Towards Precision B-physics from Non-Perturbative Heavy Quark Effective Theory

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We 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. Rather than surveying the latest results, this contribution focuses on the concept and the challenges of fully non-perturbative computations in the B-meson sector, where the b-quark is treated within an effective theory. We outline its use to determine the b-quark mass and report on the results obtained in the quenched approximation and on the status in the two dynamical flavour theory.

1 B-physics and lattice QCD

The plenty of beautiful results from recent and still ongoing B-physics experiments, which require the knowledge of QCD matrix elements for their interpretation in terms of parameters of the Standard Model and its possible extensions, motivates investigations in lattice QCD. The importance of this interplay of experiment and theory is further expressed by the fact that one of its main objectives, the phenomenon of CP violation, is closely related to the symmetry breaking mechanism the 2008’s Nobel Prize was dedicated to.

Lattice QCD represents our best founded theoretical formulation of QCD and allows for the computation of low-energy hadronic properties in the non-perturbative domain, where the usual power series expansion in the coupling constant fails, through the Monte Carlo evaluation of the Euclidean path integral after a discretization of space-time on a lattice with spacing $a$ in all 3+1 dimensions. While such numerical computations necessarily involve approximations, one of the key features of the lattice approach is that all approximations can be systematically improved. For an overview of results from the field of heavy flavour physics, which reflect some of these improvements by the small error bars quoted for many quantities, we refer to the reviews of past Lattice Conferences.

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 Fig. 1. There are many disparate physical scales to be covered simultaneously, ranging from the lightest hadron mass of $m_\pi \approx 140\,\text{MeV}$ over $m_D \approx 2\,\text{GeV}$ to $m_B \approx 5\,\text{GeV}$, plus the...
1.1 Ultraviolet cutoff

The ultraviolet cutoff of $\Lambda_{\text{UV}} = a^{-1}$ 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 $\Lambda_{\text{IR}} = L^{-1}$ so that the following scale hierarchy is met:

$$\Lambda_{\text{IR}} = L^{-1} \ll m_\pi, \ldots, m_D, m_B \ll a^{-1} = \Lambda_{\text{UV}}.$$  \hspace{1cm} (1)

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 Sec. 2, we 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\textsuperscript{9}, powerful non-perturbative approaches have been developed\textsuperscript{3, 4}, and we 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, we only mention 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\textsuperscript{10} and its lattice-specific refinements.

Regarding the algorithmic side of a lattice QCD simulation, the Hybrid Monte Carlo (HMC) as the first exact and still state-of-the-art algorithm has received considerable improvements by multiple time-scale integration schemes\textsuperscript{12, 13}, the Hasenbusch trick of mass-preconditioning\textsuperscript{14, 15}, supplemented by a sensible tuning of the algorithm’s parameters\textsuperscript{16}, and the method of domain decomposition (DD) applied to QCD\textsuperscript{17, 18}, just to name a few. In addition, low-mode deflation\textsuperscript{20} (together with chronological inverters\textsuperscript{21}) 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 (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 $N_f = 2$ dynamical quarks, using the rather simple $O(a)$ improved Wilson action\textsuperscript{4} to profit from the above algorithmic developments such as DD-HMC, and lattice spacings $a = 0.08, 0.06, 0.04 \text{ fm}$, sizes $L = (2 - 4) \text{ fm}$ and pion masses down to $m_\pi = 200 \text{ MeV}$, which altogether help to diminish systematic and statistical errors. Amongst others, charm physics\textsuperscript{23} as well as our B-physics programme outlined here are being investigated.
Non-perturbative Heavy Quark Effective Theory

Heavy Quark Effective Theory (HQET) at zero velocity on the lattice 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 (recall also Fig. 1).

Since the heavy quark mass ($m_b$) is much larger than the other scales such as its 3–momentum or $\Lambda_{\text{QCD}} \sim 500$ 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 at $O(1/m_b)$ reads:

$$S_{\text{HQET}} = a^4 \sum_x \overline{\psi}_h \left\{ D_0 + \delta m - \omega_{\text{kin}} D^2 - \omega_{\text{spin}} \sigma B \right\} \psi_h,$$

(2)

with $\psi_h$ satisfying $P_+ \psi_h = \psi_h, \ P_+ = \frac{1 + \gamma_0}{2}$, 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 $O$ and up to $1/m_b$–corrections to the operator itself (irrelevant when spectral quantities are considered), this means

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

(3)

where $\langle O \rangle_{\text{stat}}$ denotes the expectation value in the static approximation and $O_{\text{kin}}$ and $O_{\text{spin}}$ are given by $\overline{\psi}_h D^2 \psi_h$ and $\overline{\psi}_h \sigma B \psi_h$. 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.

2.) As in HQET mixings among operators of different dimensions occur, the power-divergent additive mass renormalization $\delta m \sim g_0^2/a$ already affects its leading order. Unless HQET is renormalized non-perturbatively, this divergence — and further ones arising at $O(1/m_b)$ — imply that the continuum limit does not exist owing to a remainder, which, at any finite perturbative order, 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.

It is based on a non-perturbative matching of HQET and QCD in finite volume.

Application: The b-quark mass from HQET at $O(1/m_b)$

Let us first note 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.

In the framework introduced in Ref., matching and renormalization are performed simultaneously and non-perturbatively. The general strategy, illustrated in Fig. 2, can be explained as follows. Starting from a finite volume with $L_1 \approx 0.5$ fm, one chooses lattice spacings $a$ sufficiently smaller than $1/m_b$ such that the b-quark propagates correctly up to controllable discretization errors of order $a^2$. The relation between the renormalization group invariant (RGI) and the bare mass in QCD being known, suitable finite-volume observables $\Phi_k(L_1, M_h)$ can be calculated as a function of the RGI heavy quark mass, $M_h$, and extrapolated to the continuum limit. 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 (r.h.s. of Fig. 2). At the same physical value of $L_1$ but for resolutions $L_1/a = O(10)$, the previously computed heavy-quark mass dependence of $\Phi_k(L_1, M_h)$ in finite-volume QCD may be exploited to determine the bare parameters of HQET for $a \approx (0.025 - 0.05)$ fm. 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 (SSFs) $\sigma_k$, indicated in Fig. 2. By using the knowledge of $\Phi_k(L_2, M_h)$ 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 (bottom of Fig. 2). This sequence of steps yields an expression of \( m_B \), the physical input, as a function of \( M_0 \) via the quark mass dependence of \( \Phi_k(L_1, M_0) \), 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 Review of the quenched computation of the b-quark mass\(^{30} \)

To apply this to \( M_0 \), the task is to fix \( \delta m \) and \( \omega_{\text{kin}} \) non-perturbatively by performing a matching to QCD, after restricting to spin-averaged quantities to get rid of the contributions proportional to \( \omega_{\text{spin}} \). For sensible definitions of the required matching observables, \( \Phi_1 \) and \( \Phi_2 \), we work with the Schrödinger functional (SF), i.e., QCD with Dirichlet boundary conditions in time and periodic ones in space (up to a phase \( \theta \) for the fermions): \( \Phi_1^{QCD}(L, m_h) \) exploits the sensitivity of SF correlation functions to \( \omega \)-matching to QCD, after restricting to spin-averaged quantities to get rid of the contributions in time and periodic ones in space (up to a phase \( \theta \) for the fermions): \( \Phi_2^{QCD}(L, m_h) \equiv L \Gamma_1(L, m_h) \), where \( \Gamma_1 \) is a finite-volume effective energy. When expanded in HQET, \( \Phi_1^{HQET}(L) \) is given by \( \omega_{\text{kin}} \) times a quantity defined in the effective theory (called \( R_1^{\text{kin}}(L, \theta, \theta') \)), whereas \( \Phi_2^{HQET}(L) \) is a function of \( \omega_{\text{kin}} \) and \( m_{\text{bare}} = \delta m + m_h \), involving two other HQET quantities, \( \Gamma_1^{\text{stat}}(L) \) and \( \Gamma_1^{\text{kin}}(L) \). According to the strategy sketched above, by equating \( \Phi_k^{QCD}(L_1, m_h) \) and \( \Phi_k^{HQET}(L_1) \) one can determine the bare parameters \( m_{\text{bare}} \) and \( \omega_{\text{kin}} \) as functions of \( m_h \) at the lattice spacings belonging to the volume \( L_1^4 \). To employ the spin-averaged B-meson mass, \( m_B^{\text{av}} \), as phenomenological input, the \( \Phi_k \) are evolved to larger volumes through proper SSFs, where the resulting \( \Phi_k^{HQET}(2L_1, m_h) \) still carry the dependence on \( m_h \) inherited from the matching to QCD in \( L_1^4 \). After 2 evolution steps (and taking continuum limits), linear extents of \( \gtrsim 1.5 \text{ fm} \) are reached, and \( m_{\text{bare}} \) and \( \omega_{\text{kin}} \), expressed in terms of SSFs, \( \Phi_k^{QCD}(L_1, m_h) \) as well as \( R_1^{\text{kin}} \), \( \Gamma_1^{\text{stat}} \) and \( \Gamma_1^{\text{kin}} \), are obtained — again as functions of \( m_h \). Now, the b-quark mass is extracted by solving

\[
m_B^{\text{av}} = E^{\text{stat}} + \omega_{\text{kin}}(m_h) E^{\text{kin}} + m_{\text{bare}}(m_h)
\]

for \( m_h \), with \( E^{\text{stat}} = \lim_{L \to \infty} \Gamma_1^{\text{stat}}(L) \) and \( E^{\text{kin}} = -\langle B | a^3 \sum_z O_{\text{kin}}(0, z) | B \rangle_{\text{stat}}. \) All quantities entering eq. (4) have a continuum limit either in QCD or HQET, which implies that all power divergences have been subtracted non-perturbatively.

In case of the leading-order, static approximation, where only \( m_{\text{bare}} \) needs to be determined, the small- and large-volume matching conditions simplify to \( \Gamma_1(L_1, m_h) = \Gamma_1^{\text{stat}}(L_1) + m_{\text{bare}} \) and \( m_B^{\text{av}} = E^{\text{stat}} + m_{\text{bare}}, \) respectively. To be able to solve the first equation for \( m_{\text{bare}} \) and replace it in the second, we bridge the volume gap in two steps by inserting a SSF \( \sigma_m(L_1) = 2L_1[F_1^{\text{stat}}(2L_1) - \Gamma_1^{\text{stat}}(L_1)] \) and arrive at the master equation

\[
L_1 \left[ m_B^{\text{av}} - (E^{\text{stat}} - \Gamma_1^{\text{stat}}) \right] - \frac{\sigma_m(L_1)}{2} = L_1 \Gamma_1(L_1, m_h),
\]

where \( \Gamma_1 \) originates from QCD in \( L_1^4 \) and any reference to bare parameters has disappeared. Its graphical solution is reproduced in Fig. 3 and yields \( m_B^{\text{stat}} = 6.806(79) \text{ GeV}. \)

The inclusion of the sub-leading \( 1/m_h \)-effects is technically more involved and exploits the freedom of choices for the angle(s) \( \theta \) and an alternative set of matching observables\(^{30} \). We just quote the final value \( m_B^{\text{stat}}(m_h) = 4.347(48) \text{ GeV} \) with the remark that, upon including the \( 1/m_h \)-terms, differences among the static results w.r.t. the matching condition chosen are gone, which signals practically negligible higher-order corrections.

\(^{30}\)Here, \( \delta m = 0 \) in the action; its effect is accounted for in the overall energy shift \( m_{\text{bare}} \) in HQET versus QCD.
3.2 Status in two-flavour QCD

The renormalization of HQET through the non-perturbative matching to $N_f = 2$ QCD in finite volume, to do the power-divergent subtractions, is under way. As an important prerequisite, the calculated non-perturbative relation between the RGI and subtracted bare heavy quark mass enables to fix RGI heavy quark masses in the matching volume $L_1^4$:

$$L_1 M = Z_M(g_0) Z(g_0) (1 + b_m(g_0) a m_{q, h}) L_1 m_{q, h}, \quad M = M_h.$$  \hspace{1cm} (6)

The extent $L_1$ is defined via a constant SF coupling, $\bar{g}^2(L_1/2) = 2.989$, and the PCAC masses of the dynamical light quarks are tuned to zero.

Figure 4 shows two examples for the heavy quark mass dependence of finite-volume QCD observables in the continuum limit, which enter the non-perturbative matching.

These results also allow to perform non-perturbative tests of HQET in the spirit of the corresponding quenched investigation. The calculation of the step scaling functions in HQET is expected to be finished soon, and the large-volume part of our strategy is currently being implemented within the CLS effort.
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. The striking agreement, for example, between the decay constant $F_{B_s}$ computed including $1/m_b$–corrections and the value resulting from the interpolation between the static number and data around the charm [36, 37], though still in the quenched approximation, provides a strong internal check of the approach. In addition, the HQET parameters at $O(1/m_b)$ calculated non-perturbatively by the ALPHA Collaboration [37] can be employed for several other quantities. The programme aiming to reach the same accuracy in the $N_f = 2$ dynamical case is well advanced and progressing fast [33].

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