Towards precision heavy flavour physics from lattice QCD

Jochen Heitger
Westfälische Wilhelms-Universität Münster, Institut für Theoretische Physik
Wilhelm-Klemm-Straße 9, D-48149 Münster, Germany

Abstract
I convey an idea of the significant recent progress, which opens up good perspectives for high-precision ab-initio computations in heavy flavour physics based on lattice QCD. This report focuses on the strategy and the challenges of fully non-perturbative investigations in the B-meson sector, where the b-quark is treated within an effective theory, as followed by the ALPHA Collaboration. As an application, I outline its use to determine the b-quark mass and summarize the status of our ongoing project in the two dynamical flavour theory.

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Jochen Heitger\textsuperscript{a} (ALPHA Collaboration)

\textsuperscript{a}Westfälische Wilhelms-Universität Münster, Institut für Theoretische Physik, Wilhelm-Klemm-Straße 9, D-48149 Münster, Germany

I convey an idea of the significant recent progress, which opens up good perspectives for high-precision ab-initio computations in heavy flavour physics based on lattice QCD. This report focuses on the strategy and the challenges of fully non-perturbative investigations in the B-meson sector, where the b-quark is treated within an effective theory, as followed by the ALPHA Collaboration. As an application, I outline its use to determine the b-quark mass and summarize the status of our ongoing project in the two dynamical flavour theory.

1. B-physics and lattice QCD

For the plenty of beautiful results from recent and current B-physics experiments \cite{1,2} — as well as from what is to be expected from LHC —, to lead to feasible precision tests of the Standard Model and trials of several New Physics scenarios, requires the knowledge of QCD matrix elements for their interpretation in terms of parameters of the Standard Model and its possible extensions. Unfortunately, the uncertainty on the theoretical side in this interplay of experiment and theory in flavour physics predominantly originates from hardly computable long-distance effects of the strong interaction that confines quarks and gluons within hadrons. This potentially limits the impact of future experimental measurements on New Physics models and motivates calculations in lattice QCD, which is a powerful approach to reach a few-% theoretical error on those non-perturbative hadronic contributions.

Still, some care is needed to obtain reliable results for b-quark physics from a Monte Carlo evaluation of the discretized Euclidean path integral. One has to keep under control simultaneously the finite-size effects and, particularly, the discretization effects, since the lattice spacing should not be larger than the Compton length of the b-quark. In practice, it is not possible to control both effects by brute force numerical simulations such that dedicated methods have to be devised.

While the numerical computations in lattice QCD necessarily involve approximations, one of the key features of the lattice approach is that all approximations can be systematically improved. For an overview of the different formulations of heavy quarks on the lattice that have been proposed in the literature and are being used today, and of results from the field of heavy flavour physics, which reflect some of these improvements by the small error bars quoted for many quantities, I refer to the reviews of past Lattice Conferences \cite{3,4,5,6,7} and references therein.

1.1. Challenges

Among the various considerable challenges one faces in an actual lattice QCD calculation on the theoretical and technical levels, let us only highlight the multi-scale problem, which is also particularly relevant in view of B-physics applications. This is illustrated in Figure 1. There are many disparate physical scales to be covered simultaneously, ranging from the lightest hadron mass of $m_\pi \approx 140$ MeV over $m_D \approx 2$ GeV to $m_B \approx 5$ GeV, plus the ultraviolet cutoff of...
\[ \Lambda_{UV} = a^{-1} \]
of the lattice discretization that has to be large compared to all physical energy scales for the discretized theory to be an approximation to the continuum one. Moreover, the finiteness of the linear extent of space-time, \( L \), in a numerical treatment entails an infrared cutoff \( \Lambda_{IR} = L^{-1} \) so that the following scale hierarchy is met:

\[
\begin{align*}
\Lambda_{IR} = L^{-1} \ll m_{\pi}, \ldots, m_{D}, m_{B} \ll a^{-1} = \Lambda_{UV}.
\end{align*}
\]

This implies \( L \gtrsim 4/m_{\pi} \approx 6 \text{fm} \) to suppress finite-size effects in the light quark sector and \( a \lesssim 1/(2m_{D}) \approx 0.05 \text{fm} \) to still properly resolve the propagation of a c-quark in the heavy sector. Lattices with \( L/a \gtrsim 120 \) sites in each direction would thus be needed to satisfy these constraints, and since the scale of hadrons with b-quarks was not even included to arrive at this figure, it is obvious that the b-quark mass scale has to be separated from the others in a theoretically sound way before simulating the theory. In Section 2.1 briefly describe, how this is achieved by recoursing to an effective theory for the b-quark.

Another non-trivial task is the renormalization of QCD operators composed of quark and gluon fields, which appear in the effective weak Hamiltonian, valid at energies far below the electroweak scale. Besides perturbation theory (see, e.g., [9]), powerful non-perturbative approaches have been developed (and reviewed, e.g., in [10]), and I will come back to the non-perturbative subtraction of power-law divergences in the context of the effective theory for the b-quark later.

1.2. Perspectives

As for the challenges with light quarks, it should only be noted that the condition \( L \gtrsim 6 \text{fm} \) may be relaxed by simulating at unphysically large pion masses, combined with a subsequent extrapolation guided by chiral perturbation theory [11] and its lattice-specific refinements.

Regarding the algorithmic side of a lattice QCD simulation, the Hybrid Monte Carlo [12] (HMC) as the first exact and still state-of-the-art algorithm has received considerable improvements by multiple time-scale integration schemes [13,14], the Hasenbusch trick of mass-preconditioning [15,16], supplemented by a sensible tuning of the algorithm’s parameters [17], and domain decomposition (DD) applied to QCD [18,19,20], just to name a few. In addition, low-mode deflation [21] (together with chronological inverters [22]) has led to a substantial reduction of the critical slowing down with the quark mass in the DD-HMC.

Finally, in parallel to the continuous increase of computer speed (at an exponential rate) over the last 25 years and the recent investments into high performance computing at many places of the world, the Coordinated Lattice Simulations [23] (CLS) initiative is a community effort to bring together the human and computer resources of several teams in Europe interested in lattice QCD. The present goal are large-volume simulations with \( N_{t} = 2 \) dynamical quarks, using the rather simple \( O(a) \) improved Wilson action to profit from the above algorithmic developments such as DD-HMC, and lattice spacings \( a = (0.08 - 0.05) \text{fm} \), sizes \( L = (2 - 4) \text{fm} \) and pion masses down to \( m_{\pi} = 250 \text{MeV} \), which altogether help to diminish systematic and statistical errors. Amongst others, the B-physics programme outlined here is investigated on these lattices.

2. Non-perturbative HQET

Heavy Quark Effective Theory (HQET) at zero velocity on the lattice [24] offers a reliable solution to the problem of dealing with the two disparate intrinsic scales encountered in heavy-light systems involving the b-quark, i.e., the lattice spacing \( a \), which has to be much smaller than \( 1/m_{b} \) to allow for a fine enough resolution of the states in question, and the linear extent \( L \) of the lattice volume, which has to be large enough for finite-size effects to be under control (Figure 1).

Since the heavy quark mass \( (m_{b}) \) is much larger than the other scales such as its 3–momentum or \( \Lambda_{QCD} \sim 500 \text{MeV} \), HQET relies upon a systematic expansion of the QCD action and correlation functions in inverse powers of the heavy quark mass around the static limit \( (m_{b} \to \infty) \). The lattice HQET action \( S_{\text{HQET}} \) at \( O(1/m_{b}) \) reads:

\[
a^{4}\sum_{x} \bar{\psi}_{h}\left\{ D_{0} + \delta m - \omega_{\text{kin}}D^{2} - \omega_{\text{spin}}\sigma B \right\} \psi_{h},
\]

with \( \psi_{h} \) satisfying \( P_{+}\psi_{h} = \psi_{h}, \) \( P_{+} = \frac{1 + \gamma_{5}}{2} \), and the parameters \( \omega_{\text{kin}} \) and \( \omega_{\text{spin}} \) being formally \( O(1/m_{b}) \). At leading order (static limit), where
the heavy quark acts only as a static colour source and the light quarks are independent of the heavy quark’s flavour and spin, the theory is expected to have $\sim 10\%$ precision, while this reduces to $\sim 1\%$ at $O(1/m_b)$ representing the interactions due to the motion and the spin of the heavy quark. As crucial advantage (e.g., over NRQCD), HQET treats the $1/m_b$–corrections to the static theory as space-time insertions in correlations functions. For correlation functions of some multi-local fields $\mathcal{O}$ and up to $1/m_b$–corrections to the operator itself (irrelevant when spectral quantities are considered), this means

$$
\langle \mathcal{O} \rangle = \langle \mathcal{O} \rangle_{\text{stat}} + a^4 \sum_x \left\{ \omega_{\text{kin}} \langle \mathcal{O} \mathcal{O}_{\text{kin}}(x) \rangle_{\text{stat}} + \omega_{\text{spin}} \langle \mathcal{O} \mathcal{O}_{\text{spin}}(x) \rangle_{\text{stat}} \right\},
$$

where $\langle \mathcal{O} \rangle_{\text{stat}}$ denotes the expectation value in the static approximation and $\mathcal{O}_{\text{kin}}$ and $\mathcal{O}_{\text{spin}}$ are given by $\bar{\psi}_h D^2 \psi_h$ and $\bar{\psi}_h \sigma B \psi_h$. In this way, HQET at a given order is (power-counting) renormalizable and its continuum limit well defined, once the mass counterterm $\delta m$ and the coefficients $\omega_{\text{kin}}$ and $\omega_{\text{spin}}$ are fixed non-perturbatively by a matching to QCD.

Still, for lattice HQET and its numerical applications to lead to precise results with controlled systematic errors in practice, two shortcomings had to be left behind first.

1.) The exponential growth of the noise-to-signal ratio in static-light correlators, which is overcome by a clever modification of the Eichten-Hill discretization of the static action [25].

2.) As in HQET mixings among operators of different dimensions occur, the power-divergent additive mass renormalization $\delta m \sim \frac{g_0^2}{a}$ already affects its leading order. Unless HQET is renormalized non-perturbatively [26], this divergence — and those $\sim \frac{g_0^2}{a^2}$ arising at $O(1/m_b)$ — imply that the continuum limit does not exist owing to a remainder, which, at any finite perturbative order [27][28], diverges as $a \to 0$. A general solution to this theoretically serious problem was worked out and implemented for a determination of the b-quark’s mass in the static and quenched approximations as a test case [29]. It is based on a non-perturbative matching of HQET and QCD in finite volume. Applications of this strategy to the determination of the b-quark mass and (a subset of all) HQET parameters at $O(1/m_b)$ [30][31], to a study of the $B_s$-meson spectrum [32] and to a computation of the $B_s$-meson decay constant [33] were realized in the quenched approximation by our collaboration and have been extended to the more realistic $N_f = 2$ situation [34][35][36][37].

3. The b-quark mass via HQET at $O(1/m_b)$

We first note [38] that in order not to spoil the asymptotic convergence of the series, the matching must be done non-perturbatively — at least for the leading, static piece — as soon as the $1/m_b$–corrections are included, since as $m_b \to \infty$ the perturbative truncation error from the matching coefficient of the static term becomes much larger than the power corrections $\sim \Lambda_{\text{QCD}}/m_b$ of the HQET expansion.
renormalization group invariant (RGI) and the bare mass in QCD being known, suitable finite-volume observables $\Phi_k(L_1, M_b)$ can be calculated as a function of the RGI heavy quark mass, $M_b$, and extrapolated to the continuum limit. $S_2$: Next, the power-divergent subtractions are performed non-perturbatively by a set of matching conditions, in which the results obtained for $\Phi_k$ are equated to their representation in HQET. At the same physical value of $L_1$ but for resolutions $L_1/a = O(10)$, the previously computed heavy-quark mass dependence of $\Phi_k(L_1, M_b)$ in finite-volume QCD may be exploited to determine the bare parameters of HQET for $a \approx (0.025 - 0.05)$ fm. $S_3$: To evolve the HQET observables to large volumes, where contact with some physical input from experiment can be made, one also computes them at these lattice spacings in a larger volume, $L_2 = 2L_1$. The resulting relation between $\Phi_k(L_1)$ and $\Phi_k(L_2)$ is encoded in associated step scaling functions denoted as $\sigma_k$. $S_4, S_5$: By using the knowledge of $\Phi_k(L_2, M_b)$ one fixes the bare parameters of the effective theory for $a \approx (0.05 - 0.1)$ fm so that a connection to lattice spacings is established, where large-volume observables, such as the B-meson mass or decay constant, can be calculated. This sequence of steps yields an expression of $m_B$, the physical input, as a function of $M_b$ via the quark mass dependence of $\Phi_k(L_1, M_b)$, which eventually is inverted to arrive at the desired value of the RGI b-mass within HQET. The whole construction is such that the continuum limit can be taken for all pieces.

3.1. Computation of HQET parameters

Following the strategy sketched above and applied to the quenched case in [31], the determination of the parameters of the HQET Lagrangian and of the time component of the isovector axial current is performed within the Schrödinger functional, i.e., QCD with Dirichlet boundary conditions in time and periodic ones in space, where suitable matching observables $\Phi_k$, such as finite-volume meson energies and matrix elements, can be readily defined. Relativistic quarks are simulated as clover-improved Wilson fermions with $N_f = 2$ dynamical quarks; for the static quark we use the so-called HYP1/2 actions [25].

We introduce observables $\Phi_{k=1,...,5}$ casted into a vector $\mathbf{\Phi} = \Phi^{QCD}$, where in the continuum and large volume limits, the first two are proportional to the meson mass and to the logarithm of the decay constant, respectively, while $\Phi_3$ is used to fix the counterterm of the axial current and $\Phi_{4,5}$ for the determination of the kinetic and magnetic terms in $S_{HQET}$. The continuum extrapolations of $\Phi_{1,2}$ in the small QCD volume $(L_1 \approx 0.5$ fm, $S_1$ in Figure 2), for nine values $M_b \equiv M$ of the RGI heavy quark mass from the charm to beyond the bottom region [36], are shown in Figure 3.

![Figure 3. Continuum extrapolation of the finite-volume observables $\Phi_1$ and $\Phi_2$, where for $\Phi_1$ we have included the error (cross on the left) stemming from the renormalization of the quark mass.](image)

When the effective theory is simulated in the same physical volume ($S_2$ in Figure 2), a set of matching conditions for $\lim_{a \to 0} \Phi^{QCD}_i(L_1, M, a)$,

$$\Phi^{QCD}(L_1, M) = \eta(L_1, a) + \phi(L_1, a)\tilde{\omega}(M, a),$$

is imposed; the r.h.s. represents the heavy quark mass expansion of the $\Phi^{QCD}$ at $O(1/m_b)$. Having computed $\eta$ and $\phi$ from these simulations for different values of $a$, the matching equations determine the set of parameters $\tilde{\omega}(M, a)$; e.g., in the simple case of the static meson mass, and up to a kinematic constant, $\eta$ is the static energy, $\phi$ a constant and $\omega$ the bare static quark mass. After step scaling to $L_2 = 2L_1$, the observables in this volume are now obtained, thanks to the parameters $\omega(M, a)$ fixed by the previous step, as

$$\Phi(L_2, M, 0) = \lim_{a \to 0} \left[ \eta(L_2, a) + \phi(L_2, a)\tilde{\omega}(M, a) \right],$$

and the continuum limit can be taken, since the power divergences in HQET cancel out here. Figure 4 depicts examples of corresponding continuum extrapolations in the static approximation,
and the results for observables sensitive to the $1/m_b$-corrections are of similar quality [37].

![Figure 4. Continuum extrapolation of the static approximation of $\Phi_1$ and $\Phi_2$ in the volume of extent $L_2$. Red (blue) symbols refer to the HYP1 (HYP2) discretization of the static propagator.](image)

Finally, the HQET parameters to be employed in the large volume, $L_{\infty}$, are estimated from $S_5$: 

$$\omega(M, a) = \phi^{-1}(L_2, a) \left[ \Phi(L_2, M, 0) - \eta(L_2, a) \right].$$

3.2. Preliminary large-volume results

To apply the non-perturbative matching results to calculate the $b$-quark mass, we write down the HQET expansion (to first order in $1/m_b$) of $m_B$ in terms of HQET parameters and energies as

$$m_B = m_{\text{bare}} + E^{\text{stat}} + \omega_{\text{kin}} E^{\text{kin}} + \omega_{\text{spin}} E^{\text{spin}}. \tag{1}$$

HQET energies and matrix elements have been extracted from measurements on a subset of configuration ensembles produced within CLS [23] solving the Generalized Eigenvalue Problem [39], which allows for a clean quantification of systematic errors from excited state contaminations. So far, only a single lattice spacing $a \approx 0.07$ fm ($\beta = 5.3$) has been analyzed so that the size of discretization effects can not be assessed yet. Figure 5 shows elements of the computations in $L_{\infty}$.

![Figure 5. Left: Comparison of plateaux of static energies at $\beta = 5.3$ to earlier quenched results. Right: Graphical solution of (1) in static approximation; $M \equiv M_h$ is the RGI heavy quark mass.](image)

Upon chiral extrapolation in the light quark mass and including a conservative uncertainty in the lattice scale ($r_0 = 0.475(25)$ fm [40]), we quote as our preliminary result for the $b$-quark’s mass in HQET at $O(1/m_b)$ for the $N_f = 2$ theory:

$$m_b^{\text{MS}}(m_b) = 4.276(25)r_0(50)_{\text{stat+renorm}}(?)_{a} \text{ GeV}.$$  

The first error states the scale uncertainty, while the second covers the statistical errors of HQET energies, the chiral extrapolation uncertainty and the error on the quark mass renormalization entering the small-volume QCD part of the computation ($S_1$). More details are found in [37].

For comparison, we cite the previous $N_f = 0$ HQET result $m_b^{\text{MS}}(m_b) = 4.320(40)r_0(48)$ GeV by our collaboration [30] and the recent sum-rule determination, $m_b^{\text{MS}}(m_b) = 4.163(16)$ GeV [41].

4. Outlook

The non-perturbative treatment of HQET including $1/m_b$-terms can lead to results with unprecedented precision for B-physics on the lattice. It also greatly improves our confidence in the use of the effective theory. Our project to extract from $N_f = 2$ lattice simulations relevant quantities for B-phenomenology within HQET is well advanced. While the non-perturbative matching of HQET with QCD through small-volume simulations is almost done, the evaluation of HQET energies and matrix elements has started recently on the CLS ensembles, but still awaits a better control of the cutoff effects. Our first results for the $b$-quark mass in HQET at $O(1/m_b)$ are promising, and further applications of the once determined HQET parameters to calculate the $B$-meson decay constant, the spectrum of heavy-light mesons and the form factors of the $B \to \pi$ semi-leptonic decay are expected in the future.

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