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Effective heavy-light meson energies in small-volume quenched QCD

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Abstract: We study effective energies of heavy-light meson correlation functions in lattice QCD and a small volume of $(0.2\ \mathrm{fm})^4$ to non-perturbatively calculate their dependence on the heavy quark mass in the continuum limit. Our quenched results obtained here constitute an essential intermediate step of a first fully non-perturbative computation of the b-quark's mass in the static approximation that has recently been presented as an application of a new proposal to non-perturbatively renormalize the Heavy Quark Effective Theory. The renormalization constant and the improvement coefficients relating the renormalized current and subtracted quark mass are determined in the relevant parameter region at weak couplings, which allows to perform the numerical simulations at several, precisely fixed values of the renormalization group invariant heavy quark mass in a range from 3 GeV to 15 GeV.

Keywords: B-Physics, Heavy Quarks Physics, Lattice QCD.

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Contents

1. Introduction

During the last years, the elementary particle physics community has seen a growing interest and activity in the study of B-meson physics and its phenomenology. While on the experimental side this interest reflects in the various facilities that are currently running to explore CP-violation in the B-system [1, 2, 3], it is nourished on the theoretical side by the demand to determine transition matrix elements of the effective weak hamiltonian in order to interpret the experimental observations within (or beyond) the standard model and to (over-)constrain the unitarity triangle. For the computations of such matrix elements between low-energy hadron states to become valuable contributions in this field, they have to be carried out non-perturbatively, which is the domain of QCD on the lattice. However, in contrast to light quarks which as widely spread objects are predominantly exposed to large-volume limitations, heavy quarks are extremely localized ($1/m_{\mathrm{b}} \simeq 1/(4\,\mathrm{GeV}) \simeq 0.04$ fm) and thus also require very fine lattice resolutions, because otherwise one would face huge discretization errors. Mainly for this reason, realistic simulations of heavy-light systems involving a b-quark (even in the quenched approximation) are impossible so far [4].

A theoretically very appealing way out of this restriction is to recourse to the *Heavy Quark Effective Theory (HQET)* [5, 6]. This comes at a prize, though. As a consequence of its different renormalization properties, physical quantities deriving from expectation values calculated in the effective theory are affected by power-law divergences in the lattice spacing that can not be subtracted perturbatively in a clean way: the continuum limit ceases to exist, unless the theory is renormalized non-perturbatively [7].

Only recently, an approach to overcome these deficiencies has been developed from a solution for the problem of a completely non-perturbative computation of the b-quark mass in the static approximation *including* the power-divergent subtraction [8] to a new method addressing the general class of renormalization problems in HQET [9]. At its root stands the insight that these power-law divergences can be removed by a *non-perturbative matching procedure to relativistic QCD in a finite volume.* In fact, the *smallness* of the physical volume represents a characteristic feature in this strategy — since only then one is capable to incorporate and simulate the b-quark as a relativistic fermion — and motivates the investigation of QCD observables in a small-volume setup presented in this work. Here we will concentrate on the non-perturbative heavy quark mass dependence of effective heavy-light meson energies in the continuum limit, whose numerical knowledge is crucial to apply the proposal of ref. [9] to the determination of the b-quark's mass in leading order of HQET.[1] An extension to also examine the mass dependence of a few more quantities, which aims at quantitative non-perturbative tests of HQET by comparing static results with those obtained along the large quark mass limit in small-volume QCD, is in progress [12].

In section 2 we first recall the main ideas of the general matching strategy between HQET and QCD of ref. [9] (section 2.1), then introduce our observables considered (section 2.2) and finally describe how these can be calculated as functions of the (renormalized) mass of the heavy quark by numerical simulations (section 2.3). Section 3.1 is devoted to some intermediate results on a renormalization constant and improvement coefficients that are needed to renormalize the heavy quark mass in the relevant parameter range. Our central results on the mass dependence of the heavy-light meson energies are discussed in section 3.2, and we conclude in section 4.

In the calculations reported here we still stay in the quenched approximation. We want to emphasize, however, that this study of the heavy quark mass dependence of suitable observables (as an important part of the general non-perturbative approach to HQET of [9]) can be expected to be numerically implementable as well for QCD with dynamical fermions at a tolerable computing expense, because on basis of the experiences made in refs. [13, 14] the use of the QCD Schrödinger functional brings us in a favourable position where in physically small to intermediate volumes dynamical simulations are definitely easier than with the standard formulation.

2. Computational strategy

For the rest of this paper we will focus on meson observables derived from heavy-light correlation functions in finite volume and their dependence on the heavy quark mass in the continuum limit. Before we explain in detail how this dependence can be singled out in an actual numerical computation, we want to clarify the special rôle of QCD in a *finite* volume as a material component of the more general idea advocated in ref. [9] to non-perturbatively renormalize HQET; therefore, it suggests itself to briefly summarize this idea in the first subsection.

[1] For another method to determine $m_{\rm b}$ and $F_{\rm B}$, which also starts from lattice QCD in small volume but employs extrapolations of finite-volume effects in the heavy quark mass, see refs. [10, 11].

2.1 From QCD in small volume to non-perturbatively renormalized HQET

A long-standing problem with lattice computations in HQET is the occurrence of power-law divergences during the renormalization process (cf. refs. [15, 16, 17]), implied by the allowed mixings of operators of different dimensions coming with coefficients $\{c_k\}$ that contain inverse powers of the lattice spacing a. At each order of the HQET expansion parameter ($1/m$, where m is the heavy quark mass), new such free parameters c_k arise, which in principle are adjustable by a matching to QCD; but owing to incomplete cancellations when performing this matching only in perturbation theory, one is always left with a perturbative remainder that still stays divergent as $a \to 0$. Therefore, the continuum limit does not exist.

Already HQET in leading order, the static approximation, exhibits this unwanted phenomenon. In this case the kinetic and the mass terms in the static action mix under renormalization and give rise to a local mass counterterm $\delta m \propto 1/a$, the self-energy of the static quark, which causes a linearly divergent truncation error if one relies on an only perturbative subtraction of this divergence. A prominent example for a quantity suffering from it is the b-quark mass itself: past computations in the static approximation [18] were limited to finite lattice spacings, and the continuum limit was impossible to reach.

A viable strategy to solve this severe problem of power divergences is provided by a *non-perturbative matching of HQET and QCD in finite volume* [8, 9]. To integrate the present work into the broader context of ref. [9], we reproduce the central line of reasoning here. Let us consider QCD consisting of (generically $N_{\rm f}-1$) light quarks and a heavy quark, typically the b-quark. In the effective theory, the dynamics of the heavy quark is governed by the HQET action, which formally is an expansion in inverse powers of the heavy quark mass. (For further details see e.g. section 2 of ref. [9].) On the renormalized level, the effective theory discretized on a lattice can be defined in terms of parameters $\{c_k\}$ that comprise those specifying the light quark sector (e.g. the bare gauge coupling, $g_0^2 \equiv c_1$, and the masses of the light quarks) and coefficients of local composite fields in the $1/m$-expansion of the lattice action, supplemented by further coefficients belonging to local composite operators which will be needed when including their correlation functions into the renormalization program. In other words, if these parameters are chosen correctly, HQET and QCD are expected to be equivalent in the sense that $\Phi^{\rm HQET}(M) = \Phi^{\rm QCD}(M) + {\rm O}(1/M^{n+1})$ holds for suitable observables Φ in both theories, where for simplicity only the dependence on the heavy quark mass, here represented by the scheme and scale independent (and thus theoretically unambiguous) renormalization group invariant quark mass, M, is stressed. Now suppose that in some way the parameters of QCD have already been fixed to proper values. Then the parameters $\{c_k\}$ in the effective theory may just be determined through its relation to QCD by requiring a set of matching conditions:

$$\Phi_k^{\rm HQET}(L,M) = \Phi_k^{\rm QCD}(L,M)\,, \qquad k = 1,\ldots,N_n\,. \tag{2.1}$$

In this equation, the index k labels the elements of the parameter set $\{c_k\}$ defining the effective theory up to $1/M^{n+1}$-corrections (where, for instance, the additive mass renormalization δm mentioned above is amongst them), and the conditions (2.1) determine the

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c_k for any value of the lattice spacing. Moreover, we have already indicated the dependence of the observables Φ_k in eq. (2.1) on another variable which will become important in the following: the linear extent L of a *finite* volume.

To substantiate this L-dependence, we note that in order to circumvent the difficulties with the power-law divergences from the start, the matching equations (2.1) are understood as *non-perturbative conditions* in which both sides are to be calculated with the aid of numerical simulations. From the practical point of view, this in turn also means that one must be able to simulate the b-quark as a relativistic fermion. Hence, the linear extent L of the matching volume (i.e. where eq. (2.1) should hold) has to be chosen with care. On the one hand, it should fulfill $LM \gg 1$ to apply HQET quantitatively on the l.h.s. of (2.1), i.e. to suppress $1/m$-corrections, and on the other hand one has to ensure $aM \ll 1$ on the r.h.s. to treat the heavy quark flavour in the relativistic theory and avoid large lattice artifacts so that the continuum limit is under control. Taking these constraints together, while at the same time keeping the number of lattice points manageable for present-day computers, one then ends up with a volume for imposing the matching conditions (2.1) that is physically small; in our application later it will turn out to be of the order of $(0.2\ \mathrm{fm})^4$.

Having highlighted QCD in finite volume as key ingredient for the practical realization of the non-perturbative matching, we close this subsection with a few remarks on the subsequent (but not less important) steps that are involved to adopt it as a general approach for non-perturbative computations using the lattice regularized HQET. These steps, together with two applications of the proposal as a whole, are also worked out in ref. [9], which the reader should consult for a thorough discussion.

- Rather than directly identifying the quantities Φ_k entering (2.1) with physical, experimentally accessible observables (by which one would sacrifice the predictability of the effective theory), they must be properly chosen as renormalized quantities computable in the continuum limit of lattice QCD, which in turn necessitates the use of a small volume as explained before. Of course, their explicit form still depends on the application in question. One may think e.g. of hadronic matrix elements or, as in the computations reported in the following sections, effective masses (respectively, energies) that are deduced from the decay of two-point heavy-light correlation functions.

- Apparently, although these matching conditions to fix the parameters of HQET are perfectly legitimate (since the underlying lagrangian does not 'know' anything about the finite volume), one still has to make contact to a physical situation, where the interesting quantities of the infinite-volume theory can be extracted at the end. Employing the same lattice resolution as in the small volume computation, however, would again demand too many lattice points. This gap between the small volume with its fine lattice resolution on the one side and larger lattice spacings, and thereby also larger physical volumes, on the other is bridged by a recursive finite-size scaling procedure inspired by ref. [19]. As a result, the Φ_k^{HQET} are obtained at some larger volume of extent $L = \mathrm{O}(1\ \mathrm{fm})$, where the resolutions a/L are such that at the same lattice spacings (i.e. at the same bare parameters) volumes with $L \simeq 2\ \mathrm{fm}$ — to accommodate physical observables in the infinite-volume theory — are affordable.

- Finally, the approach requires a physical, dimensionful input. This usually amounts to relate the observables $\Phi_k^{\rm HQET}$ of the effective theory calculated in large volume to some experimental quantity. Which quantity this actually might be has to be decided when a concrete application is addressed. (E.g., in the application to compute $\overline{m}_{\rm b}$, it is the B-meson mass [9].)

2.2 Lattice setup and observables

In our investigation of QCD in a small volume we distinguish between a light ('l') and a heavy ('h') quark flavour. The lattice regularized theory is formulated in a Schrödinger functional (SF) cylinder of extent $L^3 \times T$ [20, 21]: the gluon and quark fields are subject to periodic (Dirichlet) boundary conditions in spatial (temporal) directions, and — if not explicitly stated otherwise — we assume $T = L$ from now on. In principle, the aforementioned matching strategy between HQET and QCD is not restricted to the SF as the only possible finite-volume scheme to treat the involved heavy-light systems in the relativistic theory, but in this way its practical implementation will much profit from known non-perturbative results on the renormalized quantities that will be needed in the following.

Starting from the $\mathrm{O}(a)$ improved heavy-light axial and vector currents,

$$(A_{\rm I})_\mu(x) = \overline{\psi}_{\rm l}(x)\gamma_\mu\gamma_5\psi_{\rm h}(x) + ac_{\rm A}\frac{1}{2}(\partial_\mu + \partial_\mu^*)\left\{\overline{\psi}_{\rm l}(x)\gamma_5\psi_{\rm h}(x)\right\}, \tag{2.2}$$

$$(V_{\rm I})_\mu(x) = \overline{\psi}_{\rm l}(x)\gamma_\mu\psi_{\rm h}(x) + ac_{\rm V}\frac{1}{2}(\partial_\nu + \partial_\nu^*)\left\{i\,\overline{\psi}_{\rm l}(x)\sigma_{\mu\nu}\psi_{\rm h}(x)\right\}, \tag{2.3}$$

(where numerical values for the coefficients $c_{\rm A}$ and $c_{\rm V}$ in the quenched approximation are taken from refs. [22, 23]), we construct their correlation functions in the SF [24, 25] as

$$f_{\rm A}(x_0) = -\frac{a^6}{2}\sum_{\boldsymbol{y},\boldsymbol{z}}\left\langle (A_{\rm I})_0(x)\overline{\zeta}_{\rm h}(\boldsymbol{y})\gamma_5\zeta_{\rm l}(\boldsymbol{z})\right\rangle, \tag{2.4}$$

$$k_{\rm V}(x_0) = -\frac{a^6}{6}\sum_{\boldsymbol{y},\boldsymbol{z},k}\left\langle (V_{\rm I})_k(x)\overline{\zeta}_{\rm h}(\boldsymbol{y})\gamma_k\zeta_{\rm l}(\boldsymbol{z})\right\rangle, \tag{2.5}$$

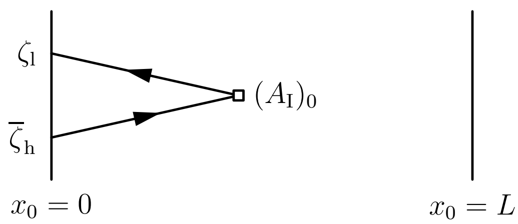

Figure 1: Illustration of the correlation function $f_{\rm A}$, while in $k_{\rm V}$ the insertion of $(A_{\rm I})_0$ is replaced by $(V_{\rm I})_k$.

schematically drawn in figure 1. Based on these, we define L-dependent energies in both channels by combining the usual forward and backward difference operators to take the logarithmic derivatives

$$\Gamma_{\rm PS}(L,M) \equiv -\frac{1}{2}\,(\partial_0 + \partial_0^*)\ln\left[\,f_{\rm A}(x_0,M)\right]\Big|_{x_0=L/2}, \tag{2.6}$$

$$\Gamma_{\rm V}(L,M) \equiv -\frac{1}{2}\,(\partial_0 + \partial_0^*)\ln\left[\,k_{\rm V}(x_0,M)\right]\Big|_{x_0=L/2}, \qquad T = L\,, \tag{2.7}$$

in which all multiplicative renormalization factors drop out. These observables also depend on the bare coupling, g_0, and — as the light quark mass is put to zero in the actual computations — on the heavy quark mass variable which, as already in section 2.1, one may conveniently set to be the *renormalization group invariant (RGI)* mass of the heavy quark, M. Having in mind the corresponding correlators in the effective theory, where in the static (i.e. infinite-mass) limit the two currents fall together owing to the heavy quark spin-symmetry, we also form their spin-averaged combination

$$\Gamma_{\rm av} \equiv \frac{1}{4}\left(\Gamma_{\rm PS} + 3\Gamma_{\rm V}\right), \tag{2.8}$$

which is expected to deviate from the static limit by the smallest $1/m$-corrections [9].

2.3 Determination of the heavy quark mass dependence

As mentioned before and detailed in refs. [8, 9], the non-perturbative matching between HQET and QCD can be applied to determine the mass of the b-quark in the static approximation. To achieve this goal, the quantities Φ_k in eq. (2.1) have to be identified with suitable observables that can be calculated by numerical simulations. Since we want to evaluate them in the continuum limit, we have to ensure a situation with fixed renormalized parameters, along which the limit $a/L \to 0$ may be performed. In regard of the (suppressed as well as indicated) dependences in the matching conditions (2.1), this means that for each value of L/a we have to make particular choices for the gauge coupling and the quark masses in the light and heavy sectors, respectively. The first two of them are immediately offered by

$$\Phi_1^{\rm HQET} = \bar{g}^2(L) = \text{constant}\,, \tag{2.9}$$
$$\Phi_2^{\rm HQET} = m_{\rm l} = 0\,, \tag{2.10}$$

where $\bar{g}^2$ denotes the renormalized finite-volume coupling in the SF scheme that runs with the box size L [26] and $m_{\rm l} \equiv m_{\rm l}^{\rm PCAC}$ is the PCAC current quark mass of the light flavour. These conditions allow to readily benefit from earlier work, because when fixing $\bar{g}^2$ to one of the values used for the (quenched) computation of the non-perturbative quark mass renormalization in [27], they translate into triples $(L/a, \beta = 6/g_0^2, \kappa_{\rm l})$ that can directly be taken over from this reference.[2]

For the computation of the b-quark's mass in leading order of HQET one yet needs one more condition in order to fix the parameter $a\delta m$ in the static lagrangian. Following [8, 9], the most natural candidates for this purpose are now the pseudoscalar and spin-averaged energies of the form (2.6) and (2.8) introduced in section 2.2. For $k = 3$, eq. (2.1) then turns into

$$L(\Gamma_{\rm stat} + m) \equiv \Phi_3^{\rm HQET}(L, M) = \Phi_3^{\rm QCD}(L, M) \equiv L\Gamma_{\rm X}\,, \tag{2.11}$$

where $\Gamma_{\rm X} = \Gamma_{\rm X}(L, M)$, $\mathrm{X} = \mathrm{PS}, \mathrm{av}$, are defined in *QCD and small volume with a relativistic b-quark* and carry the entire quark mass dependence. On the l.h.s., $\Gamma_{\rm stat}$ denotes the analogue of $\Gamma_{\rm X}$ in the effective theory, where the heavy quark entering the correlator (2.4) is treated in the static approximation, and implicitly contains the problematic, linearly divergent mass counterterm $a\delta m$. The matching equation (2.11) may be connected to a

[2] In this case the lattice action's hopping parameter associated with the light quark flavour, $\kappa_{\rm l}$, just equals the critical hopping parameter, $\kappa_{\rm c}$, as a consequence its very definition: $m_{\rm l}(\kappa_{\rm c}) = 0$, see ref. [27].

physical quantity in large volume (the B-meson mass [9]) by finite-size scaling (cf. section 2.1). But without going into further, unnecessary details we only note that this yields a (dimensionless) equation, which apart from $\Gamma_X(L,M)$ only contains energy differences computable in the static theory — such that the counterterm $a\delta m$ cancels out — and the experimental mass of the B-meson. Since all pieces in that equation can be evaluated non-perturbatively and in the continuum limit, the quantitative knowledge of $\Gamma_X(L,M)$ as a function of M in the relevant quark mass region finally allows to solve it for the desired numerical value of the non-perturbatively renormalized RGI mass of the b-quark, M_b, in the static approximation [9].

So the task is here to non-perturbatively determine the heavy quark mass dependence of the effective heavy-light meson energies $\Gamma_X(L,M)$. It thus remains to discuss how we fix the linear size of the finite volume, $L = L_0$, and a set of dimensionless quark mass values,

$$z \equiv L_0 M = \text{constant}\,, \tag{2.12}$$

at which the numerical computation of Γ_X for various lattice spacings takes place in practice.

We answer this question again on basis of the present numerical knowledge in the framework of the SF. Among the available constant values of the renormalized SF coupling that belong to different sets of triples $(L/a, \beta, \kappa_l)$ known from ref. [27] we fix, as was initially required by the condition (2.9),

$$\bar{g}^2\left(\frac{L_0}{2}\right) = 1.8811\,, \tag{2.13}$$

where the (inverse) lattice spacing varies within $6 \leq L_0/(2a) \leq 16$. This choice is particularly convenient, because from the same reference one then finds that L_0 is given in units of a certain maximal size, $L_{\max}$, of the SF box, namely

$$L_0 = \frac{L_{\max}}{2} = 0.36\,r_0 \approx 0.18 \text{ fm}\,, \tag{2.14}$$

which is implicitly defined by $\bar{g}^2(L_{\max}) = 3.48$ and, through its relation to the hadronic radius $r_0 = 0.5$ fm [28], also known in physical units: $L_{\max}/r_0 = 0.718(16)$ [29]. Indeed, from a closer inspection of the parameters corresponding to the condition (2.13) (see table 1) one may convince oneself that an accompanying volume of some small extent as (2.14) is a sensible compromise between the associated resolutions being small enough to comfortably accommodate a propagating (albeit the system size confining) b-quark and being able to consider heavy quark masses large enough to suppress $O(1/z)$-corrections (i.e. $z \gg 1$ but not too large to avoid a substantial enhancement of cutoff effects) as well as to cover the physical RGI b-quark mass scale itself.

In order to satisfy eq. (2.12) for the intended numerical values z while L/a and β are changed to approach the continuum limit, we still have to relate the RGI mass of the heavy quark, M, to the corresponding hopping parameter κ_h as the simulation parameter for the bare heavy quark mass in the lattice action. One possibility would be to employ the (O(a)

improved) relation between the RGI and the bare PCAC quark mass, m_{h}, viz.

$$M = \frac{M}{\overline{m}_{\mathrm{h}}(\mu_0)} \frac{Z_{\mathrm{A}}(g_0)(1+b_{\mathrm{A}}am_{\mathrm{q,h}})}{Z_{\mathrm{P}}(g_0,L_0)(1+b_{\mathrm{P}}am_{\mathrm{q,h}})} \times m_{\mathrm{h}} + \mathrm{O}\left(a^2\right) , \qquad \mu_0 = \frac{1}{L_0} , \tag{2.15}$$

where $\overline{m}_{\mathrm{h}}(\mu_0)$ denotes the running heavy quark mass renormalized at the scale $\mu_0 = 1/L_0$ in the SF scheme and (the inverse of) its *ratio* to the RGI mass M, the first factor on the r.h.s., is inferable from the literature as will be elaborated on after eq. (2.19). The numerator and denominator in the second factor account for the renormalization of the axial current and the pseudoscalar density in the $\mathrm{O}(a)$ improved theory, respectively. Here, the subtracted bare heavy quark mass is defined as usual by $m_{\mathrm{q,h}} = m_{0,\mathrm{h}} - m_{\mathrm{c}}$ with m_{c} the critical value of the bare quark mass $m_{0,\mathrm{h}}$, which in terms of the hopping parameters is given by $am_{\mathrm{q,h}} = \frac{1}{2}(\kappa_{\mathrm{h}}^{-1} - \kappa_{\mathrm{c}}^{-1})$. Although the involved renormalization factors are in principle known from refs. [27, 30] in the quenched case, this would demand additional simulations to appropriately tune κ_{h} — and thereby the PCAC mass m_{h} as a secondary quantity composed of correlation functions (cf. eq. (3.3)) — until the condition (2.12) is met with sufficient precision.

However, a safer (and also more economic) way to estimate κ_{h} such that a constant $z = L_0 M$ can be enforced in advance *without* any additional tuning runs is as follows. Recall that alternatively the renormalized quark mass can be written in terms of the $\mathrm{O}(a)$ improved subtracted bare quark mass, $\widetilde{m}_{\mathrm{q,h}}$, as

$$\overline{m}_{\mathrm{h}} = Z_{\mathrm{m}}\, \widetilde{m}_{\mathrm{q,h}} , \qquad \widetilde{m}_{\mathrm{q,h}} = m_{\mathrm{q,h}}(1+b_{\mathrm{m}}am_{\mathrm{q,h}}) , \tag{2.16}$$

where non-perturbative estimates on the improvement coefficient b_{m} and the finite combination of renormalization constants

$$Z(g_0) \equiv \frac{Z_{\mathrm{m}}(g_0,L)Z_{\mathrm{P}}(g_0,L)}{Z_{\mathrm{A}}(g_0)} \tag{2.17}$$

have been published in ref. [30] for the quenched approximation. The latter identity may then be used to eliminate the (in the SF scheme unknown) renormalization factor Z_{m} in eq. (2.16) in favour of numerically known ones. The decomposition of the RGI heavy quark mass analogous to (2.15) now assumes the form:

$$M = \frac{M}{\overline{m}_{\mathrm{h}}(\mu_0)} \frac{Z(g_0)Z_{\mathrm{A}}(g_0)}{Z_{\mathrm{P}}(g_0,L_0)} \times m_{\mathrm{q,h}}(1+b_{\mathrm{m}}am_{\mathrm{q,h}}) + \mathrm{O}\left(a^2\right) , \qquad \mu_0 = \frac{1}{L_0} . \tag{2.18}$$

The last piece to be addressed in this equation is the universal, regularization independent ratio of the RGI quark mass to the renormalized mass at fixed renormalization scale, which for later reference we call

$$h(L_0) \equiv \frac{M}{\overline{m}_{\mathrm{h}}(\mu_0)} , \qquad \mu_0 = \frac{1}{L_0} . \tag{2.19}$$

In a mass independent renormalization scheme such as the SF it is flavour independent and, according to ref. [27], can be expressed as

$$h(L_0) = \frac{Z_{\mathrm{P}}(L_0)}{Z_{\mathrm{P}}(2^{-6}L_{\mathrm{max}})} \times \left[2b_0\bar{g}^2(\mu)\right]^{-d_0/(2b_0)} \exp\left\{-\int_0^{\bar{g}(\mu)} \mathrm{d}g \left[\frac{\tau(g)}{\beta(g)} - \frac{d_0}{b_0 g}\right]\right\} \tag{2.20}$$

set	L/a	$\beta = 6/g_0^2$	κ_l	$\bar{g}^2(L/2)$	$\bar{g}^2(L)$	Z_P
A	12	7.4082	0.133961(8)	1.8811(22)	2.397(17)	0.6764(6)
B	16	7.6547	0.133632(6)	1.8811(28)	2.393(18)	0.6713(8)
C	20	7.8439	0.133373(2)	1.8811(22)	2.379(22)	0.6679(8)
D	24	7.9993	0.133159(4)	1.8811(38)	2.411(20)	0.6632(8)
E	32	8.2415	0.132847(3)	1.8811(99)	2.397(52)	0.6575(13)

Table 1: Our parameter sets that refer to the light quark sector and have fixed SF coupling, $\bar{g}^2(L/2) = 1.8811$. The parameters L/a, β and $\kappa_\mathrm{l} \equiv \kappa_\mathrm{c}$ of A, B, D and E are taken over from [27] without changes, whereas we performed new simulations to add with C a further lattice resolution for this work. Moreover, the renormalization constants $Z_\mathrm{P} = Z_\mathrm{P}(g_0, L/a)$ differ from those of [27] in that they have been computed in the context of [31] using the two-loop value [32] for the boundary improvement coefficient c_t.

with $L_0 = L_\mathrm{max}/2$, $\mu = 2^6/L_\mathrm{max}$ and b_0, d_0 the leading-order coefficients in the perturbative expansions of the renormalization group functions of the running coupling and quark mass, $\beta(\bar{g})$ and $\tau(\bar{g})$. In the ratio of Z_P-factors we encounter a scale evolution through changes by finite step sizes in the SF renormalization scale $L = 1/\mu$ that has been non-perturbatively computed in [27], whereas the remainder lives in the high-energy regime where the coupling is reasonably small to evaluate it in perturbation theory. Since in eq. (2.14) we just chose the linear extent L_0 of the small volume, where the non-perturbative matching to the relativistic theory is to be performed, as a proper multiple of the scale L_max, a numerical estimate for $h(L_0)$ in the continuum limit, eq. (2.19), can be directly extracted from the results already published in [27] and will be quoted in section 3.2 later on.

Our simulation parameters, which fix via eqs. (2.9), (2.10) and (2.13) the physics in the relativistic sector and via eq. (2.14) the size of the matching volume where to determine the non-perturbative heavy quark mass dependence of our observables, are summarized in table 1. Values for the other quantities, which have to be inserted into eq. (2.18) in order to obey the condition (2.12) of constant $z = L_0 M$, will be specified when we come to describe the actual calculation of the z-dependence of $\Gamma_\mathrm{X} = \Gamma_\mathrm{X}(L_0, M)$, $\mathrm{X} = \mathrm{PS}, \mathrm{av}$, in section 3.2.

At this stage we still want to direct the reader's attention to an issue that can already be foreseen to become a potential limitation in any application of the numerically computed quark mass dependence: even with eq. (2.18), the dimensionless mass parameter z can only be fixed through quantities known to a certain precision. In particular, the improvement coefficient b_m and the renormalization factor Z are only available from ref. [30][3] for $6.0 \leq \beta \leq 6.756$, which are significantly lower than the β-s of table 1 we are interested in. It hence appears quite difficult to reliably guess from the numbers in [30] values for b_m and Z in the β-region relevant here and, even more, to quantitatively assess the additional error contribution those estimates would then be afflicted with. Since this constitutes a dominant source of uncertainty, which would also propagate into any quantity that explicitly derives

[3]The β-range considered in [30] was chosen to cover values commonly used to simulate $\mathrm{O}(a)$ improved quenched QCD in physically large volumes. Similarly, the results from determinations through chiral Ward identities with mass non-degenerate quarks [33, 34] refer to this region and are not applicable here, too.

from the z-dependence of the observables studied here — such as, for instance, the b-quark mass through the matching of HQET and QCD [9] —, we first determine $b_{\rm m}$ and Z exactly for the β-values of table 1 and also improve their numerical precision.

3. Results

We now present the numerical results of our (quenched) computation of the heavy-light meson energies $\Gamma_{\rm X}(L_0,M)$, $\rm X = PS, av$, which — as outlined in the previous subsection — basically consists of two parts: first, we determine $b_{\rm m}$ and Z in the β-range relevant for a matching in physically small volume in order to be able to fix the RGI heavy quark mass to a set of desired values $z = L_0 M$ with sufficient precision, and second, the $L_0\Gamma_{\rm X}(L_0,M)$ are calculated at these values of z in the continuum limit. This will then allow for smooth representations of the energies as functions of z, which eventually may be used to interpolate them to the b-quark scale, $z_{\rm b} = L_0 M_{\rm b}$ [9].

3.1 Coefficients $b_{\rm A} - b_{\rm P}$, $b_{\rm m}$ and renormalization factor Z for $7.4 \lesssim \beta \lesssim 8.2$

Here we proceed in the spirit of ref. [30], where the idea of *imposing improvement conditions at constant physics* was advocated. In that work, which considered a range $6.0 \leq \beta \leq 6.756$ of bare couplings commonly used in large-volume simulations, this was realized by keeping constant the ratios L/r_0 and $T/L = 3/2$ (supplemented by the SF-specific choices $C = C' = 0$ and $\theta = 0.5$). However, despite $\ln(a/r_0)$ as a function of β needed to fix L/r_0 to some suitable value for given L/a is available for $5.7 \leq \beta \leq 6.92$ [35] and even beyond [36], the condition of constant L/r_0 can not be transfered to the present situation. The reason lies in the fact that for β-values in the range we are interested in, $7.4 \lesssim \beta \lesssim 8.2$, enforcing an improvement condition such as $L/r_0 = {\rm O}(1)$ would lead to prohibitively large values of L/a in the simulations. Therefore, to replace the latter, we exploit one of the already built in elements of the matching strategy between HQET and QCD as explained in the foregoing section: namely, as for the computation of the energies $\Gamma_{\rm X}$ on the QCD side we have to work along a line of constant physics in bare parameter space anyway, we can directly adopt the pairs $(L/a, \beta)$ of table 1, which correspond to $L/L_{\rm max} = 1/2 = 0.36 r_0/L_{\rm max}$ and simultaneously to a constant renormalized coupling of $\bar{g}^2(L/2) = 1.8811$ (see eqs. (2.14) and (2.13)). Within the present application, this constitutes a much more natural and equally admissible choice of improvement condition and thereby, in the same way as in ref. [30], the improvement coefficients $b_{\rm A} - b_{\rm P}$ and $b_{\rm m}$ as well as the renormalization constant Z become smooth functions of g_0^2 but exactly in the region where they are needed.

Following [30] — and also referring to this reference for any unexplained details —, the improvement coefficient $b_{\rm m}$ and the renormalization constant Z (as well as the difference of coefficients $b_{\rm A} - b_{\rm P}$, though it does not enter the subsequent computations in section 3.2) can be determined by studying QCD with non-degenerate quarks. This is particularly advantageous in case of the quenched approximation at hand, since then the structure of the ${\rm O}(a)$ improved theory stays quite simple. For instance, the improvement of the off-diagonal bilinear fields $X^{\pm} = X^1 \pm i\,X^2$, $X = A_\mu, P$, emerging as a consequence of the broken isospin symmetry, is the same as in the degenerate case, except that the b-coefficients now multiply cutoff effects proportional to the average $\frac{1}{2}(am_{\mathrm{q},i}+am_{\mathrm{q},j})$ of the subtracted bare quark masses, $m_{\mathrm{q},i}=m_{0,i}-m_{\mathrm{c}}$, which themselves are separately improved for each quark flavour:

$$\widetilde{m}_{\mathrm{q},i}=m_{\mathrm{q},i}(1+b_{\mathrm{m}}am_{\mathrm{q},i})\,. \tag{3.1}$$

(Here and below the indices i,j label the different quark flavours.) Identifying, for instance, the flavours in the isospin doublet with a light and a heavy quark as before, the corresponding PCAC relation reads

$$\partial_\mu A_\mu^{\pm}(x)=(m_{\mathrm{l}}+m_{\mathrm{h}})P^{\pm}(x)\,, \tag{3.2}$$

and the renormalization constants Z_{A} and Z_{P} that come into play upon renormalization are just those known in the theory with two mass degenerate quarks.

Accordingly, the fermionic correlation functions defined in the SF and involving the axial current and the pseudoscalar density [24] generalize to $f_{\mathrm{A}}^{ij}(x_0)=-\frac{1}{2}\left\langle A_0^{+}(x)O^{-}\right\rangle$ and $f_{\mathrm{P}}^{ij}(x_0)=-\frac{1}{2}\left\langle P^{+}(x)O^{-}\right\rangle$, with pseudoscalar boundary sources decomposed as $O^{\pm}=O^1\pm i\,O^2$ where $O^a=a^6\sum_{\boldsymbol{y},\boldsymbol{z}}\bar{\zeta}(\boldsymbol{y})\gamma_5\,\frac{1}{2}\,\tau^a\,\zeta(\boldsymbol{z})$. Then the improved bare PCAC (current) quark masses[4] as functions of the timeslice location x_0 are given by

$$m_{ij}\left(x_0;\frac{L}{a},\frac{T}{L},\theta\right)=\frac{\tilde{\partial}_0 f_{\mathrm{A}}^{ij}(x_0)+ac_{\mathrm{A}}\partial_0^*\partial_0 f_{\mathrm{P}}^{ij}(x_0)}{2\,f_{\mathrm{P}}^{ij}(x_0)}\,, \tag{3.3}$$

where only here we explicitly indicate their additional dependence on L/a, T/L and the periodicity angle θ of the fermion fields. In the degenerate case, $i=j$, the correlators assume the standard form as introduced earlier [24, 25], and m_{ij} just reduces to the current quark mass of a single quark flavour that is prepared by a corresponding choice of equal values for the associated hopping parameters, $\kappa_i=\kappa_j$. Also the precise definition of the lattice derivatives in eq. (3.3) matters. As it is written there, $\tilde{\partial}_0=\frac{1}{2}(\partial_0+\partial_0^*)$ denotes the average of the usual forward and backward derivatives, but as in ref. [30] we have employed the improved derivatives

$$\tilde{\partial}_0\to\tilde{\partial}_0\left(1-\frac{1}{6}\,a^2\partial_0^*\partial_0\right)\,,\qquad \partial_0^*\partial_0\to\partial_0^*\partial_0\left(1-\frac{1}{12}\,a^2\partial_0^*\partial_0\right) \tag{3.4}$$

as well, which (when acting on smooth functions) have $\mathrm{O}(g_0^2a^2,a^4)$ errors only.

To enable their numerical calculation, the desired coefficients $b_{\mathrm{A}}-b_{\mathrm{P}}$, b_{m} and the finite factor $Z=Z_{\mathrm{m}}Z_{\mathrm{P}}/Z_{\mathrm{A}}$ have to be isolated. This can be achieved by virtue of the identity

$$\begin{aligned} m_{ij}\;=\;Z\Big[&\frac{1}{2}\left(m_{\mathrm{q},i}+m_{\mathrm{q},j}\right)+\frac{1}{2}\,b_{\mathrm{m}}\left(am_{\mathrm{q},i}^2+am_{\mathrm{q},j}^2\right)-\\ &-\frac{1}{4}\left(b_{\mathrm{A}}-b_{\mathrm{P}}\right)a\left(m_{\mathrm{q},i}+m_{\mathrm{q},j}\right)^2\Big]+\mathrm{O}\left(a^2\right)\,, \end{aligned} \tag{3.5}$$

[4] This expression for the PCAC masses is only $\mathrm{O}(a)$ improved up to a factor $1+\frac{1}{2}(b_{\mathrm{A}}-b_{\mathrm{P}})(am_{\mathrm{q},i}+am_{\mathrm{q},j})$ for quark mass dependent cutoff effects.

which is obtained if one equates the two available expressions for the $\mathrm{O}(a)$ improved renormalized quark masses, i.e. in terms of the current quark and the subtracted bare quark masses (as they appear for the degenerate case in eq. (2.15) and thereafter). Forming ratios of suitable combinations of degenerate and non-degenerate current quark masses in the representation (3.5) allows to derive the following direct estimators for $b_{\mathrm{A}} - b_{\mathrm{P}}$, b_{m} and Z [30]:

$$R_{\mathrm{AP}} = \frac{2\,(2m_{12} - m_{11} - m_{22})}{(m_{11} - m_{22})(am_{\mathrm{q},1} - am_{\mathrm{q},2})} = b_{\mathrm{A}} - b_{\mathrm{P}} + \mathrm{O}\left(am_{\mathrm{q},1} + am_{\mathrm{q},2}\right), \tag{3.6}$$

$$R_{\mathrm{m}} = \frac{4\,(m_{12} - m_{33})}{(m_{11} - m_{22})(am_{\mathrm{q},1} - am_{\mathrm{q},2})} = b_{\mathrm{m}} + \mathrm{O}\left(am_{\mathrm{q},1} + am_{\mathrm{q},2}\right), \tag{3.7}$$

with $m_{0,3} = \frac{1}{2}(m_{0,1} + m_{0,2})$, apart from other quark mass independent lattice artifacts of $\mathrm{O}(a)$. For the renormalization constant Z an analogous expression holds even up to $\mathrm{O}(a^2)$ corrections,

$$R_Z = \frac{m_{11} - m_{22}}{m_{\mathrm{q},1} - m_{\mathrm{q},2}} + (b_{\mathrm{A}} - b_{\mathrm{P}} - b_{\mathrm{m}})(am_{11} + am_{22}) = Z + \mathrm{O}\left(a^2\right), \tag{3.8}$$

provided that the correct value for $b_{\mathrm{A}} - b_{\mathrm{P}} - b_{\mathrm{m}} = R_{\mathrm{AP}} - R_{\mathrm{m}}$ (only involving correlation functions with mass degenerate quarks) is inserted.

Concerning the simulation parameters, we argued above that it is most natural to choose L/a and β exactly as listed in table 1 of the preceding section. Moreover, values for the bare quark masses have to be selected. Here we considered two pairs of values for them,

$$\begin{aligned} &\text{choice 1}: \quad m_{0,\mathrm{l}} = m_{\mathrm{c}} \Leftrightarrow Lm_{\mathrm{l}} \approx 0\,, \quad Lm_{\mathrm{h}} \approx 0.5\,, \\ &\text{choice 2}: \quad m_{0,\mathrm{l}} = m_{\mathrm{c}} \Leftrightarrow Lm_{\mathrm{l}} \approx 0\,, \quad Lm_{\mathrm{h}} \approx 2.6\,; \end{aligned} \tag{3.9}$$

to comply with the heavy-light notation before we identify the bare quark masses as $m_{0,1} = m_{0,\mathrm{l}}$ and $m_{0,2} = m_{0,\mathrm{h}}$ with associated PCAC masses $m_{11} \equiv m_{\mathrm{l}}$ and $m_{22} \equiv m_{\mathrm{h}}$. With the first choice (corresponding to $z \approx 1$) Lm_{h} is close to the value used in ref. [30], which has the advantage that there this condition was also investigated in perturbation theory and the encountered $\mathrm{O}(a)$ ambiguities were not enormous. On the contrary, the second one (corresponding to $z \approx 5$) is motivated by the typical quark mass region that we have to deal with when probing our non-degenerate, heavy-light quark system in the next subsection. Maintaining these conditions to sufficient accuracy requires some prior simulations to tune the hopping parameter κ_{h} belonging to the heavy flavour's bare mass appropriately, whereas by $\kappa_{\mathrm{l}} = \kappa_{\mathrm{c}}$ taken over from the known values of ref. [27] the light quark mass is set to zero. The final simulation parameters to determine the quantities R_{X}, $\mathrm{X} = \mathrm{AP}, \mathrm{m}, Z$, in question can be drawn from the triples $(L/a, \beta, \kappa_{\mathrm{l}})$ of table 1 specifying the light quark sector (except that, only here, $T = 3L/2$), while the bare heavy quark mass is set through κ_{h} given in the second columns of tables 2 and 3. There one can also see that the bare current quark mass Lm_{h} has been fixed within a few percent to the values dictated by (3.9) to keep physics constant.[5]

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set	$\kappa_{\rm h}$	$Lm_{\rm h}$	$b_{\rm A}-b_{\rm P}$	$b_{\rm m}$	Z
A	0.132728	0.4778(7)	$-0.0008(14)$	$-0.6217(17)$	1.0941(3)
B	0.132711	0.4621(7)	$-0.0059(22)$	$-0.6218(27)$	1.0916(3)
C	—	0.4572(6)	$-0.0057(23)$	$-0.6228(28)$	1.0900(3)
D	0.132553	0.4539(5)	$-0.0072(21)$	$-0.6260(27)$	1.0882(2)
E	0.132395	0.4508(5)	$-0.0077(25)$	$-0.6312(32)$	1.0859(2)

Table 2: Numerical results on the improvement coefficients $b_{\rm A}-b_{\rm P}$ and $b_{\rm m}$ and on the renormalization constant Z, based on statistics varying between O(900) measurements (A) and O(200) measurements (E). These numbers refer to 'choice 1' in eq. (3.9), where the heavy quark mass is kept at $Lm_{\rm h}\approx 0.5$, while $Lm_{\rm l}$ indeed turned out to be compatible with zero up to tiny deviations of O(0.03) (A) and O(0.01) (sets B–E). For C, we interpolated results obtained with $L/a=16,24$ to $L/a=20$. Amongst others, $b_{\rm m}$ and Z are needed to fix the renormalized heavy quark mass in the simulations reported in section 3.2.

set	$\kappa_{\rm h}$	$Lm_{\rm h}$	$b_{\rm A}-b_{\rm P}$	$b_{\rm m}$	Z
A	0.126040	2.7100(6)	0.0489(3)	$-0.5401(4)$	1.0855(2)
B	0.128028	2.6112(6)	0.0239(5)	$-0.5621(7)$	1.0867(2)
C	—	2.6709(5)	0.0151(6)	$-0.5744(9)$	1.0867(2)
D	0.129595	2.5456(5)	0.0103(5)	$-0.5811(8)$	1.0859(1)
E	0.130246	2.5035(5)	0.0051(6)	$-0.5927(9)$	1.0845(1)

Table 3: The same as in table 2 but for 'choice 2' of the heavy quark mass: $Lm_{\rm h}\approx 2.6$.

The Monte Carlo simulation details and the technical aspects of the analysis to compute the observables (3.6)–(3.8) from the measured fermionic correlation functions are essentially the same as in ref. [30]. In particular, these secondary quantities have been averaged over the central timeslices $L/(2a),\dots,(T-L/2)/a$ to increase statistics, and their statistical errors were estimated by the jackknife method. Another issue that deserves to be mentioned is the occurrence of the third mass parameter $m_{0,3}$ in the determination of $b_{\rm m}$, which has to be set properly to ensure the required (but subtle) cancellation leading to the expression (3.7) for the estimator $R_{\rm m}$. As in terms of the hopping parameters this amounts to form the combination $\kappa_3=2\kappa_1\kappa_2/(\kappa_1+\kappa_2)$, the condition $\frac{1}{2}(m_{0,1}+m_{0,2})-m_{0,3}=0$ can be satisfied in practice only up to roundoff errors, which might cause a systematic uncertainty in simulations with single precision arithmetics. But in contrast to ref. [30], where this effect had to be taken into account carefully, the exact numerical value of κ_3 was now calculated in double precision directly in the simulation program itself so that a rounding error contribution (reflecting some possible remnant imperfection in the cancellation via $m_{0,3}$) to the error on $R_{\rm m}$ can be neglected here.

Our non-perturbative results on $b_{\rm A}-b_{\rm P}$, $b_{\rm m}$ and Z, which we obtained from the numerical simulation data along these lines using improved derivatives throughout, are also

[5] Similar to the situation in ref. [30], this is to a good precision equivalent to keeping fixed the corresponding renormalized masses $Lm_{\rm R}=LZ_{\rm A}m/Z_{\rm P}$, because also over our range of considered couplings the entering renormalization constant barely varies.

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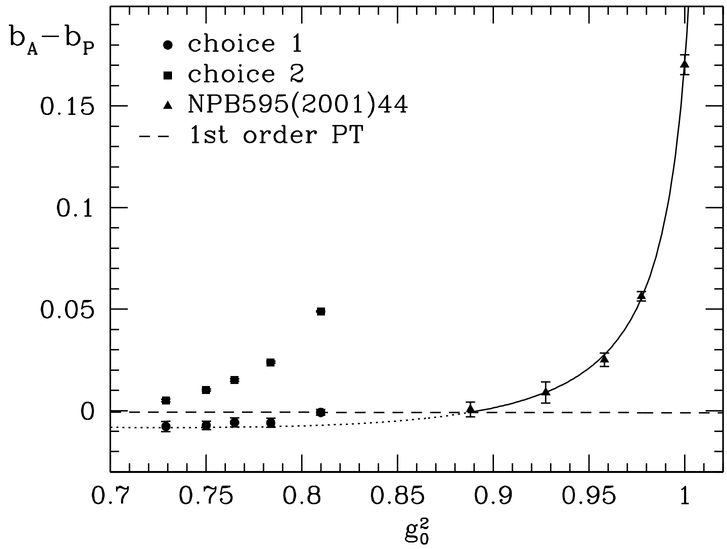

Figure 2: Non-perturbative results for $b_{\rm A} - b_{\rm P}$ in the considered region of bare couplings for our two choices of quark masses (cf. eq. (3.9)), together with the corresponding results at larger g_0^2 from [30] (triangles) and the prediction from one-loop perturbation theory. The solid line gives the rational fit function that was quoted in [30] to well describe the numerical simulation results obtained there.

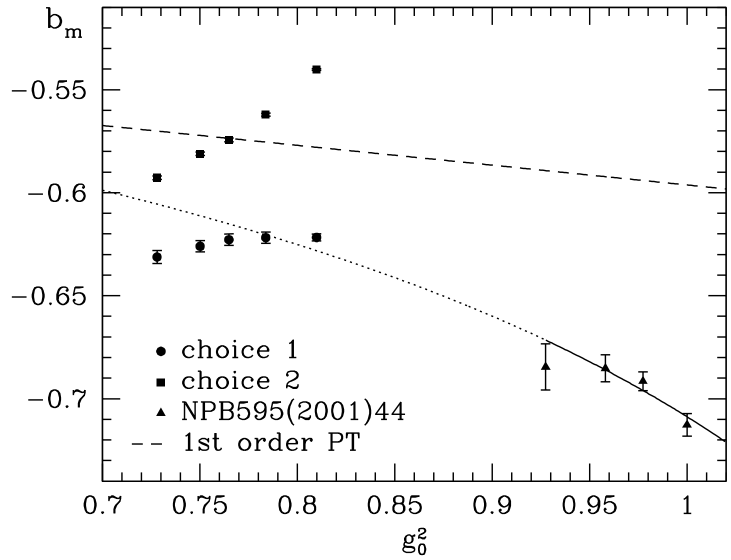

Figure 3: The same as in figure 2 but for the improvement coefficient $b_{\rm m}$. In view of the leading perturbative behaviour that one expects to be approached in the limit $g_0^2 \to 0$, the curvature seen in our results hints at a more complicated structure of (unknown) higher-order terms.

collected in tables 2 and 3.[6] As a consequence of the fact that all renormalized quantities have been fixed in units of L while the ratio $L/L_{\rm max}$ and thereby also the renormalized

[6]We note in passing that memory and processor-topology restrictions of the APEmille parallel computers in use prevented us from directly simulating $L/a = 20$ lattices at an earlier stage of our work. Therefore, we employed $16^3 \times 30$ and $24^3 \times 30$ lattices and a linear interpolation in $1/L$ to arrive at the results for set C in tables 2 and 3.

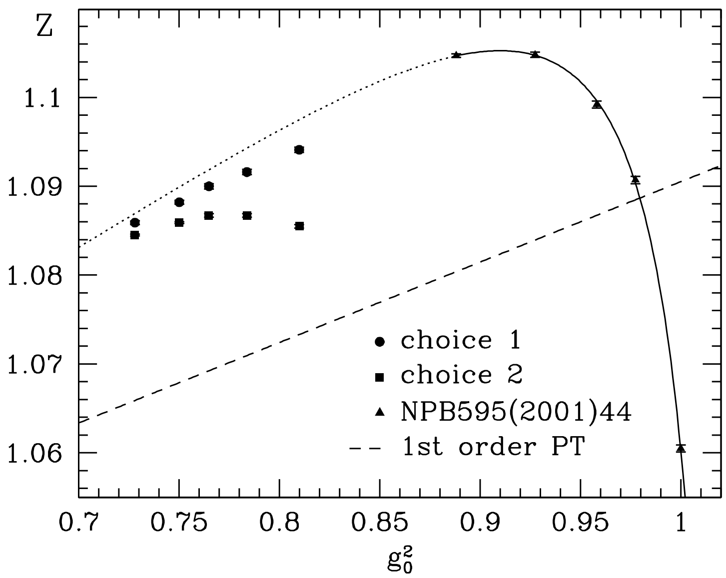

Figure 4: The same as in figure 2 but for the renormalization constant Z.

SF coupling are kept constant, the estimates R_X become smooth functions of the bare coupling, $g_0^2 = 6/\beta$. This is well fulfilled in figures 2–4, where our results are shown in conjunction with those at larger couplings of the earlier work [30] together with the one-loop perturbative predictions [37, 30]. One observes that the estimates for $b_A - b_P$ and Z corresponding to 'choice 1' of quark masses are roughly consistent with the fit functions quoted in ref. [30] for larger couplings, if one assumes them to be even valid far beyond the β-region where the underlying data were actually taken. Nonetheless, this was not obvious from the beginning, since despite the quark mass values being comparable in that case the conditions defining the associated lines of constant physics are different.

For b_m the situation is more intricate. Here a naive prolongation of the curve from [30] to weak couplings (dottet line in figure 3) does not give the right g_0^2-behaviour for this region. We infer this from the fact that the difference of the dotted line to our results does not seem to be compatible with being of $O(a)$. In other words, if the improvement condition of [30] were used also in the region of weaker couplings, the points would look quite differently, and we have to conclude that a simple approach to one-loop perturbation theory is not an adequate representation for the continuation of the triangles in figure 3. This underlines the importance of using particularly adapted improvement conditions, which may be used in the coupling range actually relevant for the desired application. The example of b_m thus illustrates that our redetermination of the b-coefficients and the Z-factor indeed eliminates a source of uncontrollable error.

On the other hand, the results from 'choice 2' (i.e. with the quark mass m_h being larger) fall significantly apart throughout, because the a-effects are generically larger in that case. But this only reveals an expected, inevitable property of the procedure applied: any other estimate R_X (e.g. stemming from a different choice of renormalization condition) may yield a different functional dependence upon g_0^2, but its differences are again smooth functions that must vanish in the continuum limit with a rate proportional to a/L (for

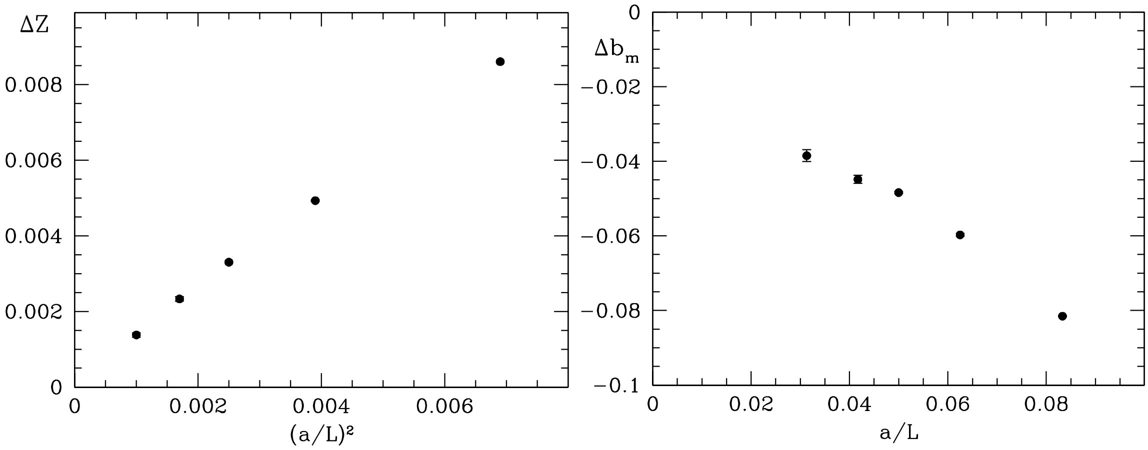

Figure 5: Left: Difference of the results on the renormalization constant Z, obtained from the two heavy quark mass choices, versus $(a/L)^2$. Right: The same for the improvement coefficient b_{m} where, however, the ambiguity inherent in any improvement condition imposed is of $\mathrm{O}(a)$.

improvement coefficients) or even $(a/L)^2$ (for renormalization constants). These intrinsic $\mathrm{O}(a^n)$ ambiguities, $n = 1, 2$, imply that rather than a numerical value at some given β, the essential information lies in the *correct* g_0^2*-dependence* of the results for the estimators R_{X}, $\mathrm{X} = \mathrm{AP}, \mathrm{m}, Z$, resulting from working at fixed physics while varying β.

To demonstrate the last statement, we also investigated a few alternative improvement conditions, which are either realized by defining the estimators R_{X} with standard instead of improved derivatives (as in [30]) or directly by the two different quark mass settings that we already have at our disposal through the choices in eq. (3.9). As an example we plot in the left part of figure 5 the difference $\Delta Z(g_0^2) = Z(g_0^2)|_{\,\mathrm{choice\,1}} - Z(g_0^2)|_{\,\mathrm{choice\,2}}$ versus $(a/L)^2$, which clearly shows a linear approach towards zero. Other cases behave similarly, e.g. the $\mathrm{O}(a)$ ambiguities for $\Delta b_{\mathrm{m}}(g_0^2) = b_{\mathrm{m}}(g_0^2)|_{\,\mathrm{choice\,1}} - b_{\mathrm{m}}(g_0^2)|_{\,\mathrm{choice\,2}}$ in the right part of figure 5 are found to be very small and rapidly decreasing in magnitude as $a/L \to 0$.

As a further (and less direct) check for the universality of the continuum limit we consider a physical quantity that depends on b_{m} and Z in a more implict way, namely the energy $L_0\Gamma_{\mathrm{PS}}(L_0, M, g_0)$ introduced in eq. (2.6) of the previous section. In fixing z while computing $L_0\Gamma_{\mathrm{PS}}$ for various lattice resolutions, the just determined results on b_{m} and Z enter via eq. (2.18), and hence it is interesting to confront the lattice spacing dependences of $L_0\Gamma_{\mathrm{PS}}|_{\,b_{\mathrm{m}},Z:\,\mathrm{choice\,1}}$ and $L_0\Gamma_{\mathrm{PS}}|_{\,b_{\mathrm{m}},Z:\,\mathrm{choice\,2}}$ with eachother. We did this exercise for $z = 9$ (where, due to the large quark mass, a-effects are already very pronounced) and anticipate results from the following section in figure 6 to display the two data sets and its continuum extrapolations linear in $(a/L)^2$. From the nice agreement of the continuum limits[7] we infer once more that our results (on b_{m} and Z) correctly model — within each choice of improvement condition separately — the respective g_0^2-dependences, entailing convergence to the continuum limit with leading corrections of $\mathrm{O}(a^2)$.

[7]The fact that in this case the cutoff effects in $L_0\Gamma_{\mathrm{PS}}$ are larger with b_{m}, Z from 'choice 1' (where the quark mass fixed is smaller) is not so surprising, since via 'choice 2' as improvement condition (where $z \approx 5$) one is closer to the line in parameter space with $z = 9$ along which $L_0\Gamma_{\mathrm{PS}}$ is computed.

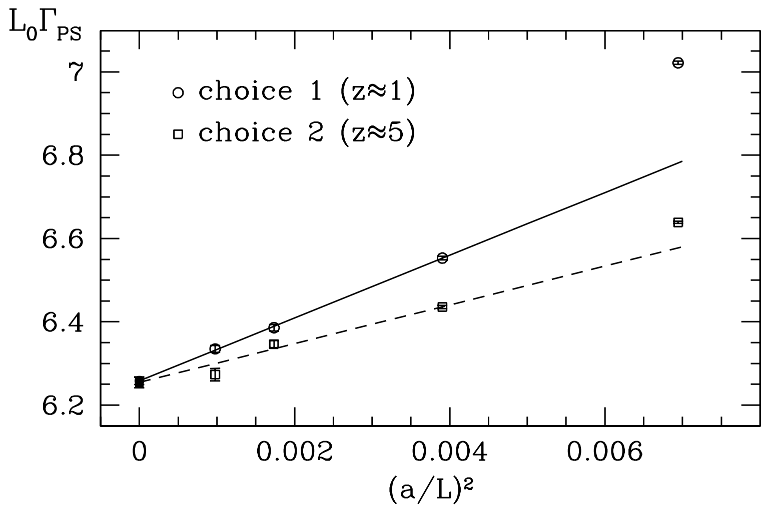

Figure 6: $L_0\Gamma_{\rm PS}(L_0, M, g_0)$, where the results on $b_{\rm m}, Z$ from both renormalization conditions corresponding to eq. (3.9) were used to keep the dimensionless RGI heavy quark mass fixed to $z = L_0 M = 9$ while varying $\beta = 6/g_0^2$ and thus a/L. Assuming quadratic scaling violations and discarding the coarsest lattice in the (unconstrained) extrapolations, the continuum limits coincide. A more thorough discussion of the continuum extrapolations of the observables $\Gamma_{\rm X}$, X = PS, av, will follow in section 3.2.

3.2 Heavy-light meson energies

Supposing the parameters β and $\kappa_{\rm l}$ at each L/a $(= L_0/a)$ to be appropriately fixed to comply with the conditions $\bar{g}^2(L_0/2) = 1.8811 = \text{constant}$ and $m_{\rm l} = 0$, eqs. (2.13) and (2.10), we still have to prescribe a sequence of dimensionless quark mass values z in order to be able to map out the heavy quark mass dependence of the observables $\Gamma_{\rm X}$, X = PS, av, over a reasonable range that encloses the RGI mass scale of the b-quark itself. To this end we split, according to the discussion around eq. (2.18) in section 2.3, $z = L_0 M$ into the product

$$z = L_0 \times h(L_0) \times Z_{\rm m} \times m_{\rm q,h}(1 + b_{\rm m} a m_{\rm q,h}) \,, \qquad Z_{\rm m} = \frac{Z\, Z_{\rm A}}{Z_{\rm P}} \,. \tag{3.10}$$

For $b_{\rm m}(g_0^2)$ and $Z(g_0^2)$ we decided to use the results of table 2 from 'choice 1' of quark mass settings, mainly because especially for $b_{\rm m}$ the g_0^2-dependence is weaker and with the corresponding value of the (heavy) quark mass fixed in their determination we more resemble the condition that in ref. [30] was found favourable also from the perturbative point of view. $Z_{\rm A}(g_0^2)$ is known in O(a) improved quenched QCD via the formula [38]

$$Z_{\rm A} = \frac{1 - 0.8496\, g_0^2 + 0.0610\, g_0^4}{1 - 0.7332\, g_0^2} \,, \qquad g_0^2 \leq 1 \,, \tag{3.11}$$

while the required values of $Z_{\rm P}(g_0, L_0/a)$ have already been quoted in the last column of table 1 and, as was said after eq. (2.20), the universal factor

$$h(L_0) = 1.531(14) \,, \qquad L_0 = \frac{L_{\rm max}}{2} \,, \tag{3.12}$$

could be extracted from the data published in ref. [27]. Given some value of z one is aiming at, the relation between the subtracted bare (heavy) quark mass and the hopping parameter,

$$am_{\rm q,h} = \frac{1}{2}\left(\frac{1}{\kappa_{\rm h}} - \frac{1}{\kappa_{\rm c}}\right), \tag{3.13}$$

then allows to straightforwardly solve eq. (3.10) for $\kappa_{\rm h}$ and, together with $\kappa_{\rm l}$ as quoted in table 1 of section 2.3, yields the pairs $(\kappa_{\rm l}, \kappa_{\rm h})$ of hopping parameters, for which the numerical simulations with the computation of the heavy-light correlation functions have been performed.[8]

Of course, the uncertainties to be associated with the various pieces entering eq. (3.10) translate into an error on z, which has to be taken into account also for any quantity regarded as a *function of* z. More precisely, the resulting error on z consists of a g_0-dependent part and a universal, g_0-independent one: while the former comes from the uncertainties of $b_{\rm m}$, Z and $Z_{\rm P}$ quoted in the tables plus an error (of 0.8% at $\beta \approx 7.4$ down to 0.4% for $\beta \geq 7.8$ [38]) on $Z_{\rm A}$, the latter stems from the overall uncertainty of 0.9% on $h(L_0)$ in the continuum limit and hence has only to be added in quadrature *after* a continuum extrapolation of the respective z-dependent quantity under study.[9]

The final parameter sets employed in the Monte Carlos simulations consist of the triples $(L/a, \beta, \kappa_{\rm l})$ in table 1 and the $\kappa_{\rm h}$-values we arrived at as described before; they are listed together with the corresponding values of the dimensionless RGI heavy quark mass, z, and the g_0-dependent error part of the latter in table 4 at the end of this section. For the technical details of the runs to produce the numerical data on the SF heavy-light meson correlators, from which the logarithmic derivatives (2.6) and (2.7) are evaluated, we refer to the simulations reported in ref. [31] (and its appendix A.2. in particular) to non-perturbatively renormalize the static-light axial current. The number of measurements in the statistical samples is comparable to what was accumulated to get the results in tables 2 and 3.

Table 4 also contains the numerical results for $L_0\Gamma_{\rm PS}$ and $L_0\Gamma_{\rm av}$ at all values of z that were considered. To ease notation, we set

$$\Omega_{\rm X}\left(u, z, \frac{a}{L}\right) \equiv L_0\Gamma_{\rm X}(L_0, M, g_0)\Big|_{\bar{g}^2(L_0/2)=u\,,\,L_0M=z}, \qquad {\rm X} = {\rm PS}, {\rm av}\,, \tag{3.14}$$

and denote its continuum limits as

$$\omega_{\rm X}(u, z) \equiv \lim_{a/L\to 0} \Omega_{\rm X}\left(u, z, \frac{a}{L}\right), \qquad {\rm X} = {\rm PS}, {\rm av}\,. \tag{3.15}$$

In table 4 both the statistical errors of $\Omega_{\rm X}$ (in square brackets) as well as the combined statistical and g_0-dependent, z-induced uncertainties (in parentheses) are given, the latter

[8] Due to the fact that the non-perturbative values for $b_{\rm m}$ in the relevant β-range lie around -0.6, the relation $z = L_0 h(L_0) Z_{\rm m} m_{\rm q,h}(1 + b_{\rm m} am_{\rm q,h})$ can not be inverted in favour of $am_{\rm q,h}$ (and thereby $\kappa_{\rm h}$) for arbitrarily high z-values. In case of our largest z $(= 13.5)$, for instance, this already restricts the possible inverse lattice spacings in table 4 to $L/a = 16 - 32$.

[9] Note that also this error can in principle be reduced further by increasing the precision of the continuum step scaling functions of ref. [27].

being obtained by including the propagation of the g_0-dependent part of the error on z. As an outcome of this error analysis we find that summing up the various errors on the factors in eq. (3.10) quadratically (since they are uncorrelated) and multiplying with the numerically estimated slopes $|[\partial\Omega_{\rm X}/\partial z]\,(g_0)|$ yields a contribution of about 0.3% or less to the final uncertainties on $\Omega_{\rm X}$.

As we work in the $\mathrm{O}(a)$ improved theory, the numbers for $\Omega_{\rm PS}$ and $\Omega_{\rm av}$ can now be extrapolated linearly in a^2 to the continuum limit.[10] However, based on the experience made in perturbation theory (see section 5 of ref. [39]) that the discretization errors primarily depend on the mass of the heavy quark, $aM = z \times a/L$, we expect some deviation from a leading linear behaviour in a^2 for the coarsest lattices as z grows. Since our non-perturbative data qualitatively confirm this picture, we again adopt perturbation theory as a guide to get a rough estimate for the quark mass value where this deviation sets in. In [39] the heavy quark mass dependence of the discretization errors in a typical matrix element of the heavy-light axial current, similarly constructed from SF correlators as our energy observables, indicates a breakdown of $\mathrm{O}(a)$ improvement beyond $(a\overline{m}_{\rm h}^{\overline{\rm MS}})^2 \approx 0.2$, which with $\overline{m}_{\rm h}^{\overline{\rm MS}} \approx 0.7M$ [40] approximately corresponds to $aM \approx 0.64$. From this we deduce the following *two-step criterium* to carefully perform the continuum extrapolations of $\Omega_{\rm X}$, $\mathrm{X} = \mathrm{PS}, \mathrm{av}$, for the various values of z:

1. In view of the z-dependence of the size of the lattice artifacts, only allow for fits which start at and beyond the minimal L/a such that $aM < 0.6$ approximately holds.

2. Among these, the n-point fit must agree with the $(n+1)$-point one within errors but the former, which omits the coarsest of the lattices meeting 1. and thereby has the larger error, gives the final estimate of the continuum limit.

The resulting continuum extrapolations for the subset $z \in \{5.15, 6.0, 9.0, 13.5\}$ of available z-values are displayed in figure 7. As it turns out when applying this fitting procedure, the continuum limits then have to be extracted from fits discarding the $L/a = 12$ lattice in case of $z \in \{3.0, 3.8, 5.15, 6.0, 6.6\}$, the $L/a = 12, 16$ lattices in case of $z = 9.0$ and even the $L/a = 12, 16, 20$ lattices for the heaviest mass, $z = 13.5$. The numbers of table 4 in Italics are the continuum limit results for all z, based on these fits.

To further corroborate our results from this prescription, we in addition considered an alternative fit ansatz that also accounts for a term cubic in a. Again, it is to some extent guided by the aforementioned finding of ref. [39] that in perturbation theory the cutoff effects in the regime of large quark masses are approximately a function of aM and not of aM and a/L separately. In the $\mathrm{O}(a)$ improved case at hand (and here for the example of $\Omega_{\rm av}$, omitting the argument u for a moment), such an ansatz may therefore be written as:

$$\Omega_{\rm av}\left(z, \frac{a}{L}\right) = \omega_{\rm av}(z)\left[1 + \rho_2\, z^3 \left(\frac{a}{L}\right)^3\right] + \rho_1(z)\left(\frac{a}{L}\right)^2, \tag{3.16}$$

where by a z-dependent parameter ρ_1 we after all admit a still more general form for the a^2-term. Performing a simultaneous fit of all available $\Omega_{\rm av}$ data (no cut on aM), we then

[10] As in [27, 31], the influence of the only perturbatively known SF-specific boundary improvement coefficients $c_{\rm t}$ and $\widetilde{c}_{\rm t}$ is negligible at the level of our precision.

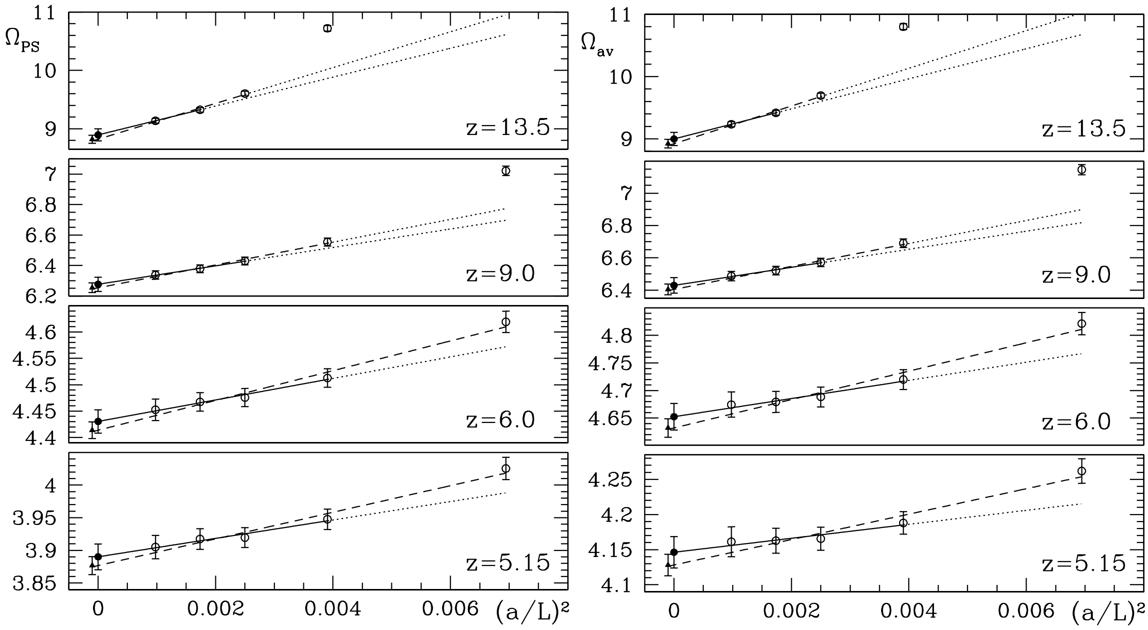

Figure 7: Continuum extrapolations of $\Omega_{\rm PS}(1.8811, z, a/L)$ (left) and $\Omega_{\rm av}(1.8811, z, a/L)$ (right) for representative values of z. As explained in the text, the number of coarsest lattices to be skipped in the fits depends on z. The final continuum limits are taken from the solid fit functions, which are compatible with the dashed extrapolations omitting one point less.

arrive at continuum limits in complete accordance with the former, having comparable or even smaller errors: $\omega_{\rm av}(z) \in \{2.86(1), 3.34(1), 4.15(3), 4.65(2), 5.00(2), 6.39(3), 8.99(6)\}$ for $z = 3.0, \ldots, 13.5$. But keeping in mind that for $aM \approx 0.6 - 0.8$ the perturbative a-expansion entirely breaks down [39], we take the continuum limits of table 4 from the linear extrapolations in $(a/L)^2$ imposing a cut on aM as a safeguard against any uncontrollable higher-order behaviour as our final results, which within their (larger) errors are moreover also consistent with the values at smallest lattice resolution. All told, we thus are confident that possible systematic uncertainties in the fitting procedure are already well covered by these estimates.

For future reference (i.e. in particular for the non-perturbative determination of the b-quark's mass in ref. [9]) we introduce for the dimensionless, spin-averaged heavy-light meson energy in small volume the further abbreviation

$$\Omega\left(u, z, \frac{a}{L}\right) \equiv \Omega_{\rm av}\left(u, z, \frac{a}{L}\right), \qquad \omega(u, z) \equiv \omega_{\rm av}(u, z)\,. \tag{3.17}$$

To parametrize the z-dependence of our continuum values $\omega(1.8811, z)$ by a smooth fit function, we make the ansatz $a_0 z + a_1 + a_2/z$, which is justified by the theoretical expectation that heavy-light meson correlation functions of the type studied here decay with a leading term proportional to the heavy quark mass, up to some low-energy scale of $\mathrm{O}(\Lambda_{\rm QCD})$ and $1/m$-corrections. Since the simulation data for the various z at given β were produced on the same gauge field backgrounds, possible correlations in z had to be taken into account in this fit. Hence weperformed it on basis of the jackknife samples that were built from the

z	set	κ_h	$z(g_0)$	Ω_PS	Ω_av
3.0	A	0.129571	3.000(12)	2.534(11)[5]	2.916(11)[6]
	B	0.130445	3.000(13)	2.485(10)[4]	2.869(11)[6]
	C	0.130876	3.000(13)	2.465(10)[5]	2.856(12)[8]
	D	0.131115	3.000(13)	2.471(11)[7]	2.863(14)[12]
	E	0.131349	3.000(13)	2.458(13)[10]	2.858(18)[16]
	CL			*2.451(13)*	*2.852(18)*
3.8	A	0.128310	3.800(16)	3.094(13)[5]	3.408(14)[6]
	B	0.129552	3.800(16)	3.039(12)[4]	3.356(13)[6]
	C	0.130185	3.800(16)	3.019(12)[5]	3.341(13)[8]
	D	0.130553	3.800(16)	3.022(12)[7]	3.345(15)[11]
	E	0.130940	3.800(17)	3.011(15)[10]	3.342(19)[16]
	CL			*3.002(16)*	*3.334(19)*
5.15	A	0.126055	5.150(21)	4.025(17)[5]	4.262(17)[6]
	B	0.127991	5.150(22)	3.948(16)[5]	4.188(16)[6]
	C	0.128989	5.150(22)	3.920(15)[5]	4.166(16)[8]
	D	0.129586	5.150(22)	3.917(16)[7]	4.163(18)[11]
	E	0.130242	5.150(23)	3.905(18)[11]	4.161(21)[16]
	CL			*3.890(20)*	*4.146(22)*
6.0	A	0.124528	6.000(25)	4.619(20)[5]	4.821(20)[6]
	B	0.126967	6.000(25)	4.513(18)[5]	4.720(18)[6]
	C	0.128214	6.000(25)	4.476(17)[5]	4.688(18)[8]
	D	0.128964	6.000(25)	4.467(18)[8]	4.679(19)[11]
	E	0.129796	6.000(27)	4.453(20)[11]	4.674(23)[15]
	CL			*4.430(22)*	*4.652(24)*
6.6	A	0.123383	6.600(27)	5.049(22)[5]	5.232(22)[6]
	B	0.126222	6.600(28)	4.912(20)[5]	5.100(20)[6]
	C	0.127656	6.600(28)	4.866(19)[5]	5.059(20)[8]
	D	0.128518	6.600(28)	4.852(19)[8]	5.045(21)[10]
	E	0.129477	6.600(30)	4.835(22)[11]	5.037(24)[15]
	CL			*4.806(24)*	*5.009(26)*
9.0	A	0.117762	9.000(39)	7.022(31)[5]	7.146(31)[5]
	B	0.122987	9.000(39)	6.554(27)[5]	6.690(27)[6]
	C	0.125309	9.000(38)	6.429(25)[6]	6.572(26)[7]
	D	0.126670	9.000(38)	6.378(26)[8]	6.521(26)[10]
	E	0.128175	9.000(40)	6.337(28)[12]	6.487(29)[15]
	CL			*6.277(47)*	*6.429(48)*
13.5	B	0.113764	13.500(69)	10.721(47)[5]	10.801(47)[5]
	C	0.120094	13.500(60)	9.603(40)[6]	9.695(40)[7]
	D	0.122808	13.500(58)	9.324(38)[8]	9.418(38)[9]
	E	0.125575	13.500(61)	9.136(40)[12]	9.235(41)[14]
	CL			*8.89(10)*	*9.00(11)*

Table 4: Heavy quark masses $z = L_0 M$ with g_0-dependent error and associated results for $\Omega_\mathrm{X}(u, z, a/L)$, $\mathrm{X} = \mathrm{PS}, \mathrm{av}$, $u = 1.8811$, with the total g_0-dependent part of the error in parentheses and the only statistical one of Ω_X in square brackets. Continuum limits (see text) are displayed in Italics.

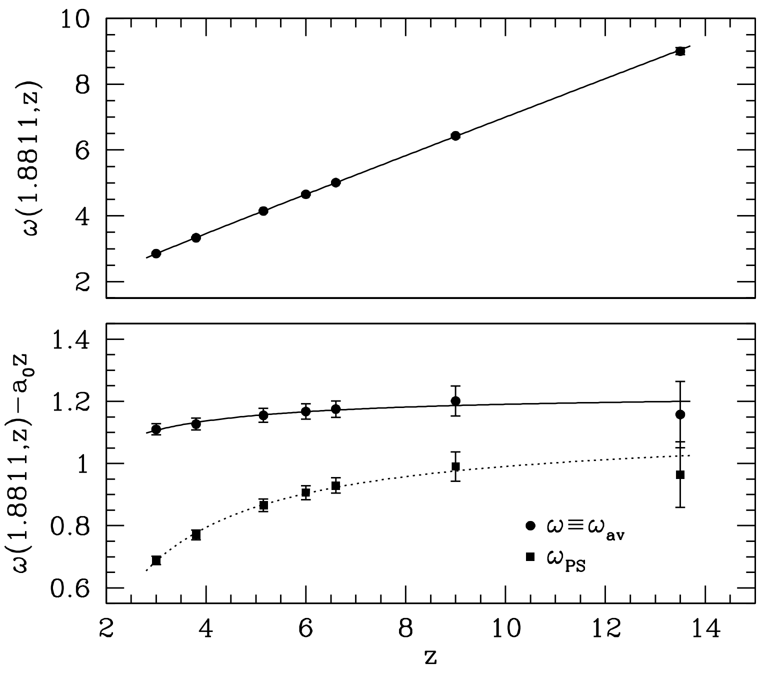

Figure 8: Continuum limit values $\omega(1.8811, z)$ of the spin-averaged energies $\Omega(1.8811, z, a/L)$, at fixed coupling $\bar{g}^2(L_0/2) = 1.8811$, as a function of $z = L_0 M$ and its fit function (top). The bottom graph has the linear term, $a_0 z$, subtracted and also includes the pseudoscalar case, $\omega_{\mathrm{PS}}(1.8811, z)$, for comparison.

raw data and passed through the whole analysis, and we end up with the parametrization

$$\omega(1.8811, z) = a_0 z + a_1 + a_2 \frac{1}{z}, \qquad a_0 = 0.581, \qquad a_1 = 1.226, \qquad a_2 = -0.358, \tag{3.18}$$

the graph of which is shown in the upper diagram of figure 8 to well represent our data. In the interval $5.2 \leq z \leq 6.6$, which for instance is the relevant z-range to calculate the RGI b-quark mass by means of the non-perturbative matching to HQET in ref. [9], this parametrization describes $\omega(1.8811, z)$ with a precision of about 0.5%. As already mentioned, a further uncertainty of 0.9% that enters only indirectly through the argument z of the function ω (and thus remains to be added in quadrature at the end) originates from the universal part $h(L_0)$ in eq. (3.10) of the renormalization factor relating the bare to the RGI quark mass.

For later use of the result (3.18) it is also necessary to have a numerical estimate for the derivative $\omega'(1.8811, z)$ w.r.t. u, in order to compensate for a possible slight mismatch in the imposed condition of fixed renormalized coupling. From an additional simulation with $L/a = 24$ and a nearby coupling of $\bar{g}^2(L_0/2) = 1.95$ (and assuming the a-effect of the derivative to be negligible) we found this derivative to be constant in the central region

$$6.0 \leq z \leq 6.6 : \qquad \frac{\partial}{\partial u}\, \omega(u, z)\bigg|_{u=1.8811} = 0.70(1)\,, \tag{3.19}$$

which is the required one in the context of the immediate application discussed in [9].

Finally, we give as well the fit result for $\omega_{\mathrm{PS}}(1.8811, z)$ for comparison, i.e. if in the definition (3.14) the effective energy in the pseudoscalar channel alone, $\Gamma_{\mathrm{PS}}(L_0, M, g_0)$, would be used instead of the spin-averaged combination. By an analogous analysis with the same ansatz for the fit function as in eq. (3.18) we obtain the coefficients

$$a_0 = 0.587\,, \qquad a_1 = 1.121\,, \qquad a_2 = -1.306 \qquad (\text{for } \Gamma_{\mathrm{X}} = \Gamma_{\mathrm{PS}})\,. \tag{3.20}$$

The fact that the absolute value of a_2 is evidently larger than in the spin-averaged case is illustrated by the shape of the subtracted fits in the bottom diagram of figure 8 and confirms our earlier claim that with $\Gamma_{\mathrm{X}} = \Gamma_{\mathrm{av}}$ the matching condition (2.11) becomes *independent of the coefficient of the chromomagnetic field strength term in the HQET lagrangian also at first order in* $1/m$. Therefore, the use of $\Omega \equiv \Omega_{\mathrm{av}} \equiv L_0\Gamma_{\mathrm{av}}$ (and eq. (3.18) for its heavy quark mass dependence in the continuum limit) is preferable for later applications to HQET, since the $1/m$-errors arising at leading order will generically be smaller then.

4. Conclusions

In this work we have computed the non-perturbative heavy quark mass dependence of effective energies derived from heavy-light meson correlation functions by means of numerical simulations. A particular aspect of this computation is the *use of a physically small volume* (of a linear extent of O(0.2 fm)): it is a prerequisite to treat the heavy quark flavour in lattice regularization as a relativistic particle and thus may be looked at as a 'device' that serves to non-perturbatively renormalize HQET with the method of matching the effective theory to small-volume QCD, proposed and applied in ref. [9].

Among the several improvement coefficients and renormalization constants that are needed to accurately keep fixed the renormalized (heavy) quark mass while the observables of interest approach their continuum limits, we determined those relating the renormalized to the subtracted bare quark mass in a range of weaker couplings relevant here ($7.4 \lesssim \beta = 6/g_0^2 \lesssim 8.2$) with high precision. Even in the region of the b-quark mass and slightly beyond we still find our results on the meson energies under study to be rather mildly cutoff dependent so that the continuum extrapolations can be well controlled.

The quenched numerical results obtained in section 3.2 directly pass into the — for the first time entirely non-perturbative — calculation of the b-quark mass in the static approximation of [9, 41]. Moreover, our quantitative investigation of the quark mass dependence in relativistic heavy-light systems in finite volume can easily be extended to other heavy-light bilinears and matrix elements, which then opens the possibility to perform genuinely non-perturbative tests of HQET and to estimate the size of the $1/m$-corrections to the static theory. We will focus on these issues in a separate publication [12].

Finally, considering the small-volume investigation presented here in the light of the more general framework [9] of a non-perturbative matching between HQET and QCD, it is an obvious practical advantage that they can be transfered to also include dynamical quarks in the (hopefully near) future without requiring exceedingly large computing resources.

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