## First Lattice Calculation of The B-meson Binding and Kinetic Energies.

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#### Abstract

We present the first lattice calculation of the B-meson binding energy  $\overline{\Lambda}$  and of the kinetic energy  $-\lambda_1/2m_Q$  of the heavy-quark inside the pseudoscalar B-meson. This calculation has required the non-perturbative subtraction of the power divergences present in matrix elements of the Lagrangian operator  $\bar{h}D_4h$  and of the kinetic energy operator  $\bar{\hbar}\vec{D}^2\hbar$ . The non-perturbative renormalisation of the relevant operators has been implemented by imposing suitable renormalisation conditions on quark matrix elements, in the Landau gauge. Our numerical results have been obtained from several independent numerical simulations at  $\beta = 6.0$  and 6.2, and using, for the meson correlators, the results obtained by the APE group at the same values of  $\beta$ . Our best estimate, obtained by combining results at different values of  $\beta$ , is  $\overline{\Lambda} = 190$   $_{-30}^{+50}$  MeV. For the  $\overline{MS}$  running mass, we obtain  $\overline{m}_b(\overline{m}_b)=4.17 \pm 0.06$  GeV, in reasonable agreement with previous determinations. From a subset of 36 configurations, we were only able to establish a loose upper bound on the b-quark kinetic energy in a B-meson,  $\lambda_1 = \langle B|\bar{h}\vec{D}^2h|B\rangle/(2M_B) < 1~{\rm GeV^2}$ . This shows that a much larger statistical sample is needed to determine this important parameter.

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## 1 Introduction

The Heavy Quark Effective Theory (HQET) [1]–[6] has proven to be an extraordinary tool for studying heavy flavour physics. In this approach, physical quantities are expanded as series in inverse powers of the heavy quark masses. The spin-flavour symmetries, appearing in the infinite mass limit, are then used to relate different hadron masses or weak amplitudes which control heavy meson and baryon decays [6]. For example, in the infinite mass limit, the set of six hadronic form factors, which parameterize the matrix elements of the flavour changing vector and axial vector current in  $B \to D, D^*$  semileptonic decays, can be reduced to a single universal one: the so called the Isgur-Wise function [3]. Spinflavour symmetries, however, are not sufficient to predict all the properties of the weak form factors and of other important quantities such as the meson decay constants and the velocity dependence of the Isgur-Wise function. Among the quantities that cannot be predicted on the basis of the HQET only, there are several parameters which characterize the dynamics of strong interactions, such as the heavy quark binding energy, relevant for higher order corrections to the semileptonic form factors, and the heavy quark kinetic energy, which enters in the predictions of many inclusive decay rates [6, 7].

The lattice formulation of the HQET offers the possibility of a numerical, non-perturbative determination of these quantities from first principles and without free parameters [8, 9]. For example, the most important achievement of lattice simulations of the HQET has been the computation of the B-meson decay constant in the static limit,  $f_B^{stat}$ . In this work, we present the first lattice calculation of the B-meson binding energy,  $\overline{\Lambda}$ , and of the kinetic energy of the heavy quark in the B-meson  $-\lambda_1/(2m_Q)$ , where  $\lambda_1 = \langle B|\bar{h}\vec{D}^2 h|B\rangle/(2M_B).$ 

The parameter  $\overline{\Lambda}$  denotes the asymptotic value of the difference between the hadron and the heavy quark "pole" mass  $m_Q$ 

$$
\overline{\Lambda} = \lim_{m_Q \to \infty} (M_H - m_Q). \tag{1}
$$

It has been recently shown that the pole mass is ambigous due to the presence of infrared renormalon singularities [10, 11]. At lowest order in  $1/m_Q$ , the infrared renormalon ambiguity appearing in the definition of the pole mass is closely related to the ultra-violet renormalon singularity present in the matrix elements of the operator  $hD_4h$ . This singu-

larity is due to the linear power divergence of  $\bar{h}D_4h$ , induced by its mixing with the lower dimensional operator  $\bar{h}h$ . In perturbation theory, using dimensional regularization, the power divergence is hidden by the absence of an intrinsic scale in the computation. On the lattice, because of the hard cut-off, renormalon poles are absent [11]. In this case, the linear divergence manifests itself as a power divergence in the inverse lattice spacing  $1/a$ , which appears in the mixing coefficient of the operator  $\bar{h}h$ . In ref. [12] it was stressed that these divergences must be subtracted non-perturbatively since factors such as

$$
\frac{1}{a}\exp\left(-\int^{g_0(a)}\frac{dg'}{\beta(g')}\right) \sim \Lambda_{\text{QCD}},\tag{2}
$$

which do not appear in perturbation theory, give non-vanishing contributions as  $a \to 0$ (see also refs. [13, 14]). In this sense, power divergences in theories with a hard cut-off and renormalon poles in dimensional regularization are closely related. For a more detailed discussion see ref. [15]. The intrinsic ambiguity of  $O(\Lambda_{\rm QCD})$ , present in the renormalisation of  $\bar{h}D_4h$ , implies an ambiguity in the definition of a finite  $\overline{\Lambda}$  and hence of  $m_Q$ .

Falk, Neubert and Luke [16] have proposed a different definition of  $\overline{\Lambda}$ ,

$$
\overline{\Lambda} = \frac{-\langle 0 | \bar{h} \Gamma D_4 q | M_H \rangle}{\langle 0 | \bar{h} \Gamma q | M_H \rangle} \tag{3}
$$

where h (q) is the effective heavy-quark (light-quark) field,  $\Gamma$  is a Dirac matrix and  $M_H$ a meson annihilated (created) by the operator  $J_{\Gamma} = \bar{h} \Gamma q$  ( $J_{\Gamma}^{\dagger} = \bar{q} \Gamma h$ ). This definition contains the same renormalon ambiguities as that in eq. (1).

In the lattice HQET, the "binding energy" computed in numerical simulations corresponds to the definition given in eq. (3). Consider the two-point function

$$
C(t) = \sum_{\vec{x}} \langle 0 | J_{\Gamma}(\vec{x}, t) J_{\Gamma}^{\dagger}(\vec{0}, 0) | 0 \rangle = \sum_{\vec{x}} \langle 0 | \bar{h}(\vec{x}, t) \Gamma q(\vec{x}, t) \ \bar{q}(\vec{0}, 0) \Gamma h(\vec{0}, 0) | 0 \rangle \tag{4}
$$

For sufficiently large Euclidean time t,

$$
C(t) \to Z^2 \exp(-\mathcal{E}t)
$$
 (5)

where Z is a constant. The definition (3) implies that  $\overline{\Lambda} = \mathcal{E}$ : indeed  $\mathcal{E}$  can be interpreted as the difference  $M_H - m_Q$  where  $M_H$  is the mass of the lightest meson which can be created by the operator  $J_{\Gamma}^{\dagger}$ . It is clear, however, that  $\mathcal E$  cannot be a "physical" quantity because it diverges linearly as  $a \to 0$ . This can be checked in one-loop perturbation theory and is a consequence of the mixing of the operator  $\bar{h}D_4h$  with  $\bar{h}h$ , as mentioned above.

It has been argued that it is possible to subtract the divergent term by computing the coefficient of  $\bar{h}h$  in perturbation theory [17]. Although it is true that with a hard (i.e. dimensional) ultraviolet cut-off, such as the lattice spacing or the Pauli-Villars regulator, the matrix elements of the bare operators have no renormalon ambiguities, the subtraction of the power divergences using perturbation theory reintroduces renormalons [18]. In other words, the perturbation series for the power-divergent counterterms contain renormalon ambiguities, which, as always, manifest themselves as terms which are exponentially small in the coupling constant eq. (2). Thus the subtraction of power divergences has to be performed non-perturbatively if the resulting matrix elements, such as  $\overline{\Lambda}$ , are to be unambiguous.

The matrix elements of the kinetic energy operator,  $\lambda_1$ , also contain power divergent contributions. In this case, the origin of the divergences is the mixing of  $\bar{h}\vec{D}^2h$  with the operator  $\bar{h}D_4h$ , with a coefficient that diverges linearly, and with the scalar density  $\bar{h}h$ , with a quadratically divergent coefficient [12].  $\lambda_1$  determines the  $1/m_Q$  corrections to the heavy quark mass and hence enters many theoretical expressions of weak decay factors. As in the case of  $\overline{\Lambda}$ , the quadratic and linear divergences of  $\lambda_1$  must be subtracted nonperturbatively.

The numerical values of  $\overline{\Lambda}$  and  $\lambda_1$ , presented in this paper, have been obtained by using the non-perturbative method proposed in ref. [18]. In that work, it has been shown that a non-perturbative renormalisation prescription, which can be implemented in lattice simulations, exists such as to avoid simultaneously both power divergences and renormalon ambiguities, in matrix elements and coefficient functions separately. In a theory regulated by a dimensionful cut-off, it is consistent not to perform the subtractions of the power divergent terms at all, but to work with the bare operators and to compute the coefficient functions (which will therefore contain powers of the cut-off) in perturbation theory [11]. In this case however, the matrix elements in the effective theory are divergent in the ultraviolet cut-off and depend on the regularization. Therefore they cannot be interpreted as "physical" quantities, in contrast to the approach that we adopt here.

The linear divergence in  $\overline{\Lambda}$  is eliminated by a suitable redefinition of the operator  $h_1h_2$ . This definition corresponds to the same normalization condition that one usually imposes in perturbation theory. We require that the matrix element of a combination

of  $\bar{h}D_4h$  and  $\bar{h}h$ ,  $\bar{h}D_4^s h = \bar{h}D_4h + \delta \overline{m} \bar{h}h$ , is zero for given external heavy quark states, in the Landau gauge:  $\langle h(p_4 = 0) | hD_4^s h | h(p_4 = 0) \rangle = 0$ <sup>1</sup>. Contrary to the perturbative procedure, which reintroduces the renormalon ambiguities in the matrix elements of the subtracted operator, the non-perturbative renormalization condition is unambigous, though prescription dependent, and independent of the regularization procedure. It is also quite natural in the sense that it allows a "physical" definition of  $\overline{\Lambda}$  that is finite and independent of the ultraviolet cut-off. This procedure can be extended to the operators appearing in higher orders of the  $1/m_Q$  expansion. Moreover it allows the matching of the operators of the HQET to those in the full theory (QCD) to be performed, via a combination of perturbative and non-perturbative calculations, in such a way that the Wilson coefficient functions are free of non-perturbative ambiguities at any given order in the  $1/m_Q$  expansion.

We show below that accurate results are obtained for the binding energy to this order. Our best estimate is

$$
\bar{\Lambda} = 190 \, \, {+50 \atop -30} \, \text{MeV} \, \, , \tag{6}
$$

where the error has been obtained by combining the statistical and systematic errors, as will be discussed below. Our results show that, as expected [18],  $\Lambda$  is indeed independent of the ultra-violet cut-off  $a^{-1}$ , within reasonably small statistical and systematic errors.

In order to remove the power divergences from the kinetic energy operator, we have imposed on the relevant operator a renormalisation condition which corresponds to the "physical" requirement  $\langle h(\vec{p} = 0) | \bar{h} \vec{D}_s^2 h | h(\vec{p} = 0) \rangle = 0$ , where  $\bar{h} \vec{D}_s^2 h$  is the subtracted kinetic energy operator [18]. This renormalisation condition, which will be explained in detail in the next section, has been used to extract the values of the mixing coefficients of the kinetic energy operator with the lower dimensional ones with a small statistical error. Unfortunately, after the subtraction of the power divergences, we were unable to obtain a precise value for  $\lambda_1$ , because of the large cancellations between the operator matrix element and its counterterm. We can only put a loose upper bound of 1 GeV<sup>2</sup> on  $\lambda_1$ . Nevertheless, the results of this study are so encouraging that we are implementing this procedure on the APE100 computer to perform a high statistics lattice calculation of both

<sup>&</sup>lt;sup>1</sup>This requires certain assumptions on the infrared behaviour of the heavy quark propagator that will be discussed below, see also [18].

 $\overline{\Lambda}$  and  $\lambda_1$ , whose results will be published elsewhere. We believe that the present results demonstrate the feasibility of the method proposed in ref. [18] to compute quantities relevant in heavy flavour phenomenology. In this way, it will still be possible to use the HQET and the notion of a "pole" mass, now defined non-perturbatively, which seemed to be ruined by the presence of the renormalons. Preliminary results of the present study can be found in ref. [19].

The plan of the paper is the following. In sec. 2 we introduce the relevant formulae which define the non-perturbative procedure for renormalising the operators  $\bar{h}D_4h$  and  $\bar{h}\bar{D}^{2}h$  [18]; in sec. 3 we describe the numerical calculation of  $\overline{\Lambda}$  and  $\lambda_1$  and discuss the main results of this study; in the conclusion we present the outlook for future developments and applications of the method discussed in this paper.

## 2 Non-perturbative definition of  $\overline{\Lambda}$  and  $\lambda_1$

In this section we define the renormalisation prescription which we will use to calculate "physical" values of  $\overline{\Lambda}$  and  $\lambda_1$ . The prescription involves imposing appropriate renormalisation conditions on the quark matrix elements of the operators  $\bar{h}D_4h$  and  $\bar{h}\vec{D}^2h$ , such that all their matrix elements are free of power divergences [18]. Similar methods have been used for light quark operators in refs. [20]–[22].

In numerical simulations, quark and gluon propagators can be computed non-perturbatively by working in a fixed gauge, typically the Landau gauge [20]–[23]. The heavy quark propagator, at lowest order in  $1/m_Q$ , has the form

$$
S(\vec{x},t) = \langle S(\vec{x},t|\vec{0},0)\rangle = \delta(\vec{x})\,\theta(t)\,\delta^{ij}\,A(t)\,\exp(-\lambda t) \tag{7}
$$

where  $i, j$  are colour indices;

$$
S(\vec{x}, t | \vec{y}, w) = \delta(\vec{x} - \vec{y}) \theta(t - w) \exp\left(i \int_{w}^{t} A_0(t') dt'\right)
$$
 (8)

is the non-translationally invariant propagator for a given gauge field configuration, computed in a given smooth gauge, typically the Landau gauge, and  $\langle \ldots \rangle$  represents the average over the gauge field configurations.  $A(t)$  is an unknown function of t, and we assume that it decreases more slowly than an exponential at large times, specifically we require that

$$
\lim_{t \to \infty} \frac{1}{a} \ln \left( \frac{A(t+a)}{A(t)} \right) \sim \lim_{t \to \infty} \frac{d}{dt} \ln A(t) = 0.
$$
\n(9)

Below we will show that, within the precision of our simulations, our results for the heavy quark propagator are consistent with the condition in eq. (9). As will also be explained below, the condition (9) is not strictly required for the definition and determination of  $\Lambda$ , since this can be done using the values of the propagator at small times  $t$ . However in that case it no longer has a direct interpretation as a binding energy, and our preferred definition of  $\overline{\Lambda}$  does use the behaviour of the propagator at large t.

The constant  $\lambda$  in eq. (7) is linearly divergent in  $1/a$  and would correspond, in dimensional regularisation, to an ultraviolet renormalon in the effective heavy-quark propagator. Since the linear divergence in  $\lambda$  is due to the mixing of the operator  $\bar{h}D_4h$  with the conserved scalar density operator  $\bar{h}h$ , we can remove it by adding to the Lagrangian of the lattice HQET

$$
\mathcal{L}_{\text{eff}} = \bar{h}(x) D_4 h(x) \tag{10}
$$

a counter-term of the form  $\delta m \bar{h}(x) h(x)$ . The HQET Lagrangian then becomes

$$
\mathcal{L}'_{\text{eff}} = \frac{1}{1 + a \,\delta m} \Big( \bar{h}(x) \, D_4 \, h(x) + \delta m \, \bar{h}(x) \, h(x) \Big), \tag{11}
$$

where the factor  $1/(1 + a \delta m)$  has been introduced to ensure the correct normalization of the heavy quark field h. With the action  $\mathcal{L}'_{\text{eff}}$ , the heavy-quark propagator is given by:

$$
S'(\vec{x},t) = \delta(\vec{x})\,\theta(t)\,\delta^{ij}\,A(t)\,\exp\left(-\left[\lambda + \frac{\ln(1+a\,\delta m)}{a}\right]\,t\right). \tag{12}
$$

The mass counter-term is defined by the behaviour of  $S(\vec{x}, t)$  at large values of the time

$$
-\delta \overline{m} \equiv \frac{\ln(1 + a \delta m)}{a} = \lim_{t \to \infty} \frac{1}{a} \ln \left[ \frac{\text{Tr}\Big(S(\vec{x}, t + a)\Big)}{\text{Tr}\Big(S(\vec{x}, t)\Big)} \right] =
$$

$$
\lim_{t \to \infty} \left[ \frac{1}{a} \ln \left( \frac{A(t + a)}{A(t)} \right) - \lambda \right] = -\lambda,
$$
(13)

where the traces are over the colour quantum numbers, and we have assumed the validity of the condition in eq. (9). Our numerical results, support the validity of this condition and the use of eq. (13) is our preferred determination of  $\delta \overline{m}$ .

We now define the renormalised binding energy by

$$
\overline{\Lambda} \equiv \mathcal{E} - \delta \overline{m}, \qquad (14)
$$

which corresponds to the following relation between the meson and the heavy quark mass

$$
M_H = m_Q + \mathcal{E} - \delta \overline{m} \tag{15}
$$

 $m_Q$  can be interpreted as a subtracted pole mass, and contains no renormalon effects. A similar relation can be found in the case of a heavy baryon.

The definition of  $\delta \overline{m}$  given in eq. (13) is not unique. A possible alternative definition would be, for example,

$$
-\delta \overline{m}(t^*) \equiv \frac{1}{a} \ln \left[ \frac{\text{Tr}\Big(S(\vec{x}, t^* + a)\Big)}{\text{Tr}\Big(S(\vec{x}, t^*)\Big)} \right] = -\lambda + \frac{1}{a} \ln \left( \frac{A(t^* + a)}{A(t^*)} \right),\tag{16}
$$

where  $t^*$  is a given time at which we perform the subtraction. The corresponding definition of  $\overline{\Lambda}$ , see eq. (14) above, will clearly depend on the choice of  $t^*$ :  $t^*$  parametrizes the renormalisation prescription dependence and can be considered as the renormalisation point in coordinate space. For physical matrix elements, the residual mass appears only through the combination  $m_Q - \delta \overline{m}$ , in such a way that different choices of  $\delta \overline{m}$  are compensated by different values of  $m_Q$  [16]. The use of the propagator at small times,  $t^*\Lambda_{QCD} \ll 1$ , to define  $\delta \overline{m}(t^*)$ , and hence  $\overline{\Lambda}(t^*)$  does not require any assumption about the behaviour of  $A(t)$  at large times, and in section 3.2 we present the results for  $\overline{\Lambda}(t^*)$ obtained in this way.

In addition to the non-perturbative contribution of  $O(\Lambda_{QCD})$  to  $\delta \overline{m}(t^*)$ , there is a perturbative one proportional to  $1/t^*$  [18],

$$
-\delta \overline{m}_{\text{pert}}(t^*) = -\frac{\alpha_s C_F}{4\pi} \frac{\gamma_\psi}{t^*} + O(\alpha_s^2)
$$
\n(17)

where  $\gamma_\psi$  is the one-loop contribution to the anomalous dimension of the heavy quark field ( $\gamma_{\psi} = -6$  in the Landau gauge) and  $C_F$  is the quadratic Casimir operator in the fundamental representation ( $C_F = 4/3$ ). Thus the definition of  $\overline{\Lambda}(t^*)$  defined, at small times cannot readily be identified as a physical binding energy. Nevertheless, computed values of  $\overline{\Lambda}(t^*)$  can be used to determine standard short-distance heavy quark masses (such as the MS one) using perturbation theory (as will be explained in section 3.1 below). This, together with the fact that no assumption about the infra-red behaviour of the heavy quark propagator is necessary, is of fundamental importance.

#### 2.1 Non-perturbative subtractions for  $\lambda_1$

The renormalised kinetic operator  $\bar{h}\vec{D}_{S}^{2}h$ , free of power divergences, has the form

$$
\bar{h}(x) \,\vec{D}_S^2 \, h(x) = \bar{h}(x) \,\vec{D}^2 \, h(x) - \frac{c_1}{a} \frac{1}{(1 + a \,\delta m)} \Big( \bar{h}(x) \, D_4 \, h(x) + \delta m \,\bar{h}(x) \, h(x) \Big) - \frac{c_2}{a^2} \,\bar{h}(x) \, h(x),\tag{18}
$$

where the constants  $c_1$  and  $c_2$  are functions of the bare lattice coupling constant  $g_0(a)$ . They have been computed in one loop perturbation theory in ref. [12]. Notice that we have preferred to express  $\bar{h}\vec{D}_{S}^{2}h$  in terms of the subtracted operator which explicitly contains the residual mass  $\delta m$ . In this way we can use the equations of motion of the Lagrangian  $\mathcal{L}'$  given in eq. (11). This will prove useful below. The constant  $c_2$  enters in the renormalisation of the heavy quark mass. Therefore, it will contribute to the relation between  $M_H$ ,  $m_Q$  and  $\overline{\Lambda}$  at order  $1/m_Q$  (see below). On the other hand, the constant  $c_1$  contributes to the renormalisation of the heavy quark wave-function and hence to the renormalisation of all the operators containing a heavy quark field, but not to the relation for the quark mass.

In order to eliminate the quadratic and linear power divergences, a possible nonperturbative renormalisation condition for  $\bar{h}\vec{D}_{S}^{2}h$  is that its subtracted matrix element, computed for a quark at rest in the Landau gauge, vanishes

$$
\langle h(\vec{p}=0)|\bar{h}\vec{D}_{S}^{2}h|h(\vec{p}=0)\rangle = 0.
$$
\n(19)

This is equivalent to defining the subtraction constants through the relation (in the following we will work in lattice units, setting  $a = 1$ )

$$
\rho_{\vec{D}^2}(t) = c_1 + c_2 t,\tag{20}
$$

where

$$
\rho_{\vec{D}^2}(t) \equiv \frac{\sum_{\vec{x}} \langle S^a'(\vec{x},t|\vec{0},0)\rangle}{\sum_{\vec{x}} \langle S'(\vec{x},t|\vec{0},0)\rangle} = \frac{\sum_{t'=0}^t \sum_{\vec{x},\vec{y}} \langle S'(\vec{x},t|\vec{y},t') \vec{D}_y^2(t') S'(\vec{y},t'|\vec{0},0)\rangle}{\sum_{\vec{x}} \langle S'(\vec{x},t|\vec{0},0)\rangle} \tag{21}
$$

By fitting the time dependence of  $\rho_{\vec{D}^2}(t)$  to eq. (20), one obtains  $c_1$  and  $c_2$ .

The heavy-quark propagator that enters in eq. (21) is the subtracted one, i.e. it is calculated with the action (11) instead of (10). We now demonstrate that  $\rho_{\vec{D}^2}(t)$  can be expressed in terms of unsubtracted propagators only:

$$
\rho_{\vec{D}^2}(t) = \frac{\sum_{t'=0}^t\sum_{\vec{x},\vec{y}}\langle (S'(\vec{x},t|\vec{y},t')\vec{D_y^2}(t')\,S'(\vec{y},t'|\vec{0},0)\rangle)}{\sum_{\vec{x}}\langle S'(\vec{x},t|\vec{0},0)\rangle} =
$$

$$
\frac{\sum_{t'=0}^{t} \sum_{\vec{x},\vec{y}} \langle (S(\vec{x},t|\vec{y},t')e^{\delta \overline{m}(t-t')}\vec{D}_{y}^{2}(t') S(\vec{y},t'|\vec{0},0) e^{\delta \overline{m}t'} \rangle)}{\sum_{\vec{x}} \langle S(\vec{x},t|\vec{0},0) e^{\delta \overline{m}t} \rangle} = \frac{\sum_{t'=0}^{t} \sum_{\vec{x},\vec{y}} \langle (S(\vec{x},t|\vec{y},t')\vec{D}_{y}^{2}(t') S(\vec{y},t'|\vec{0},0) \rangle)}{\sum_{\vec{x}} \langle S(\vec{x},t|\vec{0},0) \rangle}
$$
(22)

Notice that this argument holds for any operator which does not contain a time derivative.

For some important applications it is only the constant  $c_2$  which is required.  $c_2$  can also be determined directly by eliminating the sum over  $t'$  in eq. (21):

$$
c_2 = \rho_{\vec{D}^2}(t',t) = \frac{\sum_{\vec{x},\vec{y}} \langle (S'(\vec{x},t|\vec{y},t')\vec{D}_y^2(t')\,S'(\vec{y},t'|\vec{0},0)\rangle)}{\sum_{\vec{x}} \langle S'(\vec{x},t|\vec{0},0)\rangle}
$$
(23)

for  $t' \neq 0, t$ .

The relation between the mass of the meson and the mass of the quark to order  $1/m_Q$ is then given by

$$
M_H = m_Q + \mathcal{E} - \delta \overline{m} - \left(1 - \frac{\alpha_s}{4\pi} X_{\overrightarrow{D}_S^2}\right) \left(\frac{\lambda_1^{\text{bare}} - c_2}{2 m_Q}\right) + O(\frac{1}{m_Q^2}),\tag{24}
$$

where  $\lambda_1^{\text{bare}} = \langle B|\bar{h}\vec{D}^2h|B\rangle/(2M_B)$ .  $\lambda_1^{\text{bare}}$  can be determined from a computation of twoand three-point correlation functions in the standard way. Consider the meson three-point correlation function (the extension of this discussion to baryons is entirely straightforward)

$$
C_{\vec{D}^2}(t',t) = \sum_{\vec{x},\vec{y}} \langle 0|J_{\Gamma}(\vec{x},t) \ \bar{h}(\vec{y},t') \vec{D}_y^2 h(\vec{y},t') J_{\Gamma}^{\dagger}(\vec{0},0)|0\rangle \tag{25}
$$

For sufficiently large values of  $t'$  and  $t - t'$ 

$$
C_{\vec{D}^2}(t',t) \to Z^2 \lambda_1^{\text{bare}} \exp\left(-(\mathcal{E} - \delta \overline{m})t\right). \tag{26}
$$

A convenient way to extract  $\lambda_1^{\text{bare}}$  is to consider the ratio

$$
R(t',t) = \frac{C_{\vec{D}^2}(t',t)}{C(t)} \to \lambda_1^{\text{bare}} \tag{27}
$$

As usual  $\lambda_1^{\text{bare}}$  must be evaluated in an interval in which  $R(t', t)$  is independent of the times  $t'$  and  $t$ , so that the contribution from excited states and contact terms can be neglected.

The term proportional to  $X_{\vec{D}_S^2}$  in eq. (24) is absent in continuum formulations of the HQET, and is a manifestation of the lack of reparametrisation invariance in the lattice version. It has been calculated in ref.  $[12]$ . Notice that only the constant  $c_2$  enters the eq.  $(24)$  because  $c_1$  is eliminated by using the equations of motions.  $c_1$  only modifies the wave function renormalisation of the heavy quark, thus contributing to the  $O(1/m_Q)$ corrections of the hadronic matrix elements.

simulation	volume	β	Number of configurations
<u>set A</u>	$16^3 \times 32$	6.0	36
set B	$16^3 \times 32$	6.0	300
set C	$20^3 \times 32$	6.2	50
set D	$18^3 \times 64$	6.0	210
set E	$18^3 \times 64$	6.2	420

Table 1: Parameters of the numerical simulations, the results of which have been used for the present study.

# 3 Numerical implementation of the renormalisation procedure

As explained in the previous section, the determination of  $\overline{\Lambda}$  and  $\lambda_1$  requires the computation of the quark propagator and matrix elements between quark states in a fixed gauge (in order to obtain the subtracted operators), as well as the evaluation of matrix elements between hadronic states. We have obtained our results using five independent numerical simulations, whose main parameters are given in table 1.

Our best value of the subtracted binding energy,  $\overline{\Lambda} = \mathcal{E} - \delta \overline{m}$ , has been determined by combining the values of  $\delta \overline{m}$  obtained using set B and set C with the calculation of E performed by the APE collaboration at  $\beta = 6.0$ , <u>set D</u>, and 6.2, <u>set E</u> [25, 26]. *E* had been determined using the SW-Clover fermion action for the light quarks. The calculations were performed at several masses of the light quark, so that extrapolations to the chiral limit are possible. We also present the results for the subtraction constants  $c_1$  and  $c_2$  obtained with <u>set B</u> and set C.

So far we have only computed  $\lambda_1^{\text{bare}}$  using <u>set A</u>. Again, for the light quarks the improved SW-Clover action [27] was used in the quenched approximation. These exploratory calculations were performed at one value of the mass of the light quark,  $\kappa = 0.1425$ , for which the mass of the corresponding "pion" is about 900 MeV. The details of the simulation can be found in refs. [20, 24]. Preliminary results for both  $\overline{\Lambda}$  and  $\lambda_1$  for mesons, evaluated using this dataset have been presented in ref. [19].

All the errors have been computed with the jacknife method by decimating one configuration at a time (set  $\underline{A}$  and set  $\underline{C}$ ) or five configurations at a time (set  $\underline{B}$ ). The error on  $\mathcal E$  was computed with the jacknife method also and we refer the reader to refs. [25, 26] for details.

#### 3.1 Determination of the residual mass  $\delta \overline{m}$

A possible lattice expression for the forward heavy-quark propagator, to leading order in the heavy quark mass, is given by

$$
S(x|0) = \delta(\vec{x}) \,\theta(x^4) \,\mathcal{P}_{\vec{x}}(x^4 \,|\, 0) \tag{28}
$$

where  $\mathcal{P}_{\vec{x}}(x^4 | y^4)$  is the lattice path ordered exponential from  $(\vec{x}, y^4)$  to  $(\vec{x}, x^4)$ , cf. eq. (8), usually called "P-line",

$$
\mathcal{P}_x(x^4 \mid y^4) = \prod_{n=1}^{\left[\frac{x^4 - y^4}{a}\right]} U^{\dagger}(\vec{x}, x^4 - n a), \quad x^4 > y^4
$$
\n
$$
\mathcal{P}_x(x^4 \mid y^4) = 1 \quad x^4 = y^4 \tag{29}
$$

This propagator corresponds to the following choice for the covariant time derivative,  $D_4 f(t) = 1/a (f(t) - U_4^{\dagger}(t - a)f(t - a)).$ 

In order to reduce the statistical noise, we have computed, in the lattice Landau gauge, the quantity

$$
S_H(t) = \frac{1}{3V} \sum_{\vec{x}} \langle \text{Tr} \left[ \mathcal{P}_{\vec{x}}(x^4 = t \, | \, 0) \right] \rangle,\tag{30}
$$

where the trace is over the colour indices and  $V$  denotes the spatial volume of our lattice. It is this averaged propagator  $S_H(t)$ , which has been used in the computations below.

There is a subtle point that we would like to discuss briefly. It can be demonstrated that  $O(a)$  effects in heavy-light operator matrix elements between physical states are cancelled by improving the light quark propagators only [28]. On the other hand, in order to improve off-shell matrix elements, which is the case when renormalising the operators between quark states, it is necessary to use an improved version of the heavy quark propagator in the effective theory, for example

$$
\mathcal{P}_x^I(x^4 \, | \, y^4) = \left[1 - \left(\frac{1}{3}\right)^{y^4 - x^4 + 1}\right] \mathcal{P}_x(x^4 \, | \, y^4). \tag{31}
$$

Notice that the improved P-line tends very rapidly to the unimproved one as  $x^4 - y^4$ increases. The propagator in eq.(31) corresponds to the following time derivative  $D_4 f(t) =$  $1/a (3/2f(t) - 2U^{\dagger}(t-a)f(t-a) + 1/2U^{\dagger}(t-a)U^{\dagger}(t-2a)f(t-2a))$ . It is also possible to add a residual mass term to the heavy quark action in such a way that it modifies the propagator (31) by an exponetial in time (up to an overall normalisation factor). Such as mass term takes the form  $3/2 (1/\lambda - 1) \bar{h}(t)h(t) + 1/2 (\lambda - 1) \bar{h}(t)h(t-2a)$ . In the following, when discussing the improved heavy quark propagator, we will implicitly assume that the mass term is of this form.

To determine the residual mass, we have to compute the effective mass of the propagator  $S_H(t)$ , defined by

$$
a\,\delta\overline{m}(t) = -\ln\left(\frac{S_H(t+a)}{S_H(t)}\right) \tag{32}
$$

In figs. 1 (from <u>set B</u>) and 2 (from <u>set C</u>), we present the values of  $\delta \overline{m}(t)$  for the improved and unimproved propagators as a function of  $t/a$ . The effective mass is indistinguishable in the two (improved and unimproved) cases, for  $t/a > 4-5$ . Thus, in order to minimize lattice artefacts, we have only used the results obtained for  $t/a \geq 5$ . Inspired by the results of one-loop perturbation theory [18], we made a fit to  $\delta \overline{m}(t)$  using the expression

$$
a\,\delta\overline{m}(t) = a\,\delta\overline{m} + \gamma\frac{a}{t} \tag{33}
$$

In order to mimic higher order effects, we have also used different expressions to fit  $\delta \overline{m}(t)$ , e.g.

$$
a\,\delta\overline{m}(t) = a\,\delta\overline{m} + \gamma'\ln\left(\frac{t+a}{t}\right) \tag{34}
$$

or

$$
a\,\delta\overline{m}(t) = a\,\delta\overline{m} - \gamma''\ln\left(\frac{\alpha_s[\mathcal{K}/(t+a)]}{\alpha_s[\mathcal{K}/t]}\right) \to a\,\delta\overline{m} + \gamma''\ln\left(\frac{\ln[(t+a)]+\mathcal{C}}{\ln[t]+\mathcal{C}}\right),\tag{35}
$$

and changed the interval of the fits in order to check the stability of the determination of  $\delta \overline{m}$ . In eqs. (33)–(35),  $\delta \overline{m}$ ,  $\gamma, \ldots, \gamma''$  and C are free parameters of the fit. The curves shown in fig. 1 and 2 correspond to fits of the improved heavy quark propagator to eq. (34), in the interval  $5 \le t/a \le 12$ .

From the different results obtained by varying the fitting functions and the time intervals, see tables 2 and 3, we quote

$$
a\,\delta\overline{m} = 0.521 \pm 0.006 \pm 0.010 \text{ at } \beta = 6.0\tag{36}
$$

Figure 1: Effective mass of the heavy-quark propagator  $S_H(t)$ , at  $\beta = 6.0$ , as a function of the time. The curve represents a fit of the numerical results (in the improved case) to the expression  $given\ in\ eq.\ (34).$ 

Figure 2: Effective mass of the heavy-quark propagator  $S_H(t)$ , at  $\beta = 6.2$ , as a function of the time. The curve represents a fit of the numerical results (in the improved case) to the expression given in eq. (35).

Subtraction constant $a\delta\overline{m}$ at $\beta = 6.0$						
Fit	$t = 4 - 12$	$t = 5 - 12$			$t = 5 - 14$ $t = 6 - 14$ $t = 7 - 14$	$t = 8 - 14$
eq. (33)	0.507(4)	0.515(6)	0.515(6)	0.52(1)	0.52(2)	0.51(3)
$\chi^2/\text{dof}$	1.50	0.56	0.86	0.84	0.96	1.05
eq. $(34)$	0.515(4)	0.521(6)	0.521(6)	0.53(1)	0.53(2)	0.51(3)
$\chi^2/\text{dof}$	0.97	0.46	0.81	0.85	0.98	1.05
eq. $(35)$	0.513(4)	0.521(6)	0.520(6)	0.51(3)	0.51(1)	0.50(2)
$\chi^2/\text{dof}$	1.20	0.56	0.93	0.97	1.10	1.28

Table 2: Numerical values of the constant  $a\delta\overline{m}$  found by using the results of <u>set B</u>, at  $\beta = 6.0$ . The results are from several fits in different time intervals. We also give the uncorrelated  $\chi^2/dof$  in the different cases. The numbers given in this table refer to the improved heavy quark propagator only.

Subtraction constant $a\delta\overline{m}$ at $\beta = 6.2$						
Fit	$t = 4 - 12$	$t = 5 - 12$	$t = 5 - 14$	$t = 6 - 14$	$t = 7 - 14$	$t = 8 - 14$
eq. $(33)$	0.437(5)	0.441(7)	0.440(8)	0.45(1)	0.46(2)	0.45(2)
$\chi^2/\text{dof}$	0.50	0.93	0.80	0.75	0.70	0.83
eq. $(34)$	0.442(5)	0.445(8)	0.445(8)	0.45(1)	0.46(2)	0.46(3)
$\chi^2/\text{dof}$	0.40	0.85	0.74	0.73	0.70	0.83
eq. $(35)$	0.443(6)	0.445(8)	0.445(8)	0.45(1)	0.45(5)	0.46(3)
$\chi^2/\text{dof}$	0.50	1.02	0.85	0.85	0.84	1.05

Table 3: Numerical values of the constant  $a\delta\overline{m}$  found by using the results of <u>set C</u>, at  $\beta = 6.2$ . The results are from several fits in different time intervals. We also give the uncorrelated  $\chi^2/dof$  in the different cases. The numbers given in this table refer to the improved heavy quark propagator only.

$$
a\,\delta\overline{m} = 0.445 \pm 0.008 \pm 0.010 \text{ at } \beta = 6.2\tag{37}
$$

where in both cases the first error is statistical, and the second is an estimate of the systematic uncertainty, based on the spread of results obtained using different time intervals and fitting functions.

The determination of the mass counter-term at fixed  $t = t^*$ , requires no fitting, and the results obtained using  $\underline{\text{set }B}$  and  $\underline{\text{set }C}$  are presented in table 4 below.

### 3.2 Determination of  $\overline{\Lambda}$

We are now ready to present our prediction for  $\overline{\Lambda}$ . In order to evaluate the subtracted  $\overline{\Lambda}$ , we have used the results of the high statistics calculations of  $\mathcal E$  given in refs. [25, 26] (set D and  $set E$ ). We will also make use of the results obtained by using the standard Wilson action, on a  $18^3 \times 64$  lattice, at  $\beta = 6.0$ , with a statistical sample of 200 configurations [25].

In order to obtain  $\bar{\Lambda}$  we have used:

- $\delta \overline{m}$  from eqs. (36) and (37);
- the SW-Clover determination of  $\mathcal E$  of the APE collaboration,  $a\mathcal E = 0.61 \pm 0.01$  at  $\beta = 6.0$  and  $a\mathcal{E} = 0.52 \pm 0.01$  at  $\beta = 6.2$  [25, 26];
- $a^{-1}(\beta = 6.0) = 2.0 \pm 0.2$  GeV and  $a^{-1}(\beta = 6.2) = 2.9 \pm 0.3$  GeV. The calibration of the lattice spacing in quenched simulations typically has an uncertainty of  $O(10\%)$ , depending on the physical quantity which is used to set the scale. We take these results as a fair representation of the spread of possible values.

We then find

$$
\overline{\Lambda} = \mathcal{E} - \delta \overline{m} = 180 \pm 35 \text{ MeV at } \beta = 6.0 \tag{38}
$$

$$
\overline{\Lambda} = \mathcal{E} - \delta \overline{m} = 220 \pm 55 \text{ MeV at } \beta = 6.2 \tag{39}
$$

where the statistical errors have been combined in quadrature with those due to the uncertainty in the lattice spacing.

Within the uncertainties, the results in eqs. (38) and (39) are compatible with the expected independence of  $\Lambda$  of the lattice spacing. Given the intrinsic uncertainty in the value of the lattice spacing in quenched simulations it is difficult however, to check this more precisely. Indeed, using different physical quantities to set the scale can increase

or decrease the difference in the central values of  $\overline{\Lambda}$  at  $\beta = 6.0$  and 6.2. For example, using the string tension to set the scale one finds  $a^{-1}(\beta = 6.0) = 1.88$  GeV and  $a^{-1}(\beta = 6.0)$ 6.2) = 2.55 GeV, giving  $\overline{\Lambda} = 170 \pm 30$  MeV at  $\beta = 6.0$  and  $\overline{\Lambda} = 190 \pm 40$  MeV at  $\beta$ =6.2, whereas using the mass of the  $\rho$ -meson to set the scale the APE collaboration finds  $a^{-1}(\beta = 6.0) = 1.95 \pm 0.07$  GeV and  $a^{-1}(\beta = 6.2) = 3.05 \pm 0.20$  GeV [25, 26], which corresponds to  $\overline{\Lambda} = 176 \pm 30$  MeV at  $\beta = 6.0$  and  $\overline{\Lambda} = 228 \pm 50$  MeV at  $\beta = 6.2$  <sup>2</sup>. Nevertheless in both cases the results are compatible at the two values of  $\beta$ .

Assuming that  $\Lambda$  is indeed constant in a, we combine the results in eqs. (38) and (39) to obtain

$$
\bar{\Lambda} = (190 \pm 30) \text{ MeV} \tag{40}
$$

Before quoting our final result, we need to estimate the discretisation error.

From a comparison of the values of  $\delta \overline{m}$  obtained with the improved and unimproved heavy quark propagators, we believe that discretisation effects are negligible for this quantity. Indeed discretisation errors in quantities which only depend on the gauge fields are of  $O(a^2 \Lambda_{\text{QCD}}^2)$ , when evaluated using the Wilson gauge action. However, in the computation of  $\overline{\Lambda}$  (and  $\lambda_1$ ), correlation functions which contain the light quark propagator are evaluated, and with the SW-Clover and Wilson fermion actions this introduces errors of  $O(\alpha_s a \Lambda_{\text{QCD}})$  and  $O(a \Lambda_{\text{QCD}})$  respectively. Notice that these effects are formally larger than the higher order  $1/m_Q$  corrections to  $\overline{\Lambda}$  (we work in the approximation  $a^{-1} \ll m_Q$ ). To obtain an estimate of the size of the discretisation errors, we compare  $\mathcal E$  obtained with the standard Wilson action and the SW-Clover action at the same value of  $\beta$ ,  $\beta = 6.0$ . In the Wilson case, by working at four different values of the light quark mass, the bare binding energy, extrapolated to the chiral limit in the light quark mass, was found to be  $a \mathcal{E}_W = 0.608(8)$ . In the SW-Clover case, by working at three different values of the light quark mass, the result for the bare binding energy, extrapolated to the chiral limit in the light quark mass, was found to be  $a \mathcal{E}_{SW} = 0.616(4)^3$ . The difference between the central values obtained with the two actions  $\mathcal{E}_{SW} - \mathcal{E}_W = (0.616 - 0.608) a^{-1} \sim 16$  MeV. We

<sup>&</sup>lt;sup>2</sup>Notice that, using the mass of the  $\rho$ -meson, the UKQCD collaboration found  $a^{-1}(\beta = 6.2) \sim 2.7(1)$  GeV [30], corresponding to  $\overline{\Lambda} = 203 \pm 45 \,\text{MeV}$ .

 $3$ As a check of our calculations with set A, we have verified that on these configurations, at the value of the mass where we have computed the light quark propagator  $(K = 0.1425)$ , our results for  $\mathcal E$  agree with those of refs. [25, 26].

deduce that +20MeV is a reasonable estimate of the discretisation error in the determination of  $\overline{\Lambda}$ . We therefore quote as our final result for  $\overline{\Lambda}$ 

$$
\bar{\Lambda} = 190 \, \, {+50 \atop -30} \, \text{MeV} \tag{41}
$$

The prediction given in eq. (41) can be compared with other results that have been presented in the literature. In perturbation theory one finds

$$
a\,\delta\overline{m}_{\text{pert}} = \frac{\alpha_s}{3} \int \frac{d^3q}{(2\pi)^2} \left(\frac{1}{\sum_{i=1}^3 \sin^2(q_i/2)}\right) = 2.12 \times \alpha_s \tag{42}
$$

By using values for  $\alpha_s$  which are commonly proposed in the literature for the "boosted" coupling [29, 31],  $\alpha_s = 0.13{\text -}0.18$  at  $\beta = 6.0$ , eq. (42) would give  $a\delta\overline{m}_{\text{pert}} = 0.28 - 0.38$ . Thus, even in the most favourable case,  $\delta \overline{m}_{\text{pert}}$  is about 280 MeV smaller (i.e.  $\Lambda_{\text{pert}}$  is about 280 MeV larger) than our non-perturbative determination.

In ref. [31], the bare binding energy  $\mathcal E$  has been determined, using the Wilson action for light quarks, on a variety of lattice volumes and at several values of  $\beta$ ,  $\beta = 5.7, 5.9, 6.1$ and 6.3. The results are consistent with a linear dependence

$$
a\,\mathcal{E}(a) = \mathcal{E}_0 + a\,\overline{\Lambda}_{\text{FNAL}}\tag{43}
$$

where  $\mathcal{E}_0$  and  $\overline{\Lambda}_{\text{FNAL}}$  are parameters of the fit,  $\mathcal{E}_0 = 0.351(14)$  and  $\overline{\Lambda}_{\text{FNAL}} = 0.481(25)$  GeV. The value of  $\mathcal{E}_0$  is consistent with  $a \, \delta \overline{m}_{\text{pert}}$  computed using an "effective"  $\alpha_s = 0.166$  (this value may be considered as an average of the values of the strong coupling constant on the points in  $\beta$  where  $\mathcal E$  has been computed). On the other hand, the value of the "finite" binding energy  $\overline{\Lambda}_{\text{FNAL}}$  is about 300 MeV larger than ours <sup>4</sup>. Our interpretation is that, up to possible  $O(a)$  effects, the two determinations differ because of the finite nonperturbative contribution of  $O(\Lambda_{\text{QCD}})$  that has been subtracted only in our case. Using the definition of ref. [31] however, it is not clear how to match the full and the effective theories, since their definition includes non-perturbative, uncalculable effects.

A further demonstration of the existence of the non-perturbative effects is provided by the comparison of  $a\delta\overline{m}$  and  $a^{-1}$  at  $\beta = 6.0$  and 6.2. In the absence of non-perturbative terms of  $O(\Lambda_{\rm QCD})$ , i.e. if  $\delta \overline{m}$  is given only by the linearly divergent contribution, we should find  $R_m \equiv a \delta \overline{m}(\beta = 6.0) / a \delta \overline{m}(\beta = 6.2) \simeq R_{\alpha_s} = \alpha_s(\beta = 6.0) / \alpha_s(\beta = 6.2)$ . Numerically

<sup>&</sup>lt;sup>4</sup>Given the presence of terms of  $O(a)$  the stability of the results with respect to a quadratic fit of the form  $a \mathcal{E}(a) = \mathcal{E}_0 + \overline{\Lambda}_{\text{FNAL}} a + \mathcal{E}_2 a^2$ , where  $\mathcal{E}_2$  is a constant, remains to be checked.

$\beta$	$t^*/a$	$a\delta\overline{m}(t^*)$	$\pi/t^*$ (GeV)	$\bar{\Lambda}(t^*)$ (MeV)
6.0	3	0.3670(6)	$2.1 \pm 0.2$	$490 \pm 20 \pm 50$
	$\overline{4}$	0.3980(8)	$1.6 \pm 0.2$	$420 \pm 20 \pm 40$
	5	0.4177(9)	$1.3 \pm 0.1$	$390 \pm 20 \pm 40$
	6	0.4328(13)	$1.0 \pm 0.1$	$350 \pm 20 \pm 40$
6.2	$\overline{4}$	0.3484(13)	$2.3 \pm 0.2$	$500 \pm 30 \pm 50$
	5	0.3663(16)	$1.8 \pm 0.2$	$450 \pm 30 \pm 50$
	6	0.3773(20)	$1.5 \pm 0.2$	$410 \pm 30 \pm 40$
	7	0.3842(27)	$1.3 \pm 0.1$	$390 \pm 30 \pm 40$

Table 4: Results for  $\bar{\Lambda}(t^*) = \mathcal{E} - \delta \overline{m}(t^*)$  for different normalization times  $t^*$ , using the results from <u>set B-set E</u>. The first error on  $\bar{\Lambda}(t^*)$  is obtained by combining the errors on  $\mathcal E$  and  $\delta \overline{m}(t^*)$ in quadrature; the second error (and the error on  $\pi/t^*$ ) comes from the calibration of the lattice spacing.

we find  $R_m = 1.16(4)$  to be compared with  $R_{\alpha_s} = 1.03 - 1.06$ : 1.03 is simply 6.2/6.0; 1.06 has been estimated from  $R_{\alpha_s^{\text{eff}}}$ , where  $\alpha_s^{\text{eff}} = \alpha_s^{\text{latt}}/\langle \Box \rangle$  with  $\alpha_s^{\text{latt}} = (6/\beta)/(4\pi)$  and  $\langle \Box \rangle$  is the expectation value of the plaquette.

We now present the results for  $\overline{\Lambda}$  defined at a fixed value of  $t^*$   $(\overline{\Lambda}(t^*))$ . In order to be able to use perturbation theory to determine values corresponding to standard short distance definitions of the heavy quark mass,  $t^*$  must be chosen to be sufficiently small. In table 4 we present the results for the mass counterterm  $\delta \overline{m}(t^*)$  at both  $\beta = 6.0$  and 6.2, obtained using the configurations of  $\underline{\text{set }B}$  and  $\underline{\text{set }C}$  respectively, for small values of  $t^*$ . We then combine the results for  $\delta \overline{m}(t^*)$  with those for  $\mathcal E$  obtained by the APE collaboration (set D and set E) to obtain  $\overline{\Lambda}(t^*)$ . These results for  $\overline{\Lambda}(t^*)$  will be used in section 3.3 to determine the  $\overline{MS}$  mass.

We end this subsection with an obvious but important remark.  $\bar{\Lambda}$  can be defined in many different ways, which correspond to different renormalization prescriptions for the renormalized  $hD_4h$  operators. The presentation of results or bounds for  $\Lambda$  must therefore be accompanied by the definition of the prescription to which they correspond.

## 3.3 The  $\overline{MS}$  mass of the b-quark

We now give the relevant formulae necessary to match the subtracted mass of the quark  $m_Q^S$  to the running mass  $\overline{m}_Q$ , computed in the  $\overline{MS}$  scheme at the scale  $\mu = \overline{m}_Q$ . We introduce the following quantities

$$
m_Q^S(t^*) = M_H - \bar{\Lambda}(t^*) = M_H - \mathcal{E} + \delta \overline{m}(t^*)\,,\tag{44}
$$

$$
\overline{C}_m(t^*) = 1 - \frac{4\alpha_s(\overline{m}_Q)}{3\pi} - \frac{1}{\overline{m}_Q} \left( \delta \overline{m}(t^*) - \alpha_s(a) \frac{X}{a} \right).
$$
 (45)

It is straightforward to show, that, at order  $\alpha_s$ , the relation between  $\overline{m}_Q$  and  $m_Q^S(t^*)$  is given by

$$
\overline{m}_Q = m_Q^S(t^*) \times \overline{C}_m(t^*).
$$
\n(46)

Equation (46) holds also for  $t^* \to \infty$ , provided at the same time  $\delta \overline{m}(t^*) \to \delta \overline{m}$ .

At this order in  $\alpha_s$  we can write

$$
\overline{m}_Q = \left(M_H - \mathcal{E} + \alpha_s(a)\frac{X}{a}\right)\left(1 - \frac{4\alpha_s(\overline{m}_Q)}{3\pi}\right) \tag{47}
$$

which is equivalent to the procedure where the linearly divergent term is subtracted in perturbation theory. Now both factors in eq. (47) contain renormalon singularities. We can also rewrite eq. (47) in the form corresponding to the procedure where we use the unsubtracted, linearly divergent "pole" mass  $M_H - \mathcal{E}$ ,

$$
\overline{m}_Q = \left(M_H - \mathcal{E}\right) \left(1 - \frac{4\alpha_s(\overline{m}_Q)}{3\pi} + \alpha_s(a)\frac{X}{a\overline{m}_Q}\right) ,\qquad (48)
$$

where the divergent dependence on  $\alpha$  in the pole mass is compensated by that in the coefficient function. In this case no renormalon singularities arise in higher orders, but the unsubtracted pole mass and the coefficient function both contain power divergences. As required, the relation (48) is independent of the subtraction constant  $\delta \overline{m}(t^*)$ .

In the numerical evaluation of  $\overline{m}_Q$  from eqs. (46) and (47), we used  $M_B = 5.278$ ;  $\mathcal E$  from the APE results, see subsection 3.2;  $a \, \delta \overline{m}(t^*)$  from eqs. (36) and (37) and table 4;  $\alpha_s(a)$  was taken in the range 0.13 and 0.18. To obtain a distribution of values, we varied  $\mathcal{E}, \Lambda_{\text{QCD}}$  and  $a \, \delta \overline{m}(t^*)$  according to a gaussian distribution;  $a^{-1}$  was varied with flat distribution within its error, while  $\alpha_s(a)$  was written in terms of the leading quenched expression of the running coupling constant, evaluated at the scale  $\pi/a$ , with  $\Lambda_{\text{QCD}}$  distributed according to a flat distribution of width  $\sigma$  and such that  $\alpha_s = 0.13$  for  $\Lambda_{\rm QCD} - \sigma$ 

Figure 3: The ditribution of values of the  $\overline{MS}$  b-quark mass  $\overline{m}_b$ , for  $t^* \to \infty$ , at  $\beta = 6.0$  and  $\beta = 6.2$ . Similar distributions are obtained for  $\overline{m}_b$  using  $t^* = 3-7$ .

and  $\alpha_s = 0.18$  for  $\Lambda_{\rm QCD} + \sigma$ . The resulting distribution is a pseudo-gaussian, as can been seen from fig. 3 where two histograms of values of  $\overline{m}_b$ , corresponding at  $\beta = 6.0$  and 6.2, are shown. From the width of the distribution we estimate the average value and error on  $\overline{m}_b$ . Using eq. (46), we obtain at  $\beta = 6.0$ ,

$$
\overline{m}_b = 4.18 \pm 0.07 \text{ GeV for } t^* \to \infty \tag{49}
$$

and

$$
\overline{m}_b = 4.21 \pm 0.07 \text{ GeV for } t^* = 3 - 6. \qquad (50)
$$

The corresponding numbers at  $\beta = 6.2$  are

$$
\overline{m}_b = 4.11 \pm 0.09 \text{ GeV for } t^* \to \infty \tag{51}
$$

and

$$
\overline{m}_b = 4.13 \pm 0.09 \text{ GeV for } t^* = 4 - 7. \qquad (52)
$$

Using eq. (47), we obtain instead

$$
\overline{m}_b = 4.22 \pm 0.07 \text{ GeV at } \beta = 6.0, \n\overline{m}_b = 4.15 \pm 0.08 \text{ GeV at } \beta = 6.2
$$
\n(53)

The difference between the results of eqs.  $(49)$ – $(52)$  and  $(53)$  can be interpreted as due to higher order corrections in  $\alpha_s$ . By combining the above results together we estimate

$$
\overline{m}_b = 4.17 \pm 0.05 \pm 0.03 \text{ GeV} \tag{54}
$$

where the second error is the systematic error coming from the different methods used to extract  $\overline{m}_b$  at this order in  $\alpha_s$ .

#### **3.4** Determination of  $c_1$  and  $c_2$

We have computed the ratio  $\rho_{\vec{D}^2}(t)$ , defined in eq. (21), using unsubtracted heavy-quark propagators, as explained in section 2.2. In order to do this calculation, we need the expression of the heavy-quark propagator with the insertion of  $\bar{h}\vec{D}^2h$ 

$$
S^{a}(x|y) = \sum_{w^{4}=y^{4}}^{x^{4}} S(x, |w) \, \vec{D}_{w}^{2}(w^{4}) \, S(w | y) \,, \tag{55}
$$

where the lattice heavy quark propagator  $S(x|w)$  has been defined in eq. (28), and in the improved case, we have used the definition of the P-line given in eq. (31). For the discretised version of  $\vec{D}^2$  we have taken

$$
\left[\vec{D}_x^2\right]_{\alpha\beta} = \frac{1}{a^2} \sum_{k=1}^3 \left( U_{\alpha\beta}^k(x) \,\delta_{x,x+a\,\hat{k}} + U_{\alpha\beta}^{k\dagger}(x-a\,\hat{k}) \,\delta_{x,x-a\,\hat{k}} - 2 \,\delta_{\alpha\beta} \,\delta_{x,x} \right), \tag{56}
$$

In fig. 4, we plot  $\rho_{\vec{D}^2}(t)$ , as defined in eq. (21), as a function of the time t, at  $\beta = 6.0$ from <u>set B</u>. In the same figure, we also give the result of a linear fit of  $\rho_{\vec{D}^2}(t)$  to eq. (20) in the interval  $6 \le t/a \le 12$ . Similar results were obtained at  $\beta = 6.2$  using the data of set C. The dependence of  $\rho_{\vec{D}^2}(t)$  on t is in remarkable agreement with the predicted linear behaviour <sup>5</sup>. In order to monitor the stability of the results, we have fitted  $\rho_{\vec{D}^2}(t)$  using different time intervals and in table 5 we show our results for  $c_1$  and  $c_2$ , in the improved

 $5$ As expected, we found that the results for  $c_2$  in the improved and unimproved case are completely compatible. The latter are not reported here.

$\beta$	time interval	c <sub>1</sub>	c <sub>2</sub>	$\chi^2/\text{dof}$
6.0	$4 - 12$	0.06(2)	$-0.759(6)$	1.24
6.0	$5 - 12$	0.01(5)	$-0.748(10)$	0.98
6.0	$5 - 14$	0.01(5)	$-0.748(10)$	1.09
6.0	$6 - 14$	$-0.16(13)$	$-0.724(22)$	0.80
6.2	$4 - 12$	0.10(4)	$-0.698(9)$	1.01
6.2	$5 - 12$	0.16(9)	$-0.708(18)$	0.98
6.2	$5 - 14$	0.17(9)	$-0.710(17)$	0.95
6.2	$6 - 14$	0.37(18)	$-0.739(29)$	0.62

Table 5: Results for the improved renormalisation constants of the operator  $\bar{h}\vec{D}^2 h$  obtained by a linear fit to  $\rho_{\vec{D}^2}(t)$ . The time interval of the fit is also given.

Figure 4: The ratio  $\rho_{\vec{D}^2}(t)$  (improved case) as a function of the time, at  $\beta = 6.0$  from set B. A linear fit of  $\rho_{\vec{D}^2}(t)$  to the expression in eq. (20) in the interval  $6 \le t/a \le 12$ , is also given.

Figure 5: The ratio  $\rho_{\vec{D}^2}(t',t)$  defined in eq. (23), in the improved case, at  $\beta = 6.0$  from <u>set B</u>, as a function of t', at several values of t,  $t = 6-10$ .

case, at  $\beta = 6.0$  and 6.2. At  $\beta = 6.0$ , we observe a shift of the value of  $c_2$  towards smaller values as we increase the minimum t-distance  $(t_{min} = 4, 5, 6)$  at which the fit is performed. Since at  $\beta = 6.2$ , we find the opposite behaviour, i.e. the value of  $c_2$  is shifted towards larger values as  $t_{min}$  is increased, we believe that the shift is a statistical effect rather than a systematic one. From table 5, we also observe that it is very difficult to determine the value of  $c_1$ , which, for the improved propagator, seems to be small, with a large relative error, and is very unstable with respect to a change of the fitting interval. We expect that this instability, which is correlated to the shift of the value of  $c_2$  with  $t_{min}$ , will be reduced with more accurate data for  $\rho_{\vec{D}^2}(t)$ . Notice that  $c_1$ , unlike  $\mathcal E$  and  $c_2$ which are long-distance quantities, depends on the lattice regularization, i.e. is different for the unimproved or the improved heavy quark propagator.

We also present the results for  $c_2 = \rho_{\vec{D}^2}(t', t)$ , at  $\beta = 6.0$ , obtained by using eq. (23).

$\beta$	t	t'	c <sub>2</sub>	$\chi^2/\text{dof}$
6.0	6	$3 - 5$	$-0.748(3)$	17.00
6.0	$\overline{7}$	$3 - 5$	$-0.735(6)$	0.76
6.0	8	$3 - 5$	$-0.727(9)$	0.14
6.0	9	$3 - 6$	$-0.713(15)$	0.11
6.0	10	$3 - 7$	$-0.698(27)$	0.16
6.2	6	$3 - 5$	$-0.674(4)$	2.2
6.2	$\overline{7}$	$3 - 5$	$-0.670(8)$	0.03
6.2	8	$3 - 5$	$-0.680(12)$	0.02
6.2	9	$3 - 6$	$-0.693(18)$	0.40
6.2	10	$3 - 7$	$-0.723(29)$	0.22

Table 6: Results for the renormalisation constant  $c_2$  computed from a weighted average of  $\rho_{\vec{D}^2}(t',t)$  in t', at fixed t.

In fig. 5, we show  $\rho_{\vec{D}^2}(t',t)$ , as a function of  $0 \leq t' \leq t$ , at several fixed values of t,  $t = 6{\text -}10$ . Up to contact terms, we expect  $\rho_{\vec{D}^2}(t',t)$  to be a constant in  $t'$ , at fixed  $t$ , and also to be independent of t. If the contact terms were entirely due to the mixing of the kinetic energy operator with the inverse propagator, eq. (18), we should find two spikes, at  $t' = 0$  and  $t' = t$ , and a constant value of  $\rho_{\vec{D}^2}(t', t)$  for  $t' \neq 0, t$ . The presence of operators of higher dimension, due to discretisation errors, introduces terms which behaves as derivatives of δ-functions (in time), giving rise to the bell-shape behaviour of  $\rho_{\vec{D}^2}(t',t)$  shown in fig. 5. Thus in order to obtain  $c_2$ , we have to look for a plateau in the central region in  $t'$ , at large values of  $t$ . From the figure, we see that it is possible to recognize a plateau in  $t'$  for  $t = 8$ –10. At values of t smaller than  $t = 8$ , the contact terms are visible at all values of t; at values of t larger than  $t = 10$  the statistical error become quite large. There is a slight shift towards larger values of  $c_2$  as t is increased. As discussed above, since the effect is opposite at  $\beta = 6.2$ , we do not believe that this is a systematic effect. In table 6 we present the values of  $c_2$ , computed from a weighted average of values of  $\rho_{\vec{D}^2}(t',t)$  for different  $t'$ , at fixed t. The average has been performed only in the central region, where there appears to be a plateau. For the sake of comparison, we present the results for several values of t, including small ones.

From the results given in tables 5 and 6, and taking into account the previous discussion, we believe that the best estimate of  $c_2$  is obtained from  $\rho_{\vec{D}^2}(t',t)$ , with  $t = 8$  and  $t' = 3-5$ 

$$
c_2 = -0.73 \pm 0.01 \pm 0.02 \text{ at } \beta = 6.0, \qquad (57)
$$

$$
c_2 = -0.68 \pm 0.01 \pm 0.02 \text{ at } \beta = 6.2, \qquad (58)
$$

where the second error comes from the variation of the values of  $c_2$  with t. These results can be compared with perturbation theory, which gives  $c_2 = -5.19 \times \alpha_s \sim -(0.67-\alpha_s)$ 0.93) for  $\alpha_s = -.13-0.18$ . For  $c_1$  using the improved propagator, such a comparison is impossible, due to the relatively large uncertainties in the non-perturbative determination.

### 3.5 Determination of the kinetic energy  $\lambda_1$

The results for  $\lambda_1$  have been obtained with limited statistics, using the data of <u>set A</u>. As explained in subsection 2.1, the value of  $\lambda_1^{\text{bare}}$  can be obtained from  $R(t', t)$  as defined in eq. (27). In principle, we should evaluate  $R(t', t)$  using the subtracted propagators S'. However, the argument used in section 2.2 for  $\rho_{\vec{D}^2}(t)$  is also valid for  $R(t', t)$ , and implies that we can obtain  $R(t', t)$  by using the unsubtracted heavy-quark propagators. In order to compute  $R(t', t)$  we have used single and double cubic smeared interpolating operators  $J = \bar{h}\gamma_0\gamma_5q$ , with smearing size  $L_s = 7$ , by using the heavy and light quark propagators rotated into the Coulomb gauge.  $L_s = 7$  was found to be the optimal value of  $L_s$  for isolating the lightest meson state at  $\beta = 6.0$  [25, 26].

The procedure to extract operator matrix elements is standard. It is the same as the second method that we used in the previous subsection to determine  $c_2$ . At fixed t, we study the behaviour of the ratio  $R(t', t)$  as a function of t', searching for a plateau in t'.  $\lambda_1^{\text{bare}}$  is defined by the weighted average of the data points in the central plateau region, if this exists. We will take as our best determination of  $\lambda_1^{\text{bare}}$ , the value evaluated in a time interval where the ratio  $R(t', t)$  appears to be independent of both t and t'. In addition, we have to require that the lightest state has been isolated. With the smeared sources used in the present case, we know that this happens at a time distance  $(t-t')/a$ and  $t'/a \geq 4-5$  from the source. This implies that the total time distance  $t/a$  for

Figure 6: The ratio  $R(t',t)$  at  $t/a = 8$  as a function of the time t'. We show the value of  $\lambda_1^{\text{bare}} = \sum_{t'/a=3,5} R(t',t)$  (full orizontal line) and the relative band of error (dashed orizontal lines).

 $R(t',t)$  has to be at least 8–10. Moreover, using  $(t-t')/a$  and  $t'/a \geq 4-5$ , we eliminate the contact terms, which on the basis of the discussion in the previous subsection, cf. fig. 5, are expected to be present up to distances of order 2–3. As an example of our results, we show in fig. 6 the ratio  $R(t', t)$ , at  $t/a = 8$ , as a function of t', the time at which the kinetic operator is inserted. With the present statistical errors, it is not easy to identify the plateau region<sup>6</sup>. If we assume that we can use the central points  $(t' = 3, 4, 5)$  to extract the value of the matrix element, we obtain for the unrenormalised value  $a^2 \lambda_1^{\text{bare}} = -0.72 \pm 0.14$ . This implies that there is a large numerical cancellation in the subtracted kinetic energy,  $a^2 \lambda_1 = a^2 \lambda_1^{\text{bare}} - c_2 = 0.1 \pm 0.14$ , cf. eq. (24). Due to the large statistical and systematic errors and to the difficulty in the clear identification of

<sup>&</sup>lt;sup>6</sup>At larger time distances,  $t/a \ge 10$  the errors are even larger.

the plateau, it is not possible to obtain a value for the renormalised kinetic energy from this simulation. We can only impose the loose upper bound  $\lambda_1 < 1 \text{ GeV}^2$ . Notice that in order to reduce the statistical error to 0.1  $\text{GeV}^2$ , we need a sample about 50–100 times larger than our current one, corresponding to 1500–3000 gluon configurations. Moreover, we would eventually also like to be able to extrapolate the results to the chiral limit. For these reason, we are implementing the method described in this paper on the 24 Gigaflops APE100 computer.

One could argue that the subtraction is not really necessary, since the effective theory on the lattice does not have renormalons. Even though this is indeed true, the difficulty in the determination of corrections of order  $1/m_Q$  related to the kinetic energy operator would remain the same. The argument goes as follows. The bare kinetic energy operator has a very large matrix element  $a^{-2} \times (a^2 \lambda_1^{\text{bare}}) \sim 2^2 \times (-0.72) \text{ GeV}^2 = -2.88 \text{ GeV}^2$ , while one expects a correction due to the kinetic energy of the heavy quark of the order of the squared Fermi momentum  $p_F^2 \sim \Lambda_{\rm QCD}^2 \sim 0.1 \text{ GeV}^2$ . Thus the huge contribution of the matrix element of the bare operator has to be compensated by the corresponding term in the coefficient function of  $\bar{h}h$ . This require an extreme accuracy in the perturbative calculation of the coefficient function. This remains true in the subtracted as well as in the unsubtracted case.

## 4 Conclusions

In this study we have shown that the method for the non-perturbative renormalisation of the lattice operators  $\bar{h}(x) D_4 h(x)$  and  $\bar{h}(x) \bar{D}^2 h(x)$ , proposed in ref. [18], is feasible in current computer simulations. We have been able to obtain the subtraction constants of the operators  $\bar{h}(x) \vec{D}^2 h(x)$  and  $\bar{h}(x) D_4 h(x)$  with a small statistical error (in the former case, particularly for the constant  $c_2$  which is needed for many physical applications). The binding energy of the B-meson,  $\overline{\Lambda}$ , has been also calculated with an error of about 15% and was found to be significantly smaller than other estimates, based on different definitions [31, 32]. We have also computed the kinetic energy of the heavy quark in the B-meson. With our current statistical sample we can only impose the bound on  $\lambda_1$  < 1  $GeV<sup>2</sup>$ , on the matrix element of the kinetic energy operator. This is due to the large

numerical cancellation when the counter-term is subtracted. We are planning to improve the precision of our results by using a much larger sample of gluon configurations, and hopefully to obtain a significant result for  $\lambda_1$ .

Our preferred determination of  $\overline{\Lambda}$  was based on the behaviour of the heavy quark propagator at large times. It is important to verify the validity of the condition (9) by extending the calculation of  $\delta \overline{m}(t)$  to larger values of t. This requires a high-statistics simulation on a large lattice, and we are currently undertaking such a study. The results will be reported elsewhere.

The present study concerned some important matrix elements which appear in the HQET. We were able to determine  $\overline{\Lambda}$ , defined in different prescriptions, with good precision. This encourages us to extend the calculation to other matrix elements which appear at  $O(1/m_Q)$ , and beyond, in the HQET. The main limitation to the matching to the full theory is due to the fact that the relevant Wilson coefficients have only been computed at first order in  $\alpha_s$ . We are planning to extend these calculations to higher orders. One may also extend the present approach to matrix elements which appear at higher orders in other important operator expansions, such as the non-leading twist operators in deep inelastic scattering or higher dimensional condensates used in QCD sum-rules.

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