In ultrarelativistic collisions of heavy nuclei such as Au or Pb, an extreme high temperature and energy density environment can be produced around the collision point, where allows to form a new state of nuclear matter consisting of the deconfined quarks and gluons, namely the quark-gluon plasma, QGP [1, 2]. To investigate its properties, the experiments using the Au and Pb as the colliding beams have been carried at the Relativistic Heavy Ion Collider (RHIC) at BNL and at the Large Hadron Collider (LHC) at CERN, respectively, in the past two decades [3–5]. The QGP was found to induce the jet quenching, as well as to exhibit the collective flow behavior among various probes [6–10]. The anisotropy of the transverse momentum.

The heavy quark propagation behavior inside the quark-gluon plasma (QGP), is usually described in terms of the Boltzmann dynamics, which can be reduced to the Langevin approach by assuming a small momentum transfer for the scattering processes between heavy quarks and the QGP constituents. In this work, the temperature and energy dependence of the transport coefficients are calculated in the framework of both Boltzmann and Langevin dynamics. The derived transport coefficients are found to be systematically larger in the Boltzmann approach as compared with the Langevin, in particular in the high temperature and high energy region. Within each of the two theoretical frameworks, we simulate the charm quark production and the subsequent evolution processes in relativistic heavy-ion collisions. We find that the total in-medium energy loss is larger from the Langevin dynamics, resulting in a smaller (larger) $R_{AA}$ at high (low) $p_T$, for both the charm quark and heavy-flavor mesons. Meanwhile, the Boltzmann model is found to induce larger $v_2$, in particular at moderate $p_T$, as well as stronger broadening behavior for the azimuthal distributions. By comparing the model calculations with available experimental measurements for D-mesons, we find that the Langevin approach is more favored by the $R_{AA}$ data while the Boltzmann approach is more favored favor by the $v_2$ data. A simultaneous description of both observables appear challenging for both models.

The collective effect can be interpolated as the strong collective expansion of QGP when its (local) thermal equilibrium state is achieved, and it can be studied by a Fourier expansion [12, 13] of the particle azimuthal distributions with respect to the reaction plane, which is defined as the plane including impact parameter and beam axis. Normally, the second coefficient, $v_2$, is called elliptic flow coefficient, which allows to describe the anisotropy of the transverse momentum.

Heavy quark (HQ), including charm and bottom, are of particular interest [14–18] since, due to their large mass, $(1)\ m_Q \gg \Lambda_{QCD}$, thus, its initial production can be well described by the perturbative Quantum ChromoDynamics (pQCD) at the next-to-leading order [19–21], in particular at high $p_T$; $(2)\ m_Q \gg T$, resulting in the negligible thermal production of HQ pairs in QGP medium with the temperature reached at RHIC and LHC energies. In addition, HQ flavor is conserved throughout the interactions with the surrounding QGP constituents, i.e. gluons and (anti-)light quarks. Therefore, the initially produced HQ pairs will experience the full evolution of QGP, and serve as its ideal probes.

During the propagating through the QGP medium, the HQ dynamics is usually described by the Boltzmann or Langevin model [22, 23]. For the Boltzmann approach, the evolution of the HQ distribution function behaves the
Boltzmann Transport Equation (BTE), where the elastic and inelastic scattering processes between HQs and the quasi-particles of QGP are quantified by the relevant scattering matrix. Consequently, it can be calculated directly in terms of the perturbative QCD. Due to large HQ mass and moderate medium temperature, the typical momentum transfers in interactions, \( q \sim gT \), are assumed small, \( gT \ll m_Q \) [24], therefore, the HQ trajectory will be changed significantly only after receiving lots of soft momentum kicks from the surrounding QGP constituents, resulting in the Brownian motion. Based on this assumption, BTE is reduced to the Fokker-Plank Transport Equation (FPTE), which can be realized stochastically by a Langevin Transport Equation (LTE). In the framework of LTE, all the interactions are conveniently encoded into three transport coefficients, satisfying the dissipation-fluctuation relation. Therefore, with LTE, all the problem reduced to the evaluation of three transport coefficients, which can be derived from the lattice QCD.

Many models were developed from the Boltzmann [25–29] and Langevin dynamics [30–34] to study the suppression and collective effect of the final heavy-flavor productions (having the charm or bottom quarks among these valence quarks) such as D mesons (\( D^0, D^+, D^{**} \)) and \( D^0 \) [35, 36]) and B mesons (\( B^0, B^+, B_s \) [37]). Comparing the theoretical calculations with available data, it was realized [38–41] that the simultaneous description of \( R_{AA} \) and \( v_2 \) of open charmed meson at low and intermediate \( p_T \) is sensitive to the temperature and energy dependence of the transport coefficients. It is necessary to mention that, in order to improve the description of the measurements, the Duke group [42, 43] develops a data-based hybrid model to extract the transport coefficient by utilizing the Bayesian model-to-data analysis. See Refs. [44–46] for the recent review.

As mentioned, the Langevin approach is a very convenient and widely used model, and it allows to establish, directly, a link between the observables and transport coefficients, which can be derived from the lattice QCD calculations. However, the condition \( m_Q \gg gT \) may not always justified, in particular for charm quark with the medium temperature close to its initial value, resulting in the possible modification of the heavy meson \( R_{AA} \). So, in this work, we focus on the discussion related to the “benefits and limitations for Boltzmann vs. Langevin implementations of the heavy-flavor transport in an evolving medium” [44]. Both the BTE and LTE will be employed to investigate the temperature and energy dependence of the various transport coefficients, as well as to study the charm quark transport behaviors in the QGP medium.

The paper is organized as follows. In Sec. II we summarize the employed Boltzmann and Langevin dynamics, as well as the comparison for the derived transport coefficients. Sec. III is dedicated to the description of the hybrid model, including the initial state configuration, the hydrodynamic expansion of the underlying medium, heavy quark propagation and hadronization via fragmentation and “heavy-light” coalescence mechanisms. Sec. V contains the summary and discussion.

II. BOLTZMANN AND LANGEVIN TRANSPORT APPROACHES FOR HEAVY QUARKS

A. Linearized Boltzmann transport model

The linearized Boltzmann Transport Equation (BTE) reads

\[
\frac{p_Q}{E_Q} \cdot \partial f_Q = C[f_Q] \tag{3}
\]

where, \( p_Q, E_Q \) and \( f_Q \) are the HQ 4-momentum, energy and distribution function, respectively. \( C[f_Q] \) denotes the collision integral, including all the interaction mechanisms between heavy quarks and the medium partons, i.e. light quarks and gluons. Based on the Monte Carlo techniques, Eq. 3 can be solved numerically by slicing the coordinate space into a 3-dimension grid, and then the test particle method [47] is utilized to sample \( f_Q \) in each cell. The collision integral is solved by using the stochastic algorithm for evaluating the collision probability [48, 49].

In the local rest frame (LRF) of the cell, the heavy quark transport is performed within a given time-step \( \Delta t \). Concerning a desired scattering process \( l \), there are \( n(m) \) incoming (outgoing) partons, and the reaction probability \( \Delta \mathcal{P}_l \) is expressed as [43]

\[
\Delta \mathcal{P}_l = \Gamma_l(E_Q, T, t) \frac{g}{\nu} \left[ \frac{(2\pi)^3 \delta}{\delta f_Q} \int d\Phi(n, m) \prod_{\{i\}} f_i |M|^2 \right] \tag{4}
\]

where, \( \Gamma_l(E_Q, T, t) \) is the relevant scattering rate; \( g \) is the spin-color degeneracy factor of the incoming medium partons; \( \nu \) is the statistical factor that corrects for double-counting when there are identical particles in the initial/final state; \( f_i \) denotes the heavy quark (\( i = Q \)) and medium parton (\( i = q, g, \bar{g} \)) density, while the latter one follows the Maxwell–Jüttner distribution; \( |M|^2 \) is the initial state spin-color averaged scattering matrix element squared. In this analysis, following Ref. [43], we consider both elastic and inelastic scattering processes whose total cross section is calculated via the perturbative QCD at leading-order [25, 50]. Concerning the inelastic scattering, both the \( 2 \to 3 \) gluon radiation and the \( 3 \to 2 \) inverse absorption processes are taken into account to guarantee the detailed balance. Meanwhile, a Debye screening mass \( m_Q^2 = \frac{\pi^2}{3} (N_c + N_f) \alpha_s T^2 \) based on the Boltzmann statistics [51] is considered to regulate the \( t \)-channel gluon propagator. \( d\Phi(n, m) \) in Eq.4 is the \( n + m \) body phase space integration,

\[
d\Phi(n, m) = (2p_T)^4 \delta^{(4)}(p_{\text{in}} - p_{\text{out}}) \prod_{\{i_{\text{in, out}}\}} \frac{d^3 \vec{p}_i}{2E_i (2\pi)^3} \tag{5}
\]
where, $p_{\text{in}}$ ($p_{\text{out}}$) indicates the total 4-momentum of all the incoming (outgoing) partons for a given scattering process $l$. Within the time interval $\Delta t$, the total reaction probability $\Delta P_{\text{total}}$ is given by

$$
\Delta P_{\text{total}} = \sum_l (\Delta P_l) = \sum_l (\Gamma_l \cdot \Delta t).
$$

(6)

It was argued [52] that the interactions between HQs and the medium partons can be encoded into the drag and momentum diffusion coefficients:

$$
\begin{align*}
\eta_D &\equiv -\frac{d < p >}{dt} / < p >, \\
\kappa_L &\equiv \frac{1}{2} \frac{d < (\Delta p)^2 >}{dt}, \\
\kappa_T &\equiv \frac{d < (\Delta p_{\perp})^2 >}{dt},
\end{align*}
$$

(7)

which describes the average momentum/energy loss, momentum fluctuations in the direction that parallel (i.e. longitudinal) and perpendicular (i.e. transverse) to the propagation, respectively.

**B. Gluon radiation incorporated Langevin transport model**

While traversing the Quark-Gluon Plasma (QGP), HQ suffers frequent but soft momentum kicks from the medium partons, therefore, HQ behaves the Brownian motion, which can be described by the Langevin Transport Equation (LTE) [33, 41, 53]

$$
\frac{dx^i}{dt} = \frac{p^i}{E^i} \\
\frac{dp^i}{dt} = F^i_{\text{Drag}} + F^i_{\text{Diff}} + F^i_{\text{Gluon}}.
$$

(8)

The deterministic drag force reads

$$
F^i_{\text{Drag}} = -\eta_D (\vec{p}, T) \cdot \vec{p},
$$

(9)

where $\eta_D (\vec{p}, T)$ is the drag coefficient.

The stochastic force which acts on the HQ is expressed as

$$
F^i_{\text{Diff}} = \frac{1}{\sqrt{dt}} C^{ij}(t, \vec{p} + \xi d\vec{p}, T) \rho^j
$$

(10)

with the Gaussian noise $\rho^j$ follows a normal distribution

$$
P(\rho) = \left(\frac{1}{2\pi}\right)^{3/2} e^{x - \frac{\rho^2}{2}},
$$

(11)

resulting in $< \rho^j >_\rho = 0$ and $< \rho^i \rho^j >_\rho = \delta^{ij}$. Therefore, there is no correlation for the random force between two different time scales $< F^j_{\text{Diff}}(t) F^j_{\text{Diff}}(t') >_\rho = C^{ij} C^{kj}(t - t')$, indicating the uncorrelated random momentum kicks from the medium partons. During the numerical implementation, as shown in Eq. 10, the stochastic process depends on the specific choice of the momentum argument of the covariance matrix, $C^{ij}(t, \vec{p} + \xi d\vec{p}, T)$, via a parameter $\xi \in [0, 1]$. Typically, $\xi = 0$ for pre-point Ito, $\xi = 1/2$ for mid-point and $\xi = 1$ for post-point discretization scheme of the stochastic integral [54]. Finally, $C^{ij}$ can be represented in terms of the longitudinal ($\kappa_L$) and transverse momentum diffusion coefficients ($\kappa_T$) [55], i.e.

$$
C^{ij}(\vec{p}, T) \equiv \sqrt{\kappa_L (\vec{p}, T)} \rho^j + \sqrt{\kappa_T (\vec{p}, T)} (\delta^{ij} - \rho^i \rho^j),
$$

(12)

therefore, the relation between $\eta_D$, $\kappa_L$ and $\kappa_T$ is given by

$$
\eta_D = \frac{\kappa_L}{2T E} + (\xi - 1) \frac{1}{2p} \frac{\partial \kappa_L}{\partial p} + \frac{d - 1}{2p^2} \left[ \xi (\sqrt{\kappa_T} + \sqrt{\kappa_L})^2 - (3\xi - 1)\kappa_T - (\xi + 1)\kappa_L \right],
$$

(13)

where $d = 3$ denotes the spatial dimension. As pointed, HQ diffusions are conveniently encoded in the three coefficients $\eta_D$, $\kappa_L$ and $\kappa_T$. Note that Eq. 13 can be reduced to

$$
\eta_D = \frac{\kappa_L}{2T E} - \frac{d - 1}{2p^2} (\sqrt{\kappa_T} - \sqrt{\kappa_L})^2
$$

(14)

with the post-point scheme, i.e. $\xi = 1$. Following our previous analysis [41, 53], a “minimum model” by assuming a isotropic momentum dependence of the diffusion coefficient, $\kappa_L = \kappa_T \equiv \kappa$, is adopted in this work, although it is just validated at $p = 0$ and, they not exactly the same at $p \neq 0$ region from the analytical calculations [56]. Eq. 14 is therefore further reduced to

$$
\eta_D = \frac{\kappa}{2T E},
$$

(15)

which is the so-called dissipation-fluctuation relation (or Einstein relation) in the non-relativistic approximation.

The recoil force induced by the emitted gluons

$$
F^i_{\text{Gluon}} = -\frac{dp^i_{\text{Gluon}}}{dt},
$$

(16)

where, $\rho^j$ indicates the momentum of the radiated gluon. The transverse momentum together with the radiation time dependence of the radiated gluon is quantified by pQCD Higher-Twist calculations [57]:

$$
\frac{dN^{\text{Gluon}}}{dzdk_{\perp}^2 dt} = \frac{2\alpha_s C_A P(z) q_0}{\pi k_{\perp}^2} \left[ \frac{k_{\perp}^2}{k_{\perp}^2 + (zm_Q)^2} \right]^4 \sin^2 \left( \frac{t - t_0}{2\tau} \right)
$$

(17)

where, $z = \omega/E_Q$ denotes the energy fraction of the emitted gluon with respect to its parent HQ, and $k_{\perp}$ indicates the transverse momentum of gluon; $\alpha_s(k_{\perp}) = \frac{4\pi}{11N_c/3 - 2N_f/3 (\ln k_{\perp}^2 / \Lambda^2)^{-1}}$ is the strong coupling constant of QCD at leading order approximation; $P(z) = (z^2 - 2z + \frac{1}{3}) / (1 + \frac{1}{3})$.
According to its definition, \( \hat{q}_q = 2\kappa_q / \eta_D \); \( \hat{q}_q \) is the jet transport coefficient for quarks\(^4\); \( t_0 \) is the initial time for gluon radiation; \( \tau_{\text{f}} = 2E_Q z(1-z)/[k_T^2 + (zm_Q)^2] \) is the gluon formation time, with \( E_Q \) and \( m_Q \) are the HQ energy and mass, respectively. It was argued \([33]\) that an additional lower cutoff was imposed on the emitted gluon energy, \( \omega \gtrsim \pi T \), to balance the gluon radiation and the inverse absorption, so as to ensure that HQ equilibrium state can be reached after sufficiently long evolution time.

C. Boltzmann vs. Langevin

In this sub-section, we mainly focus on the comparison of the transport coefficients obtained via the Boltzmann and Langevin approaches. We show before that the scattering rate (Eq. 4) for \( c+q \rightarrow c+q \) process in Fig. 1, which is presented as a function of charm quark energy and the medium temperature. It is found that the energy dependence is weak, while the temperature dependence is stronger.

1. Boltzmann vs. Langevin: spatial diffusion coefficient

The spatial diffusion coefficient \( D_s \) \([52]\) scaled by the thermal wavelength \( 1/(2\pi T) \),

\[
2\pi T D_s = \lim_{p \rightarrow 0} \frac{2\pi T^2}{m_Q \cdot \eta_D(p)} = \lim_{E \rightarrow m_Q} \frac{2\pi T^2}{m_Q \cdot \eta_D(E)},
\]

is defined at \( p \rightarrow 0 \) limit, which can be obtained directly by substituting Eq. 7 with the Boltzmann approach. \( 2\pi T D_s \) is available from the Lattice QCD calculation, moreover, it is found \([53]\) that, according to a phenomenological fitting analysis with the Langevin approach, model predictions based on \( 2\pi T D_s = 7 \) allow to reproduce all the measured \( p_T \) dependence of the nuclear modification factor at both RHIC and LHC energies. Therefore, in the Langevin approach, the drag and the momentum diffusion coefficients (Eq. 15) can be obtained via Eq. 18 by setting \( 2\pi T D_s = 7 \). Note that, in this case, (1) the definition of spatial diffusion coefficient is extended to larger momentum values. Similar strategy is adopted in Ref. \([33, 51, 58]\); and (2) the drag and momentum diffusion coefficients in Eq. 15 can be represented in terms of \( 2\pi T D_s \) as

\[
\eta_D = \frac{1}{2\pi T D_s} \cdot \frac{2\pi T^2}{E},
\]

\[
\kappa = \frac{1}{2\pi T D_s} \cdot 4\pi T^3.
\]

The temperature dependence of the spatial diffusion coefficient \( 2\pi T D_s \) is presented in Fig. 2. The results from the Boltzmann (only \( c+q \rightarrow c+q \) and \( c+g \rightarrow c+g \)) and Langevin (only collisional) approaches are displayed as the dashed red and solid black curves, respectively. Lattice QCD calculations, i.e. Banerjee (pink circles \([59]\)), Kaczmarek (blue square \([60]\)) and Ding (red triangles \([61]\)) are shown as well as for comparison. Within the significant systematic uncertainties, both Boltzmann (dashed red curve) and Langevin predictions (solid black curve) are consistent with the Banerjee calculations. Similar behavior can be found by comparing with the CUJET3 predictions (red region \([28]\), as well as the results based on the Bayesian model-to-data analysis (green region \([43]\).

\[
\tau_{\text{charm}} = \lim_{p \rightarrow 0} \frac{m_{\text{charm}}}{\eta_D(p)}^{-1} = \frac{m_{\text{charm}}}{2\pi T c} \frac{(2\pi T D_s)}{(T/T_c)^2},
\]

\( \eta_D \) \([52]\) scaled by the thermal wavelength \( 1/(2\pi T) \),

\[
2\pi T D_s = \lim_{p \rightarrow 0} \frac{2\pi T^2}{m_Q \cdot \eta_D(p)} = \lim_{E \rightarrow m_Q} \frac{2\pi T^2}{m_Q \cdot \eta_D(E)},
\]

is defined at \( p \rightarrow 0 \) limit, which can be obtained directly by substituting Eq. 7 with the Boltzmann approach. \( 2\pi T D_s \) is available from the Lattice QCD calculation, moreover, it is found \([53]\) that, according to a phenomenological fitting analysis with the Langevin approach, model predictions based on \( 2\pi T D_s = 7 \) allow to reproduce all the measured \( p_T \) dependence of the nuclear modification factor at both RHIC and LHC energies. Therefore, in the Langevin approach, the drag and the momentum diffusion coefficients (Eq. 15) can be obtained via Eq. 18 by setting \( 2\pi T D_s = 7 \). Note that, in this case, (1) the definition of spatial diffusion coefficient is extended to larger momentum values. Similar strategy is adopted in Ref. \([33, 51, 58]\); and (2) the drag and momentum diffusion coefficients in Eq. 15 can be represented in terms of \( 2\pi T D_s \) as

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\eta_D = \frac{1}{2\pi T D_s} \cdot \frac{2\pi T^2}{E},
\]

\[
\kappa = \frac{1}{2\pi T D_s} \cdot 4\pi T^3.
\]

The temperature dependence of the spatial diffusion coefficient \( 2\pi T D_s \) is presented in Fig. 2. The results from the Boltzmann (only \( c+q \rightarrow c+q \) and \( c+g \rightarrow c+g \)) and Langevin (only collisional) approaches are displayed as the dashed red and solid black curves, respectively. Lattice QCD calculations, i.e. Banerjee (pink circles \([59]\)), Kaczmarek (blue square \([60]\)) and Ding (red triangles \([61]\)) are shown as well as for comparison. Within the significant systematic uncertainties, both Boltzmann (dashed red curve) and Langevin predictions (solid black curve) are consistent with the Banerjee calculations. Similar behavior can be found by comparing with the CUJET3 predictions (red region \([28]\), as well as the results based on the Bayesian model-to-data analysis (green region \([43]\).

\[
\tau_{\text{charm}} = \lim_{p \rightarrow 0} \frac{m_{\text{charm}}}{\eta_D(p)}^{-1} = \frac{m_{\text{charm}}}{2\pi T c} \frac{(2\pi T D_s)}{(T/T_c)^2},
\]

\( \eta_D \) \([52]\) scaled by the thermal wavelength \( 1/(2\pi T) \),

\[
2\pi T D_s = \lim_{p \rightarrow 0} \frac{2\pi T^2}{m_Q \cdot \eta_D(p)} = \lim_{E \rightarrow m_Q} \frac{2\pi T^2}{m_Q \cdot \eta_D(E)},
\]

is defined at \( p \rightarrow 0 \) limit, which can be obtained directly by substituting Eq. 7 with the Boltzmann approach. \( 2\pi T D_s \) is available from the Lattice QCD calculation, moreover, it is found \([53]\) that, according to a phenomenological fitting analysis with the Langevin approach, model predictions based on \( 2\pi T D_s = 7 \) allow to reproduce all the measured \( p_T \) dependence of the nuclear modification factor at both RHIC and LHC energies. Therefore, in the Langevin approach, the drag and the momentum diffusion coefficients (Eq. 15) can be obtained via Eq. 18 by setting \( 2\pi T D_s = 7 \). Note that, in this case, (1) the definition of spatial diffusion coefficient is extended to larger momentum values. Similar strategy is adopted in Ref. \([33, 51, 58]\); and (2) the drag and momentum diffusion coefficients in Eq. 15 can be represented in terms of \( 2\pi T D_s \) as

\[
\eta_D = \frac{1}{2\pi T D_s} \cdot \frac{2\pi T^2}{E},
\]

\[
\kappa = \frac{1}{2\pi T D_s} \cdot 4\pi T^3.
\]

The temperature dependence of the spatial diffusion coefficient \( 2\pi T D_s \) is presented in Fig. 2. The results from the Boltzmann (only \( c+q \rightarrow c+q \) and \( c+g \rightarrow c+g \)) and Langevin (only collisional) approaches are displayed as the dashed red and solid black curves, respectively. Lattice QCD calculations, i.e. Banerjee (pink circles \([59]\)), Kaczmarek (blue square \([60]\)) and Ding (red triangles \([61]\)) are shown as well as for comparison. Within the significant systematic uncertainties, both Boltzmann (dashed red curve) and Langevin predictions (solid black curve) are consistent with the Banerjee calculations. Similar behavior can be found by comparing with the CUJET3 predictions (red region \([28]\), as well as the results based on the Bayesian model-to-data analysis (green region \([43]\).
which is about 2.27 and 3.07 fm/c for Boltzmann and Langevin approach, respectively, with $T = 2T_c \approx 330$ MeV and $m_{\text{charm}} = 1.5$ GeV.

2. **Boltzmann vs. Langevin: transport diffusion coefficients**

In Fig. 3, the drag coefficient (left), longitudinal (middle) and transverse momentum diffusion coefficients (right), are presented as a function of the medium temperature (upper) at a given energy $E \approx 10$ GeV, and as a function of the charm quark energy (bottom) at fixed temperature $T = 0.3$ GeV. The results obtained with the Boltzmann (Eq. 7) and Langevin model (Eq. 19) are shown as dashed red and solid black curves, respectively, in each panel.

Concerning the drag coefficient $\eta$ [(a), (d)], the two models show an increasing temperature dependence and a decreasing behavior for the energy. The results with the Boltzmann approach (dashed red curve) is systematically larger than that with the Langevin approach (solid black curve). Both the longitudinal $\kappa_L$ [(b), (e)] and transverse momentum diffusion coefficient $\kappa_T$ [(c), (f)] increases strongly with increasing the energy and temperature via the Boltzmann approach, while they change slowly, as expected (Eq. 19), via the Langevin approach.

### III. METHODOLOGY

In the previous analysis [41], we construct a theoretical framework to study the charm quark propagation in ultrarelativistic heavy-ion collisions. The general modules of the hybrid model are discussed in the following.

#### A. Initial state configuration

The initialization of the heavy quark pairs is performed in the spatial and momentum space, respectively. In the transverse direction, the initial spatial distribution is sampled according to the initial binary collision density that is modeled by a Glauber-based approach [62], while in the longitudinal direction, it is described by a data-inspired phenomenological function [41]. The initial momentum distribution of $c\bar{c}$ pairs is predicted by the FONLL calculations [19–21], assuming a back-to-back azimuthal correlation between $c$ and $\bar{c}$ ($|\Delta\phi^{c\bar{c}}| = \pi$). For nucleus-nucleus collisions, e.g. Pb–Pb, the nuclear modification of the parton distribution functions (nPDFs) is taken into account by utilizing the EPS09 NLO parametrization approach [63].

The above initial state configuration allows providing the relevant entropy density distribution, which will be taken as the input of the subsequent hydrodynamical evolution. All the parameters in this procedure are tuned by the model-to-data comparison [41].

#### B. Hydrodynamic description

The underlying medium evolution is modeled by a 3+1D relativistic viscous hydrodynamics, vHLLE [64], with the initial time scale $\tau_0 = 0.6$ fm/c, shear viscosity $\eta/s = 1/(4\pi)$ and critical temperature $T_c = 165$ MeV in both Au–Au and Pb–Pb collisions. Note that the hydrodynamical simulation provides the space-time evolution of the temperature and the flow velocity field, which will be used in the HQ Boltzmann and Langevin dynamics.

The QGP medium expands and cools down, and the (local) temperature drops below the critical one $T_c$, resulting in the transition from the QGP phase to hadrons gas, namely hadronization. After the transition, the hadron gas can in principle continue to interact inelastically until the chemical freeze-out, subsequently, the hadronic system continues to expand and interact elastically until the kinetic freeze-out. In this work, we neglect the chemical freeze-out procedure and consider, only, the kinetic freeze-out (or freeze-out since now) occurs at $T_c = 165$ MeV. An instantaneous approach across a hypersurface of constant temperature, namely isothermal freeze-out, is utilized and modeled by a widely used approach, Cornelius [65].

#### C. Heavy quark propagation in medium

We refer to Ref. [41] for the detailed discussion about the numerical framework of charm quark Langevin evolution, which is coupled with the expanding hydrodynamic medium. For the Boltzmann case, it is quite similar except the procedure to update the charm quark momentum in a discrete time-step. In the following, we show the general strategy for both cases:

1. sample a given number of HQ pairs at the position and momentum $(x^\mu, p^\mu)$, in the laboratory frame (LAB), according to the previous initial phase space configurations $(\tau \sim 0)$;
2. move all the HQs from $\tau \sim 0$ to $\tau_0 = 0.6$ fm/c as free streaming particles, and modify the positions $x^\mu$ correspondingly;
3. search the fluid cell at the same position as HQ, $x^\mu$, and extract its temperature $T$ and velocity $u^\mu$ from the hydrodynamic simulations; then, boost the current HQ to the local rest frame (LRF) of the fluid cell and get the HQ momentum in this frame;
4. make a discrete time-step $\Delta t = 0.01$ fm/c for the HQ in order to update its momentum $p^\mu$:

   - Boltzmann dynamics: for the current HQ with $p_{old}^\mu$, calculate its reaction probability $\Delta P_l$ for each possible scattering channel $l$ (Eq. 4); the target channel is selected according to the relative reaction probabilities $\Delta P_l/\Delta P_{total}$ (Eq. 6), meanwhile, the 4-
momentum $p_{new}^\mu$ of the heavy quark after the scattering can be obtained according to the relevant scattering kinematics;

- Langevin dynamics: fix the drag and momentum diffusion coefficient with the fluid cell temperature $T$ (Eq. 19), as well as the drag (Eq. 9) and thermal force (Eq. 10); the momentum of the radiated gluon is given by the higher-twist model (Eq. 17), together with the recoil force (Eq. 16); and then, modify the HQ momentum $p^\mu$ according to the Langevin transport equation (Eq. 8);

(5) update the HQ position after the time step $\Delta t$

$$x(t + \Delta t) - x(t) = \frac{p(t)}{E_p(t)} \Delta t$$

with the $p^\mu$ obtained in the previous step, and then boost back the HQ to the LAB frame;

(6) repeat the above steps (3)-(5) when the local temperature $T \gtrsim T_c$.

D. Heavy quark hadronization via fragmentation and coalescence

The heavy quark will suffer the instantaneous hadronization procedure via a “dual” approach, including fragmentation and heavy-light coalescence mechanisms, when the local temperature drops below the critical one $T_c = 165$ MeV. In this work, we follow the previous analysis [41] and use this “dual” model for the final heavy-flavor meson productions.

Concerning the universal fragmentation function, the Braaten approach [66] is employed, and the fragmentation fractions for the various hadron species are $f(c \rightarrow D^0) = 0.566$, $f(c \rightarrow D^+) = 0.227$, $f(c \rightarrow D^{*+}) = 0.230$, and $f(c \rightarrow D^{*0}) = 0.081$ [41], respectively.

The momentum distributions of heavy-flavor mesons ($Q\bar{q}$) reads

$$\frac{dN_M}{d^3p_M} = g_M \int d^3\vec{x}_Q d^3\vec{p}_Q d^3\vec{x}_\bar{q} d^3\vec{p}_{\bar{q}} f_Q(\vec{x}_Q, \vec{p}_Q) f_{\bar{q}}(\vec{x}_\bar{q}, \vec{p}_{\bar{q}}) \times W_M^{(n)}(\vec{y}_M, \vec{k}_M) \delta^{(3)}(\vec{p}_M - \vec{p}_Q - \vec{p}_{\bar{q}})$$

where, $g_M$ is the spin-color degeneracy factor; $f_Q(\vec{x}_Q, \vec{p}_Q)$ is the phase-space distributions of heavy quark, which can be obtained after the HQ propagate through the underlying QGP medium; $f_{\bar{q}}(\vec{x}_\bar{q}, \vec{p}_{\bar{q}})$ is the one for light antiquark, which follows the Boltzmann-Jüttner distribution in the momentum space and it is spatially distributed on the freeze-out hypersurface. The coalescence probability for $Q\bar{q}$ combination to form the heavy-flavor meson in the $n^{th}$ excited state, is quantified by the overlap integral of the Wigner function of the meson and the $Q\bar{q}$ pair [67],

$$W_M^{(n)}(\vec{y}_M, \vec{k}_M) = \int \frac{d^3\vec{x}_Q d^3\vec{p}_Q}{(2\pi)^3} \frac{d^3\vec{x}_\bar{q} d^3\vec{p}_{\bar{q}}}{(2\pi)^3} W_M(\vec{x}_Q, \vec{p}_Q) W_{\bar{q}}(\vec{x}_\bar{q}, \vec{p}_{\bar{q}})$$

$$\times W_M^{(n)}(\vec{y}_M, \vec{k}_M) = \frac{1}{\sigma_M^2} \frac{\gamma_M^2 + \sigma_M^2 \vec{k}_M^2}{\sqrt{\sigma_M^2 + \sigma_M^2 \vec{k}_M^2}}$$

$$\exp\left\{-\frac{1}{2} \left(\frac{\vec{y}_M^2}{\sigma_M^2} + \sigma_M^2 \vec{k}_M^2\right)\right\} / n!$$

where, $\vec{y}_M = (\vec{x}_Q - \vec{x}_\bar{q})$ and $\vec{k}_M = (m_\bar{q}\vec{p}_Q - m_Q\vec{p}_{\bar{q}})/(m_Q + m_\bar{q})$ are the relative coordinate and the relative momentum, respectively, in the center-of-mass frame of $Q\bar{q}$ pair.
$W_Q(\vec{x}_Q, \vec{p}_Q^2)$ and $W_{\bar{q}}(\vec{x}_{\bar{q}}, \vec{p}_{\bar{q}}^2)$ are, respectively, the Wigner functions of heavy quark and light anti-quark with their centroids at $(\vec{x}_Q, p_Q^2)$ and $(\vec{x}_{\bar{q}}, p_{\bar{q}}^2)$, and they are both defined by taking the relevant wave function to be a Gaussian wave packet [68]. $W^{(n)}_M(\vec{y}_M^t, E_M^t)$ denotes the Wigner function of heavy-flavor meson, which is based on the well-known harmonic oscillator [68]. The width parameter $\sigma_M$ is expressed as [41]

$$\sigma_M^2 = \begin{cases} \frac{2}{3} \frac{(e_Q + e_{\bar{q}})(m_Q + m_{\bar{q}})^2}{e_Q m_Q^2 + e_{\bar{q}} m_{\bar{q}}^2} \cdot (r_M^2) & \text{for } n = 0 \\ \frac{2}{5} \frac{(e_Q + e_{\bar{q}})(m_Q + m_{\bar{q}})^2}{e_Q m_Q^2 + e_{\bar{q}} m_{\bar{q}}^2} \cdot (r_M^2) & \text{for } n = 1 \end{cases}$$

(23)

where, $(r_M^2) \approx (0.9 \text{ fm})^2$ is the mean-square charge radius of D-meson; $e_Q$ and $e_{\bar{q}}$ are the absolute values of the charge of heavy quark and light anti-quark, respectively; the light (anti-)quark mass takes $m_{u/d} = m_{d/u} = 300 \text{ MeV}$ and $m_{s/\bar{s}} = 475 \text{ MeV}$. We consider the various heavy-flavor meson species up to their first excited states ($n \leq 1$), see the Tab. II shown in Ref. [41] for details.

As displayed in Fig. 4, the hadronization of charm quark is divided into three channels: fragmentation, coalescence to form D mesons at ground state and at first excited state. During the implementation, we generate a random number, using the Monte Carlo techniques, with flat distribution between zero and one, and then compare it to the above three probabilities. Finally, the target channel can be selected, and the momentum of the relevant heavy-flavor meson will be obtained by assuming the energy-momentum conservation in the $Q$ and $\bar{q}$ combination procedure. See Ref. [41] for details.

IV. SUPPRESSION AND ELLIPTIC FLOW OF CHARM QUARK AND HEAVY MESON

A. Momentum distribution inside a static hydrodynamic medium

In order to study the difference between the Boltzmann and Langevin dynamics, in this sub-section, we focus on the time evolution of the charm quark momentum distribution, which is obtained inside a static hydrodynamic medium with temperature fixed at $T = 0.3 \text{ GeV}$, as well as the momentum initialized at $p = 10 \text{ GeV}$.

In Fig. 5, the charm quark momentum distribution $dN/dp$ based on the Boltzmann model [(a)], is calculated at various times during the hydrodynamic evolution of the medium, showing as different styles. At the starting time $\tau_0 = 0.6 \text{ fm}/c$ (solid black curve), as expected, the initial $dN/dp$ behaves a delta distribution at $p = 10 \text{ GeV}$. During the evolution up to $\tau = 8 \text{ fm}/c$, $dN/dp$ is broadened comparing with the initial distribution, meanwhile, the average momentum is shifted toward low $p$, which is mainly induced by the drag force. This is caused by the fact that the initial momentum spectrum of charm quark is much harder that of medium constituent, and the multiple elastic scatterings are therefore dominated by the drag term. The results based on the Langevin approach [(b)] present a different broadening behavior, which follows a Gaussian-like shape, as expected in the construction (Eq. 11). Similar results can be found in Ref. [69]. Comparing Boltzmann with Langevin calculations, it is observed that the momentum broadening profile is stronger with the Boltzmann model, since the scatterings with large momentum transfer are allowed in this approach, which are discarded with the Langevin approach. Consequently, the relevant azimuthal angular distribution with the Boltzmann model, is expected to show a stronger broadening behavior as compared to the Langevin model. Note that, for both Boltzmann and Langevin dynamics, $dN/dp(p, \tau)$ (dotted red curve) is followed by a tail in the range $p > 10 \text{ GeV}$, where the interaction processes allow the charm quark to gain more energy respect to the lost term.

![Graph](image-url)
dynamics, which is consistent with results shown in (a) similar as panel (a) but with the Langevin approach.

FIG. 5. (Color online) (a) Charm quark momentum distribution based on the Boltzmann dynamics at different times during the hydrodynamical evolution of the medium with a constant temperature $T = 0.3$ GeV (see legend for details). (b) similar as panel (a) but with the Langevin approach.

B. Energy loss inside a realistic medium

Figure 6 shows the average in-medium energy loss of charm quark as a function of initial energy, displaying separately the contributions of elastic (or collisional) and inelastic (or radiative) mechanisms as the dashed black and long dashed blue curves, respectively, while the combined results are shown as the solid red curves. The results with the Boltzmann and Langevin dynamics are presented as the thick and thin curves, respectively. We can see that the inelastic energy loss (think blue curve) with the Boltzmann approach, is dominated at high energy, while the elastic component (thick black curve) is significant at low energy. Similar behavior is observed with the Langevin approach (thin curves). When comparing the Boltzmann with Langevin results, the total energy loss for the latter one is slightly larger at high energy, resulting in a softer charm quark spectrum in this region.

C. $R_{AA}$ and $v_2$ for charm quarks

Figure 7 shows the nuclear modification factor $R_{AA}$ ($v_2$) of charm quark obtained with the Boltzmann (solid red curves) and Langevin approach (dashed black curve) in central (semicentral) Pb–Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV. It is observed that $R_{AA}$, as displayed in the panel (a), is enhanced (suppressed) at low (high) $p_T$ with the Langevin approach as compared to the Boltzmann approach. Therefore, charm quark loses more its initial energy while traversing the medium in the Langevin dynamics, which is consistent with results shown in

FIG. 6. (Color online) Energy loss of charm quarks obtained via Boltzmann approach (thick curves) and Langevin approach with $2\pi T D_\phi = 7$ (thin curves) after the propagation through a realistic hydrodynamic medium. For each approach, the elastic and inelastic contributions are shown separately as dashed black and long dashed blue curves, respectively. The combined results are shown as the solid red curves.

Concerning the relative azimuthal angle distribution, the yields of the initially back-to-back generated $c\bar{c}$ pairs can be described by a delta distribution at $|\Delta \phi| = \pi$. After propagating through the medium, it is argued [41] that the above $|\Delta \phi| = \pi$ distribution is broadened within different initial transverse momentum interval $p_T^{c/\bar{c}}$, in particular the one in the range $p_T^{c/\bar{c}} < 1.5$ GeV, which is almost flat, indicating the corresponding initially back-to-back properties are largely washed out throughout the interactions with the surrounding medium constituents. Meanwhile, the broadening behavior tends to decrease with increasing $p_T^{c/\bar{c}}$. Similar results can be found with the Boltzmann approach in this analysis. For comparison, Fig. 8 shows a ratio ($R = \text{Langevin}/\text{Boltzmann}$) obtained in central (0–10%) Pb–Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV. The different curves refer to different $p_T^{c/\bar{c}}$ intervals. Note that the nuclear (anti-)shadowing effect is not included. It is clearly shown that, as expected, $R$ is almost flat in the range $p_T^{c/\bar{c}} < 1.5$ GeV (dotted black curve), meanwhile, $R > 1$ means the broadening behavior is stronger with the Langevin approach in this region. The flat behavior of $R$ is significantly destroyed toward larger $p_T^{c/\bar{c}}$, where $R < 1$ ($R > 1$) at small (large) $|\Delta \phi|$, depending on $p_T^{c/\bar{c}}$. This can be explained by the fact that the broadening behavior is stronger with the Boltzmann approach as compared to the Langevin approach, which is consistent with the result observed in Fig. 5.
D. $R_{AA}$ and $v_2$ for heavy-flavor mesons

Figure 9 presents the average $R_{AA}$ [(a)] and $v_2$ [(b)] of the nonstrange D-meson ($D^0$, $D^+$, and $D^{++}$) in central (0–10%) and semicentral (30–50%) Pb–Pb collisions at $\sqrt{s_{NN}} = 5.02$ TeV, respectively, with the Boltzmann (solid red curves) and Langevin approach (dashed black curves). The bands denote the theoretical uncertainties, which are mainly contributed by the QCD scales and the EPS09 NLO parameterization [41]. It is observed that $R_{AA}$ is enhanced (suppressed) at low (high) $p_T$ for the Langevin dynamics as compared to the Boltzmann, while $v_2$ is systematically higher at moderate $p_T$ ($2 \lesssim p_T \lesssim 3$ GeV). This behavior is consistent with the results found at parton level (see Fig. 7). The available measurements for $R_{AA}$ and $v_2$ (boxes) are shown for comparison. The calculations with the Langevin approach seem to give a better description of the measured $R_{AA}$ [70] as compared to those with Boltzmann approach, in particular in the range $p_T \gtrsim 10$ GeV. Meanwhile, nonstrange D-meson $v_2$ calculated with the Boltzmann approach is closer to the available data [71] at $p_T \lesssim 4$ GeV. The comparison of $R_{AA}$ and $v_2$ gives the opposite indications about the two models, confirming that it is challenging to describe well $R_{AA}$ and $v_2$ simultaneously, as observed in Ref. [39].
Au–Au collisions at $\sqrt{s_{NN}} = 200$ GeV (panel b and e in Fig. 10). The predictions for the average $R_{AA}$ and $v_2$ of nonstrange D-meson in central (0–10%) and semicentral (30–50%) Xe–Xe collisions at $\sqrt{s_{NN}} = 5.44$ TeV, are displayed as well (panel c and f in Fig. 10).

V. CONCLUSION AND DISCUSSION

In this work, we investigated the charm quark evolution via the Boltzmann and Langevin dynamics in relativistic heavy-ion collisions. The derived drag coefficient ($\eta_D$), momentum diffusion coefficients ($\kappa_L$ and $\kappa_T$) and spatial diffusion coefficient ($2\pi T D_s$) are calculated as a function of charm quark energy and the medium temperature, and further compared between the two approaches. The relevant in-medium energy loss together with its effect on the nuclear modification factor ($R_{AA}$) and elliptic flow coefficient ($v_2$) at parton and hadron level, are discussed and compared with the available measurements at RHIC and LHC energies.

It is found that $\eta_D$, $\kappa_L$ and $\kappa_T$ calculated from the Boltzmann dynamics ($2\pi T D_s < 7$ in the range $1 < T/T_c < 3$), are systematically larger than the ones obtained with the Langevin approach ($2\pi T D_s = 7$). The total in-medium energy loss is larger with the Langevin approach, resulting in a smaller (larger) charm quark $R_{AA}$ at high (low) $p_T$, as compared to the Boltzmann. Meanwhile, Boltzmann dynamics is more efficient in producing $v_2$, in particular at moderate $p_T$, as well as in developing the broadening effect for the relative azimuthal angle distributions. The above $R_{AA}$ and $v_2$ behaviors observed at parton level are well inherited by the corresponding heavy-flavor hadrons. Comparing with the available data at RHIC and LHC energies, the model calculations for D-meson $R_{AA}$ favor the Langevin approach, while $v_2$ prefer the Boltzmann approach. A simultaneous description of both $R_{AA}$ and $v_2$ remains a challenge for both models.

The resolution of such challenge may require the inclusion of nonperturbative dynamics in the medium. It may be noted that a similar challenge was previously investigated for light flavor jet energy loss and a viable solution was previously proposed by introducing a nontrivial medium color structure that includes both chromoelectric and chromo-magnetic degrees of freedom [76, 77] and that leads to a strong temperature dependence of transport coefficients [28, 78, 79]. Whether a similar strategy may help address the $R_{AA}$ and $v_2$ challenge in the heavy flavor sector would be an interesting problem for future investigation. More detailed studies will be reported in forthcoming publications.

ACKNOWLEDGMENTS

The authors are grateful to Weiyao Ke for providing the Boltzmann module in Duke model, as well as the data shown in Fig. 2. S. Li is supported by National Science Foundation of China (NSFC) under Grant Nos.11847014 and 11875178, China Three Gorges University (CTGU) Contracts No.1910103, Hubei Province Contracts No.B2018023, China Scholarship Council (CSC) Contract No.201807620007, and the Key Laboratory of Quark and Lepton Physics Contracts No.QLPL2018P01. C. W. Wang acknowledges the support from the NSFHB No.2012FFAO85. R. Z. Wan acknowledges support from NSFC under Project No.11505130. J. F. Liao is supported by the National Science Foundation under Grant No.PHY-1352368. The computation of this research was performed on IU’s Big Red II cluster, which was supported in part by Lilly Endowment, Inc., through its support for the Indiana University Pervasive Technology Institute, and in part by the Indiana METACyt Initiative. The Indiana METACyt Initiative at IU was also supported in part by Lilly Endowment, Inc.

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FIG. 10. (Color online) Same as Fig. 9 but for nonstrange D-meson in Pb–Pb collisions at √sNN = 2.76 TeV [(a), (d)], D⁰ in Au–Au collisions at √sNN = 200 GeV [(b), (e)] and nonstrange D-meson in Xe–Xe collisions at √sNN = 5.44 TeV [(c), (f)]. Experimental data taken from Refs. [72–75].
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