Open heavy-flavor observables at the LHC and the importance of higher-order flow harmonics

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Abstract. Heavy-quark dynamics in the quark-gluon plasma provide information about the medium properties and the details of the heavy-quark-medium interaction. Traditional observables like the nuclear modification factor and the elliptic flow of $D$ mesons have shown suppression at intermediate and high momenta and collective flow at low momenta. Thanks to the improving accuracy of the experimental data a combined analysis of these two observables starts to have discriminating power between different heavy-quark transport coefficients or features of the energy-loss models. In this overview, we summarize the modern strategy of describing heavy-quark dynamics and show how recent advances to include more differential observables such as azimuthal correlations and higher-order flow harmonics can help us understand the properties of heavy-flavor transport.

1. Heavy-flavor observables in heavy-ion collisions
Understanding thermodynamic and transport properties of strongly interacting many-body systems is the main motivation of performing (ultra)relativistic heavy-ion collisions and the discovery of the quark-gluon plasma (QGP) as an almost perfect fluid [1] has been one of the highlights of these endeavors. Key observables are linked to probes which do not fully thermalize with the medium and thus do not lose memory of their interactions with the medium constituents. An extreme example are electromagnetic probes, like photons and dileptons, which do not reinteract strongly with the produced QCD matter and thus give us information about the circumstances of their production. High-$p_T$ jets are another important probe. They are produced in the initial hard scatterings of partons inside the nucleons of the incoming nuclei. Upon scattering with the medium constituents they lose some fraction of their energy and their final spectra are thus expected to be modified compared to elementary reactions.

The mass of heavy quarks is another scale in the system, which allows us to probe both the regime of low heavy-quark momenta, where $p_T \ll m_{HQ}$, and the high-momentum regime, where $p_T \gg m_{HQ}$. The dynamics of heavy quarks at low momenta is mostly governed by diffusive processes and one may ask about the degree of thermalization inside the medium. At high momenta, the heavy quarks behave similarly to light partons and the contributions from...
different energy loss mechanisms are the main subject of interest. The intermediate-momentum regime is especially interesting, because most experimental data exist in this kinematic region.

Partial thermalization can be studied in terms of collective flow pattern of heavy flavor compared to the flow of the bulk medium consisting of light partons. Most models give relaxation times for charm quarks which are much longer than the evolution of the QGP \cite{2}. Surprisingly, the measured light-flavor and heavy-flavor elliptic flow coefficients are quite similar within the large experimental error bars on the latter \cite{3}.

While nowadays the nuclear modification factor $R_{AA}$ is mostly used to calibrate parameters in the energy loss models - explicitly or implicitly - in connection with the model of the medium evolution, the $v_2$ as well as higher-order flow harmonics for the low-$p_T$ sector and more differential observables like azimuthal correlations provide further opportunities to distinguish between energy loss models and exclude some of them.

In this overview, we will first present the current strategies to model heavy-flavor dynamics in heavy-ion collisions in section 2 and then discuss recent theoretical advances in heavy-flavor observables in particular higher-order flow harmonics in section 3.

2. Heavy-flavor dynamics

One of the main questions is how to get access to fundamental properties of the QGP from a comparison of theoretical models to experimental data and which observables can serve which purpose. It needs to be distinguished between the purpose of tomography, i.e. learning about medium properties, such as temperature, viscosity, but also about initial state fluctuations, expansion velocities, density distributions, etc., and studying the heavy-quark-medium interaction itself to learn about the individual processes of the underlying theory. In \cite{4} it has been pointed out that jet observables can to some extent be classified in one or the other category, but both aspect remain very much entangled. Neither tomography of the medium nor studies of the energy loss model can be achieved alone but one needs to well calibrating the other.

pQCD and pQCD inspired models of collisional \cite{5, 6, 7} and radiative processes \cite{8}, as well as non-perturbative resonance scattering \cite{9, 10} and strong-coupling approaches \cite{11, 12} have been proposed and studied to great detail in the past decades. Most of the mentioned models are derived in some limit or kinematic region. Usually, however, experimental observables are not sensitive to only one asymptotic limit and span over various kinematic regions including several scales. Most models are therefore not applicable over the whole kinematic range mostly in the intermediate $p_T$ regime, which is most interesting. However, even if the underlying theory for heavy-quark-medium interaction could be fully solved, there are many other sources of uncertainties involved, as will become clear by outlining the complete strategy of modeling heavy-flavor dynamics in heavy-ion collisions in the following:

In the initial hard scatterings the heavy quarks are produced according to partonic cross sections. The most elaborate model for inclusive spectra is provided by the FONLL (first-order next-to-leading log) \cite{13} pQCD framework. One has to remember, however, that the comparison with data is only possible, when the pQCD production cross sections are folded with the parton distribution functions and a fragmentation function. For the FONLL framework the fragmentation functions in \cite{14} work best to reproduce the data. This should be kept in mind and done consistently for the heavy-quark fragmentation after the evolution stage in the medium as described below. For more exclusive spectra, like $Q\bar{Q}$ azimuthal correlations, NLO pQCD matrix elements are coupled to parton shower event generators \cite{15, 16}. Thanks to the heavy-quark mass the virtuality is significantly reduced compared to light partons and the charm and bottom quarks can be assumed onshell at the equilibration time of the QGP medium. The stage of preequilibrium dynamics remains the least understood phase during a heavy-ion collision and this is no different for the heavy-flavor sector.
The interaction of the heavy-quarks with the QGP constituents can occur via elastic or inelastic scattering processes. The elastic processes, also called collisional energy loss processes, in the perturbative regime need to be regularized in the $t$-channel. This is usually done schematically by the Debye mass and can be extended to replacing the bare gluon propagator with the full hard-thermal loop (HTL) resummed propagator at small momentum exchange. In the nonperturbative QCD regime, however, it turns out that the energy loss will not be independent of the intermediate scale between bare and HTL-propagators. Here, it is necessary to resort to modeling in order to extend the validity to the full kinematic regime, e.g. like in [28], or use nonperturbative approaches, such as resonance scattering effective theory [9, 10] or the strong-coupling AdS/CFT correspondance [11, 12]. For very energetic partons the radiative gluon emission resulting from the scattering with the medium constituents is considered the dominant contribution to energy loss. The gluon formation in this regime is long and thus several scatterings contribute coherently to the emission spectra. For heavy quarks at intermediate energies, the gluon formation time gets reduced by the mass and the radiative energy loss can be described by several incoherent scatterings [17, 18]. Such a prescription can be readily applied in Monte-Carlo simulations for heavy-quark dynamics. Several theoretical descriptions have addressed the radiative energy loss of light and heavy quarks in various kinematic regimes [8] resulting in averaged formulas assuming a medium at constant temperatures. As pointed out above, however, it is crucially important to assume a most realistic background evolution of the medium in order to compare to experimental data in a meaningful way. The QGP medium provides the scattering partners of the heavy-quarks, which can either be described by a Boltzmann parton cascade [19], a fluid dynamical evolution or a microscopic off-shell transport model [20]. Most importantly the medium description needs to be well tested for and constraint by the light and soft bulk observables. Factor-of-2 differences in the $R_{AA}$ at intermediate and high $p_T$ can solely stem from using a simplistic versus realistic medium. Another source of inconsistency in the coupling between light- and heavy-flavor sectors can be the choice of the active degrees of freedom [21]. In a fluid dynamical evolution at LHC and top-RHIC energies the equation of state comes from lattice QCD [22, 23]. In the temperature regime of interest a gas of massless, noninteracting partons, as it is often sampled from via thermal distributions, does not reproduce the lattice equation of state. A representation of the medium quasi-particles which matches the lattice equation of state [24] can affect the scattering cross sections and the extracted transport coefficients [25]. Further aspects of the medium evolution, including initial state fluctuations [26] and viscous corrections are also of importance.

Once the medium has expanded and cooled down the heavy quarks hadronize via either recombination [30] at low momenta or fragmentation [14] at higher momenta. Both descriptions as well as their respective probabilities have a couple of parameters, which ideally one would like to obtain from other experiments. This is to some degree possible for the fragmentation process, as it is constraint by the initial production mechanisms and comparison to data from elementary reactions. After hadronization the final-state hadronic interaction are expected to affect the heavy-flavor observables on the order of 10-20% [27].

3. Recent advances in heavy-flavor observables
Traditional heavy-flavor observables are the nuclear modification factor, $R_{AA}$, and the elliptic flow $v_2$. As mentioned in the introduction the $R_{AA}$ with its rather generic $p_T$ dependence, has become a good observable to fix the overall normalization of the energy loss model in conjunction with the medium evolution model. Various approaches with different ingredients and largely different heavy-quark transport coefficients are so able to describe the available $R_{AA}$ data remarkably well. For a review and collection of data-to-model comparisons, see [33].

In the light-flavor sector, important contributions have become possible by looking into correlations and higher-order flow harmonics. For example, the better understanding of the
Figure 1. Higher-order flow harmonics of D mesons for the 20 − 30% most central Pb+Pb collisions at $\sqrt{s} = 2.76$ TeV. Calculations are done in the MC@sHQ+EPOS2 model for a collisional+radiative(+LPM) energy loss mechanism.

initial conditions for fluid dynamical modeling in correspondance with the extracted values for the ratio of shear viscosity over entropy density $\eta/s$ was made possible by the exact measurement of $v_n$ [34, 35, 36, 37, 38].

In recent works [39, 40] it has been pointed out that azimuthal correlations of $Q\bar{Q}$ pairs are promising observables for disentangling purely elastic and inelastic contributions to the energy loss mechanisms. There are, however, a couple of challenges, that need to be overcome, before a meaningful comparison between theory and experiment can be achieved. From the theory side already the $c\bar{c}$ proton-proton baseline is not well understood, as can be seen in the differences between NLO pQCD + parton shower calculations and available $D\bar{D}$ measurements in proton-proton collisions [41]. Since experimentally the feasibility of measuring $D\bar{D}$ correlations directly will only become possible with data from future runs, theoretical tools need to couple the light- and the heavy-flavor sectors more consistently in order to get reliable results for correlations between $D$ mesons and hadrons or heavy-flavor decay electrons and hadrons. This would in particular concerns the initial production of heavy quarks and the soft bulk matter, the fragmentation process, as well as the final state hadronic interactions.

In [42] we have predicted a finite triangular flow of $D$ mesons for RHIC and LHC energies using the MC@sHQ+EPOS2 model [28]. It couples a Boltzmann propagation of heavy quarks to a fluid dynamical evolution with the event-by-event EPOS initial conditions [43, 44]. This bulk description yields an excellent agreement with the available light hadron sector and can thus be considered a realistic modeling of the QGP medium. This is in particular true for LHC energies. With the upcoming coupling of MC@sHQ to EPOS3 the reliability will be extended to lower energies and different collision systems. The energy loss mechanism can describe either be a purely elastic or inelastic scatterings. The elastic scattering cross sections are obtained from the the Born approximation of pQCD and includes a running strong coupling coupling $\alpha_s$ [45]. The $t$-channel infrared divergence is regularized by the Debye screening mass, which is calculated self-consistently [46], albeit as the reduced semi-hard gluon propagator tuned
Figure 2. The contribution of hadronization (recombination) to the $B$ meson elliptic (solid) and triangular (dashed) flow (left plot) and the contribution of the bulk flow to the bottom quark elliptic (solid) and triangular (dashed) flow (right plot) for the $30-50\%$ most central Pb+Pb collisions at $\sqrt{s} = 2.76$ TeV. Calculations are done in the MC@sHQ+EPOS2 model for a collisional+radiative(+LPM) energy loss mechanism to reproduce the HTL+semi-hard energy loss [28]. The radiative processes are included as stemming from incoherent scatterings. The emission spectra are an extension of the calculation in [29] to finite quark masses [18]. Coherent emission is accounted for in form of a suppression of the power spectra at high $p_T$ [47]. This model reproduces well the $R_{AA}$ at RHIC and LHC after rescaling the scattering rates by a global factor $K$, which is $K_{\text{coll}} = 1.5$ in the case of purely elastic scatterings and $K_{\text{coll+rad}} = 0.8$ in the case of both elastic and inelastic scatterings, which is close to unity. While the collective flow observables of the light charged hadrons are determined by the initial state geometry and fluctuations, the flow of the charm quarks comes from the interaction with the medium constituents. The stronger the charm quarks couple to the medium the more they thermalize inside the flowing medium and pick up the momentum anisotropy from the bulk. We could show that the $v_3$ of $D$ mesons is more sensitive to the decoupling of the charm quarks from the medium evolution than the $v_2$.

In Fig. 1 we can now present the higher-order coefficients $v_4$ and $v_5$, which require to run many more events for sufficient statistics. Calculations are performed for the collisional plus radiative(+LPM) energy loss mechanism. The expected D meson $v_4$ has a maximal value of $\sim 1-2\%$, while the values of charged hadron $v_4$ measured by the ALICE and ATLAS collaborations [38] show a maximal value of $\sim 8\%$. The decoupling of heavy quarks from the bulk is thus clearly seen.

Our calculations show that the elliptic flow of the much heavier bottom quarks is already significantly lower than that for charm quarks or the light charged hadrons. In the left plot of Fig. 2 we can further demonstrate that the $v_3$ of bottom quarks is vanishingly small. Furthermore, the $v_2$ of $B$ mesons is almost entirely due to the flow of the bottom quarks. The hadronization mechanism of recombination adds only a small contribution to the overall $v_2$. Due to the path length difference in an spatially anisotropic medium heavy quarks are expected to be more strongly deflected from their original azimuthal direction along the long axis than along the short axis, which leads to a $v_2$ signal independent of the flow of the medium.

Theoretically one can mimick this situation by artifically neglecting the local fluid velocity in the scattering processes. At low momenta this contribution to the $v_2$ signal is negligible for the $D$ mesons, but is the dominant source of $v_2$ at higher momenta. We repeat the same analysis for the bottom quarks and see in the right plot of Fig. 2, that the energy loss along the path
length anisotropy does not lead to a substantial contribution to the bottom quark $v_2$.

Both the $D$ meson triangular flow and the $B$ meson elliptic flow would be valuable experimental data to enhance our understanding of heavy-flavor dynamics beyond the current level.

4. Conclusions

Heavy quarks probe partial thermalization with the QGP at low $p_T$ and in-medium energy loss at high $p_T$. In the most interesting region around intermediate $p_T$, many aspects play an important role, in particular the onset of coherent gluon emission, gluon thermal mass and width [48], finite path length and the importance of nonperturbative scatterings.

Modern models propagate heavy quarks by either the Langevin or the Boltzmann equation, where the former is a good approximation for bottom quarks but its reliability for charm quarks is questionable [49]. These approaches couple the heavy-flavor dynamics to dynamical evolutions of the QGP, which are well tested in the light-flavor sector and are able to reproduce $p_T$ spectra and flow coefficients of charged hadrons.

Yet, the traditional observables of heavy flavor, the $D$ meson $R_{AA}$ and $v_2$ are described well by many models with to some extent very different ingredients and transport coefficients. It is therefore important to go beyond these observables in $AA$ collisions. Currently, effort goes into the study of systems like proton-lead collisions, where initial shadowing effects at low transverse momenta play a role and first experimental data do not see a suppression at higher $p_T$.

More differential observables like $Q\bar{Q}$ correlations and higher-order flow coefficients of $D$ mesons as well as the elliptic flow of $B$ mesons indicate to have a larger discriminating power and are good candidates for reaching another level of understanding of the heavy-flavor dynamics and its relation to the bulk medium evolution. They can thus help us to identify most dominant features of the heavy-quark-medium interaction in order to connect experimental data to fundamental properties of QCD.

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