Challenges in heavy-quark fragmentation

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Abstract: I discuss some open issues concerning the fragmentation of heavy quarks in e^+e^- annihilation, from LEP/SLD to FCC-*ee*. In particular, I review the state of the art of resummed calculations and Monte Carlo event generators and underline some of the challenging objectives of FCC-*ee* in the heavy-flavour sector.

Introduction

Heavy-quark (charm, bottom, top) phenomenology in different environments is one of the most challenging topics in high-energy physics, from both theoretical and experimental viewpoints, as it allows tests of QCD, parton model, factorization and power corrections. In fact, when calculating the cross section for heavy-quark production, the heavy-quark mass (m) regularizes the collinear singularity, but nevertheless differential distributions exhibit large logarithmic corrections, which need to be resummed to all orders, such as contributions $\sim \alpha_S \ln(m^2/Q^2)$, Q being a typical scale. Calculations resumming such large logarithms are available [1] [2], as well as Monte Carlo parton shower algorithms, such as the HERWIG [3] [4] and PYTHIA [5] [6] codes, which have lately been matched to NLO calculations in the aMC@NLO [7] and POWHEG [8] frameworks, for a number of hard-scattering processes, including heavy-quark production. As for hadronization, resummed calculations typically use non-perturbative fragmentation functions depending on few parameters which are to be tuned to experimental data [9]; alternatively, one can model power corrections by including them in an effective [10] or frozen [11] strong coupling constant. On the other hand, Monte Carlo generators implement phenomenological models, such as the string [12] or cluster [13] models, to turn partons into hadrons, once a scale of the order of 1 GeV is reached in the shower. When fitting hadronization parameters and using the tuned models in other processes, it is essential describing the parton-level process always within the same framework, namely resummations or Monte Carlo showers.

In the following, as a case study for heavy-quark fragmentation, I shall concentrate on bottom production in e^+e^- annihilation: I will discuss the state of art of perturbative calculations, at fixed order and resummed, review the current status of Monte Carlo generators, and finally comment on the perspectives at FCC-*ee* and make concluding remarks.

Perturbative calculations for heavy-quark fragmentation

As discussed in the introduction, fixed-order and resummed calculations are available to describe bottom production in e^+e^- annihilation and the fragmentation into b-flavoured mesons/baryons. Heavy-quark spectra are usually expressed in terms of x, the quark energy fraction in the centre-of-mass frame; the perturbative fragmentation approach, proposed in [1], factorizes the x-spectrum as the convolution of a massless, $\overline{\rm MS}$-subtracted coefficient function and a massive perturbative fragmentation function. The initial condition of the perturbative fragmentation function is process-independent [2] and, by means of the DGLAP equations, for an evolution between scales of the order of the centre-of-mass energy $\sqrt{s}$ and m, one manages to resum the large logarithms $\alpha_S \ln(m^2/s)$ appearing in the NLO mass spectrum (collinear resummation).

Furthermore, both $\overline{\text{MS}}$ coefficient function and initial condition contain terms which become large whenever the energy fraction x gets close to unity, which corresponds to soft or collinear gluon radiation. It is therefore mandatory to resum even these contributions to all orders to obtain a reliable prediction (large-x or threshold resummation).

The initial condition of the perturbative fragmentation function was computed at NLO in [1] and lately at NNLO in [14] and [15] for quark- and gluon-initiated contributions, respectively. The $\overline{\text{MS}}$ coefficient function was instead calculated at NLO in [16] and at NNLO in [17]; Ref. [18] computes the NNLO corrections to the Altarelli–Parisi splitting functions, entering in the evolution of the perturbative fragmentation function. In fact, if the splitting functions are computed at NLO, the large mass logarithms $\alpha_S \ln(m^2/s)$ are resummed at NLL, whereas collinear resummation can be carried out at NNLL once even the NNLO corrections to the splitting functions are implemented.

As for threshold resummation, large-x contribution to the coefficient function and initial condition of the perturbative fragmentation function can be resummed following standard techniques as in [19], where the calculation is carried out in the next-to-leading logarithmic approximation (NLL). By using the results in [20] and [21], one can extend threshold resummation to NNLL accuracy.

Although all the ingredients to calculate the heavy-quark spectra at NNLO, with the resummation of mass and threshold contributions to NNLL accuracy, are available, most phenomenological investigations have been carried out in the NLO+NLL approximation in [2] and [22] for e^+e^- annihilation, in [23] for b-production in top decays $t \to bW$, in [24] for $H \to b\bar{b}$ processes, H being the Standard Model Higgs boson. Extending the studies of heavy-quark fragmentation in e^+e^- annihilation is nevertheless very useful, in order to further decrease the scale uncertainty on the predictions and improve the behaviour of the energy spectra at large x, which are instead unstable and oscillating whenever $x > 1 - \Lambda_{\text{QCD}}/m$ [2].

As for the inclusion of hadronization corrections, the heavy-quark spectra yielded by resummed calculations are typically convoluted with non-perturbative fragmentation functions containing a few parameters which are to be tuned to experimental data, e.g., B-hadron production at LEP [25] [26] or SLD [27]. Details on the fitting of hadronization models can be found in [28], where the best-fitted models are also used to predict B-hadron energy distributions in top and Higgs decays.

Before concluding this section, it is worthwhile pointing out that most analyses on heavy-quark fragmentation are undertaken in the so-called non-singlet approximation and gluon splitting into heavy-quark pairs is neglected. Ref. [22] did include $g \to c\bar{c}(b\bar{b})$ splitting, but its contribution to charm/bottom fragmentation turned out to be small and not essential to fit the experimental data. In fact, LEP and SLD experiments measured the gluon branching fractions to heavy quarks, labelled as $g_{c\bar{c}}$ and $g_{b\bar{b}}$, and it was found $g_{c\bar{c}} \simeq 3 \times 10^{-2}$ [29] [30] and $g_{b\bar{b}} \simeq 2 \times 10^{-3}$ [31] [32] [33]. As will be commented later on, FCC will have a better sensitivity to $g \to c\bar{c}(b\bar{b})$ processes, thanks to expected higher statistics and more refined granularity of calorimeter and vertex detectors.

Monte Carlo parton showers and heavy-quark fragmentation

As pointed out in the introduction, Monte Carlo event generators, implementing parton showers in the soft/collinear approximation, along with non-perturbative models for hadronization, are available tools to address heavy-quark fragmentation in e^+e^- collisions. Ref. [28] discusses a tuning of HERWIG 6 [3] and PYTHIA 6 [5] event generators to LEP and SLD, taking particular care about fitting the Monte Carlo parameters which are directly related to the hadronization of the bottom quark. Those tunings were then used in [34] to estimate the Monte Carlo uncertainty on the top-quark mass due to the treatment of bottom fragmentation in top decays at the LHC. The overall result of these analyses is that it was necessary to retune both HERWIG and PYTHIA to get an acceptable description of B-hadron data at LEP and SLD. Indeed, one managed to tune PYTHIA to reproduce well the data, whereas HERWIG was only marginally consistent, although the fitting procedure improved the comparison pretty much.

Given the late progresses in Monte Carlo implementations, the results in Refs. [28] and [34] clearly need to be updated. On the one hand, both HERWIG and PYTHIA have new versions in C++, namely HERWIG 7 [4] and PYTHIA 8 [6]: Ref. [35] compares the PYTHIA 8 predictions with bottom-fragmentation data from LEP and SLD, showing that it is possible to tune PYTHIA 8 to reproduce such data. On the other hand, HERWIG 7 exhibits some discrepancies with respect to B-hadron data [36] and therefore a retuning is therefore mandatory.

As for the novel generation of NLO codes, such as aMC@NLO [7] and POWHEG [8], in principle the HERWIG and PYTHIA fragmentation parameters need to be retuned, once the hard scattering is implemented at NLO. However, HERWIG and PYTHIA standard showers are matched to NLO tree-level matrix elements, along the lines of [37] and [38], and the full virtual corrections, included in POWHEG and aMC@NLO, are relevant only at large energy fractions. Furthermore, up to power corrections $\mathcal{O}(m/\sqrt{s})^p$, the NLO K-factor for the total e^+e^--annihilation cross section is small, being $K \simeq 1 + \alpha_S(s)/\pi$. Therefore, although a thorough investigation of bottom fragmentation using POWHEG and aMC@NLO is currently in progress [39] and should be very welcome, since such programs are heavily used even for b-quark production in top or Higgs decays at the LHC, one should expect very little differences in the best-fit parametrizations with respect to the standard tunings of PYTHIA and HERWIG.

Prospects at FCC-*ee*

The perspectives of the FCC-*ee* program, with an integrated luminosity $\mathcal{L}_{\rm int}$=1 ab^{-1}, are summarized in [40], where the authors also debate the challenging objectives at different centre-of-mass energies, namely the threshold for Z, Higgs, WW, $t\bar{t}$ and HZ production.

In particular, the expected statistics will be 10^5 larger than at LEP and therefore the statistical uncertainties will be reduced by a factor of 30. Also, because of the smaller beam-spot size and the new-generation vertex detectors, much more precise measurements of the R_b ratio are foreseen. The current value is $R_b = 0.21629 \pm 0.00066$, whereas a precision about 2-5 $\times 10^{-5}$ is the goal of FCC-*ee* [41].

Furthermore, while the LEP and SLD fragmentation measurements were carried out essentially for inclusive spectra (B-mesons and possibly Λ_b baryons) and chains like $B \to D^*\ell\nu$, $D^* \to D\pi$, $D \to K(n\pi)$, the high FCC-*ee* statistics will make it possible to distinguish b- and c-flavoured hadrons and separate fragmentation spectra (charged vs neutral, spin 1 vs spin 0, baryons vs mesons). In this way, one will be able to extract the non-perturbative fragmentation function very precisely, which is crucial to carry out any program of precision physics even in the Higgs and top-quark sectors. Moreover, according to the FCC project, one will be sensitive to rare B-decays, such as $B \to J/\psi X$, which, albeit the small branching ratio, can be easily discriminated from the backgrounds, after suitable cuts are set.

Finally, as commented above, the higher statistics and granularity of calorimeters and vertex detectors will allow one to disentangle the $g \to b\bar{b}$ and $g \to c\bar{c}$ splittings, through a double tagging of the jets originated from the $b(c)$ and $\bar{b}(\bar{c})$ quarks. Therefore, FCC-*ee* will be a unique environment to perform precise measurements of gluon-initiated contributions to heavy-quark fragmentation functions and thus perform further tests of QCD and factorization.

Conclusions

I discussed heavy-quark fragmentation in e^+e^- collisions, in the perspective of Future Circular Colliders, and briefly reviewed the state of the art of theoretical calculations and Monte Carlo generators. As for resummations, although phenomenological analyses have been so far carried out in the NLO+NLL approximation, all ingredients to promote them to NNLO+NNLL accuracy are available and such an extension will be certainly desirable in order to meet the precision goals of FCC-*ee*. Particular care will have to be taken to include in a consistent way non-perturbative corrections, once the higher-order corrections to the parton-level process are implemented. Futhermore, the large statistics and more refined detectors which are foreseen at FCC will allow more accurate determinations of the gluon branching fractions into heavy-quark pairs.

Thanks to lively activity in the latest years, much progress has been undertaken in the implementation of Monte Carlo generators. The new object-oriented versions of HERWIG and PYTHIA contain improved hadronization models and have been matched to NLO hard-scattering processes provided by POWHEG and aMC@NLO. A systematic investigation of heavy-quark/hadron production in e^+e^- annihilation with the NLO+shower codes is currently in progress. Although NLO corrections to shapes and normalization of e^+e^--annihilation cross section should be small, retuning non-perturbative models and studying heavy-hadron production with POWHEG and aMC@NLO will be nonetheless very interesting.

In summary, FCC-*ee* will be a great opportunity to study heavy-quark phenomenology with high precision, from the viewpoint of both perturbative and non-perturbative QCD. The late advances in QCD calculations and Monte Carlo implementations, as well as the ongoing work on heavy-quark phenomenology, should make the challenging objectives of the FCC-*ee* project reachable.

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