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Theoretical view on Heavy Flavour schemes

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Processes involving heavy quarks are crucial at the LHC, for flavour physics and Higgs physics and as backgrounds for new physics searches. In this brief contribution, I outline the main theoretical challenges involved in the theoretical description of this kind of processes, both at the inclusive and exclusive levels, and highlight a few examples that testify the enormous progress that has been made in the field over the past five years.

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Processes featuring heavy quarks either in the initial or final states are a natural playground to test our understanding of perturbative Quantum Chromodynamics (QCD) in the presence of several energy scales. There are at least two scales that enter these processes: the heavy-quark mass m and the (invariant) mass M of the particle(s) produced along with the heavy quark. Large collinear logarithms of the ratio M/m may jeopardise the convergence of the perturbative expansion of theoretical predictions. Fortunately, the impact of these logarithmic contributions can be controlled by resumming them to all orders in the strong coupling constant, via a scheme in which the heavy quark mass m is neglected at the level of the matrix element. Such a scheme is often referred to as massless or five-flavour scheme (5FS), in case the heavy quark is identified with the bottom quark. As far as heavy quarks in the initial state are concerned, this procedure amounts to introducing a suitable parton distribution function (PDF) for the heavy quark. An analogous procedure for heavy quarks in the final state involves the use of fragmentation functions. The resummation of powers of $\log(M/m)$ in a 5FS is performed by solving the DGLAP evolution equations, at the price of discarding power corrections of $O(m^2/M^2)$, and thus of yielding less accurate theoretical predictions for the observables related to the heavy-quark degrees of freedom. A scheme in which the heavy quark is produced at the matrix-element level and is not treated on the same footing as the light quarks is dubbed as massive scheme or four-flavour scheme (4FS). In this scheme, the potentially large collinear logarithms are not resummed to all orders, however they appear order-by-order in the perturbative expansion.

In Refs. [1, 2] it was shown that processes in which the heavy quarks (more specifically bottom quarks) are dominantly produced via initial-state (space-like) splittings, the theoretical predictions in 4FS are typically not spoiled by initial-state collinear logarithms. This is due to two main factors, one of dynamical and the other of kinematical origin. The first is that the effects of the resummation of the initial-state collinear logarithms are relevant mainly at large x and, in general, keeping only the explicit logs appearing at next-to-leading order (NLO) in the 4FS is a good approximation. The second reason is that the scale which appears in the collinear logarithms turns out to be proportional to the hard scale of the process but is suppressed by universal phase space factors that, at hadron colliders, reduce the size of the logarithms for processes taking place. This result makes it not only possible, but also advisable – owing to the better perturbative description of the differential observables involving the heavy quark(s) – to employ the 4FS for the exclusive description of these processes. This has been shown explicitly to be the case for several processes including single-top production [3, 4], bottom-initiated Higgs production [5, 6] and bottom-initiated Z/γ production [7, 8], and also for BSM processes, such as heavy charged Higgs boson production in a two-Higgs doublet model or in supersymmetry [9, 10]. On the other hand, the calculations of the total cross sections in the 5FS display a faster perturbative convergence and exhibit a smaller scale uncertainty associated with missing higher orders.

In this contribution, I briefly summarise the current status of our understanding of processes involving heavy flavours and highlight some of the recent progress in their theoretical calculation, both at the level of inclusive and exclusive observables.

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1. Matched calculations for inclusive observables

Methods that combine the 4F and the 5F schemes, retaining the advantages of both, are widely available. A well-known approach is FONLL, which is based on standard QCD to match 4FS and 5FS calculations at all orders and for all processes, matching fixed order calculation at N^pLO with DGLAP resummed N^qLL. First devised for the transverse momentum spectrum of bottom quarks produced in hadronic collisions [12], the FONLL scheme has been extended to the matching of Deep-Inelastic-Scattering cross sections [13] and subsequently applied to the computation of the total cross section for Higgs and Z production in bottom-quark fusion [14, 15]. In these studies it was observed that the 4FS calculations have a very mild dependence on the factorisation scale, while the dependence on the renormalisation scale is much stronger. Moreover, the choice of a lower factorisation scale in both the 5FS and 4FS calculations helps improving the perturbative stability of the 4FS calculations and brings the predictions in the two schemes closer to each other. On the other hand, while the perturbative expansion is not very stable in the 4FS, increasing the perturbative order of the 4FS calculation in the FONLL matched calculation yields remarkably stable results. Overall the FONLL results end up being much closer to the 5FS and to the experimental data. Quite recently, in Ref. [16], the FONLL scheme has been used to combine analytic results for the 5FS partonic cross sections for the production of a Higgs boson via the fusion of two bottom quarks at N^3LO in QCD perturbation theory with NLO accurate predictions in the 4FS that include the full bottom quark mass dependence, by appropriately removing any double-counting stemming from contributions included in both predictions. While the difference between this state-of-the-art matched calculation and the 5FS results is not large in absolute value, it becomes rather significant when compared to the very small 1% theory uncertainty of the 5FS N^3LO calculation [17] .

2. Matched calculations for exclusive observables

Prior to recent developments that will be highlighted in this section, matched 4FS and 5FS calculations were not available for generic exclusive observables. A practical recipe that was typically suggested was to use the 4FS for the prediction of the shapes of differential distributions that are sensitive to the bottom quark kinematics, while using the less scale-dependent 5FS calculation for the prediction of the total cross section, hence of the normalisation of the distributions. This suggestion was motivated by the strong dependence on Parton Shower (PS) models that was often observed in the 5FS exclusive calculations [5, 9]. Another simple option that has been investigated in [18] is to switch from 4FS to 5FS at a b-quark matching scale $\mu_b > m_b$, so that the switching between the 4FS and the 5FS takes place in a region where neither the mass effects nor the resummation of collinear logs are crucial. In practice one may choose the value (or functional form) of the factorization scale μ_F and decide on the value of the matching scale μ_b. Then, events with kinematics for which $\mu_F < \mu_b$ are computed in the 4FS scheme and full mass dependence is to be retained; events with kinematics for which $\mu_F > \mu_b$ are to be evaluated in a 5FS and the bottom mass m_b is set to zero. Clearly the procedure does yield discontinuities in the theoretical predictions, that are however within experimental error.

In the past five years, several new ideas have been developed to match 4FS and 5FS at the level of exclusive observables. In this contribution, I briefly highlight two of those, while I point to

Ref. [19] for a methodology based on the idea of vetoing B-hadrons, and to Refs. [20, 21], for the formulation of a massive 5FS with consistent b-quark PDFs to be used in association with massive initial states [22]. A promising avenue for matching 4FS and 5FS at the level of exclusive observable is based on multi-jet merging: the simulations in the 5FS are merged with the calculations of the production of b-quark associated final states in the 4FS [23]. Taking Z and b-quark associated production as a testing ground, the idea is to generate showered events for $Z + j$, use clustering to determine whether the core hard process is $Z + b\bar{b}$ or $Z + j$, and throw away events if the core process belongs to the first type. Afterwards, one generates $Z + b\bar{b}$ events in the 4FS and sums up the two samples, which by construction do not overlap. An alternative methodology was presented in Ref. [24] for the calculation of Z-boson production in association with a b-jet at $O(\alpha_s^3)$. The first calculation of a hadronic scattering process involving the direct production of a flavoured-jet at NNLO accuracy in massless QCD was extended by applying FONLL techniques, to also account for the impact of finite heavy-quark mass effects.

3. Heavy flavour splitting in the final states

While initial-state collinear logarithms have been studied in details, the situation is much less clear for processes in which final-state (time-like) splittings into heavy quarks contribute significantly to the process. While the importance of the resummation of collinear logarithms has been partially investigated for $b \to bg$ splittings [25], the first assessment of the impact of the collinear logarithms of M/m, as far as the $g \to b\bar{b}$ splittings are concerned, was only done in Ref. [26], where the impact of missing powers of $\log(M/m)$ associated to final-state splittings was estimated by means of fragmentation functions. There the resummation of collinear logarithms was shown to be extremely large. Clearly, while fragmentation functions are the most exclusive observables, the importance of final-state collinear logarithms on a realistic process requires devoted phenomenological studies. If the resummation of these logarithms was found to have a strong impact in relevant observables, such as for example the associated production of top and bottom quark pairs [27], this would point to the need for a matched calculation that could solve the observed discrepancies in the comparison between different NLO calculations performed in the 4FS.

4. Conclusions

Recently, an enormous progress has been made in comparing theoretical predictions obtained in different heavy flavour schemes. For inclusive observables, there exists a general and well-tested framework to match predictions in different schemes, although not yet available for all processes, that points to heavy quark mass effects that are typically small but surely relevant at the current precision level. For exclusive observables many new exciting developments have been achieved, which I highlighted in this contribution. As far as final states are concerned, a better insight on the interplay between parton shower and collinear resummation in final states would be desirable. Studies based on fragmentation functions hint to possible pathologies in the simulation of final-state $g \to b\bar{b}$ splittings at the matrix-element level for exclusive observables. Devoted studies in assessing their impact in realistic processes would shed further light on this highly relevant topic.

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