $P_{0,2}$ is computed to 2- (blue line) and 4-loops (black line). The error on the factorization formula comes from $Q_{0,2}^{\sqrt{t_0}} = [\sqrt{t_0(0)}\Lambda]_{N_q=2}/[\sqrt{t_0}\Lambda]_{N_q=0} \simeq 1.19(13)$ and is displayed by the dashed blue lines only for the 2-loop curve. The value of $Q_{0,2}^{\sqrt{t_0}}$ is obtained from $Q_{0,2}^{r_0} = [\Lambda r_0(0)]_{N_q=2}/[\Lambda r_0]_{N_q=0} = 1.30(14)$ known from previous works [15, 16] and $[\sqrt{t_0(0)}/r_0(0)]_{N_q=2}/[\sqrt{t_0}/r_0]_{N_q=0} \simeq 0.915$ from [17]. Within 10% accuracy, the perturbative prediction for the mass dependence of $\sqrt{t_0(M)/t_0(0)}$ agrees with our simulation results at $\beta = 5.7$ for masses of about half the charm quark mass. For completeness, in Fig. 2 the red line to the right shows the mass dependence in the chiral limit [17, 14].

5. Conclusions

Perturbation theory seems to be reliable for decoupling of heavy quarks at leading order in $1/M$ even at the charm quark mass. Our data from simulations of $N_q = 2$ O(a) improved Wilson quarks shown in Fig. 2 match the factorisation formula Eq. (2.2) for the mass dependence of hadronic scales. A careful continuum limit of the data in Fig. 2 will be addressed in the near future combined with twisted mass simulations.

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