On the effects of heavy sea quarks at low energies

(ALPHA collaboration)

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(Dated: October 31, 2014)

We present a factorisation formula for the dependence of light hadron masses and low energy hadronic scales on the mass M of a heavy quark: apart from an overall factor Q, ratios such as $r_0(M)/r_0(0)$ are computable in perturbation theory at large M. The mass-independent factor Q is obtained from the theory in the limit $M \to 0$ and the decoupled theory with the heavy quark removed. The perturbation theory part is stable concerning different loop orders and our non-perturbative results match on quantitatively to the perturbative prediction.

Upon taking ratios of different hadronic scales at the same mass, the perturbative function drops out and the ratios are given by the decoupled theory up to M^{-2} corrections. Our present numerical results are obtained in a model calculation where there are no light quarks and a heavy doublet of quarks is decoupled. They are limited to masses a factor two below the charm. This is not large enough to see the M^{-2} scaling predicted by the theory, but it is sufficient to verify – in the continuum limit – that the sea quark effects of quarks with masses around the charm mass are very small.

INTRODUCTION

One usually presumes that the low energy dynamics of QCD, such as the hadron mass spectrum, is rather insensitive to the physics of heavy quarks. One can then work with QCD with just the three or four light quarks in order to understand it.[1] While large N_c (color) arguments suggest a general suppression of quark loop effects, and then a particular one for heavy quarks, so far there has not been any non-perturbative investigation determining the typical magnitude of these effects. This is understandable, since lattice gauge theory with heavy quarks generically has enhanced discretisation errors and it is a non-trivial task to separate the physical effects from those unwanted errors. It is thus of high interest for the lattice community to understand whether it is already time to include a charm sea quark in the simulations. Note that one has to be precise about the meaning of the decoupling of heavy quarks [1, 2]. They do leave traces through renormalisation, which we discuss below.

The theoretical tool to understand these questions is the low energy effective theory [2, 3] describing the physics with one or more heavy quarks decoupled. We denote this theory by decQCD. The leading order effective theory is just QCD with one or more quark flavors

less. The gauge coupling $\overline{g}_{\mathrm{dec}}$ and quark masses of dec-QCD are adjusted such that decQCD (approximately) reproduces the physics of the (more) fundamental theory at an energy sufficiently below the mass of the decoupled quark [4]. This adjustment is referred to as matching.

We consider the situation with N_l light quarks and N_q quarks in total. Indicating the flavor content N_f of the theory by a subscript, the fundamental theory is QCD_{N_q}. The theory with only the light quarks is QCD_{N_l}. Hadronic quantities, the couplings and the Λ-parameters in these theories are distinguished by subscripts q and l.

In this letter we briefly present the effective theory from the non-perturbative point of view, discuss the perturbative matching of its parameters in terms of renormalisation group invariants (RGI) and point out the factorisation formula

$$\frac{m_q^{\mathrm{had}}(M)}{m_q^{\mathrm{had}}(0)} = Q_{l,q}^{\mathrm{had}} \times P_{l,q}(M/\Lambda_q) + \mathrm{O}((\Lambda_q/M)^2). \quad (1)$$

It gives the mass-dependence of hadron masses or hadronic scales such as r_0 [5] or t_0, w_0 [6, 7] in terms of two factors. The first factor, $Q_{l,q}^{\mathrm{had}}$, depends on the hadron mass or hadronic scale and involves only information from the theories with N_q and N_l mass-less quark flavors.[2] The second factor, $P_{l,q}(M/\Lambda_q)$, gives the relation of the Λ-parameters of these two theories, deter-

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[1] Of course, in higher energy processes the heavier quarks play a relevant role, e.g. in the fundamental parameters of QCD for LHC physics, or more generally the Λ-parameter of the 5-flavor theory.

[2] We here use the language of a theoretical situation where all light quarks are mass-less. Light quark masses can be added with trivial changes, such as additional arguments in several functions.

mined such that the low energy physics of the fundamental theory, $\mathrm{QCD}_{N_{\mathrm{q}}}$ with $N_{\mathrm{q}} - N_{\mathrm{l}}$ quarks of RGI mass M, is the same as the one of $\mathrm{QCD}_{N_{\mathrm{l}}}$ up to power corrections $\mathrm{O}((\Lambda_{\mathrm{q}}/M)^2)$. Throughout this letter we take the Λ-parameters to be defined in the $\overline{\mathrm{MS}}$ scheme, but this choice is irrelevant, namely Q, P have a trivial scheme dependence in regular schemes.[3] Interestingly, the asymptotics of $P_{\mathrm{l,q}}(M/\Lambda_{\mathrm{q}})$ for large mass M, is computable in perturbation theory. The formula thus provides a factorisation into a non-perturbative piece, Q, and a "perturbative" one. In particular, the mass-dependence is "perturbative". We here use quotation marks since the precise meaning is that the *asymptotics* is perturbative.

We further report on our investigation of the numerical precision of perturbation theory for P and then compare eq. (1) to a first non-perturbative investigation for $N_{\mathrm{q}} = 2$, $N_{\mathrm{l}} = 0$, which we expect to be a quite realistic model for real QCD. In this case, the lowest order effective theory is the Yang-Mills Theory, as long as we look at the gluonic sector only, which we do here. Finally we argue through our numerical simulations that the effects of a charm quark, which are missed by simulating just QCD with N_{l} quarks, are small in typical ratios of hadronic scales.

THE EFFECTIVE THEORY: decQCD

The leading order low energy effective theory is $\mathrm{QCD}_{N_{\mathrm{l}}}$. Next-to-leading order (NLO) correction terms in the local effective Lagrangian are gauge-, Euclidean- and chiral-invariant local fields. These invariances allow only for fields, $\Phi_i(x)$, of at least dimension six.[4] The Lagrangian may then be written as

$$\mathcal{L}_{\mathrm{dec}} = \mathcal{L}_{\mathrm{QCD}_{N_{\mathrm{l}}}} + \frac{1}{M^2} \sum_i \omega_i \Phi_i + \mathrm{O}(M^{-4}), \quad (2)$$

with dimensionless couplings ω_i which depend logarithmically on the mass M.

At the lowest order in $1/M$, a single coupling[5], $\bar{g}_{\mathrm{dec}}$, is adjusted such that the low energy physics of $\mathrm{QCD}_{N_{\mathrm{l}}}$ and $\mathrm{QCD}_{N_{\mathrm{q}}}$ match for energies $E \ll M$. It then suffices to require one physical low-energy observable to match,

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[3] In regular schemes the couplings are related to, say, the $\overline{\mathrm{MS}}$ one by $\bar{g}^2 = \bar{g}_{\overline{\mathrm{MS}}}^2 + \mathrm{O}(\bar{g}_{\overline{\mathrm{MS}}}^4)$.

[4] To be precise, we here assume that either $N_{\mathrm{l}} = 0$ where light quark fields are absent, or $N_{\mathrm{l}} \geq 2$ where there is a non-anomalous chiral symmetry in the light sector. The statement also holds for theories with light quark masses if we define light-quark mass-factors to be included in $\Phi_i(x)$. We thank Martin Lüscher for a clarification on the use of chiral symmetry in this context.

[5] Again we refer to the theoretical situation where the first N_{l} flavors are mass-less. In general, also the light quark masses have to be matched.

e.g. a physical coupling. Discussing the issue in perturbation theory [4], Bernreuther and Wetzel chose the MOM-coupling as a physical coupling and worked out the matching of the $\overline{\mathrm{MS}}$ coupling. Meanwhile, the matching of the latter is known to high perturbative order. We use this information below.

For now, we remain with the lowest order theory, i.e. all terms $\mathrm{O}(E^2/M^2)$ are neglected and the Lagrangian is $\mathcal{L}_{\mathrm{dec}} = \mathcal{L}_{\mathrm{QCD}_{N_{\mathrm{l}}}}$. We just make use of the fact that there is a single coupling, the gauge coupling $\bar{g}_{\mathrm{dec}}$. Specifying a renormalisation scheme, its β-function is fixed and the coupling is a unique function $\bar{g}_{\mathrm{dec}} = \bar{g}_{\mathrm{l}}(\mu/\Lambda_{\mathrm{l}})$, where μ is the renormalisation scale. Therefore the matching condition between $\bar{g}_{\mathrm{dec}}$ and $\bar{g}_{\mathrm{q}}$ is equivalent to a relation between the Λ-parameters. Considering only RGIs, the only additional parameter is the quark mass M of the fundamental theory. Therefore, we have to set

$$\Lambda_{\mathrm{l}} = \Lambda_{\mathrm{dec}}(M, \Lambda_{\mathrm{q}}) \quad (3)$$

in order to match the two theories. For dimensional reasons the unknown function Λ_{dec} can be written as

$$\Lambda_{\mathrm{dec}}(M, \Lambda_{\mathrm{q}}) = P_{\mathrm{l,q}}(M/\Lambda_{\mathrm{q}}) \Lambda_{\mathrm{q}}. \quad (4)$$

In general the Λ-parameter of an asymptotically free theory is a free, dimensionful, constant, which is to be fixed from outside, usually by matching the theory to experiment. In the present case, experiment for $\mathrm{QCD}_{N_{\mathrm{l}}}$ is replaced by $\mathrm{QCD}_{N_{\mathrm{q}}}$ where the overall energy scale Λ_{q} remains free as before.

The factorisation eq. (1) is a simple consequence of eq. (4): consider low energy scales of the theory, in particular hadron masses m^{had}. After matching (and neglecting terms of order $\Lambda_{\mathrm{q}}^2/M^2$) they are equal in the fundamental and in the effective theory, $m_{\mathrm{l}}^{\mathrm{had}} = m_{\mathrm{q}}^{\mathrm{had}}$. We note further, that in $\mathrm{QCD}_{N_{\mathrm{l}}}$ there are no mass parameters, the only scale is Λ_{l} and hence hadron masses are $m_{\mathrm{l}}^{\mathrm{had}} = \rho^{\mathrm{had}} \Lambda_{\mathrm{l}}$ with pure numbers ρ^{had}. Thus $m_{\mathrm{l}}^{\mathrm{had}}/\Lambda_{\mathrm{l}}$ is independent of M. In the fundamental theory $m_{\mathrm{q}}^{\mathrm{had}}(M)/\Lambda_{\mathrm{q}}$ does of course depend on M, but Λ_{q} is by definition independent of M. Together these facts entail the relation eq. (1) with

$$Q_{\mathrm{l,q}}^{\mathrm{had}} = \frac{m_{\mathrm{l}}^{\mathrm{had}}/\Lambda_{\mathrm{l}}}{m_{\mathrm{q}}^{\mathrm{had}}(0)/\Lambda_{\mathrm{q}}} \quad (5)$$

defined entirely through the two mass-less theories.

Even though the physics of the two theories is matched at energy scales far below the mass, the perturbative matching of the couplings is in fact best done with a renormalisation scale μ of the order of the mass [2, 4]. Higher order perturbative corrections then vanish asymptotically as $M \to \infty$ and the matching of the couplings is indeed perturbative. This entails that $P_{\mathrm{l,q}}$ can be computed in perturbation theory when the mass is large.

The Bernreuther-Wetzel relation between the $\overline{\text{MS}}$ couplings $\bar{g}_{\text{dec}} = \bar{g}_1(m_*/\Lambda_l)$ and $\bar{g}_q \equiv \bar{g}_q(m_*/\Lambda_q)$ is meanwhile known to four loops [8, 9],

$$\bar{g}_{\text{dec}}^2 = \bar{g}_q^2 \times \left[1 + c_2\bar{g}_q^4 + c_3\bar{g}_q^6 + \ldots\right],\qquad(6)$$

where $c_2 = (N_q - N_l)\frac{11}{72}(4\pi^2)^{-2}$, and $c_3 = \left[\frac{572437}{62208} - \frac{84185}{13824}\zeta_3 - \frac{2633}{15552}N_l\right](4\pi^2)^{-3}$ for $N_q - N_l = 2$, and $c_3 = \left[\frac{564731}{124416} - \frac{82043}{27648}\zeta_3 - \frac{2633}{31104}N_l\right](4\pi^2)^{-3}$ for $N_q - N_l = 1$. In this relation, the $c_1\bar{g}_q^2$ term in the brackets is missing since c_1 vanishes for our choice of renormalisation scale, $\mu = m_*$, where m_* satisfies $\overline{m}_{\overline{\text{MS}}}(m_*/\Lambda_q) = m_*$ with $\overline{m}_{\overline{\text{MS}}}$ the quark mass in the $\overline{\text{MS}}$ scheme.

From now on we suppress indices l, q on Λ and $\bar{g}$, since the effective theory only appears implicitly through the previously defined quantities Q, P. We define a renormalisation group invariant mass scaling function by the logarithmic derivative $(P'(x) = \frac{d}{dx}P(x))$

$$\eta^{\text{M}}(M) \equiv \frac{M}{P}\frac{\partial P}{\partial M}\bigg|_\Lambda = \frac{M}{\Lambda}\frac{P'}{P} \stackrel{M\to\infty}{\sim} \eta_0 + \eta_1^{\text{M}}\bar{g}^2 + \ldots\,(7)$$

with respect to the RGI mass M. Just like M itself, $\eta^{\text{M}}(M)$ is independent of the scheme. Residual dependences only result when it is evaluated approximately, e.g. at a finite order of perturbation theory. We worked out its perturbative expansion [10], using eq. (6) and the known expansions of the QCD β-function and the mass anomalous dimension in the $\overline{\text{MS}}$ scheme up to 4-loop [11–14]. Here we only report

$$\eta_0 = 1 - \frac{b_0(N_q)}{b_0(N_l)} > 0,\qquad(8)$$

$$\eta_1^{\text{M}} = -\frac{b_0(N_q)}{b_0(N_l)}\left(\frac{b_1(N_q)}{b_0(N_q)} - \frac{b_1(N_l)}{b_0(N_l)}\right) - \frac{\eta_0}{2\pi^2},\quad(9)$$

with $b_0(n) = (11 - 2n/3)/(4\pi)^2$, $b_1(n) = (102 - 38n/3)/(4\pi)^4$ and refer the reader to [10] for the general expressions and details of the perturbation theory. Integrating eq. (7) gives an asymptotic expression $(\tau = \log(M/\Lambda))$

$$P = \frac{1}{k}\exp(\eta_0\tau)\,\tau^{\eta_1^{\text{M}}/2b_0(N_q)} \times \left(1 + \text{O}\!\left(\frac{\log\tau}{\tau}\right)\right),(10)$$

where the constant k is fixed by our conventions for the Λ parameter and the RGI mass M [15] to $\log k = \frac{b_1(N_q)}{2(b_0(N_q))^2}\log 2 - \frac{b_1(N_l)}{2(b_0(N_l))^2}\log(2b_0(N_q)/b_0(N_l))$. It turns out that in the $\overline{\text{MS}}$ scheme the higher order corrections to η^{M} as well as the function P are very small as far as they are known, namely up to an impressive 4-loop level, $\eta_3^{\text{M}}g^6$. We discuss an example below.

We now turn to a non-perturbative investigation of the question how well the mass-dependence at intermediate masses M matches onto the asymptotic perturbative prediction. For this purpose we simulate a model, namely QCD with two heavy, mass-degenerate quarks. The effective theory, decQCD, then is the Yang-Mills theory up to $1/M^2$ corrections $(N_q = 2, N_l = 0)$.
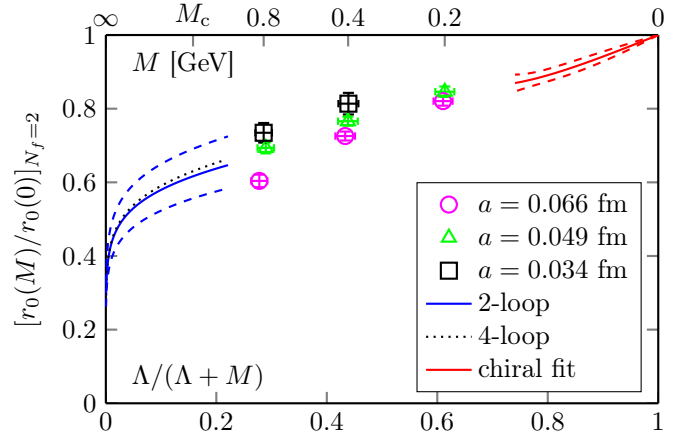

FIG. 1. The mass-dependence of $r_0(M)/r_0(0)$ in the $N_f = 2$ theory. Monte Carlo data (symbols) are compared with the perturbative predictions for $1/(QP)$ at large M. A fit to data close to the chiral limit is also shown.

In Monte Carlo simulations of QCD with $N_f = 2$ mass-degenerate O(a) improved Wilson fermions [16] we compute hadronic scales, e.g. $r_0(M)/a$, at three values of the lattice spacing $a = 0.066\,\text{fm}$, $0.049\,\text{fm}$ and $0.034\,\text{fm}$. The RGI mass M is obtained along the lines of [17]. For details about the numerical computations, performed with MP-HMC [18], openQCD [19] and the package https://github.com/to-ko/mesons, and the methods applied we refer to [10, 20].

For the hadronic scale r_0 [5], eq. (1) takes the form $r_0(0)/r_0(M) = Q \times P(M/\Lambda) + \text{O}((\Lambda/M)^2)$ with $Q = [\Lambda r_0(0)]_{N_f=2}/[\Lambda r_0]_{N_f=0}$. The ratios $r_0(M)/r_0(0)$ for $N_f = 2$ are plotted in figure 1 as a function of $\Lambda/(\Lambda+M)$. The value $r_0(0)/a$ in the chiral limit is taken from [17] for $a = 0.066\,\text{fm}$ and $0.049\,\text{fm}$, and we estimate it to $13.06(42)$ at $0.034\,\text{fm}$.

The red curve in figure 1 shows the mass-dependence close to the chiral limit as fitted in [17] with the dashed red lines representing the error of the fit. At large M/Λ the blue curve in figure 1 is drawn using the 2-loop perturbative formula for P in eq. (10) and $Q = 0.789(52)/0.602(48) = 1.30(14)$ known from previous work [15, 17]. The dashed blue lines represent the uncertainty of Q. The dotted black curve is drawn using the 4-loop value of P and shows that higher perturbative orders are very small. They are negligible in comparison to the uncertainty of Q. As our present non-perturbative results, we take the values at the smallest lattice spacing ($a = 0.034\,\text{fm}$). For $M/\Lambda = 2.50$ or $M \approx 0.8\,\text{GeV}$, a rather modest value of the mass, these are consistent with the (upper error bar of the) factorisation curve. Thus within our precision, the perturbative prediction is verified.

By discretizing the derivative in eq. (7) as $\eta^{\text{M}} \approx \log(r_0(M_2)/r_0(M_1))/\log(M_2/M_1)$ we obtain from our simulations numerical estimates of η^{M}. Their values are
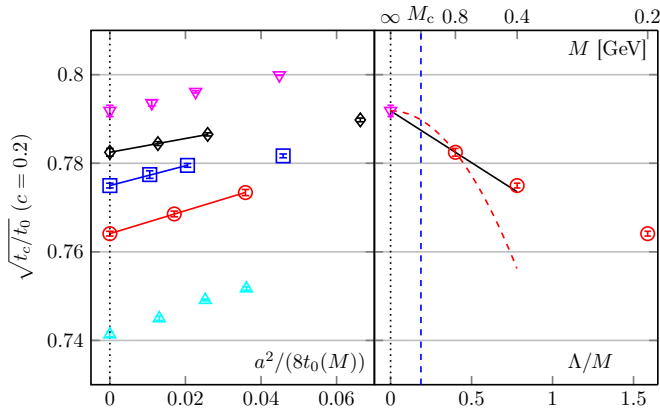
FIG. 2. Left: The continuum extrapolation of the ratio $\sqrt{t_c/t_0}$ ($c = 0.2$) at mass values (from top to bottom) $M/\Lambda = \infty$, 2.5, 1.28, 0.63, 0. Right: Its mass-dependence including a linear and quadratic interpolation in Λ/M between the largest mass and $N_f = 0$ ($M/\Lambda = \infty$).

between 0.12 and 0.17 and are very close to perturbation theory, $\eta_0 \approx 0.12$. A more precise statement needs a careful continuum limit, both for η^M and in figure 1. The lattice community should address this issue in the near future.

POWER CORRECTIONS $O(\Lambda^2/M^2)$

So far we have discussed a comparison of the full theory to the prediction of the factorisation formula resulting from the lowest order effective theory. When we take ratios of different hadron masses or different hadronic scales, the function $P(M/\Lambda)$ drops out and we have access to the $O(\Lambda^2/M^2)$ power corrections without any perturbative uncertainties. We consider ratios

$$R = \sqrt{t_0}/w_0\,,\; r_1/r_0\,,\; r_0/\sqrt{t_0}\,,\; \sqrt{t_c/t_0} \qquad (11)$$

where the scale t_c is defined through the smoothed action density [6] $E(t)$ via $t_c^2\langle E(t_c)\rangle = c$ with $c = 0.2$. It is a shorter distance cousin of t_0 [6].

We target the mass values $M/\Lambda = 0.63$, 1.28, 2.50 which correspond approximately to 0.2, 0.4, 0.8 GeV. For comparison the RGI charm mass $M_c \approx 1.6\,\text{GeV}$ [21]. We correct the ratios R for small differences between the targeted and the simulated values of the masses. In the corrections we neglect the error on M/Λ since it mainly comes from Λ and is therefore common to all points.

Our continuum extrapolations are performed by global fits,

$$R_{\text{Lat}} = R(M) + s\frac{a^2}{8t_0}\left(1 + k_1\frac{M}{\Lambda} + k_2\frac{M^2}{\Lambda^2}\right)\,, \quad (12)$$

to all the data. Where it is known, we fix the slope s (which describes the mass independent cut-off effects)

from its value determined at $M = 0$, cf. [22]. As a representative case, we show in figure 2 (left) the global fit for $R = \sqrt{t_c/t_0}$. The slope $s = 0.295$ has been determined from a continuum extrapolation of $\sqrt{t_c/t_0}$ in the chiral limit (cyan upward-facing triangles). Our fits yield k_2 compatible with zero. We drop it for our preferred continuum extrapolation, which then gives $k_1 = -0.19(6)$ and an excellent quality of the fit. The continuum limit values are very precise and allow to determine the size of the mass effects in the ratio R. For comparison, the magenta downward-facing triangles in figure 2 are the results for $N_f = 0$, which according to eq. (1) is recovered in the limit $M/\Lambda \to \infty$.

In figure 2 (right) we plot the values $R(M)$ (red circles) together with $R(\infty)$ in the $N_f = 0$ Yang-Mills theory (magenta downward-facing triangle). While the effective theory expectation is a roughly quadratic behavior in Λ/M, the full theory results are approximately linear in that variable. The natural explanation – since we do not have any doubt about the validity of the effective theory description – is that the masses of our simulations are not yet large enough to be described by NLO decQCD (Yang-Mills plus $1/M^2$ corrections). Taking the largest mass and the $N_f = 0$ value we can obtain by simple linear interpolation in $1/M$ (black line) and $1/M^2$ (red dashed line) two estimates of the mass effects at the charm mass marked by the blue vertical dashed line.

The dynamical fermion effects of these heavy quarks are very small and it is hence expected that they are strongly dominated by the contribution of a single fermion-loop (but non-perturbative in $\bar{g}$ and after renormalisation). As a result one expects a rather linear dependence on N_f. Since the relevant effect for physics is the contribution of a single heavy quark, we rescale the relative mass effect as ($N_f = 2$)

$$\frac{1}{N_f}\frac{R(M) - R(\infty)}{R(\infty)}\,. \qquad (13)$$

These numbers are listed in table I for the ratios in eq. (11).

CONCLUSIONS

In conclusion, we pointed out the factorisation formula eq. (1) for the dominating dependence of low energy dimensionful quantities such as hadron masses on the mass of a heavy (dynamical) quark. In perturbation theory, the power law $P \sim (M/\Lambda)^{\eta_0}$ is a very good approximation and we find that the non-perturbative dependence is also rather close to that law for quark masses around $\frac{1}{2}M_c \ldots \frac{1}{4}M_c$. The knowledge of this mass-dependence is expected to provide valuable information for tuning heavy quark masses to the correct point in future lattice QCD computations. We emphasise that our results are entirely sufficient to get the qualitative picture. At

$M/\Lambda \to$	M_c/Λ		2.50	1.28	0.63	0
R	$1/M$-scaled	$1/M^2$-scaled				
$\sqrt{t_0}/w_0$	0.34(5)%	0.16(2)%	0.72(11)%	1.26(12)%	2.62(14)%	5.4%
$\sqrt{t_c/t_0}$	0.28(3)%	0.13(1)%	0.59(6)%	1.06(3)%	1.74(3)%	3.2%
r_1/r_0	0.45(13)%	0.21(6)%	1.0(3)%	1.8(5)%	2.6(6)%	$\approx 4.0\%$
$r_0/\sqrt{t_0}$	0.05(28)%	0.02(12)%	0.1(6)%	0.7(5)%	1.7(5)%	3.0%

TABLE I. Relative effects eq. (13) for the ratios in eq. (11). At M_c we quote the results from interpolations in $1/M$ and $1/M^2$, see figure 2.

the quantitative level, they are limited to an accuracy of around 10%, both because of the limited precision in the mass-less theory and because we have not yet taken a true continuum limit for the finite mass points in figure 1. At least the latter should be improved soon. In principle one also has to worry about power corrections to the factorisation formula, but table I shows that these are irrelevant at the present level of precision.

The dominating effect in figure 1 originates from the mass-dependence of the gauge coupling in the effective theory. It therefore disappears in dimensionless ratios of low energy scales at fixed mass M and only leaves residual power law effects. The effective theory analysis predicts those to be of the form M^{-2} for large M. Our investigation of these power corrections has been restricted to $M \leq \frac{1}{2}M_c$. Larger masses require smaller lattice spacings, larger lattices and (due to critical slowing down) larger statistics. However, in the accessible region we have precise results. Phenomenologically they are described by an approximate M^{-1} law. We therefore interpolated between the largest simulated mass and the Yang-Mills theory to the charm mass as M^{-n} with both $n = 1$ and $n = 2$. It seems safe to assume that the true results will be in between. In any case, the thus interpolated effects are very small, between 1 and 6 permille (table I). This provides a message for today's dynamical fermion simulations. Dynamical charm effects are relevant only when one has very good precision, a very small lattice spacing and/or physical observables sensitive to higher energy scales.

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