Heavy flavors in AA collisions: production, transport and final spectra

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Abstract A multi-step setup for heavy-flavor studies in high-energy nucleus-nucleus (AA) collisions—addressing within a comprehensive framework the initial Q̅Q production, the propagation in the hot medium until decoupling and the final hadronization and decays—is presented. The initial hard production of Q̅Q pairs is simulated using the POWHEG pQCD event generator, interfaced with the PYTHIA parton shower. Outcomes of the calculations are compared to experimental data in pp collisions and are used as a validated benchmark for the study of medium effects. In the AA case, the propagation of the heavy quarks in the medium is described in a framework provided by the relativistic Langevin equation. For the latter, different choices of transport coefficients are explored (either provided by a perturbative calculation or extracted from lattice-QCD simulations) and the corresponding numerical results are compared to experimental data from RHIC and the LHC. In particular, outcomes for the nuclear modification factor RAA and for the elliptic flow v2 of D/B mesons, heavy-flavor electrons and non-prompt J/ψ’s are displayed.

1 Introduction

The purpose of our paper is to provide a comprehensive setup for the study of heavy-flavor observables in high-energy hadronic (pp) and nuclear (AA) collisions: D/B-mesons, decay electrons (D/B → X νe) and displaced J/ψ’s (i.e., non-prompt J/ψ’s from B decays, B → J/ψ + X).

The interest in heavy quarks for heavy-ion phenomenology lies in the fact that, being produced in the first instants and with an abundance low enough to guarantee a small annihilation rate, they allow a tomography of the medium formed in high-energy AA collisions, the Quark–Gluon Plasma (QGP). In fact, because of the large mass, their initial production is a short-distance process described—even in the AA case (modulo possible modifications of the Parton Distribution Functions)—by pQCD. Hence, differences in the final observables with respect to the pp benchmark reflect the presence of a dense medium formed in the collision and allow us to test its properties.

The last few years have seen remarkable experimental advances in heavy-flavor measurements in AA collisions, both at RHIC and at the LHC. Until very recently experimental information on heavy quarks in high-energy nuclear collisions was only accessible through the electrons from semileptonic decays, without the possibility of disentangling the charm and beauty contributions.

Electron studies, carried out by the PHENIX [1] and STAR [2] experiments, were however already sufficient to suggest a high degree of rescattering of the heavy quarks in the medium, leading to a quenching of their decay electron spectra and to a non-vanishing elliptic flow.

Nowadays a much richer information has become available thanks to the measurements of D0, D+ and D+ mesons in Pb–Pb collisions performed by the ALICE experiment [3] and of displaced J/ψ’s detected by CMS [4], the latter opening a new window on the understanding of the interaction of beauty in the QCD medium. Open-charm measurements in heavy-ion collisions were also recently presented by the STAR collaboration [5], based on measuring hadronic D0 decays in Au–Au collisions at RHIC. Finally, the possibility of reconstructing Ds mesons in a nuclear environment (preliminary results obtained by ALICE can be found in Ref. [6]) will allow to study changes in the heavy-flavor hadrochemistry arising from in-medium hadronization [7, 8].
On the theory side—at variance with jet-quenching (in which one simply considers the energy degradation of a high-\(p_T\) parton) and soft-physics studies based on hydrodynamics (in which one directly assumes to deal with a system at local thermal equilibrium)—heavy quark studies require to develop tools capable of describing how off-equilibrium probes tend asymptotically to thermalize with the surrounding environment (the Quark–Gluon Plasma). Transport calculations provide such a tool. Various models have been developed in the literature in the last few years [9–17], differing either in the general setup (Boltzmann, Fokker–Planck or Langevin equations) or in the way transport coefficients are evaluated.

The present study relies on a framework—based on the relativistic Langevin equation—developed by us in the past and described in detail in Refs. [18, 19], where one can also find a comparison with the PHENIX data available at that time. Predictions of our model for LHC energies were provided in Refs. [20, 21]. The calculations encompass several steps: the initial production of the heavy \(Q\bar{Q}\) pairs, taken from the next-to-leading-order pQCD event generator POWHEG [22] (supplemented with nuclear PDFs in the AA case [23]); the use of hydrodynamic codes [24–28] to describe the evolution of the medium from its formation up to the hadronization stage; the propagation, governed by the Langevin equation, of the heavy quarks in this medium; the hadronization of the heavy quarks, their decoupling from the fireball and the simulation of the final decays. Transport coefficients entering into the Langevin equation and describing the interaction of the heavy quarks with the medium have been derived within a weak-coupling thermal field theory calculation, with proper resummations of medium effects.

Here we update our findings, both for the \(pp\) and the AA cases, including new features in the setup. Concerning the initial production, the output of the POWHEG code for the hard event is now interfaced to the PYTHIA 6.4 [29] parton shower (the POWHEG-BOX [30] package provides the necessary routines to accomplish this task), simulating multiple gluon radiation from the external legs. This allows us to get, for \(pp\) collisions, \(p_T\)-spectra of heavy flavor hadrons and of their decay electrons in agreement with the experimental data and also with FONLL [31, 32] calculations (often used as a benchmark in heavy-flavor studies), but employing a more practical tool (since it is an event generator) providing at the same time a richer information on the final state. This would for instance make possible to address more differential observable, like \(Q\bar{Q}\) correlations.

For what concerns the transport coefficients, beside the perturbative values employed in past studies, here we consider also the ones provided by recent lattice-QCD calculations [33, 34]. Though being limited to the non-relativistic/static limit, so that no information on their momentum dependence is available, and in spite of the well-known difficulties in extracting real-time information from Euclidean simulations, lattice results seem to indicate values of the momentum diffusion coefficient significantly larger than perturbative predictions. Implications of this fact on the final heavy flavor spectra will be explored in the following.

The paper is organized as follows. In Sect. 2 we compare POWHEG+PYTHIA results for heavy flavor production in \(pp\) collisions to experimental data obtained at RHIC and at the LHC. In Sect. 3 we move to the AA case; after a brief summary of the formalism, we display results obtained with our Langevin setup using perturbative and non-perturbative transport coefficients and we compare them to experimental data on D mesons, heavy-flavor decay electrons and displaced \(J/\psi\)’s from the STAR, PHENIX, ALICE and CMS experiments. Finally, in Sect. 4 we draw our conclusions and suggest perspectives for future improvements of our analysis.

## 2 Heavy flavors in \(pp\) collisions

Although the main goal of our paper is to study medium effects on heavy-flavor observables in AA collisions, one needs first of all to validate the tools employed in simulating the initial \(Q\bar{Q}\) production through a comparison with the experimental data collected in \(pp\) collisions. For this purpose we rely on a standard pQCD public tool, namely POWHEG-BOX (based on collinear factorization), in which the hard \(Q\bar{Q}\) event (under control, due to the large quark mass) is interfaced with a shower stage described with PYTHIA. We start by briefly recalling the theoretical scheme upon which it is based, since this can be of interest when addressing the comparison of experimental data to various calculations.

The large mass of \(c\) and \(b\) quarks makes their partonic production cross-section accessible to pQCD calculations. Tools like POWHEG [22] and MC@NLO [35] generate hard \(Q\bar{Q}\) events according to the pQCD cross-section at next-to-leading-order (NLO) accuracy and represent the state of the art as event generators. Examples of NLO processes contributing to the \(Q\bar{Q}\) hadro-production cross-section are shown in the upper Fig. 1. The hard pairs are then showered with PYTHIA 6.4 [29], benefiting from the user-friendly interface provided by the POWHEG-BOX package [30]: this allows us to include the effects of Initial State Radiation (ISR) and Final State Radiation (FSR), resumming multiple emission of soft/collinear gluons at Leading Log (LL) accuracy. Intrinsic-\(k_T\) corrections (with \(\langle k_T^2 \rangle = 1\) GeV\(^2\)) are also included in the simulation of the heavy-quark production. The structure of a typical event resulting from the above chain is displayed in the lower panel of Fig. 1.

We now wish to illustrate how the above setup compares with the FONLL (Fixed Order Next to Leading Log) calculation of the inclusive charm/beauty production cross-section [31, 32], often regarded as the standard theoretical
benchmark in experimental heavy-flavor analysis. A particular NLO contribution comes from processes as the one displayed in Fig. 2, in which an intermediate gluon with virtuality much smaller than the (high) $p_T$ of the hard scattering splits into a $Q\bar{Q}$ pair. The process can be seen as the convolution of the cross-section for the production of an almost on-shell gluon ($gg \rightarrow gg^*$) followed by its splitting into a $Q\bar{Q}$ pair ($g^* \rightarrow Q\bar{Q}$). Integrating over the possible virtuality of the gluon from the $Q\bar{Q}$-threshold up to $p_T$ one gets that (at NLO) the average $Q\bar{Q}$ multiplicity inside a gluon-jet is of the order of

$$N(Q\bar{Q}) \sim \frac{\alpha_s}{6\pi} \ln \frac{p_T^2}{m_Q^2},$$

so that for very large $p_T$ one can have $\alpha_s \ln(p_T/M) \sim 1$ and a Fixed Order Calculation becomes no longer meaningful. One has then to resum the full DGLAP evolution of the gluon from the hard interaction up to its splitting into a $Q\bar{Q}$ pair, as shown in the lower panel of Fig. 2. This goes beyond the processes accounted for by NLO pQCD event generators, but is included in the FONLL calculation, which—employing NLO Altarelli–Parisi splitting functions—allows one to reach Next to Leading Log accuracy, resumming all $\alpha_s^n \ln^n(p_T/M)$ and $\alpha_s^{n+1} \ln^{n+1}(p_T/M)$ terms.

We shall see below that the differences between the resummation schemes adopted by POWHEG and FONLL give rise to differences between the corresponding heavy quark spectra well within the theoretical uncertainties and, generally, in fairly good agreement with the available experimental data.

Concerning the hadronization stage we adopt essentially the same fragmentation setup employed by FONLL, which was tuned by the authors to reproduce experimental $e^+e^-$ data. Heavy quarks are made hadronize by sampling different hadron species from $c$ and $b$ fragmentation fractions extracted from experimental data. Then, hadron momenta are sampled from Fragmentation Functions (FFs) calculated in heavy-quark effective theory (HQET), which entails a dependence on the parameter $r$. For charm quarks, we have used, for the $r$ parameter, the value fitted (in particular, fixing the higher moments of the FF) in the FONLL framework to ALEPH data at the LEP $e^+e^-$ collider (i.e., $r = 0.06$ for $m_c = 1.3$ GeV). For bottom fragmentation we used the functional form proposed by Kartvelishvili et al., whose single parameter $\alpha$ was fitted in the FONLL framework to ALEPH and SLD $e^+e^-$ data (namely $\alpha = 29.1$ for $m_b = 4.75$ GeV).

In order to estimate the systematic uncertainties associated to different FF choices, we have re-done the calculation with an alternative choice for the fragmentation function, namely using for the parameter $r$ the definition proposed in Ref. [39], which was $r \equiv (m_H - m_Q)/m_H$ ($m_H$ and $m_Q$ being the hadron and the heavy quark masses, respectively), resulting, e.g., in $r = 0.3$ for $D^0$ and $D^+$ mesons (using $m_c = 1.3$ GeV).

In Fig. 3 we display the outcomes of the POWHEG+PYTHIA setup for $D^0$ mesons in $pp$ collisions compared to ALICE [45] data at $\sqrt{s} = 7$ TeV, together with the FONLL uncertainty band [46]. Both data and theoretical predictions include the “primary” production ($c \rightarrow D$) as well as the $D^*$ feed-down ($c \rightarrow D^* \rightarrow D$). In the POWHEG+PYTHIA setup we have kept the default values for the renormalization and factorization scales and for the charm mass we have set $m_c = 1.3$ GeV. The results displayed have been obtained with two different values of the $r$ parameter ($r = 0.3$, entailed by the HQET calculation, and $r = 0.06$, fitted to $e^+e^-$ data)
Fig. 3 POWHEG+PYTHIA predictions for $D^0$ meson spectra at $\sqrt{s} = 7$ TeV (with different parameter choices for the fragmentation stage) compared to ALICE data [45] and to the FONLL systematic uncertainty band.

Fig. 4 POWHEG+PYTHIA predictions with for $D^0$ spectra at $\sqrt{s} = 2.76$ TeV (with different fragmentation schemes) compared with ALICE data [47].

Fig. 5 The ratio of electrons $e_b$ from beauty decays over the total number of non-photonic electrons $e_{c+b}$ in $pp$ collisions at $\sqrt{s} = 2.76$ TeV at the LHC. POWHEG+PYTHIA results are compared to preliminary ALICE data [48].

Fig. 6 POWHEG+PYTHIA predictions for $B^0$ meson spectra at $\sqrt{s} = 7$ TeV (with different fragmentation schemes) compared to CMS data [50] and to the FONLL systematic uncertainty band.

The POWHEG+PYTHIA setup predicts that the beauty contribution increases, becoming as large as the charm contribution at $p_T \sim 7$ GeV, in agreement with the ALICE preliminary data [48].

In Fig. 6 we address beauty production, comparing results for $B^0$ mesons to CMS data [50]. Again, in the POWHEG+PYTHIA setup we have kept the default values for the renormalization and factorization scales and we have used for the bottom mass $m_b = 4.8$ GeV. Two different fragmentation functions are tested: the one provided by HQET and the parametrization proposed by Kartvelishvili et al., fitted to $e^+e^-$ data. The latter is found to describe pretty well the data and will be the one employed in the rest of the paper. An analogous degree of agreement has been found for $B^+$ and $B^0_s$ mesons.

Finally, in Fig. 7 we display the outcomes of the POWHEG+PYTHIA setup (with the same parameters used...
choice is now slightly overshooting the data at FONLL uncertainty band. As it can be seen, our default present work; note that the curves are normalized to the predictions of the POWHEG+PYTHIA setup employed in the

tiations is then to reproduce within a coherent setup the rich amount of heavy-flavor data nowadays available, in partic-ular the quenching of the heavy quarks in the medium formed in heavy-
collisions working over an extended relax-ation) in the plasma in terms of uncorrelated random

To summarize, we have shown how—within the pT range of interest for heavy-flavor studies at the LHC—the POWHEG+PYTHIA setup, which will be employed in the rest of the paper, provides results in quantitative agreement with the available experimental data and also with FONLL; with respect to the latter, it is for our purposes a more practical tool, providing full information on the event, of potential interest for future less inclusive measurements, such as Q̅̅ correlations.

3 Heavy flavors in AA collisions

In this section we discuss the results of our transport setup for several heavy-flavor observables accessible in AA collisions at RHIC and at the LHC. All the experimental data so far available (namely, non-photonic electrons measured by PHENIX and ALICE, D mesons reconstructed by ALICE and STAR, heavy flavor decay muons measured by ALICE at forward rapidity, and displaced J/ψ’s from B decays measured by CMS) signal a high degree of rescattering of the heavy quarks in the medium formed in heavy-ion collisions. The challenge for the theoretical calculations is then to reproduce within a coherent setup the rich amount of heavy-flavor data nowadays available, in particular the quenching of the pT spectra—commonly studied via the nuclear modification factor (R_AA)—and the elliptic flow v_2.

At very large pT—the mass playing a negligible role—there is no reason to believe that the energy-loss mechanism of c and b quarks should be different from the one of light quarks, usually described by medium-induced gluon radiation; their final semi-leptonic decays are even proposed (and already used) as a tool to tag quark jets in a heavy-ion environment, shedding light on jet-quenching in AA collisions.

On the other hand, at small or moderate values of pT the large quark mass is expected to suppress the rate of gluon radiation, favoring the transition to a regime where collisional energy loss (in particular for beauty) plays the major role. Furthermore, in such a pT range it becomes mandatory to employ tools (transport calculations) capable of describing the asymptotic relaxation of heavy quarks to thermal equilibrium. Actually, in the case of a static medium heavy quarks—sooner or later—would always thermalize, no matter how strongly they are coupled with the plasma. The fact that in the actual experimental situation—of a medium with a finite life-time and a non-vanishing expansion rate—heavy quarks are found to follow the collective flow of the fireball can put tight constraints on their relaxation time to thermal equilibrium.

In our approach the dynamics of heavy quarks in the QGP is studied through the relativistic Langevin equation. The general setup has been presented in previous publications [18, 19] and its predictions were already compared with RHIC and first LHC data [20, 21]. Here we extend the setup along different directions. While in previous studies we relied on a microscopic derivation of the heavy-flavor transport coefficients performed within a weakly coupled scenario, here we also test the predictions obtained with the values provided by recent non-perturbative lattice-QCD simulations.

Furthermore we will put a stronger emphasis on beauty measurements (already feasible via displaced J/ψ detection by CMS and at the center of the ALICE upgrade program) and on their potentially major role in getting information on the quark-medium coupling. The large mass of b quarks makes in fact a description of their energy-loss (and thermal relaxation) in the plasma in terms of uncorrelated random collisions working over an extended pT-range; moreover, non-perturbative information on heavy-quark transport coefficients arising from lattice-QCD simulations performed in the static (M → ∞) limit, if questionable for charm, may provide a good guidance in the case of beauty.

Finally, at variance with the case of charm, for b quarks hadronization should play a minor role as a source of sys-tematic uncertainty. While in elementary collisions it occurs via fragmentation, with the final hadron carrying away a fraction z of the parent parton momentum, in AA collisions it has been pointed out that a coalescence mechanism (in which a hard parton hadronizes picking-up a companion
quark/antiquark from the thermal bath) might explain several features of hadron production at moderate $p_T$. In particular, the latter mechanism entails a momentum gain in the hadronization stage.

Medium modification of hadronization, while being an interesting research topic in itself, represents an important source of uncertainty in our studies, which are aimed at getting information on what occurred in the partonic phase. Coalescence can in fact modify hadron spectra both at the level of their shape (entailing a momentum gain, at variance with fragmentation) and of their absolute normalization, due to possible changes in the hadrochemistry (as suggested for instance by the recent ALICE $D_s$ measurements [6]). This might have a minor relevance in the case of beauty. Since its vacuum fragmentation function is very hard and the momentum-gain in case of coalescence is very small (of order $(m_q/M_b)p_T^2$), the two opposite scenarios should not entail dramatic differences for the final hadron spectra. Furthermore, measurements of displaced $J/\psi$'s should be less sensitive to changes in the relative abundances of the parent beauty hadrons. In summary: beauty measurements, being sensitive to changes in the relative abundances of the parent quark/antiquark from the thermal bath) might explain several features of hadron production at moderate $p_T$. In particular, the latter mechanism entails a momentum gain in the hadronization stage.

3.1 The relativistic Langevin equation

Within the Langevin framework, the time evolution of the momentum of a relativistic Brownian particle is provided by the following stochastic differential equation

$$\frac{\Delta \mathbf{p}}{\Delta t} = -\eta_D(p)\mathbf{p} + \xi(t),$$

where the drag coefficient $\eta_D(p)$ describes the deterministic friction force acting on the heavy quark, whereas the term $\xi$ accounts for the random collisions with the constituents of the medium. The effect of the stochastic term is completely determined once its temporal correlation function is fixed. The latter is usually assumed to be given by

$$\langle \xi^i(t)\xi^j(t') \rangle = b^{ij}(p)\delta_{tt'}/\Delta t,$$

entailing that collisions at different time-steps are uncorrelated. The tensor $b^{ij}(p)$ can be decomposed with a standard procedure according to

$$b^{ij}(p) \equiv \kappa_L(p)\hat{p}^i\hat{p}^j + \kappa_T(p)(\delta^{ij} - \hat{p}^i\hat{p}^j),$$

with the coefficients $\kappa_{L/T}(p)$ representing the squared longitudinal/transverse momentum per unit time exchanged by the quark with the medium. Finally, the drag coefficient $\eta_D(p)$ is fixed in order to fulfill equilibrium: for large times the momenta of an ensemble of heavy quarks should approach a thermal Maxwell–Jüttner distribution. This request leads to the relativistic generalization of the Einstein relation

$$\eta_D(p) \equiv \frac{\kappa_L(p)}{2T E_p} + \text{discr. corr.},$$

where the corrections on the right hand side are fixed in order to ensure that in the continuum, $\Delta t \to 0$, limit Eq. (1) reduces to the same Fokker–Planck equation, independently on the discretization scheme employed. At each time step the update of the quark momentum (and position) has to be performed in the local fluid rest frame (for more detail on the procedure see Ref. [19]), where the transport coefficients $\kappa_{L/T}(p)$ and $\eta_D(p)$ are defined. They can be in principle obtained from first-principle calculations and represent the key quantities to establish a link between the underlying microscopic theory (QCD) and the final observables accessible in $AA$ collisions. Their evaluation will be the subject of the next section.

3.2 The transport coefficients: weak-coupling vs. non-perturbative results

Heavy quark transport coefficients can be evaluated starting from their definition

$$\kappa_L = \left\{ \frac{\Delta q_L^2}{\Delta t} \right\} \quad \text{and} \quad \kappa_T = \frac{1}{2} \left\{ \frac{\Delta q_T^2}{\Delta t} \right\}. $$

We will consider the outcomes of two different approaches: weak-coupling calculations and lattice-QCD simulations. The momentum broadening (and degradation) of heavy quarks in the medium must arise from their interaction with the other constituents of the plasma: light quarks and gluons. Within a perturbative setup, the lowest order diagrams to be considered are the ones in Fig. 8. If the four-momentum exchange is sufficiently hard ($\{|t| > |t|^\ast\}$, where $t \equiv \omega^2 - q^2$) one is dealing with a short-distance process and the result is given by a kinetic pQCD calculation:

![Fig. 8 Diagrams for the hard scattering of a heavy quark off a light (anti-)quark and a gluon from the medium](image)
Scattering mediated by long-wavelength gluons require the resummation of medium effects

\[
\kappa_{L,\text{hard}}^{g/q} = \frac{1}{2E} \int \frac{n_{B/F}(k) n_{B/F}(k')}{2k} \int_{p'} \frac{\theta(|t| - |t'|^*)}{2E'} \times (2\pi)^4 \delta^4(P - K - K') |\mathcal{M}_{g/q}(s,t)|^2 |\mathbf{q}_L|^2,
\]

(6)

and

\[
\kappa_{T,\text{hard}}^{g/q} = \frac{1}{2E} \int \frac{n_{B/F}(k) n_{B/F}(k')}{2k} \int_{p'} \frac{\theta(|t| - |t'|^*)}{2E'} \times (2\pi)^4 \delta^4(P - K - K') |\mathcal{M}_{g/q}(s,t)|^2 |\mathbf{q}_T|^2.
\]

(7)

If on the contrary the momentum transfer is soft (|t| < |t'|^*), the scattering involves the exchange of a long wavelength gluon, which requires the resummation of medium effects, as displayed in Fig. 9. This can be done in hot-QCD within the Hard Thermal Loop approximation. The corresponding contribution to \(\kappa_{L/T}\) has been derived and evaluated in Refs. [18, 19], where the interested reader can find more details. Eventually, one has to sum-up the soft and hard contributions to the transport coefficients

\[
\kappa_{L/T} = \kappa_{L/T}^{\text{soft}} + \kappa_{L/T}^{\text{hard}}.
\]

(8)

checking that the final result is not too sensitive to the artificial intermediate cutoff |t'|^*: choosing |t'|^* \sim m_D^2 (the Debye-mass \(m_D\) being responsible for the screening of electric fields in the plasma) one verifies that this is actually the case [19], as it can be seen in Figs. 10 and 11. Concerning the scale of the strong coupling constant \(g\), the latter has been set at the typical thermal momentum, \(\mu \sim T\), in the soft contribution and to the squared-momentum transfer in the collisions, \(\mu \sim |t|\), in the evaluation of \(\kappa_{\text{hard}}\).

An independent way to extract the transport coefficients from the underlying microscopic theory comes from lattice-QCD simulations. The results we shall employ in the calculations have been obtained in the static (\(m_Q \to \infty\)) limit and refer to the momentum diffusion coefficient \(\kappa\). The latter is calculated [51, 52] starting from the non-relativistic limit of the Langevin equation (here written in the continuum limit):

\[
\frac{dp^j}{dt} = -\eta D p^j + \xi^j(t), \quad \text{with } \langle \xi^j(t)\xi^j(t') \rangle = \delta^{jj'} \delta(t-t') \kappa.
\]

(9)
Hence, in the $p \to 0$ limit, $\kappa$ reduces to the evaluation of the following force–force correlator:

\[
\kappa = \frac{1}{3} \int_{-\infty}^{+\infty} dt \langle [\eta(t) \eta(0)]_{HQ} \rangle,
\]

where the expectation value is taken over a thermal ensemble of states containing one Heavy Quark (HQ) (further details are provided in Appendix). In the static limit (magnetic effects being negligible) the force is nothing but the color-electric field acting on the heavy quark, namely:

\[
F(t) = g \int dx \, Q^\dagger(t, x) t^a Q(t, x) E^a(t, x),
\]

where $Q$ and $Q^\dagger$ are non-relativistic fields destroying and creating a heavy quark respectively. In Refs. [33, 34] $\kappa$ has then been extracted from Euclidean electric-field correlators, getting, within the explored temperature range, $\kappa/T^3 \sim 2.5$–4. For our calculations we shall rely on a linear interpolation of the values of $\kappa(T)$ quoted in Ref. [33]. The friction and spatial-diffusion coefficients are then set through the Einstein relation to $\eta_D = \kappa/2E_p T$ and $D = 2T^2/\kappa$.

Figures 10 and 11 summarize the essential features of the results for the heavy-quark transport coefficients. Notice in particular how the dependence on the unphysical intermediate cutoff $|t|^+$ is very mild. In these figures the weak coupling transport coefficients are compared to the ones from a lattice-QCD analysis, which provides results for $\kappa$ larger than the perturbative one by a sizable factor a low momenta, where the static approximation used in the lattice calculation is valid. Lacking any information on their momentum dependence, we are forced to use the same value also at large momenta: the growth with $p$ of the weak coupling coefficients is such that in the transverse channel they become roughly of the same size as the lattice-QCD one, whereas in the longitudinal channel they become much larger. This fact has relevant consequences on the physical observables, as we shall discuss in the following.

### 3.3 Results

In this section we present the results of our Langevin setup, comparing them with the recent experimental data obtained by the STAR, ALICE and CMS collaborations at RHIC and the LHC. The medium produced in Au–Au and Pb–Pb collisions is described through hydrodynamical calculations performed with the viscous $2+1$ code of Ref. [26], using Glauber initial conditions with $\sigma_{NN} = 42$ mb and $\sigma_{NN} = 64$ mb for RHIC and the LHC, respectively. The parameters used for the code initialization are summarized in Table 1, whereas in Table 2 we show the impact parameters corresponding to various centrality classes (results in other centrality classes have been obtained by a weighted sum of the cases of Table 2).

The initial hard $Q\bar{Q}$ production is simulated through the POWHEG+PYTHIA setup described in Sect. 2, supplemented in the AA case by EPS09 [53] nuclear corrections to the PDFs. Transverse momentum broadening in nuclear matter is also introduced, according to the procedure described in Ref. [19]. We summarize the results for the total $c\bar{c}$ and $b\bar{b}$ cross sections in Table 3.

### Table 1 Initial conditions for the hydrodynamical calculations simulating the background medium in AA collisions at RHIC and the LHC.

| Nuclei     | $\sqrt{s}_{NN}$ | $t_0$ (fm/c) | $n_0$ (fm$^{-3}$) | $T_0$ (MeV) |
|------------|-----------------|--------------|------------------|-------------|
| Au–Au     | 200 GeV         | 1.0          | 84               | 333         |
| Pb–Pb     | 2.76 TeV        | 0.6          | 278              | 475         |
| Pb–Pb     | 2.76 TeV        | 0.1          | 1688             | 828         |

### Table 2 The centrality classes and the corresponding average impact parameters at the kinematics of RHIC and the LHC.

| Collisions | $\sqrt{s}$ (MeV) | $b$ (fm) |
|------------|------------------|----------|
| Au–Au      | $\sqrt{s} = 200$ GeV | 3.27     |
| Pb–Pb      | $\sqrt{s} = 2.76$ TeV | 12.42    |

### Table 3 Total $c\bar{c}$ and $b\bar{b}$ cross sections in $pp$ and AA collisions at RHIC and the LHC, calculated with POWHEG using the default renormalization and factorization scales and the CTEQ6M PDF (supplemented by the EPS09 nuclear modifications in the case of AA collisions); $m_c = 1.3$ GeV and $m_b = 4.8$ GeV

| Collision | $\sqrt{s}$ (GeV) | $\sigma_{c\bar{c}}$ (mb) | $\sigma_{b\bar{b}}$ (mb) |
|-----------|------------------|------------------------|------------------------|
| $pp$      | 200 GeV          | 0.405                  | $1.77 \times 10^{-3}$   |
| Au–Au     | 200 GeV          | 0.356                  | $2.03 \times 10^{-3}$   |
| $pp$      | 2.76 TeV         | 2.425                  | 0.091                  |
| Pb–Pb     | 2.76 TeV         | 1.828                  | 0.085                  |
sentaing the central value of the systematic band explored in our study.

In Fig. 12 we display the outcomes of our Langevin setup (with weak coupling HTL transport coefficients as well as with lattice-QCD ones) for the nuclear modification factors $R_{AA}(p_T)$ of $D^0$ mesons in central and minimum-bias Au–Au collisions at RHIC, compared to preliminary STAR data [5]. The size of the suppression for $p_T \gtrsim 2$ GeV in central (0–10 %) events is quite well reproduced by the HTL curve. On the other hand experimental data display a bump around $p_T \approx 1.5$ GeV/c, with $R_{AA} > 1$ in the $p_T$ range 1–2 GeV/c and a depletion at smaller $p_T$, which is missed by our model.

Such a non-trivial behavior at low $p_T$ (say, for $p_T \lesssim 3$ GeV/c)—made visible by the very fine binning in the low-momentum region—might come from coalescence [54], so far not implemented in our framework: $D$ mesons in a given $p_T$-bin, in $pp$ collisions can only come from the fragmentation of $c$ quarks with higher momentum; if on the other hand coalescence were at work in the $AA$ case, the $D$ mesons in the same $p_T$ bin might come from the much more abundant $c$ quarks at lower $p_T$, leading to an enhancement of the spectrum.

The $p_T$ behavior of the quenching obtained with lattice-QCD transport coefficients on the other hand looks quite different from the one of the weak coupling calculations. In particular, the strong suppression of the spectra at moderate $p_T$ leads to a steep rise of $R_{AA}$ for $p_T \to 0$ not observed in the data: however, since, as we noticed, this is the region most affected by a possible coalescence mechanism, one cannot draw any definite conclusion. At larger momenta the lattice-QCD results show a mild growth of $R_{AA}$, at variance with both the HTL calculations and the data, but this is likely a consequence of the lack of any momentum dependence in the lattice-QCD transport coefficients.

Notably—at variance with the experimental data, which for moderate $p_T$ display a milder quenching in the 0–80 % centrality class—Langevin results for minimum-bias collisions are very similar to the ones in more central events. Actually, such a difference between central and minimum-bias events is not apparent in the PHENIX data [1] for non-photonic electrons (see Ref. [19] for a comparison with our model). Indeed, some amount of discrepancy is present between these PHENIX data and the preliminary STAR data for non-photonic electrons [58], as one can see in Fig. 13, where we compare them to our Langevin outcomes for heavy flavor decay electrons ($e_{c+b}$) in Au–Au collisions for different centrality classes.

Also in this case theory outcomes nicely reproduce the data for large enough $p_T$ (say, $p_T \gtrsim 4$ GeV/c), missing the enhancement observed in the low-momentum region. The present experimental systematic uncertainties and the moderate discrepancies between the results by the two collaborations make difficult to draw more definite conclusions.

In Figs. 14, 15 we display our results for the $D$-meson $R_{AA}$ (as a function of $p_T$ and of the centrality) in Pb–Pb collisions at the LHC compared to ALICE data [3]. In the LHC case we performed a wider systematic study exploring the sensitivity of the HTL results to the scale of the coupling. As shown in the left panel of Fig. 14, HTL transport coefficients reproduce quite nicely the data at moderate $p_T$, but at larger $p_T$ they would entail a too strong quenching of the spectra, presumably due to the rapid rise of $\kappa_L(p)$ with the quark momentum. Note that the data seem to favor the larger values of the scale $\mu$ in the QCD coupling and, interestingly, one observes a sort of saturation when increasing the value of $\mu$, thus reducing the sensitivity of the results to this unknown parameter.

On the other hand, “lattice” curves, obtained fixing $\kappa$ (independent on the momentum) through the static results of Ref. [33], display a too strong rise of $R_{AA}$ with $p_T$ compared to data, suggesting that the actual behavior stays probably in between, with a mild dependence of $\kappa_L$ on the quark momentum. This finding is also confirmed by the centrality dependence of $R_{AA}$ at high momenta (right panel of Fig. 15), whereas at moderate momenta the two theoretical models give essentially the same predictions (left panel of Fig. 15).

Preliminary ALICE results [55] on electrons from charm and beauty decays have also become available; we display them in Fig. 16 compared with the outcomes of our Langevin simulations for $R_{AA}$ in central events. The size of the suppression is quite well reproduced.

Let us now consider the azimuthal anisotropy of the momenta of the heavy flavor hadrons produced in the collision and of their decay electrons. The anisotropy is characterized by the Fourier coefficients $v_n = \langle \cos[n(\phi - \psi_{RP})]\rangle$, where $\phi$ is the particle azimuthal angle and $\psi_{RP}$ is the azimuthal
Fig. 13 Results (with HTL transport coefficients) for the R_{AA} of non-photonic electrons (e_{c+b}) from charm and beauty decays in Au–Au collisions at \( \sqrt{s_{NN}} = 200 \) GeV for various centrality classes compared to PHENIX [1] and preliminary STAR [58] data. In the upper left panel we include also the result with lattice-QCD transport coefficients.

Fig. 14 A systematic study of the D-meson nuclear modification factor for different choices of the transport coefficients. In the HTL case we let the scale of the coupling vary from \( \mu = \pi T \) to \( \mu = 2\pi T \). Results obtained with lattice-QCD transport coefficients are also shown for comparison. Our results are compared to ALICE data collected in the 0–20 % most central Pb–Pb collisions at \( \sqrt{s_{NN}} = 2.76 \) TeV [3] (left panel) and in semi-peripheral events (40–80 %, right panel).
Fig. 15 Centrality dependence of the $D$-meson $R_{AA}$ in Pb–Pb collisions. Results with different transport coefficients are compared to ALICE data [3] at moderate (left panel) and large (right panel) momenta.

Fig. 16 Predictions (with HTL and lattice-QCD transport coefficients) for heavy-flavor decay electrons from charm and beauty ($e_{c+b}$) in Pb–Pb collisions at the LHC compared to preliminary ALICE experimental data [55] in 0–10 % most central events.

angle of the reaction plane, which is defined by the impact parameter of the colliding nuclei and the beam direction. For non-central collisions, the dominant harmonic in the Fourier series is the second one, $v_2$, commonly called elliptic flow, which reflects the lenticular shape of the overlap region of the colliding nuclei. Non-zero elliptic flow of final state hadrons originates from the build-up of a collective motion of the medium constituents (dominant at low $p_T$) [56] and from the path-length dependence of in-medium parton energy loss.

In Fig. 17 we address the elliptic flow of $D$ mesons. Outcomes of our Langevin setup for the elliptic flow $v_2$ are compared to ALICE data [57] in semi-peripheral (30–50 %) Pb–Pb collisions. HTL results significantly underestimate the experimental data at low $p_T$, achieving at larger $p_T$’s an asymptotic plateau (experimentally observed also in the case of light-hadron spectra) arising from the path-length dependence of the energy loss. Lattice results on the other hand do a slightly better job at low $p_T$, but neglecting any possible energy dependence of the momentum broadening coefficient $\kappa$ leads to underestimate the flow at higher $p_T$. 

Fig. 17 Top panel: elliptic flow of $D$ meson in semi-peripheral (30–50 % centrality class) Pb–Pb collisions at the LHC compared to ALICE data [57]. Results obtained with HTL and lattice-QCD transport coefficients are displayed. Bottom panel: dependence of the $D$-meson $v_2$ on the thermalization time $\tau_0$ of the background medium.
The fact that, even with the quite large value of $\kappa$ provided by lattice-QCD simulation, one still underestimates the charm $v_2$ at small $p_T$ is a strong hint that an important contribution to the elliptic flow of $D$ mesons may come from coalescence with thermal partons at hadronization. Notably, even the quite extreme choice $\tau_0 = 0.1 \text{ fm}/c$ for the initial thermalization time of the medium leads just to a moderate increase of $v_2$ in the low-$p_T$ region, not sufficient to reproduce the amount of anisotropy displayed by the experimental data.

In Figs. 18 and 19 the elliptic flow of heavy quarks is studied through the electrons from the semi-leptonic decays of charm and beauty, $e_{c+b}$. In this case the discrepancy between Langevin outcomes and experimental data at small $p_T$ is even larger, whereas at the largest $p_T$'s accessible by ALICE the agreement between the preliminary data [55] and the HTL calculations is rather good.

Finally, we apply our setup to the study of beauty dynamics in the QGP. Measurements of $B$ mesons will become possible with the upgrade program of the ALICE detector. We display our results for $B^0$ mesons in Pb–Pb collisions in Fig. 20, where curves obtained with different sets of transport coefficients (HTL and lattice-QCD) are shown. Here, the low-$p_T$ region is especially interesting: for the reasons explained above, in the case of bottom quarks one expects the coalescence mechanism to alter the shape of $R_{AA}$ much less than in the case of charm quarks, allowing one, hopefully, to clarify whether the strong transport coefficients predicted by lattice-QCD are realistic.

Indirect information on beauty in heavy-ion collisions is however already experimentally accessible, through the non-prompt $J/\psi$ (from $B \rightarrow J/\psi + X$ decays) measurements by CMS [59]. Our results for the displaced $J/\psi$ $R_{AA}$, versus $p_T$ and centrality, are shown in Fig. 21 and compared to the CMS preliminary results. The data seem to point to a stronger quenching than predicted by theory, at variance with the charm data, whose quenching is generally overestimated at large $p_T$'s, at least in the HTL model. Here, $R_{AA}$ as a function of $N_{\text{part}}$ (shown in the right panel of Fig. 21) does not show appreciable differences between the HTL and the lattice-QCD models. On the other hand, the minimum-bias $R_{AA}$ as a function of $p_T$ (left panel of Fig. 21) shows a fair agreement with the one of the HTL calculation, although, we stress it again, no data are available at low $p_T$, where the lattice-QCD predictions are more reliable.

4 Conclusions and perspectives

In this paper we have shown a rich set of results provided by our transport setup for the study of heavy quarks in the QGP.
Theory outcomes have been compared to the most recent experimental data collected at RHIC and the LHC ($D$ mesons, non-photonic electrons and displaced $J/\psi$'s) concerning the quenching and the elliptic flow of charm and beauty in $AA$ collisions. If the experimental heavy-flavor $R_{AA}$ can be reproduced reasonably well over most of the $p_T$ range experimentally accessible, a consistent description within the same setup of the elliptic flow of charm is still lacking. In particular neither with perturbative nor with (the much larger) lattice-QCD transport coefficients we are able to reproduce the sizable elliptic flow of $D$ mesons at low $p_T$. This suggests that in order to reproduce the experimental data a modeling of the hadronization stage including the possibility of coalescence—in which the final $D$ mesons inherit part of the anisotropy from the light thermal partons—might be necessary.

We have discussed in the text how $B$ mesons should be less affected by effects arising from hadronization and how at the same time theory predictions (in particular the ones provided by lattice-QCD) should be more reliable in the case of beauty. $B$-meson measurements at low and moderate $p_T$, possible in the near future thanks to the upgrade of the ALICE detector, have the potentiality of providing information on the heavy-flavor transport coefficients favored by the experimental data.

So far, indirect information on the behavior of beauty in the medium is provided by preliminary CMS analysis of non prompt $J/\psi$'s from $B$ decays. Results for the corresponding $R_{AA}$ have been compared to the outcomes of our setup with different sets of transport coefficients: a decent agreement has been found in the HTL case; the available experimental data on the other hand refer to a too hard $p_T$-range to make meaningful a comparison with the lattice-QCD case (for which there is no information on the momentum dependence of the transport coefficients).

A few important items remain to be addressed and are left for future work. First of all, a modeling of coalescence, necessary in order to provide predictions at low $p_T$. Secondly, extending the setup to the forward-rapidity region, so that one can study also the rapidity dependence of the various heavy-flavor observables and face also the single-muon data measured by the ALICE experiment. This step would require to interface our transport setup with the output of a full $3+1$ hydrodynamic code, which is currently under development \cite{60}. Finally, addressing the study of more differential observables, like $Q\bar{Q}$ correlations (recently attempted by other groups \cite{61}), which are accessible to us thanks to the use of an event generator for the initial heavy quark production. This kind of studies is starting to trigger the interest of the experimental community.

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Appendix: Lattice transport coefficients

For the sake of self-consistency, in this appendix, following the steps of Ref. \cite{51}, we display how the heavy quark momentum-diffusion coefficient $\kappa$ can be given a general quantum field theory definition and how it can be expressed in terms of quantities accessible by lattice-QCD simulations.

One has to address the quite common situation of a “system” (the heavy quark) coupled to an “environment” (the thermal bath of gluons and light quarks). We have shown in Eq. (10) how $\kappa$ is related to the following force–force correlator:

$$
D^>(t) \equiv \frac{1}{3} \langle F^i(t) F^i(0) \rangle_{HQ}.
$$

(A.1)
Analogously, one defines \( D^<(t) \equiv (1/3)(F^i(0)F^i(t))_{\text{HQ}} \). KMS boundary conditions entail for their Fourier transforms \( D^<(\omega) = e^{-\beta \omega} D^>(\omega) \). One has then for the corresponding spectral function:

\[
\sigma(\omega) \equiv D^>(\omega) - D^<(\omega) = (1 - e^{-\beta \omega}) D^>(\omega). \tag{A.2}
\]

The momentum-diffusion coefficient reflects the \( \omega \to 0 \) limit of the above spectral density. In fact:

\[
\kappa \equiv \int_{-\infty}^{+\infty} dt \ D^>(t) = D^>(\omega = 0). \tag{A.3}
\]

Hence one has

\[
\kappa = \lim_{\omega \to 0} \frac{\sigma(\omega)}{1 - e^{-\beta \omega}} = \lim_{\omega \to 0} \frac{T}{\omega} \sigma(\omega), \tag{A.4}
\]

\( \sigma(\omega) \) being the quantity extracted from lattice-QCD simulations. For the latter one needs to consider the coupling of a (infinitely) heavy quark with the color field. The starting point is the \( M \to \infty \) limit of the NRQCD Lagrangian

\[
\mathcal{L} = \bar{Q}^\dagger (i\partial_0 + g A_0) Q, \tag{A.5}
\]

with the non-relativistic fields obeying the anticommutation relation

\[
\{ \bar{Q}_i(t, x), Q^\dagger_j(t, y) \} = \delta_{ij} \delta(x-y) \tag{A.6}
\]

and the heavy-quark evolution being described the path-ordered exponential \( U(t, t_0) \):

\[
Q_i(t) = \mathcal{P} \exp \left[ i g \int_{t_0}^{t} A_0(t') \, dt' \right] Q_j(t_0) = U_{ij}(t, t_0) Q_j(t_0). \tag{A.7}
\]

One needs then to define the expectation value in Eq. (A.1)

\[
\langle F^i(t) F^i(0) \rangle_{\text{HQ}} = \frac{\sum_s \langle s | e^{-\beta H} F^i(t) F^i(0) | s \rangle \langle s | e^{-\beta H} | s \rangle}{\sum_s \langle s | e^{-\beta H} | s \rangle}, \tag{A.8}
\]

which is taken over a thermal ensemble of states \( |s\rangle \) of the environment plus one additional heavy quark, namely:

\[
\sum_s |s\rangle \ldots |s\rangle \equiv \sum_{s'} \int d\mathbf{x} \langle s'| Q_i(-T, \mathbf{x}) \ldots Q^\dagger_j(-T, \mathbf{x}) |s'\rangle. \tag{A.9}
\]

Viewing the thermal weight \( e^{-\beta H} \) as the imaginary-time translation operator, so that

\[
Q(-T)e^{-\beta H} = e^{-\beta H} e^{\beta H} Q(-T)e^{-\beta H} = e^{-\beta H} Q(-T - i\beta), \tag{A.10}
\]

and exploiting the anticommutation relation (A.6) one gets for the HQ partition function appearing in the denominator of Eq. (A.8)

\[
Z_{\text{HQ}} = \sum_{s'} \int d\mathbf{x} \langle s'| Q_i(-T, \mathbf{x}) e^{-\beta H} Q^\dagger_j(-T, \mathbf{x}) |s'\rangle = V_{\text{PS}} \sum_{s'} \langle s'| e^{-\beta H} U_{ij}(-T - i\beta, -T) |s'\rangle = V_{\text{PS}} \langle \text{Tr} U(-T - i\beta, -T) \rangle Z_0, \tag{A.11}
\]

where now the thermal average is taken over the states of the environment only, with partition function \( Z_0 = \sum_{s'} \langle s'| e^{\beta H} |s'\rangle \), and the phase space volume arises from

\[
\int d\mathbf{x} \delta(\mathbf{x} - \mathbf{y}) = \int d\mathbf{x} \int d\mathbf{p}/(2\pi)^3 = V_{\text{PS}}.
\]

The numerator in Eq. (A.8) can be evaluated analogously starting from

\[
\sum_s \langle s | e^{-\beta H} \mathbf{F}(t) \cdot \mathbf{F}(0) |s\rangle = \sum_{s'} \int d\mathbf{x} \int d\mathbf{r} \int d\mathbf{r'} \times \langle s'| Q_i(-T, \mathbf{x}) e^{-\beta H} Q^\dagger_j(t, \mathbf{r}) gE_{jk}(t, \mathbf{r}) Q_l(t, \mathbf{r}) \times Q^\dagger_j(0, \mathbf{r'}) gE_{lm}(0, \mathbf{r'}) Q_m(0, \mathbf{r'}) Q^\dagger_j(-T, \mathbf{x}) |s'\rangle. \tag{A.12}
\]

One gets then

\[
\langle F^i(t) F^i(0) \rangle_{\text{HQ}} = \frac{\langle \text{Tr} [U(-T - i\beta, 0) gE^i(0)] [\text{Tr} U(-T - i\beta, -T)] \rangle}{\langle \text{Tr} U(-T - i\beta, -T) \rangle}. \tag{A.13}
\]

The above definition is the one used in Ref. [51], in which the AdS/CFT correspondence allows the derivation of real-time quantities in strongly coupled gauge theories (\( N = 4 \) SYM). However, in lattice-QCD one has to rely on lattice simulations carried on in Euclidean time. Equation (A.13) has to be accordingly generalized. In Refs. [33, 34] the authors evaluated then the following Euclidean electric-field correlator [52]:

\[
D_E(\tau) = -\frac{1}{3} \langle \text{Tr} [U(\beta, \tau) gE^i(\tau) U(\tau) gE^i(0)] \rangle / \langle \text{Tr} U(\beta, 0) \rangle \tag{A.14}
\]

and from the latter they extracted the spectral function \( \sigma(\omega) \) entering in Eq. (A.4) according to

\[
D_E(\tau) = \int_0^\infty d\omega \frac{\sigma(\omega) \cosh[(\beta/2 - \tau)\omega]}{\sinh(\beta\omega/2)}. \tag{A.15}
\]
